

SELENIUM TRANSFER
BETWEEN KAOLINITE OR GOETHITE SURFACES,
NUTRIENT SOLUTION AND *Oryza sativa*

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Karlsruhe, den 28.04.2015

Alexandra K. Nothstein

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Abstract

Management of Se resources is a vital topic. This metalliod trace element is essential for many organisms and has a small range between human dietary deficiency ($< 55 \mu\text{g}/\text{d}$) and chronic toxicity ($> 400 \mu\text{g}/\text{d}$). Moreover, Se is unevenly distributed throughout the world and its bioavailability is governed by many factors. Biofortification and Se toxicity risk assessment are key aspects of managing global Se resources. Therefore, detailed research is required regarding biomolecular and geochemical interactions between Se and the environment. Accordingly, the aim of this study was to describe and quantify Se transfer in the Critical Zone, i.e. at the interface between soil and plant.

For this purpose, the Critical Zone was compartmentalized into three Se reservoirs: "soil", "soil solution" and "plant". Experimentally, these were represented by the model minerals kaolinite and goethite, a nutrient solution and rice plants (*Oryza sativa*), respectively. Using identical experimental parameters, first the speciation-dependent Se transfer from solution to plant and subsequent Se partitioning within the plant was studied; then adsorption-desorption processes of selenate and selenite onto the model minerals kaolinite and goethite were investigated. After that, both experiments were combined. Quantification of Se transfer between solution and mineral substrate as well as Se-uptake into plants from the solution provided the basis for a mathematical process model.

To determine Se-uptake differences due to lack of nutrients, a series of closed plant-box systems was used; *Oryza sativa* caryopses were prepared with Se-spiked nutrient-free phytoagar or nutrient solution of 0 - 2500 $\mu\text{g}/\text{L}$ Se as selenite or selenate. Furthermore, forcing plants to grow through a Se-free agar-filled tube before reaching the Se-spiked nutrient solution or phytoagar made it possible to observe the effects of delayed Se treatment. All

plants were grown with 14 days of Se-uptake in a climate chamber. After harvest, plant bulk samples of shoot and root were freeze-dried and microwave-digested with nitric acid and hydrogen peroxide. Selenium content was measured with HG-FIAS. Agar samples were digested similarly and measured with HG-FIAS. Selenium and nutrient content of the nutrient solution was measured by ICP-MS and IC.

To characterize Se adsorption-desorption behavior, a series of 24-h sorption batch experiments was carried out with 0.5 g kaolinite or goethite in a KCl-solution resembling the nutrient solution in ionic strength. Solutions were spiked with 0 - 5000 µg/L Se as either selenite or selenate. To study competition effects, these experiments were repeated in the presence of 750 µmol/L nitrate, sulphate or phosphate. To quantify ion exchange potential, subsequent Se desorption experiments were conducted with 0.1 mol/L K₂HPO₄.

To study combined effects of Se sorption processes and Se-uptake by plants, a combined sorption-plant-box experiment was devised with *Oryza sativa* caryopses, 170 mL of Se-spiked nutrient solution between 0 and 10,000 µg/L Se as selenite or selenate and 8.5 g of kaolinite or goethite substrate. Plant-free sorption controls were prepared in glass bottles parallel to the plant-box experiments. In addition, single plants exposed to 500, 2000 and 10,000 µg/L Se as selenite or selenate were air-dried. Their speciation was determined by measuring XANES scans, while mapping of spatial Se distribution was achieved by using µXRF at ANKA, Karlsruhe.

Results for all plant Se-uptake showed a preferential partitioning of selenite to the root (70 % of total plant-Se) and selenate to the shoot (72 % of total plant-Se). Due to a lack of competing ions in a nutrient-free environment, plant Se treatment directly upon germination led to greater Se-uptake at lower Se concentration (0 - 1000 µg/L Se as selenite and 0 - 250 µg/L Se as selenate) compared to the nutrient solution uptake (maximum uptake: 177 mg/kg Se DW in roots and 75 mg/kg Se DW in shoots for selenite; and 367 mg/kg Se DW in shoots and 96 mg/kg Se DW in roots). However, this treatment induced phytotoxicity symptoms and strongly decreased Se-uptake when these lower Se concentrations were exceeded. Treating the plants with nutrients and delaying Se exposure for 5 - 7 days led to greater plant tolerance for Se and steadily increasing Se-uptake with increasing applied

Se concentration (159 mg/kg Se DW in shoots and 312 mg/kg Se DW in roots for the Se-addition of 2500 µg/L Se as selenite and 405 mg/kg Se DW in the shoots and 128 mg/kg Se DW in the roots for the Se-addition of 2500 µg/L Se as selenate). However, competition by nutrients reduced Se-uptake into the plants.

Based on µXRF data, Se was mainly present in the phloem and xylem of the plant, irrespective of selenite or selenate application. Se-speciation in the plant tissue depended on the species applied. Selenite treatment led to a mean of 93 % organic Se in roots and 72 % organic Se in shoots, the rest being selenite (7 % and 28 %, respectively). Selenate treatment led to a mean of 48 % organic Se, 16 % selenite and 36 % selenate in roots and 46 % organic Se, 15 % selenite and 39 % selenate in shoots.

In the sorption experiments, adsorption by selenite and selenate onto kaolinite and goethite was very different. Measurements of remaining Se concentrations in solution showed that selenite adsorption onto kaolinite and goethite was 61 and 99 %, respectively. Selenate's respective sorption was 72 and 42 %. Desorption showed that 71 - 96 % of previously adsorbed Se was exchangeable by ion exchange with phosphate. However, subsequent plant Se-uptake was not higher through contact with the mineral than it was in just the nutrient solution. This suggests that plants did not actively desorb Se from the mineral surface. It was also shown that the nutrient solution's effect on Se adsorption was complex and could not be described as a linear combination of the effects of single ions.

These experimental data were used to create a mass balance model of the Critical Zone. The model assumes 100 % of the Se to be distributed into the three compartments "mineral surface", "solution" and "plant". With the required input parameters limited to the concentrations of selenite and selenate, the model calculates the Se adsorption to the mineral surface, the resulting Se solution concentration and the subsequent Se concentrations in plant roots and shoots, as well as the Se speciation found in these tissues.

This model does not simply interpolate Se concentrations between experimental results, but can model the competition between selenite and selenate when both are present in solution, as well as calculate adsorption for less or more than the appointed kaolinite amounts used in the experiments. For each scenario, the complete mass balance is calculated. Un-

fortunately, goethite results could not be incorporated into the model as experimental Se concentrations did not approach maximum load capacity.

The model created here quantified key processes of Se transfer between mineral surface, solution and plant and can easily be extended using results of further experiments. This model, reproducing experimental results, is a solid basis for our ability to predict Se transfer in the Critical Zone. This is a crucial component of effective global Se resource management concerning biofortification and Se toxicity risk assessment.

Zusammenfassung

Selenressourcenverwaltung ist ein lebenswichtiges Thema. Dieses Halbmetall-Spurenelement ist für viele Organismen essentiell und weist eine geringe Spanne zwischen Mangeler-nährung ($< 55 \mu\text{g}/\text{Tag}$) und chronischer Toxizität ($> 400 \mu\text{g}/\text{Tag}$) für den Menschen auf. Überdies hinaus ist Se in der Welt ungleichmäßig verteilt und seine Bioverfügbarkeit durch viele Faktoren bestimmt. Biofortifikation und Selentoxizitäts-Risikoanalyse sind Schlüs-selaspekte der globalen Selenressourcenverwaltung. Daher sind detaillierte Untersuchungen hinsichtlich molekularbiologischer und geochemischer Wechselwirkungen zwischen Se und der Umwelt notwendig. Dementsprechend war es Ziel dieser Studie, Selentransfer in der kritischen Zone, d.h. an der Schnittstelle zwischen Boden und Pflanze, zu beschreiben und zu quantifizieren.

Zu diesem Zweck wurde die kritische Zone in drei Selenreservoir unterteilt: "Boden", "Bodenlösung" und "Pflanze". Experimentell wurden diese durch die Modellminerale Kao-linit und Goethit, eine Nährlösung und Reis (*Oryza sativa*) repräsentiert. Unter der Ver-wendung identischer Versuchsparameter wurde zunächst der speziesabhängige Selentransfer von der Lösung in die Pflanze und die darauffolgende Selenpartitionierung innerhalb der Pflanze untersucht. Dann wurden Adsorptions-Desorptionsprozesse von Selenat und Selenit an den Modellmineralen Kaolinit und Goethit erforscht. Danach wurden beide Experimente kombiniert. Die Quantifizierung des Selentransfers zwischen Lösung und Mineralsubstrat sowie Selenaufnahme von der Lösung in die Pflanze stellen die Basis für ein mathematisches Prozessmodell dar.

Um Unterschiede in der Selenaufnahme aufgrund von Nährstoffmangel zu bestimmen, wurde eine Serie an geschlossenen Pflanzenboxversuchen genutzt. *Oryza sativa*-Karyopsen

wurden mit einem mit Selen versetztem, nährstoffreiem Agar oder einer Nährlösung von 0 - 2500 µg/L Se als Selenit oder Selenat vorbereitet. Pflanzen zu zwingen, durch ein Se-freies, Agar-gefülltes Eppendorfgesäß zu wachsen, bevor sie mit der mit Selen versetzten Nährlösung oder Phytoagar in Kontakt kommen, ermöglichte es darüber hinaus, die Effekte verzögerter Selenbehandlung zu beobachten. Alle Pflanzen wurden mit 14-tägiger Selenaufnahme in einer Klimakammer kultiviert. Nach der Ernte wurden Pflanzensammelproben des Sprosses und der Wurzel gefriergetrocknet und mit Salpetersäure und Wasserstoffperoxid in der Mikrowelle aufgeschlossen. Selengehalte wurden mit der HG-FIAS bestimmt. Agarproben wurden ähnlich aufgeschlossen und mit der HG-FIAS gemessen. Selen- und Nährstoffgehalte in der Nährlösung wurden mit ICP-MS und IC gemessen.

Um das Selenadsorptions- und -desorptionsverhalten zu charakterisieren, wurde eine Serie von 24-h Batchsorptionsversuchen mit 0,5 g Kaolinit oder Goethit in einer der Nährlösung entsprechenden KCl-Ionenstärke durchgeführt. Die Lösungen waren mit 0 - 5000 µg/L Se in Form von Selenit oder Selenat versetzt. Um Konkurrenzeffekte zu untersuchen, wurden diese Versuche in Anwesenheit von 750 µmol/L Nitrat, Sulfat oder Phosphat wiederholt. Um das Ionenaustauschpotential zu quantifizieren, wurden anschließend Selendesorptionsversuche mit 0,1 mol/L K₂HPO₄ durchgeführt.

Um Kombinationseffekte zwischen Selensorptionsprozessen und Pflanzenselenaufnahme zu untersuchen, wurde ein kombiniertes Sorptions-Pflanzenbox-Experiment konzipiert, mit *Oryza sativa*-Karyopsen, 170 mL mit Selen versetzter Nährlösung zwischen 0 und 10.000 µg/L Se in Form von Selenit oder Selenat und 8,5 g Kaolinit- oder Goethitsubstrat. Parallel zu den Pflanzenboxexperimenten, wurden pflanzenlose Sorptionskontrollen in Glasflaschen angesetzt. Zusätzlich wurden einzelne Pflanzen, die 500, 2000 und 10.000 µg/L Se in Form von Selenit oder Selenat ausgesetzt waren, luftgetrocknet. Deren Speziation wurde durch XANES Messungen bestimmt und die Kartierung der räumlichen Selenverteilung wurde durch Verwendung von µXRF an der ANKA, Karlsruhe, erreicht.

Die Ergebnisse für die Selenaufnahme aller Pflanzen zeigte eine bevorzugte Partitionierung des Selenits in die Wurzel (70 % des gesamten Pflanzenselens) und des Selenats in den Spross (72 % des gesamten Pflanzenselens). Aufgrund fehlender Konkurrenzen in der

nährstofffreien Umgebung, führte die direkt zum Zeitpunkt der Keimung erfolgte Selenbehandlung zu größerer Selenaufnahme bei niedrigerer Selenkonzentration (0 - 1000 µg/L Se als Selenit and 0 - 250 µg/L Se als Selenat) im Vergleich zur Aufnahme in der Nährlösung (maximale Aufnahme: 177 mg/kg Se DW in der Wurzel und 5 mg/kg Se DW im Spross für Selenit, und 367 mg/kg Se DW im Spross und 96 mg/kg Se DW in der Wurzel). Diese Behandlung erzeugte jedoch Phytotoxizitätserscheinungen und stark verringerte Selenaufnahme bei Überschreitung dieser geringen Selenkonzentrationen. Pflanzenbehandlung mit Nährstoffen und einer um 5 - 7 Tage verzögerten Selenexposition führte zu größerer Seltoleranz bei Pflanzen und stetig ansteigender Selenaufnahme mit steigender zugegebener Selenkonzentration (159 mg/kg Se DW im Spross und 312 mg/kg Se DW in der Wurzel für die Zugabe von 2500 µg/L Se als Selenit und 405 mg/kg Se DW im Spross und 128 mg/kg Se DW in der Wurzel für die Selenzugabe von 2500 µg/L Se als Selenat). Konkurrenz durch Nährstoffe verringerte jedoch die Selenaufnahme in die Pflanze.

Basierend auf µXRF-Daten, war Se vor allem im Phloem und Xylem vorhanden, unabhängig von der Selenzugabe in Form von Selenit oder Selenat. Die Selenspeziation im Pflanzengewebe war von der zugegebenen Spezies abhängig. Selenitbehandlung führte zu einem Mittelwert von 93 % organischem Se in der Wurzel und 72 % organischem Se im Spross, während der Rest aus Selenit bestand (7 % und 28 %, respektive). Selenatbehandlung führte zu einem Mittelwert von 48 % organischem Se, 16 % Selenit und 36 % Selenat in der Wurzel und 46 % organischem Se, 15 % Selenit and 39 % Selenat im Spross.

In den Sorptionsversuchen war Adsorption von Selenit und Selenat an Kaolinit und Goethit sehr unterschiedlich. Messungen von Selenrestkonzentrationen in der Lösung zeigten eine Selenitadsorption an Kaolinit und Goethite von 61, bzw. 99 %. Die Selenatsorption lag bei 72 bzw. 42 %. Desorption zeigte, dass 71 - 96 % des zuvor adsorbierten Se's durch Ionenaustausch mit Phosphat austauschbar war. Die darauffolgende Pflanzenselenaufnahme war durch den Kontakt mit dem Mineral jedoch nicht höher als in der reinen Nährlösung. Dies lässt vermuten, das Pflanzen Se nicht aktiv von der Mineraloberfläche desorbiert haben. Es wurde auch gezeigt, dass der Effekt der Nährlösung auf die Adsorption komplex ist und sich nicht als eine Linearkombination der Effekte einzelner Ionen darstellen lässt.

Diese experimentellen Daten wurden verwendet, um ein Massenbilanzmodell der kritischen Zone zu erstellen. Das Modell nimmt an, dass 100 % des Se's auf die drei Kompartimente "Boden", "Bodenlösung" und "Pflanze" verteilt sind. Mit den auf die Selenit- und Selenatkonzentration beschränkten notwendigen Eingabeparameter berechnet das Modell die Selenadsorption an der Mineraloberfläche, die resultierende Selenkonzentration in der Lösung und die darauffolgenden Selenkonzentrationen in Pflanzenwurzeln und -sprossen sowie die in diesen Geweben vorhandene Selenspeziation.

Dieses Modell interpoliert nicht einfach zwischen Selenkonzentrationen experimenteller Ergebnisse, sondern kann die Konkurrenz zwischen Selenit und Selenat modellieren, wenn beide in der Lösung vorhanden sind und kann die Adsorption für geringere oder größere als in den Experimenten verwendete Mengen an Kaolinit berechnen. Für jedes Szenario wird eine vollständige Massenbilanz berechnet. Unglücklicherweise konnten Goethitergebnisse nicht in das Modell integriert werden, da bei den experimentellen Selenkonzentrationen die maximale Beladungskapazität nicht annähernd erreicht wurde.

Das Modell, das hier erstellt wurde, quantifiziert Schlüsselprozesse des Selentransfers zwischen Mineraloberfläche, Lösung und Pflanze und kann leicht durch die Einbindung weiterer Versuche erweitert werden. Dieses Modell, welches experimentell erzielte Ergebnisse reproduziert, ist eine solide Basis für die Prognose des Selentransfers in der kritischen Zone. Dies stellt eine entscheidende Komponente effektiver globaler Selenressourcenverwaltung im Hinblick auf Biofortifikation und Selentoxizitäts-Risikoanalyse dar.

"I do not know what I may appear to the world, but to myself I seem to have been only like a boy playing on the sea-shore, and diverting myself in now and then finding a smoother pebble or a prettier shell than ordinary, whilst the great ocean of truth lay all undiscovered before me."

–Sir Isaac Newton–

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1. Introduction

The story of Selenium (Se) research is one littered with serendipity [Oldfield, 2006]. It began with the accidental discovery of Se nearly 200 years ago by the Swedish chemist Jöns Jacob Berzelius [Berzelius, 1817] and continued throughout the next two centuries until the beneficial effects of Se were discovered while studying ways to avoid its toxicity in the second half of the 20th century [Oldfield, 2006]. To this day, new seleno-proteins are still being discovered and not all metabolic functions and geochemical pathways of many organic species and some inorganic species have been clarified [Khan & Hell, 2014]. The transformation that the view on Se has undergone throughout the past two centuries is indicative of the surprises and challenges scientists are faced with when studying this trace element.

1.1. The fate of Se in research

For decades, Se had been considered to be merely a toxic trace element, which was discovered to cause hair and hoof loss in animals during the 1930s [Lenz & Lens, 2009]. It wasn't until 1957 that Se deficiency was recognized as a potential cause for human disease [Schwartz & Foltz, 1957].

In 1973, it was determined that, indeed, this trace element was interesting not only due to its toxicity [Oldfield, 2006], but also because it was proven to be essential to humans, as it is an integral component of the glutathione peroxidase enzyme. This antioxidant compound is designed to protect hemoglobin from oxidative damage [Flohé et al., 1973, Rotruck

et al., 1973].

This was only the first of various seleno-proteins to be discovered in the human body which, in combination, account for a wide array of functions within the human organism [Rotruck et al., 1973]. Since then, Se has been acknowledged as having 'two faces' [Oldfield, 1987] labelled 'the essential toxin' [Lenz & Lens, 2009] or 'a double edged sword' [Fernández-Martínez & Charlet, 2009, Hartikainen, 2005] to describe its dual nature.

These two facets of Se had been known to scientists for years. However, awareness of Se as an environmental pollutant became acute in the Kesterson Reservoir controversy in the United States in the 1980s not only for scientists, but also for politicians and the general public [Terry et al., 2000]. To reduce salt build-up, agricultural drainage water, which also happened to be geogenically enriched in Se, was discharged into the reservoir. When reproductive failure, development defects and mortality were found in migratory aquatic birds and fish, these were linked to the anthropogenic activity [Terry et al., 2000, Winkel et al., 2011].

This is not the only form of anthropogenic Se-contamination of the environment; industrial activities such as oil refineries and electric utilities also generate Se-contaminated aquatic discharges [Terry et al., 2000]. Amelioration and management of such sites still present considerable research potential today [Water Education Foundation, 2014].

On the other hand, Se is considered a rare and non-renewable resource, which must be carefully managed [Haug et al., 2007]. Optimizing procedures of crop fertilization of Se-deficient areas, such as Finland, still shows great potential for improvement [Eurola et al., 2003, Winkel et al., 2011]. Therefore, Se research faces two equally important, yet entirely diverse goals:

1. securing Se nutrient resources for future generations and
2. management of current enormous Se-enriched waste deposits to protect the environment and improve the quality of life in such areas of contamination [Haug et al., 2007].

Understanding the underlying geochemical and biochemical mechanisms for Se transfer processes within the Critical Zone is, therefore, an important first step for both aspects of these vital research questions.

1.2. Study objective and approach

This study is based on the premise that due to the complexity of Se geochemistry, a much better understanding of the Se cycle, as well as the basic processes governing it, is required [Fernández-Martínez & Charlet, 2009]. The objective of this study is, therefore, to quantify and characterize Se transfer pathways and processes as part of the Se cycle within the Critical Zone. To achieve this, the concept of this study relies on the compartmentalization of the Critical Zone into three Se reservoirs: 'soil', 'soil solution' and 'plant' (Figure 1.1). With the reservoir 'soil solution' connecting the reservoirs 'soil' and 'plant', this enables the study of two main process pathways for Se cycling on a scale of laboratory experiments:

1. speciation- and concentration-dependent uptake of Se into plants using the model plant of *Oryza sativa* in the absence or presence of nutrients in agar medium or a solution with defined chemical characteristics, respectively
2. Se sorption processes between soil particles and the soil solution using the two model minerals of kaolinite and goethite with the focus on Se ad- and desorption processes in the presence of the competing plant-relevant oxy-anions nitrate, sulfate and phosphate

The combination of both of these Se transfer processes and pathways are then connected to produce an empirical process model of the biogeochemistry of the Se cycle between these compartments of the Critical Zone.

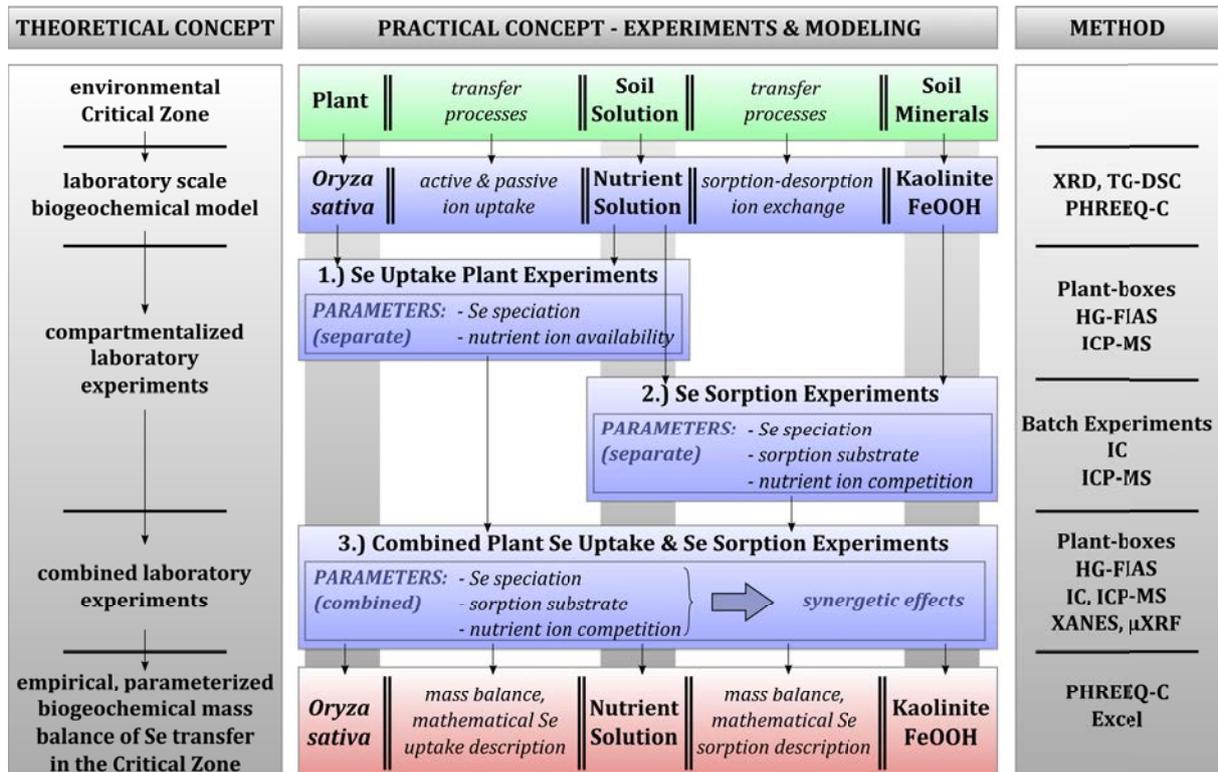


Figure 1.1.: *Research Concept: Quantification and characterization of processes between three compartments of the Critical Zone: soil, soil solution and plant. A 3-step experimental approach works toward*

- (1) *understanding Se pathways between solution and plants depending on Se speciation, nutrient availability and nutrient competition (explored by experiments A1 - A4),*
- (2) *understanding influences on Se pathways from sorption processes depending on Se speciation and ion competition (explored by experiments B1 - B3) and*
- (3) *creating a biogeochemical process model accounting for synergistic effects between both experiments (explored by experiment C).*

2. Selenium in the environment

Selenium was discovered in 1817 due to its geochemical similarity to sulfur. It was Jöns Jacob Berzelius, who, in the course of studying methods to prepare sulfuric acid from sulfur-bearing rock, came across a reddish sludge that formed when using pyrite from the mines in Falun, Sweden. This sludge contained an element that could be identified neither as sulfur, arsenic nor tellurium [Berzelius, 1817, Fernández-Martínez & Charlet, 2009].

2.1. Geochemical properties of Se

Selenium is a nonmetal trace element with the atomic number 34 and has an atomic mass of 78.96 g/mol [Fernández-Martínez & Charlet, 2009]. Like oxygen (O) and sulfur (S), it belongs to number VI of the main groups of the periodic table of elements and has an electron configuration of [Ar] 3d¹⁰ 4s² 4p⁴. Similar to S, this leads to the five natural oxidation states of Se: -II, -I, 0, +IV, +VI [Neal, 1995]. Selenium's two oxy-anions, which are the focus of this study, are the fully oxidized tetrahedral selenate and the pyramidal selenite.

Similar to sulfuric acid, selenic acid (H₂SeO₄) is a strong acid [Mortimer, 2010]. In aqueous solution, selenate (SeO₄²⁻) and the once-protonated biselenate (HSeO₄⁻) exist with a dissociation constant of pK_{a2} = 1.80 ± 0.10 (Figure 2.1a). The doubly protonated species (H₂SeO₄) has a constant of pK_{a1} = -2.01 ± 0.06 and, therefore, does not exist under natural conditions [Séby et al., 2001].

Selenous acid (H₂SeO₃), on the other hand, is a weak acid, analogous to sulfurous acid [Mortimer, 2010]. Selenite exists in solution as H₂SeO₃, HSeO₃⁻ and SeO₃²⁻ with

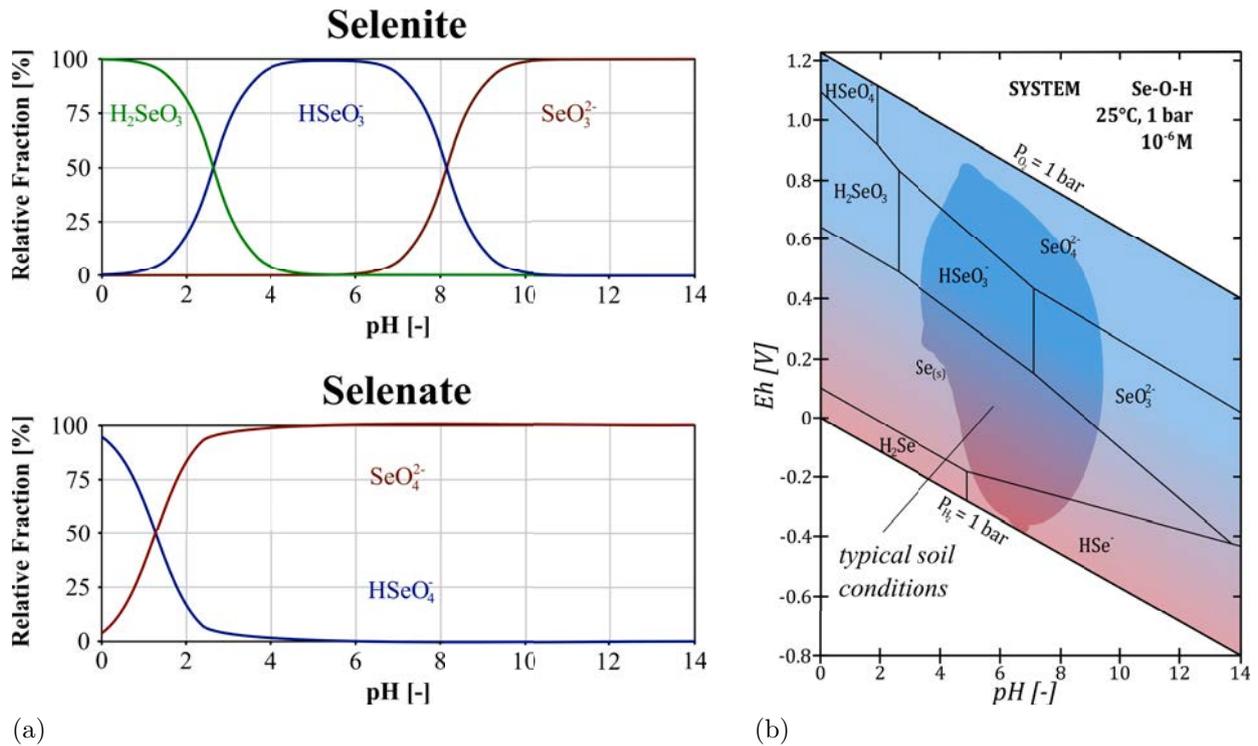


Figure 2.1.: *pH-dependent Se species*

a: Bjerrum plot for selenite and selenate: $c(\text{Se}) = 0.01 \text{ mol}$, $T = 25^\circ\text{C}$, $p = 1 \text{ bar}$ (created with PHREEQ-C, database: wateq4, Appendix A.1, A.2);

b: Pourbaix diagram of the Se-H-O system: $c(\text{Se}) = 10^{-6} \text{ mol/L}$, $T = 25^\circ\text{C}$, $p = 1 \text{ bar}$ [Brookins, 1988]; blue indicating oxic conditions, red indicating reducing conditions

dissociation constants of $\text{p}K_{\text{a}1} = 2.70 \pm 0.1$ and $\text{p}K_{\text{a}2} = 8.54 \pm 0.04$, depending on the solution pH [Séby et al., 2001] (Figure 2.1a).

As shown in Figure 2.1b, both Se oxy-anions are dominant under oxic conditions. The less oxic conditions become, however, the more elemental selenium, Se(0), is found to be prevalent (Figure 2.1b). Eleven Se(0) allotropes with various structural properties have been described [Minaev et al., 2005], all of which are believed to be present in nature in non-soluble form and, therefore, of limited bioavailability [Fernández-Martínez & Charlet, 2009]. However, recent studies have also shown plausible evidence of biological availability of Se(0) nano-particles [Terry et al., 2000, Zhang et al., 2005].

Under strongly reducing conditions, Se(-II) and Se(-I) are stable (Figure 2.1b), generally as a variety of metallic selenides and organic compounds [Fernández-Martínez & Charlet, 2009]. Also present under strongly reducing conditions is the gaseous, inorganic

compound H_2Se (Figure 2.1b), which has been shown to be a product of microbiological processes [Fernández-Martínez & Charlet, 2009].

There are five stable Se isotopes (given in order of their abundance): ^{80}Se (49.61 %), ^{78}Se (23.78 %), ^{76}Se (9.36 %), ^{77}Se (7.63 %), ^{74}Se (0.87 %). There are also multiple radioactive isotopes as well, one of which is the naturally occurring ^{82}Se which, due to its long half-life of $1.1 \cdot 10^{20}$ years, makes up 8.73 % of naturally occurring Se isotopes [Boullis, 1997, Duc et al., 2003]. Therefore, research on Se behavior in the environment is also applicable to the mobility of radioactive Se, which is of interest for long-term nuclear waste disposal [Bitterli et al., 2010].

As both are members of the VI-A chalcogen group of elements, Se and S share many properties. This means that Se can replace S in compounds, minerals and proteins. However, the Se atom has a larger radius (0.5 \AA) than the S atom (0.37 \AA), which makes a Se-Se bond approximately 1/7 longer and 1/5 weaker than a S-S bond [Sors et al., 2005].

2.2. Abundance and anthropogenic use of Se

The primary source of Se in the terrestrial system is rock [Rosenfeld & Beath, 1964, Neal, 1995]. Forty percent of the Se found in the earth's crust is bound in rocks, mainly as clay fractions in sediments, shales (Table 2.1), phosphatic rocks, coals or organic-rich deposits that contain high concentrations of Se, while sedimentary rocks are usually low in Se [Fernández-Martínez & Charlet, 2009].

Table 2.1.: *Se-contents in the environment, from [Fernández-Martínez & Charlet, 2009]*

Compartment	Se [mg/kg]	Compartment	Se [mg/kg]
Earth's Crust	0.05	Soil	0.01 - 2
Igneous & Volcanic Rock	0.35	Se-deficient Soils (China)	0.004 - 0.48
Limestone	0.03 - 0.08	Atmospheric Dust	0.05 - 10
Carbon Shale (China)	206 - 280	Freshwater [$\mu\text{g/L}$]	0.02

Selenium abundance in the earth's crust is around 0.05 mg/kg, which equals about 1/6000 of the total S content [Wang & Gao, 2001, Haug et al., 2007]. However, it is very un-

evenly distributed throughout the world, ranging from concentrations near zero up to 1250 mg/kg [Haug et al., 2007].

Selenium is often found substituting S in minerals such as chalcopyrite, pyrite or other sulfides or substituting phosphorus in phosphate minerals [Fernández-Martínez & Charlet, 2009]. However, Se-bearing minerals are too scarce to be mined [Haug et al., 2007]. Therefore, Se is produced as a by-product during electrolytic refining of copper, lead and silver or as a by-product in the manufacturing of sulfuric acid [Adriano, 1986, Stwertka, 2002].

Selenium also occurs as a by-product of radioactive decay; ^{79}Se , a long-living Se isotope has an abundance of 0.04 % in nuclear waste disposal and a relatively long half-life of $6.5 \cdot 10^4$ years, [Boullis, 1997, Duc et al., 2003, Bitterli et al., 2010].

Selenium is utilized for many purposes, such as the manufacturing of glass, plastics, ceramics and electronic components (because of its properties as a semi-conductor). It is also used in the chemical industry in pigments and lubricants or in shampoos against dandruff and also in nutritional supplements in combination with vitamin E [Adriano, 1986, Neal, 1995, Haug et al., 2007].

Because soil Se concentration is mainly influenced by the parent rock, the average world mean Se content in soils is 0.4 mg/kg (0.01 - 2 mg/kg). Soils with a Se content below 0.1 mg/kg are considered Se-deficient [Dhillon & Dhillon, 2003]. Soils above 0.5 mg/kg of Se are considered seleniferous because, in the absence of knowledge about their Se speciation, this Se concentration poses the risk of producing forage which exceeds maximum advisable Se-levels for animal consumption [Dhillon & Dhillon, 2003]. Both types of soil can exist in close proximity of each other (less than 20 km apart), presenting some countries, such as China and Brazil, with both challenges associated with this double-edged sword element [Fordyce, 2007].

As shown in Figure 2.1, Se in aerobic and neutral to alkaline environments tends to be present as selenate and selenite, whereas the major species dominating anaerobic environments are selenide and elemental Se [Adriano, 1986, Terry et al., 2000]. Volatile Se compounds are also estimated to constitute a large part of the Se cycle with 13,000 to 19,000 t cycling through the troposphere every year [Wen & Carignan, 2007] as dimethylselenide

(DMSe), dimethyldiselenide (DMDSe) and probably dimethyl selenone, dimethyl selenyl-sulfide and methaneselenol [Reamer & Zoller, 1980].

Comparing Se content in the environmental compartments listed in Table 2.1, coupled with knowledge of their abundance, it is estimated that Se-deficient environments are more widespread than Se-abundant ones [Haygarth, 1994].

2.3. Selenium in human health - requirement and toxicity

On the one hand, Se has been proven to be essential for mammals, and therefore, humans. In a wide array of 40 seleno-proteins known to be found in mammals, this trace element not only acts as an important anti-oxidant [Oldfield, 2006]. It is known to act as a growth factor as well, playing an important role in catalyzing production of thyroid hormones and in synthesising leucotrienes, which are needed to regulate immune responses. Furthermore, Se is involved in regulatory processes of a multitude of other metabolic functions [Reilly, 1997, Imai, 1998, Rayman, 2000]. To this day, an increasing number of seleno-proteins are still being discovered [Khan & Hell, 2014].

Suboptimal supply of Se is, therefore, associated with a number of adverse health effects such as myalgia, cartilage dysfunction, oxidative stress, heart failure, impaired immune function, reduced fertility and an elevated risk of certain cancers [Combs, 2001, Rayman, 2008]. Currently, an estimated 0.5 - 1 billion people are believed to be insufficiently supplied with Se [Combs, 2001]. Its essential role as a micronutrient becomes very clear in the effects of extreme Se deficiency: as shown in Figure 2.2a, low Se intake is known to lead to 'white muscle disease' in cattle [Oldfield, 2006], which is characterized by white necrosis and mineralization of calcium deposits within the heart muscle [Beytut et al., 2002]. An illness related to Se deficiency in humans is Kashin-Beck disease [Jiyun et al., 1982, Levander & Burk, 2006], which is characterized by dystrophic osteoarthritis in its first stage

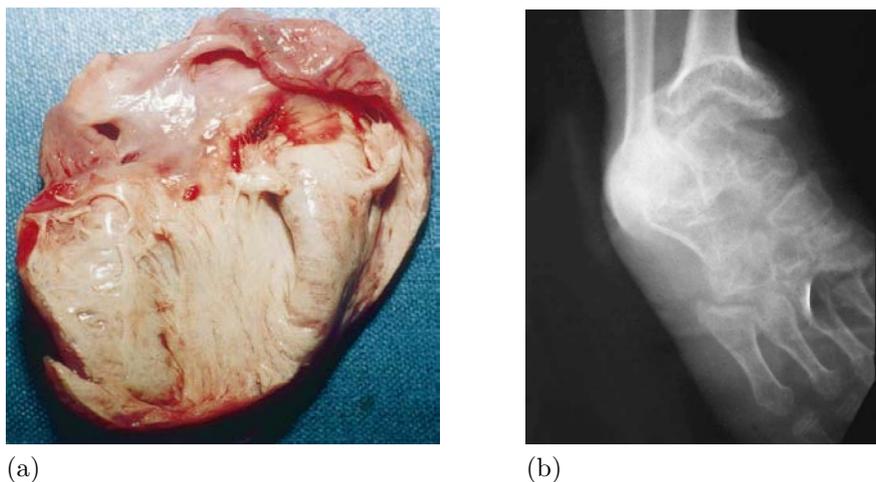


Figure 2.2.: *Pathological Se deficiency*

a: necrosis and mineralization in heart muscle tissue, [Beytut et al., 2002];

b: x-ray image of the left ankle of a 14-year old Tibetan boy with Kashin-Beck disease showing deformed bones and ligaments, [Moreno-Reyes et al., 1998]

(Figure 2.2b). On reaching the second stage, this becomes chronically painful and leads to irreversible deformities in its third stage [Nesterov, 1964].

On the other hand, Se toxicity can reach chronic or even acute poisoning levels. The so-called 'alkali disease' in livestock is attributed to chronic Se poisoning (selenosis), demonstrating symptoms such as hair loss, hoof deformity, anemia and the wasting away of the body [Lombeck et al., 1987]. Acute Se poisoning is sometimes equated to 'blind staggers', another disease described in cattle, the symptoms of which include blindness, abdominal pain, paralysis and death through loss of appetite [Lombeck et al., 1987]. However, contrary to assumptions made in the 1930s and '40s, the nosology of 'blind staggers' could not be clearly linked to Se poisoning [O'Toole & Raisbeck, 1964].

Se-related illnesses in humans are more likely to be induced by Se deficiency, although there are naturally seleniferous regions in China or Venezuela whose inhabitants have been affected by chronic selenosis [Lombeck et al., 1987]. Cases of acute Se poisoning are rare; however, there also exists a published case study of acute Se poisoning in a 2-year old child [Lombeck et al., 1987]. Toxicity symptoms of hypochromic anaemia, leucopenia and damaged nails were reported in workers with prolonged Se exposure in manufacturing, while accidental ingestion of high Se concentrations has been related to vomiting, diarrhoea and neurological disturbances [Navarro-Alarcon & Cabrera-Vique, 2008].

It wasn't until 1996 [Levander & Burk, 2006] that the World Health Organization (WHO) introduced references on Se intake, after Chinese studies were able to provide data on recommended daily allowance (RDA), accounting both for the dietary need of Se as an anti-oxidant and its adverse effects when consumed in toxic concentrations. Today's recommended Se intake - according to the 2000 Dietary Reference Intakes (DRI) - advises 20 - 30 μg Se per day for children up to the age of 8 and 55 μg of Se per day for adults, both male and female. 400 μg of Se per day is considered to be the upper tolerance limit of daily intake [Institute of Medicine, 2000, Levander & Burk, 2006].

This range between dietary deficiency ($< 55 \mu\text{g}$ per day) and toxicity ($> 400 \mu\text{g}$ per day) is one of the narrowest that can be found for any element [Finley, 2005, Fernández-Martínez & Charlet, 2009]. Some authors consider this range of health benefits to be even smaller at 55 - 200 μg Se/day [Rayman, 2000].

2.4. Biochemical properties of Se

Selenium can be taken up by organisms as selenate, selenite, organic Se compounds, such as selenomethionine (SeMet) and also as Se(0) nano-particles [Terry et al., 2000, Fernández-Martínez & Charlet, 2009].

"The bioavailability of a trace element is related to factors that make this element available to an organism, in a form that is transportable across the organisms' biological membrane."

[Reeder et al., 2006, Fernández-Martínez & Charlet, 2009]

Factors of bioavailability relate to the solubility of interacting substances, which are affected by speciation, ionic strength, pH or redox potential [Fernández-Martínez & Charlet, 2009]. These, in turn, are the result of indirect factors, such as soil type, plant species and amounts of rainfall [Girling, 1984, Haug et al., 2007]. Therefore, bioavailability is ultimately dependent on bedrock geology and climate as is apparent in the case of Se-deficient Scandinavian soils of Norway and Finland [Xue et al., 2001]. Due to the low bedrock-Se coupled

with low temperatures, high humidity and low pH as well as a high Fe content, any Se in these soils of glacial origin is present in reduced and therefore bio-unavailable form [Oliver, 1997]. Furthermore, not only soil development, but also processes of soil erosion have an impact on soil-Se bioavailability and play a key role in Se soil deficiency, as evident in Chinese soils [Oliver, 1997].

With so many factors governing Se transport and bioavailability, it comes as no surprise that total Se soil concentrations do not necessarily reflect whether plant uptake of Se will cause toxicity or deficiency [Lakin, 1972]. This explains the seemingly contradictory observation that 0.03 mg Se/kg in soils of Kars, Turkey lead to an accumulation of Se in meadow grass of 0.07 mg Se/kg dry mass on average, which then resulted in white muscle disease in cattle [Beytut et al., 2002], while in parts of Finland, 0.2 mg Se/kg soil, nearly a tenfold total concentration compared to that of the Kars region, is considered deficient in Se due to the element's reduced form, which is not readily taken up by plants [Oliver, 1997].

While organic Se as selenide (Se(-II)) is considered the most bioavailable Se form in marine environments, as it is taken up 1000 times more readily than inorganic Se by algae [Lemly, 1993], in terrestrial ecosystems, selenate (Se(VI)) is considered the most mobile and therefore most bioavailable form of Se [Haug et al., 2007]. Selenite (Se(IV)), though potentially 5 - 10 times more bioavailable and toxic than selenate [Lemly, 1993], is often retained in the soil due to fixation by soil minerals, such as ferric oxides or organic matter [Haug et al., 2007]. Elemental Se(0), on the other hand, is insoluble and therefore considered to have little toxicological significance unless perhaps as nano-particles [Fernández-Martínez & Charlet, 2009, Winkel et al., 2011].

Microorganisms are known to perform biotic transformations of Se. Organic Se compounds, selenate and selenite can be reduced actively by bacteria in the process of dissimilatory reduction (using the anion as a terminal electron acceptor) or assimilatory reduction (incorporating Se into organic compounds) to selenite, elemental Se and selenide [Fernández-Martínez & Charlet, 2009]. There are at least 16 species of bacteria or archaea known to grow under anaerobic conditions by linking the oxidation of organic substrates or H₂ to the dissimilatory reduction of selenium oxy-anions [Fernández-Martínez &

Charlet, 2009].

The environmentally most important process in this regard is dissimilatory reduction [Stolz & Oremland]. Thermodynamic data show that the free energy for SeO_4^{2-} and SeO_3^{2-} reduction into selenide (HSe^-) is -22.2 and -22.9 kcal eq $^{-1}$, respectively, which is about four times higher than that for the reduction of SO_4^{2-} to sulphide (HS^- ; -5.9 kcal eq $^{-1}$). Therefore, selenate reduction to selenite is favourable over nitrate reduction to ammonium and sulfate reduction to sulfide, which makes selenate an environmentally significant electron acceptor [Stolz & Oremland]. Selenate reduction has been found to occur in chemically disparate environments [Stolz & Oremland] and in many cases, selenite has been shown to be an intermediate product of this reduction, which is believed to subsequently adsorb onto soil minerals [Fernández-Martínez & Charlet, 2009]. However, it has also been shown that microbiological selenite reduction occurs at a faster rate than selenate reduction [Bajaj et al., 2011] which suggests rapid metabolization in cases in which it is not rapidly adsorbed.

The ability of micro-organisms to perform bio-methylation of Se is often seen as a possible remediation procedure for Se-contaminated soils. This process consists of a series of redox reactions changing the Se oxidation state from +IV or +VI to -II, by producing selenide compounds with methyl groups [Chasteen & Bentley, 2003]. These species can be volatile and are, therefore, removed from the soil. This is important because although much of plant Se-uptake occurs via soil or solution, it has also been shown that even volatile Se species can be taken up by plants via absorption through the leaf [Zieve & Peterson, 1984, Xu & Hu, 2004].

Plants are believed to take up selenate via the sulfate transporter, while uptake of selenite by sulfate, phosphate or silicone transporters is still debated [Terry et al., 2000, Li et al., 2007, Zhao et al., 2010]. Selenium can then be transformed into organic Se compounds and also volatilized [Terry et al., 2000]. Details on the uptake of Se into plants and translocation within plants are provided in Chapter 3.1.

In many vertebrates, Se is known to replace S in proteins due to similarities between these two elements, most frequently in seleno-cysteine (SeCys) compared to cysteine (Cys). In direct comparison between enzymes containing SeCys rather than Cys, the seleno-isologues

prove to be the more efficient catalysts [Birringer et al., 2002]. In the case of glutathione peroxidase (GSH), which is required by all mammals, efficiency of this enzyme for detoxifying hydroperoxides is reduced by 2 - 3 orders of magnitude when Se does not substitute S and, therefore, fails to fulfill its purpose. The reason that Se is essential to organisms is, therefore, attributed to this substitution of S in proteins with Se, which, leading to greater reactivity than in their S-counterpart, is often required for catalytic activity [Birringer et al., 2002, Sors et al., 2005].

In general, biomolecular mechanisms of Se toxicity are poorly understood [Brozmanová et al., 2010]. However, the same greater reactivity of Se-substituted proteins may also be the cause for its toxicity. As an oxidizing catalyst, Se is able to oxidize thiols producing free radicals which can damage DNA. Moreover, unwanted substitutions of S by Se in proteins leads to disfunctional proteins, causing hoof, hair, nail and feather loss when S of the keratin is substituted for Se [Spallholz & Hoffman, 2002]. SeCys provides the greatest source of Se-toxicity to humans as it leads to accumulation of hydrogen selenide due to inhibition selenium methylation [Spallholz & Hoffman, 2002].

2.5. Approaches to studying Se in the environment

Introduction of Se into the foodchain is a source of both essential nutritional supply to organisms as well as environmental toxicity hazardous to life [Lenz & Lens, 2009, Winkel et al., 2011]. Because of the narrow range between dietary deficiency and toxicity [Fernández-Martínez & Charlet, 2009], management thereof requires detailed understanding of Se transfer processes in all environments that include organisms. This concept is known as the 'Critical Zone'.

"The Critical Zone is the system of coupled chemical, biological, physical, and geological processes operating together to support life at the Earth's surface. (It) ... is defined as the volume extending from the upper limit of vegetation down to the lower limit of groundwater." [Anderson et al., 2007, Brantley et al., 2007]

This geo-science model concept includes the multitude of natural components that are interwoven with living organisms and also coincides with compartments of an element's cycle: the geosphere, pedosphere, biosphere, hydrosphere and atmosphere.

The challenge that presents itself in the environmental modelling of Se is the amount of parameters governing Se bioavailability, transfer and retention. Furthermore, Se is known to behave non-conservatively in the environment. Moreover, it cannot simply be described by applying transport pathways of sulfur [Presser & Piper, 1998]. To tackle this problem, there have been various approaches to studying Se in the environment (Figure 2.3). Selenium transfer between compartments of the Critical Zone can be studied on various scales and modelling of Se in the Critical Zone can be divided accordingly into different groups (Figure 2.3).

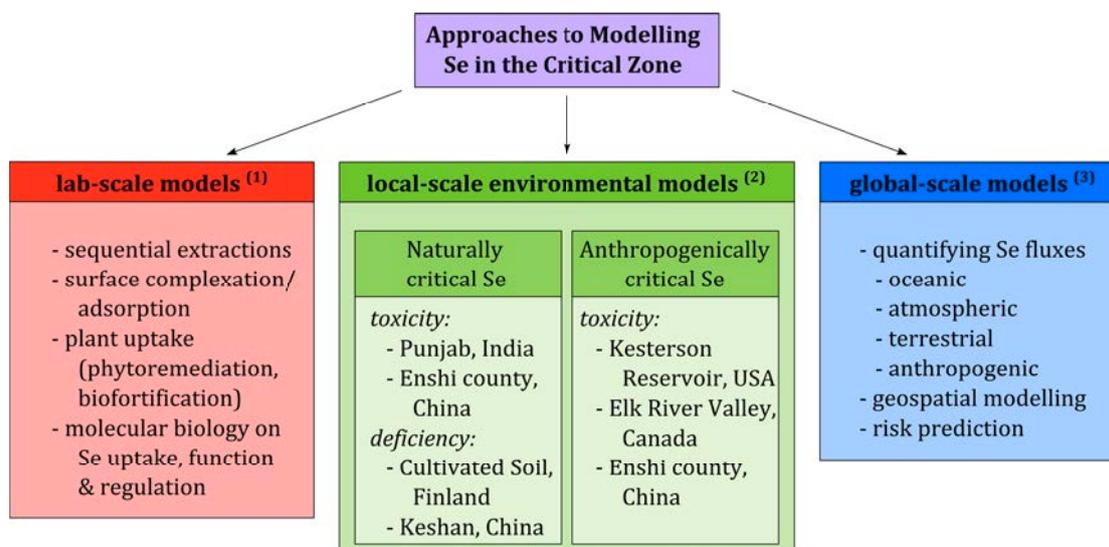


Figure 2.3.: Approaches to modelling Se in the Critical Zone on different scales:
 (1) theoretical and empirical lab-scale approaches [Balistriieri & Chao, 1990, Kulp & Pratt, 2004, Li et al., 2007, Khan & Hell, 2014],
 (2) empirical local-scale approaches [Presser & Piper, 1998, Wang & Gao, 2001, Ohlendorf, 2002, Bajaj et al., 2011],
 (3) and theoretical, empirical or spatial-numerical global-scale approaches [Haygarth, 1994, Bowie et al., 1996, Amoroux, 2001, Winkel et al., 2011]

Although there had been previous studies on lab-scale effects of Se [Lévesque, 1974, Asher et al., 1977, Howard, 1977, Tzeng & Zeitlin, 1978], it was the Kesterson Reservoir controversy in the 1980s that brought awareness of Se as an environmental pollutant to the broader public [Terry et al., 2000], thus paving the way for more interdisciplinary, holistic

approaches to Se research on a larger scale. Subsequent studies conducted on the deaths of Kesterson waterfowl and other birds have been recognized as one of the ‘gold standards’ of retrospective ecological risk assessment [Ohlendorf, 2002] with their integrated combination of field and laboratory studies that included recognising a disease syndrome, identifying the causative agent and verifying the findings in reproducing the disease syndrome in healthy individuals. It was the understanding of the complex interactions between anthropogenic effects - such as the re-routing of drainage water - in combination with geological effects - such as the naturally Se-enriched Cretaceous marine source bedrock - which gave rise to the term “Kesterson Effect” [Presser, 1994, Water Education Foundation, 2014]. This term summarizes all aspects found to contribute to the biological accumulation of Se-induced toxicity, tracing Se “from rock to duck” [Presser, 1994, Water Education Foundation, 2014].

Ideally, all three scales (lab-scale, local-scale and global-scale, Figure 2.3) of Se transfer processes merge into a coherent model of the Se cycle, supporting both theoretical and empirical study. Within the scope of this study, the goal is to merge theoretical and practical lab-scale processes at an interdisciplinary level, combining a botanical and geochemical approach.

Small lab-scale systems (Figure 2.3(1)) have the advantage of having a more limited amount of parameters and being more clearly definable than larger, environmental-scale systems. All the more so, when the study can be conducted as a closed system. However, because of this restricted amount of influencing parameters, applicability of such small-scale systems is limited in the context of modelling the Se cycle. This is especially true of mono-disciplinary approaches.

For example, results from lab-scale studies of interactions between mineral surface and solution, such as adsorption/desorption studies, are very selectively applicable only to the mineral, pH-value and ionic strength chosen in the experiment [Parks, 1990]. And on the other hand, lab-scale bio-molecular approaches on the uptake of Se by plants and microorganisms target specific enzymatic processes of Se uptake, transport and assimilation [Terry et al., 2000]. Each of these important findings, however, must be combined into a coherent model when modelling the Se cycle.

At the scale of a local-scale environment (Figure 2.3(2)), studies lacking a closed system encounter a completely different set of challenges. Areas characterized by Se deficiency such as Finland or the U.K., for example, attempt amelioration by fertilising their crops with Se. While Finish authorities closely monitored resulting Se uptake into the food chain, little emphasis was placed on the environmental impact of such Se fertilization [Winkel et al., 2011]. Although dietary intake was increased by a factor of 4, crop uptake of Se was only 5 - 20 % of the annual Se application. It is still unclear what happened to the remaining 80 - 95 % of that applied Se, since it was thought to be immobilized, yet could not be accounted for when soil Se concentration was measured [Euroala et al., 2003]. This is disquieting, as Se is known to have a strong tendency to bioaccumulate - especially in aquatic biota [Winkel et al., 2011].

Modelling global-scale processes of the Se cycle (Figure 2.3(3)) faces another set of challenges entirely. While many lab-scale processes are understood in great detail, systematic measurement of environmental Se content and speciation throughout the world is sparse [Winkel et al., 2011]. But there have been attempts at creating a world Se map [Winkel et al., 2011] and Se flux estimates on a global scale have also been published [Haygarth, 1994, Amoroux, 2001].

To combine the benefits of lab-scale research with the applicability of local environmental-scale research, this study combines an interdisciplinary approach - botanical and geochemical - with a controllable, lab-scale biogeochemical model. This enables the simulation of multiple parameters of a local environmental-scale situation, while retaining detailed quantification of lab-scale precision.

2.6. Premises and hypotheses for this study

In reference to the classification of Figure 2.3, the first premise is that a lab-scale biogeochemical model with three compartments - plants, nutrient solution and soil minerals - will be an adequate compromise between a realistic reflection of environmental processes and practical labwork. Concerning the subdivision of these experiments, the second premise

assumes that processes between each compartment can be studied separately between solution & plant and then soil & solution before synergistic effects are uncovered in combined experiments with all three compartments. This compartmentalization is what enhances the significance of results, since factors influencing Se transport between two compartments may be absent in the Se transport between two others. Furthermore, as explained earlier, smaller lab-scale compartments reduce the amount of influencing factors. The ability to quantify Se transfer beyond characterization of the Se transfer processes is crucial to creating a mass balance of Se in the Critical Zone. Therefore, the third premise is that results on Se transfer can be mathematically described, even if these mathematical descriptions might not quantify mono-causal processes.

Regarding the outcome of the experiments, the following hypotheses are included in the choice of experimental set-up, based on previous publications and knowledge of Se behaviour:

1. Se uptake of rice will be dependent on Se speciation and nutrient ion availability
2. Regarding the soil minerals, Se prevalence - and, therefore, also bioavailability - will be dependent on adsorption-desorption processes, which are influenced by Se behavior pertaining to mineral surface properties and soil solution properties
3. In combined experiments, there will be synergistic effects not observable in single experiments

3. Biochemistry - Se-uptake by *Oryza sativa*

The first part of this study is concerned with soluble Se and its uptake into and interactions with biota in the Critical Zone. While the biological components taking up Se could be either microorganisms, funghi, plants or animals such as insects or cattle - which all have a large impact on element cycles in the Critical Zone - this study focuses on biochemical properties as they pertain to the uptake of Se by plants. Given that in continental ecosystems Se is primarily introduced into the foodchain by plants, this approach targets the interface between abiotic Se and biotic Se compartments of the Se cycle.

3.1. Selenium in higher plants

Selenium content in plants generally reflects the levels of bioavailable Se in the parent soil, which is why most plant species contain less than 5 $\mu\text{g/g}$ Se dry weight (DW) [Fernández-Martínez & Charlet, 2009]. Exceptionally high amounts of Se are taken up by Se-hyper-accumulators, like those of the genera *Astragalus* and *Stanleya*, which can accumulate up to 10 - 15 mg/g Se DW from soils containing only 2 - 10 $\mu\text{g/g}$ Se DW [Virupaksha & Shrift, 1965]. It is believed that the majority of plants take up Se due to its similarity to sulfur (S), because, as of yet, Se has not been shown to be essential for the completion of the life cycle of plants [Läuchli, 1993, Pilon-Smits et al., 2009]. However, there have also been studies on possible allelopathic roles of Se-uptake by plants, such as protection from

herbivores or pathogens [Quinn et al., 2008, Cappa et al., 2014].

Selenate is accumulated in plants against its electrochemical potential gradient. Research on this fact revealed that selenate is taken up actively across the root plasma mediated by a high-affinity sulfate transporter, which is regulated positively by O-acetylserine and negatively by sulfate and reduced glutathione [Asher et al., 1977, Arvy, 1993, Terry et al., 2000].

sulfate and selenate uptake show both antagonistic and synergistic interactions when it comes to plant Se-uptake behavior. On the one hand, selenate competes with sulfate for uptake into plants and the presence of sulfate can inhibit Se-bioavailability. In Se-accumulators, on the other hand, selenate is taken up preferentially over sulfate in cases of high sulfate salinity [Terry et al., 2000]. Rice does not belong to the category of Se-accumulators. Nevertheless, rice plants have also been shown to take up Se preferentially in the presence of high sulfate [Bellet al., 1992, Terry et al., 2000].

Unlike selenate uptake, mechanisms of selenite uptake are still a matter of debate. In the past, studies suggesting passive uptake of selenite acknowledged having difficulties providing final evidence supporting their theory [Ulrich & Shrift, 1968, Asher et al., 1977]. Nonetheless, this theory is still being cited [Zhang et al., 2003]. However, more recent studies have reported uptake competition by phosphate as well as by sulphite [Hopper & Parker, 1999, Zhang et al., 2006, Li et al., 2007] and partial sensitivity to metabolic inhibitors [Li et al., 2007]. This suggests that active and specific mechanisms are responsible for selenite transport, with uptake likely to be governed by the phosphate transporter system [Li et al., 2007] and/or a silicon influx transporter system [Zhao et al., 2010].

Uptake of Se can also occur when Se is present in organic forms such as selenomethionine (SeMet) [Zayed et al., 1998]. There is also evidence that Se(0) has, until now, falsely been believed to be bio-unavailable and that Se(0)-nanoparticles might indeed be taken up as well [Fernández-Martínez & Charlet, 2009].

Translocation of Se within the plant strongly depends on the form of applied Se. Selenate was found to behave similarly to sulfate, entering plasma membranes of root cells unspecifically by the high-affinity sulfate transporters [Khan & Hell, 2014]. Throughout the plant, selenate then enters xylem transport vacuole membranes, inner plastids and tonoplasts

unspecifically by further sulfate transporters [Khan & Hell, 2014] and is, therefore, quickly transported into shoots via xylem and phloem [Carey et al., 2012]. Its similarity to sulfate causes selenate to be reduced by the same pathways as sulfate as well, yielding selenide and finally selenocysteine (SeCys), which can be specifically methylated to produce the non-protein amino acid methyl-selenocysteine (MeSeCys) [LeDuc et al., 2004, Khan & Hell, 2014]. Selenite, on the other hand, is believed to be retained in the roots, but not as selenite [Läuchli, 1993]. Rather, selenite is transformed into organic compounds, such as SeMet, MeSeCys or SeCys, which are then distributed throughout the plant at a much lower rate, exclusively via phloem [Asher et al., 1977, Zayed et al., 1998, Terry et al., 2000, Sun et al., 2010].

3.2. Rice (*Oryza sativa*) as a model plant

The model plant of choice for our experiments is rice (*Oryza sativa*) of the cultivar *nihonmasari*. Rice, also known as the 'cereal crop of the world's poor' [Cantrell & Reeves, 2002], has been cultivated as a crop for more than 7,000 years. Currently, it sustains more than half of the world's population [Izawa & Shimamoto, 1996, FAOSTAT, 2012], most of whom are desperately poor [Cantrell & Reeves, 2002]. Though there are two cultivated rice species, *Oryza sativa* – also referred to as Asian rice – and *Oryza glaberrima* – referred to as African rice –, the predominant species *Oryza sativa* is the main staple of rice-growing countries as well as the main focus of subsequent research.

Oryza sativa is a diploid, annual, short-day monocotyledonous cereal plant which self-fertilizes [Izawa & Shimamoto, 1996]. What makes rice so interesting as a model plant is the fact that its genome is much shorter than comparable monocotyledonous cereals such as maize and wheat, although it shares much genetic similarity with these other crop-relevant plants [Cantrell & Reeves, 2002]. Due to its tremendous importance for human nutrition, the rice plant has been of great interest to research, leading to early genome sequencing [Goff et al., 2002] and detailed molecular mapping which, in turn, makes it an even better model

plant for further research [Cantrell & Reeves, 2002].

However, the genetics of Se-accumulation are barely investigated, although it is well documented that inter- and intraspecific variations in Se accumulation in plants exists [Zhu et al., 2008]. Moreover, biofortification of food plants with Se is generally problematic. On the one hand, simultaneous fortification with Se together with other nutrient elements such as S is challenging due to uptake competition and metabolic crosstalk [Khan & Hell, 2014]. On the other hand, rice is able to take up Se beyond the recommended limits of human Se intake, so that fortification may lead to toxicity [Huang et al., 2013]. Therefore, our study was focused on clarifying antagonistic influences of nutrient addition and Se-fortification on one of human nutrition's most vital crops.

Previous research on Se-uptake into cereals has focused on agricultural water management [Li et al., 2010] and Se biofortification, such as uptake from Se-supplemented soils by barley [Gissel-Nielsen, 1973], wheat and ryegrass [Keskinen et al., 2010], durum wheat [Kikkert et al., 2013] and rice [Hu et al., 2002, Li et al., 2010]. In addition, mechanistic biomolecular studies on inner-plant transportation or single-ion competition have been conducted on excised barley roots [Leggett & Epstein, 1956, Ferrari & Renosto, 1972] and rice [Mikkelsen & Wan, 1990, Zhao et al., 2010, Carey et al., 2012].

Experimental set-ups vary greatly between these studies, depending on research focus. On the one hand, selenium addition to soils, which resemble the situation in real-world environmental conditions more closely, is a meaningful strategy to study biofortification. However, this approach is not appropriate to investigate the mechanisms of speciation or ion competition, because these are obscured by the complex interactions of Se and other nutrient components with multiple soil minerals. As major constituents of natural soils, organic matter, clay minerals and iron oxides or hydroxides, for example, add considerable sorption and complexation processes, which influence Se availability to the plant depending on pH-values and speciation of the added Se [Bar-Yosef & Meek, 1987, Balistrieri & Chao, 1990, Neal, 1995, Fernández-Martínez & Charlet, 2009]. Moreover, rice is unique in that it has specifically adapted to flooded conditions [Bellet al., 1992], where Se is most likely to be present as selenite [Zhao et al., 2010], elemental Se or selenide [Li et al., 2010]. Approaches

such as these are intermediate- or long-term experiments (weeks or months), in which microbiological activity or plant growth-related changes create a dynamic equilibrium difficult to model in its complexity.

On the other hand, short-term excision experiments (hours or days) are the best solution for specifically focused bio-molecular studies on inner-plant transposition [Leggett & Epstein, 1956, Ferrari & Renosto, 1972]. However, plants in such experiments are usually exposed to Se after pre-cultivation in Se-free medium, which does not address the agronomically important aspect of germination and early seedling development in the presence of Se. Although the effect of Se on rice germination itself has been addressed [Liu & Gu, 2009], subsequent plant growth was not part of that study, so that an integrated view on early development in the presence of Se is lacking so far. A more holistic approach on the complexity of speciation-dependent uptake, translocation and distribution exists for wheat [Li et al., 2007]. Their focus, however, was on single-ion competition.

Therefore, neither Se-toxicity in early-stage rice seedlings nor nutrient supply effects thereupon have yet been explored. In this study, rice is considered to be most suitable for the plant-box studies, as it is an easily cultivated and well-known model organism with great relevance to human nutrition. This provides the basis for experiments on Se bioavailability and toxicity in early-stage seedling growth depending on Se concentration and Se species (Chapter 3.3.2), nutrient competition effects on Se uptake (Chapter 3.3.3) and influences on Se-bioavailability due to soil sorption processes dependent on mineral surface properties and Se species (Chapter 6.5c).

3.3. Experimental set-ups

Quantifiable characterization of an element in an intricate system such as the Critical Zone requires a maximum of controllable parameters concerning in- and output to and from this system.

To determine the variables influencing Se uptake into plants, it was essential to create

an environment with ideal growth conditions so that ailments due to external factors unrelated to Se-uptake, such as nutrient deficiency, lack of light or insufficient temperature and water provisions could be excluded. Otherwise, signs of malnutrition in plants might be misinterpreted as Se toxicity symptoms or malnutrition might induce other metabolic pathways in the plants uncommon in healthy agricultural crops.

Plant requirements provided in this study are: sufficient photosynthetically usable light, CO₂ partial pressure, optimal temperature and humidity appropriate for the species' growth, all of which can be adjusted in a climate chamber or restricted area green houses with special lighting.

Furthermore, plants require water, nutrients and a substrate firm enough to offer rooting support for the plant. This has direct implications for this study. To determine plant-dependent parameters in the Se cycle in the Critical Zone, four plant experiments were conducted differing in nutrient supply and germination Se exposure (Exp. A1, A2, A3 and A4), the first of which is an open culture, while the following three are closed plant-box cultures.

3.3.1. Exp. A1 - open rice cultures in Se-nutrient solution

In this first plant-based experiment, emphasis was placed on the nutritional and water supply requirements of *Oryza sativa* plants. These were monitored and quantified for future closed-system-experiments.

To this purpose, cultures of *Oryza sativa* of the cultivar of *nihonmasari* were sterilized, grown on agar to a size large enough for re-potting, and then transferred to the actual experimental set-up, which consisted of flower pots filled with chemically nearly inert quartz sand. This experiment focused on plant uptake of nutrients and water provided by a specially devised nutrient solution.

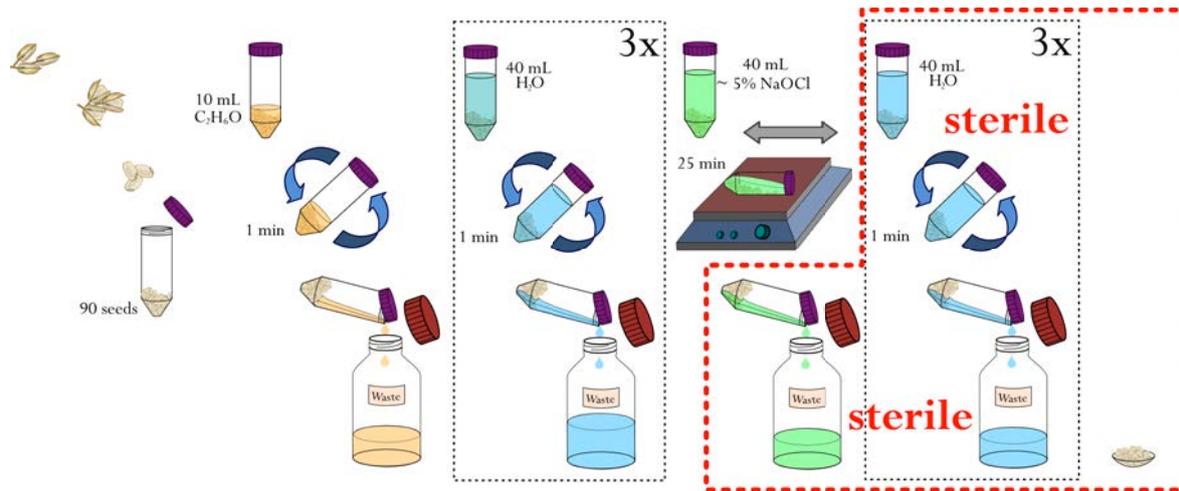


Figure 3.1.: *Sterilization procedure for 40 - 100 rice caryopses in a 50-mL-PP-centrifuge tube (VWR 525-0155): removal of the husks (palm husker, Ambala Associates), pre-sterilising in ethanol for 1 min before decanting (10 mL of 70 % ethanol, mixed as 700 mL p.a. ethanol absolute (Roth, Art. No. 9065.4) and 300 mL of double-deionized water), rinsing with double-deionized water three times, sterilising in 40 mL of 5 % NaOCl (as 400 mL NaOCl stock solution (Roth Art. No. 9062.3, 12 % active Cl) and 600 mL double-deionized water), shaking at 120 rpm for 25 min; subsequent NaOCl decanting and 3 times rinsing in 40 mL of autoclaved double-deionized water are done under sterile conditions*

Rice pre-cultivation in plant-boxes

The sterilization of caryopses for all experiments in the course of this study followed the same standardized explant-surface sterilization protocol used in most laboratories [Oyebanji et al., 2009], which was adjusted empirically in terms of durations and solution amounts as shown schematically in Figure 3.1.

In preparation for planting, two assembled plant-box sets, each with a lower half (Sigma Aldrich, Art. No. V8380) and an upper half (Sigma Aldrich, Art. No. V8505) connected with a coupler (Sigma Aldrich, Art. No. C0667), were autoclaved in a Systec VE-95 at 123.5 °C and 210.4 kPa for a sterilization time of 15 minutes along with 200 mL 0.4 % (=0.8 g) phytoagar (Duchefa Direct, CAS # 9002-18-0) in a 500 mL Schott duran glass bottle. Under cleanbench conditions, 100 mL of the autoclaved, warm liquid agar were poured into the smaller half of each of the magenta box sets and left to cool down to room temperature. Twenty caryopses were planted into each box in rows of four with the embryo facing upwards just below the surface of the cooled agar.



Figure 3.2.: *Seedlings grown in agar in plant-boxes;*
a: experimental set-up schematic (Inkscape);
b: Photo taken 30.04.2012 (3 days after sowing);
c: Photo taken 07.05.2012 (10 days after sowing)

Boxes were sealed under cleanbench conditions and then kept in a PAR (**P**hotosynthetically **A**ctive **R**adiation)-light chamber for 2 weeks to promote optimal growth (Figure 3.2).

Transfer into open cultivation in quartz sand

As shown in Figure 3.2 (right), the first plants reached plant-box height (ca. 13 cm) after 10 days. Therefore, it was not deemed advisable to keep them growing in such boxes for longer than a maximum of 2 - 3 weeks. Furthermore, with only phytoagar as a substrate, nutrient supply was not sufficient for further growth without risking malnutrition.

For transfer into a new experimental set-up, the following aspects were taken into account:

- available root space, which was varied by using two different pot sizes: ca. 300 mL and 900 mL flower pots (geli Thermo Plastic, PP Pflanzkübel Blumentopf Standard rund)
- inert substrate choice; to quantify nutrient and water uptake, quartz was chosen as a geochemically fairly inert substrate
- nutrient supply; to be able to control details of the nutrient solution composition, a specifically designed nutrient solution was required
- *Oryza sativa*-specific climate was attained by growing plants under greenhouse con-

ditions

Out of the 40 seedlings planted into agar on April 27th, 2012, 35 developed normally and were re-potted into quartz sand (Dorsillit No. 98 0.1-0.6 mm) on May 11th, 2012.



Figure 3.3.: *Preparation of open culture experiments*

a: flower pot taped with gauze;

b: watering the freshly re-potted seedlings with 35 mL of nutrient solution;

c: reference plants with nutrient solution filled to 400 mL

To keep the quartz sand from flowing out through the water holes of the plant pots due to liquefaction, these holes were taped with fishing gauze (Figure 3.3a).

The quartz sand was moistened with once-deionized water before filling ca. 750 mL into the large pots and ca. 250 mL into the small pots. As shown in Figure 3.3b, each of the 35 seedlings was planted separately into a pot and then watered with 35 mL of nutrient solution (preparation described below). After that, pots were organized into 6 green drainage boxes and each plant was labelled with a box number and plant letter in alphabetical order (Figure 3.4).

Nutrient supply and watering regime

The nutrient solution was composed specifically for this experiment, with nutrient content and concentrations based roughly on the Murashige & Skoog medium [Murashige & Skoog, 1962] and nutrient solutions used in other, similar experiments [Bellet et al., 1992] [Clement et al., 1977] [Asher et al., 1977]. Although rice can take up Fe(III) by using special chelating agents, Fe(II), is more soluble and more bioavailable [Ogo et al., 2007]. Therefore, Fe is the only element, which was added as the organic complex ferric citrate; all other elements

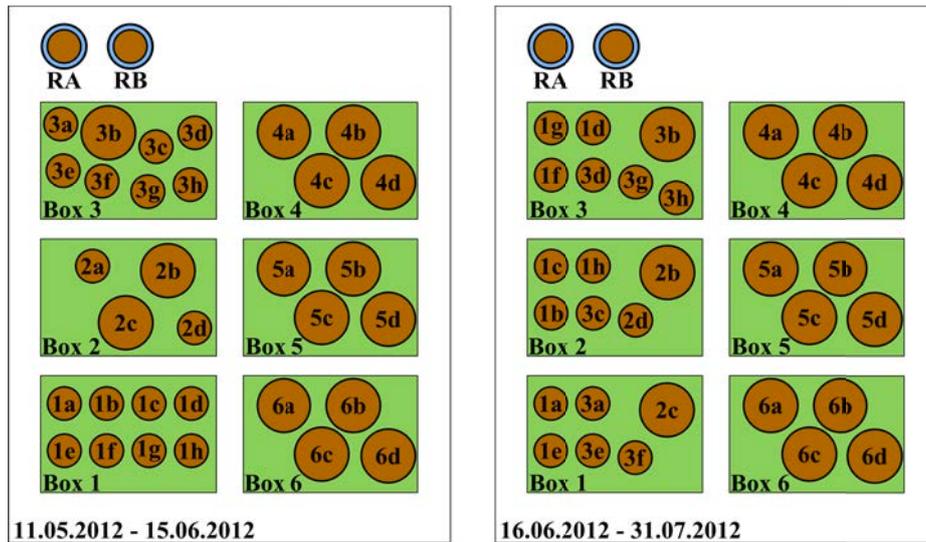


Figure 3.4.: Schematic drawing of plant order and labelling in *Exp. A1* (*RA*, *RB* = reference plants *A* and *B*);
 left: Plant order 11.05.2012 - 15.06.2012;
 right: change in plant order after change in watering regime 16.06.2012 - 31.07.2012

were added as inorganic compounds, primarily as sulfates, nitrates or phosphates.

Table 3.1 lists the compounds of this nutrient solution, which were all dissolved in double-deionized water. CuSO_4 , $\text{ZnSO}_4 \cdot \text{H}_2\text{O}$ and $\text{MnSO}_4 \cdot \text{H}_2\text{O}$ were dissolved together in 10 mL of double-deionized water. Except for ferric citrate, which was heated in an oven to 80 °C, all components were dissolved at room temperature.

The nutrient solution was stored at -20 °C as two concentrated stock solutions (factor 200), separating Ca-containing components and sulfates to avoid CaSO_4 precipitation (PhreeqC-modelling of solution saturation indices, Appendix Table A.4).

To be able to quantify the amount of water required by the plants through evapotranspiration, two plants were chosen as reference plants, *RA* and *RB*. As shown in Figure 3.3c, these plants in small pots were hung into 500 mL glass beakers. Each time the plants were watered, the amount of nutrient solution needed to bring the solution level back to the 400 mL line was noted for both plants.

Unlike the large drainage boxes, the small pots fit into the beaker without leaving the solution surface openly exposed to evaporation, therefore making it possible to determine the amount needed solely due to evapo-transpiration directly related to the plant. These

Table 3.1.: *Nutrient solution compounds of Exp. A1; inweight for target concentration of 100 L and required minimal dissolution volume of double-deionized water for the concentrate*

compound	product name	final solution concentration [mg/L]	in-weight for 100 L [mg/L]	disolving volume [mL]
Ca(NO ₃) ₂ · 4H ₂ O	Sigma-Aldrich, p.a. C1396-500G	236.145	23.596	40
K ₂ SO ₄	Merck, p.a. 1.05153.0500	65.346	6.532	120
MgSO ₄ · 6H ₂ O	Fluka, p.a. 00627	74.248	7.435	30
KH ₂ PO ₄	Merck, p.a. 1.04873.1000	13.608	1.360	40
H ₃ BO ₃	Sigma-Aldrich, p.a. B6768-500G	0.495	0.049	25
CuSO ₄	Sigma-Aldrich, p.a. 61230-100G	0.032	0.003	10
ZnSO ₄ · H ₂ O	Sigma-Aldrich, p.a. 96495-250G	0.090	0.001	10
MnSO ₄ · H ₂ O	Sigma-Aldrich, p.a. M7634-100G	0.034	0.003	10
CaCl ₂	Merck, p.a. 1.02378.0500	5.549	0.555	20
Na ₂ MoO ₄ · 2H ₂ O	Merck, p.a. 1.06521.0100	0.012	0.002	15
C ₆ H ₅ O ₇ Fe	Sigma-Aldrich, p.a. F6129-250G	12.247	1.224	200

amounts were used to determine nutrient solution volume for all plants.

Using a Schott bottle cap (27 mL ± 3 mL), plants were watered three times a week (Mondays, Wednesdays and Fridays) with nutrient solution, which was both the plant's sole source of water and only source of nutrients. Half of the plants were watered with 27 mL/day of nutrient solution, while the other half was watered with 55 mL/day of nutrient solution to quantify vitality differences due to lower nutrient uptake. Plants were grown in this fashion from May 11th, 2012 to July 15th, 2012. Table A.3 (Appendix) lists the volumes of nutrient solution used for a single plant in each of the boxes.

Addition of Se

The open culture experiment had to be modified due to some plants showing fungal infection, loss of vitality and overall inhomogenous plant development (Figure 3.5). Plants were categorized into "low nutrient solution supply" and "high nutrient solution supply" as well as into "big pot" and "small pot". On July 16th, 2012, 65 days after transfer into open cultures, plant pots were re-arranged (Figure 3.4) to distribute plants of each category evenly among the drainage boxes. A 1000 mg/L Se-stock solution was prepared of sodium selenate decahydrate, Na₂SeO₄·10H₂O (VWR BDH Prolabo, 302113L) in 100 mL

of double-deionized water. As shown in Figure 3.5, for the following 2 weeks, boxes 3 and 4 and reference plant RB were watered with nutrient solution, boxes 2 and 5 were watered with nutrient solution spiked with 2.5 mg/L Se and boxes 1 and 6 as well as reference plant RA were watered with nutrient solution spiked with 5 mg/L Se.

Plants were harvested on July 31st 2012 as described below (Chapter 3.4.1).

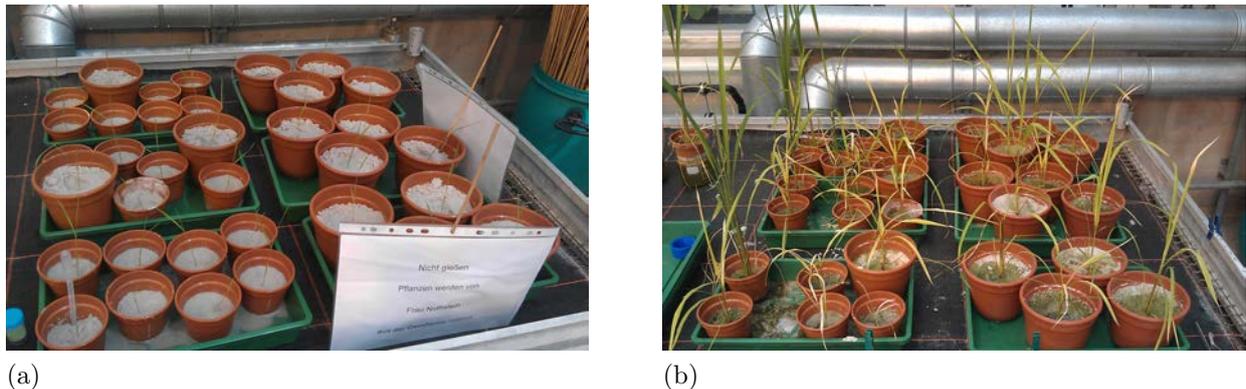


Figure 3.5.: *Photos of A1 experimental set-up for Se addition to open culture rice plants*
a: beginning of experiment (Photo taken 14.05.2012)
b: plant growth until addition of Se (Photo taken 27.07.2012)

3.3.2. Exp. A2 - plant-box rice cultures in Se-agar

The second set of experiments focused on Se uptake directly during germination and toxicity in early-stage growth of rice plants. Since quantifying input and output is easiest in closed systems, a plant-box solution was chosen. As mentioned in Exp. A1 (Chapter 3.3.1), this restricted the plant growth period to a maximum of three weeks.

For the first set of plant-box experiments (Figure 3.6a), 10 assembled Magenta box sets (Sigma Aldrich, Art. No. V8380, V8505 & C0667) were autoclaved in a Systec VE-95 at 123.5 °C and 210.4 kPa for a sterilization time of 15 min, together with 1200 mL 0.4 % (= 4.8 g) phytoagar (Duchefa Direct, CAS # 9002-18-0), a 100-mL measuring cylinder and 200 mL of double-deionized water. Ninety rice caryopses were sterilized according to the procedure described above in Chapter 3.3.1.

From a 1000 mg/L Se stock solution (in double-deionized water, either $\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$ [VWR BDH Prolabo 302113L], or Na_2SeO_3 [AlfaAesar 012585], respectively), 10 mL of a

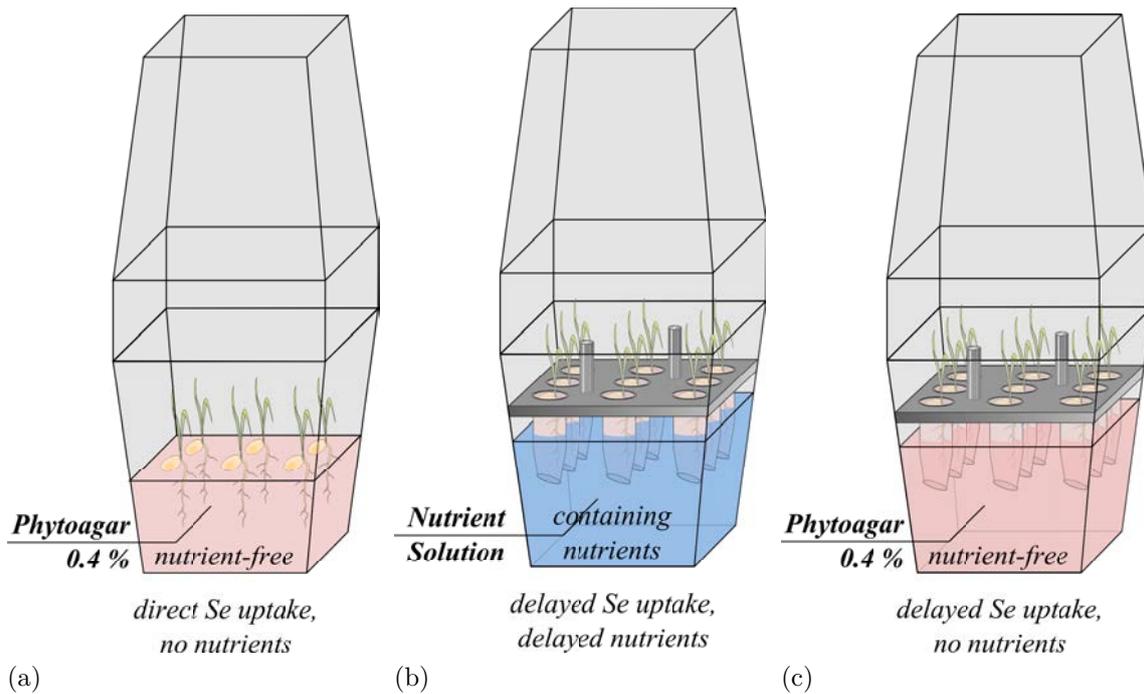


Figure 3.6.: Schematics of Exp. A2, A3 & A4

a: Se-agar experiments contained 6 rice plants grown in 100 mL Se-agar for 16 days with Se concentrations of 0, 5, 10, 25, 50, 100, 250, 500, 1000 and 2500 $\mu\text{g/L}$ Se added as either selenate or selenite.

b: Se-nutrient solution experiments contained 9 rice plants grown for 19 days, sprouting first in Se-free agar in Eppendorf tubes before reaching 170 mL of Se-spiked nutrient solution (0 – 2500 $\mu\text{g/L}$ Se) after ca. 5 days.

c: Se-agar experiments with delayed Se-uptake contained 9 rice plants grown for 19 days, sprouting first in Se-free agar in Eppendorf tubes before reaching 170 mL Se-spiked agar (0 – 2500 $\mu\text{g/L}$ Se) after ca. 5 days.

All three sets of experiments were kept in a climate chamber with an 8h-short-day rhythm, 1 h of each dusk and dawn and a temperature of 28 °C during the day period and 22 °C during the night period.

100 mg/L Se solution in double-deionized water was sterilized in the cleanbench using a 0.22- μm sterilization filter (Omnifix T550.1, Rotilabo P 666.1).

Under cleanbench conditions, plant-boxes were opened and 100 mL of the autoclaved liquid 0.4 % agar (ca. 50 °C) was poured into the smaller half of each of the plant-box sets.

While the agar was still liquid, though not hotter than 50 °C, the sterilized Se-solution was added to yield the appropriate final concentrations (0, 5, 10, 25, 50, 100, 250, 500, 1000 and 2500 $\mu\text{g/L}$ Se). Using a 5-mL pipette tip, Se was homogenized in the agar before sampling 2 mL from each box into the allotted 20-mL patho-vessels (Böttger 08-313-1001), which had been prepared with 1 mL of nitric acid (VWR 20429.320 p.a. subboiled to

suprapure quality) and 1 mL of double-deionized water and weighed (including the lid and tape covering the marker-written labels to avoid washing off by sterilising ethanol). These were weighed to determine the exact weight per volume of the agar and kept at 4 °C. Plant-boxes were then left to cool until the agar was firm. As described in Chapter 3.3.1, 6 rice plants were sown into the agar and the boxes were sealed.

For the duration of 16 days, plant-box cultures were kept in a climate chamber (YORK Refrigeration) at 70 % humidity, and a sub-tropical 8h-short-day rhythm, 1 h of dusk and dawn each and a temperature of 28 °C during the day period and 22 °C during the night period. This time frame was calculated as 2 days of sprouting and 14 days of Se-uptake. Plant growth was monitored by measuring plant height on days 5, 7, 9 and 12 for each plant.

After 16 days, magenta box cultures were harvested as described below (Chapter 3.4.1). For each experimental set-up, three independent biological replicas were conducted, one of which was conducted by bachelor student Matthias von Brasch as part of his thesis under my supervision.

3.3.3. Exp. A3 - plant-box rice cultures in Se-nutrient solution

In the second plant-box experiment (Figure 3.6b), plants were grown in the presence of all essential nutrients, similar to the nutrient solution used in Exp. A1 (Chapter 3.3.1). Because these closed plant-box systems were not to be opened during the entire duration of the experiment, nutrient solution composition had to be modified to that of Exp. A1 (Chapter 3.3.1) to provide for the growing plants for the entire duration of the experiment. Optimal nutrient solution composition (Table 3.2) was obtained empirically in preliminary experiments.

The nutrient solution was stored at -20 °C as two stocks (factor 200), separating Ca-containing components and sulfates to avoid CaSO₄ precipitation.

Ten assembled Magenta plant-box sets (Sigma Aldrich, 2 x V8505 & 1 x C0667) were

Table 3.2.: *Optimized nutrient solution compounds of Exp. A3, inweight for target concentration of 100 L and required dissolution volume of double-deionized water*

compound	product name	final solution concentration [mg/L]	in-weight for 100 L [mg]	disolving volume [mL]
Ca(NO ₃) ₂ · 4H ₂ O	Sigma-Aldrich, p.a. C1396-500G	1180.745	118.0745	200
K ₂ SO ₄	Merck, p.a. 1.05153.0500	65.346	6.532	120
MgSO ₄ · 6H ₂ O	Fluka, p.a. 00627	74.248	7.435	30
KH ₂ PO ₄	Merck, p.a. 1.04873.1000	54.432	5.443	160
H ₃ BO ₃	Sigma-Aldrich, p.a. B6768-500G	0.495	0.049	25
CuSO ₄	Sigma-Aldrich, p.a. 61230-100G	0.064	0.006	10
ZnSO ₄ · H ₂ O	Sigma-Aldrich, p.a. 96495-250G	0.135	0.014	10
MnSO ₄ · H ₂ O	Sigma-Aldrich, p.a. M7634-100G	0.204	0.020	20
CaCl ₂	Merck, p.a. 1.02378.0500	5.549	0.555	20
Na ₂ MoO ₄ · 2H ₂ O	Merck, p.a. 1.06521.0100	0.018	0.002	25
C ₆ H ₅ O ₇ Fe	Sigma-Aldrich, p.a. F6129-250G	12.247	1.224	200

prepared (Figure 3.6b) with a specially designed Eppendorf tube tray holder for 9 x 1.5-mL tubes (1.5-mL Eppendorf Safe-Lock Microcentrifuge Tube, 0030120086). The plant-box sets, 90 1.5-mL Eppendorf tubes, 250 mL 0.7 % phytoagar, 2.5 L nutrient solution (preparation as given above), a 100-mL measuring cylinder and 250 mL double-deionized water were autoclaved. Sterile rice caryopses as well as Na₂SeO₄·10H₂O and Na₂SeO₃-standards were prepared as described above (Chapter 3.3.2).

After autoclaving, 1.5-mL reaction tubes (Eppendorf, Hamburg) were placed into a tray-holder under the cleanbench and filled to the brim with the still-liquid 0.7 % phytoagar. Only after the agar had solidified, were the lid and 0.5 cm from the bottom of each reaction tube cut off using sterilized scissors. Each tube was then loaded with one sterilized caryopse.

Plant-boxes were disassembled under the cleanbench, Eppendorf trays removed and 200 mL of nutrient solution filled into each lower half of the boxes. Specified concentrations of Se (0 - 2500 µg/L Se, as described in Chapter 3.3.2) were obtained by diluting the stock into the nutrient solution. After mixing the solutions with a pipette tip, 2 x 15 mL of each solution were sampled for subsequent analysis into 20-mL patho-vessels (Böttger 08-313-1001) - 15 mL were frozen for later IC measurement (Chapter 3.4.4), the other 15 mL were acidified with 50 µL of HNO₃ (VWR 20429.320 p.a. sub-boiled) and stored at 4 °C for later ICP-MS measurement (Chapter 3.4.4). For plant-box assembly, each Eppendorf

tray was loaded with 9 rice-bearing Eppendorf tubes and placed into the plant-box with the lower half of the tubes submerged in nutrient solution before closing the plant-box. These were kept under the same climate chamber conditions as described above (Chapter 3.3.2), keeping the boxes closed until harvest (Chapter 3.4.1). Each experimental set-up was repeated independently three times.

3.3.4. Exp. A4 - plant-box rice cultures in Se-agar with delayed Se-uptake

For the purpose of comparison, an experiment was devised to separate the two parameter differences of both previous plant-box experiments (Figure 3.6c). The non-nutrient-bearing agar of experiment A2 (Chapter 3.3.2) was combined with the uptake delay of the nutrient solution plant-boxes from experiment A3 (Chapter 3.3.3).

Similarly to the nutrient solution experiments, plant-boxes were prepared with trays of 9 x 1.5-mL Eppendorf tubes filled with 0.7 % phytoagar, each planted with one rice plant. Instead of nutrient solution, tray holders were placed into 170 mL liquid 0.4 % agar spiked with 0 - 2500 µg/L Se (as described above Chapter 3.3.3) with the lower half of the tubes submerged in agar before closing the plant-box. Boxes were left until the agar solidified and then placed in the climate chamber described above (Chapter 3.3.2). Plants were harvested after 19 days as described below (Chapter 3.4.1). This experiment was conducted only once for selenate and selenite, each.

3.4. Sample preparation and analytical methods

Because harvest, digestions and subsequent HG-FIAS analysis were alike for all plant experiments, as well as the IC- and ICP-MS analysis of all nutrient solution samples, the following chapter will detail these methods once.

3.4.1. Plant harvest

After photo-documentation using a Samsung S4 mini cell phone camera (Appendix, Figure ?? - ??, A.9 - A.13, A.20 - A.21), shoot height and 2nd leaf length were measured; then harvested plant material was cleaned under running mono-deionized water to remove quartz sand substrate (Exp. A1, Chapter 3.3.1), agar (Exp. A2, A4 Chapter 3.3.2, 3.3.3) or nutrient solution residue (Exp. A3, Chapter 3.3.3). Plants were then rinsed with double-deionized water before being air-dried for 2 h at standard lab conditions (22 °C, 1 atm, 30 % humidity) and separated into shoot and root above the caryopse (Figure 3.7a) using a pair of clean scissors. Each sample was weighed (Sartorius basic BA 1105) to determine fresh root and shoot weight.

Using a Christ Alpha 1-4, 100400 freeze-dryer, plant material was freeze-dried at 0.05 mbar and -20 °C for 24 h. After warming up to lab conditions, samples were weighed anew to determine plant water loss. Samples of the open culture experiments were milled using an agate disc mill (Scheibenschwingmühle-TS, Siebtechnik) to pulverize and homogenize the entire material of each sample. In the case of plant-box studies, root and shoot plant-box bulk samples were cut into 0.2 cm pieces using a clean pair of scissors. The use of Teflon scissors and Teflon forceps was discontinued due to massive static charge.

All plant samples were stored in 20-mL patho-vessels (Böttger 08-313-1001) at lab conditions until digestion (Chapter 3.4.2). To sample the viscous agar during the preparation of Exp. A2 (Chapter 3.3.2), the top 1 cm of a 5-mL pipette tip was cut off and using an adjustable 0.5-5-mL pipette, amounts of 2 mL of the still-liquid agar were directly pipetted and weighed (Sartorius basic BA 1105) into 20-mL patho-vessels (Böttger 08-313-1001) prepared with an in-weighed 1 mL of nitric acid (VWR 20429.320 p.a. subboiled to suprapure quality) and 1 mL of double-deionized water. To sample the cooled agar at the end of the experiment, agar was sampled directly from the plant-box after stirring it with a pipette tip. Due to the large amount of air within the cooled, stirred agar, patho-vessels were placed on a balance (Sartorius 1712MP8) and a weight of 2 g was sampled, rather than a volume of 2 mL. All plant and agar samples were stored in the refrigerator at 4 °C until

digestion.

From the nutrient solution experiments, 2 x 15 mL of nutrient solution was sampled from the plant boxes into 20-mL patho-vessels (Böttger 08-313-1001) - 15 mL were frozen for later IC measurement (Chapter 3.4.4), the other 15 mL were acidified with 50 μL of HNO_3 (VWR 20429.320 p.a. sub-boiled) and stored at 4 $^\circ\text{C}$ for later ICP-MS measurement (Chapter 3.4.4).

3.4.2. Microwave digestions

For the plant digestion, small adjustments were made to the procedure described in previous studies [Bellet al., 1992]. In-weights (Sartorius 1712MP8) of 0.1 g or less were filled into Teflon vessels (Figure 3.7b,c,d) of an MLS START 1500 Microwave System preconditioned with 3 mL of double-deionized water and 3 mL HNO_3 p.a. (VWR 20429.320) at 150 $^\circ\text{C}$ for 1 h on a hotplate (Ceran 500, LHG).

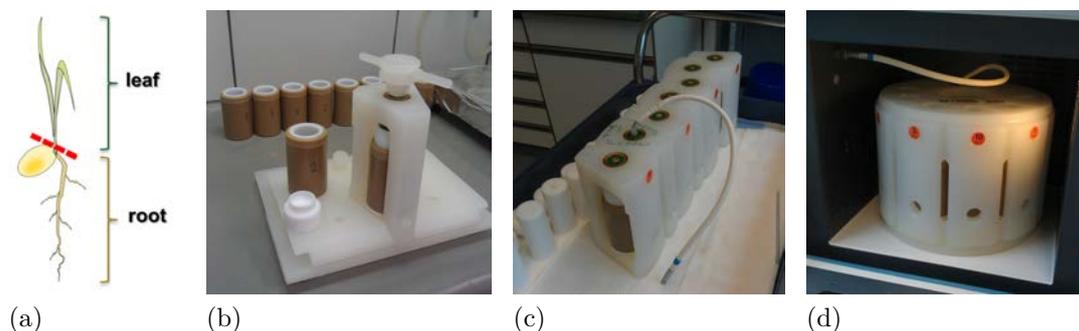


Figure 3.7.: *Plant digestion with a microwave system;*
a: separation of shoot and root (Inkscape illustration);
b: Teflon lid fixation onto Teflon vessels with pressure ring and vessel holders;
c: Teflon vessels in holders ready to be mounted;
d: Teflon vessels mounted in microwave

Samples were digested with 1 mL of double-deionized water, 3 mL HNO_3 conc. (VWR 20429.320 p.a. sub-boiled) and 1 mL of 30 % H_2O_2 (p.a. Rotipuran 8070.3). Each batch of 10 digestion samples included one Teflon vessel blank and one plant standard (0.1 g NBS SRM 1567a Wheat Flour) to verify digestion quality.

Applying the temperature program shown in Table 3.3, samples were digested in the microwave at up to 220 $^\circ\text{C}$ and 1000 W for 33 min. To avoid volatile Se loss, samples were

Table 3.3.: Digestion temperature program for microwave system START 1500

	t(min)	T (°C)	E (W)
	3	75	600
	8	130	700
	10	210	1000
	12	220	1000
	45	cooling	
total	1 h 18 min		

left in the microwave overnight to cool completely.

All digested samples, standards and blanks were quantitatively transferred into a 10-mL glass flask with a glass funnel and filled to volume with double-deionized water. Samples were then transferred and stored in 15-mL-centrifuge tubes (VWR 525-0149) in the refrigerator at 4 °C until analysis.

Agar digestions were prepared similarly to plant digestions, albeit with the additional difficulty of transferring the agar sample quantitatively into the Teflon vessels. This was achieved by using the remaining digestion ingredients (2 x 1 mL HNO₃ conc. and 1 mL of 30 % H₂O₂) to rinse all of the agar sample into the Teflon vessels.

3.4.3. Plant-Se and agar-Se analysis with HG-FIAS

Se-content of digestion samples was analysed with HG-FIAS (Hydride Generation Flow Injection Atomic Absorption Spectroscopy) with a Perkin Elmer AAnalyst200 coupled with a FIMS-400 Hydride Generation System and Autosampler. Before measurement, a reduction of selenate to selenite was necessary for the hydride to be able to form H₂Se, which could then be atomized in the quartz tube and measured [Bye & Lund, 1988]. To achieve concentrations within calibration range, samples were diluted by a factor of 2 to 1200 in 6 mol/L HCl (Merck, 37 %, low-Hg HCl 1.13386.2500). From a 1000 mg/L Se standard solution (Roth Rotistar ICP), 10 mL of calibration standard (1000 µg/L Se) were prepared in a 15-mL centrifuge tube (VWR 525-0149). A sample volume of 3 mL each in 15-mL centrifuge tubes (VWR 525-0149) and the calibration standard were reduced to selenite for 15 min in a water bath (Dinkelberg analytics, E30U) pre-heated to 75 °C.

After cooling, calibration concentrations of 0.5, 0.75, 1, 2, 4, 5, and 6 $\mu\text{g/L}$ Se (for open culture samples: 0, 0.5, 1, 2 and 5 $\mu\text{g/L}$) were prepared with 1 mol/L low-Hg HCl from the reduced Se solution. Then all samples were diluted to 12 mL with double-deionized water before measurement. Using a reducing agent of 0.2 % NaBH_4 (Merck 8.06373.0500) in 0.05 % NaOH solution, a carrier solution of 1 mol/L HCl (Merck, 37 %, low-Hg HCl 1.13386.2500) and an argon carrier gas flow rate of 50 - 70 mL/min, Se concentration was measured with 5 replicates (3 for open culture samples) as the peak height of atomic absorption at a wavelength of 196.2 nm (background subtraction: off, a 260-V EDL-lamp, slit width: 2.7/2.3, quartz cell temperature: 900 °C).

To verify measurement quality, a multi-element drinking water standard (PromoChem Trace Metals QCP 050-1 and QCP 050-2 combined, with 252 $\mu\text{g/L}$ Se) was included with a dilution factor of 120, as well as a reduction blank of 6 mol/L HCl. For the purpose of quality control, within each measurement, all standards were re-measured as samples after every 10 samples for linear interpolation of drifts and the trace metal standard was measured at the beginning and end of the measurement.

3.4.4. Nutrient solution analysis with IC and ICP-MS

Ion chromatography (IC) analysis of anions was conducted using a Dionex ICS 1000 with an IonPac AS14 column coupled with an IonPac AG14 pre-column. The eluent consisted of a mixture of 3.5 mmol/L Na_2CO_3 and 1.0 mM NaHCO_3 with an eluent flow rate of 1.10 mL /min. Frozen nutrient solution samples were thawed prior to measurement and diluted by a factor of 4 with double-deionized water before being filled into IC-vials covered with filter caps.

A multi-ion IC-standard calibration solution (Alfa Aesar, Specpure) containing fluoride, chloride, bromide, nitrate, phosphate and sulfate in proportions of 1 : 2 : 4 : 4 : 6 : 4, respectively, was diluted to calibration standards containing 1, 2.5, 5, 10 and 20 mg/L fluoride. Using an Anion Self-Regenerating Suppressor (ASRS 300), conductivity of samples was detected at an applied current of 25 mA for an injection volume of 25 μL .

Computer-aided peak analysis over the detection span of 14 min was manually adjusted for optimal standard comparability. Sample standard deviation (SD) was calculated by applying the 1σ percentile of repeated calibration solution measurements to all samples for each ion. A river water standard (BATTLE-02, Environment Canada; 42.4 mg/L Cl⁻, 0.194 mg/L F⁻, 149 mg/L SO₄²⁻) was measured with a dilution factor of 2 to confirm analytical accuracy. For the purpose of quality control, within each measurement batch, one calibration standard was re-measured as a sample after every 8 - 12 samples for linear interpolation of drifts and the river water standard (to determine analytical reproducibility) was measured once per measurement batch.

Analysis of ¹¹B, ²³Na, ²⁵Mg, ²⁶Mg, ³¹P, ³⁹K, ⁴²Ca, ⁴³Ca, ⁵⁵Mn, ⁵⁶Fe, ⁶³Cu, ⁶⁵Cu, ⁶⁴Zn, ⁶⁶Zn, ²⁵Mg, ⁷⁷Se, ⁷⁸Se, ⁸²Se, ⁹⁵Mo, ⁹⁸Mo, was performed using an inductively coupled plasma mass spectrometer (ICP-MS) X-Series 2 (Thermo Fisher Scientific). Five mL of sample were diluted by factors of 2 - 10 in 1 % subboiled HNO₃. Each sample was spiked with 50 µL of internal standard (10 µg/L Sc, Merck 1.70349.100; 10 µg/L Rh, Merck 1.70345.0100; 10 µg/L In, Merck 1.70324.0100; 10 µg/L Tm, Merck 1.70361.0100), which were measured as ⁴⁵Sc, ¹⁰³Rh, ¹¹⁵In and ¹⁶⁹Tm. Calibration was carried out using the ICP multi-element standard solution VI Certipur (Merck 1.09493.0100) in dilution factors of 20,000, 10,000, 4000, 2000, 1000, 400, 200, 100, 20 and 10. Added to the multi-element standard, P (Merck 1.70340.0100) was calibrated with 5, 10, 25, 50, 100, 250, 500, 1000, 5000 and 10,000 µg/L. Calibration was extended to 5 and 10 mg/L Na (Merck 1.70353.0100), Mg (Merck 1.703331.0100), K (Merck 1.70342.0100) and Fe (Merck 1.70326.0100), as well as 25 and 50 mg/L Ca (Merck 1.70308.0100) using single element standards. Verification of analysis quality was achieved by measuring a trace metal standard CRM-TMDW-A (High Purity Standards) with a dilution factor of 5. For the purpose of quality control, within each measurement batch, one standard was re-measured as a sample after every 8 - 12 samples for linear interpolation of drifts and the trace metal standard was measured at the beginning and end of the measurement batch.

Gas flow of the argon sample carrier gas (nebulizer gas) was 0.87 L/min, flow of argon fuel gas (auxiliary gas) was 0.68 L/min and flow of argon cooling gas was 13 L/min. Each sample

was measured in three different modes. First, a survey scan of 10 sweeps with a dwelling time of 13 seconds was performed to obtain a general overview of the sample's content. Then, the main peak jump was determined by measuring in CCT-ED mode (Collision Cell Technology – Energy Discrimination), with 3 times 40 sweeps and a dwelling time of 14 seconds for the remaining elements Na, P, K, Mn, Fe, Cu, Zn and Se. In CCT-ED measuring mode, the detection limit was lowered by including a collision cell between the plasma torch and the quadrupole mass spectrometer, in which collision gas, a mixture of 92 % He and 8 % H₂, was injected at an intercepting angle, colliding with the ionized sample gas. Compound clusters between argon and hydrogen with themselves, each other and sample elements were thereby slowed or destroyed and did not interfere with the actual sample measurement. After that, the main peak jump was measured for the elements B, Mg, Ca and Mo in standard measuring mode with 3 times 40 sweeps of 25 seconds dwelling time per isotope and 30 seconds of acquisition per run. In solutions, in which only Se was measured, 3 times 40 sweeps with a dwelling time of 25 seconds per isotope resulted in an acquisition time of 14 seconds per run.

3.5. Results for the Se treatment of rice plants

In the following chapter, results on the Se content of rice shoots and roots are given for each of the experiments listed above and combined with results on further parameters of plant health, such as plant mass, shoot height and heights of the second leaf.

3.5.1. Exp. A1 - open rice cultures in Se-nutrient solution

Quality measures for experiment A1 (Chapter 3.3.1) showed that harvested plant yield was 91 % of transferred seedlings. Digestion standard retrieval was 85 % (± 24 %) and drinking water standard retrieval during HG-FIAS measurement was 105 % (± 9 %).

Selenium concentrations for the additions of 2.5 or 5 mg/L measured in the rice plants of experiment A1 ranged from 23 to 113 mg/kg DW for shoots (Figure 3.8a) and 4 to 207 mg/kg DW for roots (Figure 3.8b). Mean values and standard deviation ($\pm 1s$) did not

differ significantly between shoot Se-uptake after 2.5 mg/L Se addition (55 mg/kg DW, \pm 35) and shoot Se-uptake after 5 mg/L Se addition (51 mg/kg DW, \pm 31).

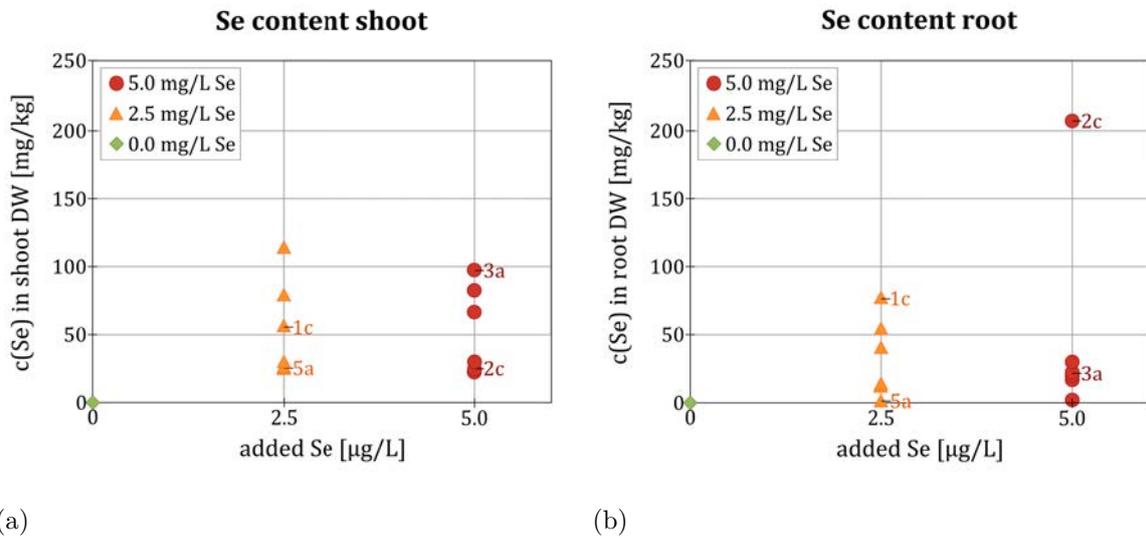


Figure 3.8.: Plant Se content after addition of 0, 2.5 or 5 mg/L Se to open culture rice plants for 2 weeks after 63 days of Se-free growth
 a: Se content in shoots
 b: Se content in roots

Similarly, no significant difference was found in the mean values between root Se-uptake after 2.5 mg/L Se addition (40 mg/kg DW, \pm 27) or after 5 mg/L Se addition (48 mg/kg DW, \pm 71). Standard deviation was higher for the values of 5 mg/L root uptake, due to the outlier 2c, which had a very high Se content compared to all other samples (Figure 3.8b). When excluding the outlier 2c, however, mean root uptake was lower for 5 mg/L Se addition (21 mg/kg DW, \pm 10) compared to 2.5 mg/L Se addition. Therefore, differences in Se shoot content were negligible for both Se concentrations, but not for root Se content. Here, addition of 5 mg/L Se resulted in only 53 % of root content compared to the addition of 2.5 mg/L. Furthermore, Se content of the root was lower than in the shoot. Root-Se for the addition of 2.5 mg/L Se was 72 % of shoot-Se and root-Se for the addition of 5 mg/L is 42 % of that in the shoots, excluding the outlier 2c.

When plants were differentiated according to experimental conditions (Figure 3.9), a Se-content distribution pattern emerged. Plants 1c and 2c were defined as outliers because their root Se-content was higher than their shoot Se-content. For all others, it was found

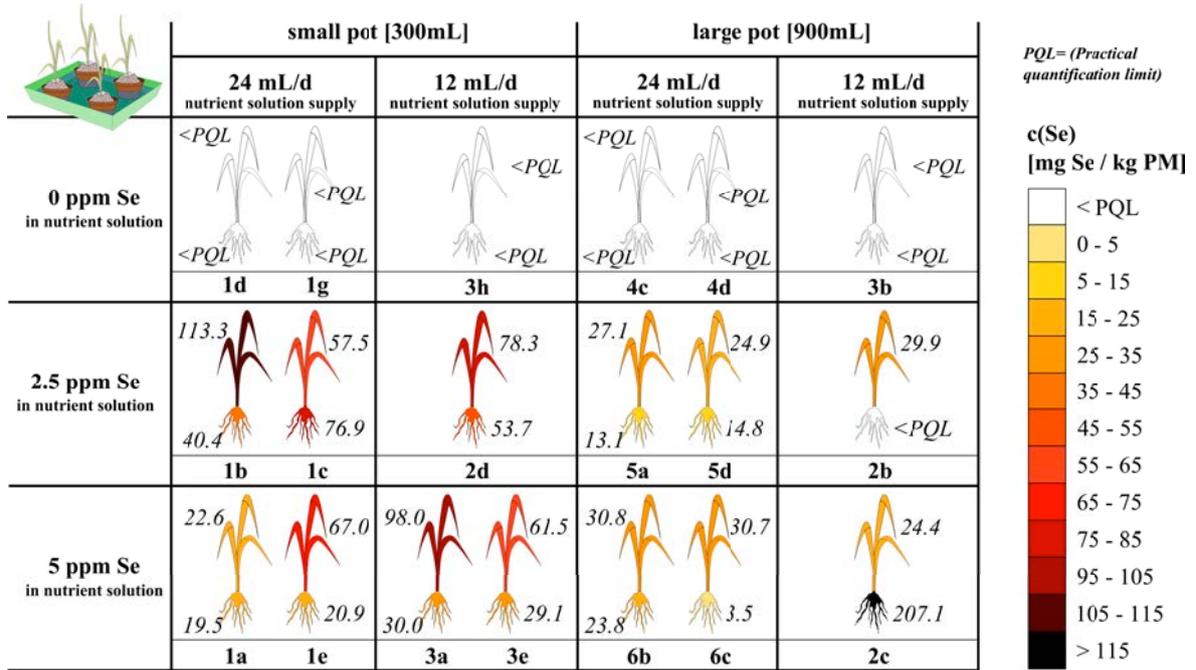


Figure 3.9.: Single-plant Se content in shoots and roots of experiment A1

that not only did pot-size play a role in the Se-uptake, but plant mass as well. Values for the two outliers 1c and 2c, as well as values for plant 3a and 5a representing 5 and 2.5 mg/L Se addition, respectively, are highlighted in each of the following graphs for better orientation.

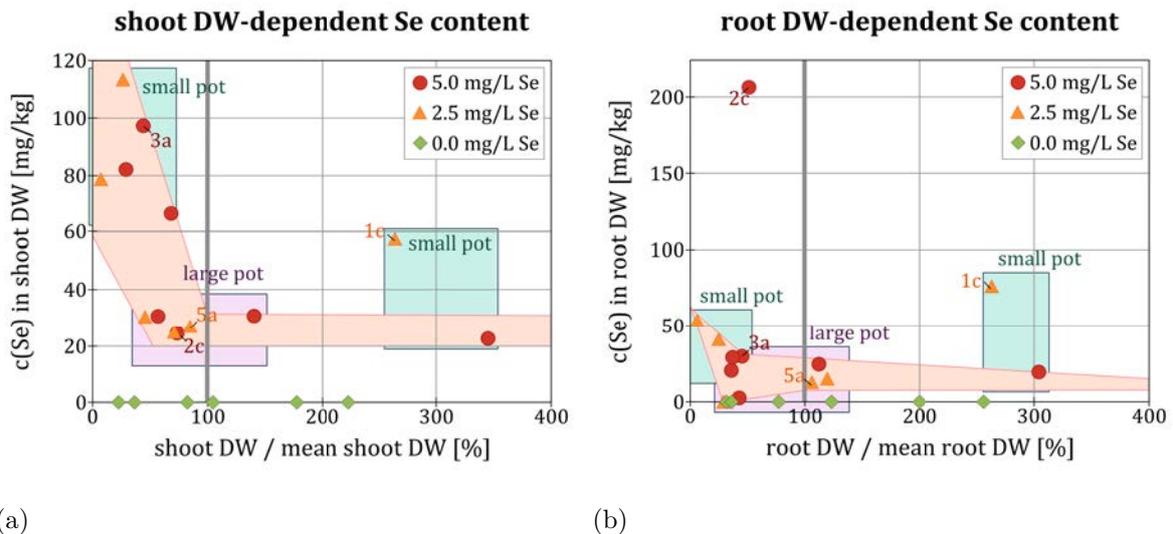


Figure 3.10.: Tissue Se content per percentage of average mass as an indicator of plant health

- a: Shoot Se content per percentage of average shoot mass
- b: Root Se content per percentage of average root mass

Figure 3.10a shows that plants with a lower-than-average shoot mass (7 - 44 %) - which were all found in small pots - showed the highest Se-shoot content (78 - 113 mg/kg DW). Selenium content decreased (67 - 24 mg/kg DW) as shoot mass approached average values (45 - 84 %), which was typical of plants from large pots. Selenium content remained low (31 - 23 mg/kg DW) in plants of higher-than-average mass grown in small pots, except for the outlier 1c (57 mg/kg DW for 265 % of average mass). For roots, disregarding the outliers 1c and 2c, this trend was similar, with plants of lower-than-average root mass (6 - 35 %) reaching the highest Se content (54 - 21 %) and plants with root mass closer to average (29 - 45 %) reaching the lowest Se content (0 - 30 mg/kg DW). For plants with above-average root mass (106 - 120 %), Se content remained low (13 - 24 mg/kg DW). Pot-size classification of root-Se was similar to that of shoots.

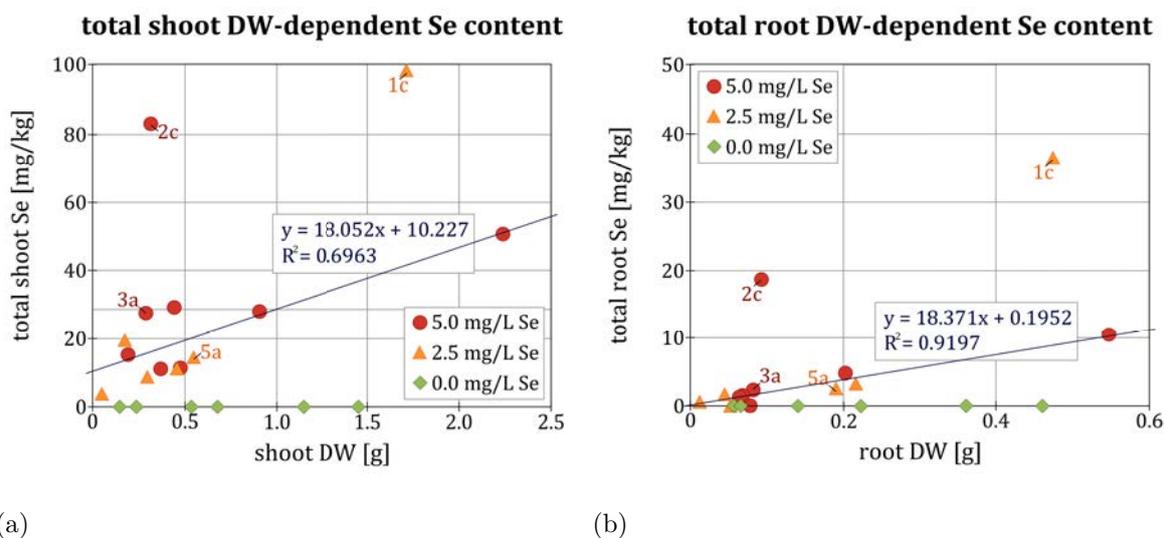


Figure 3.11.: *Independence of Se-uptake of plant health*
 a: linear correlation between total shoot Se and shoot DW
 b: linear correlation between total root Se and root DW

In cases in which Se-uptake is similar for two plants of different masses, pure plant mass could lead to dilution effects that have nothing to do with Se-uptake properties. Any non-linear correlation of Se content with plant mass is, therefore, a sign of either dilution effects or defective mechanisms in uptake regulation due to impaired plant health. Figure 3.11 shows there was no evidence of non-linear behavior. Instead, linear correlations between Se content and plant mass for both shoots and roots showed a good linear fitting ($R^2 =$

0.6933) for shoot-DW-dependent Se content and a very good fitting for root-DW-dependent Se content ($R^2 = 0.9197$) for both Se concentrations added.

3.5.2. Exp. A2 - plant-box rice cultures in Se-agar

Quality measures for experiment A2 (Chapter 3.3.2) showed that harvested plant yield was 84 % (± 6 %) of planted caryopses for selenite and 88 % (± 6 %) for selenate. Digestion standard retrieval was 84 % (± 9 %) and 85 % (± 19 %) for selenite and selenate, respectively, and drinking water standard retrieval during HG-FIAS measurement was 102 % (± 7 %) for all samples of experiment A2.

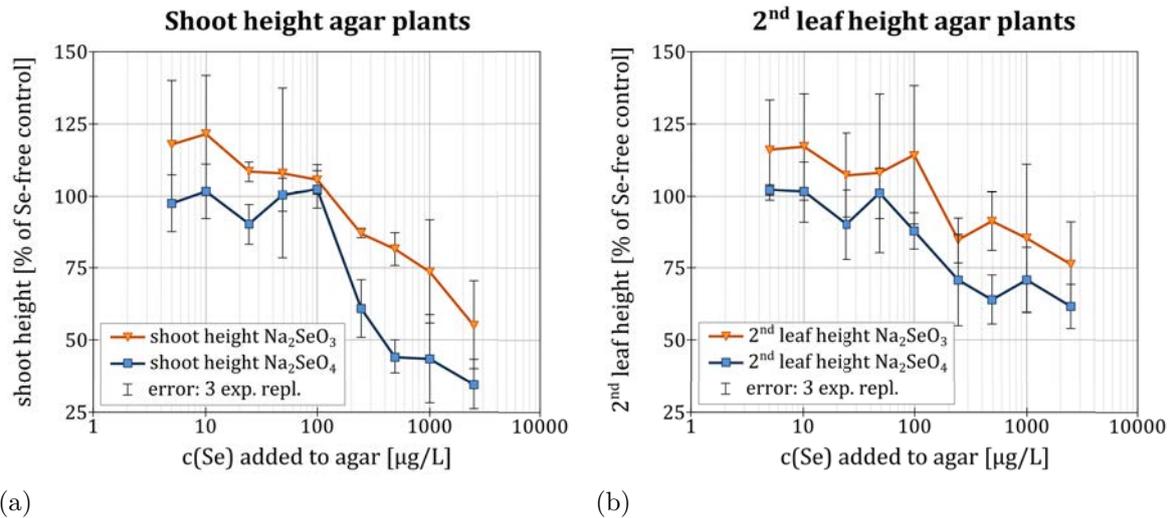


Figure 3.12.: *Plant growth expressed as percentage of Se-free blank plants for experiment A2*
 a: total shoot height on harvest day (Day 16)
 b: total length of 2nd leaf on harvest day (Day 16)

As shown in Figure 3.12a, total shoot height increased with the addition of Se as selenite between 0 and 10 µg/L, with 10.7 cm (122 %) being the maximum height reached, compared to 8.9 cm (100 %) height in the Se-free blank. If the concentration of selenite in the medium was 100 µg/L or higher, total shoot height decreased down to 5.0 cm when adding 2500 µg/L Se as selenite to the agar. Thus, selenite-treated plants reached only 55 % of the original plant height for 2500 µg/L Se. With the addition of Se as selenate, total shoot height remained similar for Se concentrations up to 100 µg/L, between 9.3 (90 %) and 10.5

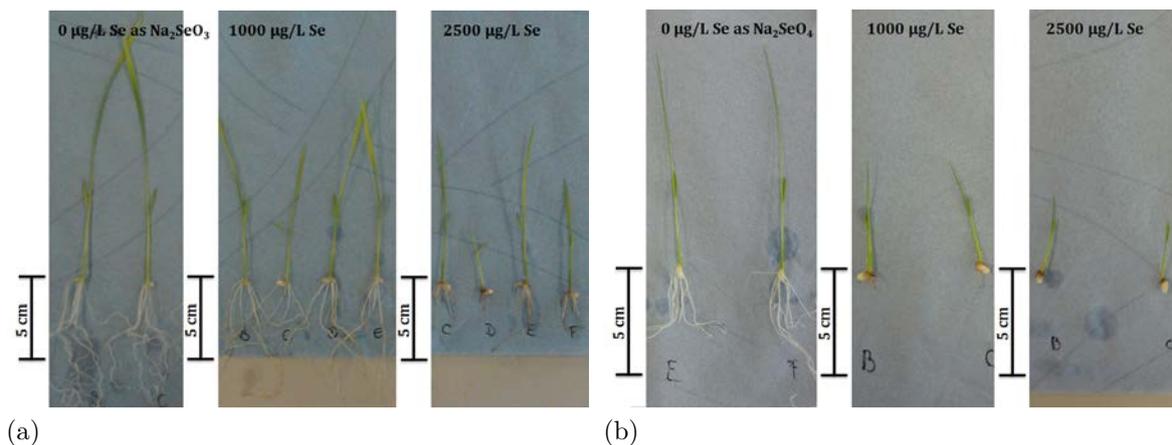


Figure 3.13.: *Root growth and toxicity symptoms for the addition of 0, 500, 1000 and 2500 µg/L Se to agar as*
a: selenite
b: selenate

cm (102 %), compared to the untreated plant height. Concentrations beyond that led to a sharp decrease in total shoot height, resulting in an overall decrease of 6.7 cm, from 10.2 cm (100 %) to 3.5 cm (35 %) when adding 2500 µg/L Se.

Similarly to total height, the length of the 2nd leaf (Figure 3.12b) was also affected by the same concentrations of selenite and selenate added to the agar. Low concentrations of selenite in the medium promoted growth (114 % for 100 µg/L Se), while concentrations above 100 µg/L were clearly inhibitory, with 76 % growth height for 2500 µg/L Se. Growth of the 2nd leaf was also negatively affected by selenate concentrations in the agar higher than 100 µg/L Se. At the highest selenate concentration, 2nd leaf height was 61 % of the untreated leaf height and the third leaf of the seedlings was almost entirely covered. Overall, selenite and selenate affected seedling growth similarly, with selenate being more effective.

Root lengths remained similar at 5 - 7 cm for the addition of 0 - 100 µg/L Se for both Se species (Figure 3.13). After that, root length decreased steadily to below 1 cm when Se was added as selenate. Additional selenite, however, resulted in decreased root length (1-2 cm) only for 2500 mg/L Se. Toxicity symptoms of stunted root growth, lack of secondary roots and brown-spotted discoloration were found for the addition of 250 to 2500 µg/L Se as selenate (Figure 3.13b), but only for 2500 µg/L Se as selenite (Figure 3.13a).

Unfortunately, measurements of Se content in agar by acid digestion were not precise

Table 3.4.: Calculated absolute Se uptake (Se as Na_2SeO_4) by plants from agar Se-content of Exp. A2 using HG-FIAS measurement data

Se added [$\mu\text{g/L}$]	initial agar			final agar			uptake/plant box	
	$c(\text{Se})_{\text{FIAS}}$ [$\mu\text{g/L}$]	inweight [g]	$c(\text{Se})_{\text{agar}}$ [$\mu\text{g/L}$]	$c(\text{Se})_{\text{FIAS}}$ [$\mu\text{g/L}$]	inweight [g]	$c(\text{Se})_{\text{agar}}$ [$\mu\text{g/L}$]	$\Delta c(\text{Se})$ [$\mu\text{g/L}$]	absol. Se [μg]
0	< PQL	1.5558	< PQL	< PQL	4.3209	< PQL	< PQL	< PQL
5	< PQL	1.6793	< PQL	< PQL	4.3049	< PQL	< PQL	< PQL
10	< PQL	1.2469	< PQL	< PQL	4.3184	< PQL	< PQL	< PQL
25	< PQL	1.9685	< PQL	< PQL	4.2925	< PQL	< PQL	< PQL
50	7.29	1.6599	43.90	4.06	4.3150	9.40	34.50	0.15
100	15.95	1.7854	89.33	7.78	4.3120	18.04	71.29	0.31
250	43.01	2.1887	196.51	19.10	4.2611	44.83	151.68	0.65
500	31.82	1.1443	278.08	64.75	4.3154	150.04	128.04	0.55
1000	134.39	1.4243	943.55	132.78	4.2699	310.96	632.59	2.70
2500	344.93	1.5222	2265.97	396.48	4.3136	919.13	1346.84	5.81

enough to be significant. No Se could be detected for additions of 25 $\mu\text{g/L}$ Se or lower, which indicates a method error of at least 25 $\mu\text{g/L}$, which is insufficient for the determination of plant uptake from the agar via Se loss from 100 mL of agar. Values calculated for absolute Se uptake (Table 3.4) are, therefore, not considered trustworthy and absolute Se uptake could only be determined for plants of Exp. A3 (Chapter 3.3.3), because the nutrient solution could be directly measured by ICP-MS.

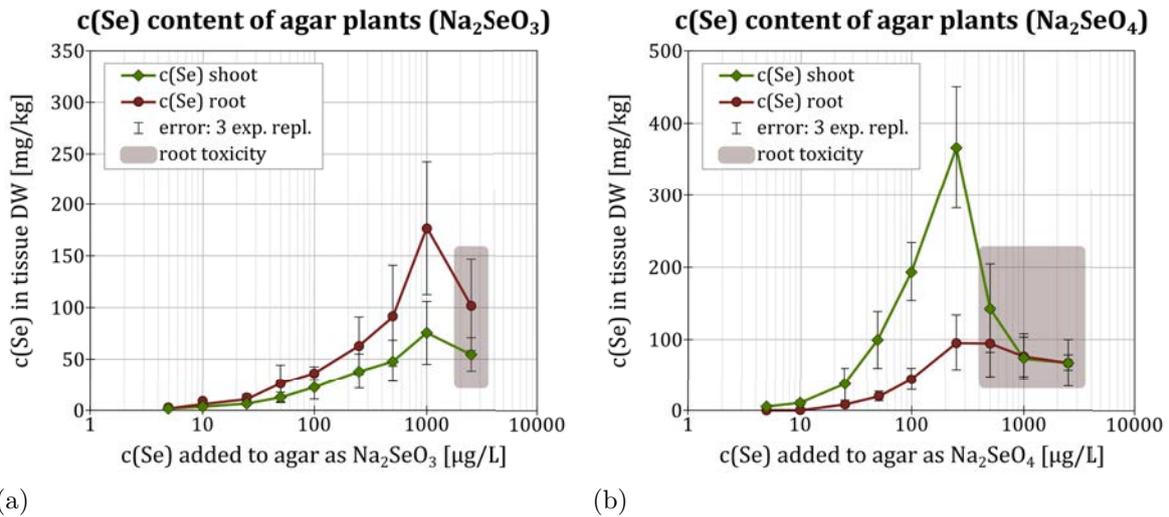


Figure 3.14.: Se content in roots and shoots of experiment A2
 a: addition of Se as Na_2SeO_3
 b: addition of Se as Na_2SeO_4

As shown in Figure 3.14a, when adding selenite to agar at a concentration of 1000 $\mu\text{g/L}$, Se concentrations in both roots and shoots steadily increased to 177 mg/kg Se plant dry

Table 3.5.: Se distribution for uptake of selenate and selenite into root and shoot in both experimental set-ups A2 and A3 ($d_{shoot} [\%] = c(Se)_{shoot} [mg/kg] / (c(Se)_{shoot} [mg/kg] + c(Se)_{root} [mg/kg]) \cdot 100$), standard deviation (SD) given as 1s

added c(Se) [μ g/L]	agar experiments						nutrient solution experiments					
	Na ₂ SeO ₃			Na ₂ SeO ₄			Na ₂ SeO ₃			Na ₂ SeO ₄		
	shoot [%]	root [%]	SD [1s]									
5	38	62	7	77	23	6	28	72	8	62	38	28
10	32	68	7	76	24	8	33	67	1	78	22	19
25	37	63	7	81	19	11	30	70	8	74	26	21
50	32	68	10	82	18	7	20	80	11	70	30	1
100	38	62	16	81	19	9	26	74	12	73	27	7
250	38	62	8	79	21	11	34	66	3	70	30	10
500	34	66	3	60	40	5	30	70	3	73	27	9
1000	30	70	8	49	51	16	36	64	3	75	25	6
2500	35	65	6	50	50	16	34	66	3	76	24	8

weight in the roots and 75 mg/kg Se DW in the shoots. If selenite concentration was increased further (i.e. 2500 μ g/L), Se content in roots (102 mg/kg Se DW) and shoots (55 mg/kg Se DW) decreased, which is consistent with toxicity symptoms found only for 2500 μ g/L Se. Of all Se found within the plant when adding it as selenite, 30 - 38 % of the Se was found in the shoots, while 62 - 80 % was found in the roots (Table 3.5). With the addition of Se as selenate, Se concentrations in shoots were generally greater than in roots (Figure 3.14b). Selenium concentrations for both roots and shoots increased with additional Se to the agar until a maximum of plant-Se was reached at the addition of 250 μ g/L Se for shoots (367 mg/kg Se DW) and roots (96 mg/kg Se DW). In the shoots, additional Se led to a decrease in plant-Se to 143 mg/kg Se DW for 500 μ g/L Se until reaching a plant-Se value of 67 mg/kg Se DW when plants were raised in 2500 μ g/L Se. This was below the Se concentration of 98 mg/kg Se DW found in the plant when adding 50 μ g/L Se. In the roots, a decrease of plant Se concentration was found if the added concentration of Se exceeded 1000 μ g/L. This is also consistent with root toxicity symptoms found at added Se concentrations between 500 and 2500 μ g/L Se. Of all Se found within the plant when adding it as selenate, 50 - 82 % of the Se was found in the shoots, while 18 - 50 % was found in the roots (Table 3.5).

3.5.3. Exp. A3 - plant-box rice cultures in Se-nutrient solution

Quality measures for experiment A3 (Chapter 3.3.3) showed that harvested plant yield was 71 % (± 9 %) of planted caryopses for selenite and 63 % (± 6 %) for selenate. Digestion standard retrieval was 89 % (± 13 %) and 84 % (± 7 %) for selenite and selenate, respectively, and drinking water standard retrieval during HG-FIAS measurement was 104 % (± 5 %) for all samples of experiment A3.

Figure 3.15a shows that for the nutrient solution experiments, the addition of 2500 $\mu\text{g/L}$ Se as selenite resulted in an apparent decrease of 5 cm from 24 cm to 19 cm of the total shoot height, which equalled 79 % of the height of plants grown in the absence of additional Se. This overall decrease, however, was still within 1s-error margin, even when normalized to untreated plant height. This lack of trend was also reflected in the 2nd leaf heights (Figure 3.15b), which remained constant between 93 % and 104 % of untreated leaf height.

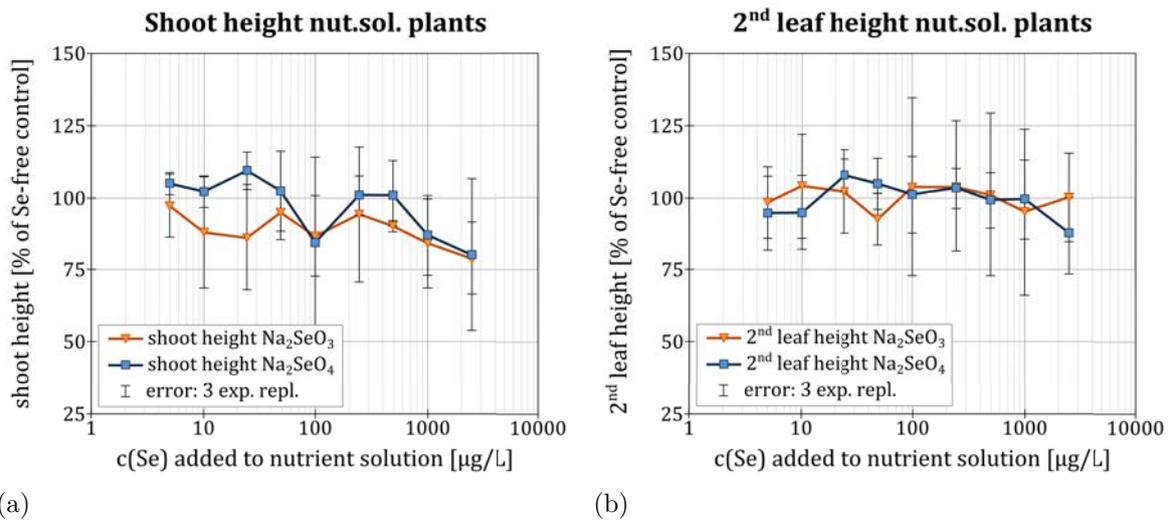


Figure 3.15.: *Plant growth expressed as a percentage of Se-free blank plants for experiment A3*

a: total shoot height on harvest day (Day 19)

b: total length of 2nd leaf on harvest day (Day 19)

Similarly, total shoot heights showed an overall decrease of 5 cm (from 23 cm to 18 cm) with the addition of selenate into the nutrient solution (Figure 3.15 a). Although this equalled 80 % of the untreated plant height, this decrease was also still within the 1s-error margin when normalized to untreated plant height and 2nd leaf heights (Figure 3.15 b) remained between 108 % and 88 % of untreated leaf height. This showed that –

unlike the results in the agar experiments – neither selenite nor selenate addition had any significant effect on plant growth in nutrient solution experiments. The lack of root toxicity symptoms in nutrient solution experiments, which, in contrast, were pronounced in the agar experiments, confirmed this. A comparison of shoot height of the untreated plants on Day 9 between both experiments showed that agar plant shoots grew to a height of 3.4 cm (± 0.8), while nutrient solution plants grew to a height of 6.6 cm (± 2.5) when no Se was present.

As shown in Figure 3.16a, increasing the addition of Se as selenite to the nutrient solution resulted in an almost linear increase in Se concentration in both shoots and roots. Selenium concentrations reached 312 mg/kg Se DW in roots and 159 mg/kg Se DW in shoots for the Se-addition of 2500 $\mu\text{g/L}$ Se. This pattern of uptake differed from the agar experiment uptake, where an uptake peak was observed at a concentration of 100 $\mu\text{g/L}$ of added Se, but additional Se led to lower plant-Se. Maximum uptake into the rice plant in the agar experiments was, therefore, lower than in the nutrient experiments. Figure 3.16b shows a similar linear increase for plant-Se in plants grown in nutrient solution with added selenate. Here, Se concentrations reached 405 mg/kg Se DW in the shoots and 128 mg/kg Se DW in the roots.

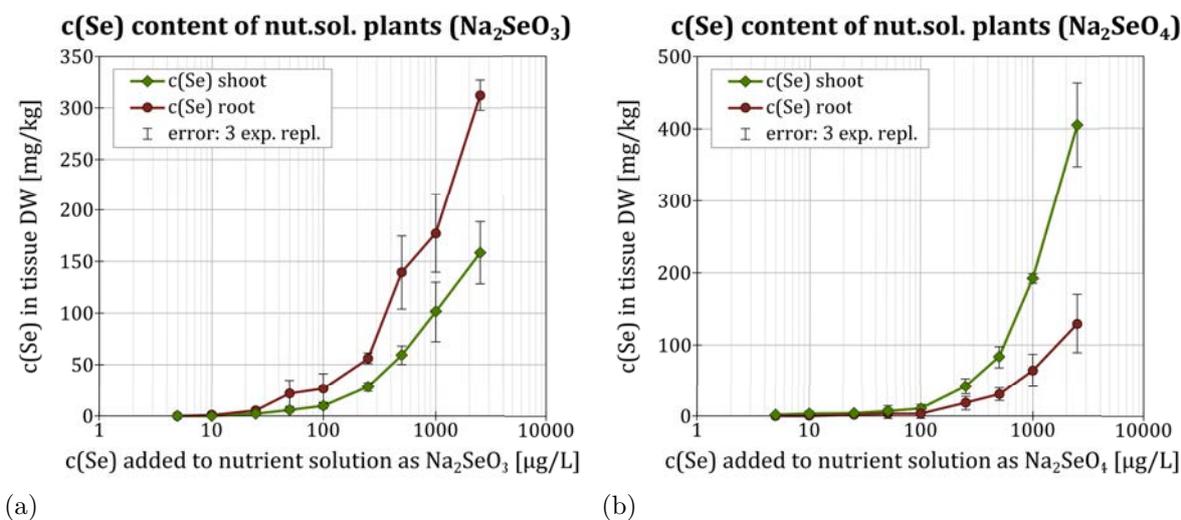


Figure 3.16.: Se content in roots and shoots of experiment A3

a: addition of Se as Na_2SeO_3

b: addition of Se as Na_2SeO_4

Table 3.6.: Fresh weight accumulation factors (AF) of selenate and selenite into shoots in both experimental set-ups (AF [-] = $c(\text{Se})$ medium [mg/L] / $c(\text{Se})$ plant [mg/kg])

added c(Se) [µg/L]	agar experiments				nutrient solution experiments			
	AF-Na ₂ SeO ₃		AF-Na ₂ SeO ₄		AF-Na ₂ SeO ₃		AF-Na ₂ SeO ₄	
	shoot [%]	root [%]	shoot [%]	root [%]	shoot [%]	root [%]	shoot [%]	root [%]
5	75.35	198.12	273.80	108.36	21.54	80.31	27.22	21.71
10	53.15	134.48	263.10	99.13	26.67	81.57	16.20	8.03
25	59.27	129.49	390.10	130.07	26.47	99.16	20.88	9.68
50	50.37	145.38	465.25	154.76	31.59	211.88	26.74	12.68
100	52.89	146.66	513.57	175.22	26.97	104.61	19.00	10.20
250	33.14	92.40	366.44	132.03	28.98	94.10	41.13	19.86
500	28.14	76.26	93.92	79.82	33.61	116.47	39.99	21.66
1000	22.98	68.02	25.19	37.00	30.68	84.81	53.35	25.53
2500	7.22	17.68	8.36	13.09	22.15	57.82	40.87	22.51

Again, an uptake peak and subsequent decrease, similar to the agar experiments, was not observed and maximum uptake was higher than in agar experiments. Furthermore, significant root length differences between added Se concentrations were not found, irrespective of the Se species added to the medium. Error (error bars over all three experimental runs, Figure 3.16) decreased with the addition of Se in Exp. A3, with an error over all plant-Se of 48 % (as Na₂SeO₃ and Na₂SeO₄) with the addition of 10 - 50 µg/L Se, 30 % with the addition of 100 - 500 µg/L Se and 20 % with the addition of 1000 - 2500 µg/L Se.

Selenium accumulation factors (Table 3.6) of fresh plant weight showed that on average, accumulation of Se as selenite in the roots was 2.7 (± 0.2) times higher than in the shoots for Exp. A2 and 3.3 times higher (± 0.4 when excluding the outlier at 50 µg/L Se) than in the shoots in Exp. A3. In contrast, Se added as selenate led to an accumulation factor of 2.8 (± 0.2 when excluding the toxicity outliers) and 1.9 (± 0.3) times higher in the shoots than in roots in Exp. A2 and A3, respectively. For the addition of 1000 and 2500 µg/L Se as selenate to agar, shoot accumulation was lower than in roots (factor 1.5). Accumulation of Se in plant tissue differed between Exp. A2 and Exp. A3. Selenium present as selenite in Exp. A2 showed an overall decrease in accumulation factors with higher concentrations of initial Se from 75 - 7.2 and 198 - 18 for the addition of 5 - 2500 µg/L Se for shoots and roots, respectively (Table 3.6). When present as selenate, Se accumulation in the plant tissue in Exp. A2 showed an increase from 274 - 514 and 108 - 175 for the addition of 5 - 100 µg/L

Se for shoots and roots, respectively. Addition of Se in concentrations between 100 and 2500 $\mu\text{g/L}$ Se, however, led to a decrease in Se accumulation in the plant tissue from 514 to 8.4 and 175 to 13 for shoots and roots, respectively (Table 3.6). Selenium accumulation in Exp. A3 was similar across a large range of initial Se concentrations with 22 - 34 and 80 - 117 for shoots and roots, respectively, when Se was added as selenite and 19 - 41 and 9.7 - 23 for shoots and roots, respectively, when Se was added as selenate.

Data on the uptake of nutrients by the plant showed no significant trends when plotted as a function of added Se (Appendix, Figures A.18, A.19). Neither selenite nor selenate had a measurable effect on nutrient uptake of N, P, K, S, Ca, Mg, Mn, Zn, Cu or Fe, as all fluctuations were well within error range of the 3 runs of the experiment. Two elements, Na and Cl, were not included because, due to climate chamber humidity operation, Na and Cl data could not be interpreted. This is because their presence in the water, which was used to maintain humidity in the climate chamber, led to an increase in Na and Cl content in the nutrient solution over the time period of the experiment, rather than a decrease due to plant uptake. Furthermore, B was found to be leached from lab equipment and the plant-boxes, leading to greater nutrient solution content of B after the experiment than initially supplied. It appears that with the addition of selenate, plant uptake of Mn and Zn showed a slightly decreasing trend at concentrations of 1000 and 2500 $\mu\text{g/L}$. However, as demonstrated in Table A.5 (Appendix), all nutrient solution phases including Fe are metastable from a thermodynamic point of view, which makes co-precipitation of such small amounts of Mn and Zn that were added to the solution highly probable. Therefore, data on nutrient uptake is considered uncorrelated with addition of Se in all measured cases.

3.5.4. Exp. A4 - plant-box rice cultures in Se-agar with delayed Se-uptake

Quality measures for experiment A4 (Chapter 3.3.4) showed that harvested plant yield was 48 % (± 13 %) of planted caryopses for selenite and 72 % (± 21 %) for selenate. Digestion standard retrieval was 101 % (± 4 %) and 95 % (± 7 %) for selenite and selenate, respect-

ively, and drinking water standard retrieval during HG-FIAS measurement was 118 % (\pm 7 %) for all samples of experiment A4.

Although there was no standard deviation for experimental data of experiment A4 because there were no repeats, conditions were similar to experiments A2 and A3, which is why results are also given as percentages of untreated plant growth for comparison.

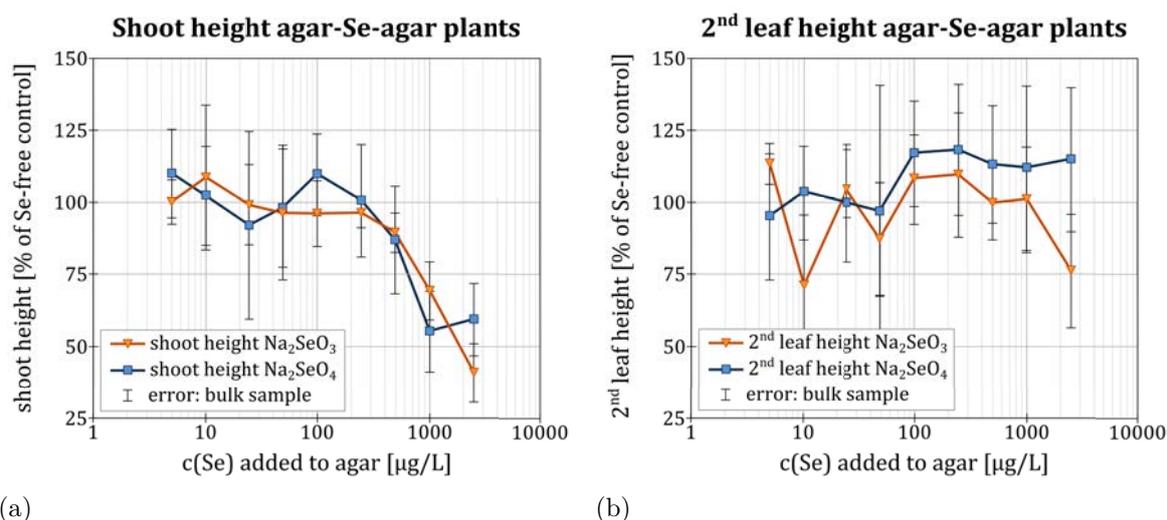


Figure 3.17.: *Plant growth expressed as percentage of Se-free blank plants for experiment A4 (note: error bars refer to single plant deviations from bulk mean)*
 a: total shoot height on harvest day (Day 19)
 b: total length of 2nd leaf on harvest day (Day 19)

With this in mind, Figure 3.17a still exhibited a trend in total shoot heights with the addition of 500 µg/L Se or more to the agar from 17 cm (100 %) to 10 cm (59 %) for selenite and 19 cm (100 %) to 8 cm (41 %) for selenate. Additions of 250 µg/L Se or less showed no change in shoot height for either speciation. Second leaf heights, as shown in Figure 3.17b, however, showed no significant decrease compared to untreated or low-Se leaf heights.

When Se was applied as selenite (Figure 3.18a), Se content in roots increased sharply between 0 and 250 µg/L of added Se from 0 to 164 mg/kg DW. Selenium content increased less strongly with the addition of more than 250 µg/L Se, resulting in 269 mg/kg DW Se with the addition of 2500 µg/L Se. In shoots, Se content peaked with the addition of 1000 µg/L Se as selenite at 93 mg/kg DW and decreased to 67 mg/kg with the addition of 2500 µg/L. As shown in Figure 3.18b, Se applied as selenate resulted in increased Se content with increasing Se addition until peaking in both shoots (1040 mg/kg DW) and roots (505

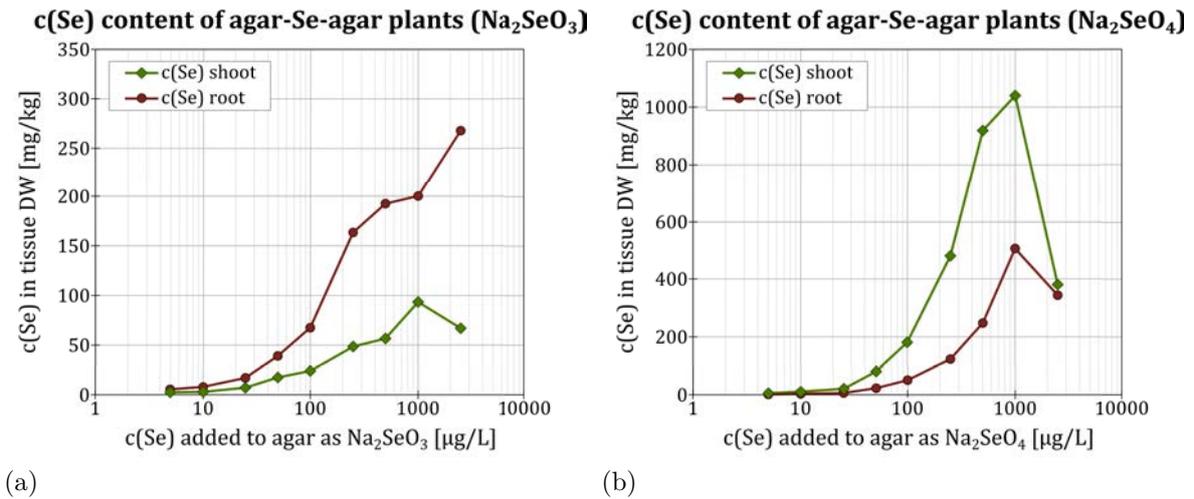


Figure 3.18.: Se content in roots and shoots of experiment A4

a: addition of Se as Na_2SeO_3

b: addition of Se as Na_2SeO_4

mg/kg DW) with the addition of 1000 $\mu\text{g/L}$ Se. A higher Se concentration of 2500 $\mu\text{g/L}$ in the agar led to a decrease in Se content in shoots (382 mg/kg DW) and roots (345 mg/kg DW).

Because two plants in the 2500 $\mu\text{g/L}$ plant-box of the selenite experiment were unusually small and exhibited discoloring around the caryopse even though their roots had not reached the Se-agar, these were sampled separately. Together with agar samples from the top 2 cm of the non-Se-bearing Eppendorf tube, these were separately tested for stray traces of Se. Agar digestion as well as plant digestion of these samples revealed Se-content to be below detection limit. Therefore, the 0.7 % agar in the Eppendorf tubes can definitely be considered Se-free at plant germination.

When directly compared to results from experiments A2 and A3, experimental data of A4 for selenite (Figure 3.19) exhibited three characteristics. The first was that for uptake of selenite, data on shoot-Se followed the trend observed in results of experiment A2, with a decrease in shoot Se-content at concentrations greater than 1000 $\mu\text{g/L}$ (Figure 3.19a). While the trend was similar, uptake concentrations for experiment A4 were between 17 % and 26 % higher than in the A2 experiment. However, as a second characteristic, for uptake of selenite (Figure 3.19b), data on root-Se followed the trend of experiment A3, in which there was no collapse in Se-uptake at concentrations greater than 1000 $\mu\text{g/L}$. The increase in

uptake between the addition of 1000 and 2500 $\mu\text{g/L}$ Se, however, was only 25 %, compared to 45 % in experiment A3.

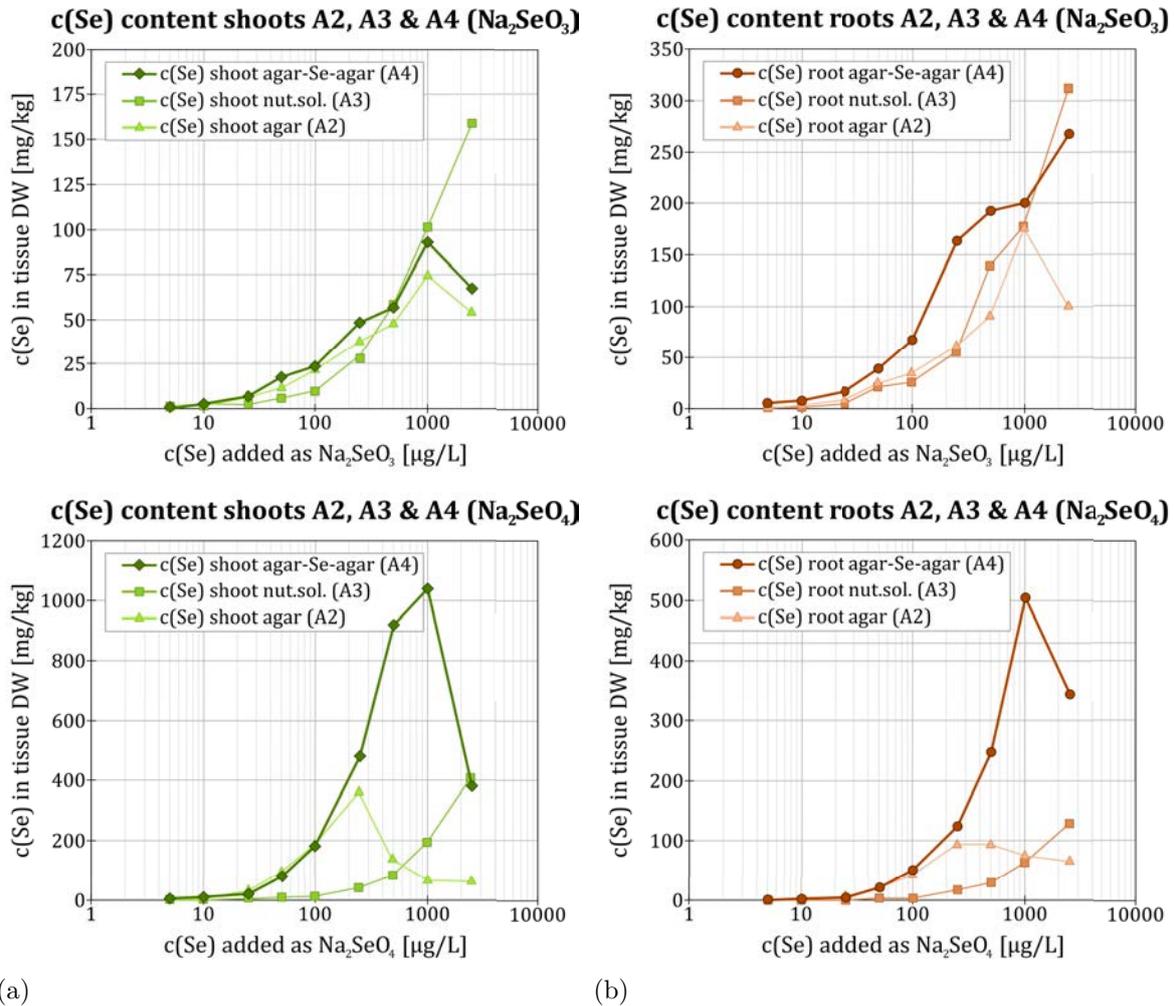


Figure 3.19.: Comparison of Se content of experiment A2, A3 and A4 after uptake as Na_2SeO_3 (top) and Na_2SeO_4 (bottom) (error bars for A2 and A3 not included for better visibility)

a: shoot-Se for A2, A3 and A4

b: root-Se for A2, A3 and A4

As a third characteristic, root-Se after uptake of selenite also showed a similarly strong increase with additions of Se between 100 and 1000 $\mu\text{g/L}$ Se, as is exhibited in experiment A2 (Figure 3.19b). This allowed the conclusion that for selenite, the set-up of experiment A4, which was designed to explore the parameter of nutrient deficiency of experiment A2 combined with the delayed uptake of Se of experiment A3, reflected this intermediate set-up in the results.

For the addition of selenate, comparison of results of experiments A2, A3 and A4 reflected

the intermediate set-up of experiment A4 as well, but in a different way than was the case for selenite Figure (3.19). For both shoots and roots, plant-Se was nearly identical as for experiments A2 for added concentrations of Se between 0 and 100 $\mu\text{g/L}$. After that, however, the trend of increasing uptake was continued similarly to the trend observed in results of experiment A3 - albeit at much higher concentrations. For the addition of 1000 $\mu\text{g/L}$, Se content was about 5 and 8 times higher in shoots (Figure 3.19a) and roots (Figure 3.19b) in experiment A4 than in experiment A3, respectively. At concentrations exceeding 1000 $\mu\text{g/L}$ Se, Se content decreased sharply, following the trend for Se-uptake in experiment A2, albeit at higher additions of Se and higher plant-Se content.

3.6. Discussion on the uptake of Se into plants

The following subchapter will discuss how plant status, nutrient supply, Se-exposure at germination and Se speciation result in different plant Se-uptake and distribution in experiments A1, A2, A3 and A4. The main conclusions are derived from experiments A2 and A3, with A1 and A4 providing supporting results.

3.6.1. Influences of plant status and substrate amount on Se-uptake in rice

The greatest differences in the Se-uptake of the open rice cultures were not - as anticipated - between the two different concentrations of 2.5 or 5 mg/L , or even between the amounts of Se-nutrient solution supply, but between pot size. This is interesting, as pot size not only changed the ratio of substrate to solution and therefore diluted the applied amount of Se (which simultaneously also applies to the nutrients of the solution). Pot size also changed the ratio of root surface area to substrate. Therefore, plants in the small pots and, therefore, less substrate were more likely to come into contact with more Se, which was verified by plant-Se results.

Pot size-related substrate amount apparently played a role in plant development as well (Figure 3.9). Especially when comparing shoot mass, the larger substrate amount produced

plants that were more homogenous and average in development compared to the plant with smaller substrate amounts, which, in turn, reflected Se-uptake. The fact that plants with the lowest-to-average plant mass took up the highest Se concentrations, while plants with average and above-average plant mass plateaued in their Se content, indicates an interesting correlation between uptake and low plant health. Therefore, the hypothesis that plants with less vitality due to less watering and nutrient sustenance would be affected more by the addition of Se than plants with greater vitality was supported. Plotting the absolute Se in the plant against shoot mass as an indicator of plant health was an attempt at clarification of the cause-and-effect relationship. However, a clear separation of cause and effect between plant health and Se toxicity for the open cultures was not possible due to low sample numbers and further discussion will focus on the following experiments, which explore nutrient supply and toxicity more closely.

3.6.2. The influence of nutrient supply on Se-uptake

For application of lower Se concentrations ($< 250 \mu\text{g/L}$ as selenate), Se-uptake is much higher in the nutrient-free environment (ca. factor 12) compared to nutrient-complemented plants, a conclusion that is also supported by substantially higher (5 - 27 times) accumulation factors (Table 3.6). This conclusion is consistent with published findings [Buchner, Takahashi & Hawkesford, 2004, Li et al., 2007] that depletion of sulfate and phosphate increases the activity of the respective transporters, so that more Se is taken up into the plant. Furthermore, lack of competing ions, i.e. sulfate, is expected to further promote the efficiency of selenate uptake. This is most prominently demonstrated in the nutrient-free experiment with a delay before Se-uptake, where Se uptake for selenate by far exceeds the highest uptakes of the other experimental set-ups due to lack of nutrients (factor 2.5 and 4 for shoots and roots, respectively). However, when a threshold of Se toxicity is exceeded (250 $\mu\text{g/L}$ Se as selenate and 1000 $\mu\text{g/L}$ as selenite in experiment A2 and 1000 $\mu\text{g/L}$ as selenate in experiment A4), Se-content in the plant collapses. For plants of experiment A2 this also coincides with root toxicity symptoms, which indicates that root functionality

is impaired and therefore transporter protein activity is shut down, significantly lowering Se-uptake.

However, addition of nutrients reduced Se-uptake when Se concentrations were < 500 $\mu\text{g/L}$, which was especially evident for selenate (Figure 3.16). This is also reflected by the accumulation factors – all of which are lower than in their nutrient-free counterparts (Table 3.6). This might be caused by down-regulation of transporter activity in response to sufficient content of nutrients (i.e. S), or by competition of sulfate for binding sites at the transporters [Li et al., 2007, Khan & Hell, 2014]. Even for the highest tested concentration of Se (2500 $\mu\text{g/L}$ Se, corresponding to approximately 30 μM Se as SeO_4^{2-} or SeO_3^{2-}), the 700 μM SO_4^{2-} and 400 μM PO_4^{3-} of the nutrient solution are most likely to compete severely with Se for uptake into the plant. It is known that additional nutrient oxy-anions, especially phosphate and sulfate, influence Se-uptake by plant roots [Li et al., 2007] [Khan & Hell, 2014]. Effects of S are considered to be more pronounced than those of P, because the affinity of selenate for the sulphur transporter is higher than that of selenite for the phosphate transporter [Hopper & Parker, 1999, Li et al., 2007].

For Se concentrations above the nutrient-free toxicity-threshold (1000 $\mu\text{g/L}$ Se as selenite and 250 $\mu\text{g/L}$ Se as selenate), nutrients clearly promoted the uptake of Se. This correlates with the fact that the nutrient-complemented plants remained healthy even when exposed to high Se concentrations and thus, presumably, were capable of sustaining uptake, leading to a higher Se-uptake compared to the nutrient-free condition. This is consistent with a previous study showing that higher S content has a protective physiological effect on Se toxicity [Kikkert et al., 2013]. This protective effect of nutrition is agronomically relevant, because at 2 mg/kg DW Se, rice yield is already reduced by 10 % and this yield loss is even more pronounced if the Se is administered as selenite [Läuchli, 1993]. Therefore, application of nutrients could help lower Se toxicity and improve crop yield in general. Although Se-uptake in our experiments was facilitated because the Se was freely available in a solution rather than soil-bound, we did not observe any drop in uptake nor any significant inhibition of plant growth, even for a condition yielding 405 mg/kg Se DW in the shoots. Thus, our study suggests that plant resilience increased with nutrient availability.

Moreover, competition between anions such as sulfate and selenate as well as selenite and phosphate not only affected the uptake, but also the partitioning between shoots and roots (Chapter 3.6.4). This indicates that sulfate competition for selenate uptake might also influence the transport from roots to shoots and/or the incorporation of Se into proteins, in accordance with previous findings [Li et al., 2007].

3.6.3. Phytotoxicity triggered by direct Se-exposure and lack of nutrients

Of all three closed-box experiments, toxicity symptoms on plants were only observed for plants grown in the nutrient-free environment, in which seedlings were in direct Se contact upon germination. As plants that showed no toxicity symptoms all came into contact with Se after a delay of about 5 days, this strongly supports the hypothesis of toxicity symptoms being triggered, though not exclusively caused, by direct Se exposure.

So far, effects of Se toxicity or biofortification have only been tested on healthy, pre-germinated seedlings [Asher et al., 1977, Bellet al., 1992, Zhang et al., 2006, Li et al., 2007]. Only one study directly addressed germination of rice in the presence of Se [Liu & Gu, 2009]. However, seedling development beyond the radicle piercing the seed coat was not investigated. In that study, germination itself was not influenced significantly below 60 $\mu\text{mol/L}$ (ca. 4.74 mg/L) Se in solution, in contrast to the much lower concentration of 1 - 2.5 mg/L Se observed to impair growth in our study. This suggests that germination per se is not the most sensitive step but rather, the subsequent development of the germinated seedling, especially under conditions of nutrient deficiency. Germination of rice in the presence of Se has been proposed as a strategy of effective Se biofortification [Liu & Gu, 2009].

Experiments of this study provide strong evidence that it is the combination of a lack of nutrients, coupled with direct Se exposure above the threshold concentrations (250 $\mu\text{g/L}$ Se as Na_2SeO_4 and 1000 $\mu\text{g/L}$ Se as Na_2SeO_3), that leads to toxicity symptoms. Nutrient deficiency alone, although leading to smaller plants, did not lead to toxicity - neither in

the agar blanks of the nutrient-free experiments with germination directly in Se, nor in the agar blanks of the nutrient-free experiments with Se. Even the combination of nutrient deficiency and a delay between Se uptake and germination (as in experiment A4) did not lead to the toxicity symptoms observed in the experiments, in which seedlings germinated in Se exposure. Therefore, this study suggests that it is essential for the strategy of Se biofortification at the pre-germination stage to provide sufficient nutrients to young seedling to avoid poisoning seedlings and lowering crop yield even at low Se concentrations. The alternative strategy might be to add Se at a later growth stage, or to pre-cultivate seedlings in a Se-free environment, before subjecting them to high Se concentrations after 5 days.

3.6.4. Selenium-uptake partitioning - distribution of selenate and selenite uptake into shoots and roots

The second main observation was that the addition of Se as selenate resulted in Se accumulating predominantly in the shoots rather than the roots, whereas addition of selenite resulted in Se accumulating mainly in the roots rather than in the shoots. This was the case for all plant-box experiments (Figures 3.14, 3.16, 3.18, Table 3.5). Mean Se concentrations in shoots were up to 3.5 - 5 times higher than in roots when Se was applied as selenate. In contrast, when applied as selenite, Se concentrations were up to 2 - 4 times higher in roots compared to shoots. This inverse partitioning was independent of the mode of cultivation.

The preferential partitioning of selenate into shoots has also been reported for other plants, such as strawberry, clover and perennial ryegrass [Hopper & Parker, 1999], barley and red clover [Gissel-Nielsen, 1973], soybeans [Zhang et al., 2003] and wheat [Li et al., 2007]. This phenomenon is generally explained by selenate being taken up actively via the sulfate transporter and then readily transported via xylem into plant shoots and leaves [Carey et al., 2012]. However, the behaviour of selenite uptake is not fully understood [Khan & Hell, 2014]; selenite uptake mechanisms, for instance, are still a matter of debate.

These experiments showed that plant Se-content is nearly as high for the uptake of sel-

enite compared to selenate, which is known to be mediated by high-affinity transporters. Furthermore, accumulation factors (Table 3.6) of selenite in roots are as high or higher than accumulation factors of selenate in shoots. These findings support a model in which selenite is taken up actively via phosphate transporters against the electrochemical gradient as previously suggested [Hopper & Parker, 1999, Li et al., 2007]. The selenite taken up in both of our experimental set-ups - presumably by phosphate [Li et al., 2007] or silicon transporters [Zhao et al., 2010] - is likely to be converted into organic seleno-compounds. This was also shown by speciation analysis of plant material in this study (Chapter 5.4.3).

On the one hand, organic Se can be methylated to produce the non-proteinogenic amino acid selenomethylcysteine [Khan & Hell, 2014]. This amino acid has been shown to accumulate in chloroplasts of *Arabidopsis*, which appear to use specific methylation as a mechanism to prevent mis-incorporation of the Se-amino acid into proteins instead of S-amino acids [LeDuc et al., 2004]. On the other hand, it was found that selenomethionine (SeMet) and selenomethylselenocysteine (SeMeSeCys) were rapidly transported exclusively via the phloem to the grain, whereas selenate was transported slower via the xylem [Carey et al., 2012]. This poses the question whether that one third of selenite, which was transported to the shoots is incorporated into proteins or retained in shoot chloroplasts. It appears that rice plants harbour protective mechanisms similar to those of Se-accumulator plants to retain two-thirds of selenite as methylated compounds in the root that are not integrated in proteins. It remains to be investigated whether this apparently precise partitioning of selenite is caused passively by saturation of binding sites, or is actively regulated.

The fact that most of the selenate is partitioned to the shoots as a consequence of its unspecific transport via sulfate transporters explains the large share of selenate in the shoot. However, it does appear that a third of the selenate taken up by plant is retained in the root - most likely as organic Se as it can be reduced to selenide and then transformed into SeCys [LeDuc et al., 2004, Khan & Hell, 2014].

3.6.5. Conclusions for biogeochemical mass balance modelling

Results of this study can be implemented into the biogeochemical model (Chapter 6) for the characterization and mass balance of the Se compartments and transfer processes within the Critical Zone. Mathematical description of uptake as functions of Se concentration present in a certain species is, of course, merely a quantification of transport, and is not descriptive of any single chemical or physical property or process. Therefore, the biogeochemical model can only provide adequate description of correlations and quantification of processes.

Plant uptake processes describe one half of the predefined model transport pathways for Se and applies to the compartments of 'soil solution' and 'plant'. Conclusions from this study for this aspect of the Critical Zone are:

1. selenite and selenate are taken up readily by the rice plant, but resulting Se-accumulation within the plant tissue is partitioned differently to root and shoot
2. nutrient supply provides competition for Se-uptake, but the thereby optimally secured plant health leads to greater tolerance and ultimately higher Se-uptake for high Se concentrations
3. direct exposure to Se during plant germination leads to phytotoxicity at moderate Se concentrations, but effective Se-uptake by the plant is increased at low Se concentrations

4. Geochemistry - Se sorption processes onto kaolinite & goethite

The second part of this study is concerned with the interactions between soluble Se and soil-forming minerals, particularly adsorption and desorption. Two of the most frequent soil-forming mineral groups which play an important role in controlling Se mobility in soils are clay minerals and iron oxides or -hydroxides [Bar-Yosef & Meek, 1987, Ghose et al., 2010]. This study focuses on one representative mineral for each of these groups:

- (1) as pure a kaolinite as could be obtained to represent a highly crystalline 2:1 layer clay mineral and
- (2) an α -FeOOH (goethite), which in this case has a large share of amorphous properties.

4.1. Selenium retention in soils

Although underlying geology is one of the primary controls of soil-Se concentration due to weathering, mechanisms of soil retention determine bioavailability of the Se present in the soil [Fordyce, 2013]. During weathering, Se is readily oxidized and becomes more mobile with increased oxidation state [Neal, 1995]. Generally, in arid alkaline environments, Se is, therefore, most likely to be present as selenate, which is highly mobile, while humid regions promote the formation of selenite, which is less mobile [Neal, 1995]. At the interface between soil solution and solid phase, defining biophysical parameters such as soil mineralogy, texture and organic matter, influence and are influenced by chemical factors

such as pH, redox conditions and competing ions [Fordyce, 2013].

4.1.1. Selenium associations in soil

Selenium is known to be associated with iron, aluminum and manganese oxides and hydroxides [Balistreri & Chao, 1987, Hayes et al., 1987, Balistreri & Chao, 1990, Chan et al., 2009, Das et al., 2013], carbonates [Wijnja & Schulthess, 2002], clay minerals [Bar-Yosef & Meek, 1987, Goldberg et al., 2013] and organic matter [Kang et al., 1991, Gustafsson & Johnsson, 1992]. Adsorption of Se by clay minerals can lower Se bioavailability to as little as 50 % and iron oxides can completely adsorb Se [Fordyce, 2013]. Maximum adsorption is influenced strongly by pH and reaches its maximum at pH 3-5, decreasing with increasing pH [Neal, 1995, Fordyce, 2013]. Chemical extraction procedures have shown that, depending on soil composition, Se adsorbed onto mineral phases accounts for about 20 % of the total soil Se in soils and sediments [Fernández-Martínez & Charlet, 2009], while an estimated 50 % of Se in soils and sediments are retained by organic matter [Fernández-Martínez & Charlet, 2009]. Fixation by organometallic complexes is the reason why organic matter can also significantly lower Se bioavailability to as little as 10 % [Neal, 1995, Fordyce, 2013]. In anoxic conditions, however, it was found that elemental Se can account for 20 - 60 % of the total Se in soils and sediments [Zhang & Moore, 1996, Fernández-Martínez & Charlet, 2009].

All these general influences are helpful to assess Se bioavailability in soils. However, when studying depth profiles of Se concentration in seleniferous soils of the Kesterson reservoir [Tokunaga et al., 1994] or in Punjab, India [Dhillon & Dhillon, 2003], where Se is enriched 5 - 10-fold in the top 15 - 40 cm compared to Se content near bedrock, it becomes apparent that mechanisms of Se soil retention and Se transport affect Se soil concentrations across greater areas. Furthermore, in natural soils, generalizations of environmental redox conditions do not account for the small-scale heterogeneous redox conditions within soil aggregates. These microsites of anaerobic conditions within an environment of overall aerobic conditions are a product of slow oxygen diffusion rates and microbiological redox

processes and can lead to a great variety of Se oxidation states across the scale of around 1 mm [Tokunaga et al., 1994]. For these reasons, soils are very difficult to model in their entire complexity.

Therefore, certain aspects of natural soils were not included in this study to simplify the set-up. Since this study focuses on inorganic soil properties, the significant impact of microbiology [Neal, 1995] is not detailed here and was not included. Furthermore, the aim of this study was to provide quantification of Se adsorption and desorption processes of soil-relevant minerals specifically tailored to complement the Se-plant uptake experiments (Chapter 3.3.3). Therefore, kaolinite and goethite were chosen as model minerals: their sorption characteristics are known to strongly influence Se bioavailability, they have been studied extensively and their properties are well known, as opposed to organic matter.

4.1.2. Properties of kaolinite

Because surface functional groups influence both chemical and electrostatic properties, which are defining for the kind of sorption processes that can occur, sorption materials are classified according to these functional surface groups [Davis & Kent, 1990]. Kaolinite, one of the minerals chosen for this study, belongs to the subgroup of aluminosilicates, which do not possess permanent structural charge, while goethite belongs to the hydrous oxide-bearing minerals. Both minerals have in common that their sorption properties are determined by surface hydroxyl groups [Davis & Kent, 1990].

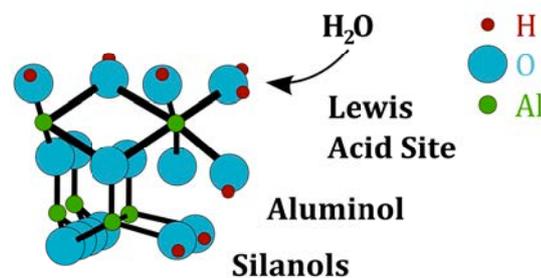


Figure 4.1.: *Types of surface hydroxyl groups on kaolinite: OH groups at the basal plane, Lewis acid sites (at which H_2O is adsorbed), aluminol and silanol groups [Sposito, 1984, Davis & Kent, 1990]*

Kaolinite ($\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$) is a phyllosilicate mineral, in which each Al(III)O_6 -containing octahedral layer is linked to an Si(IV)O_4 -containing tetrahedral layer. It is often found in soils in warm, moist climates as a result of deep weathering [Singh & Gilkes, 1998]. Kaolinite is the clay mineral of choice when studying the anion adsorption and desorption properties of clay minerals because, ideally, it has no layer charge or inter-layer cations to enable inter-layer cation exchange [Lagaly & Köster, 1993]. As a consequence of its well-packed structure, kaolinite particles are not easily broken down and the kaolinite layers are not easily separated. Therefore, Se anion adsorption onto kaolinite occurs mainly at the outer edges and surfaces of the structure [Bar-Yosef & Meek, 1987, Miranda-Trevino & Coles, 2003]. Because kaolinite is known to have a much greater proportion of its total surface area as broken edges, of all clay minerals commonly found in soils, it would be expected to adsorb more Se than any other [Dhillon & Dhillon, 2009].

The degree of ionic substitution within kaolinite layers is less than 0.01 ions per unit cell, resulting in low permanent charge [Sposito, 1984]. As shown in Figure 4.1, kaolinite has three different types of surface hydroxyl groups: aluminol ($=\text{Al-OH}$), silanol ($=\text{Si-OH}$) and adsorbed water at Lewis acid sites [Sposito, 1984, Davis & Kent, 1990]. This has direct implications for the pH_{PZC} . Often, published pH_{PZC} values for kaolinite are around 3 or 4 [Schroth & Sposito, 1997], [Appel et al., 2003] [Miranda-Trevino & Coles, 2003]. However, there is little consensus on this, as a wide array of values for kaolinite's pH_{PZC} have been published (pH 2 - 6), as well as multiple pH_{PZC} s or the possibility of none at all [Schroth & Sposito, 1997, Yukselen & Kaya, 2002]. This is attributed to the fact that the lower pH_{PZC} value, i.e. pH 4.2, corresponds to the surface groups [Hur & Schlautmann, 2003], while the higher pH_{PZC} value of 6 - 7.2 corresponds to the amphoteric edge groups [Hur & Schlautmann, 2003, Tombácz & Szekeres, 2006]. This means that above pH 7, kaolinite surface sites are negatively charged and anion adsorption is likely to occur as ligand exchange [Tombácz & Szekeres, 2006]. Below pH 6, however, adsorption is expected to be strongly dependent on the prevalence of surface over edge sites if it occurs as ligand exchange. In any case, coulombic attraction makes physisorption below pH 7 possible [Tombácz & Szekeres, 2006].

4.1.3. Properties of goethite

Goethite (α -FeOOH) is a ferric oxy-hydroxyl mineral belonging to the hydroxide minerals. It is another mineral frequently created in soils by weathering [Lagaly & Köster, 1993] and is one of the most common and reactive crystalline iron hydroxide phases found in soils and sediments [Ghose et al., 2010]. Because of goethite's importance as a ubiquitous environmental substrate, it is commonly studied to investigate interfacial processes such as sorption, dissolution, aggregation, and precipitation [Ghose et al., 2010]. Its adsorptive surface properties are described by four types of surface hydroxyl groups (Figure 4.2) [Davis & Kent, 1990]. One of these is a designated Lewis acid site, at which a water molecule is chemisorbed directly onto an Fe(III) atom. Reactivity of the other three sites is dependent on whether the O-atom in the FeOH group is coordinated with 1, 2 or 3 adjacent Fe(III) ions (Figure 4.2) [Davis & Kent, 1990]. Of these four sites, only the hydroxyl group with the once-coordinated O-atom is considered to be a basic site (proton acceptor) [Sposito, 1984].

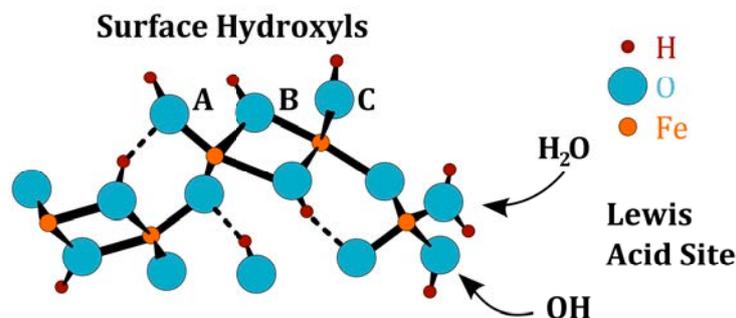


Figure 4.2.: *Types of surface hydroxyl groups on goethite: hydroxyl groups coordinated singly (A), doubly (B) and triply (C) with Fe(III) ions and one Lewis acid site [Sposito, 1984, Davis & Kent, 1990]*

Values for pH_{IEP} and pH_{PPZC} range from 7.3 to 9.4 [Parks, 1990, Kosmulski, 2002]. Therefore, the three influences on the formation of Se sorption complexes with ferric hydrates - pH, ionic strength and surface coverage - can be summarized as follows [Fukushi & Sverjenski, 2007]: (1) in general, adsorption declines with higher pH values beginning between pH 5 and 8, coinciding with the presence of the deprotonated selenate molecule in the solu-

tion;

(2) lowering the background ionic strength leads to a shift of adsorption stability toward higher pH values;

(3) raising the selenate-to-background-ion-ratio leads to a higher prevalence of the outer-sphere complex.

Depending on surface conditions, pH-range of stability for a certain surface complexation changes. For example, high pH_{PZNPC} and high BET goethite exhibits the highest stability for inner-sphere complexation for low pH values, while the outer-sphere complexation becomes more stable with neutral pH values. In contrast, low pH_{PZNPC} and low BET lead to both forms of complexation being stable at the same pH value. The importance of the outer-sphere species increases with increasing surface coverage, which means that, for equal background ionic strength and equal selenate concentration, less available goethite surface leads to a greater share of more outer-sphere complexation.

4.2. Processes at the mineral/water interface

Interaction of anions in aqueous solution with a mineral surface can be divided into three main categories: (ad)sorption, co-precipitation and surface precipitation processes, the latter two of which are determined by solubility constants [Fernández-Martínez & Charlet, 2009]. Adsorption, in general, is defined as

"the process through which a chemical substance accumulates at the common boundary layer of two contiguous phases." [Sposito, 2004, Fernández-Martínez & Charlet, 2009].

There are two main types of modelling adsorption-desorption equilibria at mineral surfaces [Davis & Kent, 1990, Goldberg et al., 2007]: (1) empirical partitioning relationships, such as the Langmuir or Freundlich isotherm, which are used to describe natural systems; (2) surface complexation models based on ion association used to gain thermodynamic understanding of coordinative properties. The difficulty with either description type is that they each require the state of equilibrium to be applicable [Davis & Kent, 1990].

4.2.1. The Langmuir and Freundlich isotherms

The Langmuir isotherm (Figure 4.3a) was originally developed to describe monomolecular chemisorption of gasses onto mineral surfaces [Langmuir, 1918] but is now also used to describe adsorption processes in aqueous solution (Equation 4.1) [Davis & Kent, 1990].



with

- $\equiv X$ as the adsorptive surface site
- A_{aq} as the adsorbing solute in aqueous solution
- $\equiv XA$ as the adsorbed solute species

The following equation (Equation 4.2), known as the Langmuir isotherm (Figure 4.3a), is based on the assumptions that (1) all surface sites have the same affinity for the solute, (2) X is the only adsorbing solute, (3) there is no lateral solute interaction and (4) the surface site density is finite [Davis & Kent, 1990, Dörfler, 2002].

$$\Gamma_A = \Gamma_{max} \frac{K_L c(A_{aq})}{1 + K_L c(A_{aq})} \quad (4.2)$$

for

$$K_L = \frac{\Gamma_A}{c(A_{aq}) \Gamma_X} \quad (4.3)$$

with

- Γ_A as the adsorption density of the solute [g/kg]
- Γ_{max} as the maximum surface site density [g/kg]
- Γ_X as the surface density of uncomplexed sites [g/kg]
- K_L as the conditional Langmuir equilibrium constant [-]
- $c(A_{aq})$ as the concentration of solute in the solution [g/L]

Although the Langmuir isotherm is a mathematical formula based on equilibrium phase

observations, a good fit of experimental data to the Langmuir isotherm provides no insight on the actual mechanisms on the mineral surface [Davis & Kent, 1990]. Special cases of precipitation, for instance, have also been shown to confirm to the Langmuir isotherm [Davis & Kent, 1990].

Not only does the Langmuir isotherm not exclusively describe adsorption processes but, furthermore, not all sorption processes are described by the Langmuir isotherm. Inorganic anions, for example, frequently are not described by the Langmuir isotherm as the requirement of a monolayer adsorption is not met [Davis & Kent, 1990, Dörfler, 2002]. Therefore, the data is either fitted to a multiple-site Langmuir expression or to a generalized exponential term such as the Freundlich isotherm (Figure 4.3b, Equation 4.4) [Davis & Kent, 1990, Dada et al., 2012].

$$\Gamma_A = K_F c(A_{aq})^n \quad (4.4)$$

with

Γ_A	as the adsorption density of the solute [g/kg]
K_F	as the conditional Freundlich equilibrium constant [-]
$c(A_{aq})$	as the concentration of solute in the solution [g/L]
n	as the conditional Freundlich exponent [-]

Two other frequently used isotherms are the Temkin isotherm, which takes into account adsorbent-adsorbate interactions and the Dubinin-Radushkevich isotherm, which is often successful for high solute activities [Dada et al., 2012]. Although these empirical approaches are simple and can easily be fitted to many data sets, there are drawbacks as well. For instance, the statistically-based empirical approach does not typically lead to a general mechanistic understanding [Goldberg et al., 2007]. Furthermore, calculated values for constants such as K_F or K_L are only valid for the specific experimental conditions under which the data was obtained, making general conclusions sketchy at best.

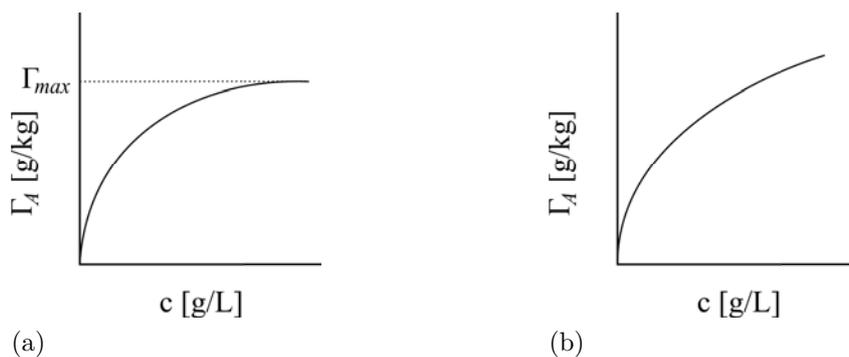


Figure 4.3.: *Empirical modelling of adsorption-desorption equilibria at mineral surfaces* [Goldberg et al., 2007]
 a: *Langmuir isotherm*
 b: *Freundlich isotherm*

4.2.2. The Electrical Double Layer Model (EDL)

In contrast to empirical adsorption fittings, surface complexation models such as the Electrical Double Layer Model (EDL) have a more mechanistic approach and are, therefore, generally more robust and apply to a greater variety of geochemical conditions. Using mass action laws, chemical speciation and competitive adsorption can be taken into account [Davis & Kent, 1990, Goldberg et al., 2007].

When submerged in aqueous solution, any mineral surface becomes an interface between bulk mineral and bulk water properties [Parks, 1990]. This leads to hydroxylation, in which water dissociates and charged, dangling bonds of the mineral's surface form chemical bonds with the resulting hydroxyl groups (OH^-) or protons (H^+). Layered around these hydroxyl or proton bonds to the mineral surface, clusters of water molecules form by hydrogen-bonding, a phenomenon called hydration [Parks, 1990]. While the first monolayer of water is chemically bound to the mineral, the following monolayers are bound increasingly loosely, until water molecules reach bulk water properties.

There are three types of mineral surface charge [Davis & Kent, 1990]: (1) permanent structural charge σ_s , usually as a result of isomorphic substitution (i.e., Al^{3+} instead of Si^{4+}); (2) coordinative surface charge σ_o as a result of potential-determining ions coordinated with surface functional groups; (3) dissociated surface charge σ_d , which is provided by counter-ions and preserves electroneutrality when the net particle charge σ_p is not zero, as

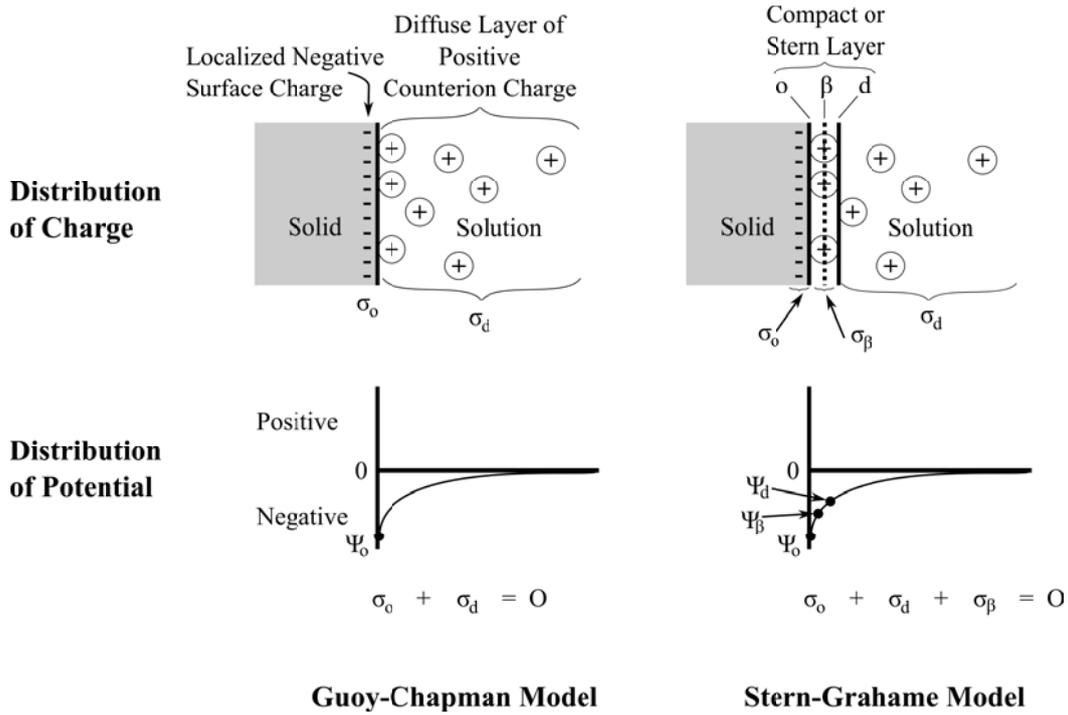


Figure 4.4.: Schematic drawing of the electrical double layer of the classical Guoy-Chapman and Stern-Grahame models under the assumption that $\sigma_s = 0$ [Davis & Kent, 1990]

shown in Equation 4.5.

$$\sigma_p + \sigma_d = 0 \tag{4.5}$$

and

$$\sigma_p = \sigma_s + \sigma_o \tag{4.6}$$

with

- σ_p as the net particle charge [C/m²]
- σ_d as the dissociated surface charge [C/m²]
- σ_s as the permanent structural charge [C/m²]
- σ_o as the coordinative surface charge [C/m²]

The surface layer and disassociated layer are referred to as the EDL. Separation of charges in the EDL leads to an electrical potential difference across the particle-water interface

[Davis & Kent, 1990]. In the Guoy-Chapman theory (Figure 4.4), this charge potential decays exponentially with the distance from the surface, as the diffuse layer of counter-ions are arranged according to their polarity in coulombic interaction around the charged surface, in effect shielding the surface charge from the surrounding bulk solution [Parks, 1990, Davis & Kent, 1990]. This theory was later refined in the Stern-Grahame theory (Figure 4.4), in which a layer of specific adsorption - or compact layer ("Stern" layer) - was added to account for finite ion size and counter-ion interactions directly at the surface [Davis & Kent, 1990].

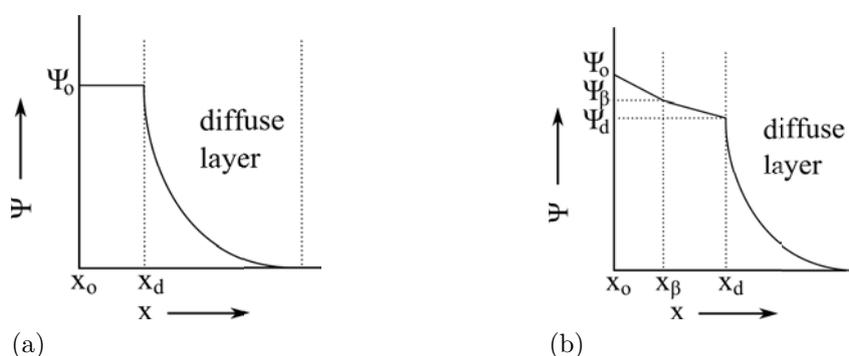


Figure 4.5.: Comparison between two surface complexation models [Davis & Kent, 1990, Goldberg et al., 2007]
 a: the Electrical Double Layer model (EDL)
 b: the Triple Layer Model (TLM)

In EDL models, all chemical adsorption is accounted for at the x_o plane (Figure 4.5a), which can be equated with chemical bonding directly at the particle surface. However, different types of sorption result in different distances from the particle surface. The triple layer model (TLM) includes a second plane x_β (Figure 4.5b), at which outer-sphere complexes or ions with a greater crystallographic radius are accounted for, as opposed to the inner-sphere complexes and ions of smaller crystallographic radius, which are located at the x_o plane [Goldberg et al., 2007].

4.2.3. Points of Zero Charge

Due to a charged surface or dangling bonds, when a solid is submerged in a solution, the initial solution pH value (pH_i) is likely to change unless it equals the so-called critical pH

value (pH_{crit}). According to the Stern-Grahame theory, protons and hydroxyl groups act as the coordinative surface charge (Equation 4.7).

$$\sigma_H = \Gamma_{H^+} - \Gamma_{OH^-} \quad (4.7)$$

with

σ_H as proton surface charge [C/m^2]

Γ_{H^+} as positive charge from adsorbed protons [C/m^2]

Γ_{OH^-} as negative charge from adsorbed hydroxyl groups [C/m^2]

If pH_i is greater than pH_{crit} , the solid is an H^+ donor (or OH^- acceptor); if pH_i is smaller than pH_{crit} , the solid is an OH^- donor (or H^+ acceptor). If the exchanged ions include only OH^- or H^+ , this pH_{crit} is also known as the Point of Zero Net Proton Charge (PZNPC or pH_{PZNPC}) and describes the pH value at which $\sigma_H = 0$ [Parks, 1990, Davis & Kent, 1990, Sposito, 1998].

Under natural conditions, however, the solution surrounding the solid includes ions other than H^+ or OH^- which shield the surface charge from the surrounding bulk solution. Therefore, protons and hydroxyl groups are only a part of the coordinative surface charge σ_o (Equation 4.8) [Parks, 1990, Davis & Kent, 1990].

$$\sigma_o = \sigma_H + \sigma_{CC} \quad (4.8)$$

with

σ_o as the coordinative surface charge [C/m^2]

σ_H as the proton surface charge [C/m^2]

σ_{CC} as the coordinative complex surface charge [C/m^2]

This means that in an environment of strongly adsorbing ions, the pH_{PZNPC} may shift considerably. This made the definition of the pristine point of zero charge (pH_{PPZC}) necessary, which is defined for the condition $\sigma_o = 0$ [Davis & Kent, 1990, Sposito, 1998].

If a particle and its diffuse layer moves through an electric field or fluid flows past it, an immobile hydrodynamic boundary layer forms. When counter-ions of the diffuse layer around the particle are not within this boundary layer, they are stripped away from the particle, resulting in a charge separation. The particle is then left with a net charge (electrokinetic net charge σ_{ek}), leading to the formation of a potential gradient (zeta potential ζ or Ψ_z) in movement direction [Parks, 1990].

The pH value at which a colloidal particle is electro-kinetically uncharged ($\sigma_{ek} = 0$) and at which, therefore, the potential gradient is also zero ($\Psi_z = 0$) is defined as the iso-electrical point (IEP or pH_{IEP}). At pH_{IEP} or at any pH in the presence of high ionic strength, the diffuse layer collapses ($\sigma_d = 0$) and agglomeration or flocculation of particles can occur. With pH_{IEP} defined as $\sigma_{ek} = 0$ (also $\sigma_d = 0$), pH_{PPZC} defined as $\sigma_o = 0$ and pH_{PZNPC} defined as $\sigma_H = 0$, all these critical pH values are analogous in concept, but quantitatively not identical [Parks, 1990]. Furthermore, either is difficult to determine experimentally [Sposito, 1998].

4.2.4. Selenium adsorption & complexation

When a mineral surface is surrounded by aqueous solution, (ad)sorption is defined as

"chemical species attachment to a mineral surface" [Hochella & White, 1990].

Depending on the nature of this attachment, adsorption can be categorized into two basic types [Manceau & Charlet, 1994], outer-sphere and inner-sphere complexes, resulting as a consequence of the two concepts of zero charge, the pH_{IEP} and pH_{PZNPC} .

1. *no presence of strongly adsorbing ions* $\rightarrow \text{pH}_{PZNPC} = \text{pH}_{IEP}$.

These two points of zero charge can be equal only if strong adsorption of electrolyte ions by a charged colloid does not occur [Sposito, 1998]. In this case, anions adsorb when $\text{pH} < \text{pH}_{PZNPC}$ and Ψ_z is positive (cations adsorb when $\text{pH} > \text{pH}_{PZNPC}$). There is minimal adsorption at $\text{pH} = \text{pH}_{PZNPC}$ when the surface is uncharged because adsorption occurs predominantly through coulombic attraction and part of the diffuse

layer remains between the ion and particle surface [Parks, 1990]. This leads to outer-sphere surface complexation, which describes the process of non-specific adsorption (physical adsorption), in which a water molecule is retained between the adsorbing ligand and the surface site. The water molecule is thus part of the adsorption complex, which means that the bonding of the ligand to the surface is of electrostatic nature rather than co-valent or ionic. Characterized by hydrogen bridge bonds or van-der-Vaals interactions, this type of complex is, therefore, less stable than the inner-sphere complex [Parks, 1990].

2. *in the presence of strongly adsorbing ions* $\rightarrow pH_{PZNPC} \neq pH_{IEP}$.

In the presence of strongly adsorbing ions, adsorption is insensitive to surface charge and allows super-equivalence, which describes adsorption of greater density than the electrical equivalent of the surface charge density [Parks, 1990]. Ion adsorption on surfaces of like charge is electrostatically repelled, which is why the strength of the bond must exceed this electrostatic repulsion [Parks, 1990]. This leads to inner-sphere surface complexation, which describes the process of specific adsorption (chemical adsorption), in which an aqueous ligand, i.e. an anion, exchanges for a surface group, i.e. hydroxyl group. First, the surface hydroxyl group is protonated by a proton of the positively charged aqueous hull around the adsorbing molecule. Then, the protonated hydroxyl group is split off as a water molecule and replaced by the adsorbing anion [Parks, 1990]. The chemical bond between the surface site and the ligand can be co-valent or ionic or in-between, which explains the greater stability of this complex [Fernández-Martínez & Charlet, 2009].

Both selenite and selenate are known to adsorb onto ferric hydroxides [Dhillon & Dhillon, 2009]. However, affinity of each anion toward these solids differs. For a long time, anions were simply classified according to their affinity to oxide surfaces, which was believed to determine the nature of the chemical attachment [Manceau & Charlet, 1994]. High-affinity anions including selenite and phosphate were thought to be bound strongly to the sorbent by inner-sphere surface complexes. Low-affinity anions like nitrate, selenate and sulfate

were thought to be bound weakly to the sorbent by an outer-sphere complex.

This convenient explanation holds true for selenite, which, in general, is adsorbed to oxy-hydroxides as shown in Figure 4.6a by a bidentate inner-sphere surface complex [Manceau & Charlet, 1994, Su & Suarez, 2000, Fernández-Martínez & Charlet, 2009]. However, while many authors have confirmed that selenate has less affinity to ferric oxy-hydroxides than selenite [Davis & Kent, 1990, Hayes et al., 1987], through the use of modern spectroscopic techniques, such as EXAFs, it was discovered in 1994 that the traditionally accepted macroscopic link between ionic dependence of adsorption and outer-sphere complexation did not always apply. While it is true that outer-sphere complexes are strongly dependent on ionic strength and are much more sensitive to competing ions which can replace the outer-sphere-adsorbed ligand, the inverse conclusion was shown to be false. Sensitivity to ionic strength is not an adequate macroscopic criterion with which outer-sphere complexation can be determined [Manceau & Charlet, 1994].

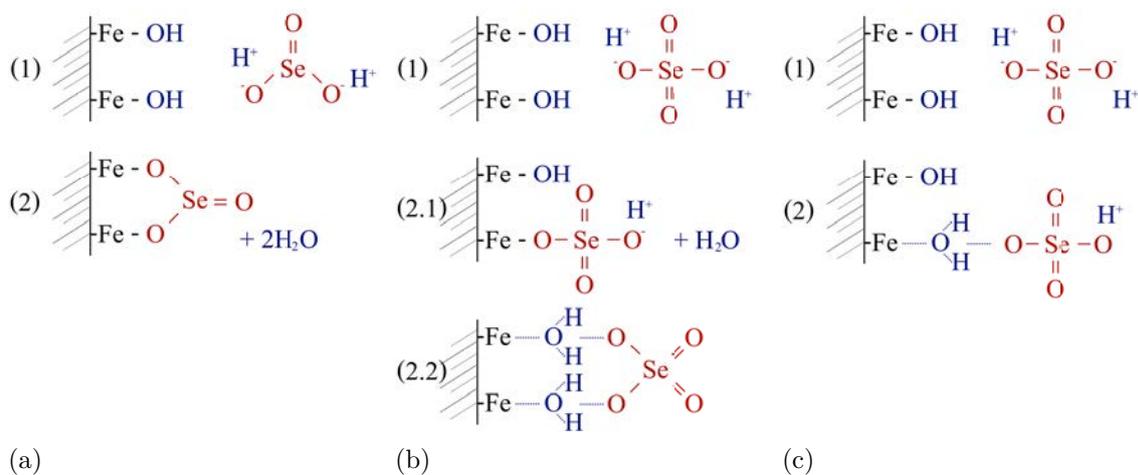


Figure 4.6.: Adsorption of Se oxy-anions in 2 steps; step 1 shows the free anion in solution, step 2 shows resulting surface complexation [Fukushi & Sverjenski, 2007]
 a: Specific adsorption of selenite as ligand exchange forming a bidentate-mononuclear inner-sphere complex
 b: Complexation of selenate, either as specific adsorption as a monodentate-mononuclear inner-sphere complex (step 2.1) or as non-specific adsorption as a bidentate-binuclear outer-sphere complex (step 2.2)
 c: Selenate adsorption onto amorphous ferric oxide as bidentate-mononuclear outer-sphere complex

In an attempt to reconcile conflicting data on selenate complexation on goethite from ATR-FTIR and EXAFS studies [Hayes et al., 1987, Manceau & Charlet, 1994, Su & Suarez,

2000], the extended triple layer model (ETLM) took into account the substantial electrostatic work associated with the desorption of water dipoles during ligand exchange reactions [Fukushi & Sverjenski, 2007]. As shown in Figure 4.6b, selenate shows two main adsorption mechanisms onto goethite, a monodentate-mononuclear inner-sphere and a bidentate-binuclear outer-sphere (or H-bonded) complex, the relative proportions of which are functions primarily of pH and ionic strength [Fukushi & Sverjenski, 2007]. However, as shown in Figure 4.6c, selenate adsorption onto hydrous ferric oxide, an amorphous goethite relative, is characterized by a bidentate-mononuclear outer-sphere complex (also H-bonded).

4.2.5. Se adsorption competition by nutrient anions

For the purpose of this study, the following main nutrient anions are of great interest: sulfate (SO_4^{2-}), phosphate (PO_4^{3-}) and nitrate (NO_3^-). In natural soil solutions, each of these anions is present in much higher concentration than either selenite or selenate. While Se in soils is roughly 0.1 - 2 mg/kg [Fernández-Martínez & Charlet, 2009], concentrations of S as sulfate are generally 2 - 20 mg/kg [Horneck et al., 2011], extractable concentrations of P are usually 10 - 100 mg/kg [Horneck et al., 2011] and plant-available concentrations of N are generally around 2-10 mg/kg as NH_4^+ and 10-30 mg/kg as NO_3^- [Marx et al., 1999]. Therefore, competition by these ions is an important aspect of Se sorption processes and influences the Se cycle.

In order to determine how these anions affect selenite and selenate adsorption, redox behaviour and pH-dependent speciation information is necessary. While Se occurs both as selenite and selenate in typical oxidized soil conditions at pH 4 - 10, S is mainly found as sulfate, P is protonated either as di-hydrogen or hydrogen phosphate and N is found as nitrate or ammonium (Figure 4.7). As shown in Figure 4.8, these anions also all exhibit distinct structural properties. Selenite is pyramidal with its two free electron pairs forming a semi-tetrahedral structure, while selenate, sulfate and phosphate are all tetrahedral in structure [Kálmán, 1971, Séby et al., 2001, Mortimer, 2010]. Nitrate, on the other hand, is a trigonal planar molecule [Paul & Pryor, 1972]. Electronegativity differences between the

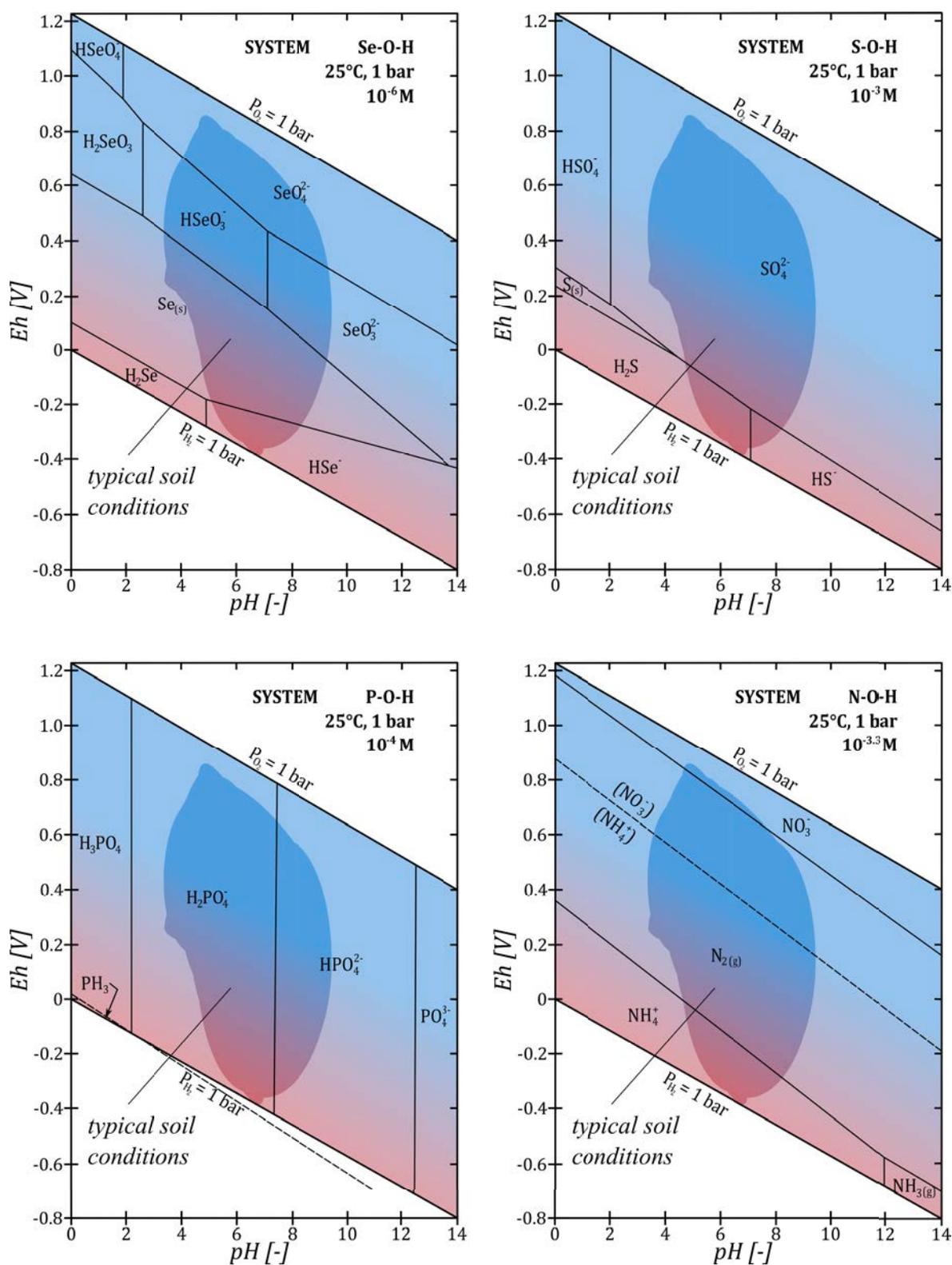


Figure 4.7.: *Eh-pH* diagrams for thermodynamic data of Se (10^{-6} mol), S (10^{-3} mol), P (10^{-4} mol) and N ($10^{-3.3}$ mol) within the stability field of water at 25°C at 1 bar [Brookins, 1988] with typical soil conditions added according to [Neal, 1995]; blue indicates oxidizing conditions in natural soils, red indicates reducing conditions with a transitional zone between

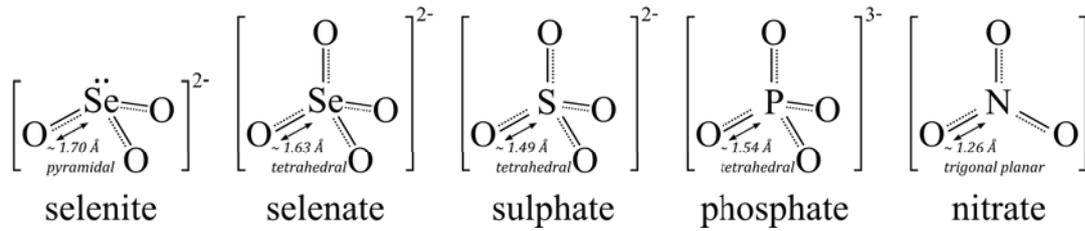
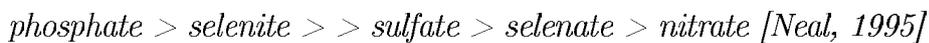


Figure 4.8.: 3D structure and X-O bond lengths of Se oxy-anions selenite and selenate as well as the three main nutrient oxy-anions phosphate, sulfate and nitrate [Kálmán, 1971, Paul & Pryor, 1972, Séby et al., 2001, Mortimer, 2010]

central atom and the O-atom in these anions, which, according to Pauling [Mortimer, 2010] account for polarizability of a molecule are the highest in phosphate (P-O bond, $\text{EN}_{\text{diff}} = 1.2$) and the lowest in nitrate (N-O bond, $\text{EN}_{\text{diff}} = 0.2$). sulfate and selenate are alike (S-O and Se-O bond, $\text{EN}_{\text{diff}} = 0.8$), but selenite has an additional free electron pair (Figure 4.8), which increases its molecular polarization [Mortimer, 2010].

Structural and electrochemical similarity between sulfate and selenate is expected to lead to similar sorption behaviour [Fernández-Martínez & Charlet, 2009]. Competition effects between selenite and phosphate have been observed, leading to the conclusion that sorption mechanisms of ligand exchange are similar between these two ions [Neal, 1995]. Due to greater differences in structure and size between nitrate and Se oxy-anions, nitrate is not expected to show the same competition effects as phosphate or sulfate. Nitrate is, therefore, believed to bind as an outer-sphere complex [Neal, 1995]. In conclusion, the affinity sequence for selected anion adsorption of nutrient oxy-anions and Se oxy-anions onto soils is considered to be the following:



4.3. Material characterization of kaolinite and goethite

Characterization of sorption processes onto the surface of a mineral requires a certain degree of purity in order to exclude interfering sorption phenomena and/or leaching of the chosen

Table 4.1.: *Industrial products tested for quality as sorption material*

sample name	main mineral	company
Kaolin AKW KN 83	kaolinite	Amberger Kaolinwerke
Kaolin KBS Opal Alpha	kaolinite	Kruse Bassermann Specialties
Kaolin KBS Burgess Thermo-Glace HB	kaolinite	Burgess Pigment
FeOOH Bayoxide E 216	ferric oxy-hydroxide	Bayferrox
FeOOH Bayoxide 920 Z	ferric oxy-hydroxide	Bayferrox
Dors 9S 1-0.6	quartz	Dorsillit

element from the substrate. Therefore, the materials used for the following experiments were analyzed for their purity. Table 4.1 summarizes the obtained industrial products, which were assessed for their quality with standard analytical procedures. A total of three industrial kaolin samples was ordered from two different companies with the request for good sorption properties and high kaolinite purity. Two different industrial goethite samples and a quartz sample were also analyzed for their purity and sorption properties. Since kaolin is a natural material containing varying quantities of kaolinite and the goethite ordered was an industrial product of unknown refinery, quality assessment was a prerequisite for all the following experiments. Of the three kaolinite and two goethite products, one product of each mineral with the greatest purity was selected.

4.3.1. Sample preparation

All materials were analyzed for their chemical components by means of full acid digestion in Teflon beakers, with 0.1 g sample incubated with 2 mL of 65 % HNO₃ (VWR 20429.320 p.a. sub-boiled) at 200 °C for 30 min before being concentrated in multiple steps with 40 % HF (Merck 1.00335.1000, suprapure) and HClO₄ (VWR 1.00517.1000, suprapure). Digested solutions were then measured with ICP-MS (Chapter 3.4.4). Furthermore, fused beads of the samples were analyzed with Wavelength dispersive X-ray spectroscopy (WDX). Sample preparation of the fused beads follows a standardized method [DIN EN ISO 12677:2013], using 0.5 g of freshly ground sample dried at 40 °C with 5 g of 65.5 % dilithiumtetraborate and 34.5 % lithiummetaborate fluxing agent (111802 Spectromelt A12 from Merck).

In-depth kaolinite analysis was conducted with thermogravimetry coupled with differ-

ential scanning calorimetry (TG-DSC) in cooperation with members of the Competence Centre for Material Moisture (CMM, KIT) using an STA 449C Jupiter (NETSCH). After a reference measurement run-through with the empty Pt-crucible, 100 mg of sample powder was tared, measured isothermally at a temperature of 35 °C for room-temperature water evaporation and then analyzed for its temperature profile from 35 - 1100 °C. To verify that the weight loss attributed to kaolinite restructuralization was indeed due to crystal water loss, the resulting gas flow during the TG-DSC measurement was analyzed with an MS (Infrared mass spectrometer, 2MS 403C Aëolas). This was used to identify ion counts for masses $M=18$ (H_2O), $M=44$ (CO_2), $M=16$ (O) and $M=64$ (SO_2) in 50 mL of sample gas combined with 20 mL N_2 protective gas.

Further evidence of clay mineral content in the kaolin samples was obtained by measuring texture samples [Tributh, 1976, Lagaly & Köster, 1993], prepared as follows: 50 mg of sample powder was filled into a 15-mL glass test tube, submerged in 10 mL of diluted NH_4OH (10 mL NH_4OH / 1 L double-deionized water), shaken and put into an ultra-sound bath for 15 min. After shaking, the sample was left to sediment for 1 h. With the non-clay particles sedimented and the clay particles held in submersion by NH_4OH , 3 1-mL samples of the supernatant were pipetted onto a glass object slide (diameter: 2 cm). The first of these three samples was air-dried for 24 h as a reference, the second was treated with ethylene glycol for 24 h to test for expanding layers of non-kaolinite clays and the third was burnt at 550 °C for 3 h to test for the kaolinite-typical collapse of the reference kaolinite peak after structural change due to water loss.

For the final step in the kaolin material characterization, an extensive x-ray diffraction scan (XRD) was performed at CMM using a Siemens D5000 X-ray Powder Diffraction System (angular range: 3 - 100 °, stepsize: 0.01 °, time step 0.1 s, anode material: Cu) Using DIFFRAC.SUITE EVA (Bruker) in combination with AutoQuan (BGMN), the mineral phases found in any of the three different kaolin powders (kaolinite, muscovite, orthoclase, cristobalite, quartz, tridymite, calcite, magnetite, anatase and rutile) were used for the computation of a theoretical XRD diffractogram, which can be subtracted from the measured diffractogram to account for unidentified phases.

Goethite characterization was achieved by x-ray diffraction (Siemens D500 X-ray Powder Diffraction System, angular range: 2 - 22°, stepsize: 0.01°, time step 1 s, blinds: 1.54, anode material: Cu) for both industrial FeOOH samples. After choosing the purest kaolinite and goethite, their surface areas were calculated using a N₂-Brunauer-Emmett-Teller scan (BET) performed by Peter Weidler, IFG (KIT), using a Quantachrome Autosorb 1-MP instrument. Additionally, scanning electron microscopy images (SEM) were taken in cooperation with Frank Zibat, LEM, (KIT).

4.3.2. Material characterization results for kaolinite and goethite

Figure 4.9 shows component percentages as oxide-equivalents corrected by the loss of mass by ignition LOI₁₀₅₀, with the exception of quartzsand, for which loss by ignition was not analyzed since it was assumed to be zero. For better comparison, minor component percentages (< 5 %) are shown separately.

The Dorsillit quartz sample showed a high degree of purity (99.1 %) and was used for experiments with open rice cultures (Chapter 3.3.1). Kaolin samples KBS BTG HB and AKW KN 83 were similar in purity according to WDX- and ICP-MS analysis (Figure 4.9), while the kaolin sample KBS 0 alpha was clearly less pure than the others due to a high K content. In the goethite samples, a large quantity of quartz in the 920 Z sample significantly lowered the goethite percentage of the substrate after loss by ignition.

Figure 4.10 shows the resulting TG-DSC curve (analyzed with NETSCH Proteus-Thermal-Analysis Version 5.1.0 Software) for kaolin powder AKW KN 83. Results for kaolin powders KBS 0 alpha and KBS BTG HB are shown in the Appendix (Figure B.2, B.3) Using the weightloss at 550 °C to calculate kaolinite purity (Figure 4.10), the AKW KN 83 sample was chosen for its purity of 89 % kaolinite, compared to 78 % for KBS 0 alpha and 86 % for KBS BTG HB for all future sorption experiments. Verification of the nature of the evaporated gases (H₂O, O₂, SO₄ and CO₂) through the coupled MS (Appendix, Figure B.4, B.5, B.6) showed that for AKW KN 83, gas loss was mainly water and a small amount of

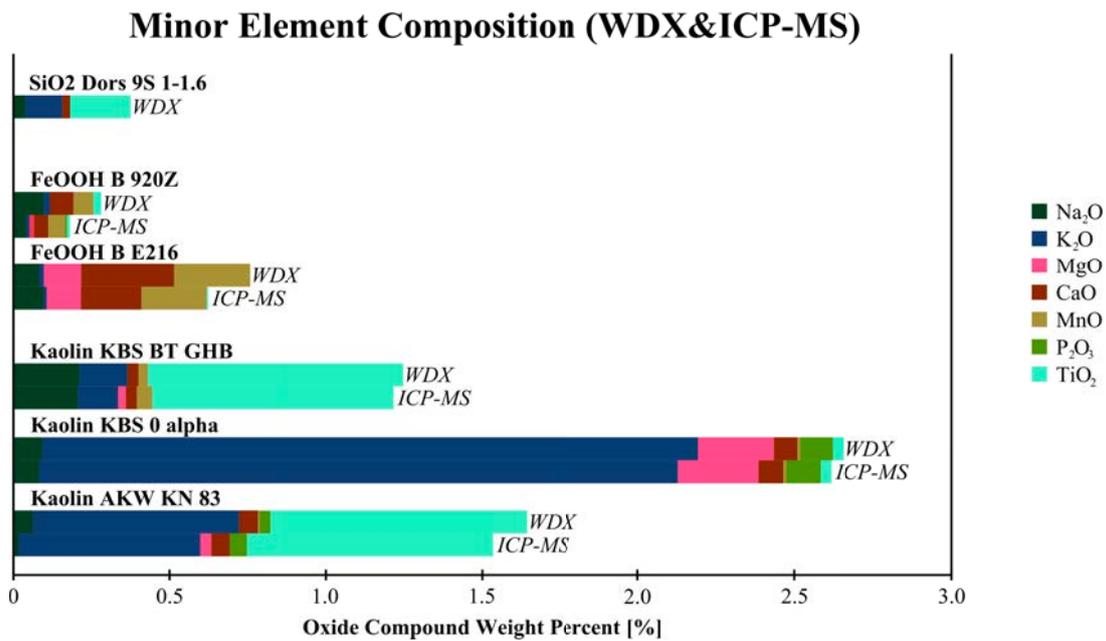
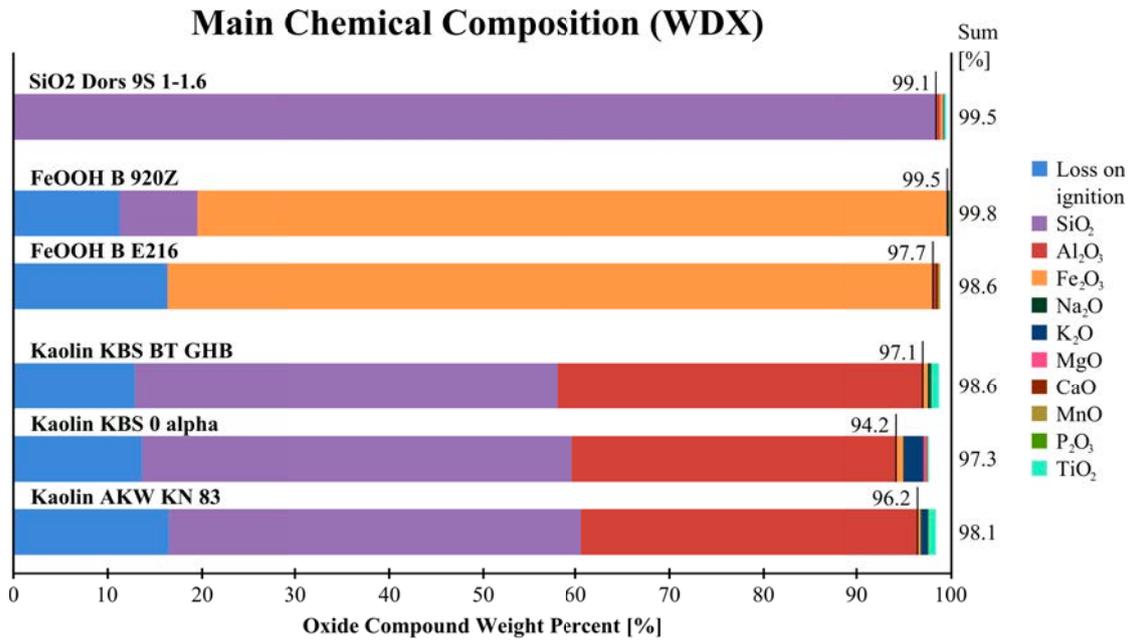


Figure 4.9.: Main chemical composition (top) and minor element composition (bottom) of sorption materials in oxide-equivalents as measured with WDX and ICP-MS after full HF-digestion

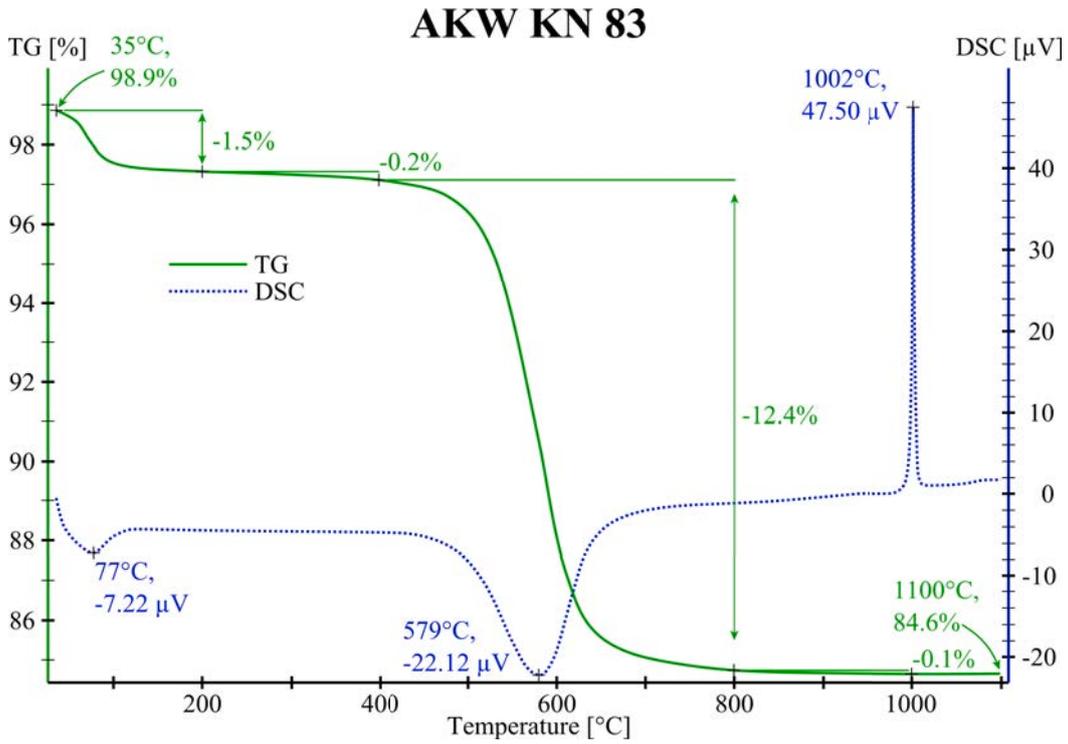


Figure 4.10.: TG-DSC curve of kaolin powder AKW KN 83 measured at CMM (100 % kaolinite yields a weight loss at 550°C of 13.95 %, therefore 12.4 % weightloss indicate a Kaolinite purity of 89 % for this sample

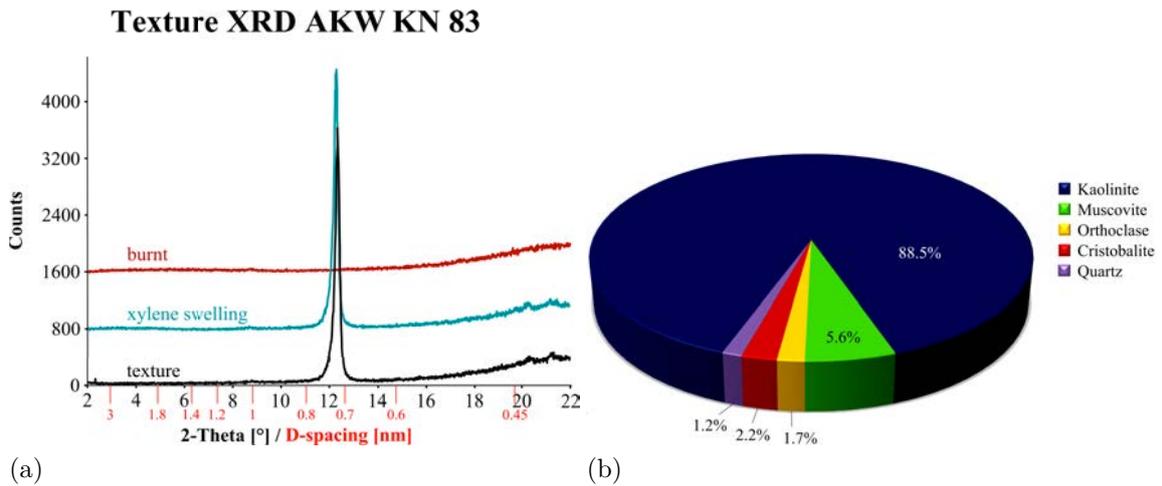


Figure 4.11.: Characterization of kaolin sample AKW KN 83
 a: XRD analysis of texture samples untreated, burnt and swelled
 b: AutoQuan-calculated mineral composition, calculated total: 99.2 % ±0.5

natural soils and the higher share of goethite in the sample, the following sorption studies were conducted with the more amorphous and purer E216.

The BET scans of both goethite samples yielded a surface of $126.4 \text{ m}^2 \pm 1.8$ for E216 and $10.0 \text{ m}^2 \pm 0.5$ for 920Z, while kaolinite was found to have a surface of $9.4 \text{ m}^2/\text{g} \pm 0.1$. The SEM images of the mineral surfaces for kaolinite (Figure 4.13a) and goethite (Figure 4.13b) shows typical, well-crystallized surfaces for kaolinite with sheet-like structures, while the large amorphous share and much larger surface area is visible for goethite.

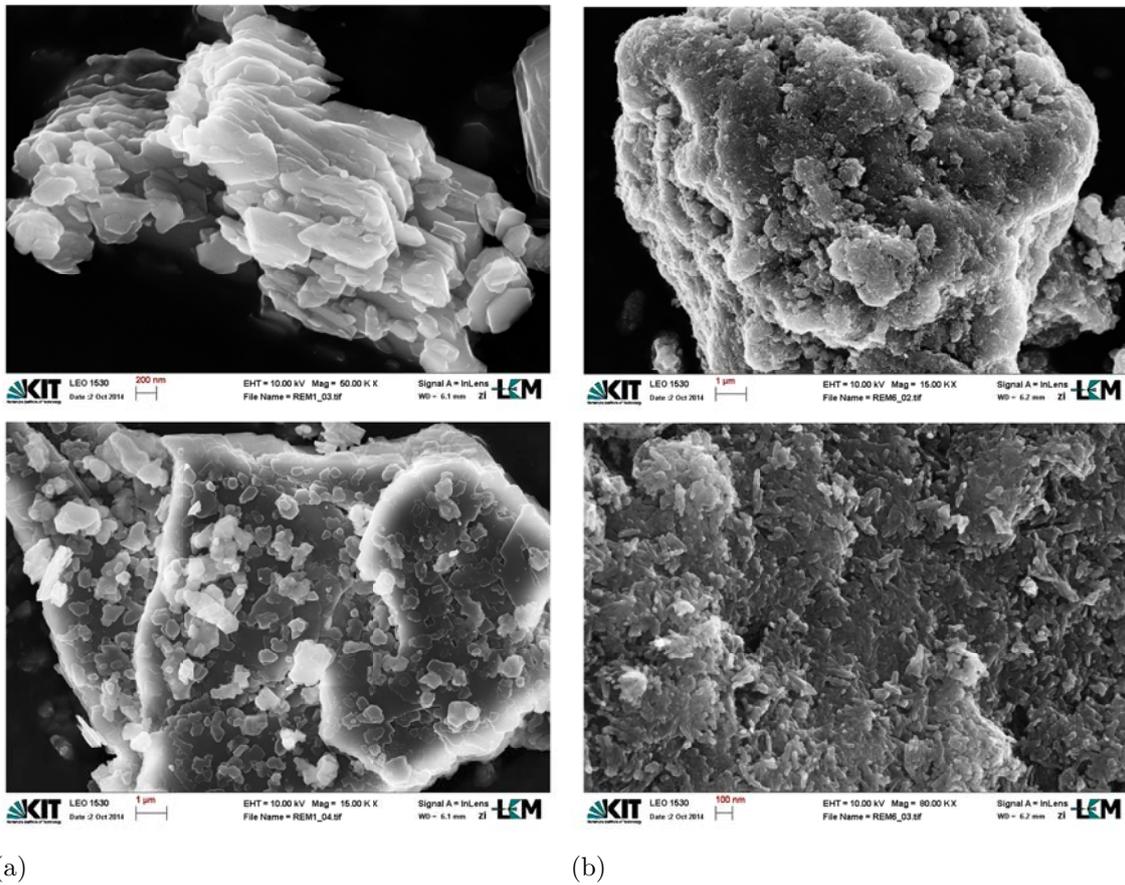


Figure 4.13.: SEM images taken from sorption materials (electrical conductivity provided by thin Pt-coating)
 a: kaolinite AKW KN 83, magnification 15 K (above), 50 K (below)
 b: goethite E216, magnification 15 K (above), 80 K (below)

4.4. Experimental set-ups

The following sorption studies are divided into 4 main parts:

- (1) preliminary tests;
- (2) pure selenite and selenate adsorption onto the substrates kaolinite and goethite;
- (3) subsequent desorption of previously adsorbed Se from kaolinite and goethite;
- (4) selenite and selenate adsorption in the presence of the competing anions phosphate, sulfate and nitrate.

Based on results from the preliminary tests, experimental set-ups were optimized.

4.4.1. Preliminary tests

In order to predict which sorption concentrations and substrate amounts might yield measurable results in later experiments the following sets of preliminary tests were conducted.

Substrate reaction to double-deionized water

Before sorption experiments were conducted, pH value changes due to mineral surface properties were measured using 0.5 g (Sartorius 1712MP8) of either kaolinite or goethite and 10 mL of double-deionized water in 20-mL patho vessels (Böttger 08-313-1001). The pH values of two double-deionized water blanks, two kaolinite samples and two goethite samples were measured in five replicates with two pH electrodes (WTW SenTix 41, WTW SenTix V), due to the difficulties of measuring the pH value of double-deionized water.

Sorption influence of substrate amount vs. Se concentration

For the sorption experiments, kaolinite and goethite powders were milled for 5 min to a homogeneous powder using an agate mill (Siebtechnik, Scheibenschwingmühle-TS). The first set of preliminary sorption studies was carried out using kaolinite or goethite amounts of 50, 100, 500 and 1000 mg (Sartorius basic BA 1105) weighed into 15-mL-centrifuge tubes (VWR 525-0149). Concentrations of 50, 500 or 5000 $\mu\text{g/L}$ Se as selenate were achieved by pipetting 10, 100 or 1000 μL of 500 mg/L Se stock solution (in an Eppendorf reaction

tube: 1 mL of double-deionized water and 1 mL of $\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$, VWR BDH Prolabo 302113L) into 100 mL glass flasks prepared with 3.536 mmol CaCl_2 solution (194.6285 mg CaCl_2 in 500 mL of double-deionized water) as background ionic strength comparable to the nutrient solution (Chapter 3.3.3). Ten mL of sorption solution was added to each substrate sample and shaken for 24 h at 180 rpm. After sorption tubes were centrifuged at 40,000 rpm for 5 min (Rotofix 32 A), 9.5 mL of sorption solution from kaolinite samples and 9.25 mL from goethite samples was extracted, pipetted into labelled 15-mL-centrifuge tubes (VWR 525-0149) and prepared for HG-FIAS measurement (Chapter 3.4.3).

Experimental desorption properties

In this set of preliminary tests, Se losses due to the substrate washing step preceding the desorption experiment needed to be quantified. Furthermore, the ability of an extraction step [Kulp & Pratt, 2004], [Bacon & Davidson, 2007] as desorption agent for easily exchangeable Se was explored.

After sampling sorption solution, Se-sorbed kaolinite and goethite samples were prepared for desorption. A washing step to remove residual sorption solution was conducted by re-submerging the substrate in 9.5 mL of double-deionized water for 1 min. After centrifuging at 40,000 rpm for 5 min (Rotofix 32 A), sorption solution (9.5 mL from kaolinite solutions and 9.25 mL from goethite solutions) was sampled into labelled 15-mL-centrifuge tubes (VWR 525-0149). Remaining substrate was then resubmerged in double-distilled water (amounts equal to the sampled sorption solution), manually shaken for 1 min before being centrifuged at 40,000 rpm for 5 min (Rotofix 32 A). This double-distilled water was sampled into labelled 15-mL-centrifuge tubes (VWR 525-0149) as well in order to verify any unintended Se loss during this step. Both sorption samples and wash samples were prepared for HG-FIAS measurement (Chapter 3.4.3).

A desorption solution of 0.1 mol/L K_2HPO_4 [Kulp & Pratt, 2004, Bacon & Davidson, 2007] was prepared as follows: in a 500-mL glass bottle (Schott), 8.7087 g of K_2HPO_4 were dissolved in 500 mL of double-deionized water and then brought to a pH of 8.0 using 100 μL (± 30) 37 % HCl (Merck, p.a. 1.00317.2500). Each sample was re-submerged in 9.5

mL of desorption solution and placed on the shaking table at 180 rpm for 24 h. After centrifuging at 40,000 rpm for 5 min, 9.5 mL of sorption solution was sampled into labelled 15-mL-centrifuge tubes (VWR 525-0149) and prepared for HG-FIAS measurement (Chapter 3.4.3).

Experimental up-scaling effects

Keeping the ratio of sorption solution volume per substrate amount constant, the following up-scaling experiments were designed to identify whether sorption results were affected by experimental conditions such as bottle size or if a constant ratio between solution volume and substrate amount yielded the same results on different scales. The experiment was carried out using 1, 5, 10, 50 and 100 g of milled kaolinite or goethite and 10, 50, 100, 500 and 1000 mL of 5000 µg/L Se as selenate ($\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$, VWR BDH Prolabo 302113L) in 3.536 mmol CaCl_2 in screw-lid PP bottles, respectively. Samples were placed on a shaking table at 180 rpm for 24 h. After centrifuging at 40,000 rpm for 5 min (Rotofix 32 A), 7.5 mL of sorption solution was sampled into labelled 15-mL-centrifuge tubes (VWR 525-0149) and prepared for HG-FIAS measurement (Chapter 3.4.3).

4.4.2. Exp. B1 - pure Se sorption onto kaolinite and goethite

The following batch experiment was designed to determine selenite and selenate adsorption properties of kaolinite and goethite in the presence of ionic strength similar to the nutrient solution used in experiments A3 (Chapter 3.3.3).

As shown in Figure 4.14a, for every batch of 36 samples, 0.5 g of either milled kaolinite (18 samples) or milled goethite (18 samples) were weighed (Sartorius 1712MP8) into labelled 20-mL patho vessels (Böttger 08-313-1001). To ensure that the sampled initial solution was identical for each Se concentration of the respective kaolinite and goethite sorption batch as well as their sampled solution for analysis, each of the 18 sorption solutions of 30 mL (10 mL for kaolinite sorption + 10 mL for goethite sorption + 10 mL for analysis) was prepared in 50-mL glass beakers. Because the range of Se concentrations in this study was so large

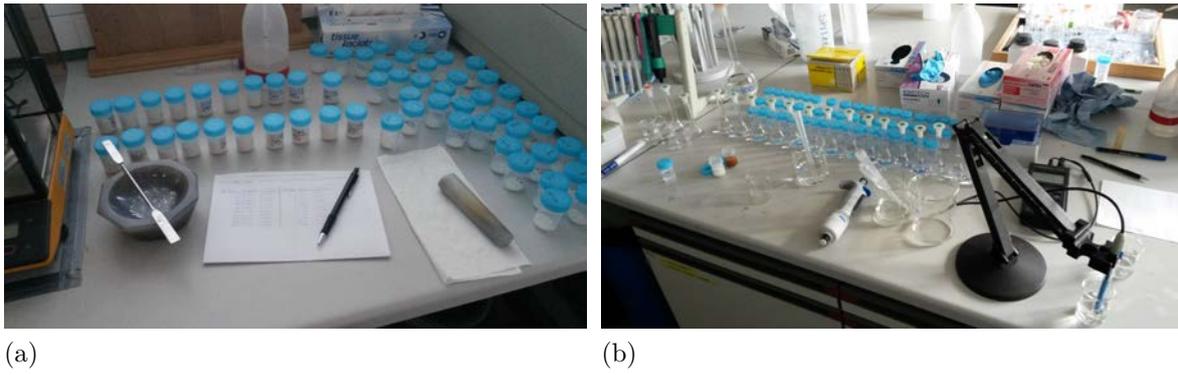


Figure 4.14.: *Photos of sorption experiment preparations*
a: weighing kaolinite for selenite adsorption studies (photo taken on 07.07.2014)
b: distribution of 30 mL of sorption solution of selenate adsorption experiments into goethite, kaolinite and sampling patho-vessels with pH measurement (photo taken on 14.05.2014)

(0, 10, 25, 50, 75, 100, 150, 200, 250, 350, 500, 750, 1000, 1500, 2000, 2500, 3500 and 5000 $\mu\text{g/L}$), two Se stock solutions of 10 mg/L and 1000 mg/L Se had to be used; in 7.735 mmol KCl, either as $\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$ (VWR BDH Prolabo 302113L), or as Na_2SeO_3 (AlfaAesar 012585), respectively. Background ionic strength was 7.735 mmol/L KCl, the calculated equivalent to nutrient solution ionic strength (Chapter 3.3.3): $6500 \mu\text{mol Ca}(\text{NO}_3)_2 + 375 \mu\text{mol K}_2\text{SO}_4 + 325 \mu\text{mol MgSO}_4 + 400 \mu\text{mol K}_2\text{HPO}_4 + 8 \mu\text{mol H}_3\text{BO}_3 + 50 \mu\text{mol CaCl}_2 + 75 \mu\text{mol C}_6\text{H}_5\text{O}_7\text{Fe} = 7.735 \text{ mmol ions}$ (contributions smaller than 8 μmol were excluded). KCl was chosen instead of CaCl_2 because comparable experiments would be performed with additional ions (Chapter 4.4.4), such as sulfate and any Ca present would lead to precipitation (Chapter 3.3.1).

To avoid disproportional distortion due to different pipetting amounts of Se, the 18 Se solutions were prepared in double-deionized water in 25-mL glass flasks at double their appointed concentrations. Likewise, the KCl solution was prepared at 15.47 mmol/L (576.8 mg KCl, Merck, p.a. 1.04936.1000, in 500 mL double-deionized water). To achieve appointed Se and KCl concentrations, 15 mL of the respective Se solution and 15 mL of KCl were pipetted into a 50-mL glass beaker for each Se sorption solution, diluting each other into appointed concentrations. Solutions were homogenized, temperature and pH values were measured (WTW SenTix 81) and the solution was then evenly distributed, pipetting 10

mL each into the goethite and kaolinite patho-vessels (Figure 4.14b). The remaining 10 mL were transferred into a sampling patho-vessel and frozen at -20°C until measurement. Kaolinite and goethite samples were shaken at room temperature for 24 h at 180 rpm; as the shape of patho-vessels allowed 10 mL of liquid to be homogenously shaken in an upright position.

After sorption, patho-vessels were centrifuged (Rotofix 32 A) at 40,000 rpm for 5 min. Because the patho-vessels are not guaranteed to withstand centrifuging, each patho-vessel was placed into a 50-mL centrifuge tube; however, none of the patho vessels broke. 9.5 mL of kaolinite sorption solution (9.25 mL of goethite sorption solution) were then sampled into labelled patho vessels with a pipette and frozen at -20°C for later measurement. Sample analysis of Se was conducted with ICP-MS (Chapter 3.4.4).

4.4.3. Exp. B2 - Se desorption from kaolinite and goethite

The desorption of Se by means of the extraction step [Kulp & Pratt, 2004, Bacon & Davidson, 2007] as a desorption agent for easily exchangeable Se was intended to represent the amount of plant-available adsorbed Se.

With only 9.5 mL (9.25 mL) retrieved from the 10 mL initially added, directly adding desorption solution would dilute the remaining sorption solution and Se measured could not be monocausally identified; in the case of $5000\ \mu\text{g/L}$ Se, by pipetting off 9.5 mL out of 10 mL, $250\ \mu\text{g/L}$ Se would be measurable simply by filling up to 10 mL again from 0.5 mL. Therefore, a wash step was included, but not sampled for measurement; 9.5 mL of double-deionized water was pipetted onto the substrate, shaken for 1 min, centrifuged (40,000 rpm, 5 min) and pipetted off, thereby reducing even the highest-possible Se concentration in the event of no sorption from $5000\ \mu\text{g/L}$ down to $12.5\ \mu\text{g/L}$ Se.

For the actual desorption experiment, 9.5 mL of desorption solution was pipetted onto each of the previous sorption samples (desorption solution preparation: 500 mL of $0.1\ \text{mol/L}$ $\text{K}_2\text{HPO}_4 = 8.709\ \text{g}$, resulting $\text{pH} = 9.23$, brought down to $\text{pH} 8.04$ by $300\ \mu\text{L}$ $9\ \text{mol/L}$ HCl , Merck, p.a. 1.00317.2500) as described in soil extraction procedures [Bacon & Davidson,

2007]). Again, samples were shaken for 24 h at 180 rpm at room temperature. Samples were then centrifuged (40,000 rpm, 5 min, Rotofix 32 A), 7 mL sampled and frozen at -20°C for later measurement. Sample analysis of Se was conducted with ICP-MS (Chapter 3.4.4) with a dilution factor of 10 due to high K_2HPO_4 sample salt load.

4.4.4. Exp. B3 - ion competition of Se sorption onto kaolinite and goethite

With the following experiment, competitive adsorption of selenite and selenate was determined for each of the major oxy-anion constituents of the nutrient solution used in experiment A3 (Chapter 3.3.3). The nutrient solution contained ca. 700 $\mu\text{mol/L}$ of sulfate, ca. 12,000 $\mu\text{mol/L}$ of nitrate and ca. 400 $\mu\text{mol/L}$ of phosphate. For comparison between these ions within the sorption experiments and semi-comparison of sorption experiments to the nutrient solution, 750 $\mu\text{mol/L}$ of each of the three main nutrient ions, nitrate, sulfate and phosphate, was separately added to the previous sorption set-up for competition sorption experiments as KNO_3 (Merck p.a. 1.05063.0500), K_2SO_4 (Merck, p.a. 1.05153.0500) or KH_2PO_4 (Merck, p.a. 1.04873.1000), respectively. Experiments were carried out with the same ionic strength of 7.735 mmol KCl for kaolinite and goethite in the presence of 750 μmol of either competing ion sulfate, nitrate or phosphate. Appointed Se concentrations (0, 10, 25, 50, 100, 250, 500, 1000, 2500 and 5000 $\mu\text{g/L}$) were again pipetted from 1000 mg/L stock solutions of $\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$ (VWR BDH Prolabo 302113L) and Na_2SeO_3 (AlfaAesar 012585).

Similar to the sorption experiment described above, for every batch of 20 samples, 0.5 g of either milled kaolinite (10 samples) or goethite (10 samples) were weighed (Sartorius 1712MP8) into labelled 20-mL patho vessels (Böttger 08-313-1001). Again, Se solutions were prepared in 25 mL glass flasks at double their appointed concentrations in double-deionized water. The KCl-oxy-anion solution was also prepared at double the appointed concentration in a 500-mL glass flask (15.47 mmol/L KCl = 576.8 mg KCl; 1500 $\mu\text{mol/L}$ oxy-anion: 75.83 mg KNO_3 , 130.70 mg K_2SO_4 , 130.64 mg KH_2PO_4). To achieve appointed

concentrations of Se, oxy-anions and KCl, 15 mL of the respective Se solution and 15 mL of the KCl-oxy-anion solution were pipetted into a 50-mL glass beaker for each Se sorption solution, diluting each other into appointed concentrations.

Again, these were homogenized, temperature and pH values were measured (WTW Sentix 81) and solutions were then distributed into a kaolinite sample (10 mL) and a goethite sample (10 mL). The remaining 10 mL (the initial reference sample) were transferred into a sampling patho-vessel and frozen at -20°C until measurement. Kaolinite and goethite samples were shaken at room temperature for 24 h at 180 rpm, centrifuged (40,000 rpm, 5 min, Rotofix 32 A) and sampled (5 mL). Samples were frozen at -20°C until analysis of Se was conducted with ICP-MS and analysis of nitrate, sulfate and phosphate was conducted by IC (Chapter 3.4.4).

4.5. Results on Se adsorption onto kaolinite and goethite

Although preliminary experiments are usually not discussed in great detail, because they are generally not conducted under the exact conditions as the subsequent experiments (i.e. ionic strength being slightly different), they are included in the results in this case, as they have implications for the later discussion concerning the wash step and up-scaling of experiments. Furthermore, sorption results in the presence of nutrient solution of Exp. C (Chapter 6.5c) are also included.

4.5.1. Preliminary tests

As shown in Table 4.2, pH values were measured with an accuracy of ± 0.3 and values for blank, kaolinite and goethite converged consistently to 5.5, 6.8 and 7.8, respectively. The calculated proton concentration difference, which establishes between both minerals and double-deionized water (in equilibrium with CO_2 at 1 atm) at pH_{init} . 5.5 was found to be nearly proportional to surface area, with a factor of 13.5 between surface areas of kaolinite

and goethite and a factor of 12.9 - 13.2 between their respective changes in $c(\text{H}^+)/\text{m}^2$.

Table 4.2.: *pH values for kaolinite (K) and goethite (G) in double-deionized water (Bl) after shaking for 24 h at 180 rpm and pH-calculated proton concentration change normalized per substrate surface area (pH_1 , pH_3 and pH_5 measured with SentixV, pH_2 and pH_4 measured with Sentix41)*

ID	Kaolinite [g]	Goethite [g]	Surface [m ²]	pH ₁ [-]	pH ₂ [-]	pH ₃ [-]	pH ₄ [-]	pH ₅ [-]	Mean [-]	SD [-]	$c(\text{H}^+)$ [mol/L]	$\Delta c(\text{H}^+)/\text{surface}$ [mol/m ²]
Bl 1	x	x	x	5.0	5.5	5.7	5.5	5.9	5.5	0.3	$3.162 \cdot 10^{-6}$	x
Bl 2	x	x	x	5.4	5.4	5.4	5.5	5.8	5.5	0.2	$3.162 \cdot 10^{-6}$	x
K 1	0.4942	x	4.6455	6.7	7.0	6.6	6.7	6.8	6.8	0.2	$1.585 \cdot 10^{-7}$	$6.466 \cdot 10^{-9}$
K 2	0.5040	x	4.7376	6.5	7.2	6.4	7.0	6.9	6.8	0.4	$1.585 \cdot 10^{-7}$	$6.466 \cdot 10^{-9}$
G 1	x	0.4972	62.8461	7.5	8.0	7.3	7.9	7.9	7.7	0.3	$1.995 \cdot 10^{-8}$	$5.000 \cdot 10^{-10}$
G 2	x	0.5081	64.2239	7.5	8.1	7.4	8.0	7.9	7.8	0.3	$1.585 \cdot 10^{-8}$	$4.899 \cdot 10^{-10}$

As shown in Figure 4.15a, when plotted against two logarithmic axes, selenate sorption showed a nearly linear trend, with goethite about twice as active as kaolinite. This means that both parameters - Se concentration in the solution and the amount of substrate added and, therefore, available sorption surface area - were nearly equally exponential in their influence. The highest adsorption in this study occurred at the lowest available surface area (50 mg $\hat{=}$ 0.47 m² kaolinite, 6.32 m² goethite) and the highest added Se concentration (5000 $\mu\text{g}/\text{L}$), leading to a load of 154 and 504 mg/kg Se on goethite and kaolinite, respectively.

Results from the wash solution (Figure 4.15b) are normalized to 100 % of the Se expected to be found due to dilution of the remaining sorption solution (only 9.5 and 9.25 mL of the original 10 mL were sampled to avoid substrate loss, leaving 0.5 and 0.75 mL of residual Se in the sorption solution to be diluted to 10 mL). Figure 4.15b shows that no Se recovery of more than 100 % was found and this is interpreted to indicate no Se desorption via the wash step, which means that for further experiments, the wash solution step was not analyzed. However, although wash loss was below the maximum Se concentration calculated for dilution, it was shown to be 4 - 20 times higher for goethite than for kaolinite. This is attributed to pipetting error, as goethite was found to bind more water than kaolinite after centrifuging and the extraction of 9.25 mL was not always precisely possible without pipetting substrate as well. Moreover, analytically, only values for 5000 $\mu\text{g}/\text{L}$ Se are above blind due to high analytically required dilution, Therefore, the factor of 3 - 7 compared to

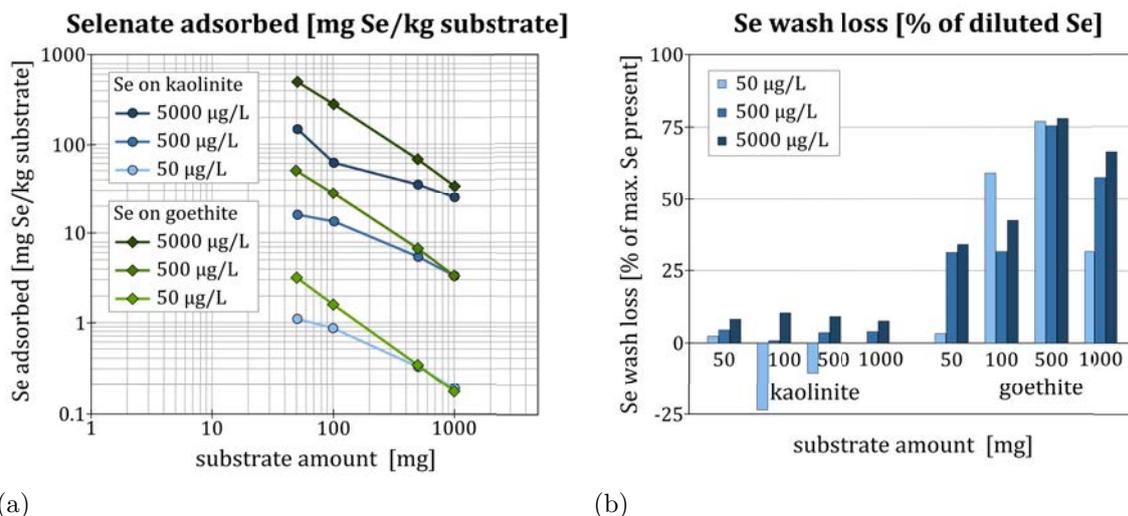


Figure 4.15.: *Se adsorption and wash results for preliminary sorptions tests*
a: Selenate adsorption dependency on Se concentration and substrate amount compared for kaolinite and goethite
b: Measured Se loss through the wash/dilution step before desorption; with 0.5 mL and 0.75 mL in kaolinite and goethite samples remaining after sorption solution sampling are diluted by factor (20 and 13.3) to 10 mL with double-deionized water, Se content above 100 % is considered Se desorption

kaolinite can be explained by experimental and analytical conditions.

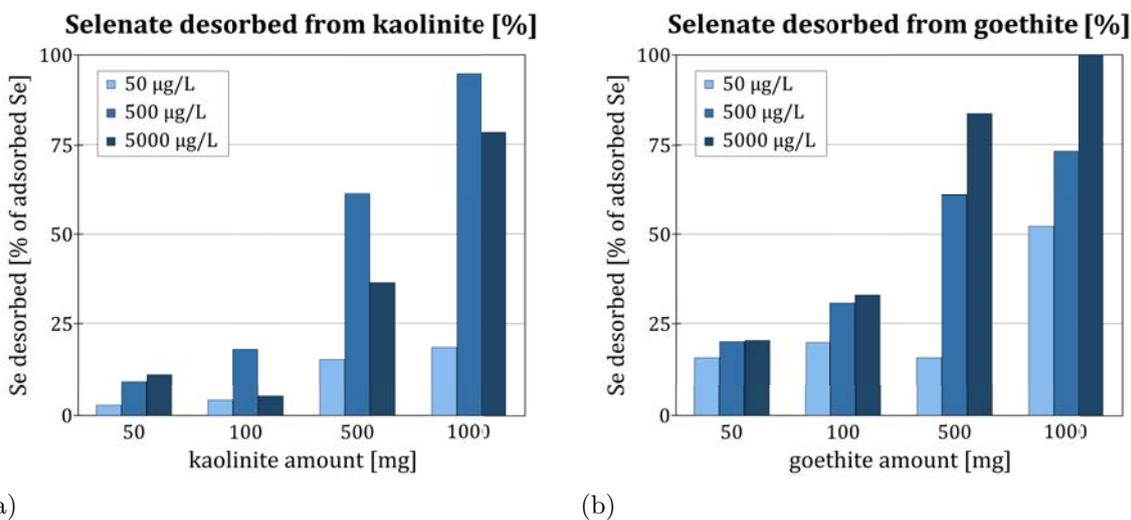


Figure 4.16.: *Se desorption results for preliminary sorptions tests as percentage of the previously adsorbed Se*
a: desorption from kaolinite
b: desorption from goethite

None of the desorption percentages of previously adsorbed selenate exceed 100 % (Figure 4.16). There is a clear trend, however, with desorption lowest (below 25 %) for the lowest

substrate amounts (50 - 100 mg kaolinite and 50 mg goethite) and increasing for greater substrate amount until reaching >75 % for 1000 mg kaolinite and goethite for desorption of 500 - 5000 $\mu\text{g/L}$ Se.

Analytical difficulties in the reducing step of the HG-FIAS sample preparation procedure due to high concentrations of phosphate (from the 0.1 mol/L K_2HPO_4) required a change of analytical method and further experiments were analyzed by ICP-MS (Chapter 3.4.4).

4.5.2. Exp. B1 - Se sorption onto kaolinite and goethite

Se sorption onto kaolinite and goethite in this experiment differed between the substrates (Figure 4.17).

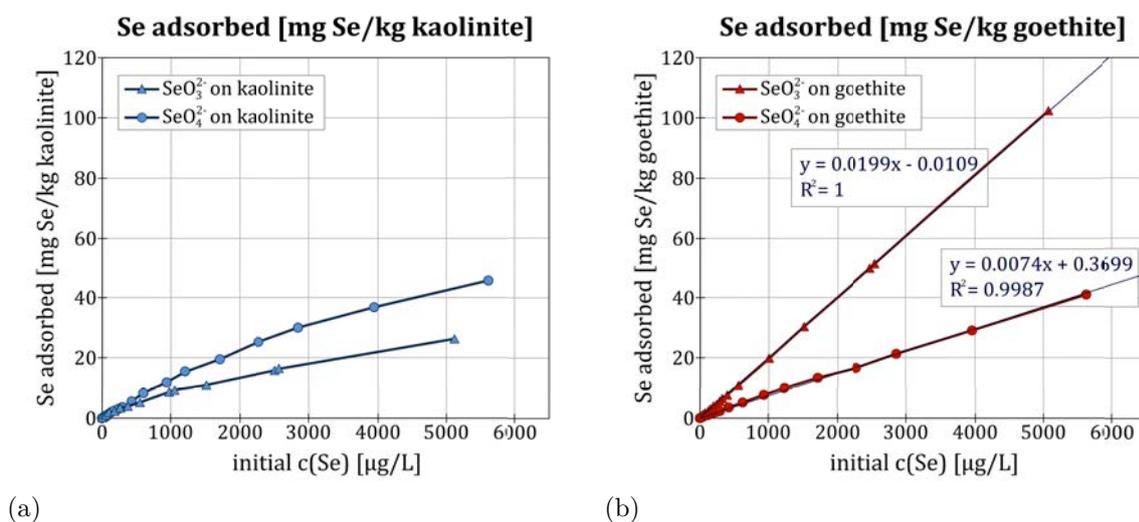


Figure 4.17.: Se adsorption results of 0 - 5000 $\mu\text{g/L}$ Se as $\text{Na}_2\text{SeO}_4^{2-}$ or $\text{Na}_2\text{SeO}_3^{2-}$
 a: onto kaolinite
 b: onto goethite

While kaolinite showed logarithmic curvature in both adsorption isotherms for selenite and selenate, suggesting that the surface could reach its maximum load at approximately a 3 - 5-fold concentration of Se, Se sorption onto goethite was completely linear with Se concentration increase, suggesting little usage of its surface capacity.

Adsorption also differed between the anions selenite and selenate. Loss of Se from the solution due to sorption onto kaolinite decreased from 62 to 26 % for increasing selenite concentrations from 0 to 10,000 $\mu\text{g/L}$ Se compared to decreasing from 74 to 40 % for

increasing selenate concentrations from 0 to 10,000 $\mu\text{g/L}$ Se (Figure 4.18). So while selenate appeared to have a higher affinity to kaolinite (30 - 47 % higher adsorption load) than selenite did, the opposite was true for goethite.

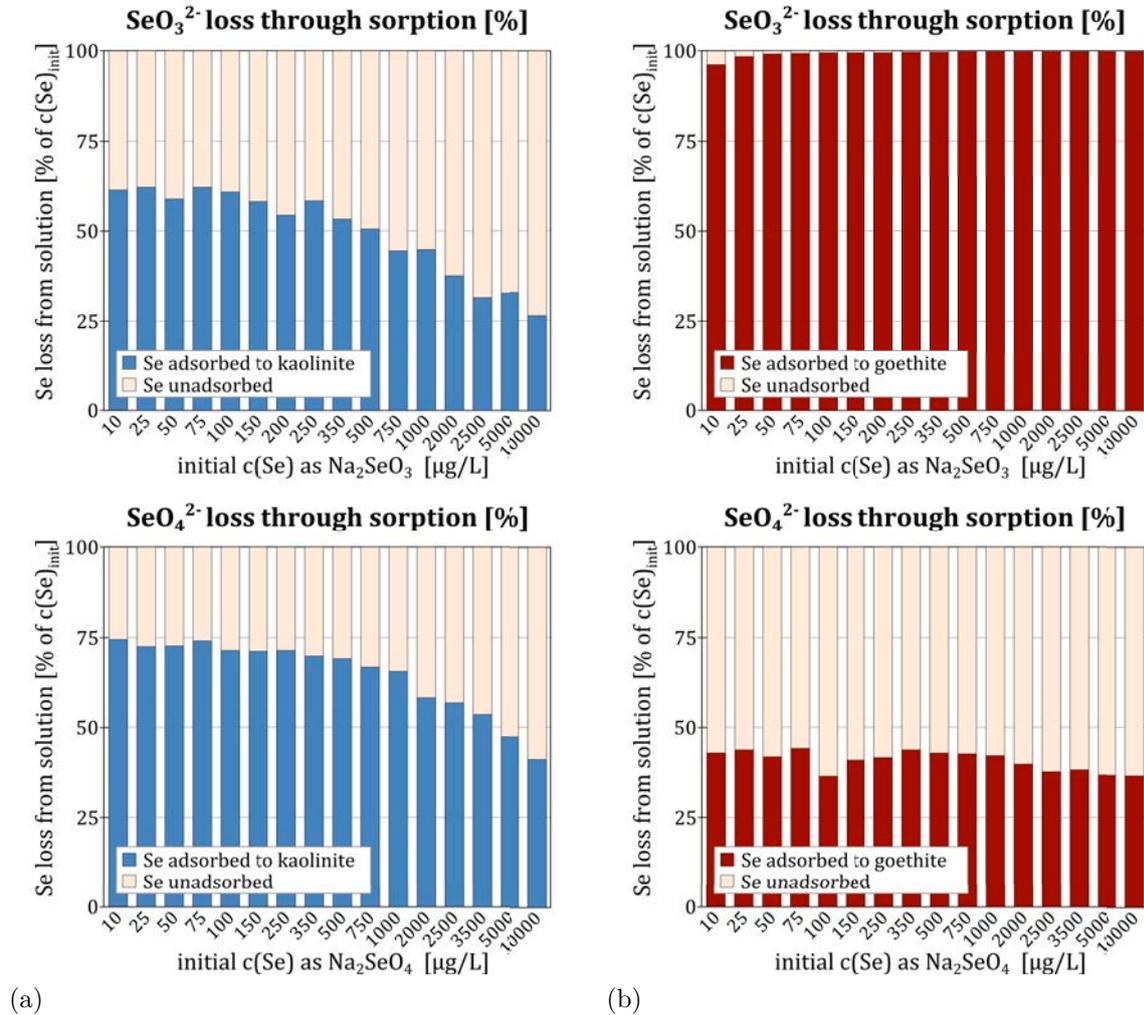


Figure 4.18.: *Se loss from solution through sorption*
 a: *after sorption onto kaolinite*
 b: *after sorption onto goethite*

As shown in Figure 4.18b, selenite in solution was nearly completely (96 - 97 %) adsorbed onto goethite (≥ 97 % when ≥ 500 $\mu\text{g/L}$ Se was added), while only 43 - 36 % of the selenate in solution was adsorbed onto the goethite surface. There is little point in defining a coefficient for the difference in selenate and selenite sorption onto goethite, as the total adsorption of selenite to goethite indicates that selenite sorption onto the goethite surface was limited by the Se concentration provided in the solution.

Upon measuring the pH values before the sorption experiment, the Se-free initial solution

blank had a pH value of 5.8 and 5.2 (Figure 4.19a), which corresponds well with the pH 5.6 predicted by PHREEQ-C (PHREEQ-C for Windows Version 2.18.00, wateq database) when the Se-free KCl-solution was equilibrated with typical air-content of 400 ppm of carbon dioxide [CO₂Now, 2014]. When adding Se to the solutions, pH values did not change significantly for the addition of selenate. With selenite, however, pH values increased with increasing Se addition, as shown in Figure 4.19 a, and has been modelled by PHREEQ-C (Appendix B.8, B.11).

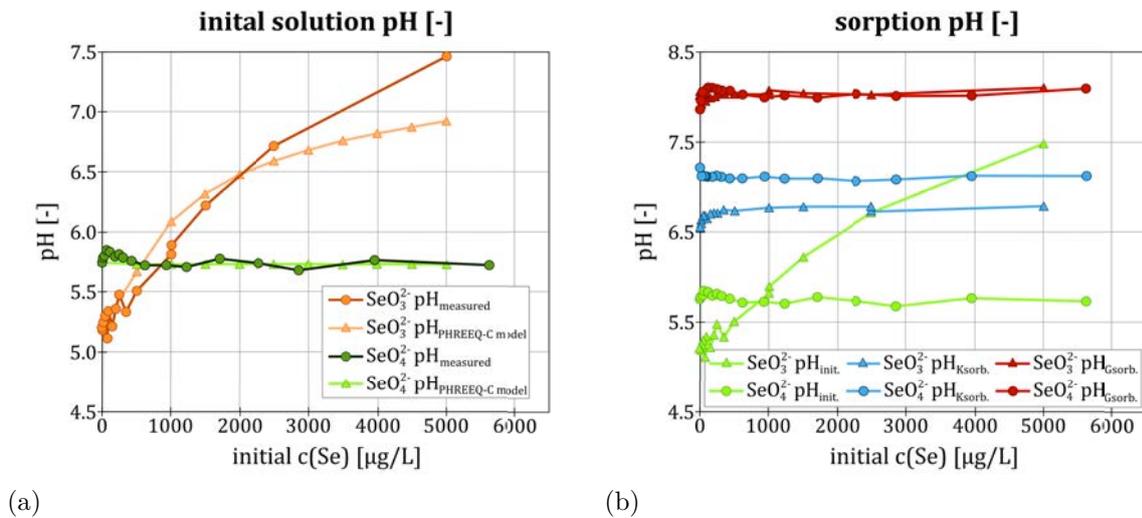


Figure 4.19.: *pH values of Se sorption onto goethite and kaolinite*

a: *pH values of initial solutions as measured and calculated by PHREEQ-C (Appendix B.8, B.11)*

b: *pH values of sorption solutions before ($pH_{init.}$) and after sorption of Na₂SeO₄ or Na₂SeO₃ onto kaolinite ($pH_{Ksorb.}$) and goethite ($pH_{Gsorb.}$)*

Adsorption onto both mineral surfaces had a levelling effect on the pH regardless of the speciation. After sorption onto kaolinite, pH values rose to 6.6 - 6.8 when selenite was present, and 7.1 - 7.2 when selenate was the species being adsorbed (Figure 4.19b). After sorption onto goethite, pH values remained constant, regardless of the Se speciation between 7.9 and 8.1 (Figure 4.19b).

Concentrations of the prevalence of thermodynamically most abundant Se speciations in the modelled initial sorption solution are given in Figure 4.20. When adding Se as selenate, the most prevalent species by far in the modelled initial solution was the entirely deprotonated SeO₄²⁻. Selenite, on the other hand, was present in all stages of protonization.

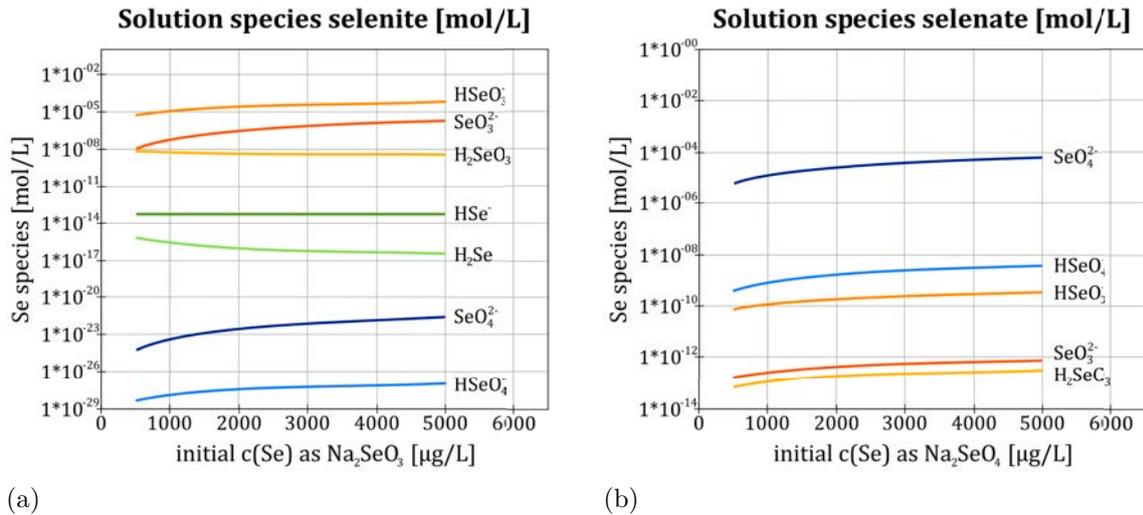


Figure 4.20.: PHREEQ-C modelling results for Se species in initial sorption solution (Appendix B.8, B.11).

a: after adding Se as selenite

b: after adding Se as selenate

4.5.3. Exp. B2 - Se desorption from kaolinite and goethite

Desorption profiles of Se from the surface to which it had previously been adsorbed to, was similar for both minerals (Figure 4.21). While desorption of selenate from kaolinite (85 - 96 %) was slightly more efficient than from goethite (71 - 94 %), desorption of selenite from kaolinite (76 - 92 %) was a little lower than that of selenate, while selenite desorption from goethite (77 - 87 %) was similar to that of selenate.

4.5.4. Exp. B3 - ion competition and Se sorption

Compared to the adsorption of pure selenite onto kaolinite, the presence of 750 $\mu\text{mol/L}$ N as nitrate or S as sulfate resulted in no significant change in selenite adsorption (Figure 4.22a). Selenite adsorption in the presence of nitrate was slightly improved compared to pure adsorption (98 - 138 %; $\bar{x} = 117 \pm 14$) and in the presence of sulfate, barely influenced (87 - 124 %; $\bar{x} = 99 \pm 14$). However, phosphate, as expected, had a great impact on selenite adsorption onto kaolinite.

In the presence of 750 $\mu\text{mol/L}$ of P as phosphate, selenite adsorption was reduced to 12 - 38 % ($\bar{x} = 20 \pm 9$). With the nutrient solution containing 400 $\mu\text{mol/L}$ P rather than 750

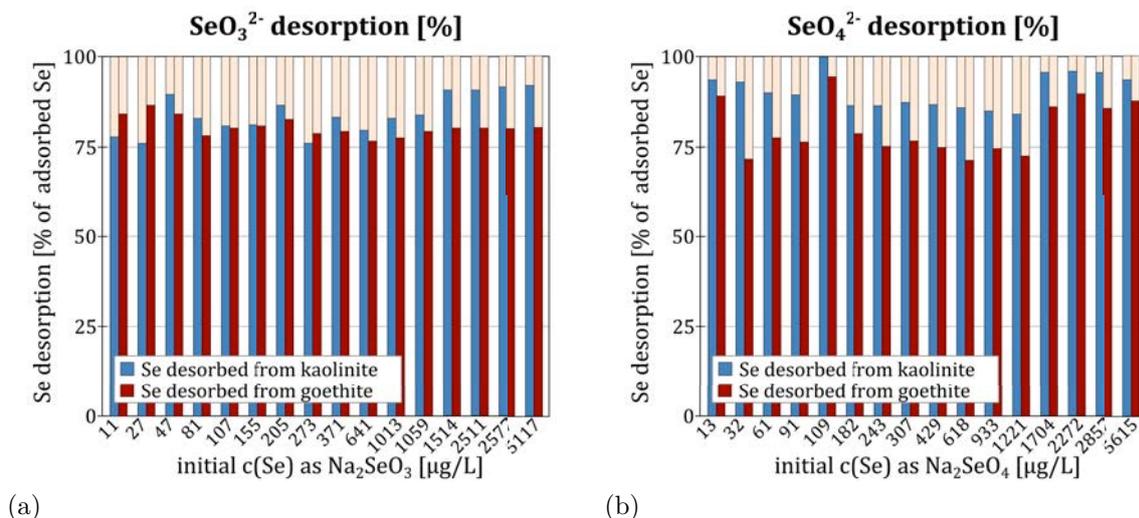


Figure 4.21.: *Se desorption profiles from kaolinite and goethite using KH₂PO₄ as percentages of previously adsorbed Se.*

a: desorption of selenite

b: desorption of selenate

µmol/L (= 53 % c(P)), the inhibition of selenite adsorption was explained in part (70 %) as phosphate-induced (Figure 4.22a).

Selenate adsorption, on the other hand, was inhibited by each of the ions to varying proportions (Figure 4.22b). While selenate adsorption was moderately inhibited (66 - 80 %; $\bar{x} = 72 \pm 5$) by 750 µmol/L N as nitrate, it was very strongly inhibited by the equivalent amount of S as sulfate (2 - 10 %; $\bar{x} = 5 \pm 3$) and P as phosphate (2 - 8 %; $\bar{x} = 6 \pm 2$). In the presence of nutrient solution (Chapter 6.5c), selenate adsorption was 22 - 42 % ($\bar{x} = 31 \pm 7$) compared to pure selenate adsorption and, therefore, inhibited less in combination of nitrate, phosphate and sulfate than with each ion individually (Figure 4.22b).

When comparing sorption on goethite between pure selenite solution and selenite solution in combination with other competing oxy-anions, Figure 4.22a clearly shows that all available selenite was always completely adsorbed, regardless of accompanying ions. This was true for all singly competing ions, as well as the nutrient solution. In all cases, goethite did not reach a maximum load.

Selenate adsorption onto goethite, on the other hand (Figure 4.22b), was inhibited by the presence of phosphate (4 - 12 %; $\bar{x} = 9 \pm 3$) and sulfate (4 - 15 %; $\bar{x} = 9 \pm 5$), with values similar to selenate adsorption onto kaolinite. While a maximum load was once again not

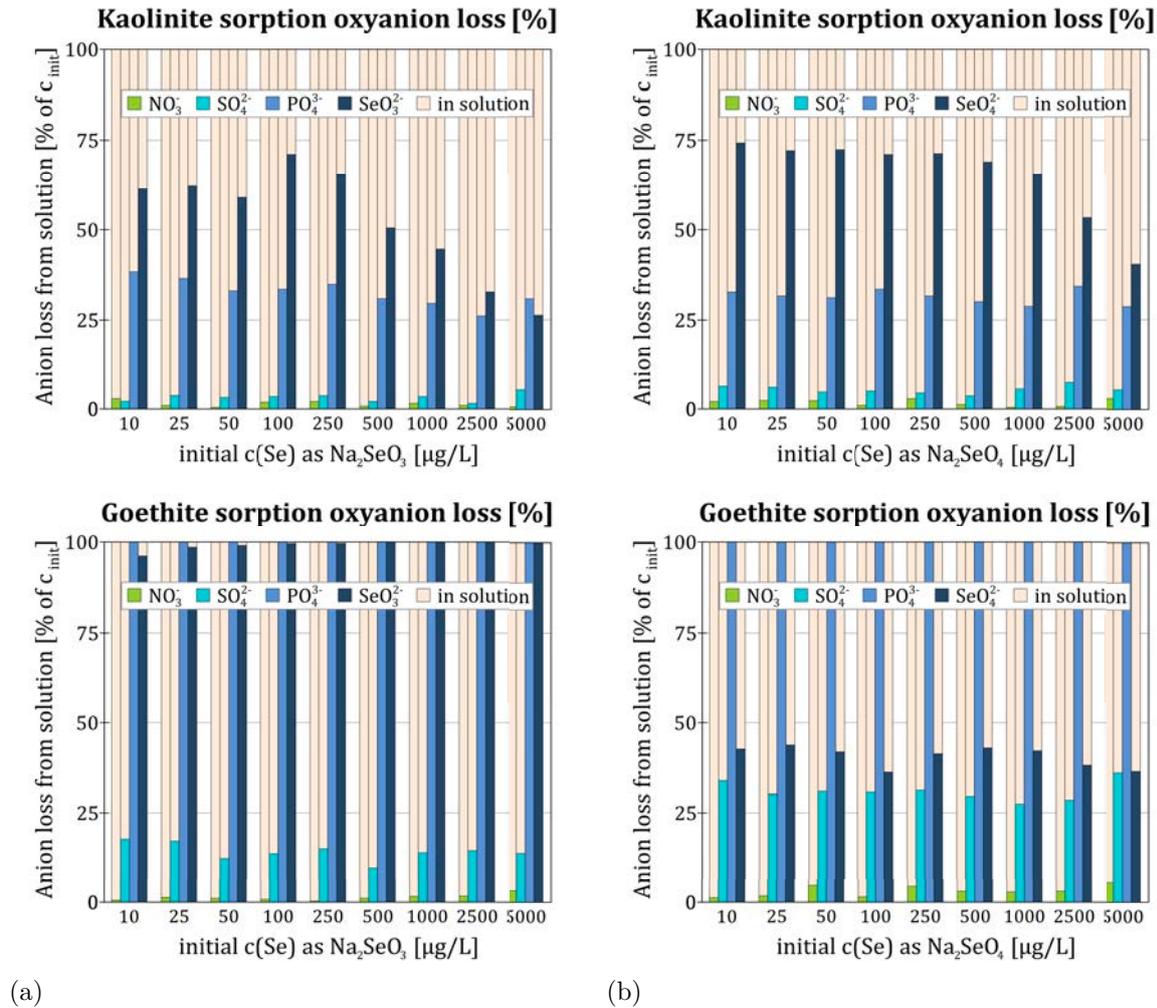


Figure 4.22.: *Se adsorption onto kaolinite (top) and goethite (bottom) in the presence of 750 µmol of competing ions nitrate, phosphate, sulfate in comparison with pure Se adsorption and Se adsorption in the presence of nutrient solution (Exp. C, Chapter 6.5c)*

a: adsorption as selenite
b: adsorption as selenate

reached, the equilibrium amount of selenate adsorbed onto the goethite surface was lower for sulfate and phosphate, but - as with adsorption onto kaolinite - selenate adsorption was not negatively influenced by nitrate, but rather increased (105 - 157 %; $\bar{x} = 118 \pm 24$). Selenate adsorption in the experiment with nutrient solution showed the highest adsorption (278 - 387 %; $\bar{x} = 283 \pm 75$).

Adsorption of the oxy-anions is shown as loss of nitrate, phosphate and sulfate from solution due to adsorption onto kaolinite and goethite in Figure 4.23. Consistent with its small influence on Se adsorption, nitrate loss from solution due to adsorption onto kaolinite was

nearly insignificant (0.4 - 3.2 %; $\bar{x} = 1.3 \pm 0.8$ and $\bar{x} = 1.85 \pm 1.0$ for selenite and selenate, respectively). Loss of sulfate from solution was only slightly higher, with about twice as much (2 - 7.5 %; $\bar{x} = 3.2 \pm 1.2$ and $\bar{x} = 5.4 \pm 1.1$ for selenite and selenate, respectively). Phosphate loss, however, was quite significant (26.0 - 38.3 %; $\bar{x} = 32.6 \pm 3.8$ and $\bar{x} = 31.5 \pm 2.0$ for selenite and selenate, respectively), which was also consistent with the adsorption of selenite and selenate being affected by phosphate presence.

With goethite, again, loss of nitrate was nearly insignificant (0.2 - 5.5 %; $\bar{x} = 1.2 \pm 0.9$ and $\bar{x} = 3.2 \pm 1.5$ for selenite and selenate, respectively), albeit up to twice as high as with kaolinite. Loss of phosphate from all experimental solutions was always 100 % (Figure 4.23). Contrary to kaolinite results, loss of competing sulfate from solution due to adsorption onto goethite was dependent on the prevalent Se species. Loss of sulfate in the presence of selenite was 9.5 - 17.5 %; $\bar{x} = 14.1 \pm 2.4$, while in the presence of selenate it was 27.4 - 36.0 %; $\bar{x} = 30.9 \pm 2.6$. This is consistent with its previously reported influence on selenite and selenate.

4.6. Discussion on Se sorption properties and effects ion competition

Apart from the obvious differences between the surface area of both minerals used, the main points of discussion for the adsorption of selenite and selenate on kaolinite and goethite address the difference in Se oxy-anion affinity for the substrates. Beyond that, the differences in competition posed by the anions sulfate, phosphate and nitrate are detailed in particular. The discussion concludes with the major points required for the following biogeochemical model and the mass balance calculations.

As the greater goal of this study was primarily concerned with characterizing and quantifying processes in the Se cycle within the Critical Zone, the following experiments were not designed to fulfill requirements on which to base a detailed, numerical sorption complexation model. Moreover, such data on microscopic mechanisms of Se oxy-anion complexation

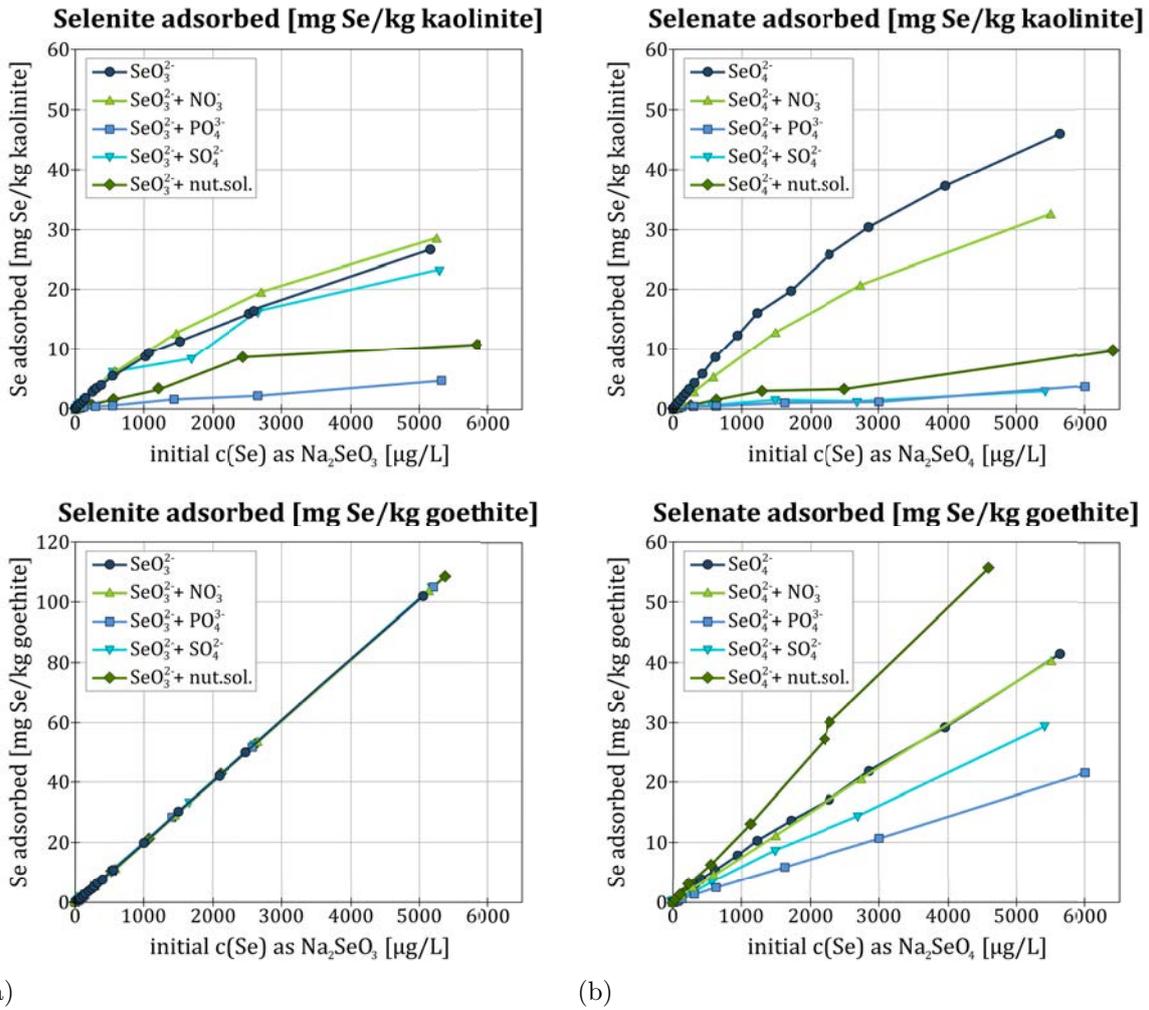


Figure 4.23.: Loss of anion concentration from solution through adsorption onto kaolinite (top) and goethite (bottom)
 a: adsorption of selenite
 b: adsorption of selenate

on mineral surfaces has already been published in various other studies [Manceau & Charlet, 1994, Wijnja & Schulthess, 2000, Peak, 2006, Chan et al., 2009]. Therefore, only macroscopic observations are used to answer questions related to this study. Since this study’s purpose was to combine sorption studies with plant uptake studies, ionic strength, pH value and the concentrations of competing ions used are specifically tailored to this goal and have not been used in previous studies.

4.6.1. Selenium complexation with kaolinite and goethite surfaces

While there is no dissent in the literature on selenite complexation, there is uncertainty about the details of selenate adsorption. It is widely accepted that selenate's type of complexation varies, depending on surrounding parameters, such as solution pH and ionic strength as well as substrate surface [Fernández-Martínez & Charlet, 2009]. Selenate is not the only oxy-anion which can bind both inner- and outer-spherically; arsenate and sulfate, for example, share this property as well [Catalano et al., 2008, Chan et al., 2009].

Selenate's behavior during the washing step (Figure 4.15b) shows no macroscopic evidence for selenate being bound as loosely as would be expected of an outer-sphere complex. Outer-sphere complexes are expected to be more susceptible to ionic strength variations than inner-sphere complexes because, according to the TLM (Chapter 4.5), background electrolyte ions are placed in the same plane as the outer-sphere complexes [Wu et al., 2000]. A solution of double-deionized water, therefore, would be expected to lead to a partial exchange of Se anions with OH^- . This was not observed (Figure 4.15 b) - neither for the adsorption onto kaolinite, nor for the adsorption onto goethite - for which inner-spheric adsorption of selenate has been shown [Hayes et al., 1987, Manceau & Charlet, 1994, Wijnja & Schulthess, 2000].

Moreover, desorption using phosphate would be expected to exchange nearly 100 % of the adsorbed Se, which is not the case (Figure 4.21). Rather, selenate desorption from goethite is similar to selenite desorption and selenate desorption from kaolinite is only slightly higher compared to selenite desorption. For this study, selenate is, therefore, considered to be adsorbed primarily as an inner-sphere complex, like selenite. This corresponds well with literature identifying selenate an intermediately bonding anion compared to the strongly bonding selenite, which has been found to bond preferably as inner-sphere complex onto goethite [Wu et al., 2000, Wijnja & Schulthess, 2000].

4.6.2. Se-oxy-anion affinities to kaolinite and goethite

The main difference between selenite and selenate was that selenite has a very high affinity to the goethite surface, compared to selenate affinity to goethite as well as either Se species' affinity to kaolinite. While selenate has a slightly higher affinity to the kaolinite surface than selenite, its affinity to goethite is much lower (Figure 4.18) considering the vast difference in surface area.

With surface area (9.4 and 126.4 m² for kaolinite and goethite, respectively) so different, it comes as no surprise that the goethite surface was not saturated with Se or any of the other oxy-anions as opposed to kaolinite. The method used to describe surface activity in these experiments is a primitive one compared to the possibilities of obtaining values for pH_{PZC} , pH_{PZNPC} or pH_{IEP} [Sposito, 1998], [Appel et al., 2003] and gives no approximation for either value. However, this pH characterization of surface activity is representative for initial experimental conditions and sufficient for the purposes of this study.

As pH_{PZC} is an indicator of the pH range for a substrate's physisorption properties, pH_{PZC} values for goethite between 7.3 and 9.4 [Parks, 1990, Kosmulski, 2002, Appel et al., 2003] make both coulombic and chemical adsorption possible for the ions used in this experiment (pH 5.2 - 5.7). However, the final pH after adsorption, which is changed independent of Se concentration is explained, not through Se adsorption, but by the goethite surface acting as a base for the solutions protons. Thereby deprived of protons, the solution's pH value rises to 7.9 - 8.1. Due to the goethite sample's large surface area, this effect is overwhelmingly larger than the oxy-anion adsorption.

Values for kaolinite's pH_{PZC} , however, range from $\text{pH}_{\text{PZC}} = 3 - 5$, corresponding to the surface groups [Schroth & Sposito, 1997, Hur & Schlautmann, 2003] to $\text{pH}_{\text{PZC}} = 6 - 7.2$, corresponding to the amphoteric edge groups [Hur & Schlautmann, 2003, Tombácz & Szekeres, 2006]. The initial sorption solution pH of 5.2 - 5.7 means that coulombic attraction is plausible only for the surface groups, but not for the edge groups, which means that physisorption for Se oxy-anions in this environment is reduced and chemical adsorption must overcome the charge repulsion. This makes adsorption onto kaolinite less effective than onto

goethite. With final pH values of kaolinite sorption at 6.6 - 6.8 and 7.1 - 7.2 for selenite and selenate addition, respectively, there appears to be strong adsorption activity from the edge groups rather than the surface groups, while selenite may also adsorb onto surface groups, raising the final pH by 0.5 less compared to selenate adsorption.

The results of this study, although not focused on complexation modelling, are considered indicative of inner-sphere complexation of both selenite and selenate ions onto the kaolinite surface. These findings are interesting because selenate, in general, shows a lower affinity to surfaces than selenite [Wu et al., 2000, Chan et al., 2009, Fernández-Martínez & Charlet, 2009]. For adsorption onto kaolinite, however, the higher amount of selenate adsorption compared to selenite adsorption can be attributed to steric properties, since the selenite molecule is larger than the selenate molecule and, therefore, occupies more space on the surface (Figure 4.8). Unfortunately, while quite a few studies have been published on Se adsorption onto goethite [Manceau & Charlet, 1994, Rietra et al., 2001, Wijnja & Schulthess, 2002, Rovira et al., 2008, Das et al., 2013], there is little data on specific Se adsorption onto kaolinite [Fernández-Martínez & Charlet, 2009].

The finding that selenite has such an overwhelming affinity for the goethite surface is not new [Hayes et al., 1987, Lo & Chen, 1997, Chan et al., 2009, Fernández-Martínez & Charlet, 2009]. In general, there is little information on direct comparison between selenite and selenate with regard to their varying affinities to goethite because in modelling, it is incorporated as a constant derived from chemical equilibria [Wu et al., 2000, Rovira et al., 2008]. Sorption rates have been shown to be higher for selenite than for selenate [Rovira et al., 2008]. The fact that selenite and selenate exhibit different kinetic processes and that selenite binds as a bidentate, rather than a mono-dentate complex like selenate, might provide an answer to the high selenite-goethite affinity [Zhang & Sparks, 1990, Lo & Chen, 1997, Su & Suarez, 2000, Fernández-Martínez & Charlet, 2009].

For quantification purposes of this study, it can be concluded that when adsorption remains in a linear range, which means the substrate surface is not maximally loaded or sorptive transport is not hampered by extreme dilution, selenite's great affinity for kaolinite and goethite leads to 61 % and 99 % selenite loss from solution, respectively, while

selenate loss from solution is 72 % for kaolinite and 42 % for goethite.

4.6.3. Desorption

Desorption with phosphate is considered an effective way to desorb selenite [Rajan & Watkinson, 1976, Kulp & Pratt, 2004]. As shown in Figure 4.21, desorption ranges of selenite and selenate are comparable for both kaolinite and goethite. Similar to the values of desorption in the literature [Singh et al., 1981], with the exception of outliers, overall desorption is between 71 and 96 % with little indication for a difference between kaolinite desorption for either Se oxy-anion to be found. However, selenate appears to desorb slightly better from kaolinite than from goethite with the use of phosphate. This has previously been described [Singh et al., 1981] and can be explained by the mono-dentate inner-sphere complex of selenate, which is more easily exchanged than the bidentate inner-sphere complex of selenite.

KH_2PO_4 was used to determine the easily exchangeable fraction of Se, which in a natural environment might, therefore, be accessible to plants. Findings of these experiments show that around 75 % of both Se species can be desorbed by ion exchange with phosphate - even when it is adsorbed to goethite. Therefore, soils rich in ferric oxides or hydroxides might contain high concentrations of Se even if the soil solution contains only traces. This Se might then unintentionally be mobilized by large quantities of fertilizer containing phosphate. It remains to be seen, however, whether the exchangeable Se determined by this study truly also equals plant-available Se in environments without excess phosphate.

4.6.4. Oxy-anion competition

Natural waters contain many different ions. In an optimally fertilized environment of plant cultivation, adsorption of selenite and selenate are affected by oxy-anions, such as nitrate, phosphate and sulfate. Predictions for oxy-anion affinities for adsorption onto surfaces are difficult, since they are highly dependent on charge distribution between central atoms and ligand atoms of both the substrate and the anion. This and the affinity for protonization

of both reaction partners are dependent on pH value and ionic strength [Hiemstra & van Riemsdijk, 1995].

As this experiment was able to demonstrate, nitrate only affects selenate adsorption onto kaolinite and is otherwise not a factor in Se adsorption, neither in selenate adsorption onto goethite, nor in selenite adsorption onto either kaolinite or goethite. This is not surprising, as nitrate's structure was very different from that of both Se oxy-anions, since it had a much larger radius and also much lower electronegativity difference (Figure 4.8), making it much less likely to adsorb onto surfaces than Se oxy-anions. Moreover, nitrate is only onefold negatively charged, while sulfate is two- and phosphate is threefold negatively charged. In published literature, nitrate was listed with lower general adsorption affinity [Neal, 1995] and early studies already proved nitrate to be adsorbed much less than competing sulfate or phosphate [Kinjo & Pratt, 1971]. As expected, sulfate poses strong competition for selenate, and only little competition for selenite, while phosphate is strongly inhibitive of Se oxy-anion adsorption in general. This is not surprising as it was shown to be a good desorption agent for both Se oxy-anions as well [Balistrieri & Chao, 1990, Geelhoed et al., 1997, Duc et al., 2003]. This is probably due to its high charge-to-radius ratio coupled with the adsorption structure of a bidentate complexation to the surface [Hiemstra & van Riemsdijk, 1995, Geelhoed et al., 1997].

Direct comparison between both mineral substrates is difficult due to their large difference in surface area. Previous literature has described clay minerals as having low retention properties towards anionic species such as selenite and selenate [Duc et al., 2003]. When comparing selenate adsorption onto kaolinite and goethite, however, this is not necessarily true, as adsorption per area was higher on kaolinite than on goethite, despite the factor 13 in surface area difference in favor of goethite. In contrast to that, considering selenite's high affinity for goethite and goethite's large surface area, it comes as no surprise that selenite adsorption is not inhibited by anything present in the experimental nutrient solution, although phosphate shows at least the same affinity for the goethite surface as selenite and is adsorbed to 100 %. Although this behavior is not directly transferrable to conditions of natural soils, published literature suggests that selenite adsorption onto ferric

oxides is a great source of Se retention, rendering selenite bio-unavailable in the presence of ferric oxides and -hydroxides [Bar-Yosef & Meek, 1987, Howard, 1977, Fernández-Martínez & Charlet, 2009].

As a final point of discussion, the effects of combined oxy-anion competition in the nutrient solution are of great interest, since this is, arguably, the most realistic kind of natural adsorption environment. The effects of multiple ion competition cannot simply be described by the sum of single-ion effects. In the case of selenite adsorption onto kaolinite, 70 % of the nutrient solution's effect could be ascribed to the phosphate share. However, with nitrate and sulfate barely influencing selenite adsorption as single-ions, this poses the question where the other 30 % of selenite inhibition comes from. The reasons for this were not explored in detail and can, therefore, only be surmised to be related either to other constituents of the nutrient solution, i.e. borate or ferric citrate, or to other parameters such as pH value and experimental set-up, which was slightly different for the other experiments. The fact that adsorption of selenite onto goethite is by far most efficient in the nutrient solution environment might be ascribed to bridging of more than one ion onto certain Fe-sites, although there is only sparse information on this process [Hingston et al. 1971]. It is also possible that Se forms complexes in the nutrient solution and that goethite, a known scavenger [Bar-Yosef & Meek, 1987], shows a greater affinity toward sorption of complexes than to selenate alone.

4.6.5. Conclusions for biogeochemical mass balance modelling

The results of this study have direct implications for the biogeochemical model with which characterization and mass balance of the Se compartments and transfer processes within the Critical Zone can be described. Although mathematical correlations do not necessarily follow chemical or physical properties or processes, the purpose of this model is to define an adequate description of correlations and quantification of processes. Therefore, the model proposed for an experimental system must be oriented on the basis of the data produced by this system and all assumptions and boundary conditions are based on macroscopic

observation.

The sorption processes describe one-half of the pre-defined model transport pathways for Se, which was compartmentalized into "soil" and "soil solution". Conclusions from this study for this aspect of the Critical Zone are:

1. selenite and selenate both adsorb as inner-sphere complexes with species- and substrate-dependent affinities
2. the small kaolinite surface size allows isotherm modelling
3. adsorption onto the large goethite surface size can be simplified as linear adsorption
4. as plants require time to germinate, the sorption equilibrium can be modelled as pre-installed before plant-induced effects occur

5. Biogeochemistry - Se uptake

competition of minerals and plants

In this chapter, the experimental set-ups of Chapters 3 and 4 are combined to study synergistic effects of the uptake of Se into plants in the presence of competing mineral surfaces. As introductions to both plant uptake of Se (Chapter 3.1) and adsorption of Se onto minerals (Chapter 4.1) have already been presented in their respective chapters, this chapter will provide a brief overview of consequences of previous experimental results for the combined experiments.

5.1. Theoretical implications of previous results

Although Exp. A3 was combined with Exp. B3 in a closed plant-box system (Figure 5.1), Se adsorption onto kaolinite or goethite preceded the uptake of Se from the nutrient solution by the rice plants in this set-up due to germination time. As selenite and selenate have been reported to equilibrate with i.e. goethite in 25 min [Su & Suarez, 2000], Se adsorption onto the substrate already reached an equilibrium while the plant had no contact with the nutrient solution yet.

Since the same nutrient solution was used as in Exp. A3, no toxicity effects were expected for concentrations up to 2500 $\mu\text{g/L}$ Se (Figure 5.1) and uptake of Se was believed to be similar to Exp. A3, with similar partitioning between shoots and roots for selenate and selenite, respectively. Because, however, kaolinite exhibited Se adsorption between 23 and 75 % of solution-Se and goethite adsorbed between 25 and 50 % of solution selenate,

experimental set-ups were modified to provide higher Se-concentrations (0 - 10,000 $\mu\text{g/L}$ Se) than those in Exp. A3 (0 - 2500 $\mu\text{g/L}$). Nonetheless, selenite affinity to goethite was observed to be so great in Exp. B3 that no Se uptake by the rice plants was expected.

5.2. Experimental set-up

As shown in Figure 5.1, in the fourth plant-box experiment of this study, plants were grown in the presence of a nutrient solution identical to the one described in Chapter 3.3.3. Additionally, mineral substrate of kaolinite and goethite was added in the exact weight-volume ratio used in Exp. B1 and B3 (Chapters 4.4.2 and 4.4.4). For a plant-free nutrient solution sorption reference, which was directly comparable to Exp. B1 and B3, each plant-box had a sorption bottle-equivalent, with the identical solution compared to the plant-box and the same amount of mineral substrate (Figure 5.1).

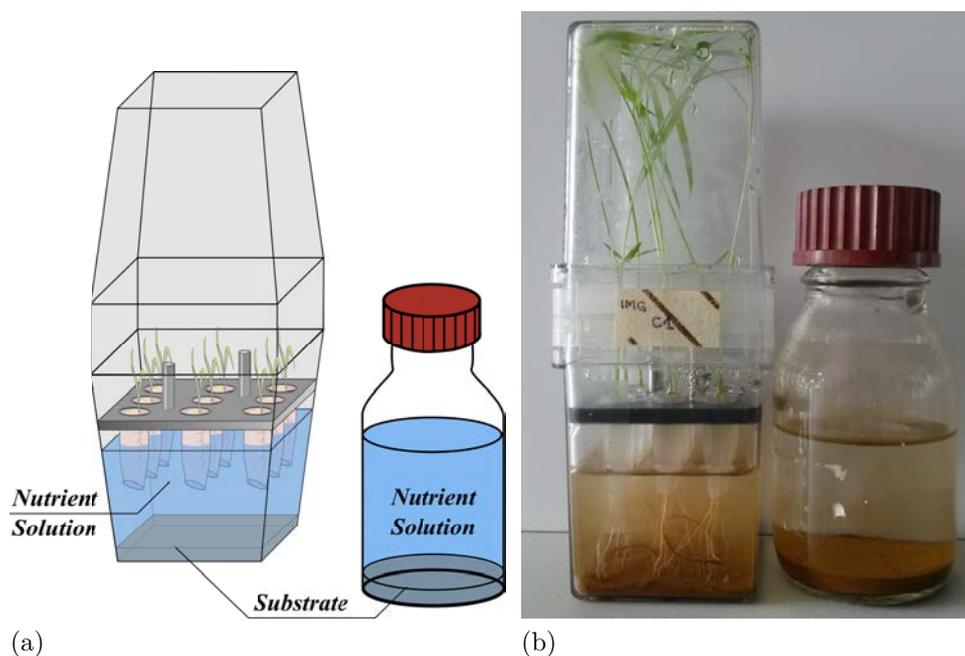


Figure 5.1.: *Se-nutrient solution experiments contained 9 rice plants growing for 19 days, sprouting first in Se-free agar in Eppendorf tubes before reaching 170 mL of Se-spiked nutrient solution (0 - 10,000 $\mu\text{g/L}$ Se) in the presence of competing Se adsorption by kaolinite or goethite mineral surface.*
a: schematic experimental set-up
b: photo taken on 03.06.2014

5.2.1. Exp. C - plant-box rice cultures with Se-nutrient solution & mineral sorption

A 1000 mg/L Se stock solution was prepared in 10 mL of double-deionized water ($\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$, VWR BDH Prolabo 302113L and Na_2SeO_3 , AlfaAesar 012585). Ninety rice caryopses were sterilized according to the procedure described in Chapter 3.3.1. 8.5 g of either kaolinite or goethite were weighed (Sartorius 1712MP8) into 10 plant-box sets (Sigma Aldrich, 2 x V8505 & 1 x C0667) and 10 250-mL Schott glass bottles.

The substrate-containing plant-box sets were prepared (Figure 5.1a) with a specially designed Eppendorf tube tray holder for 9 x 1.5-mL tubes (1.5 ml Eppendorf Safe-Lock Microcentrifuge Tube, 0030120086). Plant-box sets, substrate-containing 250-mL Schott glass bottles (all pre-labelled autoclave-proof), 90 1.5-mL Eppendorf tubes, 250 mL 0.7 % phytoagar, 10 500-mL Schott glass bottles with 400 mL nutrient solution each (preparation given in Chapter 3.3.3), a 100-mL measuring cylinder and 250 mL of double-deionized water were autoclaved.

After autoclaving, 1.5-mL reaction tubes (Eppendorf, Hamburg) were placed into a tray-holder under the cleanbench and filled to the brim with the still-liquid 0.7 % phytoagar. Only after the agar had solidified, were the lid and 0.5 cm from the bottom of each reaction tube cut off using sterilized scissors. Each tube was then loaded with one sterilized caryopse.

Due to autoclaving, nutrient solution compositions varied slightly from bottle to bottle (variation within one experimental batch 0.8 - 13.3 % , $\bar{x} = 4.9$ %). To ensure that plant-box experiments were directly comparable to their plant-free sorption references, the initial nutrient solutions were prepared in the autoclaved 500-mL Schott glass bottles as follows (Figure 5.2a), before being aliquoted into the plant-box, sorption reference bottle and sample vessels.

Under the cleanbench, Se standard was added to the nutrient solution in the autoclaved 500-mL Schott glass bottles to achieve specified concentrations (0, 20, 50, 100, 200, 500, 1000, 2000, 5000, 10 000 $\mu\text{g/L}$ Se). Solutions in the 500-mL bottles were shaken to ho-

mogenize. Autoclaved plant-boxes were disassembled under the cleanbench and Eppendorf trays removed. From the nutrient solution in the 500-mL Schott glass bottles, 170 mL of nutrient solution was filled into each lower half of the boxes and an equal 170 mL filled into its respective autoclaved reference glass bottle. Two times 15 mL of the remaining solution in the 500-mL Schott glass bottles were sampled for subsequent analysis into 20-mL patho-vessels (Böttger 08-313-1001) - 15 mL were frozen for later IC-measurement, the other 15 mL were acidified with 50 μL of HNO_3 (VWR 20429.320 p.a. sub-boiled) and stored at 4°C.

For plant-box assembly, each Eppendorf tray was loaded with 9 rice-bearing Eppendorf tubes and placed into the plant-box with the lower half of the tubes submerged in nutrient solution before closing the plant-box. The 250-mL Schott reference glass bottles were screwed shut and not shaken. Plant-boxes and reference bottles were kept under the same climate chamber conditions as described in Chapter 3.3.3, keeping the boxes and bottles closed for 19 days until harvest. In total, four experimental set-ups were conducted: two with kaolinite as the sorption substrate and Se added as selenite and another two with goethite as the sorption substrate with Se added as selenate. Each experimental set-up was conducted only once without further replicates.

5.2.2. Sample preparation and analytical methods

Plants were harvested (Figure 5.2b) as described in Chapter 3.4.1 (images Appendix C.1), shoot and root bulk samples were digested using the protocol described in Chapter 3.4.2 and subsequent analysis of plant-Se with HG-FIAS was conducted according to Chapter 3.4.3. 2 x 15 mL of nutrient solution was sampled from the plant boxes as well as from the reference sorption bottles into 20-mL patho-vessels (Böttger 08-313-1001) - 15 mL were frozen for later IC-measurement, the other 15 mL were acidified with 50 μL of HNO_3 (VWR 20429.320 p.a. sub-boiled).

As shown in Figure 5.3a, the substrate of plant-boxes and reference bottles was filtered



Figure 5.2.: *Photos of Exp. C preparation and harvest.*

a: preparation of goethite experiments under sterile conditions of the clean-bench; goethite in disassembled plant-boxes and 250-mL reference bottles (red lids) and prepared nutrient solution in 500-mL bottles (blue lids), caryopses planted into Eppendorf tubes with bottom cut off on the right, patho vessels for sampling in the front (photo taken on 08.05.2014)

b: harvest of kaolinite experiment (photo taken on 13.04.2014)

through cellulose filters (Schleicher & Schuell, 595, No. 311610), washed once with double-deionized water (comparable to the wash-step before desorption experiments in Chapter 4.4.3) and dried on the filters in an oven at 40°C for 48 h. As shown in Figure 5.3b, samples were then filled into 20-mL patho-vessels (Böttger 08-313-1001) for storage, later analysis and desorption experiments.

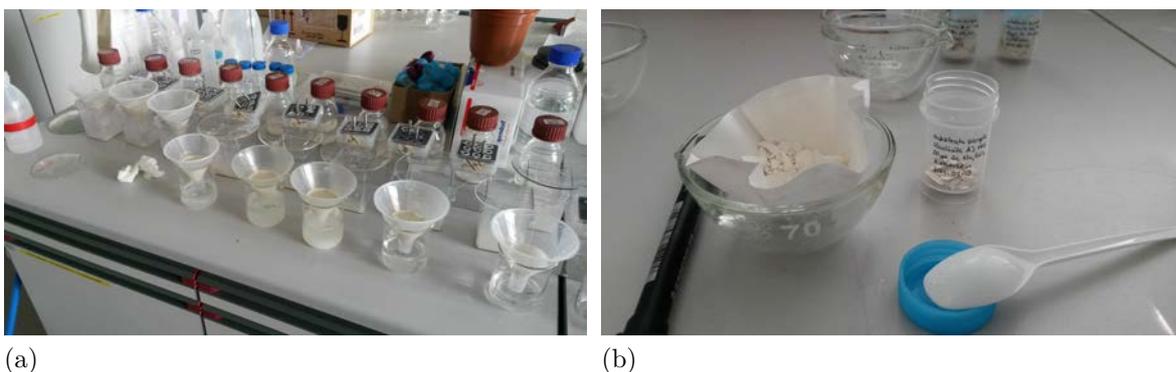


Figure 5.3.: *Photos of substrate sample preparation after harvest.*

a: filtration of substrate from nutrient solution onto cellulose filters (photo taken on 14.04.2014)

b: sampling of dried material from the filter into a patho-vessel (photo taken on 16.04.2014)

5.2.3. Desorption experiments

From the filtered sorption substrate material, desorption samples were prepared similarly to those described in Chapter 4.4.3. 0.5 mg of substrate sample were weighed into 20-mL patho-vessels (Böttger 08-313-1001) and 10 mL of desorption solution (0.1 mol/L K_2HPO_4 , prepared as in Chapter 4.4.3) was pipetted onto it. Samples were shaken for 24 h at 180 rpm at room temperature. Samples were then centrifuged (40,000 rpm, 5 min, Rotofix 32 A), 7 mL sampled into 20-mL patho-vessels (Böttger 08-313-1001) and frozen at $-20\text{ }^\circ\text{C}$ for later measurement. Sample analysis of Se was conducted with ICP-MS (Chapter 3.4.4) with a dilution factor of 10 due to a high K_2HPO_4 sample salt load.

5.2.4. Scanning Electron Microscopy analysis (SEM)

From each of the four experimental runs of Exp. C, to which 5000 $\mu\text{g/L}$ Se had been added, sorption substrate material of plant-box experiments and their respective sorption reference bottles were taken to the LEM (KIT) for SEM analysis. Samples were coated in platinum by vapor deposition to enable static discharge and measured with a LEO 1530 Gemini at 10 keV operating voltage and beam focal distance of 5.1 - 6.3 mm.

5.2.5. Synchrotron-based analysis

Synchrotron radiation is generated when accelerated electrons are redirected by the use of bending magnets. Specialized beamlines using this tangentially escaping radiation are installed around an electron storage ring, in which accelerated electrons are circulated [Newville, 2004]. Methods used for this study included x-ray absorption near edge spectroscopy (XANES) of speciation-dependent Se absorption (SUL-X beamline, ANKA, Karlsruhe) and fluorescence mappings (FLUO beamline, ANKA, Karlsruhe) of plant tissue Se content.

XANES scans detail how X-rays are absorbed by an atom at energies near ($\pm 30\text{ eV}$) the core-level binding energies of an atom and is strongly sensitive to formal oxidation state and coordination chemistry of the absorbing atom [Newville, 2004]. X-rays (ca. 500 eV to

500 keV) as part of the synchrotron radiation spectrum, are absorbed when the incoming radiation energy equals the binding energy of an electron [Newville, 2004]. The electron is thereby removed from its quantum level [Newville, 2004]. If the incoming radiation energy exceeds that of the electron binding energy, the excess energy is transferred to a photo-electron which is then ejected from the atom. Using Lambert-Beer's law, x-ray absorption can be described and calculated [Newville, 2004].

$$\mu(E) \cdot t = \ln(I_0/I_{trans}) \quad (5.1)$$

with

$\mu(E)$ as the absorption coefficient

t sample thickness

I_0 as the intensity of incident radiation

I_{trans} as the intensity transmitted through the sample

A so-called "absorption edge" is observed when the incident x-ray has an energy equal to the binding energy of a core-level electron. Core-level binding energies for electrons are specific to each atom, which makes XANES an element-specific measuring method [Newville, 2004]. After absorption, the atom is in an excited state with a core electron level vacant and an emitted photo-electron. This excited state decays within femtoseconds after absorption by either fluorescence or the Auger Effect [Newville, 2004]. Fluorescence describes the process of a higher-level electron filling the vacant electron-hole by emitting the defined excess energy as light [Newville, 2004]. In the case of Se, the $K\alpha$ energy denoting the photon energy released during an electron transition from the L to the K shell is at 11.2 keV [Tokunaga et al., 1994]. The Auger Effect, on the other hand, describes the process in which the emitted excess energy of a higher-level electron filling the vacant electron-hole is not emitted as light, but rather transferred to another electron, which is then ejected from the atom, leaving it with two electron vacancies [Newville, 2004]. These two processes do not interfere with x-ray absorption, but are directly proportional to it [Newville, 2004].

Therefore, the Auger Effect or fluorescence effect can be used to determine the absorption edge instead of directly measuring transmission, when, for example, sample thickness allows only little transmission or element concentration is very low and there is little difference between incident and transmitted radiation.

In the case of this study, fluorescence was the underlying process used both for XANES measurements and fluorescence mappings. The difference between the former and the latter was only one of analytical set-up and interpretation. While XANES use fluorescence in its proportionality to absorption when induced with a radiation spectrum of ± 30 eV around the absorption edge (for Se: 12.658 keV), fluorescence mappings are carried out with a fixed incident radiation energy and fluorescence of different atoms is distinguished by the energy increments of the emitted fluorescence (for Se: 11.222 keV).

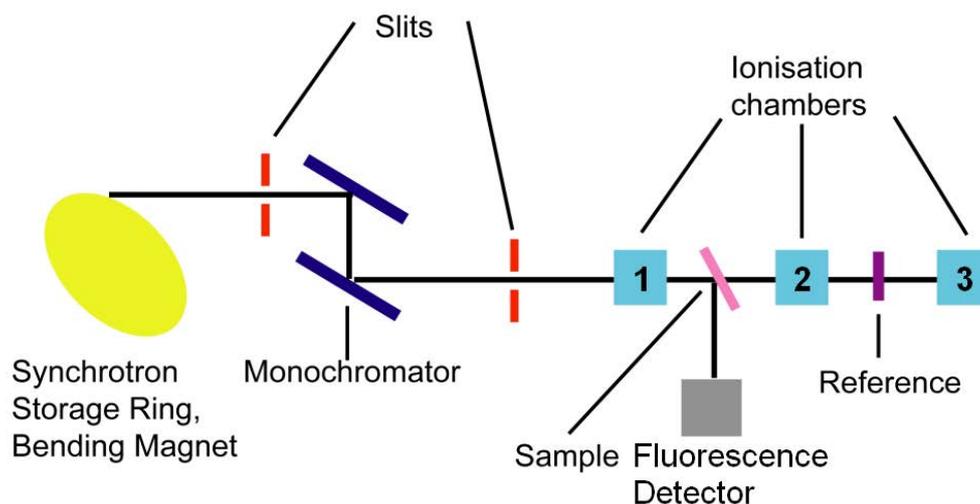


Figure 5.4.: *Scheme of the experimental setup for XANES analysis at a synchrotron facility ([Newville, 2004, Diener, 2012])*

Samples with sufficiently high concentrations, such as reference materials can be measured in transmission mode (measuring absorption of the sample by loss of intensity between ionization chamber 1 and 2, Figure 5.4). In this case, absorption is calculated as $\ln(\text{abs}) = \ln(I_0/I_{\text{trans}})$. Samples with low concentrations can be more accurately measured in fluorescence mode (measuring fluorescence of the sample, which is proportional to the absorption; Figure 5.4). In this case, absorption is calculated as $I_{\text{fluor}} = I_{\text{fluor}}/I_0$. Additionally, each measurement (reference or sample alike) can be energy-calibrated by measuring absorption of an

elemental Se standard (measuring standard absorption loss of intensity between ionization chamber 2 and 3, Figure 5.4), with which all scans can be calibrated and aligned to the energy of the element's absorption edge E_0 .

Sample preparation

From each of the kaolinite sorption plant box experiments, one rice plant was selected per box (Appendix, C.1) for measurements at the synchrotron facility ANKA, Karlsruhe. Harvested along with the other plants, these were not freeze-dried. After rinsing under once-deionized water and 2 h of drying in lab conditions, each plant was placed in a separate 15-mL centrifuge tube (VWR 525-0149) with the lid only loosely screwed on. To avoid any changes of Se speciation in the plant tissue, samples were not freeze-dried, but kept in a desiccator for 4 weeks to air-dry prior to analysis to avoid Se-loss and preserve plant structures during the drying process.

XANES analysis

XANES were measured at the SUL-X beamline (ANKA, Karlsruhe). This beamline was equipped with a 7-element fluorescence detector (e2v; Resolution: <140 eV at 5.9 keV, 1000 cps and <310 eV at 5.9 keV, 100.000 cps), three ionization chambers for absorption measurement (Oxford Instruments, IC-Plus type; active length 5 cm, Kapton windows 6 μm thick), a CCD detector (Photonic science; 80 x 120 mm^2 , Fiber optic 3.46:1, 2048 x 2048, 16 bit dynamic, readout time 3.3 s – 21 s) and an optical microscope (TSO Spezialoptik, resolution 2 μm).

Seleno-methionine (Sigma Aldrich S3132-100 MG), Na_2SeO_3 (AlfaAesar 012585) and $\text{Na}_2\text{SeO}_4 \cdot 10\text{H}_2\text{O}$ (VWR BDH Prolabo 302113 L) were prepared as reference materials by finely grinding the material in an agate mortar and spreading it over the sticky side of kapton tape (M. Newville, 2014, personal communication; IDE-13 beamline, APS, Argonne). Eight layers of this prepared tape were glued on top of each other. All reference samples (for later linear combination fitting) were measured under vacuum in transmission against the Se(0) standard prepared as a press pellet with 8 mg of elemental Se (Merck 1.07714.0050) in 100

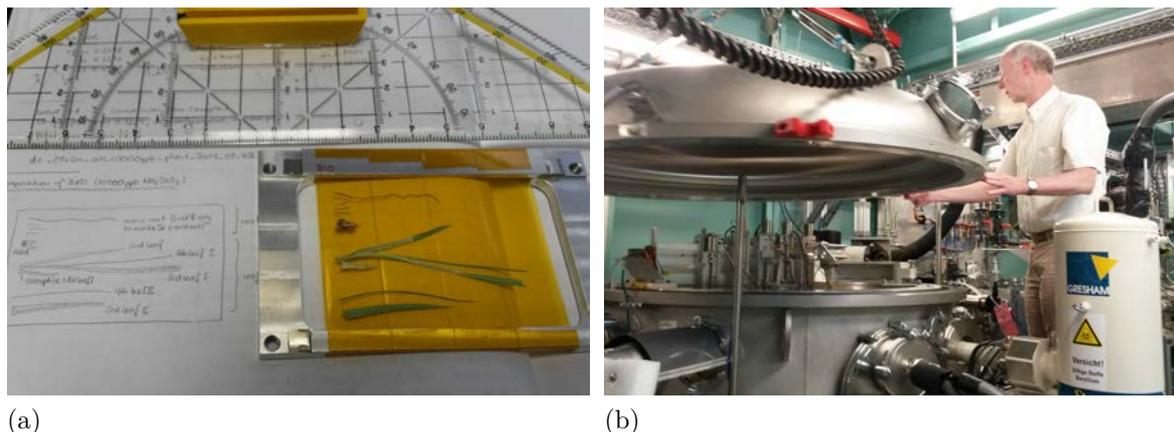


Figure 5.5.: *Sample preparation for synchrotron-based analysis of air-dried plant samples*
a: XANES plant sample on kapton-tape (right) and schematic sample documentation (left) (photo taken on 22.05.2014)
b: Ralph Steininger closing the vacuum chamber for test XANES measurements of a plant sample using a cryo-cell (photo taken on 20.05.2014)

Table 5.1.: *XANES measurement parameters: stepsize and acquisition time of pre-edge, absorption edge and post-edge*

scan	parameter	pre-edge I	pre-edge II	absorption edge: 12.658 keV	post-edge
quickscan	range	-75 to -20 eV		-20 to +20 eV	+20 to +200 eV
	acq. time	1 s		1 s	1 s
	stepsize	1 eV		0.5 eV	1.5 eV
absorption spectrum	range	-100 to -50 eV	-50 to -25 eV	-25 to +25 eV	+25 to +144 eV
	acq. time	1 s	1 s	1 s	1 s
	stepsize	5 eV	2 eV	0.5 eV	1.5 eV

mg of cellulose powder (Sigma Aldrich C8002-1KG).

Plant samples were fixed on kapton tape and placed on a metal frame (Figure 5.5a). Using an optical microscope, regions of interest (labelled 01 - 09) on the sample were calibrated relative to reference points on the sample frame and microscope images were taken of each spot. The sample holder was then installed in the measuring chamber and put under vacuum.

To locate hotspots of Se on the sample for XANES measurements, Se profiles across plant sections (measured across the point from -0.5 mm to +0.5 mm in 50 steps for 1 s) in the regions of interest (ROI) were measured at 12.661 keV. Then, absorption spectra (details below) of 2 - 8 points (labelled a - h) of the profile with sufficient Se content were measured for each ROI. Each of these points was measured twice and scans were merged for greater

Table 5.2.: Available data columns for the processing of SUL-X beamline data

data	column No.
energy	1
C_{fluo} (fluorescence counts)	56
I_0 (intensity in ionization chamber 1, incoming intensity)	59
I_{abs} (intensity in ionization chamber 2, intensity after transmission through sample)	60
I_{ref} (intensity in ionization chamber 3, intensity after transmission through reference)	61
calculated absorption	62
calculated reference absorption	63

accuracy. XANES measurements were carried out under vacuum and with short acquisition times (ca. 7 min) to minimize beam-induced redox reactions. Although references were measured in transmission mode, in many cases, Se tissue concentration was too low to measure in transmission mode, so absorption was measured in fluorescence mode for all plant samples.

To determine measurement conditions best suited to avoid beam-induced damage, one sample was measured with 3 set-ups. The same sample was measured first using atmospheric conditions, second, in a chamber under vacuum and third, using a cryo-cell cooled with liquid nitrogen in the vacuum chamber (Figure 5.5b). Beamtime measuring current during measurement varied by 5 - 15 mA, the beam spot on the sample was 30 x 50 μm in diameter and the fluorescence detector was between 60 and 80 mm away from the sample. Table 5.1 details how absorption spectra and quickscans, in which the motor changing the light energy does not pause while fluorescence is detected, were measured.

Data was processed as ".spec" data files using the Athena program of the Demeter software package (Demeter 0.9.13, B. Ravel, M. Newville). In ".spec-files" of the SUL-X beamline at ANKA, data for these calculations are given in the columns described in Table 5.2. For normalization, the pre-edge was set to -90 to -45 keV before E_0 and the post-edge was set to +90 to +245 keV after E_0 in the calibration scans. Samples were normalized to a pre-edge of -90 to -45 keV before E_0 and the post-edge was set to +90 to +190 keV after E_0 in the sample scans. Using linear combination fitting, proportional weighting of reference scans in all combinations was calculated to match the merged sample scans across -30 eV to +30 eV around the absorption edge.

High resolution μ XRF mapping

In an unsuccessful first attempt at μ XRF (micro x-ray fluorescence) mapping of Se concentration in plant material, samples were prepared using the Immuno-fluorescence fixation method into paraffin [Lützelshwab, 1990] by using a fixation agent to fix all biochemical compartments to the cell structure and then replacing - in incremental steps - tissue water by ethanol, ethanol by xylene and xylene by paraffin. Using a cutter, thin sections of the paraffin-embedded sample were manually sliced to ca. 0.5 - 1 mm thickness. However, the fluorescence measured could not be assigned to plant tissue structures, leading to the conclusion that the Immuno-fluorescence fixation method did not preserve cell structures and Se was distributed uniformly across plant tissue and in some cases bled into the paraffin embedding material.

Therefore, fluorescence of the complete air-dried plant samples used previously for XANES measurements was mapped at an excitation energy of 22 keV at the FLUO beamline at ANKA, Karlsruhe. This beamline was equipped with a double multilayer monochromator (W-Si multilayers in 2.7 nm period), CRL: 2×10^9 ph/s at 17 keV ($5 \mu\text{m} \times 2 \mu\text{m}$), 1 ionization chamber, Si(Li)-energy dispersive detector (Oxford Instruments), HPGe- High Purity Germanium detector (Princeton Gamma- Tech (PGT)) and a SiMCD-Vortex Silicon Multicathode Detector. Two undiluted press pellets of bulk plant material (Figure 5.6a) with known Se concentrations (measured with ICP-MS after acid digestion) from Punjab, India were prepared to calibrate Se concentration in the mappings: *Brassica juncea* root with 186 mg/kg Se DW and *Brassica juncea* leaf with 931 mg/kg Se DW. Plant samples were glued to slide frames (Butch, 28565348) between kapton tape to ensure as plane a surface as possible (Figure 5.6b). This was necessary, because during mesh analysis mode (meshes = 2D grids of measuring points), sample distance from detector could not be varied between measuring points.

Using a binocular, regions of interest were calibrated relative to an easily identifiable marker point. The sample slide frame was then installed in the measuring chamber. To locate exact positions of Se on the sample, Se fluorescence profiles (at 11.2222 keV for

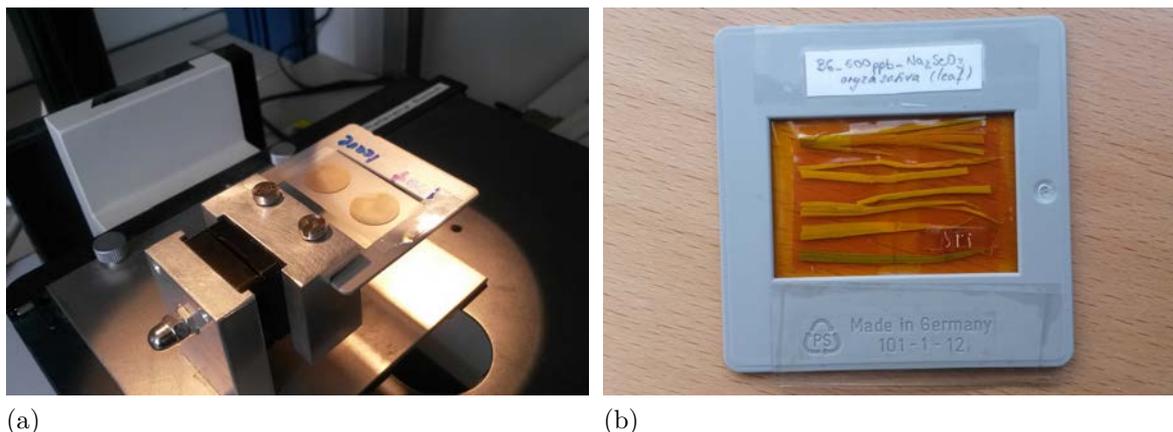


Figure 5.6.: *Sample preparation for synchrotron-based μ -XRF analysis of air-dried plant samples*

a: bulk press pellets for quantitative concentration calibration prepared on kapton tape fastened to a magnetic sample holder under the light of a binocular (photo taken on 04.06.2014)

b: fluorescence mapping samples between kapton tape on a slide frame for a maximum of planar surface (photo taken on 06.06.2014)

$k_{\alpha 1}$) across plant sections (measured across the point from -1 mm to +1 mm in 50 steps for 1 s) in the ROIs were measured at an excitation energy of 22 keV. Then, meshes were measured across ROIs. Beam spot on the sample was 16 x 11 μ m (polycapillary focus) and acquisition time was 3-4 sec. Data was analyzed using the PyMCA (version 3.9.5) software and mappings were created with Surferplot 6 (Golden Software).

5.3. Results

As these experiments are a synthesis of the previous experiments Exp. A2 - A4 (Chapters 3.3.2, 3.3.3, 3.3.4) and B1 - B3 (Chapters 4.4.2, 4.4.3, 4.4.4), results for parameters of plant health, such as plant mass, shoot height and heights of the second leaf as well as Se content results of rice shoots and roots from Exp. C, are directly compared with the respective results from Exp. B3 to determine additional effects of the possible presence of sorption in Exp. C. Furthermore, results for the adsorption of Se from the nutrient solution onto kaolinite or goethite during Exp. C are shown in Figures 4.22 in Chapter 4.5.4.

5.3.1. Plant growth of *Oryza sativa*

Shoot growth height of plants in the kaolinite experiment (Figure 5.7a) showed no correlation to added Se between initial Se concentrations of 20 - 1000 $\mu\text{g/L}$ Se, with heights of 102 - 87 % and 90 - 81 % of the untreated shoot height for Se added as selenite or selenate, respectively. With the addition of 2000, 5000 and 10,000 $\mu\text{g/L}$ Se as selenite, however, shoot height decreased to 75, 41 and 28 % of untreated shoot height, respectively. With the addition of 5000 and 10,000 $\mu\text{g/L}$ Se as selenate, shoot height decrease was not quite as pronounced at 71 and 59 % of untreated shoot height, respectively.

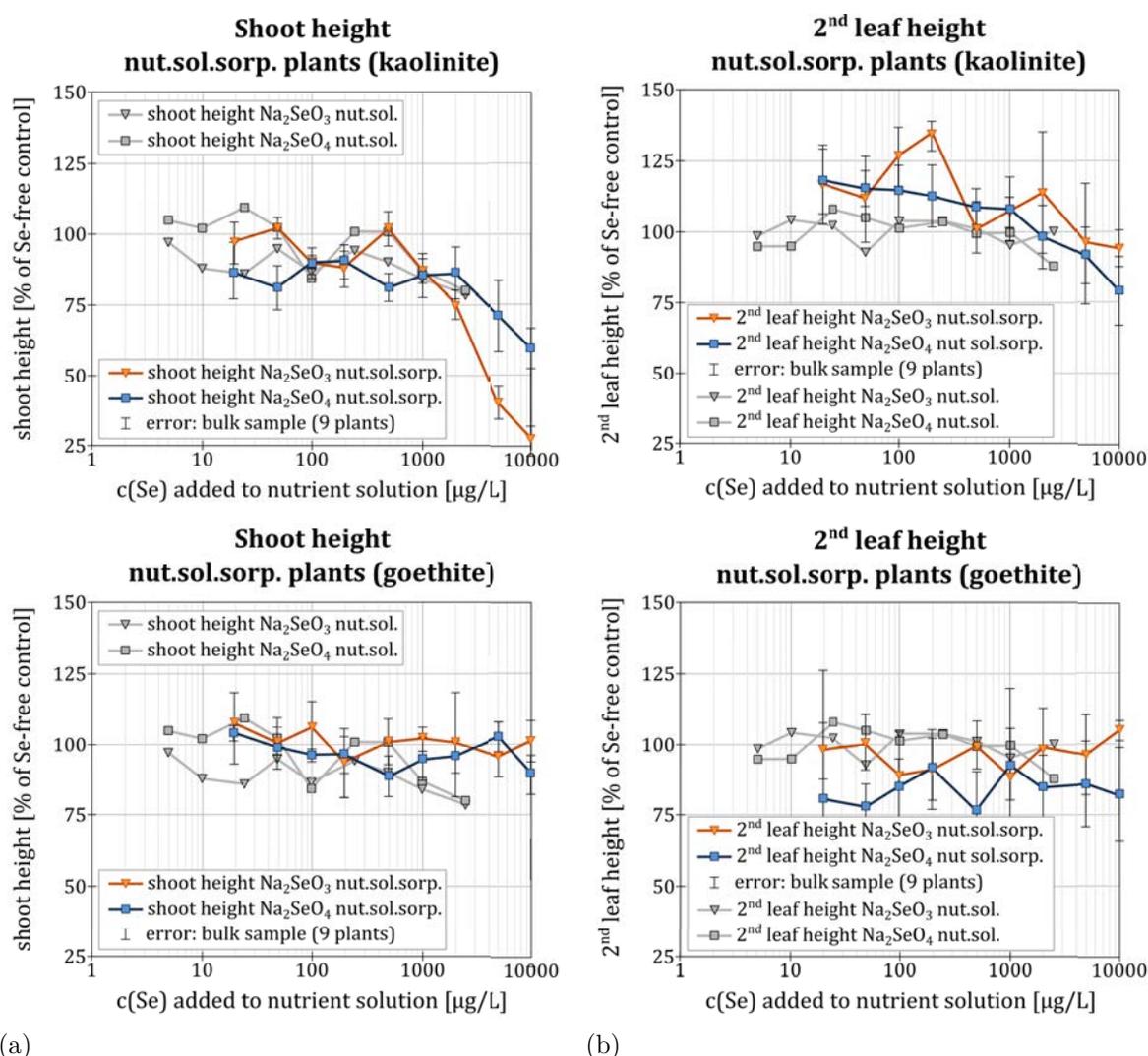


Figure 5.7.: Plant growth expressed as percentage of Se-free blank plants for experiment C in competition with kaolinite (top) and goethite (bottom) adsorption
 a: total shoot height on harvest day (Day 16)
 b: total length of 2nd leaf on harvest day (Day 16)

A similar decrease in shoot height was also found for the height of the second leaf; however (Figure 5.7b), this was less pronounced. Heights for the second leaf in the kaolinite experiment showed an overall slightly decreasing trend from 116 - 94 % and 118 - 79 % compared to the untreated plants for selenite and selenate, respectively.

Shoot height of plants in the goethite experiment (Figure 5.7a) showed no correlation with added Se across the initial concentrations 20 - 10,000 $\mu\text{g/L}$ Se, with heights of 107 - 93 % and 103 - 88 % compared to the untreated plant- height for selenite and selenate, respectively. Height of the second leaf in the goethite experiment (Figure 5.7b) also showed no correlation with added Se, with heights of 105 - 90 % and 92 - 77 % compared to the untreated plant- height for selenite and selenate, respectively. This corresponds well with the lack of correlation with added Se concentration for the experiments without substrate, since any fluctuations observed in shoot height or height of the second leaf were within 1s-error margin, as discussed in Chapter 3.5.3.

5.3.2. Selenium content in *Oryza sativa*

Quality measures for experiment C show that harvested plant yield was 85.6 % of transferred seedlings. Digestion standard retrieval was 83 % (± 13) and drinking water standard retrieval during HG-FIAS measurement was 121 % (± 9).

Selenium concentrations measured in the rice plants of Exp. C in the presence of kaolinite increased from 1.4 to 80 mg/kg DW for shoots (Figure 5.8a) and from 3.1 to 444 mg/kg DW for roots with the addition of 20 - 10,000 $\mu\text{g/L}$ Se as selenite. With the addition of Se as selenate, plant-Se in the presence of kaolinite increased from 0.8 to 1080 mg/kg DW for shoots (Figure 5.8b) and from 0.1 to 402 mg/kg DW for roots.

Selenium concentrations measured in the rice plants in the presence of goethite increased from 0.0 to 1.9 mg/kg DW for shoots (Figure 5.8a) and from 0.0 to 9.9 mg/kg DW for roots with the addition of 20 - 10,000 $\mu\text{g/L}$ Se as selenite. With the addition of Se as selenate, plant-Se in the presence of goethite increased from 0.7 to 347 mg/kg DW for shoots (Figure 5.8b) and from 0.2 to 84 mg/kg DW for roots.

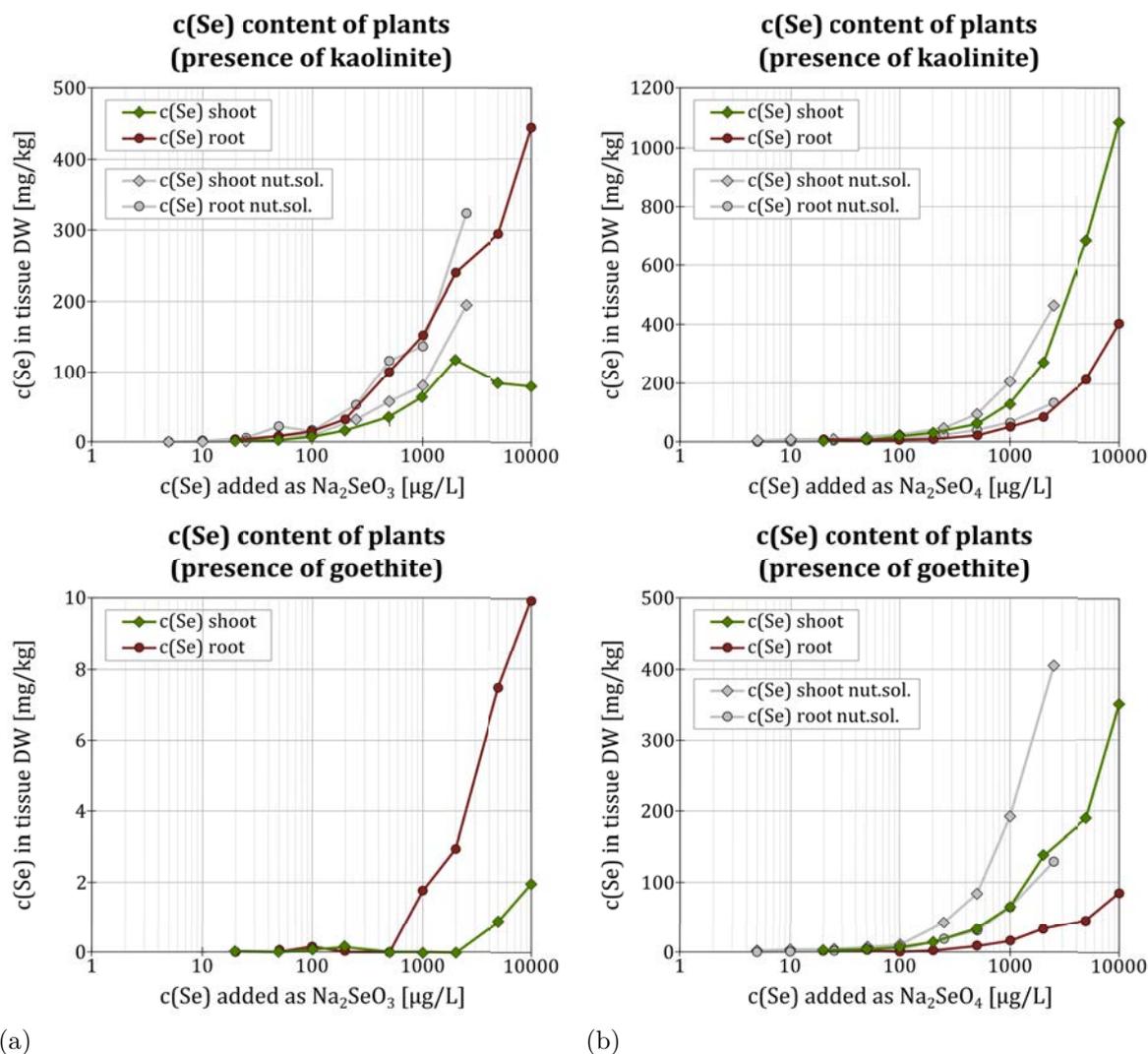


Figure 5.8.: *Se content in roots and shoots of Exp. C; Se-uptake in competition with adsorption by kaolinite (top) and goethite (bottom) compared with data from Exp. A3 without sorption (data from Exp. A3 is omitted for selenite uptake in the presence of goethite, because Se-uptake in Exp. C was too small for comparison)*
 a: addition of Se as Na_2SeO_3
 b: addition of Se as Na_2SeO_4

As in Exp. A3, overall plant-Se content increased with additional Se in the nutrient solution in all set-ups of Exp. C. For experiments in the presence of kaolinite, addition of 100, 1000 and 10,000 $\mu\text{g/L}$ Se as selenite led to 8.5, 65 and 80 mg/kg DW shoot-Se and 14, 152 and 444 mg/kg DW root-Se (Figure 5.8a). However, there was one exception. Shoot-Se content peaked at 117 mg/kg DW with the addition of 2000 $\mu\text{g/L}$ Se as selenite. For Se solution concentrations higher than that, 5000 and 10,000 $\mu\text{g/L}$ Se, shoot-Se decreased to 86 and 80 mg/kg DW, respectively.

For selenate experiments in the presence of kaolinite, additions of 100, 1000 and 10,000 $\mu\text{g/L}$ Se led to 12, 127 and 1080 mg/kg DW shoot-Se and 3.2, 49 and 402 mg/kg DW root-Se (Figure 5.8b), respectively. Here, higher Se concentration led to higher Se content in the plant.

In the presence of goethite, very little Se was taken up into the plant when it was added as selenite compared to the uptake of Se as selenate. Plant-Se in the shoots was only measurable for the addition of 5000 and 10,000 $\mu\text{g/L}$, resulting in 0.9 and 1.9 mg/kg DW, respectively. In the roots, Se-content was measurable at additions of Se greater than 500 $\mu\text{g/L}$ and increased with the concentration of added Se from 1.8 mg/kg DW with the addition of 1000 $\mu\text{g/L}$ Se to 10 mg/kg DW with the addition of 10,000 $\mu\text{g/L}$ Se.

Selenate additions in the presence of goethite showed an increase in plant-Se with added Se concentrations. Additions of 100, 1000 and 10,000 $\mu\text{g/L}$ Se as selenate led to 5.2, 63 and 347 mg/kg DW of shoot-Se and 1.1, 15 and 84 mg/kg DW of root-Se, respectively.

As with Exp. A2, A3 and A4, partitioning of selenate predominantly to the shoots and selenite predominantly to the roots was observable in the results of Exp. C as well, regardless of the addition of substrate, as shown in Table 5.3. Accumulation factors for the experiments in the presence of kaolinite with the addition of Se as selenite were 22.2 (± 3.1) in shoots in concentrations of 20 - 2000 $\mu\text{g/L}$ Se; then decreased to 6.6 and 2.9 for initial Se concentrations of 5000 and 10,000 $\mu\text{g/L}$ Se, respectively. Selenium accumulation factors in the roots when added as selenite decreased with increasing initial Se concentrations from 138 to 23.9 for initial Se concentrations of 20 to 10,000 $\mu\text{g/L}$ Se, respectively. Accumulation factors of Se in plants when added as selenate in the presence of kaolinite was 20.5 (± 4.7) and 9.1 (± 2.9) for shoots and roots, respectively. Therefore, Se accumulation in roots when added as selenite was an average of 5.7 (± 1.8) times higher than in shoots in the presence of kaolinite; accumulation of Se as selenate in shoots was an average of 2.4 (± 0.7) times higher than in roots.

For the low concentrations available for plant uptake in the goethite experiments with selenite, uptake, when measurable, showed a high accumulation factor in the roots (153 - 596), but an accumulation comparable to the kaolinite experiments in the shoots (18.2 -

Table 5.3.: *Fresh weight accumulation factors (AF) of selenate and selenite into shoots in Exp. C and Exp. A3 as calculated from measured Se content in the nutrient solution ($AF [-] = c(Se)_{medium} [mg/L] / c(Se)_{plant} [mg/kg]$)*

added c(Se) [µg/L]	Exp. C _{kaolinite}				Exp. C _{goethite}				Exp. A3			
	AF-Na ₂ SeO ₃		AF-Na ₂ SeO ₄		AF-Na ₂ SeO ₃		AF-Na ₂ SeO ₄		AF-Na ₂ SeO ₃		AF-Na ₂ SeO ₄	
	shoot	root	shoot	root	shoot	root	shoot	root	shoot	root	shoot	root
	[-]	[-]	[-]	[-]	[-]	[-]	[-]	[-]	[-]	[-]	[-]	[-]
5									21.5	80.3	27.2	21.7
10									26.7	81.6	16.2	8.0
20	24.2	138	10.6	3.8	0.3	2.9	19.6	8.3	26.5	99.2	20.9	9.7
50	22.7	148	22.6	11.4	0.2	0.7	11.3	13.1	31.6	212	26.7	12.7
100	22.7	118	27.1	10.3	26.1	153	25.0	9.8	27.0	105	19.0	10.2
200	26.8	132	24.4	8.5	18.2	0.6	34.5	6.5	29.0	94.1	41.1	19.9
500	18.2	156.6	17.4	13.5	0.1	4.8	34.3	15.7	33.6	117	40.0	21.7
1000	18.1	98.8	24.4	9.6	0.4	545	29.8	12.4	30.7	84.8	53.4	25.5
2000	22.9	55.3	18.7	9.9	1.4	554	35.7	14.0	22.1	57.8	40.9	22.5
5000	6.6	30.4	19.8	9.0	21.2	595	49.3	23.0				
10,000	2.9	23.9	19.7	5.5	26.1	469	40.5	14.6				

26.1). In the selenate experiments, Se accumulation, in the presence of goethite was 31.1 (\pm 11.3) and 13.0 (\pm 4.8) into shoots and roots, respectively. Accumulation of Se as selenate in shoots was, therefore, an average of 2.6 (\pm 1.1) times higher than in roots in the presence of goethite.

When compared to the results of Exp. A3, where there was no sorption interference, accumulation of Se as selenite in roots was an average of 3.7 (\pm 1.2) times higher than in shoots and accumulation of Se as selenate in shoots was an average of 1.9 (\pm 0.3) times higher than in roots. Partitioning of the accumulation of Se in plant tissue was, therefore, more pronounced in Exp. C.

Under the assumption that plant-Se standard deviation was comparable to that of Exp. A3 (standard deviation across all plant-Se of Exp. A3: 47.9 % for the addition of 10 - 50 µg/L Se, 30.3 % for the addition of 100 - 500 µg/L Se and 19.8 % for the addition of 1000 - 2500 µg/L Se, Figure 3.16, Chapter 3.5.3), Se-uptake into plants in the kaolinite experiments was comparable to that of Exp. A3 and within that margin of error. However, these high standard deviations mask that additional substrate had an effect on the mean values of plant-Se. With the exception of shoot-Se with the addition of 100 µg/L Se added as selenate to the kaolinite experiment, these were all below mean values of Exp. A3 (Table 5.4), in which

Table 5.4.: *Plant-Se of Exp. C given as percentage of plant-Se of Exp. A3 for respectively comparable Se additions ($c(\text{Se})_{\text{Exp. C}}/c(\text{Se})_{\text{Exp. A3}}$)*

added c(Se) [µg/L]	Na_2SeO_3				Na_2SeO_4			
	kaolinite		goethite		kaolinite		goethite	
	shoot [%]	root [%]	shoot [%]	root [%]	shoot [%]	root [%]	shoot [%]	root [%]
20	50.3	46.5	0.1	0.1	33.1	28.7	33.1	18.6
50	57.0	31.8	0.0	0.0	69.7	55.6	19.9	29.0
100	73.4	44.3	1.1	0.7	112.3	82.8	57.2	33.5
200	51.1	48.7	0.4	0.0	51.1	35.4	34.0	9.3
500	50.5	59.5	0.0	0.0	61.7	69.6	40.3	26.2
1000	53.0	70.9	0.0	1.0	55.2	65.3	33.1	24.0
2000	61.5	64.3	0.0	0.9	55.6	55.5	33.8	25.0
mean	56.68	52.27	0.22	0.38	62.65	56.14	35.90	23.66
mean-SD	8.43	13.38	0.39	0.46	24.58	18.97	11.22	7.81

there was no sorption substrate. For kaolinite experiments, plant-Se with the addition of either selenate or selenite was between half and two-thirds of the Exp. A3 plant-Se (52.27 - 62.65 %) and for goethite experiments, plant-Se was between a quarter and a third of the Exp. A3 plant-Se when added as selenate. Plant-Se when added as selenite for goethite experiments was below 1 % of comparable Exp. A3 plant-Se.

5.3.3. Root toxicity

In kaolinite-substrate experiments, addition of Se as selenite produced toxicity symptoms in the rice plants at the addition of 5000 and 10,000 µg/L Se (Appendix, Figure C.1). As shown in Figure 5.9, in the case of the addition of 5000 µg/L Se, all plant roots grew through the agar in the Eppendorf tube, but no further than 0.5 cm into the nutrient solution-containing the Se. In the case of the addition of 10,000 µg/L Se, also shown in Figure 5.9, only the main root (one root per plant) grew through the agar of the Eppendorf tube until reaching the nutrient solution. For all plants of this plant-box, this main root showed brown-spotted discoloration and discontinued growth at less than 3 mm into the nutrient solution. All other roots remained stunted at less than 1.5 cm in length and also exhibited brown discoloration despite not being directly in contact with the Se. Experiments with selenate did not show signs of toxicity, nor did the selenite experiments with goethite, since

adsorption of goethite led to strong depletion of Se from the nutrient solution (Chapter 5.3.4).



Figure 5.9.: Comparison of root growth for rice plants grown in contact with Se as Na_2SeO_3 in nutrient solution, in Se concentrations of 2000 $\mu\text{g/L}$ Se (left), 5000 $\mu\text{g/L}$ Se (middle), 10,000 $\mu\text{g/L}$ Se (right)

5.3.4. Adsorption influence of kaolinite and goethite

As expected in light of the previous results of Exp. B1 - B3, Se was not only taken up by plants, but also adsorbed onto the additional substrates kaolinite and goethite.

Under the assumption that the same amount of Se was adsorbed by the substrate in the plant boxes than in the reference bottles, initial Se content of the nutrient solution was corrected by the amount of Se adsorbed by the substrate to determine Se content at the time the plant roots reached the nutrient solution (Figure 5.10). Calculated factors ($c(\text{Se})_{\text{tissueDW}}/c(\text{Se})_{\text{nut.sol.}}$) of sorption-corrected plant-Se uptake compared to the uncorrected uptake reflected that substrate influence.

In the presence of kaolinite, sorption-corrected plant uptake of Se was calculated to be $\bar{x} = 119 \% \pm 7$ and $\bar{x} = 112 \% \pm 4$ of the uncorrected uptake for selenite and selenate, respectively. In the presence of goethite, sorption-corrected plant uptake of Se was calculated to be $\bar{x} = 27150 \% \pm 9608$ and $\bar{x} = 112 \% \pm 4$ of the uncorrected uptake for selenite and selenate, respectively. This made goethite the greater influence on either selenite or selenate uptake, with selenite uptake affected disproportionately. Kaolinite had a similar influence

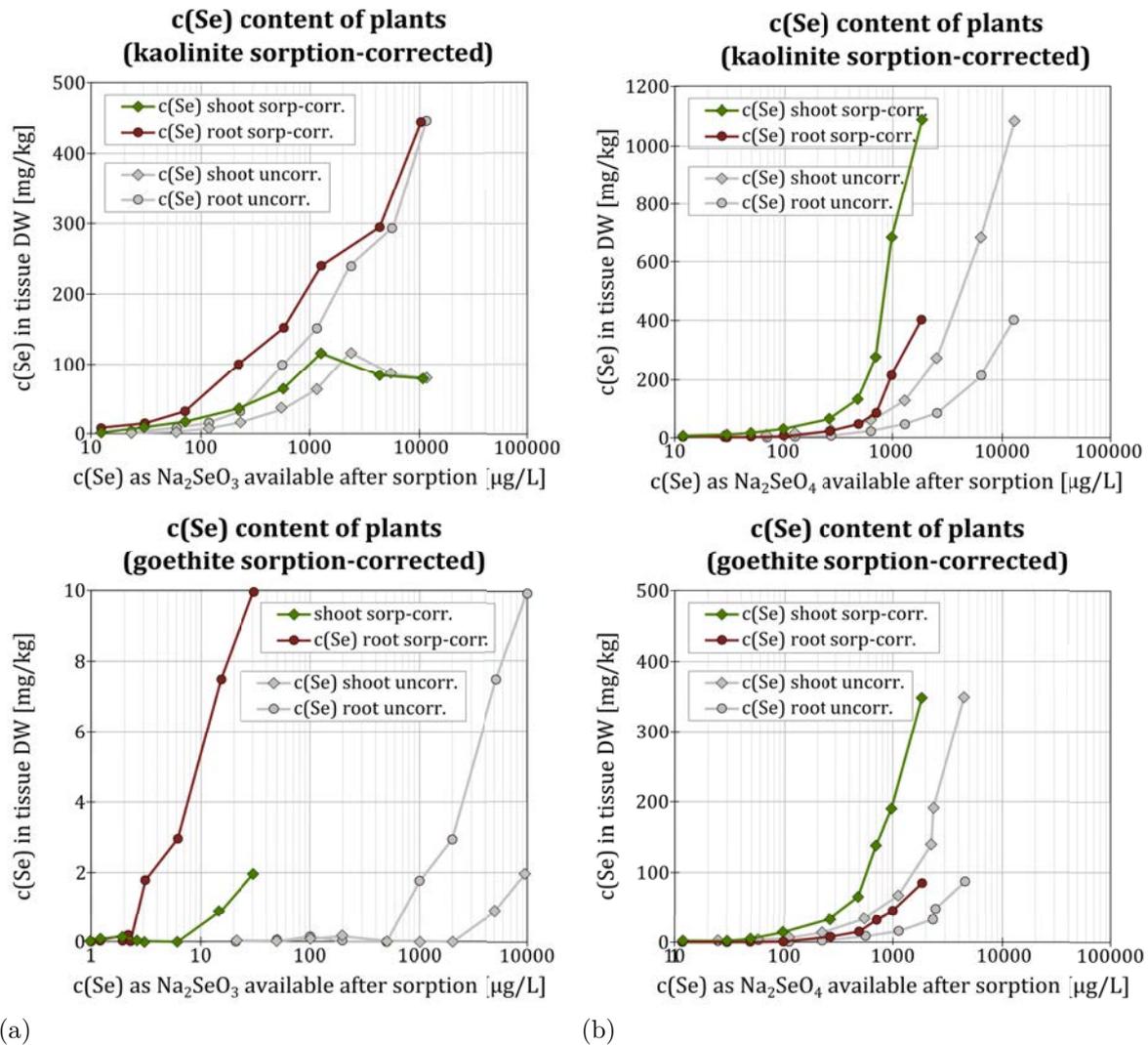


Figure 5.10.: *Se content in plant tissue with sorption competition by kaolinite (top) and goethite (bottom); initial Se concentration corrected by adsorption determined from bottle reference experiments compared to the uncorrected initial Se concentration*

a: addition of Se as Na_2SeO_3

b: addition of Se as Na_2SeO_4

on uptake of either Se oxy-anion.

With the main difference in experimental set-up being the additional ions in the nutrient solution, adsorption results of Se in Exp. C differed from those in Exp. B1 (Figure 5.11a,b). Although kaolinite adsorption (Figure 5.11a) did not reach a maximum - as was the case in Exp. B1 - adsorption of selenite compared to selenate showed only small differences, unlike results of Exp. B1, where selenate adsorption to kaolinite was higher than selenite adsorption. Moreover, adsorption in the presence of nutrients in Exp. C. was much lower

compared to Exp. B1, where the background ion concentration was comprised solely of KCl.

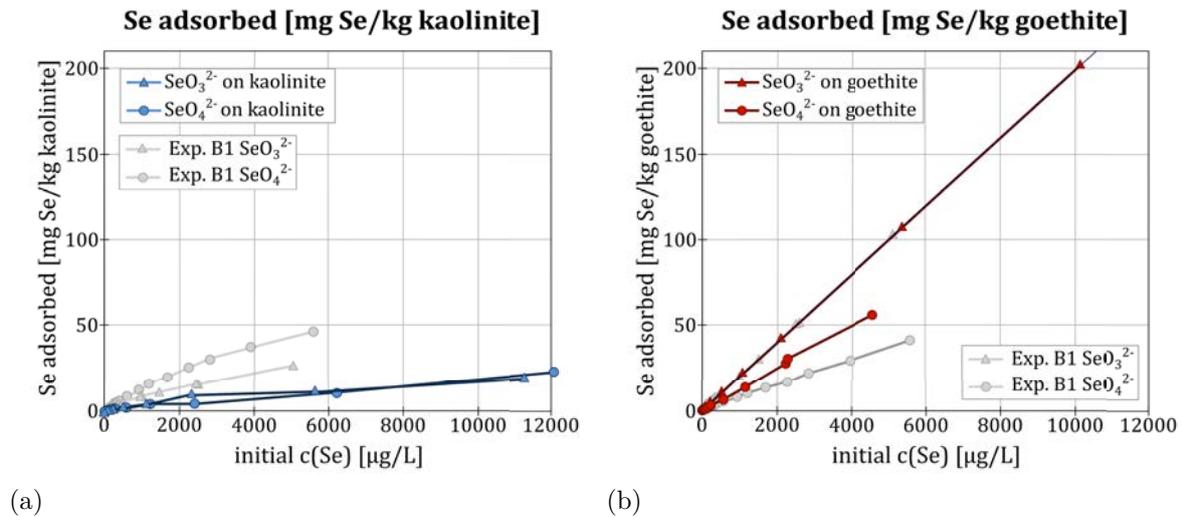


Figure 5.11.: *Se adsorption from nutrient solution as Na_2SeO_3 and Na_2SeO_4*
a: onto kaolinite
b: onto goethite

Compared to Exp. B1, in which adsorption was studied in the presence of KCl solution rather than a nutrient solution, adsorption onto kaolinite was reduced to $\bar{x} = 17\% \pm 5$ and $\bar{x} = 39\% \pm 8$ for selenate and selenite, respectively. Adsorption onto goethite (Figure 5.11b) was increased to $\bar{x} = 126\% \pm 31$ compared to Exp. B1 and remained unchanged at $\bar{x} = 99\% \pm 9$ in the presence of nutrients for selenate and selenite, respectively.

As with the results in Exp. B1, this substrate influence was visible in the Se loss of the solution. Again, assuming experimental conditions between plant boxes and reference bottles were comparable, Se loss due to kaolinite adsorption in Exp. C (Figure 5.12 (top)) was $\bar{x} = 16\% \pm 5$ and $\bar{x} = 10\% \pm 3$, while plant uptake only accounted for $\bar{x} = 12\% \pm 4$ and $\bar{x} = 6\% \pm 3$ of the Se loss for selenite and selenate, respectively.

This is much lower than in Exp. B1, where Se loss due to kaolinite adsorption was between 26 and 62% for selenite and 40 to 74% for selenate. Selenium loss due to goethite adsorption in Exp. C (Figure 5.12 (bottom)), however, showed greater similarity to that of Exp. B1. Sorption accounted for $\bar{x} = 98\% \pm 2$ and $\bar{x} = 57\% \pm 4$, while plant uptake only accounted for $\bar{x} = 0.5\% \pm 0.9$ and $\bar{x} = 7\% \pm 4$ of the Se loss for selenite and selenate, respectively. In Exp. B1, selenite in solution was nearly completely (96 - 97%) adsorbed

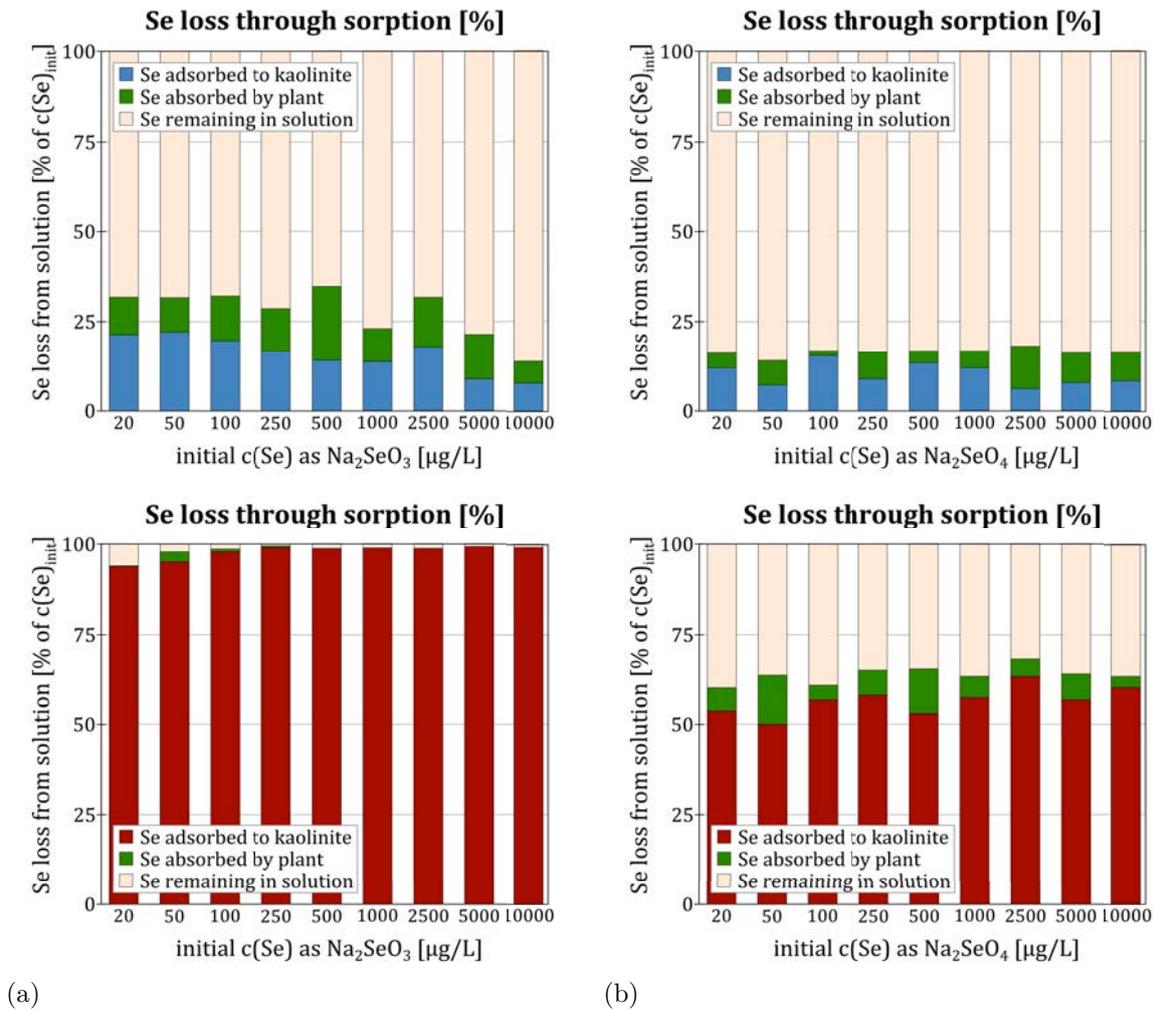


Figure 5.12.: *Loss of Se concentration from solution through adsorption onto kaolinite (top) and goethite (bottom)*
a: addition of Se as Na_2SeO_3
b: addition of Se as Na_2SeO_4

onto goethite, while Se-loss from solution was due to selenate sorption onto goethite (43 - 36 %).

Adsorption did not only affect Se concentrations in the nutrient solution. As shown in Figure 5.13, concentrations of N as nitrate, S as sulfate and P as phosphate were influenced as well; however, there was no visible correlation of nutrient adsorption with Se concentration. Kaolinite was observed to adsorb phosphate with a loss from solution of $\bar{x} = 55 \% \pm 11$ and $\bar{x} = 65 \% \pm 7$ in the selenite and selenate experiments, respectively, but no measurable amounts of nitrate ($\bar{x} = 0 \% \pm 0$ and $\bar{x} = 0 \% \pm 1$) or sulfate ($\bar{x} = 0 \% \pm 0$ and $\bar{x} = 0 \% \pm 1$). This means that Se speciation had an influence on phosphate adsorption onto kaolinite

in the presence of selenite (Figure 5.13a), lowering phosphate adsorption compared to the presence of selenate (Figure 5.13b). As shown in Figure 5.13, loss of nitrate and sulfate from these solutions was due entirely to plant uptake and not kaolinite. Plant uptake, therefore, led to a loss of nitrate of $\bar{x} = 36 \% \pm 20$ and $\bar{x} = 30 \% \pm 7$ and a loss of sulfate of $\bar{x} = 11 \% \pm 4$ and $\bar{x} = 9 \% \pm 4$ in the selenite and selenate experiments, respectively.

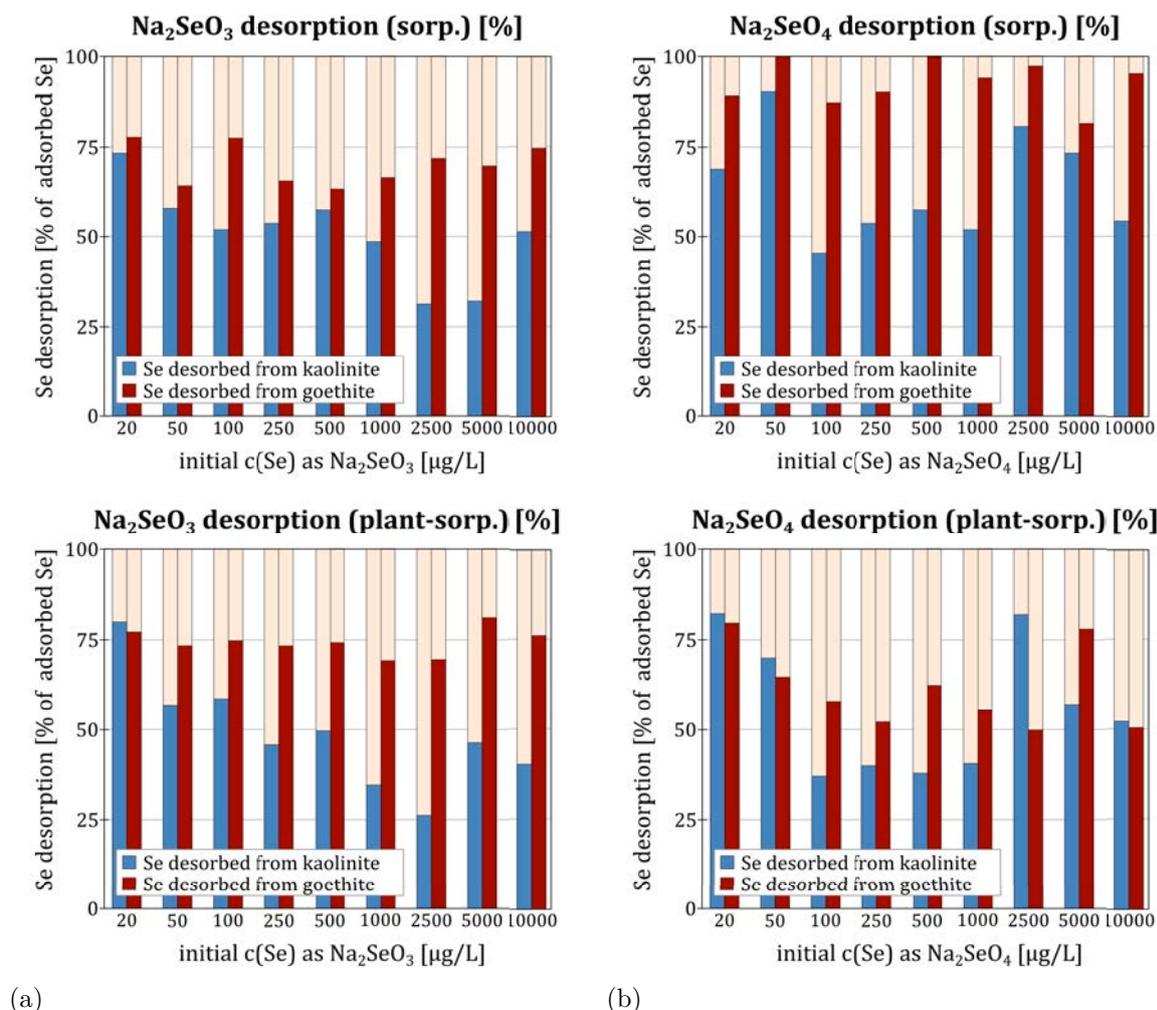


Figure 5.13.: Loss of NO_3^- , SO_4^{2-} and PO_4^{3-} concentration from solution through uptake by plants (colored bar with grey-structured filling) and substrate adsorption (colored bar) onto kaolinite (top) and goethite (bottom); plant uptake calculated from the difference between plant-less reference bottle experiments and rice plant-containing plant-box experiments.

a: addition of Se as Na_2SeO_3

b: addition of Se as Na_2SeO_4

Phosphate uptake by plants led to loss from solution of $\bar{x} = 20 \% \pm 9$ and $\bar{x} = 18 \% \pm 5$ in the selenite and selenate experiments, respectively. Being within each other's standard

deviation, this allows the conclusion that the Se speciation had no significant influence on nitrate, sulfate or phosphate uptake, although it must be noted that uptake in the presence of selenite was slightly lower in all three cases.

Goethite was observed to adsorb 100 % of all phosphate independently of the Se speciation present (Figure 5.13 (bottom)), leaving at the most trace concentrations of phosphate for plant uptake. Adsorption of nitrate and sulfate was sparse, with nitrate loss from solution at $\bar{x} = 1 \% \pm 2$ and $\bar{x} = 4 \% \pm 5$ and sulfate loss from solution at $\bar{x} = 3 \% \pm 3$ and $\bar{x} = 7 \% \pm 4$ for selenite and selenate experiments, respectively. Due to the small adsorption amount, possible Se speciation influences were not significant and sulfate uptake into plants could not be measured in the presence of goethite independent of the Se speciation. Loss of nitrate from solution due to plant uptake was $\bar{x} = 28 \% \pm 5$ and $\bar{x} = 33 \% \pm 14$ in the selenite and selenate experiments, respectively, and also showed no relation to Se speciation.

When analysing the pH-values, initial values for nutrient solution with selenite (Figure 5.14a) increased with additional Se from 4.9 - 6.3 ($\bar{x} = 5.4 \pm 0.4$) and 4.9 - 6.0 ($\bar{x} = 5.1 \pm 0.4$) for initial solutions of the kaolinite and goethite experiment, respectively - as already shown in Chapter 4.5. On the other hand, initial values for selenate solutions (Figure 5.14b) remained constant between 4.7 and 5.1 ($\bar{x} = 4.9 \pm 0.1$) and between 4.5 and 4.9 ($\bar{x} = 4.7 \pm 0.1$) for initial solutions of the kaolinite and goethite experiment, respectively.

The levelling effect of mineral adsorption already described in Exp. B1 and B2 (Chapter 4.5) was prominent for kaolinite, but less pronounced for goethite. Kaolinite sorption increased the pH-value to $\bar{x} = 6.7 \% \pm 0.1$ for both selenite and selenate adsorption, respectively, independent of initial solution pH. With the additional presence of plants, pH increased to $\bar{x} = 7.2 \% \pm 0.1$ (with one outlier at 5.8) and $\bar{x} = 7.4 \% \pm 0.1$ in the selenite and selenate experiments, respectively. Goethite sorption led to higher pH-values than kaolinite with $\bar{x} = 8.2 \% \pm 0.3$ and $\bar{x} = 7.1 \% \pm 0.3$ for selenite and selenate adsorption, respectively. The presence of plants levelled the pH to $\bar{x} = 7.6 \% \pm 0.3$ and $\bar{x} = 7.4 \% \pm 0.4$ in the selenite and selenate experiments, respectively.

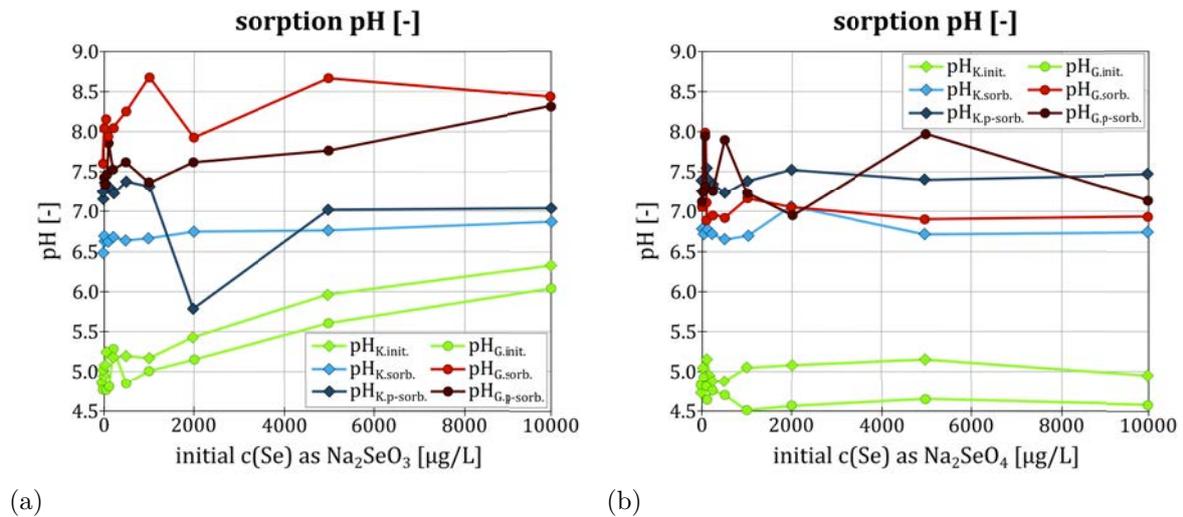


Figure 5.14.: *pH*-values before (*init.*) and after Se sorption (*sorb.*) and sorption coupled with plant-uptake (*p-sorb.*) onto kaolinite (*K*) and goethite (*G*)

a: as Na_2SeO_4

b: as Na_2SeO_3

5.3.5. Desorption properties

Desorption of previously adsorbed Se in Exp. C (Figure 5.15) was generally very inhomogenous, but without a recognizable Se concentration-dependent trend. As with Exp. B3, kaolinite desorption did not change the pH of the desorption solution ($\text{pH} = 8.0$). Selenite desorption recovery from kaolinite (Figure 5.15a) was between 32 and 74 % ($\bar{x} = 51 \% \pm 13$) for the pure adsorption in the glass reference bottles, and between 26 and 80 % ($\bar{x} = 49 \% \pm 16$) for the plant-box experiments. Selenate desorption from kaolinite (Figure 5.15b) was between 45 and 81 % ($\bar{x} = 62 \% \pm 17$) for the pure adsorption in the glass reference bottles, and between 37 and 82 % ($\bar{x} = 55 \% \pm 19$) for the plant-box experiments.

This means that Se was less homogenously recoverable after adsorption from a nutrient solution than from pure solutions, and that desorption from kaolinite was twice as homogenous when plants were present during adsorption.

Similarly to results in Exp. B3, goethite desorption changed the pH of the desorption solution from 8.0 to 9.5. Selenite desorption recovery from goethite (Figure 5.15a) was between 63 and 78 % ($\bar{x} = 70 \% \pm 6$) for the pure adsorption in the glass reference bottles, and between 69 and 81 % ($\bar{x} = 74 \% \pm 4$) for the plant-box experiments. Selenate desorption from goethite (Figure 5.15b) was between 82 and 100 % ($\bar{x} = 95 \% \pm 10$) for the pure

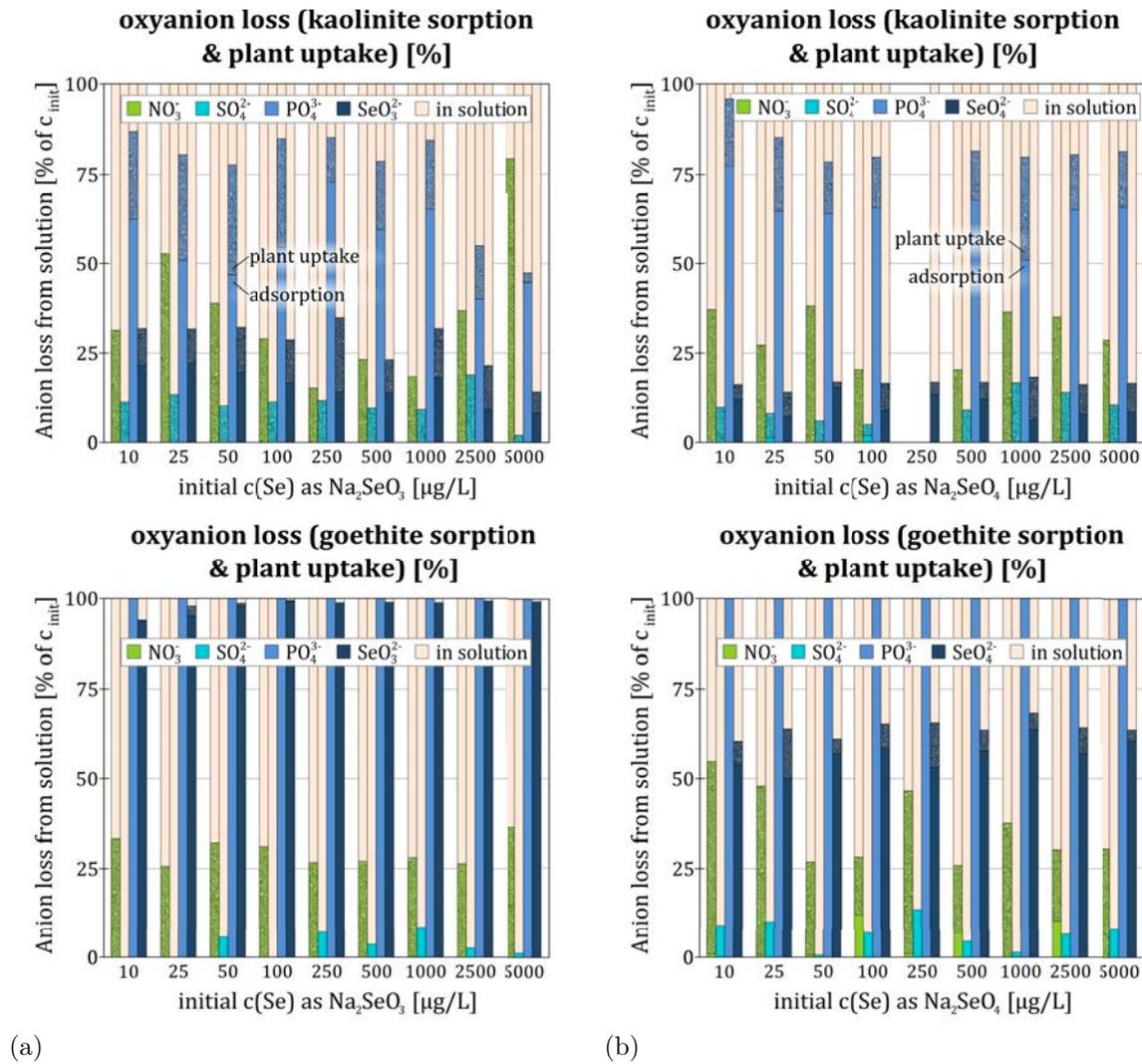


Figure 5.15.: *Se* desorption profiles from kaolinite and goethite for reference bottle experiments (top) and plant-box experiments (bottom) using KH_2PO_4 as percentages of previously adsorbed *Se*.
 a: desorption of selenite
 b: desorption of selenate

adsorption in the glass reference bottles, and between 50 and 79 % ($\bar{x} = 61 \% \pm 11$) for the plant-box experiments.

In general, therefore, desorption from goethite had a higher *Se* recovery (6 - 33 % higher) than desorption from kaolinite but overall inhomogeneity of recovery was very high (SD = 6 - 19 %) compared to Exp. B3 (SD = 3 - 8 %). Previous adsorption in the presence of plants led to slightly greater inhomogeneity of *Se* recovery (SD = 1 - 3 %).

5.3.6. SEM results

SEM analysis (Figures C.5, C.6, C.7, C.8, C.9, C.10 Appendix C.5.1) revealed no visible surface alteration due to Se sorption for either goethite or kaolinite in the presence of selenite or selenate. This was attributed to the low Se concentrations used in the experiments.

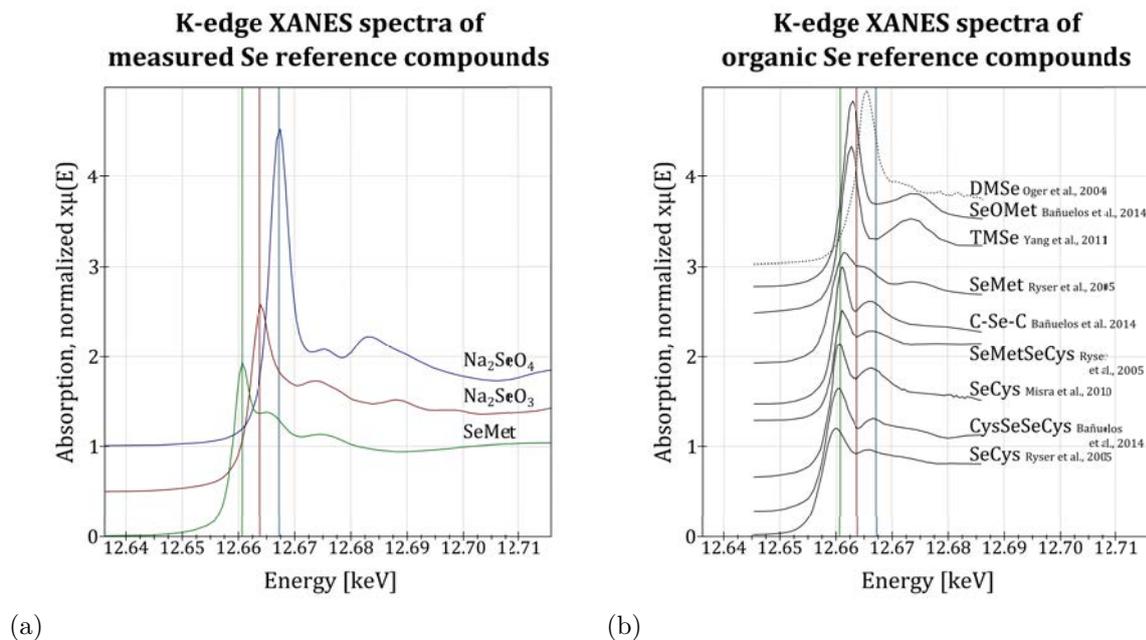


Figure 5.16.: XANES of reference materials, with lines in green, red and blue indicating the absorption edges of the measured standards;
 a: measured references selenomethionine (SeMet, absorption edge peak: 12.661 keV), selenite (12.664 keV) and selenate (12.667 keV)
 b: spectra digitized from publications for orientation and linear fitting

5.3.7. XANES results

Figure 5.16a shows that the measured references of selenite, selenate and SeMet species were easily distinguishable from one another. The absorption edge peaks were at 12.661 keV for SeMet, 12.664 keV for selenite and 12.667 keV for selenate. Peaks were distinct for each species; selenate showed the most pronounced peak (ca. 2.5 times the normed edge height), while selenite's peak was less pronounced (ca. 1 times the normed edge height), and SeMet's peak was the least pronounced (ca. 0.5 times the normed edge height). Within the XANES region (± 30 eV), the ascending peak slopes were similar, but the tailing slopes showed distinct oscillations with maxima at 12.665 and 12.675 keV for SeMet, 12.673 and

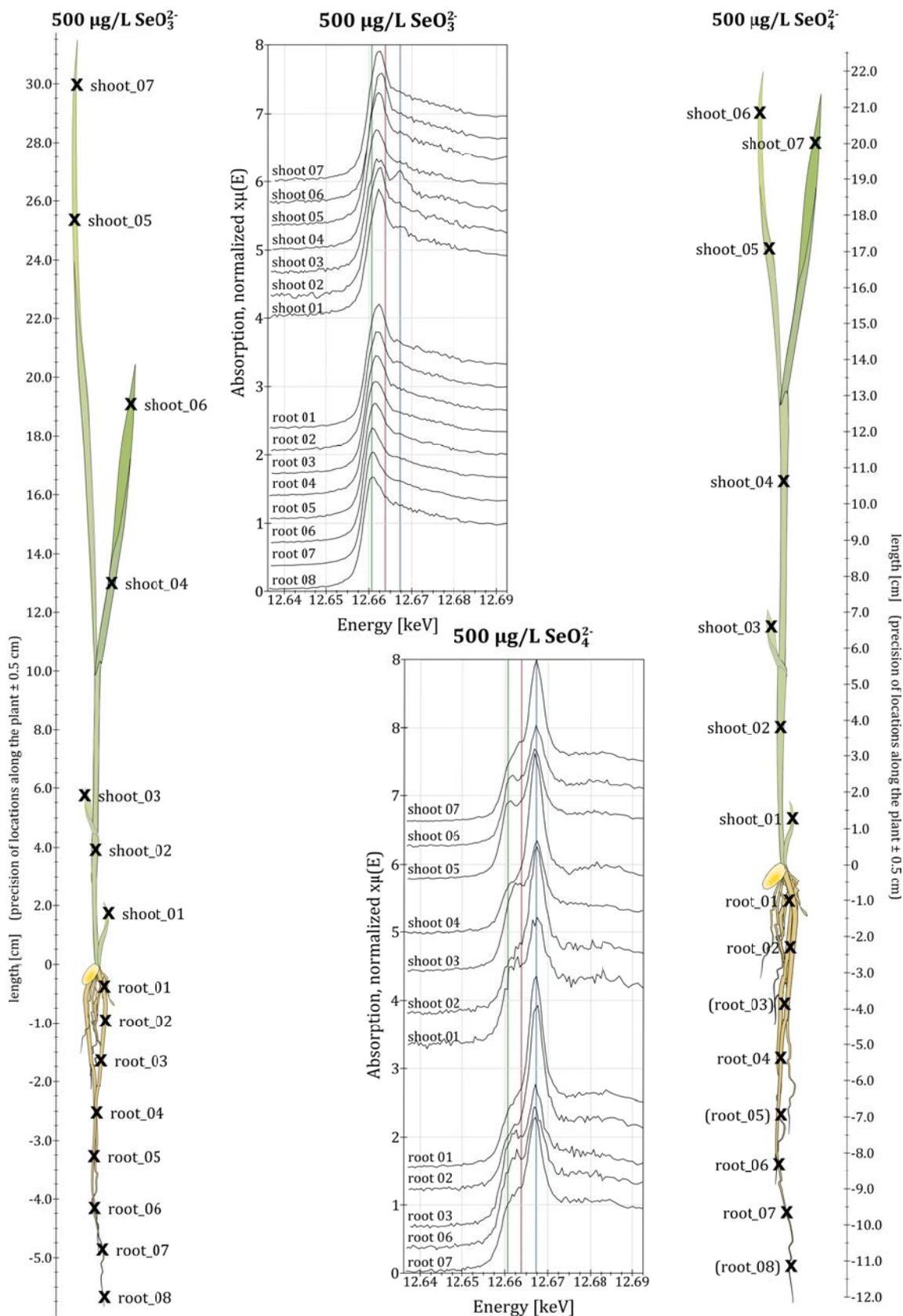


Figure 5.17.: XANES results for regions of interest (ROI) of the shoot and root of a dried rice plant treated with 500 µg/L Se as Na_2SeO_3 (left) or Na_2SeO_4 (right); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively (detailed scans: Appendix C.5.2)

12.688 keV for selenite and 12.675 and 12.683 keV for selenate.

Because there are more organic Se compounds present in a plant than the Se references measured in this study, supplementary reference data (Figure 5.16b) was acquired from various publications using a digitizing software (Engauge Digitizer, version 5.1). The range of organic Se spans peaks at 12.660 keV for SeCys [Ryser et al., 2005], 12.661 for CysSeSeCys [Bañuelos et al. 2015], SeCys [Misra, 2010] and SeMetSeCys [Ryser et al., 2005], 12.662 keV for SeMet [Ryser et al., 2005] and 12.663 keV for TMS_e [Yang et al., 2011] and SeOMet [Bañuelos et al. 2015] as well as 12.666 keV for DMSe [Oger et al., 2004]. The measured SeMet spectrum (Figure 5.16a) matched the organic Se mean referred to as Se-C-Se [Bañuelos et al. 2015], indicating that a distinction between SeMet and SeCys as well as combinations thereof would be difficult to make. After a linear combination fitting survey of 4 measured plant sample scans of selenite and selenate with all combinations of measured and acquired references, all subsequent linear fittings were conducted with the following 5 references as all the others appeared negligible: SeMet (measured), C-Se-C [Bañuelos et al. 2015], SeOMet [Bañuelos et al. 2015], selenite (measured) and selenate (measured). Results of SeMet, C-Se-C and SeOMet were combined and labelled "organic Se".

Figures 5.17, 5.18, 5.19 show that plants treated with selenite and selenate exhibited differences in the species found in XANES spectra of their respective plant tissues (all individual scans: Appendix C.5.2). When adding selenite to nutrient solution, peak energy of the XANES spectra generally suggested organic Se to be dominant within the plant (Figure 5.17, 5.18, 5.19). Furthermore, a depth-dependent trend was visible for the peak-energy. The absorption peak, though retaining its shape, shifted by 10 eV toward a higher energy the closer the scans were to the caryopse – from 12.661 keV at -6.0 cm (root 08) to 12.662 keV at -0.5 cm below the surface (root 01) when adding 500 µg/L Se (Figure 5.17). A much smaller peak shift of no more than 5 eV was observed with the addition of 2000 µg/L Se, while none at all was visible with the addition of 10,000 µg/L Se. Linear combination fitting (Appendix, Table C.19) revealed that only a small portion of selenite was found in the root; 0 - 27 % ($\bar{x} = 15 \% \pm 9$), 0 - 11 % ($\bar{x} = 3 \% \pm 4$) and 0 - 3 % ($\bar{x} =$

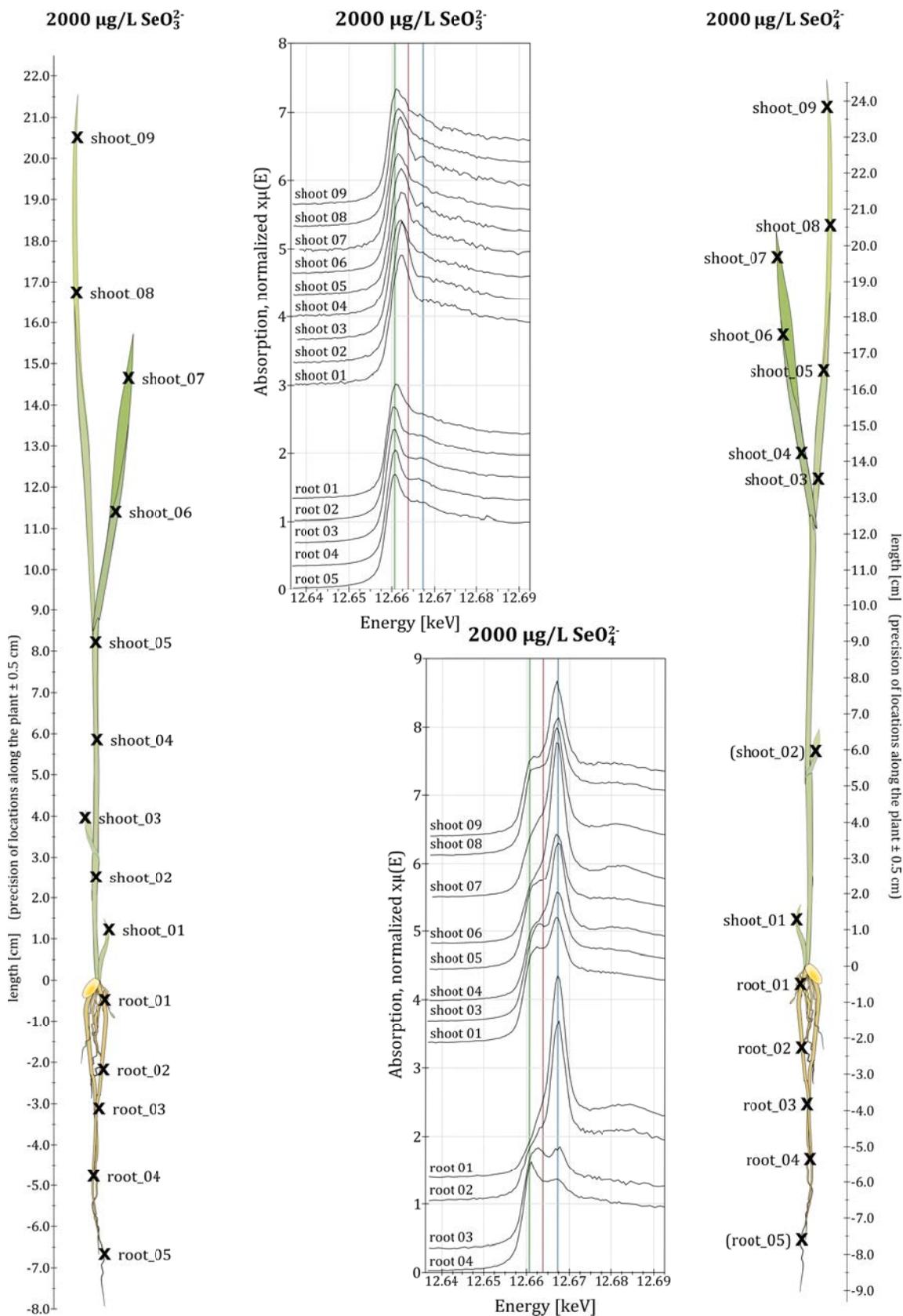


Figure 5.18.: XANES results for regions of interest (ROI) of the shoot and root of a dried rice plant treated with 2000 µg/L Se as Na₂SeO₃ (left) or Na₂SeO₄ (right); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively (detailed scans: Appendix C.5.2)

0 % \pm 1) for the additions of 500, 2000 and 10,000 $\mu\text{g/L}$ Se, respectively. The proportion of organic Se, the main species found in the root, increased toward lower root regions (root 01 - root 08; Figure 5.17, 5.18, 5.19), but also with added Se concentration as well: 73 - 100 % (between 0 and - 6 cm below surface; \bar{x} = 85 % \pm 9), 89 - 97 % (between 0 and - 4.5 cm below surface; \bar{x} = 95 % \pm 4) and 95 - 100 % (between 0 and - 3 cm below surface; \bar{x} = 99 % \pm 2) of SeMet with the additions of 500, 2000 and 10,000 $\mu\text{g/L}$ Se, respectively. The proportion of selenate was calculated to be only 1 - 3 % for isolated samples and, therefore, negligible. This corresponds very well with the peak positions and shapes that correlate with SeMet to a large degree.

In the shoots, organic Se proportion was lower than in the roots with the addition of Se as selenite and speciation did not differ significantly between tissue height above ground. Increasing in proportion to added Se concentration, organic Se comprised up to 50 - 74 % (\bar{x} = 65 % \pm 8), 63 - 76 % (\bar{x} = 74 % \pm 11) and 74 - 81 % (\bar{x} = 78 % \pm 3) of Se in the shoot tissue with the addition of 500, 2000 and 10,000 $\mu\text{g/L}$ Se, respectively. The remaining 26 - 50 % (\bar{x} = 35 % \pm 8), 24 - 37 % (\bar{x} = 27 % \pm 11) and 19 - 26 % (\bar{x} = 22 % \pm 3) of plant-Se was comprised of selenite. Shoot 09 (2000 $\mu\text{g/L}$ Se added, Figure 5.18) was an exception, showing 100 % of its Se to be organic Se, while no selenite was found. No selenate was found in the shoots when selenite was added to the nutrient solution. This corresponds very well with the peak positions and shapes that appear to be a mixture of SeMet and selenite and shift toward the SeMet position and shape as Se concentrations are increased.

When treating the plants with selenate, Se speciation in the roots differed compared to treatment with selenite. Absorption spectra of the roots changed from containing more organic Se to containing more selenate between lower root scans and scans closer to the caryopse; particularly as Se concentration increased from 500 (Figure 5.17) to 2000 (Figure 5.18) and then to 10,000 (Figure 5.19) $\mu\text{g/L}$ Se. As with selenite treatment, the proportion of organic Se increased the further below surface the root sample was taken. When adding 500 $\mu\text{g/L}$ Se as selenate (Figure 5.17), organic Se comprised 31 % of plant-Se for root 01 at -0.5 cm below the surface and increased to 50 % for root 06 at -8.0 cm below the surface. Correspondingly, selenate, the second major Se species in the plant-root, decreased with

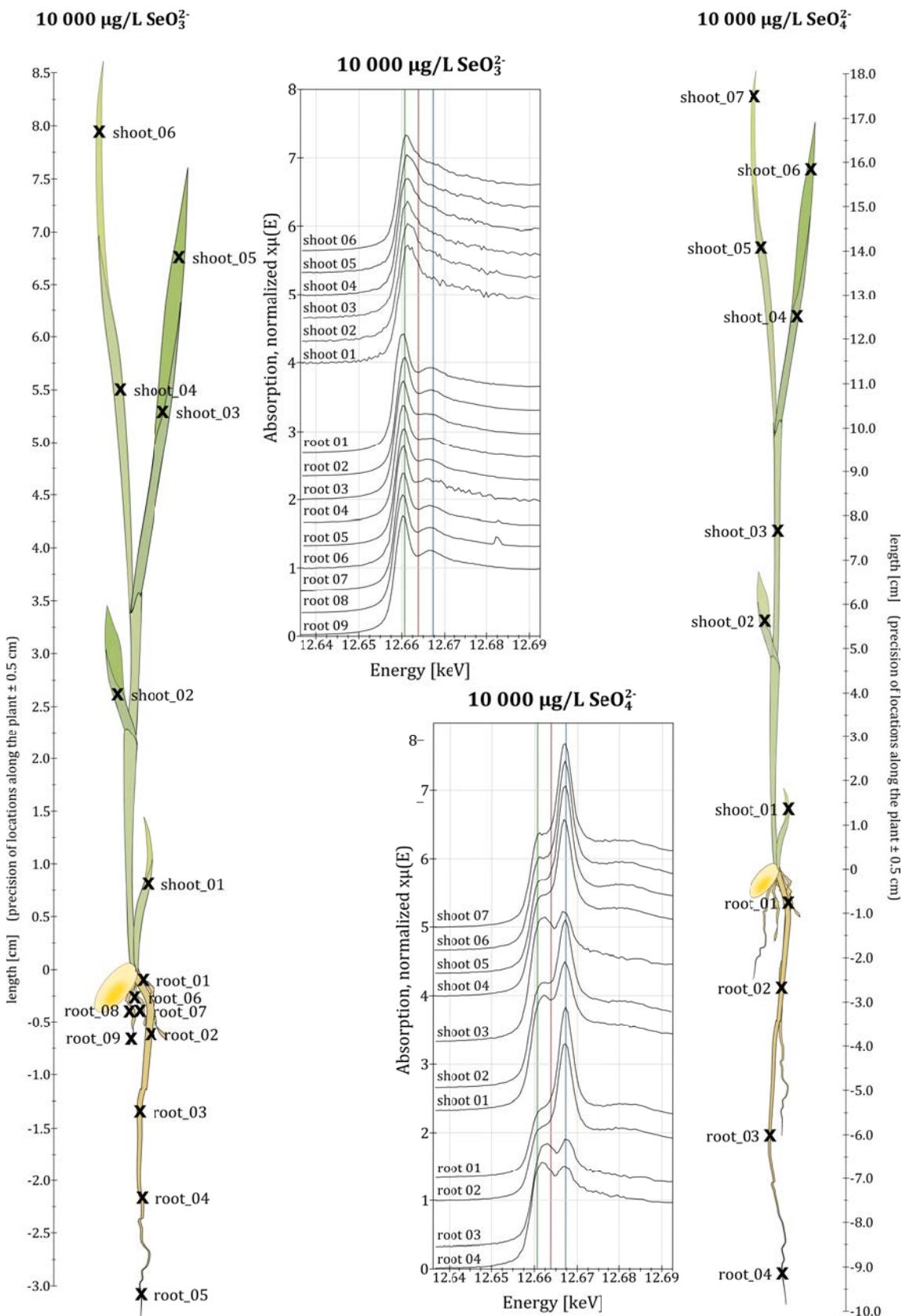


Figure 5.19.: XANES results for regions of interest (ROI) of the shoot and root of a dried rice plant treated with $10,000\ \mu\text{g/L Se}$ as Na_2SeO_3 (left) or Na_2SeO_4 (right); green, red & blue indicating peak lines for selenomethionine ($12.661\ \text{keV}$), selenite ($12.664\ \text{keV}$) and selenate ($12.667\ \text{keV}$), respectively (detailed scans: Appendix C.5.2)

root depth, from 63 % for root 01 to 32 % for root 06. The calculated proportion of selenite, however, increased with depth, similar to organic Se from 6 % for root 01 to 17 % for root 07. Mean values of organic Se proportion in the roots increased with additional Se from $\bar{x} = 42 \% \pm 10$ to $\bar{x} = 48 \% \pm 30$ and $\bar{x} = 54 \% \pm 7$ for the additions of 500, 2000 and 10,000 $\mu\text{g/L}$ Se, respectively. Similarly to the addition of 500 $\mu\text{g/L}$ Se as selenite, increased Se concentrations led to the same trends of increasing organic Se with root depth, decreasing selenate with root and increasing selenite with root depth, although this became more pronounced when increasing the added Se concentration. With the addition of 2000 $\mu\text{g/L}$ Se as selenate (Figure 5.18), root-Se between root 01 at -0.5 cm and root 05 at -8.0 cm showed an increase of organic Se from 14 % to 80 % ($\bar{x} = 48 \% \pm 30$) and a corresponding decrease in selenate from 71 % to 5 % ($\bar{x} = 36 \% \pm 34$). Selenite made up between 10 and 27 % ($\bar{x} = 17 \% \pm 7$) of plant-Se. With the addition of 10,000 $\mu\text{g/L}$ Se as selenate (Figure 5.19), root-Se between root 01 at -0.5 cm and root 04 at -9.0 cm showed an increase of organic Se from 43 % to 68 % ($\bar{x} = 54 \% \pm 11$), an increase of selenite from 6 % to 23 % ($\bar{x} = 17 \% \pm 12$) and a corresponding decrease in selenate from 51 % to 9 % ($\bar{x} = 29 \% \pm 22$).

Selenium speciation in the shoot with the addition of Se as selenate exhibited greater heterogeneity than in roots or in shoots and roots for the addition of selenite. However, there was no significant spatial trend to explain this heterogeneity. Scans show a dominance in selenate with visibly smaller peaks at the SeMet energy, which is reflected in the linear combination fitting, as well. Addition of 500 $\mu\text{g/L}$ Se led to 27 - 57 % SeMet ($\bar{x} = 38 \% \pm 10$), 6 - 28 % selenite ($\bar{x} = 14 \% \pm 8$) and 31 - 67 % selenate ($\bar{x} = 48 \% \pm 16$). Addition of 2000 $\mu\text{g/L}$ Se led to 25 - 56 % SeMet ($\bar{x} = 45 \% \pm 11$), 10 - 22 % selenite ($\bar{x} = 18 \% \pm 5$) and 22 - 65 % selenate ($\bar{x} = 31 \% \pm 13$). Addition of 10,000 $\mu\text{g/L}$ Se led to 43 - 68 % SeMet ($\bar{x} = 54 \% \pm 11$), 6 - 31 % selenite ($\bar{x} = 17 \% \pm 12$) and 8 - 51 % selenate ($\bar{x} = 29 \% \pm 22$). Heterogeneity decreased with increased Se concentration, and, as previously noted, average organic Se proportion increased with increased Se concentration as well, while proportions of selenite and selenate varied.

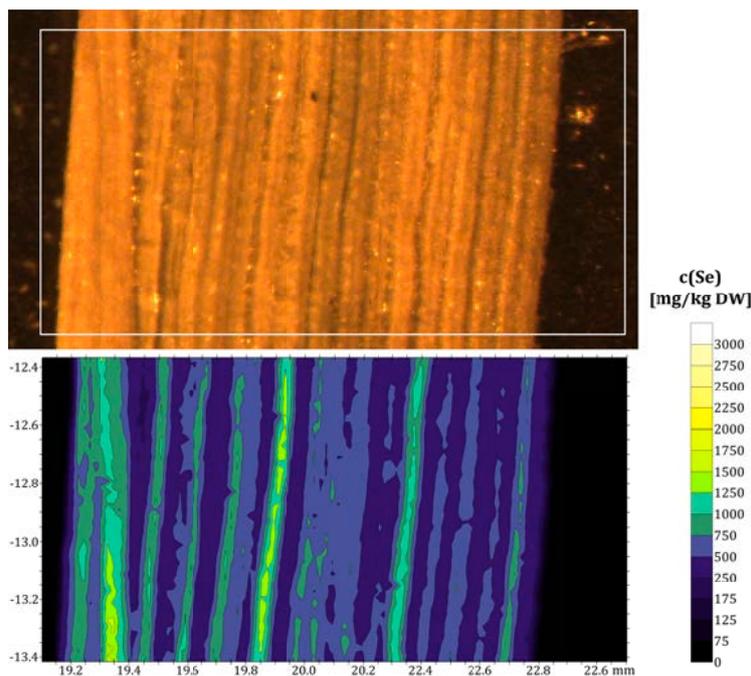


Figure 5.20.: *Selenium fluorescence mapping of air-dried shoot tissue - rice plant treated with 10,000 $\mu\text{g/L}$ Se as selenate in hydroponic culture; photo (top) taken under the binocular*

5.3.8. Results of high-resolution Se mappings using synchrotron based μXRF

The μXRF results exhibited a very distinct pattern of Se distribution, which followed the plant's vascular bundles (Figure 5.20). This was observed independently from the addition of Se as selenite or selenate. Concentrations of Se, which could be determined semi-quantitatively, were up to 2000 mg/kg DW and selectively reached 3000 $\mu\text{g/L}$ in these vascular bundles of the rice plant treated with 10,000 $\mu\text{g/L}$ Se (Figure 5.22). In between these vascular bundles, Se concentrations were below 500 mg/kg DW, but not below 50 mg/kg DW.

For plants treated with 2000 $\mu\text{g/L}$ Se as selenite, Se content in the shoots was much lower (Figure 5.21, top). Again, concentrations were highest in the vascular bundles, but only amounted to 45 mg/kg DW Se at the most and the lowest Se concentration within the plant tissue was 10 mg/kg DW.

When the rice plant was treated with 10,000 $\mu\text{g/L}$ Se as selenite (Figure 5.21, bottom), fluorescence showed vascular bundles in the shoots with Se hot spots of up to 1750 mg/kg

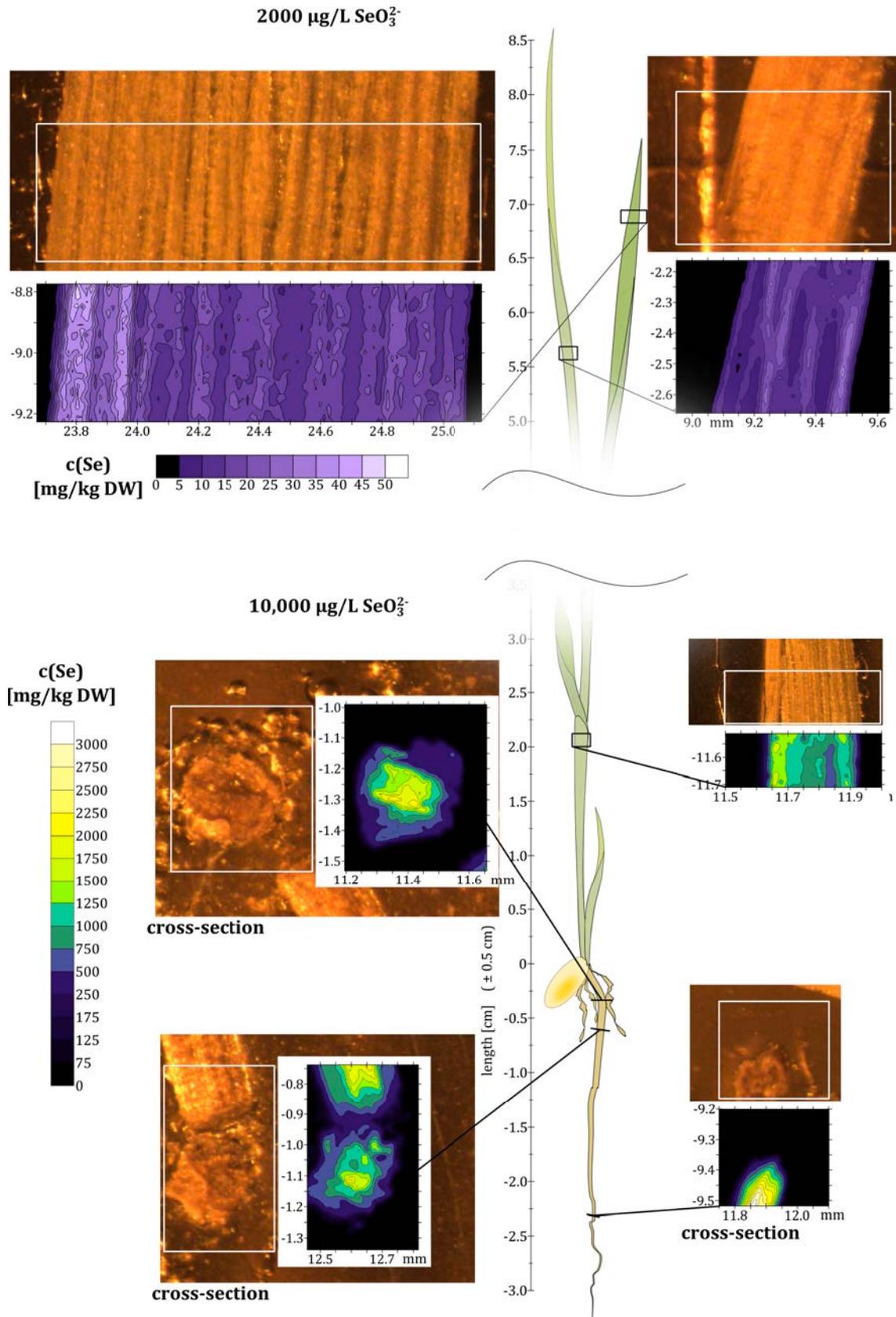


Figure 5.21.: Selenium fluorescence mappings of shoot and root tissue of a dried rice plant treated with 2000 $\mu\text{g/L Se}$ (top) and 10,000 $\mu\text{g/L Se}$ (bottom) as Na_2SeO_3 ; photos taken with a binocular

DW Se. However, overall Se content was closer to 1000 mg/kg DW. Root cross-sections also showed the highest Se concentrations to be in the middle of the root (up to 3000 mg/kg DW) where vascular bundles converge into the central cylinder, with Se decreasing toward the outer edge of the cross-section to below 500 mg/kg DW (Figure 5.21).

In some places, although slightly deformed by the pressure of the razor blade used to produce the root cross-section of the selenite-treated plant (Figure 5.21), single vascular bundles stood out with high Se concentrations of more than 2000 µg/kg DW. Selenium content appeared to be highest for root cross-sections further below the surface with 3000 mg/kg DW at -2.5 cm, compared to 2000 mg/kg DW at -0.5 cm below the surface.

When the rice plant was treated with 10,000 µg/L Se as selenate, concentrations in vascular bundles of the leaves reached up to 3000 mg/kg DW Se in tissue of 15 cm growth height. Selenium content in the highest-measured leaf (4th leaf, 17.5 cm growth height) still reached 1750 mg/kg DW. Leaf tips, such as the coleoptile or the tip of the second leaf, however, showed lower Se concentrations of 500 - 1000 mg/kg DW. Root Se concentrations for the selenate-treated plants were lower than in their selenite counterparts and reached 1250 mg/kg DW at the most. It is interesting to note that root hairs, although large enough to be resolved by the x-ray beam of 11 x 16 µm if they contained Se, show no trace of Se concentration.

5.4. Discussion

As it has already been thoroughly discussed in Chapter 3.6, selenate accumulation predominantly in shoots and selenite accumulation predominantly in roots will not be discussed deeply here. Likewise, adsorption and desorption properties of kaolinite and goethite with respect to selenite and selenate as well as the nutrient oxy-anions nitrate, sulfate and phosphate have already been discussed in Chapter 4.6.

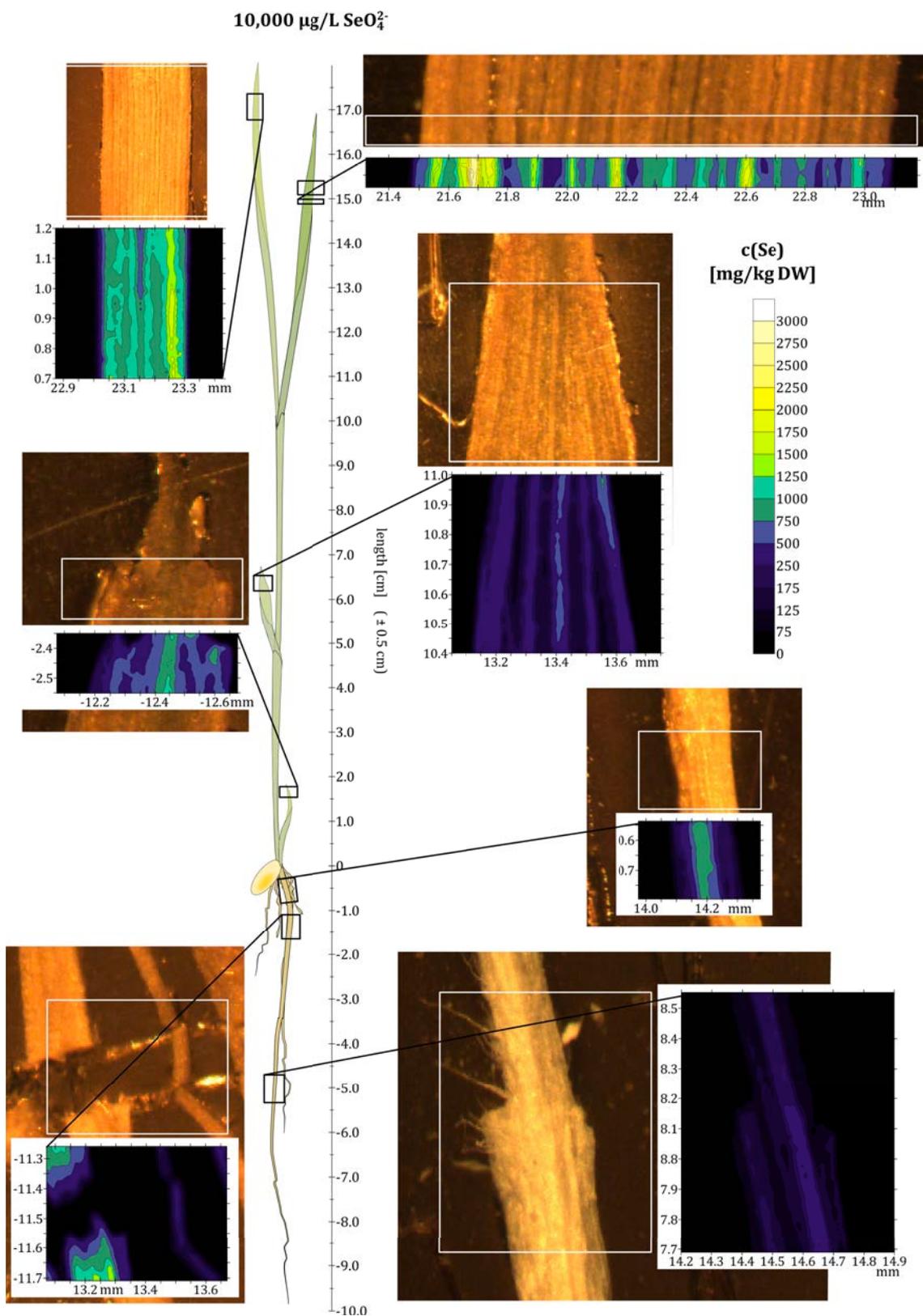


Figure 5.22.: Selenium fluorescence mappings of shoot and root tissue of a dried rice plant treated with 10,000 $\mu\text{g/L Se}$ as Na_2SeO_4 ; photos taken with a binocular

5.4.1. Selenium toxicity in plants under optimal conditions

As argued in Chapter 3.6, the availability of nutrients and germination in a Se-free environment enables the rice plant to deal with much higher Se concentrations than if grown directly in Se without nutrient supplementation. However, additions of 5000 and 10,000 $\mu\text{g/L}$ Se lead to toxicity symptoms similar to those on the agar plants despite Se-free germination and the supplement of nutrients. If the set-up in the agar experiments can be considered the maximum of adverse effects on the rice plant concerning nutrients and Se-respite during germination, these experiments constitute the minimum of adverse effects with regard to those two factors. Therefore, 2000 $\mu\text{g/L}$ Se addition as selenite is the highest tolerance limit for 2-3 week-old rice plants under optimal conditions. Since selenate shows no adverse effect on the rice plants in these concentrations, selenite is considered more toxic than selenate.

The 2000 mg/kg DW of Se considered to lead to 10 % less crop yield in rice [Läuchli, 1993] must, therefore, refer to selenate addition, since selenite shows severe toxicity already at concentrations below 100 mg/kg DW in shoots and 500 mg/kg DW in roots. Therefore, for rice plants, selenite can be considered 8 - 12 times more toxic than selenate when considering the entire plant Se concentration, which corresponds very well with present literature, in which a similar difference in toxicity has been described [Smith & Watkinson, 1984, Läuchli, 1993]. This is particularly important because much rice is cultivated in wet soil and stagnant water, therefore making selenite the more prevalent Se species [Khan & Hell, 2014].

5.4.2. Substrate influence on Se-uptake by rice

As to be expected due to results of the previous experiments, kaolinite adsorption influenced plant-Se uptake slightly, while goethite adsorption had a major influence. Kaolinite's limited sorption capacity reduced selenite availability by 16 % and selenate availability by 10 %. This largely remained within error margins of plant uptake for previous experiments of the same cultivar and is therefore not considered significant. Therefore, soils containing

kaolinite offer little protection against toxicity of high Se concentrations and are also unsuitable as a Se reservoir for Se-biofortification of plants.

Selenite and selenate adsorption to goethite, on the other hand, was significant. With 98 % Se-loss due to selenite adsorption and 57 % Se-loss due to selenate adsorption, plant-uptake of Se is strongly inhibited by goethite. Plant-uptake reflected this Se-loss. Although plant roots had physical contact with the Se-containing goethite, there is no evidence of increased uptake beyond that of pure Se content in the nutrient solution, since uptake was not elevated compared to the uptake without the presence of Se-rich sorption material. Most likely, plants which are not under stress to obtain nutrients will not desorb Se from mineral surfaces by root exudates. The fact that Se can strongly adsorb onto iron oxides and hydroxides has been noted in many publications [Balistreri & Chao, 1987, Hayes et al., 1987, Balistreri & Chao, 1990, Chan et al., 2009, Das et al., 2013]. What is noteworthy as well, however, is the wide pH range for which this is the case. Due to large quantities adsorbed to the soil, a sudden change in redox and pH conditions can re-submerge these previously adsorbed quantities of Se and make them bioavailable. This is not unrealistic for rice agriculture, as flooded conditions during early growth stages alternate with dry conditions around harvest time and this leads to frequent redox changes in the soil. As shown in the desorption experiments, phosphate can easily displace adsorbed Se, even from goethite. So, not only is a sudden change of redox conditions important to monitor in such cases, but also the agricultural application of large quantities of phosphate-bearing fertilizer. Since iron oxides will preferentially bind phosphate, not only would plants be left without phosphate, but also exposed to the possibly toxic concentrations of Se.

Another interesting observation is that adsorption onto kaolinite differed compared to the pure sorption experiments, in which there was no nutrient solution, but rather a KCl background electrolyte of similar ionic strength. The presence of further nutrient ions, especially phosphate and sulfate, diminished kaolinite adsorption capacity by a factor of 2 - 4 for selenite and by a factor of 4 - 7 for selenate. Since plant germination and root growth requires up to 5 - 7 days for roots to reach the nutrient solution, this effect of kaolinite adsorption interference must be a product of the additional nutrients. It also explains why

the effect is $7/4^{\text{th}}$ more pronounced for selenate than for selenite, as this is the ratio of molar concentrations of sulfate (700 μmol) and phosphate (400 μmol). Therefore, selenite adsorbed onto kaolinite is believed to be hindered by competing phosphate ions, while selenate adsorption is hindered by competing sulfate adsorption.

5.4.3. Se distribution within the plant

As argued previously in the literature [Sun et al., 2010, Bañuelos et al. 2015], XANES spectra of some organic species are difficult to distinguish. Moreover, different authors have measured slightly different peak energies for SeCys and SeMet, which confirms that measurement results for these compounds, in particular, are not as conservative as for example measurement results for selenite or selenate, which do not vary. In a study using a different measuring technique (HPLC-ICP-MS), species of SeMet, MeSeCys, and SeCys were discernable and a linear correlation between these species was formulated for tissue samples of fruit-bearing rice plants [Sun et al., 2010]. What XANES spectra and μXRF mappings in our study were able to show in contrast, however, is the spatial progression of species proportions along the length of the root, in particular. As shown in this study, the proportion of organic Se within the root is lowest near the caryopse and increases toward lower parts of the root for both selenite and selenate. As Se is known to be rapidly converted into organic Se when taken up as selenite [Terry et al., 2000, Khan & Hell, 2014], finding a large portion of organic Se in the roots is to be expected [Terry et al., 2000, Khan & Hell, 2014, Eiche, 2015]. Finding higher concentrations of selenite in higher parts of the plant might indicate that not all selenite was transformed in the root, but rather was transported into higher regions of the plant before being transformed into organic Se there. Formation of SeCys, which precedes formation of SeMet, is believed to take place in the chloroplasts, where methylation can render it a non-protein (SeMetSeCys), protecting against Se incorporation into enzymes without sacrificing Cys [Zayed et al., 1998, Terry et al., 2000, Finley, 2005]. An explanation for why the organic Se proportion is higher in the root than in the shoot in general and for Se addition as selenate, in particular, might be that transformation into

organic Se appears to be either more effective in the roots, or that Se is stored as organic Se in the roots as a non-protein, such as MeSeCys [Duc et al., 2003], while it is volatilized from the shoots. As methylation of Se might inhibit its incorporation into proteins, thereby providing a method to avoid toxicity [LeDuc et al., 2004], it is feasible that higher Se concentrations lead to a higher proportion of SeMet in the plant, as observed with the additions of 500, 2000 and 10,000 $\mu\text{g/L}$ Se.

It is known that selenate reduction, which also takes place in the chloroplasts, is the rate-limiting step of selenate assimilation [Terry et al., 2000]. Therefore, it is not surprising to find a large portion of Se as selenate in the shoots when adding Se as selenate. The question arises why so much selenite is also present, since selenite was shown to be rapidly converted into organic Se. Although there is a selenate reduction step to selenite [Terry et al., 2000, Finley, 2005], it is still an unanswered question why it isn't synthesized more quickly into organic Se, or if this is perhaps a different species not accounted for by the linear combination fitting. There have been similar findings in wheat, with selenite found in the shoots by linear combination fitting of XANES data [Eiche, 2015].

One possibility, of course, is beam-induced damage and therefore, reduction of selenate into selenite [Wang et al. 2013]. However, well aware of this danger, measurements were kept very short and no more than 2 scans were taken from the exact same spot and the reproducibility of such great quantities of selenite due to sudden beam-induced damage when none was previously seen is highly unlikely. It is more likely that either selenite is really transported as selenite to higher parts of the plant, which would not agree with other currently published data [Läuchli, 1993, Zayed et al., 1998, Terry et al., 2000, Sun et al., 2010], or that some vital Se reference is missing in the linear fitting. The insecurities connected with the linear fitting coupled with a probable lack of reference material is currently considered the most plausible explanation for this finding. There are multiple possible Se compounds that include S which could be part of this explanation, since their XANES spectra show peaks at multiple energies between organic species and selenite [Pickering et al., 1999]. More detailed investigations are needed to determine these spatial-speciation differences.

5.4.4. Conclusions for the biogeochemical mass balance model

In combination with results of both other sets of experiments (Chapter 3.6, 4.6), these results are incorporated into the biogeochemical model in Chapter 6. Model-relevant conclusions from this part of the study not already made in previous chapters are:

1. Se-uptake for concentrations greater than 2500 μL Se (i.e. 5000 and 10,000 $\mu\text{g/L}$ Se) can be added
2. selenite and selenate-dependent partitioning into organic Se, selenite and selenate can be mathematically formulated for shoots and roots for a range of Se concentrations
3. additionally, root depth profiles of this partitioning can be described dependent on Se speciation and concentration
4. kaolinite and goethite sorption in the presence of a nutrient solution can be compared to Se adsorption in the presence of single-ion competition
5. direct influence of substrate adsorption on bioavailable Se for plant uptake can be modelled

6. A biogeochemical model of Se transfer in the Critical Zone

In order to connect the experimental results of this study to formulate a coherent model, all key findings were transferred into mathematical terms. These mathematical arguments of this bottom-up approach do not necessarily describe processes mono-causally, but were intended to provide a good approximation for quantities of Se transfer between reservoirs in the Critical Zone.

6.1. Selenium transfer between soil solution and plant

For this part of the model, data were used in which Se was taken up from nutrient solution, including experiments A3 (Chapter 3.3.3) and C (Chapter 6.5c). Since growing rice without nutrients is highly unlikely in a practical setting, the results of experiment A2 (Chapter 3.3.2) and A4 (Chapter 3.3.4) are not included, as those experiments were conducted on nutrient-free agar instead of nutrient solution. The following assumptions were made for the model, resulting from Exp. A3 (Chapter 3.3.3) and Exp. C (Chapter 6.5c):

- differences between selenite and selenate uptake into plants made separate modelling of each species necessary
- differences between root and shoot partitioning within the rice plants required separate modelling of these plant tissues

- therefore, speciation differences also made separate modelling of root and shoot necessary
- in addition to the mean root speciation, local root speciation could be modelled as a function of depth below the surface

6.1.1. Data input

For the model of resulting Se-content in the plant, all data of measured (Exp. A3) or sorption-corrected Se (Exp. C) as selenite or selenate in the initial solution was correlated with plant uptakes into shoots and roots. To provide a large data-set for this modelling, data of all 3 replicates as well as the mean were plotted. Mathematical arguments for the fitting were achieved with Excel (Microsoft, version 14.0.7147.5001) and pre-setted trend lines were fitted. Best fits were chosen by comparing R^2 .

Since the uptake of 10,000 $\mu\text{g/L}$ Se was only covered by two data points, it was not included in the model. Because the range of Se concentration was large enough to produce two very different fits when either including or omitting data on the uptake of 5000 $\mu\text{g/L}$ Se, both types of fits were used in the model. Additionally, smaller concentration ranges (0 - 50 $\mu\text{g/L}$ Se, 50 - 500 $\mu\text{g/L}$ Se and 500 - 5000 $\mu\text{g/L}$ Se) were modelled as well, using only the mean values of Exp. A3 and Exp. C. These were included optionally in the model.

For the model of Se speciation percentages within roots and shoots, mean results of the linear combination fitting of Exp. C were used. Therefore, proportions of three species were modelled: organic Se, selenite and selenate. Data on tissue speciation distribution for 500, 2000 and 10,000 $\mu\text{g/L}$ Se in the initial solution allowed concentration-dependent speciation modelling. In the case of selenite addition, amounts of selenate found in the tissue were negligible and were set to 0. Only organic Se content was modelled over a Se concentration range of 500 - 10,000 $\mu\text{g/L}$ and extrapolated to lower Se concentrations; selenite content in the tissue was then obtained by subtracting the organic content from 100 %. In the case of selenate addition, differences in root and shoot speciation trends meant modelling had to be adapted. Therefore, roots required modelling of organic Se and selenite, while the

remaining selenate fraction was obtained by subtracting the sum of organic Se and selenite from 100 %. For the shoots, organic Se and selenate percentages were modelled, while the remaining selenite fraction was obtained by subtracting the sum of organic Se and selenate from 100 %.

Not only was concentration-dependent Se speciation modelling possible, but also depth-dependent speciation shifts in the root as well. This required a 3-step fitting. The first step was the mean root speciation dependent on Se concentration described above. In the second step, linear ($y = mx+t$) Se concentration-dependent deviation from the mean was determined for each root depth by plotting the share of organic Se at a depth of x cm per mean root organic Se against the added Se concentration. This required Se speciation to be known for 2 - 3 Se concentrations (500, 2000 and 10,000 $\mu\text{g/L}$ Se) in the same root depth (Table 6.1). Due to the depth-dependence of this speciation, each root-depth resulted in plots with different slopes (m) and y-axis intercepts (t) in its respective mathematical argument. In the third step, these (m and t) were plotted against root depth. Therefore, depth-dependent Se speciation was modelled as the linear deviation from the Se concentration-dependent root-speciation mean with slope and y-axis intercepts dependent on root depth.

Table 6.1.: *Root depth dependence of linear combination fitting results; selenite addition required only percentages of organic Se data, selenate addition required data for percentages of organic Se and selenate*

root depth [cm]	root-Se org. [%] c(Se) as SeO_3^{2-} [$\mu\text{g/L}$]			root-Se org. [%] c(Se) as SeO_4^{2-} [$\mu\text{g/L}$]			root selenate [%] c(Se) as SeO_4^{2-} [$\mu\text{g/L}$]		
	500	2000	10,000	500	2000	10,000	500	2000	10,000
0	73		100		14	43	6	10	6
-1	76			31			6	15	8
-2	79	89	100	32	32	48			
-3	84	97	100						
-4	85	100		50		57	17		31
-5	91	99	100	53	63	68		27	
-6	100				46		18	27	27
-7	92	94							23

6.1.2. Fitting results

Fitting plant-Se content over the span of 0 - 5000 µg/L Se in the nutrient solution (Figure 6.1) produced polynomial functions of the 2nd degree. Equations 6.1 and 6.2 describe shoot-Se content, which were fitted with an accuracy of $R^2 = 0.9604$ and $R^2 = 0.9859$ with the addition of 0 - 5000 µg/L Se as selenite and selenate, respectively.

$$c_{P.sh} = -2.0 \cdot 10^{-5} c_{SeO_3}^2 + 0.1013 c_{SeO_3} - 0.5859 \quad (6.1)$$

$$c_{P.sh} = -5.0 \cdot 10^{-6} c_{SeO_4}^2 + 0.147 c_{SeO_4} - 0.8039 \quad (6.2)$$

with

$c_{P.sh}$ as the mean Se shoot content [mg Se/kg DW]

c_{SeO_3} as the initial bioavailable solution selenite concentration [µg/L Se]

c_{SeO_4} as the initial bioavailable solution selenate concentration [µg/L Se]

Root-Se content was modelled as shown in Equations 6.3 and 6.4, which were fitted with an accuracy of $R^2 = 0.971$ and $R^2 = 0.9744$ with the addition of 0 - 5000 µg/L Se as selenite and selenate, respectively.

$$c_{P.r} = -2.0 \cdot 10^{-5} c_{SeO_3}^2 + 0.177 c_{SeO_3} + 5.3887 \quad (6.3)$$

$$c_{P.r} = -1.0 \cdot 10^{-6} c_{SeO_4}^2 + 0.0471 c_{SeO_4} + 0.0659 \quad (6.4)$$

with

$c_{P.r}$ as the mean Se root content [mg Se/kg DW]

c_{SeO_3} as the initial bioavailable solution selenite concentration [µg/L Se]

c_{SeO_4} as the initial bioavailable solution selenate concentration [µg/L Se]

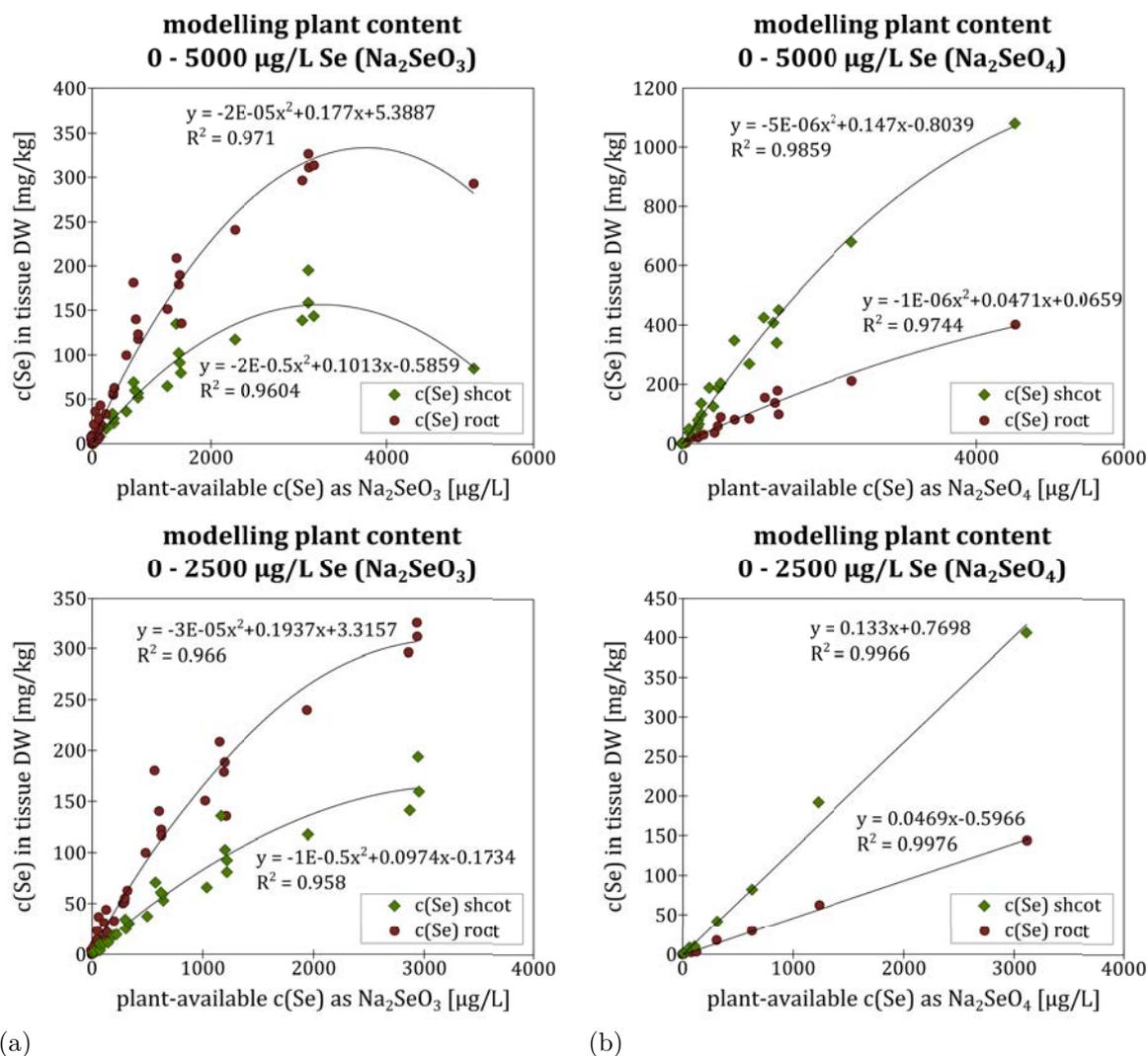


Figure 6.1.: *Excel fitting of experimental data on plant uptake in a range of 0 - 5000 $\mu\text{g/L}$ Se in the nutrient solution (top) with a polynomial and in a range of 0 - 2500 $\mu\text{g/L}$ Se in the nutrient solution (bottom) with a polynomial or straight line*
a: plant uptake of Se as Na_2SeO_3 into shoots and roots
b: plant uptake of Se as Na_2SeO_4 into shoots and roots

Mirroring the experimental results, the polynomial describing plant-Se due to selenite treatment shows a decrease in uptake at concentrations higher than 2500 $\mu\text{g/L}$ Se (Figure 6.1a). However, when fitting plant-Se content over the span of 0 - 2500 $\mu\text{g/L}$ Se rather than 0 - 5000 $\mu\text{g/L}$, thereby omitting this change of Se-uptake pattern, the accuracy of the fitting was not improved, neither for shoot-Se ($R^2 = 0.958$ vs. $R^2 = 0.9604$) nor for root-Se ($R^2 = 0.9660$ vs. $R^2 = 0.9710$).

Plant-Se uptake due to selenate treatment (Figure 6.1b) could be described by a straight line rather than a polynomial. Omitting data for the addition of 5000 $\mu\text{g/L}$ Se and using

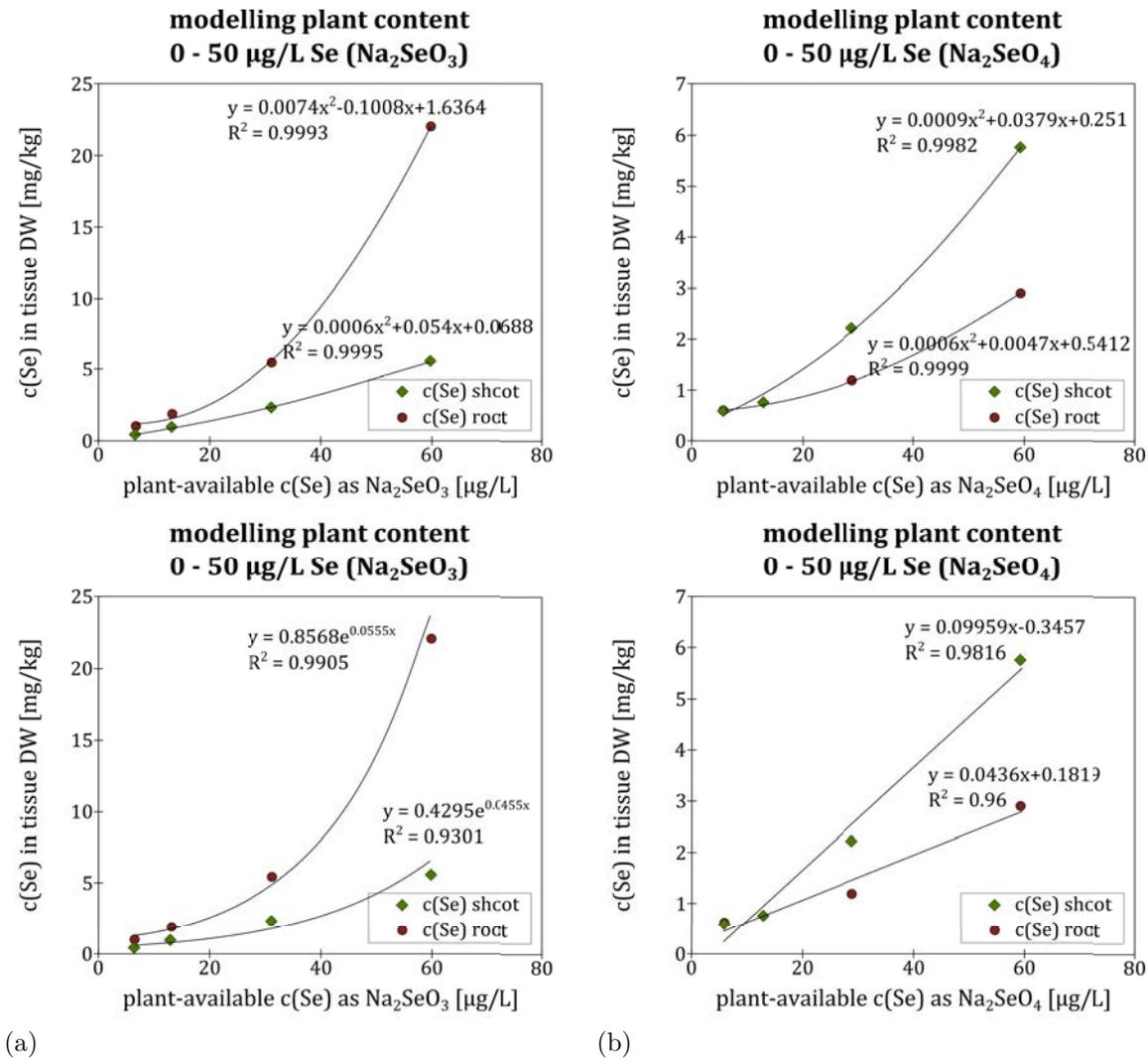


Figure 6.2.: Excel fitting of experimental data on plant uptake in a range of 0 - 50 $\mu\text{g/L}$ Se in the nutrient solution

a: plant uptake of Se as Na_2SeO_3 into shoots and roots fitted with a polynomial (top) or exponential curve (bottom)

b: plant uptake of Se as Na_2SeO_4 into shoots and roots fitted with a polynomial (top) or straight line (bottom)

only datasets of experiment C, both for shoot-Se ($R^2 = 0.9966$ vs. $R^2 = 0.9859$) and root-Se ($R^2 = 0.9976$ vs. $R^2 = 0.9744$) improved fitting. Equations 6.5 and 6.6 describe Se shoot content with an accuracy of $R^2 = 0.958$ and $R^2 = 0.9966$ with the addition of 0 - 2500 $\mu\text{g/L}$ Se as selenite and selenate, respectively.

$$c_{P.sh} = -1.0 \cdot 10^{-5} c_{\text{SeO}_3}^2 + 0.0974 c_{\text{SeO}_3} - 0.1734 \quad (6.5)$$

$$c_{P.sh} = 0.133c_{SeO_4} + 0.7698 \quad (6.6)$$

with

$c_{P.sh}$ as the mean Se shoot content [mg Se/kg DW]

c_{SeO_3} as the initial bioavailable solution selenite concentration [$\mu\text{g/L}$ Se]

c_{SeO_4} as the initial bioavailable solution selenate concentration [$\mu\text{g/L}$ Se]

Equations 6.7 and 6.8 describe Se root content with an accuracy of $R^2 = 0.966$ and $R^2 = 0.9976$ with the addition of 0 - 2500 $\mu\text{g/L}$ Se as selenite and selenate, respectively.

$$c_{P.r} = -3.0 \cdot 10^{-5}c_{SeO_3}^2 + 0.1937c_{SeO_3} + 3.3157 \quad (6.7)$$

$$c_{P.r} = 0.0469c_{SeO_4} - 0.5966 \quad (6.8)$$

with

$c_{P.r}$ as the mean Se root content [mg Se/kg DW]

c_{SeO_3} as the initial bioavailable solution selenite concentration [$\mu\text{g/L}$ Se]

c_{SeO_4} as the initial bioavailable solution selenate concentration [$\mu\text{g/L}$ Se]

Overall, fitting quality was limited most by scattering (1s error) of experimental data, which was discussed in Chapter 3.5.3.

Modelling of smaller ranges of Se treatment yielded better accuracy and worked best for polynomial functions of the 2nd degree. Addition of 0 - 50 $\mu\text{g/L}$ Se (Figure 6.2) was modelled with an accuracy of $R^2 = 0.9995$ and $R^2 = 0.9993$ in shoots and roots for selenite addition and with an accuracy of $R^2 = 0.9982$ and $R^2 = 0.9999$ in shoots and roots for selenate addition, respectively. Addition of 50 - 500 $\mu\text{g/L}$ (Figure 6.3) Se was modelled with an accuracy of $R^2 = 0.9999$ in shoots and roots for selenate and selenite addition, respectively. Addition of 500 - 5000 $\mu\text{g/L}$ Se (Figure 6.4) was modelled with an accuracy of

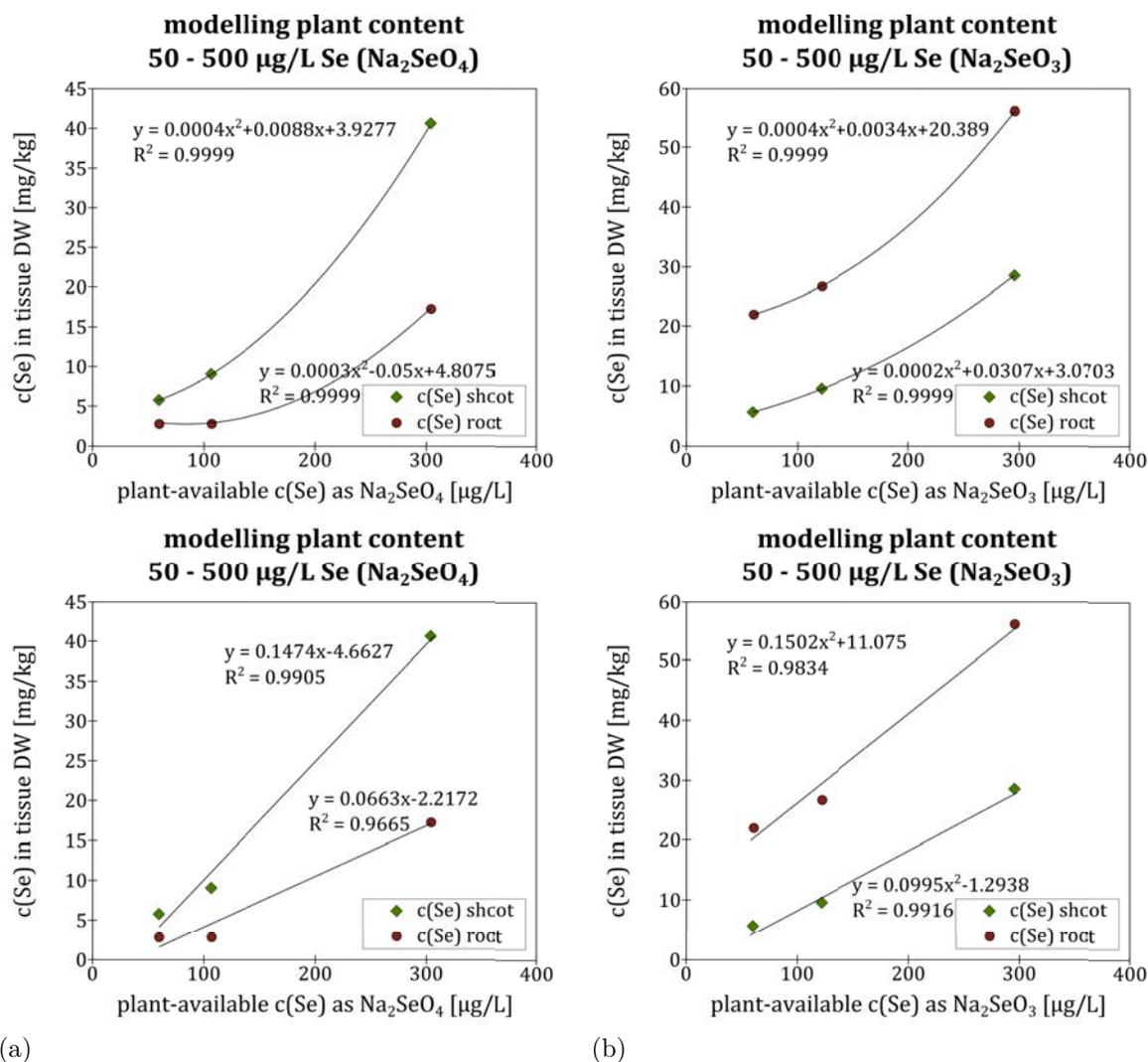


Figure 6.3.: *Excel fitting of experimental data on plant uptake in a range of 50 - 500 $\mu\text{g/L}$ Se in the nutrient solution*
a: plant uptake of Se as Na_2SeO_3 into shoots and roots fitted with a polynomial (top) or power function (bottom)
b: plant uptake of Se as Na_2SeO_4 into shoots and roots fitted with a polynomial (top) or straight line (bottom)

$R^2 = 0.9997$ and $R^2 = 0.9731$ in shoots and roots for selenite addition and with an accuracy of $R^2 = 0.9984$ and $R^2 = 0.9992$ in shoots and roots for selenate addition, respectively.

While plant-Se in shoots and roots resulting from the addition of Se as selenite was alternatively modelled using an exponential fitting (0 - 50 $\mu\text{g/L}$ Se, Figure 6.2), a squared function (50 - 500 $\mu\text{g/L}$ Se, Figure 6.3) and a logarithmic function (500 - 5000 $\mu\text{g/L}$ Se, Figure 6.4), the resulting plant-Se in shoot and root after addition of Se in the form of selenate was alternatively fitted linearly for each concentration range. However, in general,

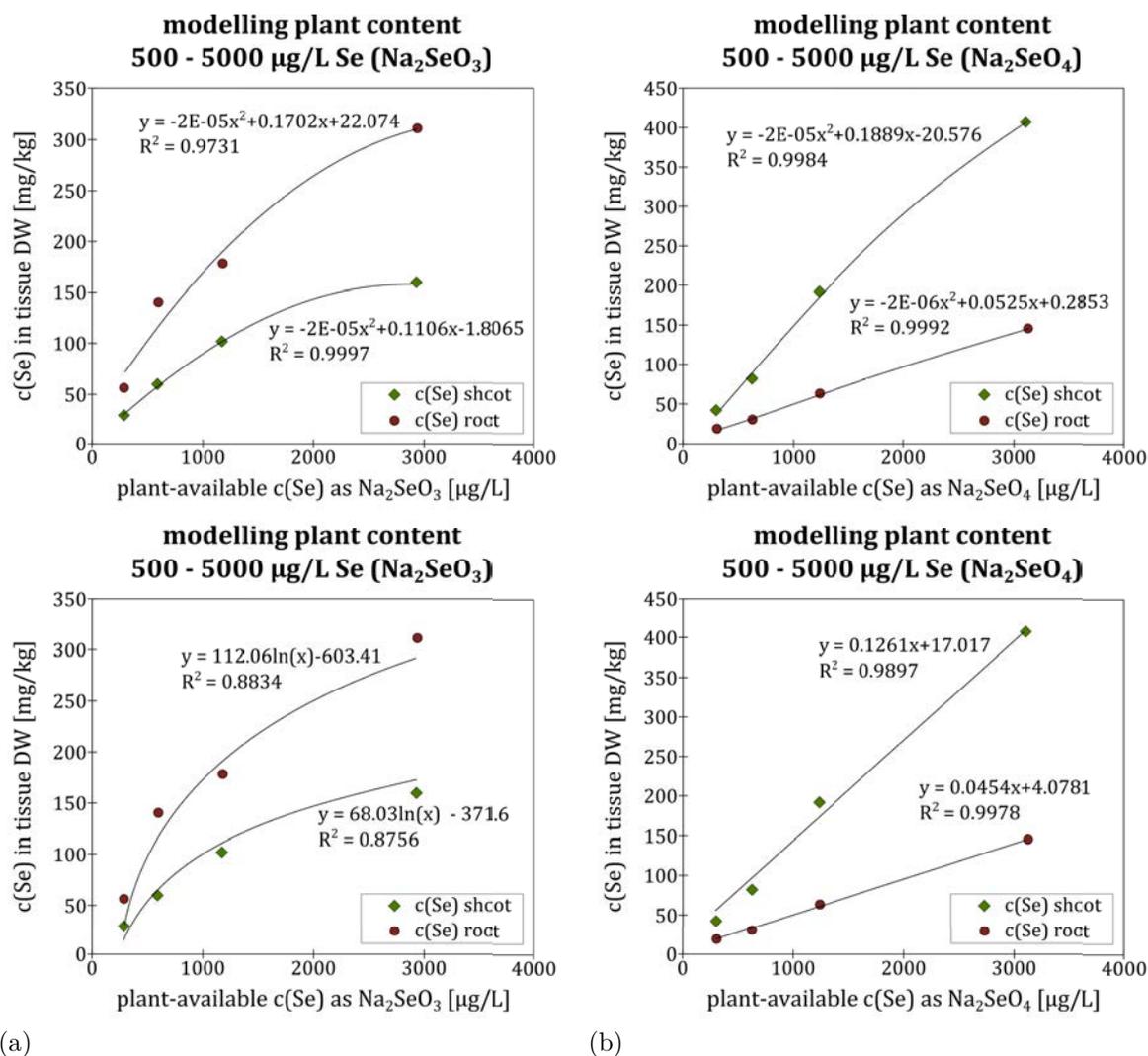


Figure 6.4.: *Excel fitting of experimental data on plant uptake in a range of 500 - 5000 µg/L Se in the nutrient solution*
 a: *plant uptake of Se as Na_2SeO_3 into shoots and roots fitted with a polynomial (top) or logarithmic function (bottom)*
 b: *plant uptake of Se as Na_2SeO_4 into shoots and roots fitted with a polynomial (top) or straight line (bottom)*

polynomial fitting of the 2nd degree provided the best accuracy. In the overall model, a mean of the fittings for plant-Se in ranges of Se addition of 0 - 5000 µg/L Se and 0 - 2500 µg/L Se was primarily used. However, results for all fittings of the smaller Se ranges are given as well for purposes of comparison.

Fitting the mean XANES results for Se speciation after Se uptake resulted in a much lower accuracy than plant-Se content modelling. As shown in Figure 6.5, a logarithmic fitting showed greater accuracy than linear fittings; organic Se in shoots was fitted with an accuracy

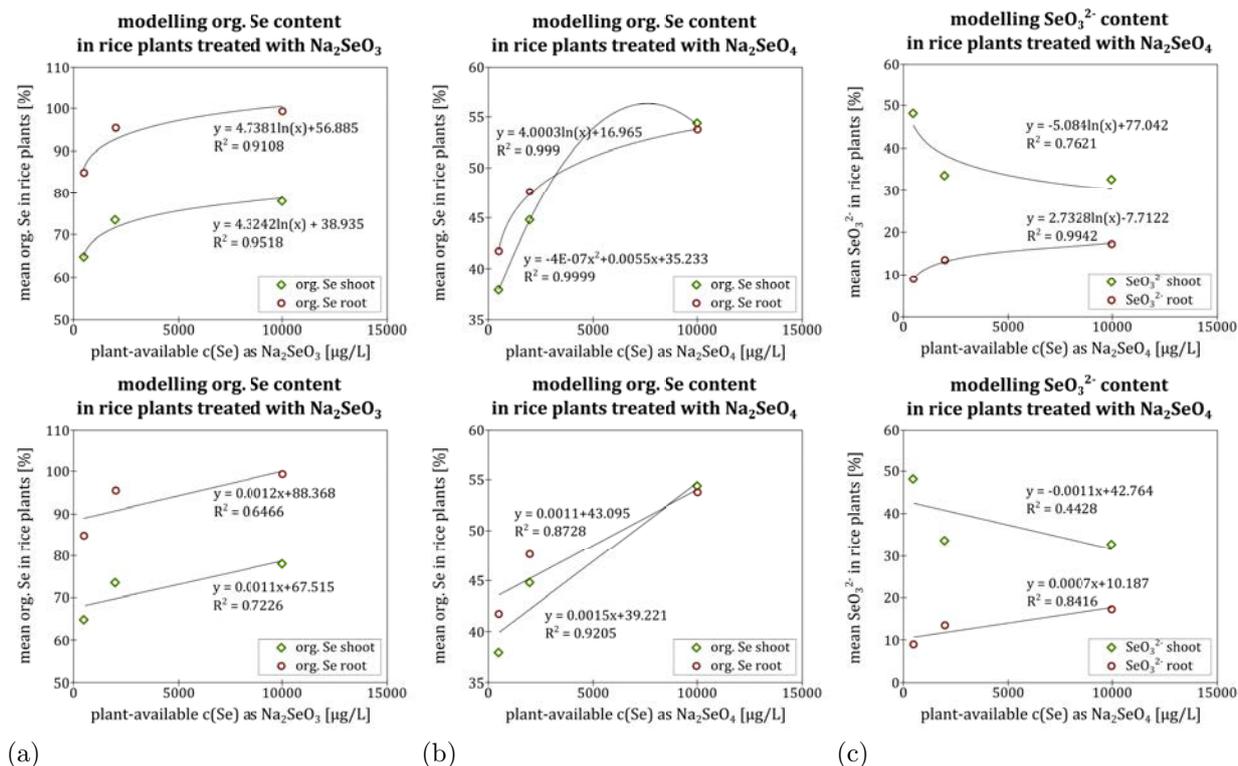


Figure 6.5.: *Excel fitting of plant tissue speciation according to XANES data with plant uptake for nutrient solution concentrations of 500, 2000 and 10,000 µg/L Se*
 a: mean percentage of organic Se in shoots and roots when Se is added as Na_2SeO_3 fitted with logarithmic function (top) or straight line (bottom)
 b: mean percentage of organic Se in shoots and roots when Se is added as Na_2SeO_4 fitted with logarithmic function (top) or straight line (bottom)
 c: mean percentage of selenite in shoots and roots when Se is added as Na_2SeO_4 fitted with logarithmic function (top) or straight line (bottom)

of $R^2 = 0.9518$ and $R^2 = 0.9999$ with the addition of selenite and selenate, respectively, while organic Se in roots was fitted with an accuracy of $R^2 = 0.9108$ and $R^2 = 0.9990$ for the addition of selenite and selenate, respectively, As shown in Figure 6.5b, polynomial fitting for organic Se in shoots of rice plants treated with selenate demonstrated the best fitting. For all other data sets, the 3rd degree polynomial fitting - although exhibiting the highest accuracy in describing the three data points - resulted in a curve progression highly unlikely to represent speciation and was, therefore, discarded. With XANES data sets providing speciation information in the plant tissue only for 500, 2000 and 10,000 µg/L Se, however, any attempted extrapolation of this information on speciation in plant tissue for lower Se concentrations, therefore, has an unquantifiable error.

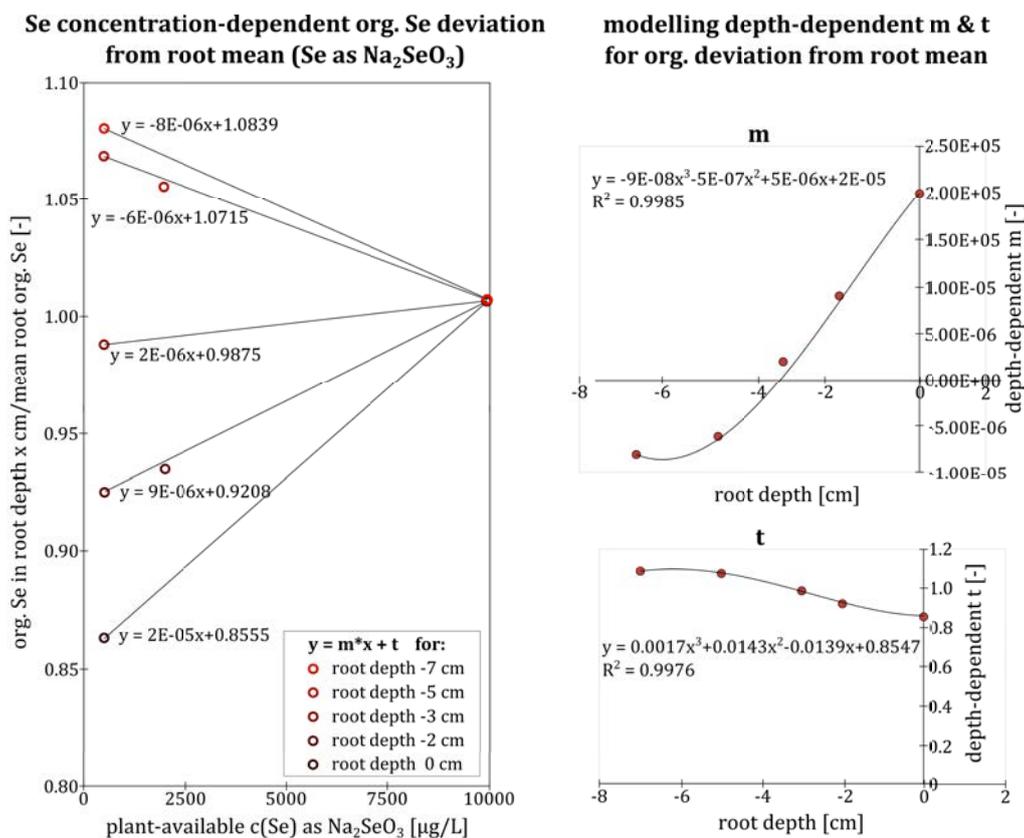


Figure 6.6.: *Root speciation modelling for additions of Se as Na_2SeO_3 ; left: fitting of the deviation of local organic Se content compared to the root mean organic Se content for 5 root depths as measured for 500 and 10,000 $\mu\text{g/L}$ Se added as selenite. right: root depth-correlated fitting of parameters (m , t) describing the organic Se speciation pattern of all local deviations from root mean*

As shown in Figure 6.6, the pattern for localized root speciation along the length of the root when the plant was treated with selenite was fitted linearly with 2 - 3 data points per Se concentration. Parameters of depth dependence for this linear concentration-dependent fitting had a high accuracy for both m ($R^2 = 0.9985$) and t ($R^2 = 0.9976$). For the model of the organic percentage of depth-dependent root-Se, parameters m and t were substituted by these fittings, making distribution of organic Se - and, therefore, the distribution of selenite as well - dependent on three parameters: Selenium concentration in the solution, the previously calculated mean root organic Se (which is dependent only on the Se concentration in the solution), and the local root depth below the surface.

The resulting modelled functions (Equations 6.9, 6.10, 6.11, 6.12) for the percentage of organic Se in any root depth between 0 and -7 cm below the surface for a known selenite

concentration in the nutrient solution were therefore:

$$p_{org.Se_r} = P_{\bar{x}_{Se_r}} \cdot (m \cdot c_{SeO_3} + t) \quad (6.9)$$

and

$$P_{\bar{x}_{Se_r}} = \frac{(4.7381 \ln c_{SeO_3} + 56.885) + ((0.0012c_{SeO_3} + 88.368))}{2} \quad (6.10)$$

and

$$m = -9.0 \cdot 10^{-7} d_r^3 - 5.0 \cdot 10^{-7} d_r^2 + 5.0 \cdot 10^{-5} d_r + 2.0 \cdot 10^{-4} \quad (6.11)$$

and

$$t = 0.0017d_r^3 + 0.0143d_r^2 - 0.0139d_r + 0.83357 \quad (6.12)$$

with

- $p_{org.Se_r}$ as the local percentage of organic Se in the root [%]
- $P_{\bar{x}_{Se_r}}$ as the mean percentage of organic Se in the root [%]
- c_{SeO_3} as the initial bioavailable solution selenite concentration [$\mu\text{g/L Se}$]
- d_r as the root depth below the surface [cm]

The local percentage of organic Se in the root when Se is added as selenate was calculated, fitted and modelled in similar fashion. However, Se concentration dependence was fitted with the greatest accuracy when using a power function (Figure 6.7). Resulting function parameters needed to model depth-dependence, were, therefore, m_1 , m_2 and t .

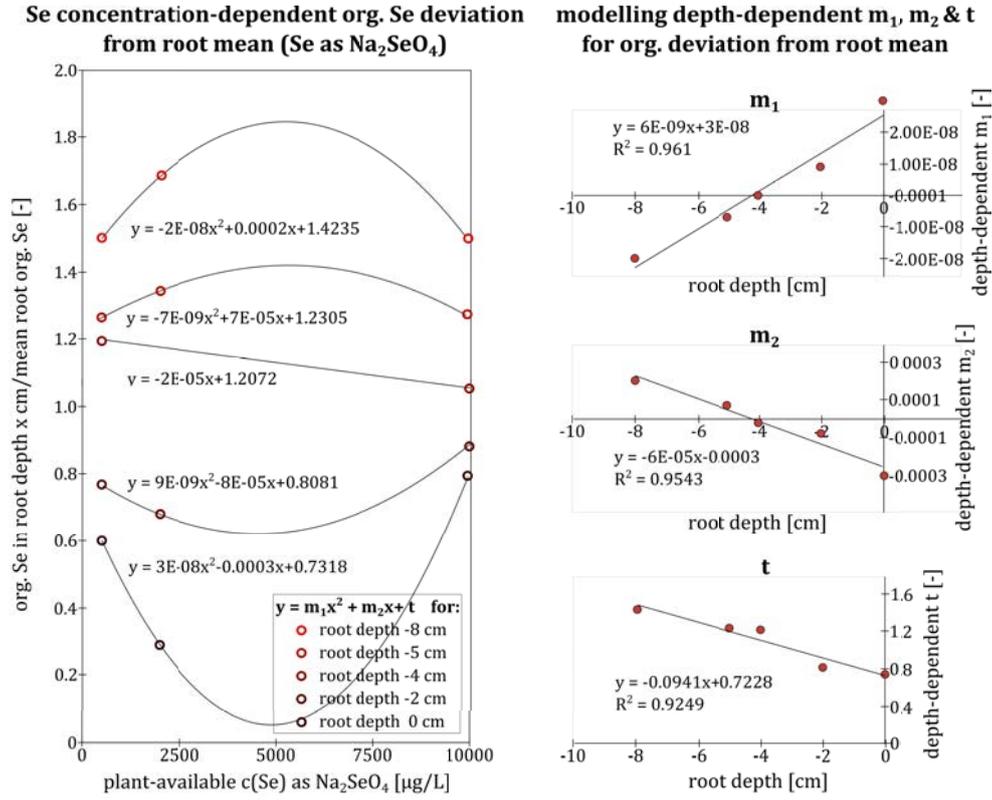


Figure 6.7.: *Root speciation modelling for additions of Se as Na₂SeO₄; left: fitting of the deviation of local organic Se content compared to the root mean organic Se content for 5 root depths as measured for 500, 2000 and 10,000 µg/L Se added as selenate. right: root depth-correlated fitting of parameters (m, t) describing the organic Se speciation pattern of all local deviations from root mean*

These were fitted with linear functions yielding accuracy measures of $R^2 = 0.9610$, 0.9543 and 0.9249 for m_1 , m_2 and t , respectively. Equations 6.13, 6.19, 6.15, 6.16 and 6.17 describe the local organic Se distribution in the root with the addition of selenate.

$$p_{org.Se_r} = P_{\bar{x}_{Se_r}} \cdot (m_1 c_{SeO_4}^2 + m_2 c_{SeO_4} + t) \quad (6.13)$$

and

$$P_{\bar{x}_{Se_r}} = \frac{(4.0003 \ln c_{SeO_4} + 16.965) + (0.0011 c_{SeO_4} + 43.095)}{2} \quad (6.14)$$

and

$$m_1 = 6.0 \cdot 10^{-8} d_r + 3.0 \cdot 10^{-7} \quad (6.15)$$

and

$$m_2 = -6.0 \cdot 10^{-4}d_r + 3.0 \cdot 10^{-3} \quad (6.16)$$

and

$$t = -0.0941d_r + 0.7228 \quad (6.17)$$

with

- $p_{org.Se_r}$ as the local percentage of organic Se in the root [%]
- $P_{\bar{x}_{Se_r}}$ as the mean percentage of organic Se in the root [%]
- c_{SeO_4} as the initial bioavailable solution selenate concentration [$\mu\text{g/L Se}$]
- d_r as the root depth below the surface [cm]

This fitting approach was also applied to the local percentage of selenite in the root when Se was added as selenate. This needed to be calculated separately, as well, because selenate treatment yielded three species in the root, rather than two, as for selenite treatment. As previously found with organic Se, Se concentration dependence was fitted with the greatest accuracy when using a power function (Figure 6.8) and the resulting function parameters needed to model depth-dependence were m_1 , m_2 and t .

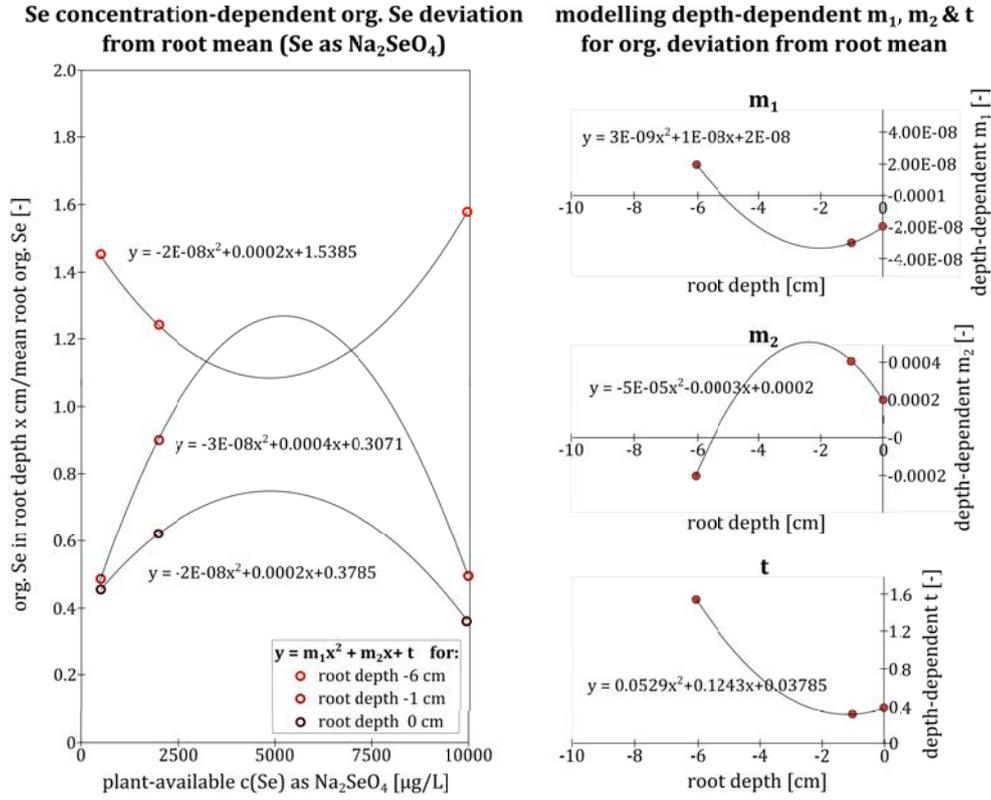


Figure 6.8.: *Root speciation modelling for additions of Se as Na_2SeO_4 ; left: fitting of the deviation of local selenite content compared to the root mean selenite content for 5 root depths as measured for 500, 2000 and 10,000 $\mu\text{g/L}$ Se added as selenite. right: root depth-correlated fitting of parameters (m , t) describing the selenite speciation pattern of all local deviations from root mean*

However, these could not be fitted with linear functions and were also described by power functions instead. Equations 6.13, 6.19, 6.15, 6.16 and 6.17 describe the local organic Se distribution in the root with the addition of selenate.

$$p_{\text{SeO}_3r} = P_{\bar{x}_{\text{Se}_r}} \cdot (m_1 c_{\text{SeO}_4}^2 + m_2 c_{\text{SeO}_3} + t) \quad (6.18)$$

and

$$P_{\bar{x}_{\text{Se}_r}} = \frac{(2.7328 \ln c_{\text{SeO}_4} - 7.7122) + (0.0007 c_{\text{SeO}_4} + 10.187)}{2} \quad (6.19)$$

and

$$m_1 = 3.0 \cdot 10^{-8} d_r^2 + 1.0 \cdot 10^{-7} d_r - 2.0 \cdot 10^{-7} \quad (6.20)$$

and

$$m_2 = -5.0 \cdot 10^{-4}d_r^2 - 3.0 \cdot 10^{-3}d_r - 2.0 \cdot 10^{-3} \quad (6.21)$$

and

$$t = 0.0529d_r^2 + 0.1243d_r + 0.3785 \quad (6.22)$$

with

- p_{SeO_3r} as the local percentage of selenite in the root [%]
- $P_{\bar{x}_{Se_r}}$ as the mean percentage of organic Se in the root [%]
- c_{SeO_4} as the initial bioavailable solution selenate concentration [$\mu\text{g/L Se}$]
- d_r as the root depth below the surface [cm]

6.1.3. Model output

With the input of the Se concentration in solution either as selenite or as selenate between 0 and 5000 $\mu\text{g/L}$, the model provides results on Se content and speciation distribution in shoots and in roots. Furthermore, the model predicts the depth profile of speciation in the roots. Figure 6.9 exemplifies model output for 35 $\mu\text{g/L Se}$ in the nutrient solution, which is a concentration not covered by the experiments. Model output values for Se content and speciation in shoots and roots were designed to be valid for input Se concentration between 0 and 5000 $\mu\text{g/L Se}$. However, input of low Se concentrations and very high concentrations are less reliable; Se content modelling with the addition of Se as selenite, for example, yields negative results for shoot-Se below an input of 6 $\mu\text{g/L Se}$ when using a mean result of Equations 6.1 and 6.5. This is not the case for the more precise modelling limited to the range of 0 - 50 $\mu\text{g/L Se}$; however, the model by default uses the overall fitting for the large concentration range.

Since this mean shoot-Se result is then used for the calculation of shoot speciation, this results in unrealistic speciation distribution and, therefore, mean-Se input needs to be adjusted to using the model more suitable for lower concentrations (Figure 6.2). Because it is so difficult to model plant-Se for the entire Se concentration range and subdivisions can be

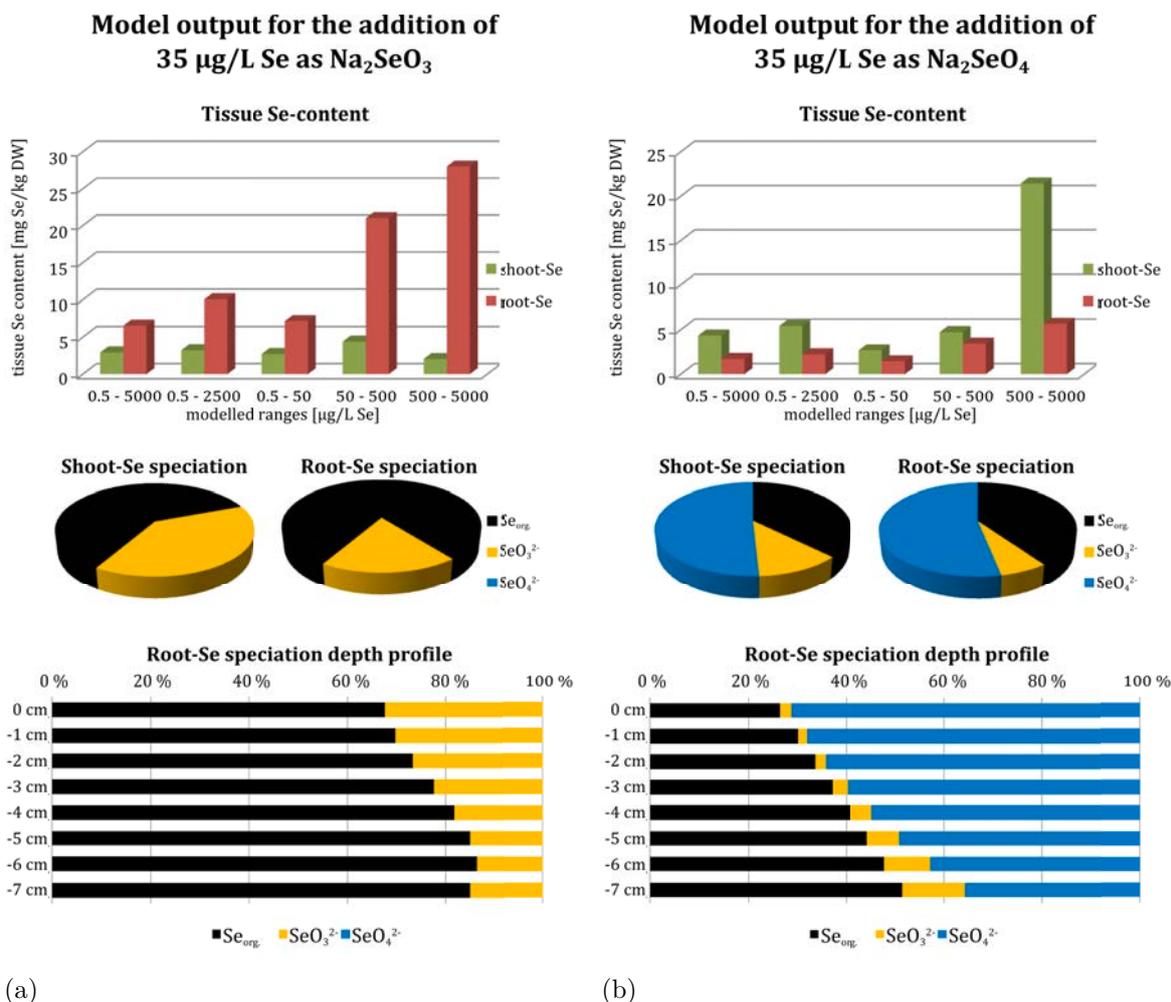


Figure 6.9.: Model output for plant Se-content and speciation
 a: for the addition of 35 µg/L Se as selenite
 b: for the addition of 35 µg/L Se as selenate

modelled with very different functions, this suggests a Se concentration-dependent change in plant Se uptake. Fitting results suggest that low Se concentrations (up to 50 µg/L Se) are taken up readily and can therefore be fitted nearly exponentially, while concentrations greater 50 µg/L can be modelled linearly with a smaller slope and concentrations greater than 1000 µg/L Se as selenite show a logarithmically describable tendency to approach an uptake maximum. Selenate concentrations between 1000 and 5000 µg/L, however, can still be described with a linear function, suggesting a load maximum at higher concentrations than the ones modelled here.

Model coherency, expressed as the standard deviation of two function results describing the same process for any given value, varies significantly across species and plant tissue;

results for Se content using the models for the ranges 0 - 5000 and 0 - 2500 $\mu\text{g/L}$ Se (Equations 6.2 - 6.8) are modelled with a standard deviation of 10 % or lower for selenite concentrations of 27 - 1450 $\mu\text{g/L}$ Se for shoots and 220 - 3300 $\mu\text{g/L}$ Se for roots and selenate concentrations of 45 - 5000 $\mu\text{g/L}$ Se for shoots and 68 - 5000 $\mu\text{g/L}$ Se for roots. If a standard deviation of 33 % or lower is sufficient, model results can be used for inputs of selenite concentrations of 12 - 3000 $\mu\text{g/L}$ Se for shoots and 30 - 4800 $\mu\text{g/L}$ Se for roots and selenate concentrations of 20 - 5000 $\mu\text{g/L}$ Se for shoots and 17 - 5000 $\mu\text{g/L}$ Se for roots.

Within these concentration ranges, modelled mean speciation appears plausible as well. Unfortunately, speciation was not experimentally obtained for low Se concentrations and error below 500 $\mu\text{g/L}$ Se input Se concentration is not quantifiable. This means that speciation modelling on this sparse data basis is highly speculative, unlike the Se content in the plant, which is backed by a larger amount of experimental data. Nonetheless, this sort of modelling can provide estimations for comparison that might be helpful for future research. Although fitting results were best with logarithmic approaches (Figure 6.5), the progression of logarithmic fitting toward lower Se concentrations was considered unrealistic, as this would lead to near-zero percentages of organic Se compared to near-100 of selenite due to low Se in the solution. Therefore, mean results of linear and logarithmic fittings were considered more realistic, but cannot be verified.

As the error of modelling mean-Se is incalculable, modelling localized depth-dependent speciation in the root, which is dependent on this mean value, provides seemingly realistic results with an uncalculable error. However, results of negative speciation are not realistic. Therefore, input Se concentrations yielding negative speciation for either organic Se or selenite are considered to be outside of the range of valid Se concentration input. Localized root speciation profiles for depths of -1 cm to -7 cm are available with this model only for inputs of 12 - 2500 $\mu\text{g/L}$ Se as selenite and 20 - 1350 $\mu\text{g/L}$ Se as selenate.

6.2. Selenium transfer between soil minerals and soil solution

For this part of the model, adsorption data from Exp. C (Chapter 6.5c) were primarily used. Unfortunately, data from Exp. B1 - B3 (Chapter 4.4.2, b2, b3) could not be used for this model, as influences of nutrient components did not add up linearly and data on the competing oxy-anions were insufficient to plot ion-concentration dependencies. Furthermore, goethite could not be used for the model, since it did not reach its loading capacity in the experiments performed and maximum sorption remained unknown for this study. Therefore, no mixtures of kaolinite and goethite could be modelled, since it remained unknown how small amounts of goethite would need to be in order to show kaolinite contribution to sorption in the case of selenite. The following assumptions resulting from Exp. C (Chapter 6.5c), were made for the model:

- as shown in Exp. B1 and Exp. B3, kaolinite adsorption produced an isotherm shape, even if this was not evident from the pure data of Exp. C
- therefore, the general mathematical formula of all Se adsorption isotherms of kaolinite should be the same with only factors and constants changing, depending on experimental parameters
- selenite and selenate adsorption are modelled separately, but with the same general mathematical formula
- lower kaolinite amounts show a linear decrease of sorption capacity

6.2.1. Data input

Model input for adsorption was derived solely from data of Exp. C (Chapter 6.5c), as data of experiments performed in Exp. B1 - B3 were not conducted in a nutrient solution. However, general information on isotherm shape observed in Exp. B1 and B3 for different sorption influences determined the choice of fitting function. In addition to fitting with pre-setted

trend line options of Excel (Microsoft, version 14.0.7147.5001) and respective outputs of R^2 , the fitting of a Freundlich isotherm (Equation 4.4) was compared as well. Functions describing the adsorption were by default fitted to cross the y-axis at $y = 0$. As previously discussed, neither ion competition, nor goethite adsorption were integrated into the model.

6.2.2. Fitting results

As shown in Figure 6.10, from a mathematical point of view, the Freundlich isotherm described the experimental data adequately with $R^2 = 0.9907$ and 0.9801 for selenite and selenate treatment, respectively. Regardless of R^2 values, however, kaolinite was shown to have limited adsorption capacity for the Se concentrations used in Exp. B1 and B3 (Chapter 4.5.2). Therefore, the modelled Freundlich isotherms, which did not reflect this, were discarded for both selenite and selenate adsorption onto kaolinite.

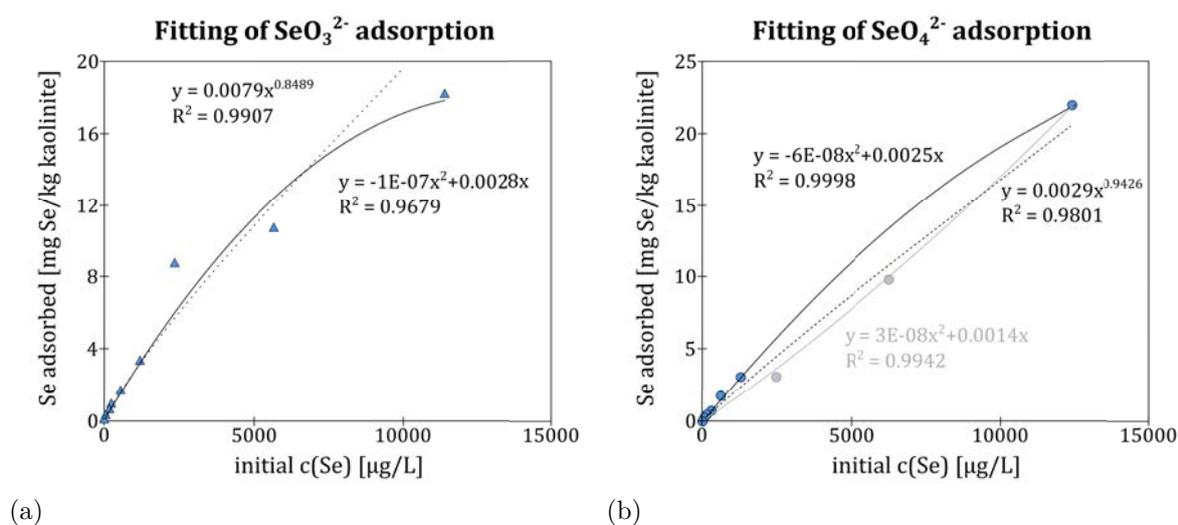


Figure 6.10.: *Fitting of Freundlich isotherms with exponential arguments (dotted line) and polynomial to model Se adsorption onto kaolinite using isotherm-conform data (solid line) or using all data points (light grey solid line)*
a: adsorption of selenite
b: adsorption of selenate

Instead, adsorption of Se onto kaolinite was fitted with a polynomial of the 2nd degree, which more closely resembled the isotherm shape observed in general for kaolinite adsorption, although R^2 was only 0.9679 and 0.8735 for adsorption of selenite and selenate, respectively. Furthermore, two data points of the selenate adsorption experiment (Figure

6.10b) were discarded as outliers as well, as the polynomial calculated in their presence did not resemble an isotherm shape. Moreover, all other data points correlated very well with an isotherm shape approaching load maximum and the polynomial describing it ($R^2 = 0.9998$). Adsorption of Se was therefore modelled using Equation 6.23 for selenite and Equation 6.24 for selenate.

$$c_{sorpSeO_3} = -1.0 \cdot 10^{-7} c_{SeO_3}^2 + 0.0028 c_{SeO_3} \quad (6.23)$$

$$c_{sorpSeO_4} = -6.0 \cdot 10^{-8} c_{SeO_4}^2 + 0.0025 c_{SeO_4} \quad (6.24)$$

with

$c_{sorpSeO_3}$	as the selenite concentration load on kaolinite [mg Se/kg kaolinite]
c_{SeO_3}	as the initial bioavailable solution selenite concentration [$\mu\text{g/L}$ Se]
$c_{sorpSeO_4}$	as the selenate concentration load on kaolinite [mg Se/kg kaolinite]
c_{SeO_4}	as the initial bioavailable solution selenate concentration [$\mu\text{g/L}$ Se]

6.2.3. Model output and mathematical extrapolations

As long as adsorption of selenite and selenate is modelled by their respective isotherms dependent only on the added Se concentration, the sorption model output is described precisely by those functions. However, optional mathematically estimated parameters were included as well, as described in the following. Since these were not verified in experiments, their errors cannot be determined.

For crude estimations, the amount of kaolinite can be varied as the percentage of the experimental conditions (100 % being the 8.5 g used in the experiment with the solution unchanged at 170 mL). Although helpful for estimations, a simple percentage or factor cannot take kinetic processes into account, such as longer diffusion pathways for fewer molecules. This means that error increases, the less experimentally evaluated the kaolinite

amount is. Since ion competition in Exp. B2 showed the isotherm shape to remain stable for a great number of adsorption-lowering processes, values for $> 25\%$ of the experimental kaolinite amount are considered reasonably reliable. A similar problem is encountered at values $> 100\%$ of the kaolinite amount used in the experiment. This is especially difficult because the maximum load capacity is unknown. Maximum load capacity calculated from sorption modelling showed a maximum Se adsorption for 14,500 $\mu\text{g/L}$ Se as selenite and 21,000 $\mu\text{g/L}$ Se as selenate. Although this is 3 and 4 times the amount considered to be a valid input for the model, inhibitory kinetic processes such as diffusion competition are not included and the load capacity is only extrapolated. Therefore, input values for kaolinite amounts should not exceed 150% for the model to be considered reasonably reliable.

A second mathematically implemented parameter is that of competition between selenite and selenate. Without this implementation, adsorption of selenite and selenate were modelled separately and their combined effect was described by adding their sorption. This is reasonable as long as one of both ions is dominant in its concentration or concentrations of both ions are low. It is unreasonable, however, to expect high concentrations of each species to be adsorbed as though the other were not present, especially since kaolinite has a limited adsorption capacity and both ions adsorb at the same binding sites, albeit in a different manner (Figure 4.6).

$$c_{X\text{sorpSeO}_3} = c_{\text{sorpSeO}_3} - \left(\frac{c_{\text{SeO}_4}}{c_{\text{SeO}_4} + c_{\text{SeO}_3}} \cdot c_{\text{sorpSeO}_3} \frac{c_{\text{sorpSeO}_4}}{c_{\text{MAXsorpSeO}_4}} \right) \quad (6.25)$$

with

$c_{X\text{sorpSeO}_3}$	as selenite sorption with selenate competition [mg Se/kg kaolinite]
c_{sorpSeO_3}	as selenite sorption without selenate competition [mg Se/kg kaolinite]
c_{sorpSeO_4}	as selenate sorption without selenite competition [mg Se/kg kaolinite]
c_{SeO_3}	as the initial bioavailable solution selenite concentration [$\mu\text{g/L}$ Se]
c_{SeO_4}	as the initial bioavailable solution selenate concentration [$\mu\text{g/L}$ Se]
$c_{\text{MAXsorpSeO}_4}$	as the maximum selenate sorption load [mg Se/kg kaolinite]

Therefore (Equation 6.25), adsorption amounts in competition between both ions were calculated as the pure anion adsorption, from which the proportion of the percentage of the competing ion of its respective maximum load was subtracted proportional to its concentration and vice versa.

6.3. Mass balance model

Using the modelled compartments "mineral surface", "nutrient solution" and "plant", a mass balance model was created (Equation 6.26). The model assumed 100 % of the Se to be distributed into these three compartments and resulting Se content of those three compartments was given either as a percentage of total Se in the system or in μg as absolute Se amounts. To keep the model simple, the only input parameters required were the concentrations of selenite and selenate in the initial solution. Model calculations started with Se adsorption onto the mineral surface (Equation 6.27) in the presence of both competing ions (Equation 6.25). The adsorbed Se amount was then subtracted from the Se in the initial solution (Equation 6.29). The resulting solution Se concentration was then used as the initial solution for subsequent Se-uptake into plant roots and shoots (Equation 6.28). This amount of Se is then subtracted from the solution, yielding the final Se concentration in the solution in the mass balance (Equation 6.29).

$$m_{totalSe} = m_{Se_{sorp}} + m_{Se_{plant}} + m_{Se_{sol}} \quad (6.26)$$

and

$$m_{Se_{sorp}} = ((c_{SeO_3} + c_{SeO_4}) - ((c_{SeO_3} - \frac{m_K \cdot c_{X_{sorp}SeO_3}}{V_{exp}}) + (c_{SeO_4} - \frac{m_K \cdot c_{X_{sorp}SeO_4}}{V_{exp}}))) \cdot V_{exp} \quad (6.27)$$

and

$$m_{Se_{plant}} = \frac{N_{PB} \left(\frac{m_{sh}}{V_{exp}} \cdot c_{P.sh} + \frac{m_r}{V_{exp}} \cdot c_{P.r} \right) (c_{SeO_3} + c_{SeO_4})}{\left(c_{SeO_3} - \frac{m_K}{V_{exp}} \cdot c_{X_{sorpSeO_3}} \right) + \left(c_{SeO_4} - \frac{m_K}{V_{exp}} \cdot c_{X_{sorpSeO_4}} \right)} \cdot V_{exp} \quad (6.28)$$

and

$$m_{Se_{sol}} = m_{totalSe} - (m_{Se_{sorp}} + m_{Se_{plant}}) \quad (6.29)$$

with

$m_{totalSe}$	as the total Se amount in the modelled system [μg]
$m_{Se_{sorp}}$	as the Se amount adsorbed to kaolinite [μg]
$m_{Se_{plant}}$	as the Se amount taken up into the plant [μg]
$m_{Se_{sol}}$	as the Se amount remaining in solution [μg]
c_{SeO_3}	as the initial solution selenite concentration [$\mu\text{g/L Se}$]
c_{SeO_4}	as the initial solution selenate concentration [$\mu\text{g/L Se}$]
$c_{X_{sorpSeO_3}}$	as selenite sorption with selenate competition [mg/kg]
$c_{X_{sorpSeO_4}}$	as selenate sorption with selenate competition [mg/kg]
m_K	as the substrate amount in experiment [= 8.5 g]
V_{exp}	as the nutrient solution volume in experiment [= 0.17 L]
N_{PB}	as the mean number of plants per box [= 7.5]
$c_{P.sh}$	as the mean Se shoot content [mg Se/kg DW]
$c_{P.r}$	as the mean Se root content [mg Se/kg DW]
m_{sh}	as the mean shoot mass [= 0.01121582 g]
m_r	as the mean root mass [= 0.00621504 g]

6.4. Requirements for model extensions

This model offers a number of possibilities for extension. Criteria which must be met for this to be possible depend on the kind of extension proposed; six of which will be explored here:

1. volatilization of Se by rice plants can be added to the model using experimental measurements of rice seedlings in a comparable setting: similar growth stage, closed-

box system, constant air volume and similar concentration range of Se uptake; the presence of substrate is not required; however, nutrient concentrations comparable to the nutrient solution are

2. change in uptake behavior due to a lack of nutrients can be integrated; however, this must be coupled with adsorption studies of those same ions
3. different plant species can be integrated as well if growth stage permits cultivation in closed plant-box systems; nutrient uptake must be monitored hereby as well
4. goethite or other sorption substrates can be added if solution volume-to-substrate mass ratios are similar to those used in experiments and maximum load capacity is known or can be modelled; plants are not necessarily required to be part of the experimental set-up
5. ion competition can be integrated into the model when measuring the influence on Se adsorption of multiple concentrations of multiple ions for a span of Se concentrations at a solution volume-to-substrate mass ratio comparable to the experiments carried out in this study; in this case, detailed studies in the presence and absence of rice plants are required as well, as nutrient uptake and competition affect Se uptake
6. likewise, pH influences can be measured as well; in this case, detailed studies both in the presence and absence of rice plants are required, as nutrient uptake and competition affect Se uptake

6.5. Evaluation and application of the mass-balance model

The model presented in this study can serve several purposes. For one, it can simply be used to interpolate results between the experimentally determined results, i.e. plant uptake calculations for 600 $\mu\text{g/L}$ Se instead of the measured increments of 500 and 1000 $\mu\text{g/L}$ Se or adsorption of 1800 $\mu\text{g/L}$ Se onto kaolinite rather than the increments of 1000 and 2000

$\mu\text{g/L}$ Se. Together with speciation information provided by the model, potential toxicity to livestock when used in fodder can be estimated, as well as the return of Se into the soil, if plants are not removed. Using data from a study on Se speciation in rice grain compared to the rest of speciation in rice [Sun et al., 2010], this model can be used to estimate grain Se content as well. The fact that different functions were required to fit the plant-Se data depending on the added Se concentration, is indicative of regulatory mechanisms of Se uptake in the plant. Even if the model cannot provide mechanistic understanding in this case, estimates for Se concentration ranges of interest can be obtained by applying the model.

While all these applications are useful, however, this model also attempted to interpolate results not obtained by the experiments, such as solutions containing a mixture of Se species or varied amounts of kaolinite. The difficulty of using such purely empirical mathematical extrapolations is that the error is uncalculable and model output must first be verified by experimental results. Therefore, this model still requires a number of validation experiments. The mean Se speciation in plant tissue needs to be verified for small Se concentrations. Moreover, more detailed data are needed to improve upon the localized root speciation.

Additional extensions to the model that can improve upon its significance would be further substrates that are frequently encountered in soils, such as iron oxides and hydroxides, other clay minerals and calcite at varying pH-values and competing nutrient anions. If experimental data was acquired with the same parameters, mixtures of minerals can be modelled to simulate a large variety of soils. An interesting further step would be to integrate organic matter as well. With the exception of microorganisms, this would constitute a complete synthetic soil. Furthermore, a greater variety of plant models would prove useful in detailed uptake modelling. Not only could additional agronomically important plants, such as wheat or corn be investigated, but also, if the experiments were to be extended over a longer time period, the fruit-bearing stage would provide insight into Se cycling throughout the entire crop cycle.

To extend the model into another compartment of the Critical Zone, trapping experiments for volatile Se species should be conducted as well. Current experiments did not

focus on this aspect, as the method of volatile Se trapping was not established, yet. Therefore, the current model works under the assumption that Se not accounted for in plants or by adsorption must have remained in the solution. As previous publications have shown, however, rice is known to produce volatile Se species [Terry et al., 2000], for example, 50 - 80 % of Se added as SeMet can be volatilized. Rates indicate that selenite and selenate volatilization are lower by a factor of 40 and 20, respectively [Zayed et al., 1998].

This model provides a basis for investigations of Se transfer in the Critical Zone and can be used with a limited amount of data input. Therefore, it provides a quick overview of expected Se concentrations in kaolinite-dominated soil, solution and rice plants and is, therefore, a practical tool for first-stage assessments of Se inventory.

7. Conclusions

The objective of this study was to quantify and characterize Se transfer pathways and processes as part of the Se cycle within the Critical Zone. The strength of this integrated approach was to connect all findings by using the same experimental parameters for all aspects of this study in order to create an empirical process model of the Se biogeochemistry in the Critical Zone. This included, in particular, the substrate-to-solution ratio of sorption experiments and plant experiments as well as the ionic strength, pH-value and chemical composition of the nutrient solution in adsorption and plant uptake experiments.

By using an experimental set-up that reduces secondary influences on the Se transfer processes usually present in natural systems, such as microbiological activity, multiple adsorbing substrates or organic matter, this study was able to focus on the core transfer processes and their immediate effects. Compartmentalization of the Critical Zone proved to be a good means to explore Se transfer processes and quantification of Se transfer was possible due to the experimental set-up of closed-box systems. The two main pathways of Se transfer were investigated: the speciation- and concentration-dependent uptake of Se into rice plants and the speciation-, ion competition- and concentration-dependent Se adsorption-desorption processes between soil and nutrient solution. This study has increased knowledge and provided quantitative data on the following points:

1. Se sorption processes are an important factor controlling bioavailability and are highly dependent on mineral substrate, pH-value and nutrient ion competition. Goethite, with its large sorption capacities and a great affinity for selenite adsorption, reduces selenate bioavailability to 40 % and selenite bioavailability to 0 %, while kaolinite

reduces selenate bioavailability to 85 % and selenite bioavailability to 90 %. Ion competition of phosphate is strongest for both selenite and selenate adsorption, reducing Se adsorption to 15 - 50 % while sulphate reduces selenate adsorption to 15 - 75 %, but has little effect on selenite adsorption.

2. Se uptake into plants and its partitioning into different plant tissue are highly dependent on bioavailable Se concentration, Se species and oxy-anion competition in the solution as well as the plant's state of health and plant stage at the time of Se addition. Direct germination in Se and nutrient-deficiency significantly lower plant tolerance to Se and result in toxicity effects and reduced uptake at solution-Se concentrations above 250 $\mu\text{g/L}$ Se as selenate and 1000 $\mu\text{g/L}$ Se as selenite, while healthy plants are able to take up Se in the presence of 10,000 $\mu\text{g/L}$ Se. Treatment with different Se species leads to preferential partitioning of selenite to the root (70 %) and selenate to the shoot (72 %) as well as species-dependent tissue speciation. Selenite treatment led to 85 - 100 % org. Se in roots and 64 - 80 % organic Se in shoots, the rest being selenite, and selenate treatment led to 42 - 54 % org. Se and 29 - 36 % selenate in roots and 38 - 54 % org. Se and 33 - 48 % selenate in shoots, the rest being selenite.
3. The biogeochemical process model showed plant uptake to be influenced by the sorption processes and showed inhibition of Se adsorption onto mineral surfaces by competing ions in the nutrient solution to be a non-additive process.

The mass balance model created with the data of this study can be used as a basis for further model extensions and optimizations. The model can be extended with single parameter that influence Se bioavailability, such as pH-values, ionic strength, temperature, etc., and with additional compartments of the Critical Zone, such as the atmosphere with its Se transfer path of Se volatilization by plants. Moreover, other plants and substrates can be modelled in a similar fashion and integrated into the model as well. Other agricultural plants such as maize, beans, potatoes and tomatoes as well as Se accumulators such as mustard might be attractive expansions to the model due to different uptake and parti-

tioning ratios, which is of interest depending on the plant tissue used for consumption or animal feed. In combination with additional substrates, such as ferric oxides and hydroxides, other clay minerals, carbonates and organic matter, this model might prove a useful tool to compare differences between Se bioavailability in soils comprised of these materials in various proportions without needing to experimentally investigate every iteration. Future research might benefit from the continuous development of such a model to assess optimal Se biofortification as well as Se toxicity or deficiency hazards in the field and the management thereof. All in all, Se remains an element full of challenges to science, with great potential for analytical improvements and biogeochemical pathway clarifications, toward which this study has provided one stepping stone for the improved management of the world's Se resources.

Bibliography

- [Adriano, 1986] D.C. Adriano: *Chapter 12: Selenium*, 1986, in D.C. Adriano: (Ed.): *Trace Elements in Terrestrial Environments*, Springer-Verlag, New York, pp. 707-758.
- [Amoroux, 2001] D. Amoroux, P.S. Liss, E. Tessier, M. Hamren-Larsson, O.F.X. Donard: *Role of oceans as biogenic sources of selenium*, 2001, *Earth and Planetary Science Letters*, Vol. 189, pp. 277-283.
- [Anderson et al., 2007] S.P. Anderson, F. von Blanckenburg, A.F. White: *Physical and chemical controls on the Critical Zone*, 2007, *Elements*, Vol. 3, pp. 315-319.
- [Appel et al., 2003] C. Appel, L.Q. Ma, R.D. Rhue, E. Kennelley: *Point of zero charge determination in soils and minerals via traditional methods and detection of electroacoustic mobility*, 2003, *Geoderma*, Vol. 113, pp. 77-93.
- [Arvy, 1993] M.P. Arvy: *Selenate and selenite uptake and translocation in bean plants (*Phaseolus vulgaris*)*, 1993, *Journal of Experimental Botany*, Vol. 44, pp. 1083-1087.
- [Asher et al., 1977] C.J. Asher, G.W. Butler, P.J. Peterson: *Selenium Transport in Root Systems of Tomato*, 1977, *Journal of Experimental Botany*, Vol. 28, pp. 279-291.
- [Bacon & Davidson, 2007] J.R. Bacon, C.M. Davidson: *Is there a future for sequential chemical extraction?*, 2007, *The Analyst*, Vol. 133, pp. 25-46.
- [Bajaj et al., 2011] M. Bajaj, E. Eiche, T. Neumann, J. Winter, C. Gallert: *Hazardous concentrations of selenium in soil and groundwater in North-West India*, 2011, *Journal of Hazardous Materials*, Vol. 189, pp. 640-646.
- [Balistrieri & Chao, 1987] L.S. Balistrieri, T.T. Chao: *Selenium Adsorption by Goethite*, 1987, *Soil Science of America Journal*, Vol. 51, pp. 1145-1151.
- [Balistrieri & Chao, 1990] L.S. Balistrieri, T.T. Chao: *Adsorption of selenium by amorphous iron oxyhydroxide and manganese dioxide*, 1990, *Geochimica et Cosmochimica Acta*, Vol. 54, pp. 739-751.
- [Bañuelos et al. 2015] G.S. Bañuelos, I. Arroyo, I.J. Pickering, S.I. Yang, J.L. Freeman: *Selenium biofortification of broccoli and carrots grown in soil amended with Se-enriched hyperaccumulator *Stanleya pinnata**, 2015, *Food Chemistry*, Vol. 166, pp. 603-608.
- [Bar-Yosef & Meek, 1987] B. Bar-Yosef, D. Meek: *Selenium Sorption By Kaolinit And Montmorillonite*, 1987, *Soil Science*, Vol. 144, pp. 11-19.
- [Bellet al., 1992] P.F. Bell, D.R. Parker, A.L. Page: *Contrasting Selenate-sulphate Interactions in Selenium-Accumulating and Non-accumulating Plant Species*, 1992, *Soil Science Society of America Journal*, Vol. 56, pp. 1818-1824.

- [Berzelius, 1817] J.J. Berzelius: *Lettre de M. Berzelius a M. Berthollet sur deux metaux nouveaux*, 1817, Annales de Chimie et de Physique, Vol. 7, pp. 199-207.
- [Beytut et al., 2002] E. Beytut, F. Karatas, E. Beytut: *Lambs with White Muscle Disease and Selenium Content of Soil and Meadow Hay in the Region of Kars, Turkey*, 2002, The Veterinary Journal, Vol. 163, pp. 214-217.
- [Birringer et al., 2002] M. Birringer, S. Pilawa, L. Flohé: *Trends in selenium biochemistry*, 2002, Natural Product Reports, Vol. 19, pp. 693-718.
- [Bitterli et al., 2010] C. Bitterli, G.S. Bañuelos, R. Schulin: *Use of transfer factors to characterize uptake of selenium by plants*, 2010, Journal of Geochemical Exploration, Vol. 107, pp. 206-216.
- [Boullis, 1997] B. Boullis: *Retraitement et séparation des radionucléides à vie longue*, 1997, in R. Turkey (Ed.): *Les déchets nucléaires*, Lesitions de Physique, Paris, pp. 69-91.
- [Bowie et al., 1996] G.L. Bowie, J.G. Sanders, G.F. Riedel, C.C. Gilmour, D.L. Breitburg, G.A. Cutter, D.B. Porcella: *Assessing Selenium cycling and accumulation in aquatic systems*, 1996, Water Air Soil Pollution, Vol. 90 pp. 93-104.
- [Brantley et al., 2007] S.L. Brantley, M.B. Goldhaber, K.V. Ragnarsdottir: *Crossing Disciplines and Scales to Understand the Critical Zone*, 2007, Elements, Vol. 3, pp. 307-314.
- [Broadley et al., 2010] M.R. Broadley, J. Alcock, J. Alford, P. Cartwright, I. Foot, S.J. Fairweather-Tait, D.J. Hart, R. Hurst, P. Knott, S.P. McGrath, M.C. Meacham, K. Norman, H. Mowat, P. Scott, J.L. Stroud, M. Tovey, M. Tucker, P.J. White, S.D. Young, F.J. Zhao: *Selenium biofortification of high-yielding winter wheat (*Triticum aestivum* L.) by liquid or granular Se fertilisation*, 2010, Plant Soil, Vol. 332 pp. 5-18.
- [Brookins, 1988] D.G. Brookins (Ed.): *Eh-pH Diagrams for Geochemistry*, 1988, Springer Berlin-Heidelberg.
- [Brown & Shrift, 1982] T.A. Brown, A. Shrift: *Selenium: Toxicity And Tolerance In Higher Plants*, 1982, Biological Reviews, Vol. 57, pp. 65-81.
- [Brozmanová et al., 2010] J. Brozmanová, D. Mániková, V. Vlčková, M. Chovanec: *Selenium: a double-edged sword for defense and offence in cancer*, 2010, Vol. 84, pp. 919-938.
- [Buchner, Takahashi & Hawkesford, 2004] P. Buchner, H. Takahashi, M.J. Hawkesford: *Plant sulphate transporters: co-ordination of uptake, intracellular and long-distance transport*, 2004, Journal of Experimental Botany, Vol. 55, pp. 1765-1773.
- [Burk & Hill, 1993] R.F. Burk, K.E. Hill: *Regulation of Selenoproteins*, 1993, Annual Review of Nutrition, Vol. 13, pp. 59-84.
- [Bye, 1983] R. Bye: *Critical Examination of some common Reagents for Reducing Selenium Species in Chemical Analysis*, 1983, Talanta, Vol. 30, pp. 993-996.
- [Bye & Lund, 1988] R. Bye, W. Lund: *Optimal conditions for the reduction of selenate to selenite by hydrochloric acid*, 1988, Fresenius' Journal of Analytical Chemistry, Vol. 332, pp. 242-224.

- [Cantrell & Reeves, 2002] R.P. Cantrell, T.G. Reeves: *The Cereal of the World's Poor Takes Center Stage*, 2002, Science, Vol. 296 p. 53.
- [Cappa et al., 2014] J.J. Cappa, C. Yetter, S. Fakra, P.J. Cappa, R. DeTar, C. Landes, E.A.H. Pilon-Smits, M.P. Simmons: *Evolution of selenium hyperaccumulation in Stanleya (Brassicaceae) as inferred from phylogeny, physiology and X-ray microprobe analysis*, 2014, New Phytologist, Vol. 285 pp. 583-595.
- [Carey et al., 2012] A. Carey, K.G. Scheckel, E. Lombi, M. Newville, Y. Choi, G.J. Norton, A.H. Price, A.A. Meharg: *Grain Accumulation of Selenium Species in Rice (Oryza sativa L.)*, 2012, Environmental Science and Technology, Vol. 46, pp. 5557-5564.
- [Catalano et al., 2008] J.G. Catalano, C. Park, P. Fenter, Z. Zhang: *Simultaneous inner- and outer-sphere arsenate adsorption on corundum and hematite*, 2008, Geochimica et Cosmochimica Acta, Vol. 72, pp. 1986 - 2004.
- [Chan et al., 2009] Y.T. Chan, W.H. Kuan, T.Y. Chen, M.K. Wang: *Adsorption mechanisms of selenate and selenite on the binary oxide systems*, 2009, Water Research, Vol. 43 pp. 4412-4420.
- [Chasteen & Bentley, 2003] T.G. Chasteen, R. Bentley: *Biomethylation of selenium and tellurium: microorganisms and plants*, 2003, Chemical Reviews, Vol. 103, pp. 1-26.
- [Christensen et al., 1989] B.T. Christensen, F. Bertelsen, G. Gissel-Nielsen: *Selenite fixation by soil particle-size separates*, 1989, Journal of Soil Science, Vol. 40 p. 641-647.
- [Clement et al., 1977] C.R. Clement, M.J. Hopper, L.H.P. Jones: *The Uptake of Nitrate by Lolium perenne from Flowing Nutrient Solution*, 1977, Journal of Experimental Botany, Vol. 29, pp. 453-464.
- [Combs, 2001] G.F. Combs: *Selenium in global food systems*, 2001, British journal of Nutrition, Vol. 85, pp. 517-547.
- [CO₂Now, 2014] CO₂Now.org: *Earth's CO₂ Home Page*, 2014, <http://co2now.org>, (page visited 15:25, Jan. 19th, 2015).
- [Dada et al., 2012] A.O. Dada, A.P. Olalekan, A.M. Olatunya, O. Dada: *Langmuir, Freundlich, Temkin and Dubinin-Radushkevich Isotherms Studies of Equilibrium Sorption of Zn²⁺ Unto Phosphoric Acid Modified Rice Husk*, 2012, IOSR Journal of Applied Chemistry, Vol. 3, pp. 38-45.
- [Das et al., 2013] S. Das, M.J. Henry, J. Essilfie-Dughan: *Adsorption of selenate onto ferrihydrite, goethite, and lepidocrocite under neutral pH conditions*, 2013, Applied Geochemistry, Vol. 28, pp. 185-193.
- [Davis & Kent, 1990] J.A. Davis, D.B. Kent: *Surface Complexation modelling in Aqueous Geochemistry*, 1990, in M.F. Hochella, Jr., A.F. White (Eds.): *Reviews in Mineralogy Vol. 23: Mineral-Water interface Geochemistry*, Mineralogical Society of America, Washington D.C., pp. 177-260.
- [Dhillon & Dhillon, 2003] K.S. Dhillon, S.K. Dhillon: *Distribution and Management of Seleniferous Soils*, 2003, in D. Sparks (Ed.): *Advances in Agronomy*, 1st edn. Elsevier, Amsterdam, pp. 119-184.

- [Dhillon et al., 2007] S.K. Dhillon, B.K. Hundal, K.S. Dhillon: *Bioavailability of selenium to forage crops in a sandy loam soil amended with Se-rich plant materials*, 2007, Chemosphere, Vol. 66, pp. 1734-1743.
- [Dhillon & Dhillon, 2009] K.S. Dhillon, S.K. Dhillon: *Chemical Processes controlling the mobility of Se in soils*, 2009, in K.S. Dhillon, S.K. Dhillon: (Ed.): *Characterisation and management of Seleniferous Soils of Punjab*, Research Bulletin 1/2009, Ludhiana, pp. 13-15.
- [Diener, 2012] A. Diener: *Structural Incorporation of Selenium into Pyrite and Mackinawite*, 2012, Dissertation, Karlsruhe Institute für Technologie, Karlsruhe.
- [DIN EN ISO 12677:2013] *Chemische Analyse von feuerfesten Erzeugnissen durch Röntgenfluoreszenz-Analyse (RFA) – Schmelzaufschluss-Verfahren*, 2013.
- [Dörfler, 2002] H. Dörfler: *Grenzflächen und kolloid-disperse Systeme: Physik und Chemie*, 2002, Springer, Berlin Heidelberg.
- [Dove et al., 1997] M.T. Dove, D.A. Keen, A.C. Hannon, I.P. Swainson: *Direct measurement of the Si–O bond length and orientational disorder in the high-temperature phase of cristobalite*, 1997, Physical Chemistry of Minerals, Vol. 24, pp. 311-317.
- [Duc et al., 2003] M. Duc, G. Lefevre, M. Federoff, J. Jeanjean, J.C. Rouchaud, F. Monteils-Rivera, J. Dumonceau, S. Milonjic: *Sorption of selenium anionic species on apatites and iron oxides from aqueous solutions*, 2003, Journal of environmental radioactivity, Vol. 70, pp. 61-72.
- [Eiche, 2015] E. Eiche, F. Bardelli, A.K. Nothstein, L. Charlet, J. Göttlicher, R. Steininger, K.S. Dhillon, U.S. Sadana: *Selenium distribution and speciation in plant parts of wheat (*Triticum aestivum*) and Indian mustard (*Brassica juncea*) from a seleniferous area of Punjab, India*, 2015, Science of the Total Environment, Vol. 505, 952-961.
- [Euroola et al., 2003] M. Euroola, G. Alfhan, A. Aro, P. Ekholm, V. Hietaniemi, H. Rainio, R. Rankanen, E.R. Venäläinen: *Results of Finnish Selenium Monitoring Program 2000-2001*, 2003, Agrifood Research Report 36; MTT Agrifood Research Finland, Jokioinen, 2003; p 42.
- [FAOSTAT, 2012] FAOSTAT, Food and Agricultural Organisation of the United Nations (FAO), Statistics Division: *PART 3 – Feeding the world, Trends in the crop sector.*, 2012, pp. 182-197.
- [Fernández-Martínez & Charlet, 2009] A. Fernández-Martínez, L. Charlet: *Selenium environmental cycling and bioavailability: a structural chemist point of view*, 2009, Reviews in Environmental Science and Biotechnology, Vol. 8, pp. 81-110.
- [Ferrari & Renosto, 1972] G. Ferrari, F. Renosto: *Regulation of sulphate Uptake by Excised barley Roots in the Presence of Selenate*, 1972, Plant Physiology, Vol. 49, pp. 114-116.
- [Finley, 2005] J.W. Finley: *Selenium Accumulation in Plant Foods*, 2005, Nutrition Reviews, Vol. 63, pp. 196-202.

- [Flohé et al., 1973] L. Flohé, W.A. Günzler, H.H. Schock: *Glutathione peroxidase: a selenoenzyme*, 1973, FEBS letters, Vol. 32, pp. 132-134.
- [Fordyce, 2007] F. Fordyce: *Selenium Geochemistry and Health*, 2007, AMBIO: a journal of the human environment, Vol. 36, pp. 94-97.
- [Fordyce, 2013] F. Fordyce: *Selenium Deficiency and Toxicity in the Environment*, 2013, AMBIO: a journal of the human environment, Vol. 36, pp. 94-97.
- [Fukushi & Sverjenski, 2007] K. Fukushi, D.A. Sverjenski: *A surface complexation model for sulphate and selenate on iron oxides consistent with spectroscopic and theoretical molecular evidence*, 2007, Geochimica et Cosmochimica Acta, Vol. 71, pp. 1-24.
- [Geelhoed et al., 1997] J.S. Geelhoed, T. Hiemstra, W.H. van Riemsdijk: *Phosphate and sulphate adsorption on goethite: Single anion and competitive adsorption*, 1997, Geochimica et Cosmochimica Acta, Vol. 61, pp. 2389-2396.
- [Ghose et al., 2010] S.K. Ghose, G.A. Waychunas, T.P. Trainor, P.J. Eng: *Hydrated goethite (α -FeOOH) (1 0 0) interface structure: Ordered water and surface functional groups*, 2010, Geochimica et Cosmochimica Acta, Vol. 74, pp. 1943-1953.
- [Girling, 1984] C.A. Girling: *Selenium in agriculture and the environment*, 1984, Agriculture, Ecosystems and Environment, Vol. 11, pp. 37-65.
- [Gissel-Nielsen, 1973] G. Gissel-Nielsen: *Uptake and Distribution of Added Selenite and Selenate by Barley and Red Clover as Influenced by Sulphur*, 1973, Journal of the Science of Food and Agriculture, Vol. 24, pp. 649-655.
- [Glass, 1954] H.D. Glass: *High-Temperature Phases from Kaolinite and Halloysite*, 1954, American Mineralogist, Vol. 39, pp. 193-207.
- [Goff et al., 2002] S.A. Goff, D. Rieke, T. Lan, G. Presting, R. Wang, M. Dunn, J. Glazebrook, A. Sessions, P. Oeller, H. Varma, (. . .) S. Briggs: *A Draft Sequence of the Rice Genome (Oryza sativa L. ssp. japonica)*, 2002, Science, Vol. 296, pp. 92-100.
- [Goldberg et al., 2007] S. Goldberg, L.J. Criscentib, D.R. Turner, J. A. Davis, K.J. Cantrelle: *Adsorption-Desorption Processes in Subsurface Reactive Transport Modelling*, 2007, Vadose Zone Journal, Vol. 6, pp. 407-435.
- [Goldberg et al., 2013] S. Goldberg: *modelling Selenite Adsorption Envelopes on Oxides, Clay Minerals, and Soils using the Triple Layer Model*, 2013, Soil Science Society of America Journal, Vol. 77, pp. 64-71.
- [Gustafsson & Johnsson, 1992] J.P. Gustafsson, L. Johnsson: *Selenium retention in the organic matter of Swedish forest soil*, 1992, Journal of Soil Science, Vol. 43, pp. 461-472.
- [Hagarová, Žemberyová & Bajčan, 2005] I. Hagarová, M. Žemberyová, D. Bajčan: *Sequential and Single Step Extraction Procedures Used for Fractination of Selenium in Soil Samples*, 2005, Chemical Papers, Vol. 59, pp. 93-98.

- [Hartikainen, 2005] H. Hartikainen: *Biogeochemistry of selenium and its impact on food chain quality and human health*, 2005, Journal of Trace Elements in Medicine and Biology, Vol. 18, pp. 309-318.
- [Haug et al., 2007] A. Haug, R.D. Graham, O.A. Christopherson, G.H. Lyons: *How to use the world's scarce selenium resources efficiently to increase the selenium concentration in food*, 2007, Microbial Ecology in Health and Disease, Vol 19, pp. 209-228.
- [Hayes et al., 1987] K.F. Hayes, A.L. Roe, G.E. Brown, Jr., K.O. Hodgson, J.O. Leckie, G.A. Parks: *In-situ X-Ray absorption study of surface complexes: Selenium oxy-anions on FeOOH*, 1987, Science, Vol. 238, pp. 783-786.
- [Haygarth, 1994] P.M. Haygarth: *Global Importance and Global Cycling of Selenium*, 1994, in W.T. Frankenberger, Jr., S. Benson (Eds.): *Selenium In The Environment*, Marcel Dekker, Inc., Hong Kong, pp. 1-28.
- [Hiemstra & van Riemsdijk, 1995] T. Hiemstra, W.H. van Riemsdijk: *A Surface Structural Approach to Ion Adsorption: The Charge Distribution (CD) Model*, 1995, Journal of Colloid and Interface Science, Vol. 179, pp. 488-508.
- [Hingston et al. 1971] F.J. Hingston, A.M. Posner, J.P. Quirk: *Competitive Adsorption of Negatively Charged Ligands on Oxide Surfaces*, 1971, Discussions of the Faraday Society, Vol. 52, pp. 334-342.
- [Hochella & White, 1990] M.F. Hochella, Jr., A.F. White: *Mineral-Water interface Geochemistry: An Overview*, 1990, in M.F. Hochella, Jr., A.F. White (Eds.): *Reviews in Mineralogy Vol. 23: Mineral-Water interface Geochemistry*, Mineralogical Society of America, Washington D.C., pp. 1-5.
- [Holben & Smith, 1999] D.H. Holben, A.M. Smith: *The diverse role of selenium within selenoproteins: a review*, 1999, Journal of the American Dietetic Association, Vol. 99, pp. 836-843.
- [Hopper & Parker, 1999] J.L. Hopper, D.R. Parker: *Plant availability of selenite and selenate as influenced by the competing ions phosphate and sulphate*, 1999, Plant and Soil, Vol. 210, pp. 199-207.
- [Horneck et al., 2011] D.A. Horneck, D.M. Sullivan, J.S. Owen, J.M. Hart: *Soil Test Interpretation Guide*, 2011, Oregon State University Extension Service, EC1478.
- [Howard, 1977] J.H. Howard: *Geochemistry of selenium: formation of ferroselite and selenium behavior in the vicinity of oxidizing sulfide and uranium deposits*, 1977, Geochimica et Cosmochimica Acta, Vol. 41, pp. 1665-1678.
- [Hu et al., 2002] Q. Hu, L. Chen, J. Xu, Y. Zhang, G. Pang: *Determination of selenium concentration in rice and the effect of foliar application of Se-enriched fertiliser or sodium selenite on the selenium content of rice*, 2002, Journal of the Science of Food and Agriculture, Vol. 82, pp. 869-872.
- [Huang et al., 2013] Y. Huang, Q. Wang, J. Gao, Z. Lin, G.S. Bañuelos, L. Yuan, Z. Yin: *Daily Dietary Selenium Intake in a High Selenium Area of Enshi, China*, 2013, Nutrients, Vol. 5, pp. 700-710.

- [Hur & Schlautmann, 2003] J. Hur, M. Schlautmann: *Molecular weight fractionation of humic substances by adsorption onto minerals*, 2003, Journal of Colloid and Interface Science, Vol. 64, pp. 313-321.
- [Imai, 1998] H. Imai, K. Narashima, M. Arai, H. Sakamoto, N. Chiba, Y. Nakagawa: *Suppression of Leukotriene Formation in RBL-2H3 Cells That Overexpressed Phospholipid Hydroperoxide Glutathione Peroxidase*, 1998, The Journal of Biological Chemistry, Vol. 273, pp.1990-1997.
- [Institute of Medicine, 2000] Institute of Medicine: *Selenium*, 2000, in Panel on Dietary Antioxidants and Related Compounds (Ed.): *Dietary reference intakes for vitamin C, vitamin E, selenium, and carotenoids*, National Academy Press, Washington, pp. 284-324.
- [Izawa & Shimamoto, 1996] T. Izawa & K. Shimamoto: *Becoming a model plant: The importance of rice to plant science* , 1996, Trends in Plant Science, Vol. 1, pp. 95-99.
- [Jiyun et al., 1982] L. Jiyun, R. Shangxue, C. Daizhong: *A Study of Kashin-Beck Disease Associated with Environmental Selenium in Shanxi Area*, 1982, Acta Scientiae Circumstantiae, Vol. 2, pp. 91-101.
- [Kálmán, 1971] A. Kálmán: *Mean X-O bond lengths of the XO₄ⁿ⁻ tetrahedral oxy-anions*, 1971, Journal of the Chemical Society A: Inorganic, Physical, Theoretical, Vol. 1, pp. 1857-1859.
- [Kang et al., 1991] Y. Kang, H. Yamada, K. Kyuma, T. Hattori, S. Kigasawa: *Selenium in Soil Humic acid*, 1991, Soil Science Plant Nutrition, Vol. 37, pp. 2441-248.
- [Keskinen et al., 2010] R. Keskinen, M. Turakainen, H. Hartikainen: *Plant availability of soil selenate additions and selenium distribution within wheat and ryegrass*, 2010, Plant and Soil, Vol. 333, pp. 301-313.
- [Khan & Hell, 2014] M.S. Khan, R. Hell: *Applied Cell Biology of Sulphur and Selenium in Plants*, in P. Nick, Z. Opatrny (eds.) *Applied Plant Cell Biology*, 2014, Springer, Berlin Heidelberg, pp. 247-272.
- [Kikkert et al., 2013] J. Kikkert, B. Hale, E. Berkelaar: *Selenium accumulation in durum wheat and spring canola as a function of amending soils with selenite, selenate and or sulphate*, 2013, Plant Soil , Vol. 372, pp. 629-641.
- [Kinjo & Pratt, 1971] T. Kinjo, P.F. Pratt: *Nitrate Adsorption: II. In Competition with Chloride, sulphate, and Phosphate*, 1971, Soil Science Society of America Journal, Vol. 35, pp. 725-728.
- [Kosmulski, 2002] M. Kosmulski: *The pH-Dependent Surface Charging and the Points of Zero Charge*, 2002, Journal of Colloid and Interface Science, Vol. 253, pp. 77-87.
- [Kulp & Pratt, 2004] T. Kulp, L. Pratt: *Speciation and weathering of selenium in upper cretaceous chalk and shale from South Dakota and Wyoming, USA*, 2004, Geochimica et Cosmochimica Acta, Vol. 68, pp. 3687-3701.

- [Lakin, 1972] H. W. Lakin: *Selenium accumulation in soils and its absorption by plants and animals*, 1972, Geological Society of America Bulletin, Vol. 83, pp. 181-190.
- [Lagaly & Köster, 1993] G. Lagaly, H.M. Köster: *Tone und Tonminerale*, 1993, in G. Lagaly, H.M. Köster (Eds.): *Tonminerale und Tone - Struktur, Eigenschaften, Anwendungen und Einsatz in Industrie und Umwelt*, Steinkopff Verlag, Darmstadt, pp. 1-32.
- [Langmuir, 1918] I. Langmuir: *The adsorption of gases on plane surfaces of glass, mica and platinum*, 1918, Journal of the American Chemical Society, Vol. 40, pp. 1361-1403.
- [Läuchli, 1993] A. Läuchli: *Selenium in Plants: Uptake, Functions, and Environmental Toxicity*, 1993, Botanica Acta, Vol. 106, pp. 455-485.
- [LeDuc et al., 2004] D.L. LeDuc, A.S. Tarun, M. Montes-Bayon, J. Meija, M.F. Malit, C.P. Wu, M. Adelsamie, C. Chiang, A. Tagmount, M. deSouza, B. Neuhierl, A. Böck, J. Caruso, N. Terry: *Overexpression of selenocysteine methyltransferase in Arabidopsis and Indian mustard increases selenium tolerance and accumulation*, 2004, Plant Physiology, Vol. 135, pp. 377-383.
- [Leggett & Epstein, 1956] J.E. Leggett, E. Epstein: *Kinetics of sulphate absorption by barley roots*, 1956, Plant Physiology, Vol. 31, pp. 222-226.
- [Lemly, 1993] A.D. Lemly: *Guidelines for evaluating selenium data from aquatic monitoring and assessment studies*, 1993, Environmental Monitoring and Assessment, Vol. 28, pp. 83-100.
- [Lenz & Lens, 2009] M. Lenz, P.N.L. Lens: *The essential toxin: The changing perception of selenium in environmental sciences*, 2009, Science of the Total Environment, Vol. 407, pp. 3620-3633.
- [Levander & Burk, 2006] O.A. Levander, R.F. Burk: *Update of human dietary standards for selenium*, 2006, in D.L. Hatfield, M.J. Berry, V.N. Gladyshev (Eds.): *Selenium: Its molecular biology and role in human health*, 2nd edn., Springer, New York, pp 399-410.
- [Lévesque, 1974] M. Lévesque: *Selenium distribution in Canadian soil profiles*, 1974, Canadian Journal of Soil Science, Vol. 54, pp. 63-68.
- [Li et al., 2007] H. Li, S.P. McGrath, F. Zhao: *Selenium uptake, translocation and speciation in wheat supplied with selenate or selenite*, 2007, New Phytologist, Vol. 178, pp. 92-102.
- [Li et al., 2010] H. Li, E. Lombi, J.L. Stroud, S.P. McGrath, F. Zhao: *Selenium speciation in soil and rice - influence of water management and selenium fertilisation*, 2010, Journal of Agricultural Food Chemistry, Vol. 58, pp. 11837-11843.
- [Liu & Gu, 2009] K. Liu, Z. Gu: *Selenium Accumulation in Different Brown Rice Cultivars and Its Distribution in Fractions*, 2009, Journal of Agricultural and Food Chemistry, Vol. 57, pp. 695-700.
- [Lo & Chen, 1997] S. Lo, T. Chen: *Adsorption of Se(IV) and Se(VI) on an iron-coated sand from water*, 1997, Chemosphere, Vol. 35, pp. 919-930.
- [Lombeck et al., 1987] I. Lombeck, H. Menzel, D. Frosch: *Acute selenium poisoning of a 2-year-old child*, 1987, European Journal of Pediatrics, Vol. 146, pp. 308-312.

- [Lussier et al., 2003] C. Lussier, V. Veiga, S. Baldwin: *The geochemistry of selenium associated with coal waste in the Elk River Valley, Canada*, 2003, Environmental Geology, Vol. 35, pp. 919-930.
- [Lützelshwab, 1990] M. Lützelshwab: *Biochemische und immunologische Charakterisierung von Funktionen der Plasmamembran in Curcubita pepo L.: Evidenz für Heterogenität der Plasmamembran*, 1990, Dissertation, Albert-Ludwig-Universität, Freiburg.
- [Manceau & Charlet, 1994] A. Manceau, L. Charlet: *The mechanism of selenate adsorption on goethite and hydrous ferric oxide*, 1994, Journal of Colloid and Interface Science, Vol. 168, pp. 87-93.
- [Marx et al., 1999] E.S. Marx, J. Hart, and R.G. Stevens: *Soil Test Interpretation Guide*, 1999, Oregon State University Extension Service, EC1478.
- [Minaev et al., 2005] V.S.Minaev, S.P. Timoshenkov, V.V. Kalugin: *Structural and phase transformations in condensed selenium*, 2005, Journal of Optoelectronics and Advanced Materials, Vol. 7, pp. 1717-1741.
- [Miranda-Trevino & Coles, 2003] J.C. Miranda-Trevino, C.A. Coles: *Kaolinite properties, structure and influence of metal retention on pH*, 2003, Applied Clay Science, Vol. 23, pp. 133-139.
- [Misra, 2010] S. Misra, D. Peak, S. Niyogi: *Application of XANES spectroscopy in understanding the metabolism of selenium in isolated rainbow trout hepatocytes: insights into selenium toxicity*, 2010, Metallomics, Vol. 2, pp. 710-717.
- [Moreno-Reyes et al., 1998] R. Moreno-Reyes, C. Suetens, F. Mathieu, F. Begaux, D. Zhu, M. T. Rivera, M. Boelaert, J. Nève, N. Perlmutter, J. Vanderpas: *Kashin-Beck Osteoarthropathy in Rural Tibet in Relation to Selenium and Iodine Status*, 1998, The New England Journal of Medicine, Vol. 339, pp. 1112-1120
- [Mortimer, 2010] C. Mortimer, U. Müller: *Die Elemente der 5 Hauptgruppe*, 2010, in C. Mortimer, U. Müller (Eds.): *Chemie - Basiswissen der Chemie*, 10th edn., Georg Thieme Verlag, Stuttgart, pp. 421-445.
- [Murashige & Skoog, 1962] T. Murashige, F. Skoog: *A Revised Medium For Rapid Growth And Bio Assays With Tobacco Tissue Cultures*, 1962, Physiologia Plantarum, Vol. 15, pp. 473-497.
- [Mikkelsen & Wan, 1990] R.L. Mikkelsen, H.F. Wan: *The effect of selenium on sulfur uptake by barley and rice*, 1990, Plant and Soil, Vol. 121, pp. 151-153.
- [Navarro-Alarcon & Cabrera-Vique, 2008] M. Navarro-Alarcon, C. Cabrera-Vique: *Selenium in food and the human body: A review*, 2008, Science of the Total Environment, Vol. 400, pp. 115-141.
- [Neal, 1995] R.H. Neal: *Chapter 12. Selenium*, 1995, in B.J. Alloway (Ed.): *Heavy Metals In Soils*, Blackie Academic and Professional, London, pp. 260-283.

- [Nesterov, 1964] J. Trofast: *Berzelius' Discovery of Selenium*, 2011, Chemistry International, Vol. 33, pp. 16-19.
- [Newville, 2004] M. Newville: *Fundamentals of XAFS*, 2004, http://xafs.org/Tutorials?action=AttachFile&do=view&target=Newville_xas_fundamentals.pdf, (page visited 15:18, Mar. 15th, 2015).
- [O'Toole & Raisbeck, 1964] D. O'Toole, M.F. Raisbeck: *Pathology of experimentally induced chronic selenosis (alkali disease) in yearling cattle*, 1995, Journal of Veterinary Diagnostic, Vol. 7, pp. 364-373.
- [Oger et al., 2004] P.M. Oger, I. Daniel, B. Cournoyer, A. Simionovici *In situ micro X-ray absorption near edge structure study of microbiologically reduced selenite (SeO_2^{2-})*, 2004, Spectrochimica Acta Part B, Vol. 59, pp. 1681-1686.
- [Ogo et al., 2007] Y. Ogo, R.N. Itai, H. Nakanishi, T. Kobayashi, M. Takahashi, S. Mori, N.K. Nishizawa: *The rice bHLH protein OsIRO2 is an essential regulator of the genes involved in Fe uptake under Fe-deficient conditions*, 2007, The Plant Journal, Vol. 51, pp. 366-377.
- [Ohlendorf, 2002] H.M. Ohlendorf: *The birds of Kesterson Reservoir: a historical perspective*, 2002, Aquatic Toxicology, Vol. 57, pp. 1-10.
- [Oldfield, 2006] J.E. Oldfield: *Chapter 1. Selenium: A historical perspective*, 2006, in D.L. Hatfield, M.J. Berry, V.N. Gladyshev (Eds.): *Selenium: Its molecular biology and role in human health*, 2nd edn. Springer, New York, pp. 1-6.
- [Oldfield, 1987] J.E. Oldfield: *The Two Faces of Selenium*, 1987, Journal of Nutrition, Vol. 117, pp. 2002-2008.
- [Oyebanji et al., 2009] O. B. Oyebanji, O. Nweke, O. Odebunmi, N. B. Galadima, M. S. Idris, U. N. Nnodi, A. S. Afolabi, G. H. Ogbadu: *Simple, effective and economical explant-surface sterilisation protocol for cowpea, rice and sorghum seeds*, 2009, African Journal of Biotechnology, Vol. 8, pp. 5395-5399.
- [Oliver, 1997] M. A. Oliver: *Soil and human health: a review*, 1997, European Journal of Soil Science, Vol. 48, pp. 573-592.
- [Papp, 2007] L.V. Papp, J. Lu, A. Holmgren, K.K. Khanna: *From Selenium to Selenoproteins: Synthesis, Identity, and Their Role in Human Health*, 2007, Antioxidants & Redox Signaling, Vol. 9, pp. 775-806.
- [Parks, 1990] G.A. Parks: *Surface Energy and Adsorption at Mineral-Water Interfaces: An Introduction*, 1990, in M.F. Hochella, Jr., A.F. White (Eds.): *Reviews in Mineralogy Vol. 23: Mineral-Water interface Geochemistry*, Mineralogical Society of America, Washington D.C., pp. 133-175.
- [Paul & Pryor, 1972] G.L. Paul, A.W. Pryor: *The Study of Sodium Nitrate by Neutron Diffraction*, 1972, Acta Crystallographica Section B: Structural Crystallography and Crystal Chemistry, Vol. 28, pp. 2700-2702.

- [Peak, 2006] D. Peak: *Adsorption mechanisms of selenium oxy-anions at the aluminum oxide/water interface*, 2006, Journal of Colloid and Interface Science, Vol. 303, pp. 337-345.
- [Pickering et al., 1999] I.J. Pickering, G.N. George, V. Van Fleet-Stalder, T.G. Chasteen, R.C. Prince: *X-Ray absorption spectroscopy of selenium-containing amino acids*, 1999, Journal of Biological Inorganic Chemistry, Vol. 4, pp. 791-794.
- [Pilon-Smits et al., 2009] E. Pilon-Smits E., C.F. Quinn, W. Tapken, M. Malagoli, M. Schiavon: *Physiological functions of beneficial elements.*, 2009, Current Opinion in Plant Biology, Vol. 12, pp. 267-274.
- [Presser, 1994] T.S. Presser: *The Kesterson Effect*, 1994, Environmental Management, Vol. 18, pp. 437-454.
- [Presser & Luomo, 2009] T.S. Presser, S.N. Luoma: *modelling of Selenium for the San Diego Creek Watershed and Newport Bay, California*, 2009, U.S. Geological Survey Open-File Report 2009-1114, Reston, Virginia.
- [Presser & Ohlendorf, 1987] T.S. Presser, H.M. Ohlendorf: *Biogeochemical Cycling of Selenium in the San Joaquin Valley, California, USA*, 1987, Environmental Management, Vol. 11, pp. 805-821.
- [Presser & Piper, 1998] T.S. Presser, D.Z. Piper: *Mass balance approach to selenium cycling through the San Joaquin Valley: From source to river to bay* 1998, in W.T. Frankenber, R.A. Ingberg (Eds.) *Environmental chemistry of selenium*, 1998, Marcel Dekker, Inc. New York, pp.153-182.
- [Quinn et al., 2008] C.F. Quinn, J.L. Freeman, M.L. Galeas, E.M. Klamper, E.A.H. Pilon-Smits: *The role of selenium in protecting plants against prairie dog herbivory: implications for the evolution of selenium hyperaccumulation*, 2008, Oecologia, Vol. 155, pp. 267-275.
- [Rajan & Watkinson, 1976] S.S.S. Rajan, J.H. Watkinson: *Adsorption of Selenite and Phosphate on an Allophane Clay*, 1976, Soil Science Society of America Journal, Vol. 40, pp. 51-54.
- [Ramesh & Riyazuddin, 2010] K. A. Ramesh, P. Riyazuddin: *Chemical Interferences in hydride generation atomic spectrometry*, 2010, Trends in Analytical Chemistry, Vol. 29, p. 166-176.
- [Rayman, 2000] M.P. Rayman: *The importance of selenium to human health*, 2000, The Lancet, Vol. 356, pp. 233-241.
- [Rayman, 2008] M.P. Rayman: *Food-chain selenium and human health: emphasis on intake*, 2008, British Journal of Nutrition, Vol. 100, pp. 254-268.
- [Reamer & Zoller, 1980] D.C. Reamer, W.H. Zoller: *Selenium Biomethylation Products from Soil and Sewage Sludge*, 1980, Science, Vol. 208, pp. 500-502.
- [Reeder et al., 2006] R.J. Reeder, M.A.A. Schoonen, A. Lanzirotti: *Metal speciation and its role in bioaccessibility and bioavailability*, 2006, in J.J. Rosso (Ed.): *The emergent field of medical mineralogy and geochemistry*, 1st edn. Mineralogical Society of America and the Geochemical Society, New York, pp 59–113.

- [Reilly, 1997] C. Reilly: *Selenium Metabolism* 1997, in C. Reilly (Ed.) *Selenium in Food and Health*, 1997, Blackie Academic & Professional, London, pp.43-66.
- [Rietra et al., 2001] R.P.J.J. Rietra, T. Hiemstra, W.H. van Riemsdijk: *Comparison of Selenate and sulphate Adsorption on Goethite*, 2001, Journal of Colloid and Interface Science, Vol. 260, pp. 384-390.
- [Rosenfeld & Beath, 1964] I. Rosenfeld, O.A. Beath: *Selenium. Geobotany, biochemistry, toxicity, and nutrition*. 1964, Academic Press, New York.
- [Rotruck et al., 1973] J. T. Rotruck, A.L. Pope, H.E. Ganther, A.B. Swanson, D.G. Hafeman, W.G. Hoekstra: *Selenium: Biochemical Role as a Component of Glutathione Peroxidase*, 1973, Science, Vol. 179, pp. 588-590.
- [Rovira et al., 2008] M. Rovira, J. Giménez María Martínez, Xavier Martínez-Lladó, J. de Pablo, V. Martí, L. Duro: *Sorption of selenium(IV) and selenium(VI) onto natural iron oxides: Goethite and hematite* 2008, Journal of Hazardous Materials, Vol. 150, pp. 279-284.
- [Ryser et al., 2005] A.L. Ryser, D.G. Strawn, M.A. Marcus, J.L. Johnson-Maynard, M.E. Gunter, G. Möller: *Micro-spectroscopic investigation of selenium-bearing minerals from the Western US Phosphate Resource Area*, 2005, Geochemical Transactions, Vol. 1, pp. 1-11.
- [Schroth & Sposito, 1997] B.K. Schroth, G. Sposito: *Surface charge properties of kaolinite*, 1997, Clays and Clay Minerals, Vol. 45, pp. 85-91.
- [Schwartz & Foltz, 1957] K. Schwartz, C.M. Foltz: *Selenium as an integral part of factor 3 against dietary necrotic liver degeneration*, 1957, Journal of the American Chemical Society, Vol. 79, pp. 3292-3293.
- [Séby et al., 2001] F. Séby, M. Potin-Gautier, E. Giffaut, G. Borge, O.F.X. Donard: *A critical review of thermodynamic data for selenium species at 25°C*, 2001, Chemical Geology, Vol. 171, pp. 173-194.
- [Pezzarossa & Petruzelli, 2001] B. Pezzarossa, G. Petruzelli, H.M. Selim, D.L. Sparks: *Selenium contamination in soil: sorption and desorption processes*, 2001, in H.M. Selim, D.L. Sparks (Eds.): *Heavy metals release in soils*, CRC Press, New York, pp. 191-206.
- [Singh & Gilkes, 1998] B. Singh, R.J. Gilkes: *Properties of soil kaolinites from south-western Australia*, 1992, Journal of Soil Science, Vol. 43, pp. 645-667.
- [Singh et al., 1981] M. Singh, N. Singh, P.S. Relan: *Adsorption and Desorption of Selenite and Selenate Selenium on Different Soils*, 1981, Soil Science, Vol. 132, pp. 134-141.
- [Smith & Watkinson, 1984] G.S. Smith, J.H. Watkinson: *Selenium toxicity in perennial ryegrass and white clover*, 1984, New Phytologist, Vol. 97, pp. 557-564.
- [Sors et al., 2005] T.G. Sors, D.R. Ellis, D.E. Salt: *Selenium uptake, translocation, assimilation and metabolic fate in plants*, 2005, Photosynthesis Research, Vol. 86, pp. 373-389.
- [Spallholz & Hoffman, 2002] J.E. Spallholz, D.J. Hoffman: *Selenium toxicity: cause and effects in aquatic birds*, 2002, Aquatic Toxicology, Vol. 57, pp. 27-37.

- [Sposito, 1984] G. Sposito: *The surface Chemistry of Soils*, 1984, in G. Sposito (Ed.): *The Surface Chemistry of Soils*, Oxford University Press, New York, pp. 106-108.
- [Sposito, 1998] G. Sposito: *On points of zero charge*, 1998, Environmental Science and Technology, Vol. 32, pp. 2815-2819.
- [Sposito, 2004] G. Sposito: *The surface chemistry of natural particles*, 2004, Oxford University Press, New York.
- [Stelling, 2010] M. Stelling: *Stable iron isotope variations in higher plants - systematics and controls*, 2010, Dissertation, Gottfried Wilhelm Leibniz Universität Hannover.
- [Stolz & Oremland] J.F. Stolz, R.S. Oremland: *Bacterial respiration of arsenic and selenium*, 1999, Federation of European Microbiological Societies Microbiology Reviews, Vol. 23, pp. 615-627.
- [Stumm & Morgan, 1996] W. Stumm, J. Morgan: *Aquatic Chemistry - Chemical Rate and Equilibria in natural waters*, 1996, Wiley Inter-Science, New York.
- [Stwertka, 2002] A. Stwertka: *Selenium*, 2002, in A. Stwertka (Ed.): *A Guide To The Elements* 2nd edn., Oxford University Press, New York, pp. 106-108.
- [Su & Suarez, 2000] C. Su, D.L. Suarez: *Selenate and Selenite Sorption on Iron Oxides: An Infrared and Electrophoretic Study*, 2000, Soil Science, society America Journal, Vol. 64, pp. 101-111.
- [Sun et al., 2010] G. Sun, X. Liu, P.N. Williams, Y. Zhu: *Distribution and Translocation of Selenium from Soil to Grain and its Speciation in Paddy Rice (*Oryza sativa* L.)*, 2010, Environmental Science and Technology, Vol. 44, pp. 6706-6711.
- [Tamai & Ma, 2003] K. Tamai, J.F. Ma: *Characterisation of silicon uptake by rice roots*, 2003, New Phytologist, Vol. 158, pp. 431-436.
- [Terry et al., 2000] N. Terry, A.M. Zayed, M.P. de Souza, A.S. Tarun: *Selenium in Higher Plants*, 2000, Annual Review of Plant Physiology and Plant Molecular Biology, Vol. 51, pp. 401-432.
- [Tombácz & Szekeres, 2006] E. Tombácz, M. Szekeres: *Surface charge heterogeneity of kaolinite in aqueous suspension in comparison with montmorillonite*, 2006, Applied Clay Science, Vol. 34, pp. 105-124.
- [Tokunaga et al., 1994] T.K. Tokunaga, S.R. Sutton, S. Bajt: *Mapping of Selenium Concentrations in Soil Aggregates with Synchrotron X-Ray Fluorescence Microprobe*, 1994, Soil Science, Vol. 158, pp. 421-434.
- [Tributh, 1976] H. Tributh: *Die Umwandlung glimmerartiger Schichtsilikate zu aufweitbaren Dreischichttonmineralen*, 1976, Zeitschrift für Pflanzenernährung und Bodenkunde, Vol. 139, pp. 7-25.
- [Trofast, 2011] J. Trofast: *Berzelius' Discovery of Selenium*, 2011, Chemistry International, Vol. 33, pp. 16-19.

- [Tzeng & Zeitlin, 1978] J. Tzeng, H. Zeitlin: *The separation of selenium from sea water by Adsorption colloid flotation*, 1978, *Analytica Chimica Acta*, Vol. 101, pp. 71-77.
- [Ulrich & Shrift, 1968] J.M. Ulrich, A. Shrift: *Selenium Absorption by Excised Astragalus Roots*, 1968, *Plant Physiology*, Vol. 43, pp. 14-20.
- [Virupaksha & Shrift, 1965] T.K. Virupaksha, A. Shrift: *Biogeochemical differences between selenium accumulator and non-accumulator Astragalus species* 1965, *Biochimica Biophysica Acta*, Vol. 107, pp. 69-80.
- [Wang & Gao, 2001] Z.J. Wang, Y.X. Gao: *Biogeochemical cycling of selenium in Chinese environments*, 2001, *Applied Geochemistry*, Vol. 16, pp. 1345-1351.
- [Wang et al. 2013] P. Wang, N.W. Menzies, E. Lombi, B.A. McKenna, M.D. de Jonge, D.J. Pateron: *In situ speciation and distribution of toxic selenium in hydrated roots of cowpea*, 2013, *Plant Physiology*, Vol. 163, pp. 407-418.
- [Water Education Foundation, 2014] Water Education Foundation: *Kesterson Reservoir*, 2014, <http://www.watereducation.org/aquapedia/kesterson-reservoir>, (page visited 20:25, Jan. 18th, 2015).
- [Wen & Carignan, 2007] H. Wen, J. Carignan: *Reviews on atmospheric selenium: Emissions, speciation and fate*, 2007, *Atmospheric Environment*, Vol. 41, pp. 7151-7165.
- [Wijnja & Schulthess, 2000] H. Wijnja, C.P. Schulthess: *Vibrational Spectroscopy Study of Selenate and sulphate Adsorption Mechanisms on Fe and Al (Hydr)oxide Surfaces*, 2000, *Journal of Colloid and Interface Science*, Vol. 229, pp. 286-297.
- [Wijnja & Schulthess, 2002] H. Wijnja, C.P. Schulthess: *Effect of Carbonate on the Adsorption of Selenate and sulphate on Goethite*, 2002, *Soil Science American Journal*, Vol. 66, pp. 1190-1197.
- [Winkel et al., 2011] L.H.E. Winkel, C.A. Johnson, M. Lenz, T. Grundl, O.X. Leupin, M. Amini, L. Charlet: *Environmental Selenium Research: From Microscopic Processes to Global Understanding*, 2011, *Environmental Science And Technology*, Vol. 46, pp. 571-579.
- [Wu et al., 2000] C. Wu, S. Lo, C. Lin: *Competitive adsorption of molybdate, chromate, sulphate, selenate, and selenite on γ - Al_2O_3* , 2000, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, Vol. 166, pp. 251-259.
- [Xue et al., 2001] T. Xue, H. Hartikainen, V. Piironen: *Antioxidative and growth-promoting effects of selenium on senescing lettuce*, 2001, *Plant and Soil*, Vol. 61, pp. 237-255.
- [Xu & Hu, 2004] J. Xu, Q. Hu: *Effect of foliar application of Selenium on antioxidant activity of aqueous and ethanolic extracts of Selenium-enhanced rice*, 2004, *Journal of Agricultural and Food Chemistry*, Vol. 52, pp. 1759-1763.

- [Yang et al., 2011] S.I. Yang, J.R. Lawrence, G.D.W. Swerhone, I.J. Pickering: *Biotransformation of selenium and arsenic in multi-species biofilm*, 2011, Environmental Chemistry, Vol. 8, pp. 543-551.
- [Young et al., 2009] T.F. Young, K. Finley, W.J. Adams, J. Besser, W.D. Hopkins, D. Jolley, E. McNaughton, T.S. Presser, D.P. Shaw, J. Unrine: *What you need to know about selenium*, 2009, in P.M. Chapman, W.J. Adams, M.L. Brooks, C.D. Gelos, S.N. Luoma, W.A. Maher, H.M. Ohlendorf, T.S. Presser, D.P. Shaw (Eds.) *Ecological Assessment of Selenium in the Aquatic Environment*, CRC Press, New York, pp. 7-45.
- [Yukselen & Kaya, 2002] Y. Yukselen, A. Kaya: *Zeta Potential of Kaolinite in the Presence of Alkali, Alkaline Earth and Hydrolyzable Metal Ions*, 2002, Water, Air and Soil Pollution, Vol. 145, pp. 155-168.
- [Zayed et al., 1998] A. Zayed, C.M. Lytle, N. Terry: *Accumulation and volatilisation of different chemical species of selenium by plants*, 1998, Planta, Vol. 206, pp. 284-292.
- [Zhang & Sparks, 1990] P. Zhang, D.L. Sparks: *Kinetics of Selenate and Selenite Adsorption/Desorption at the Goethite/Water Interface*, 1990, Environmental Science and Technology, Vol. 24, pp. 1848-1856.
- [Zhang & Moore, 1996] Y.Q. Zhang, J.N. Moore: *Selenium fractionation and speciation in a wetland system*, 1996, Environmental Science and Technology, Vol. 30, pp. 2613-2619.
- [Zhang et al., 2003] J. Zhang, G. Pan, J. Chen, Q. Hu: *Uptake and transport of selenite and selenate by soybean seedlings of two genotypes*, 2003, Plant and Soil, Vol. 253, pp. 437-443.
- [Zhang et al., 2005] E.S. Zhang, H.L. Wang, X.X. Yan, L.D. Zhang: *Comparison of short-term toxicity between Nano-Se and selenite in mice*, 2005, Life Science, Vol. 76, pp. 1099-1109.
- [Zhang et al., 2006] L.H. Zhang, W. Shi, X. Wang: *Difference in selenite absorption between high- and low-selenium rice cultivars and its mechanism*, 2006, Plant and Soil, Vol. 282, pp. 183-193.
- [Zhao et al., 2010] X.Q. Zhao, N. Mitani, N. Yamaji, R.F. Shen, J.F. Ma: *Involvement of Silicon Influx Transporter OsNIP2;1 in Selenite Uptake in Rice*, 2010, Plant Physiology, Vol. 153, pp. 1871-1877.
- [Zhu et al., 2008] Y. Zhu, E.A.H. Pilon-Smitts, F. Zhao, P. Williams, A.A. Meharg: *Selenium in higher plants - understanding mechanisms for biofortification and phytoremediation*, 2008, Trends in Plant Science, Vol. 14, pp. 436-442.
- [Zieve & Peterson, 1984] R. Zieve, P.J. Peterson: *The accumulation and assimilation of dimethylselenide by four plant species*, 1984, Planta, Vol. 160, pp. 180-184.

A. Se uptake by Rice - Data

Table A.1.: *PHREEQ-C Input file for Bjerrum plot of selenite*

```
1  DATABASE wateq4f.dat
2  TITLE Bjerrumplot Selenite
3
4  SOLUTION 1
5  units mol/L
6  pH 13
7  pe -8
8  Na 0.1 charge
9  Se(4) 0.01
10
11 REACTION 1 # addition of 34 mmol HCl in 1200 steps simulating pH change
12 HCl 1
13 0.34 in 1200
14
15 USER_GRAPH
16 -chart_title "species of selenite"
17 -axis_titles "pH" "mol/L"
18 -axis_scale x_axis 1 13 2
19 -axis_scale y_axis 0 0.011 0.001
20 -initial_solutions false
21 -headings pH SeO3-2 HSeO3- H2SeO3
22 -start
23 10 graph_x -la("H+")
24 20 graph_y mol("SeO3-2")
25 30 graph_y mol("HSeO3-")
26 40 graph_y mol("H2SeO3")
27 -end
28 END
```

Table A.2.: PHREEQ-C Input file for Bjerrum plot of selenate

```
1  DATABASE wateq4f.dat
2  TITLE Bjerrumplot Selenate
3
4  SOLUTION 1
5  units mol/L
6  pH 13
7  Na 0.01 charge
8  Se(6) 0.01
9
10 REACTION 1 # addition of 1.4 mol HCl in 340 steps to simulate pH change
11 HCl 1
12 1.4 in 340
13
14 USER_GRAPH
15 -chart_title "species of selenate"
16 -axis_titles "pH" "mol/L"
17 -axis_scale x_axis 1 13 2
18 -axis_scale y_axis 0 0.011 0.001
19 -initial_solutions false
20 -headings pH HSeO4- SeO4-2
21 -start
22 10 graph_x -la("H+")
23 20 graph_y mol("HSeO4-")
24 30 graph_y mol("SeO4-2")
25 -end
26 END
```

A.1. Datasheets experiment A1

Table A.3.: *watering regime for open plant cultures*

	watering date	Box 1	Box 2, 3	Box 4, 5, 6	reference plants
Fr.	11.05.	55 mL	55 mL	55 mL	x
Mo.	14.05.	55 mL	55 mL	55 mL	x
Mi.	16.05.	55 mL	55 mL	55 mL	x
Fr.	18.05.	55 mL	55 mL	55 mL	x
Mo.	21.05.	55 mL	27 mL	55 mL	27 mL
Mi.	23.05.	27 mL	27 mL	55 mL	27 mL
Fr.	25.05.	27 mL	27 mL	55 mL	27 mL
Mo.	28.05.	27 mL	27 mL	55 mL	40 mL
Mi.	30.05.	27 mL	27 mL	55 mL	27 mL
Fr.	01.06.	27 mL	27 mL	55 mL	35 mL
Mo.	04.06.	27 mL	27 mL	55 mL	50 mL
Mi.	06.06.	27 mL	27 mL	55 mL	27 mL
Fr.	08.06.	55 mL	27 mL	55 mL	55 mL
Mo.	11.06.	55 mL	27 mL	55 mL	55 mL
Mi.	13.06.	55 mL	27 mL	55 mL	55 mL
Fr.	15.06.	55 mL	27 mL	55 mL	35 mL
Mo.	18.06.	55 mL	27 mL	55 mL	70 mL
Mi.	20.06.	55 mL	27 mL	55 mL	35 mL
Fr.	22.06.	55 mL	27 mL	55 mL	55 mL
Mo.	25.06.	55 mL	27 mL	55 mL	70 mL
Mi.	27.06.	55 mL	27 mL	55 mL	70 mL
Fr.	29.06.	70 mL	55 mL	70 mL	55 mL
Mo.	02.07.	70 mL	55 mL	70 mL	80 mL
Mi.	04.07.	70 mL	55 mL	70 mL	70 mL
Fr.	06.07.	70 mL	55 mL	70 mL	70 mL
Mo.	09.07.	70 mL	55 mL	70 mL	70 mL
Mi.	11.07.	70 mL	55 mL	70 mL	55 mL
Fr.	13.07.	70 mL	55 mL	70 mL	70 mL

Table A.4.: PHREEQ-C calculation input file for nutrient solution composition

```

1  DATABASE wateq4f.dat
2  TITLE Nut_Sol_2012_11_21
3
4  SELECTED_OUTPUT
5  -reset false
6  -pH
7  -saturation_indices
8
9  SOLUTION 1
10 temp 25
11 units mg/L
12
13 REACTION 1
14
15 Ca(NO3)2:4H2O 235.960
16 K2SO4 65.320
17 MgSO4:6H2O 74.348
18 KH2PO4 13.598
19 H3BO3 0.493
20 CuSO4 0.032
21 ZnSO4:H2O 0.088
22 MnSO4:H2O 0.033
23 CaCl2 5.552
24 #Na2MoO4:2H2O 0.018
25 C6H5OFe 12.242
26
27 END

```

Table A.5.: saturation indices >0 for non-gaseous nutrient solution compounds

phase	chemical formula	NS _{conc}	saturation index		
			NS _{concA}	NS _{concB}	NS _{dil}
Anhydrite	CaSO ₄	1.13	-	-	-1.93
Aragonite	CaCO ₃	2.13	-	-	-1.62
Calcite	CaCO ₃	2.28	-	-	-1.47
Dolomite	CaMg(CO ₃) ₂	4.03	-	-	-3.50
Iron(III)oxide-hydroxide (a)	Fe(OH) ₃ (a)	3.97	-	3.95	2.47
Goethite	FeOOH	9.91	-	9.85	8.36
Gypsum	CaSO ₄ * 2H ₂ O	1.26	-	-	-1.71
Hematite	Fe ₂ O ₃	21.87	-	21.70	18.73
Hydroxyapatite	Ca ₅ (PO ₄) ₃ OH	15.19	15.71	-	2.70
Jarosite-K	KFe ₃ (SO ₄) ₂ (OH) ₆	9.98	-	-	0.54
Rhodocrosite	MnCO ₃	0.86	-	0.81	-2.71
Siderite	FeCO ₃	2.93	-	2.96	-0.70
Vivianite	Fe ₃ (PO ₄) ₂ *8H ₂ O	9.29	-	-	2.24

Table A.6.: A1 experimental data

plant tissue	added Se	fresh	dry	ratio			1s	digestedc	c(Se)	FIAS	1s	c(Se)	FIAS	1s	c(Se)	total Se		total	
		weight (FW)	weight (DW)	loss	total DW	tissue DW/total DW										digested amount	volume	20.12.12	29.12.12
		± 0.0001	± 0.0001													[µg]	[µg]	[µg]	[µg]
		[µg/L]	[g]	[g]	[%]	[g]	[g]	[mL]	[µg/L]	[µg/L]	[µg/L]	[µg/L]	[mg/kg]	[mg/kg]		[µg]	[µg]	[µg]	[µg]
1a shoot	5	3.1338	2.2351	71.3	2.7829	0.80	0.1997	0.0001	10	< PQL	< PQL	450.41	17.71	22.55	0.89	50.41	1.98	61.08	10.76
root	5	0.6043	0.5478	90.7	2.7829	0.20	0.2040	0.0001	10	390.64	237.35	404.27	11.44	19.48	6.10	10.67	3.34	61.08	10.76
1b shoot	2.5	0.2011	0.1696	84.3	0.2134	0.79	0.1021	0.0001	10	> calib	> calib	1156.67	21.95	113.29	2.15	19.21	0.36	20.98	0.76
root	2.5	0.0454	0.0438	96.5	0.2134	0.21	0.0061	0.0001	10	< PQL	< PQL	24.67	1.33	40.44	2.18	1.77	0.10	20.98	0.76
1c shoot	2.5	2.4447	1.7147	70.1	2.1896	0.78	0.0999	0.0002	10	574.50	41.27	< PQL	< PQL	57.48	4.13	98.57	7.08	135.10	11.83
root	2.5	0.5067	0.4749	93.7	2.1896	0.22	0.0997	0.0002	10	767.10	79.24	< PQL	< PQL	76.93	7.95	36.54	3.77	135.10	11.83
1d shoot	0	1.4825	1.1524	77.7	1.5140	0.76	0.1002	0.0002	10	x	x	x	x	x	x	x	x	x	x
root	0	0.3771	0.3616	95.9	1.5140	0.24	0.1003	0.0002	10	x	x	x	x	x	x	x	x	x	x
1e shoot	5	0.5145	0.4383	85.2	0.5017	0.87	0.2017	0.0005	10	1318.14	204.00	1383.71	80.48	66.99	7.05	29.36	3.09	30.68	3.93
root	5	0.1031	0.0634	61.5	0.5017	0.13	0.0050	0.0005	10	< PQL	< PQL	10.36	1.57	20.85	3.15	1.32	0.20	30.68	3.93
1f shoot	0	0.6522	0.5474	83.9	0.6677	0.82	0.1005	0.0002	10	x	x	x	x	x	x	x	x	x	x
root	0	0.1267	0.1203	94.9	0.6677	0.18	0.0307	0.0002	10	x	x	x	x	x	x	x	x	x	x
1g shoot	0	1.9392	1.4504	74.8	1.9121	0.76	0.2034	0.0001	10	x	x	x	x	x	x	x	x	x	x
root	0	0.4792	0.4617	96.3	1.9121	0.24	0.1652	0.0001	10	x	x	x	x	x	x	x	x	x	x
1h shoot	2.5	0.4737	0.4008	84.6	0.5066	0.79	0.1000	0.0005	10	542.49	29.96	x	x	54.25	3.00	21.75	1.20	27.09	2.24
root	2.5	0.1107	0.1058	95.6	0.5066	0.21	0.0214	0.0005	10	108.15	11.89	x	x	50.56	5.56	5.35	0.59	27.09	2.24
2a shoot dead																			
root dead																			
2b shoot	2.5	0.3551	0.2933	82.6	0.3451	0.85	0.2121	0.0001	10	> calib	> calib	635.82	3.85	29.98	0.18	8.79	0.05	x	x
root	2.5	0.0531	0.0518	97.6	0.3451	0.15	0.0014	0.0001	10	< PQL	< PQL	< PQL	< PQL	x	x	x	x	x	x
2c shoot	5	0.5949	0.4723	79.4	0.5632	0.84	0.1974	0.0001	10	492.69	22.23	470.42	12.44	24.39	0.88	11.52	0.41	30.34	1.12
root	5	0.095	0.0909	95.7	0.5632	0.16	0.0161	0.0001	10	< PQL	< PQL	333.37	12.61	207.06	7.83	18.82	0.71	30.34	1.12
2d shoot	2.5	0.0506	0.0459	90.7	0.0564	0.81	0.0042	0.0003	10	< PQL	< PQL	32.50	1.55	78.32	3.73	3.59	0.17	4.16	1.01
root	2.5	0.0111	0.0105	94.6	0.0564	0.19	0.0024	0.0003	10	12.79	5.59	< PQL	< PQL	53.72	23.51	0.56	0.25	4.16	1.01
3a shoot	5	0.3309	0.2818	85.2	0.3628	0.78	0.1888	0.0001	10	1834.52	9.32	1850.25	60.67	97.58	1.85	27.50	0.52	29.93	0.48
root	5	0.0827	0.081	97.9	0.3628	0.22	0.0188	0.0001	10	< PQL	< PQL	56.45	0.74	30.03	0.39	2.43	0.03	29.93	0.48
3b shoot	0	0.157	0.1447	92.2	0.2103	0.69	0.0463	0.0001	10	x	x	x	x	x	x	x	x	x	x
root	0	0.0693	0.0656	94.7	0.2103	0.31	0.0056	0.0001	10	x	x	x	x	x	x	x	x	x	x
3cleaves	2.5	0.1357	0.1242	91.5	0.1539	0.81	too little material												
roots	2.5	0.03	0.0297	99.0	0.1539	0.19	too little material												
3d leaves	0	0.0444	0.0411	92.6	0.0486	0.85	too little material												
roots	0	0.0091	0.0075	82.4	0.0486	0.15	too little material												
3e shoot	5	0.2057	0.1852	90.0	0.2517	0.74	0.1148	0.0005	10	966.97	108.61	922.99	32.79	82.31	6.16	15.24	1.14	17.18	0.84
root	5	0.0992	0.0665	67.0	0.2517	0.26	0.0150	0.0005	10	< PQL	< PQL	43.74	1.02	29.12	0.68	1.94	0.05	17.18	0.84
3f leaves	5	0.1555	0.1408	90.5	0.1728	0.81	0.0296	0.0005	10	x	x	x	x	x	x	x	x	x	x
roots	5	0.0335	0.032	95.5	0.1728	0.19	0.0038	0.0005	10	x	x	x	x	x	x	x	x	x	x
3g leaves	0	0.0945	0.0316	33.4	0.0637	0.50	0.0212	0.0015	10	x	x	x	x	x	x	x	x	x	x
roots	0	0.0392	0.0321	81.9	0.0637	0.50	0.0011	0.0015	10	x	x	x	x	x	x	x	x	x	x
3h shoot	0	0.2698	0.2328	86.3	0.2890	0.81	0.0998	0.0015	10	x	x	x	x	x	x	x	x	x	x
root	0	0.0574	0.0562	97.9	0.2890	0.19	0.0045	0.0015	10	x	x	x	x	x	x	x	x	x	x
4a leaves	0	0.3259	0.1881	57.7	0.2826	0.67	0.0998	0.0015	10	x	x	x	x	x	x	x	x	x	x
roots	0	0.0959	0.0945	98.5	0.2826	0.33	0.0268	0.0015	10	x	x	x	x	x	x	x	x	x	x
4b leaves	0	0.7379	0.6803	92.2	0.7983	0.85	0.1004	0.0003	10	x	x	x	x	x	x	x	x	x	x
roots	0	0.122	0.118	96.7	0.7983	0.15	0.0298	0.0003	10	x	x	x	x	x	x	x	x	x	x
4c shoot	0	0.8161	0.6776	83.0	0.9001	0.75	0.1960	0.0001	10	x	x	x	x	x	x	x	x	x	x
root	0	0.2259	0.2225	98.5	0.9001	0.25	0.1356	0.0001	10	x	x	x	x	x	x	x	x	x	x
4d shoot	0	0.6296	0.5356	85.1	0.6758	0.79	0.1003	0.0015	10	x	x	x	x	x	x	x	x	x	x
root	0	0.144	0.1402	97.4	0.6758	0.21	0.0622	0.0015	10	x	x	x	x	x	x	x	x	x	x
5a shoot	2.5	1.3478	0.547	40.6	0.7373	0.74	0.2005	0.0001	10	554.06	36.76	533.68	12.64	27.12	1.23	14.83	0.67	17.34	1.27
root	2.5	0.3175	0.1903	59.9	0.7373	0.26	0.1096	0.0001	10	145.66	26.17	142.32	2.86	13.14	1.32	2.50	0.25	17.34	1.27
5b leaves	2.5	0.6742	0.2964	44.0	0.3419	0.87	0.1005	0.0005	10	553.22	4.37	x	x	55.05	0.43	16.32	0.13	x	x
roots	2.5	0.0611	0.0455	74.5	0.3419	0.13	0.0020	0.0005	10	< PQL	< PQL	3419	x	x	x	x	x	x	x
5c leaves	2.5	1.6735	0.6616	39.5	0.8972	0.74	0.0992	0.0003	10	448.00	27.59	x	x	45.15	2.78	29.87	1.84	36.97	2.91
roots	2.5	0.4556	0.2356	51.7	0.8972	0.26	0.1003	0.0003	10	302.14	29.01	x	x	30.12	2.89	7.10	0.68	36.97	2.91
5d shoot	2.5	1.1373	0.4577	40.2	0.6733	0.68	0.1002	0.0005	10	261.87	26.41	236.95	4.83	24.90	1.56	11.40	0.71	14.59	0.80
root	2.5	0.3126	0.2156	69.0	0.6733	0.32	0.0998	0.0005	10	158.82	9.14	136.61	4.95	14.81	0.71	3.19	0.15	14.59	0.80
6a leaves	5	0.5308	0.4295	80.9	0.5386	0.80	0.2019	0.0005	10	< PQL	< PQL	x	x	x	x	x	x	x	x
roots	5	0.1137	0.1091	96.0	0.5386	0.20	0.1096	0.0005	10	< PQL	< PQL	x	x	x	x	x	x	x	x
6b shoot	5	1.2058	0.9056	75.1	1.1079	0.82	0.1005	0.0005	10	< PQL	< PQL	309.42	14.04	30.80	1.40	27.89	1.27	32.70	1.64
root	5	0.2078	0.2023	97.4	1.1079	0.18	0.1000	0.0005	10	< PQL	< PQL	237.65	13.03	23.76	1.30	4.81	0.26	32.70	1.64
6c shoot	5	0.4487	0.3654	81.4	0.4419	0.83	0.1005	0.0005	10	< PQL	< PQL	308.29	6.17	30.68	0.61	11.21	0.22	11.48	0.26
root	5	0.0781	0.0765	98.0	0.4419	0.17	0.1000	0.0005	10	< PQL	< PQL	34.97	0.86	3.50	0.09	0.27	0.01	11.48	0.26
6d leaves	5	0.3469	0.2931	84.5	0.3530	0.83	0.0992	0.0003	10	< PQL	< PQL	x	x	x	x	x	x	x	x
roots	5	0.0621	0.0599	96.5	0.3530	0.17	0.0038	0.0003	10	< PQL	< PQL	x	x	x	x	x	x	x	x
RA leaves	5	3.2292	2.323	71.9	3.4242	0.68	0.2005	0.0001	10	642.18	27.97	x	x	32.03	1.39	74.40	3.24	314.12	8.21
roots	5	1.1936	1.1012	92.3	3.4242	0.32	0.2037	0.0001	10	4434.19	38.66	x	x	217.68	1.90	239.71	2.09	314.12	8.21
RB leaves	0	3.3602	2.2272	66.3	3.2053	0.69	0.1990	0.0001	10	x	x	x	x	x	x	x	x	x	x
roots	0	1.4242	0.9781	68.7	3.2053	0.31	0.1990	0.0001	10	x	x	x	x	x	x	x	x	x	x
WP leaves	0	2.1407	1.6036	74.9	2.4244	0.66	0.1001	0.0002	10	x	x	x	x	x	x	x	x	x	x
roots	0	2.7085	0.8208	30.3	2.4244	0.34	0.1005												

Table A.7.: A1 analytical data - HG-FIAS measurement I

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Pflanzenaufschlüsse		
Results Data Set	Nothstein_2012_12_20_b		
Date Measured	20.12.2012		
Method Name	Se Nothstein		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.997384	LOQ (= 7-wash)	0.251	
calib. slope	LOD (= 3-wash)	0.107	
0.0171	analytical quality [%]	111.052	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0012	0.0	0.00	0.00
2	0.5 ppb	0.0059	0.0005	0.5	0.34	0.03
3	1.0 ppb	0.0166	0.0005	1.0	0.97	0.03
4	2.0 ppb	0.0311	0.0008	2.0	1.82	0.05
5	5.0 ppb	0.0869	0.0014	5.0	5.08	0.08

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.125	0.111	-0.125	0.111	1	-0.13	0.11
2	wash	0.007	0.050	0.007	0.050	1	0.01	0.05
3	HCl Blank	0.049	0.048	0.028	0.027	6	0.17	0.16
4	Trace Metal 252µg/L	1.322	0.202	1.199	0.183	240	287.77	43.97
5	wash	0.078	0.055	0.078	0.055	1	0.08	0.06
6	Se_Std_0	0.046	0.042	0.046	0.042	1	0.05	0.04
7	Se_Std_0.5	0.492	0.009	0.492	0.009	1	0.49	0.01
8	Se_Std_1.0	1.064	0.071	1.064	0.071	1	1.06	0.07
9	Se_Std_2.0	1.763	0.133	1.763	0.133	1	1.76	0.13
10	Se_Std_5.0	4.869	0.073	4.869	0.073	1	4.87	0.07
11	wash	0.083	0.017	0.083	0.017	1	0.08	0.02
12	wash	0.090	0.021	0.090	0.021	1	0.09	0.02
13	1h_leaves	4.346	0.240	4.521	0.250	120	542.49	29.96
14	1h_roots	0.955	0.105	0.901	0.099	120	108.15	11.89
15	5b_leaves	4.432	0.035	4.610	0.036	120	553.22	4.37
16	5b_roots	0.154	0.151	0.083	0.081	120	< PQL	< PQL
17	5c_leaves	3.589	0.221	3.733	0.230	120	448.00	27.59
18	5c_roots	2.500	0.240	2.518	0.242	120	302.14	29.01
19	5d_leaves	2.310	0.233	2.182	0.220	120	261.87	26.41
20	5d_roots	1.401	0.081	1.324	0.076	120	158.82	9.14
21	5a_leaves	4.893	0.325	4.617	0.306	120	554.06	36.76
22	5a_roots	1.564	0.281	1.214	0.218	120	145.66	26.17
23	wash	0.057	0.117	0.059	0.122	1	0.06	0.12
24	Se_Std	0.113	0.099	0.113	0.099	1	0.11	0.10
25	Se_Std_0.5	0.514	0.031	0.514	0.031	1	0.51	0.03
26	Se_Std_1.0	0.992	0.172	0.992	0.172	1	0.99	0.17
27	Se_Std_2.0	1.853	0.320	1.853	0.320	1	1.85	0.32
28	Se_Std_5.0	4.883	0.715	4.883	0.715	1	4.88	0.72
29	wash	0.230	0.535	0.230	0.535	1	0.23	0.54
30	wash	0.030	0.050	0.030	0.050	1	0.03	0.05
31	1b_leaves	9.820	1.622	10.930	1.805	120	> calib	> calib
32	1b_roots	0.370	0.004	0.218	0.002	120	< PQL	< PQL
33	1c_leaves	4.302	0.309	4.788	0.344	120	574.50	41.27
34	1c_roots	5.744	0.593	6.392	0.660	120	767.10	79.24
35	2b_leaves	6.319	0.426	7.033	0.474	120	> calib	> calib
36	2b_roots	0.136	0.063	0.080	0.037	120	< PQL	< PQL
37	2d_leaves	0.377	0.071	0.222	0.042	120	< PQL	< PQL
38	2d_roots	0.181	0.079	0.107	0.047	120	12.79	5.59
39	1a_leaves	0.457	0.039	0.269	0.023	1200	< PQL	< PQL
40	1a_roots	0.553	0.336	0.326	0.198	1200	390.64	237.35
41	wash	0.007	0.011	0.007	0.011	1	0.01	0.01
42	Se_Std_0	0.138	0.102	0.138	0.102	1	0.14	0.10
43	Se_Std_0.5	0.457	0.088	0.457	0.088	1	0.46	0.09
44	Se_Std_1	0.858	0.125	0.858	0.125	1	0.86	0.13
45	Se_Std_2	1.536	0.248	1.536	0.248	1	1.54	0.25
46	Se_Std_5	4.129	0.822	4.129	0.822	1	4.13	0.82
47	wash	0.426	0.735	0.426	0.735	1	0.43	0.74
48	wash	0.033	0.032	0.033	0.032	1	0.03	0.03
49	1e_leaves	1.092	0.169	1.098	0.170	1200	1318.14	204.00
50	1e_roots	0.053	0.124	0.040	0.093	1200	< PQL	< PQL
51	2c_leaves	0.549	0.025	0.411	0.019	1200	492.69	22.23
52	2c_roots	0.090	0.113	0.067	0.085	1200	< PQL	< PQL
53	3a_leaves	1.809	0.009	1.529	0.008	1200	1834.52	9.32
54	3a_roots	0.132	0.129	0.099	0.097	1200	< PQL	< PQL
55	3e_leaves	1.077	0.121	0.806	0.091	1200	966.97	108.61
56	3e_roots	0.166	0.111	0.124	0.083	1200	< PQL	< PQL
57	3f_leaves	0.078	0.123	0.058	0.092	1200	< PQL	< PQL
58	3f_roots	0.083	0.139	0.062	0.104	1200	< PQL	< PQL
59	wash	-0.030	0.014	-0.030	0.014	1	-0.03	0.01
60	Se_Std_0	0.145	0.137	0.145	0.137	1	0.15	0.14
61	Se_Std_0.5	0.404	0.156	0.404	0.156	1	0.40	0.16
62	Se_Std_1	1.077	0.015	1.077	0.015	1	1.08	0.01
63	Se_Std_2	1.787	0.201	1.787	0.201	1	1.79	0.20
64	Se_Std_5	4.509	0.276	4.509	0.276	1	4.51	0.28
65	wash	0.201	0.144	0.201	0.144	1	0.20	0.14

Table A.8.: A1 analytical data - HG-FIAS measurement I (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
66	wash	0.034	0.053	0.034	0.053	1	0.03	0.05
67	6a_leaves	0.234	0.035	0.227	0.034	1200	< PQL	< PQL
68	6a_roots	-0.030	0.011	-0.029	0.010	1200	< PQL	< PQL
69	6b_leaves	0.295	0.055	0.286	0.053	1200	< PQL	< PQL
70	6b_roots	0.221	0.048	0.214	0.047	1200	< PQL	< PQL
71	6c_leaves	0.246	0.049	0.238	0.048	1200	< PQL	< PQL
72	6c_roots	0.143	0.168	0.139	0.163	1200	< PQL	< PQL
73	6d_leaves	0.188	0.156	0.182	0.151	1200	< PQL	< PQL
74	6d_roots	0.042	0.069	0.041	0.067	1200	< PQL	< PQL
75	RA_leaves	0.552	0.024	0.535	0.023	1200	642.18	27.97
76	RA_roots	3.812	0.033	3.695	0.032	1200	4434.19	38.66
77	wash	0.131	0.197	0.131	0.197	1	0.13	0.20
78	wash	0.015	0.022	0.015	0.022	1	0.02	0.02
79	HCl_Blank	0.118	0.018	0.131	0.020	6	0.79	0.12
80	Trace Metal 252 µg/L	0.960	0.086	1.133	0.101	240	271.93	24.25
81	wash	-0.021	0.061	-0.021	0.061	1	-0.02	0.06
82	Se_Std_0	0.003	0.091	0.003	0.091	1	0.00	0.09
83	Se_Std_0.5	0.305	0.003	0.305	0.003	1	0.31	0.00
84	Se_Std_1.0	0.797	0.119	0.797	0.119	1	0.80	0.12
85	Se_Std_2.0	1.438	0.519	1.438	0.519	1	1.44	0.52
86	Se_Std_5.0	4.674	1.356	4.674	1.356	1	4.67	1.36
87	wash	0.965	1.409	0.965	1.409	1	0.97	1.41
88	wash	0.049	0.095	0.049	0.095	1	0.05	0.10

Table A.9.: A1 analytical data - HG-FIAS measurement II

Technique	AA FIAS-MHS	
Spectrometer Model	Aanalyst 200 S/N 200S6110908	
Autosampler Model	AS-90plus	
Batch ID	Pflanzenaufschlüsse	
Results Data Set	Nothstein_2013_04_29	
Date Measured	29.04.2013	
Method Name	Se Nothstein 5repl	
correl. coeff.	PQL (= lowest calib-10 %)	0.450
0.999409	LOQ (= 7-wash)	-0.140
calib. slope	LOD (= 3-wash)	-0.060
0.03272	analytical quality [%]	98.893

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0017	0.0	0.00	0.00
2	0.5 ppb	0.0146	0.013	0.5	0.45	0.40
3	1.0 ppb	0.0323	0.013	1.0	0.99	0.40
4	2.0 ppb	0.0687	0.0010	2.0	2.10	0.03
5	5.0 ppb	0.1624	0.0039	5.0	4.97	0.12

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.008	0.049	-0.008	0.049	1	-0.01	0.05
2	wash	-0.023	0.042	-0.023	0.042	1	-0.02	0.04
3	HCl Blank	-0.016	0.019	-0.016	0.019	6	-0.10	0.11
4	Trace Metal 252 µg/L	4.181	0.053	4.090	0.051	60	245.42	3.09
5	wash	-0.021	0.031	-0.021	0.031	1	-0.02	0.03
6	Se_Std_0	-0.008	0.028	-0.008	0.028	1	-0.01	0.03
7	Se_Std_0.5	0.444	0.025	0.444	0.025	1	0.44	0.03
8	Se_Std_1	1.030	0.039	1.030	0.039	1	1.03	0.04
9	Se_Std_2	2.163	0.049	2.163	0.049	1	2.16	0.05
10	Se_Std_5	5.073	0.085	5.073	0.085	1	5.07	0.09
11	wash	-0.003	0.041	-0.003	0.041	1	0.00	0.04
12	wash	-0.005	0.019	-0.005	0.019	1	-0.01	0.02
13	2012-09-27 Wheat Std 1567a	0.635	0.041	0.621	0.040	12	7.45	0.49
14	2012-10-19 Wheat Std 1567a	0.969	0.045	0.925	0.043	12	11.10	0.52
15	2012-09-21 1a Shoot	1.908	0.075	1.877	0.074	240	450.41	17.71
16	2012-09-21 1a Root	1.712	0.048	1.684	0.048	240	404.27	11.44
17	2012-09-24 1b Shoot	4.607	0.087	4.819	0.091	240	1156.67	21.95
18	2012-09-24 1b Root	2.090	0.113	2.056	0.111	12	24.67	1.33
19	2012-10-16 1c Shoot	0.140	0.023	0.137	0.023	2400	< PQL	< PQL
20	2012-10-16 1c Root	0.172	0.032	0.168	0.031	2400	< PQL	< PQL
21	2012-09-24 1e Shoot	1.179	0.069	1.153	0.067	1200	1383.71	80.48
22	2012-09-24 1e Root	0.905	0.137	0.864	0.130	12	10.36	1.57
23	wash	-0.027	0.030	-0.027	0.030	1	-0.03	0.03
24	Se_Std_0	-0.043	0.019	-0.043	0.019	1	-0.04	0.02
25	Se_Std_0.5	0.468	0.036	0.468	0.036	1	0.47	0.04
26	Se_Std_1	1.034	0.064	1.034	0.064	1	1.03	0.06
27	Se_Std_2	2.105	0.188	2.105	0.188	1	2.11	0.19
28	Se_Std_5	4.400	0.069	4.400	0.069	1	4.40	0.07
29	wash	0.008	0.067	0.008	0.067	1	0.01	0.07
30	wash	-0.015	0.061	-0.015	0.061	1	-0.01	0.06
31	2012-09-25 2b Shoot	2.732	0.017	2.649	0.016	240	635.82	3.85
32	2012-09-25 2b Root	0.056	0.020	0.051	0.018	12	< PQL	< PQL
33	2012-09-24 2c Shoot	2.021	0.053	1.960	0.052	240	470.42	12.44
34	2012-09-24 2c Root	1.508	0.057	1.389	0.053	240	333.37	12.61
35	2012-10-10 2d Shoot	2.793	0.133	2.709	0.129	12	32.50	1.55
36	2012-10-10 2d Root	0.149	0.019	0.135	0.017	12	< PQL	< PQL
37	2012-09-24 3a Shoot	1.590	0.052	1.542	0.051	1200	1850.25	60.67
38	2012-09-24 3a Root	4.486	0.059	4.704	0.062	12	56.45	0.74
39	2012-09-27 3e Shoot	0.847	0.030	0.769	0.027	1200	922.99	32.79
40	2012-09-27 3e Root	3.475	0.081	3.645	0.085	12	43.74	1.02
41	wash	-0.018	0.018	-0.018	0.018	1	-0.02	0.02
42	Se_Std_0	-0.019	0.018	-0.019	0.018	1	-0.02	0.02
43	Se_Std_0.5	0.506	0.051	0.506	0.051	1	0.51	0.05
44	Se_Std_1	1.095	0.025	1.095	0.025	1	1.10	0.03
45	Se_Std_2	2.222	0.096	2.222	0.096	1	2.22	0.10
46	Se_Std_5	5.045	0.066	5.045	0.066	1	5.04	0.07
47	wash	-0.054	0.029	-0.054	0.029	1	-0.05	0.03
48	wash	-0.053	0.028	-0.053	0.028	1	-0.05	0.03
49	2012-10-19 5a Shoot old	4.626	0.110	4.447	0.105	120	533.68	12.64
50	2012-10-19 5a Root old	1.290	0.026	1.186	0.024	120	142.32	2.86
51	2012-10-19 5d Shoot old	2.054	0.042	1.975	0.040	120	236.95	4.83
52	2012-10-19 5d Root old	1.238	0.045	1.138	0.041	120	136.61	4.95
53	2012-10-19 5d Shoot new	10.927	0.168	10.504	0.161	12	> calib	> calib
54	2012-10-19 5d Root new	7.784	0.164	7.483	0.158	12	> calib	> calib
55	2012-10-19 6b Shoot	1.421	0.065	1.289	0.059	240	309.42	14.04
56	2012-10-19 6b Root	1.091	0.060	0.990	0.054	240	237.65	13.03
57	2012-10-19 6c Shoot	1.416	0.028	1.285	0.026	240	308.29	6.17
58	2012-10-19 6c Root	3.031	0.074	2.914	0.072	12	34.97	0.86
59	wash	-0.054	0.031	-0.054	0.031	1	-0.05	0.03
60	HCl Blank	-0.010	0.032	-0.008	0.026	6	-0.05	0.16
61	Trace Metal 252 µg/L	4.492	0.080	4.217	0.075	60	253.00	4.53
62	wash	-0.017	0.031	-0.017	0.031	1	-0.02	0.03
63	Se_Std_0	-0.017	0.009	-0.017	0.009	1	-0.02	0.01
64	Se_Std_0.5	0.521	0.043	0.521	0.043	1	0.52	0.04
65	Se_Std_1	1.062	0.036	1.062	0.036	1	1.06	0.04
66	Se_Std_2	2.318	0.024	2.318	0.024	1	2.32	0.02
67	Se_Std_5	5.269	0.076	5.269	0.076	1	5.27	0.08
70	wash	-0.014	0.050	-0.014	0.050	1	-0.01	0.05
71	wash	0.004	0.027	0.004	0.027	1	0.00	0.03

A.2. Datasheets experiment A2

A.2.1. A2 Plant Growth Data

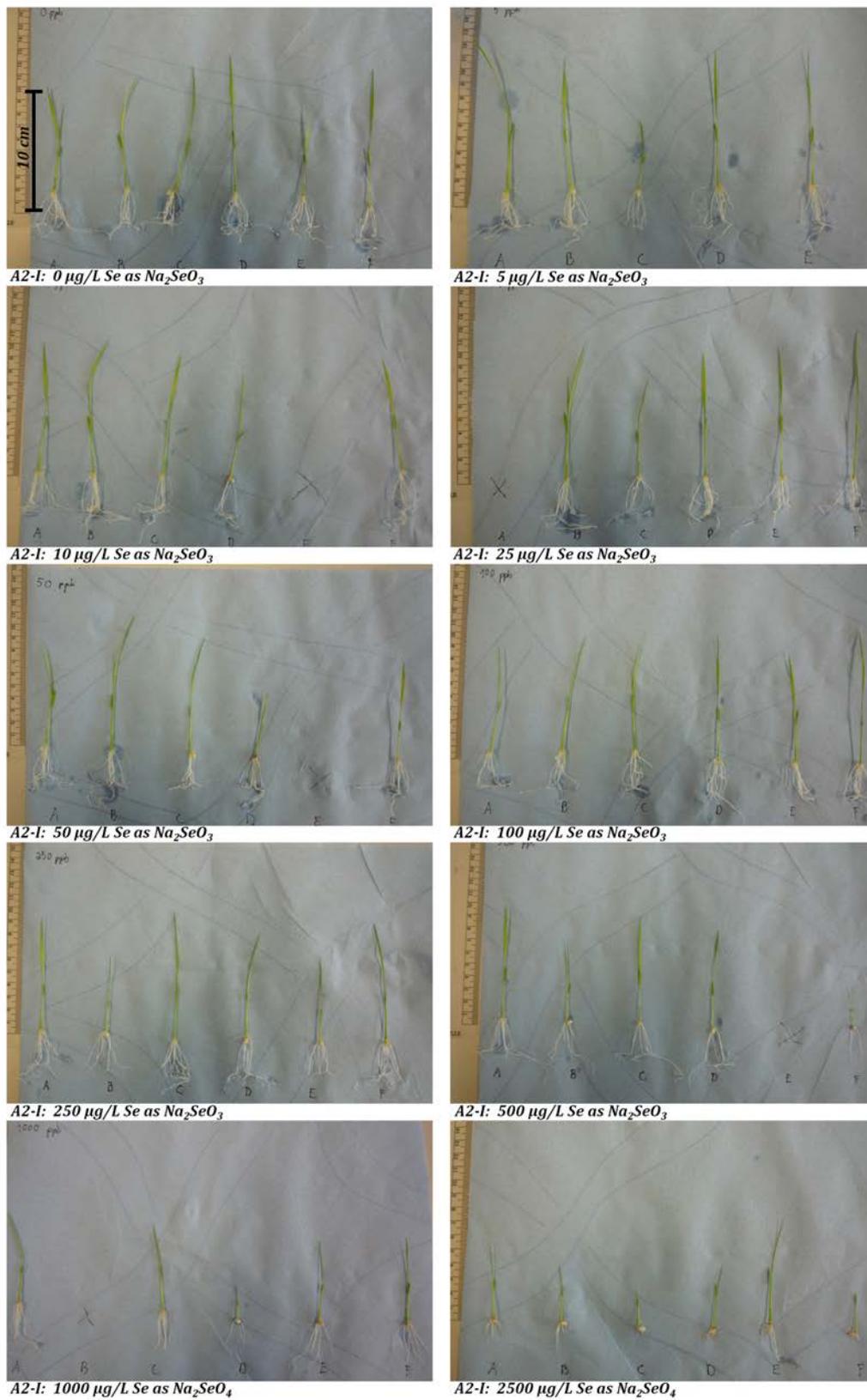
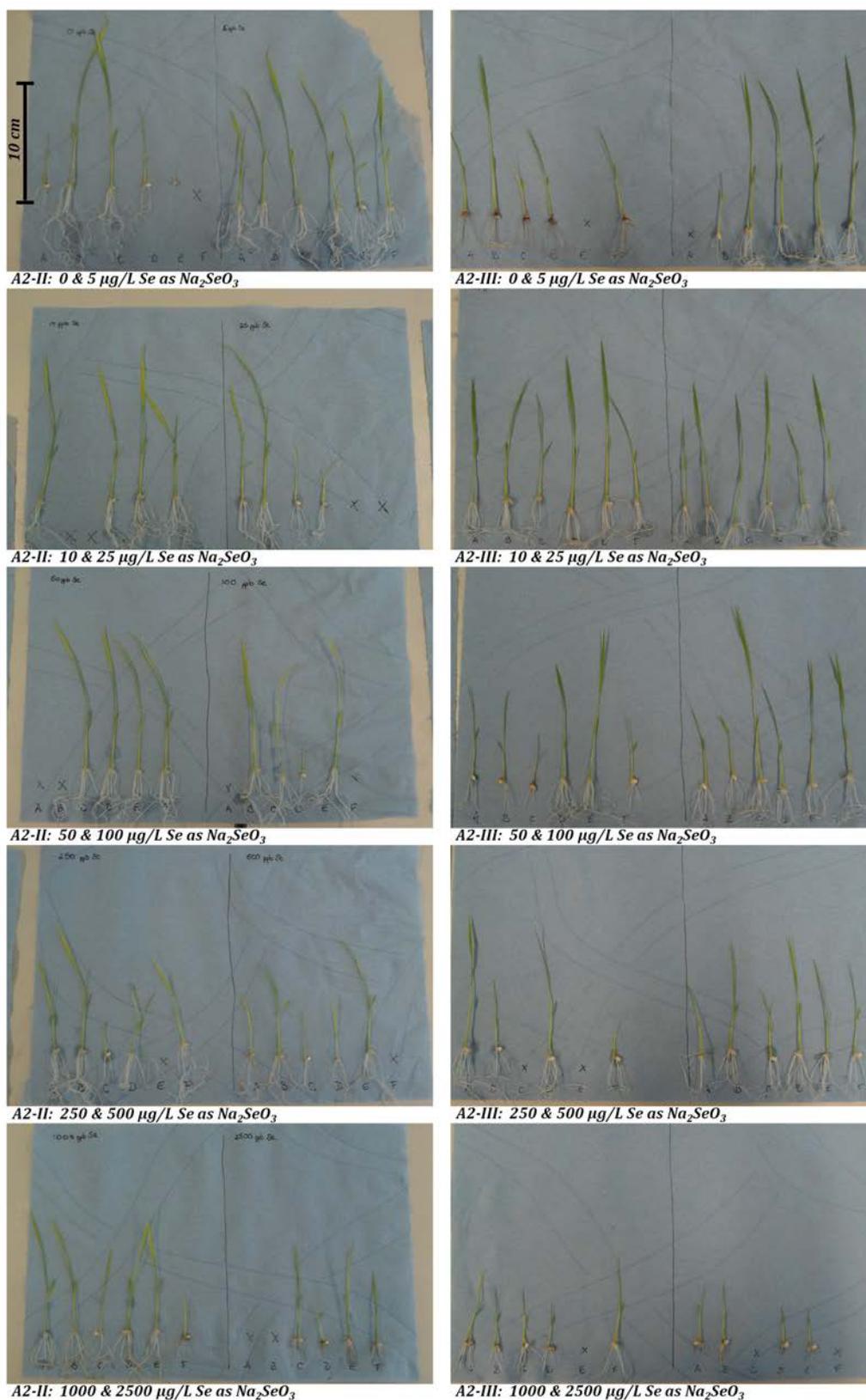


Figure A.1.: A2 photos of harvested plants treated with Na_2SeO_3

Figure A.2.: A2 photos of harvested plants treated with Na_2SeO_3

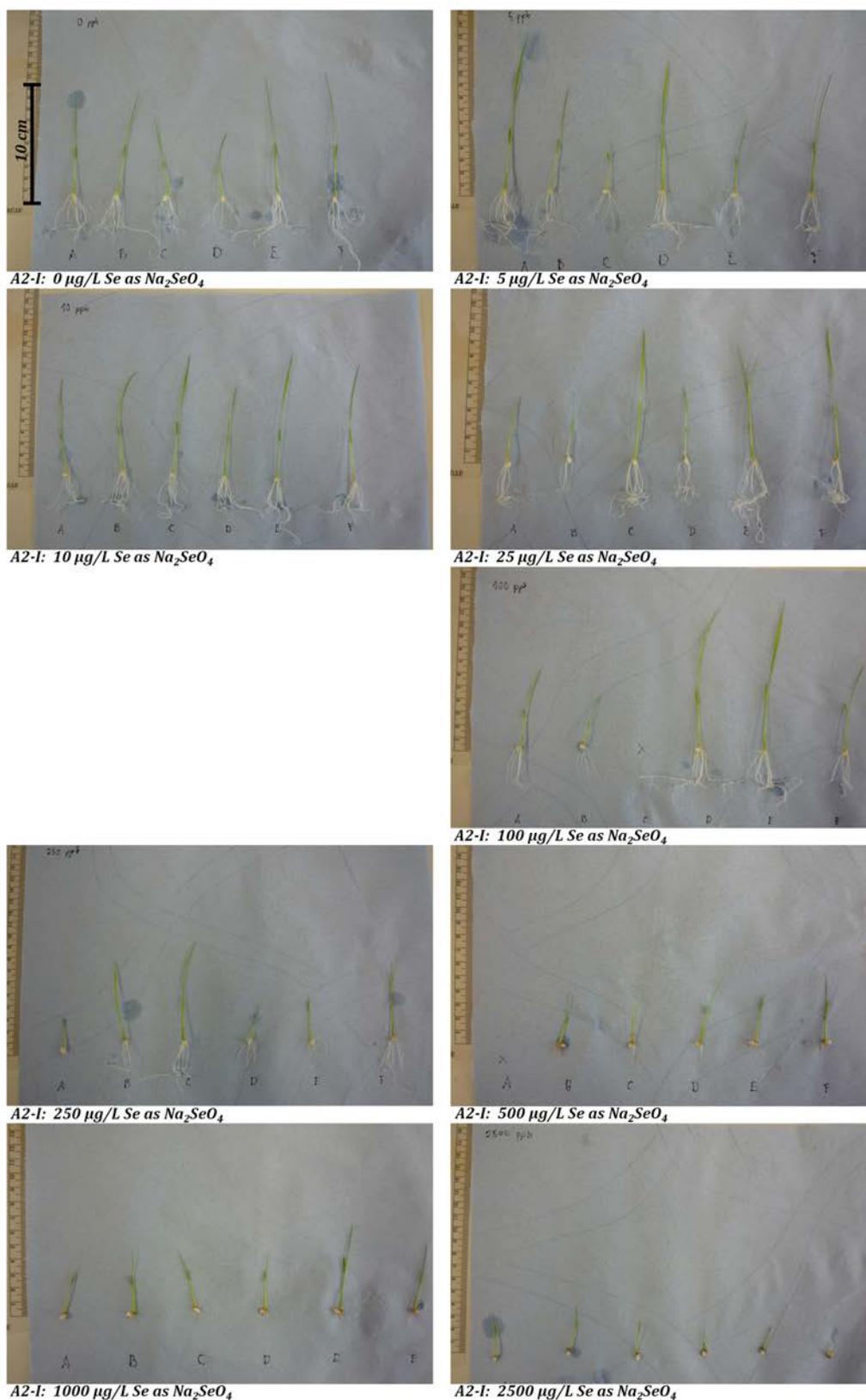


Figure A.3.: A2 photos of harvested plants treated with Na_2SeO_4

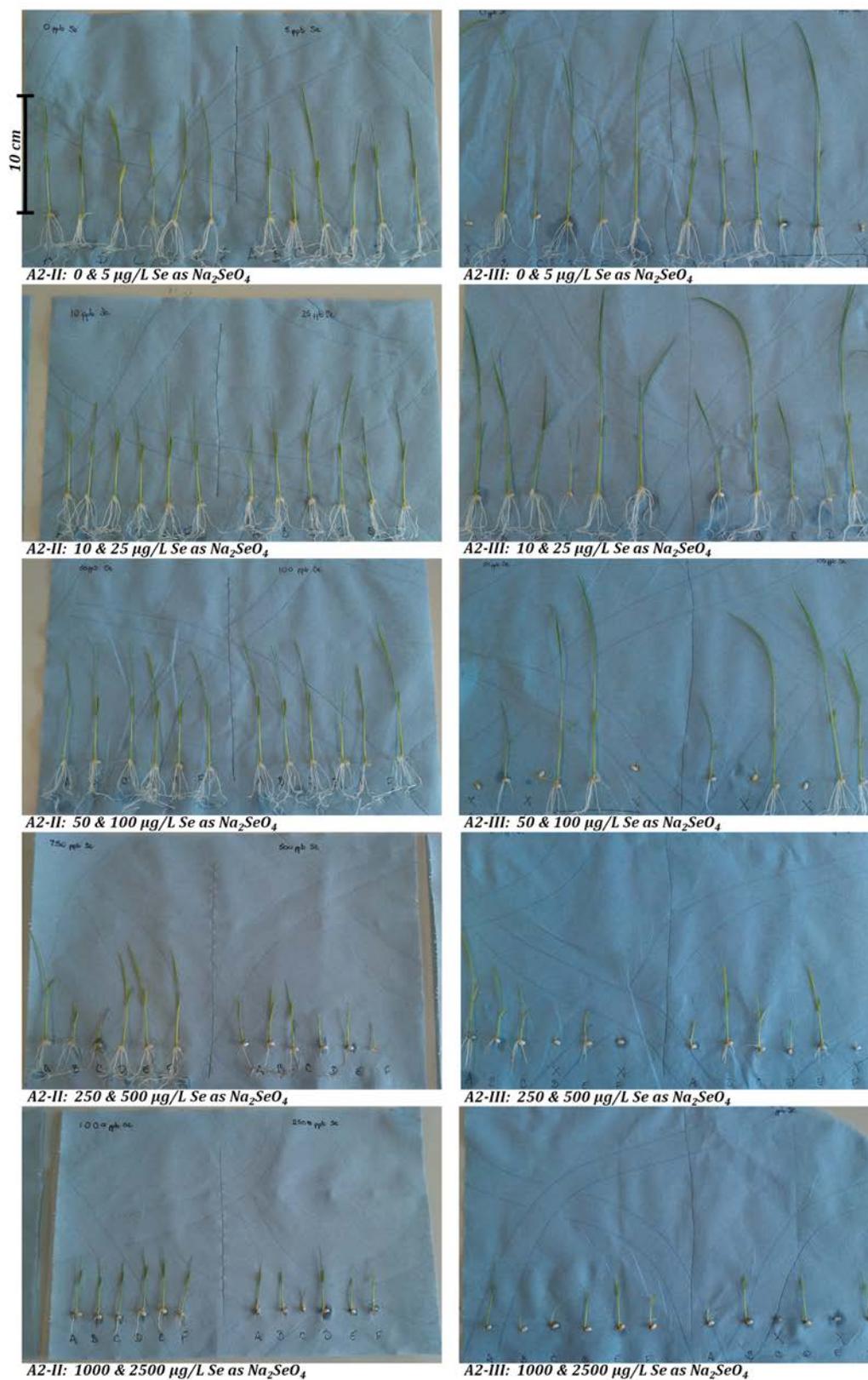


Figure A.4.: A2 photos of harvested plants treated with Na_2SeO_4

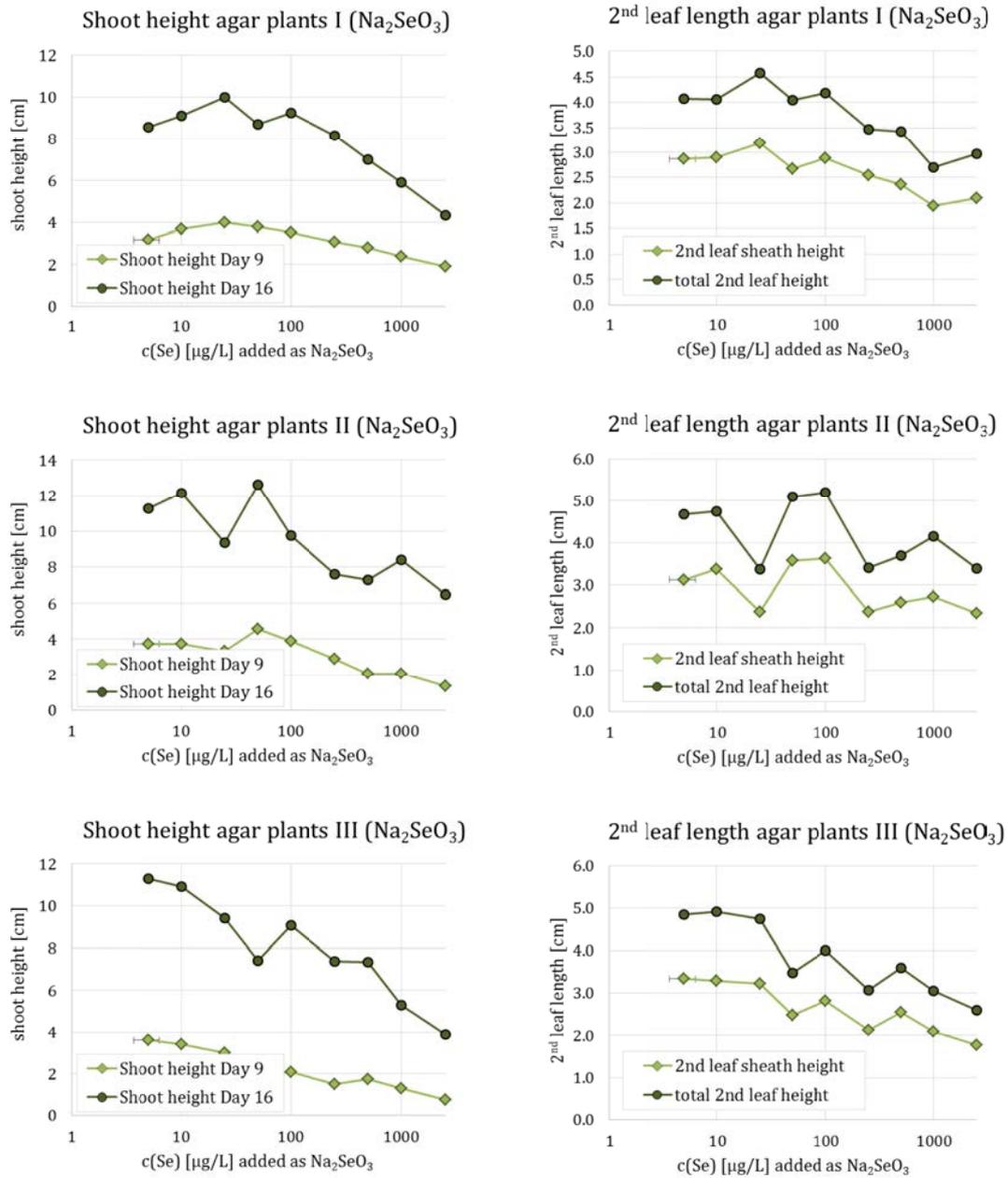


Figure A.5.: A2 shoot heights and 2nd leaf length for Na₂SeO₃ experiments

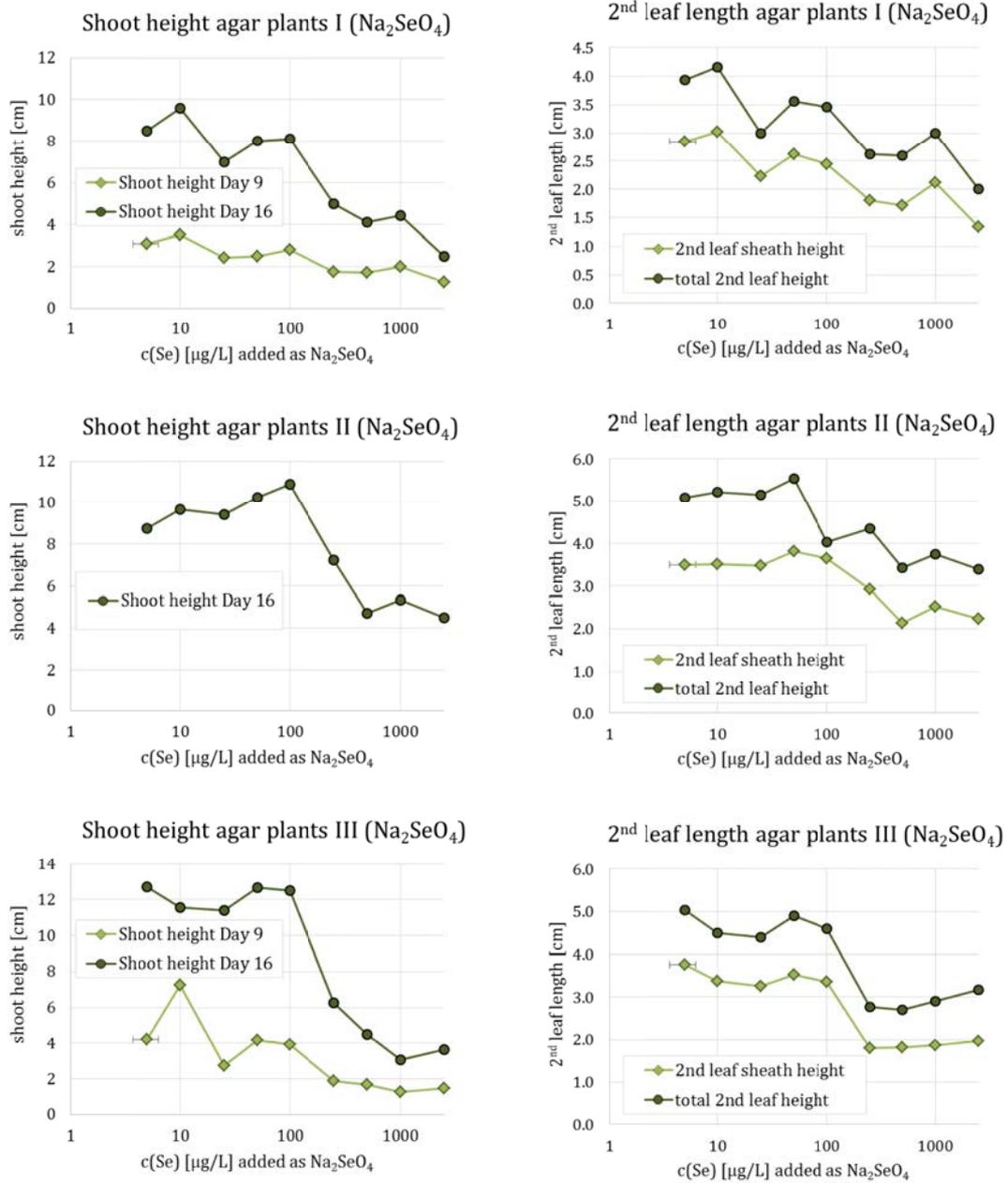


Figure A.6.: A2 shoot heights and 2nd leaf length for Na₂SeO₄ experiments

Table A.10.: A2 plant growth data for Na_2SeO_3 I (Planting Date: 09.01.2013, Bachelor Thesis Matthias von Brasch)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	2.6	1.1	3.7	8.0	0.0327	0.0549	0.0061	0.0084	81.35	84.70
0000B	0	3.0	1.3	4.3	9.0	0.0273	0.0470	0.0046	0.0073	83.15	84.47
0000C	0	3.2	1.4	4.6	10.0	0.0312	0.0608	0.0065	0.0088	79.17	85.53
0000D	0	3.4	1.6	5.0	11.0	0.0401	0.0609	0.0074	0.0104	81.55	82.92
0000E	0	2.5	0.9	3.4	7.0	0.0247	0.0469	0.0042	0.0063	83.00	86.57
0000F	0	3.0	1.4	4.4	10.5	0.0306	0.0309	0.0071	0.0077	76.80	75.08
<i>0000_sum</i>	<i>0</i>	<i>17.7</i>	<i>7.7</i>	<i>25.4</i>	<i>55.5</i>	<i>0.1866</i>	<i>0.3014</i>	<i>0.0359</i>	<i>0.0489</i>	<i>485.00</i>	<i>499.26</i>
<i>0000_mean</i>	<i>0</i>	<i>3.0</i>	<i>1.3</i>	<i>4.2</i>	<i>9.3</i>	<i>0.0311</i>	<i>0.0502</i>	<i>0.0060</i>	<i>0.0082</i>	<i>80.83</i>	<i>83.21</i>
<i>0000_SD</i>	<i>0</i>	<i>0.3</i>	<i>0.2</i>	<i>0.6</i>	<i>1.5</i>	<i>0.0053</i>	<i>0.0113</i>	<i>0.0013</i>	<i>0.0014</i>	<i>2.44</i>	<i>4.16</i>
0005A	5	3.4	1.4	4.8	11.0	0.0338	0.0368	0.0056	0.0081	83.43	77.99
0005B	5	3.0	1.2	4.2	9.5	0.0264	0.0411	0.0072	0.0119	72.73	71.05
0005C	5	1.8	0.7	2.5	5.0	0.0086	0.0239	0.0015	0.0115	82.56	51.88
0005D	5	3.1	1.4	4.5	10.0	0.0224	0.0253	0.0057	0.0062	74.55	75.49
0005E	5	2.9	1.2	4.1	9.5	0.0217	0.0288	0.0053	0.0100	75.58	65.28
0005F	5	3.0	1.3	4.3	6.5	0.0153	0.0316	0.0042	0.0120	72.55	62.03
<i>0005_sum</i>	<i>5</i>	<i>17.2</i>	<i>7.2</i>	<i>24.4</i>	<i>51.5</i>	<i>0.1282</i>	<i>0.1875</i>	<i>0.0295</i>	<i>0.0597</i>	<i>461.40</i>	<i>403.72</i>
<i>0005_mean</i>	<i>5</i>	<i>2.9</i>	<i>1.2</i>	<i>4.1</i>	<i>8.6</i>	<i>0.0214</i>	<i>0.0313</i>	<i>0.0049</i>	<i>0.0100</i>	<i>76.90</i>	<i>67.29</i>
<i>0005_SD</i>	<i>5</i>	<i>0.6</i>	<i>0.3</i>	<i>0.8</i>	<i>2.3</i>	<i>0.0087</i>	<i>0.0067</i>	<i>0.0019</i>	<i>0.0024</i>	<i>4.86</i>	<i>9.64</i>
0010A	10	3.1	1.0	4.1	9.0	0.0223	0.0263	0.0051	0.0073	77.13	72.24
0010B	10	2.9	1.3	4.2	10.5	0.0326	0.0351	0.0068	0.0086	79.14	75.50
0010C	10	2.9	1.0	3.9	9.5	0.0228	0.0165	0.0049	0.0050	78.51	69.70
0010D	10	2.7	1.2	3.9	8.5	0.0130	0.0181	0.0020	0.0047	84.62	74.03
0010E	10	x	x	x	x	x	x	x	x	x	x
0010F	10	2.9	1.3	4.2	8.0	0.0220	0.0172	0.0048	0.0070	78.18	59.30
<i>0010_sum</i>	<i>10</i>	<i>14.5</i>	<i>5.8</i>	<i>20.3</i>	<i>45.5</i>	<i>0.1127</i>	<i>0.1132</i>	<i>0.0236</i>	<i>0.0326</i>	<i>397.58</i>	<i>350.77</i>
<i>0010_mean</i>	<i>10</i>	<i>2.9</i>	<i>1.2</i>	<i>4.1</i>	<i>9.1</i>	<i>0.0225</i>	<i>0.0226</i>	<i>0.0047</i>	<i>0.0065</i>	<i>79.52</i>	<i>70.15</i>
<i>0010_SD</i>	<i>10</i>	<i>0.1</i>	<i>0.2</i>	<i>0.2</i>	<i>1.0</i>	<i>0.0069</i>	<i>0.0080</i>	<i>0.0017</i>	<i>0.0016</i>	<i>2.94</i>	<i>6.44</i>
0025A	25	x	x	x	x	x	x	x	x	x	x
0025B	25	3.5	1.5	5.0	11.0	0.0364	0.0399	0.0082	0.0098	77.47	75.44
0025C	25	3.2	1.5	4.7	8.0	0.0157	0.0273	0.0044	0.0102	71.97	62.64
0025D	25	3.0	1.3	4.3	9.5	0.0274	0.0297	0.0059	0.0072	78.47	75.76
0025E	25	3.1	1.3	4.4	10.0	0.0248	0.0265	0.0060	0.0064	75.81	75.85
0025F	25	3.1	1.4	4.5	11.5	0.0263	0.0235	0.0069	0.0062	73.76	73.62
<i>0025_sum</i>	<i>25</i>	<i>15.9</i>	<i>7.0</i>	<i>22.9</i>	<i>50.0</i>	<i>0.1306</i>	<i>0.1469</i>	<i>0.0314</i>	<i>0.0398</i>	<i>377.48</i>	<i>363.30</i>
<i>0025_mean</i>	<i>25</i>	<i>3.2</i>	<i>1.4</i>	<i>4.6</i>	<i>10.0</i>	<i>0.0261</i>	<i>0.0294</i>	<i>0.0063</i>	<i>0.0080</i>	<i>75.50</i>	<i>72.66</i>
<i>0025_SD</i>	<i>25</i>	<i>0.2</i>	<i>0.1</i>	<i>0.3</i>	<i>1.4</i>	<i>0.0074</i>	<i>0.0063</i>	<i>0.0014</i>	<i>0.0019</i>	<i>2.66</i>	<i>5.68</i>
0050A	50	2.9	1.5	4.4	8.5	0.0225	0.0292	0.0049	0.0081	78.22	72.26
0050B	50	3.3	1.8	5.1	11.5	0.0341	0.0344	0.0077	0.0085	77.42	75.29
0050C	50	2.3	1.1	3.4	9.5	0.0231	0.0359	0.0056	0.0086	75.76	76.04
0050D	50	2.6	1.6	4.2	5.5	0.0211	0.0277	0.0034	0.0067	83.89	75.81
0050E	50	x	x	x	x	x	x	x	x	x	x
0050F	50	2.3	0.8	3.1	8.5	0.0250	0.0314	0.0055	0.0085	78.00	72.93
<i>0050_sum</i>	<i>50</i>	<i>13.4</i>	<i>6.8</i>	<i>20.2</i>	<i>43.5</i>	<i>0.1258</i>	<i>0.1586</i>	<i>0.0271</i>	<i>0.0404</i>	<i>393.29</i>	<i>372.34</i>
<i>0050_mean</i>	<i>50</i>	<i>2.7</i>	<i>1.4</i>	<i>4.0</i>	<i>8.7</i>	<i>0.0252</i>	<i>0.0317</i>	<i>0.0054</i>	<i>0.0081</i>	<i>78.66</i>	<i>74.47</i>
<i>0050_SD</i>	<i>50</i>	<i>0.4</i>	<i>0.4</i>	<i>0.8</i>	<i>2.2</i>	<i>0.0052</i>	<i>0.0034</i>	<i>0.0015</i>	<i>0.0008</i>	<i>3.08</i>	<i>1.75</i>
0100A	100	2.9	1.2	4.1	8.0	0.0154	0.0273	0.0036	0.0105	76.62	61.54
0100B	100	2.8	1.9	4.7	9.0	0.0223	0.0292	0.0063	0.0080	71.75	72.60
0100C	100	3.1	1.3	4.4	9.5	0.0284	0.0290	0.0066	0.0082	76.76	71.72
0100D	100	2.7	1.2	3.9	10.0	0.0280	0.0400	0.0072	0.0111	74.29	72.25
0100E	100	2.9	1.2	4.1	8.5	0.0234	0.0243	0.0056	0.0067	76.07	72.43
0100F	100	2.9	1.0	3.9	10.5	0.0319	0.0417	0.0090	0.0104	71.79	75.06
<i>0100_sum</i>	<i>100</i>	<i>17.3</i>	<i>7.8</i>	<i>25.1</i>	<i>55.5</i>	<i>0.1494</i>	<i>0.1915</i>	<i>0.0383</i>	<i>0.0549</i>	<i>447.27</i>	<i>425.60</i>
<i>0100_mean</i>	<i>100</i>	<i>2.9</i>	<i>1.3</i>	<i>4.2</i>	<i>9.3</i>	<i>0.0249</i>	<i>0.0319</i>	<i>0.0064</i>	<i>0.0092</i>	<i>74.55</i>	<i>70.93</i>
<i>0100_SD</i>	<i>100</i>	<i>0.1</i>	<i>0.3</i>	<i>0.3</i>	<i>0.9</i>	<i>0.0058</i>	<i>0.0072</i>	<i>0.0018</i>	<i>0.0018</i>	<i>2.33</i>	<i>4.75</i>
0250A	250	2.8	0.8	3.6	8.5	0.0190	0.0262	0.0051	0.0068	73.16	74.05
0250B	250	1.9	0.6	2.5	6.0	0.0119	0.0239	0.0032	0.0110	73.11	53.97
0250C	250	3.1	1.4	4.5	10.0	0.0272	0.0354	0.0076	0.0099	72.06	72.03
0250D	250	2.6	1.2	3.8	8.5	0.0167	0.0221	0.0049	0.0114	70.66	48.42
0250E	250	1.9	0.4	2.3	6.5	0.0096	0.0212	0.0027	0.0119	71.88	43.87
0250F	250	3.0	1.1	4.1	9.5	0.0232	0.0267	0.0076	0.0085	67.24	68.16

Table A.11.: A2 plant growth data for Na_2SeO_3 I (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250_sum	250	15.3	5.5	20.8	49.0	0.1076	0.1555	0.0311	0.0595	428.10	360.50
0250_mean	250	2.6	0.9	3.5	8.2	0.0179	0.0259	0.0052	0.0099	71.35	60.08
0250_SD	250	0.5	0.4	0.9	1.6	0.0067	0.0051	0.0021	0.0020	2.21	12.96
0500A	500	2.8	1.3	4.1	9.0	0.0238	0.0294	0.0065	0.0076	72.69	74.15
0500B	500	2.2	1.1	3.3	6.5	0.0101	0.0194	0.0021	0.0073	79.21	62.37
0500C	500	2.9	1.4	4.3	8.5	0.0168	0.0155	0.0061	0.0051	63.69	67.10
0500D	500	2.6	1.1	3.7	8.0	0.0118	0.0174	0.0030	0.0106	74.58	39.08
0500E	500	x	x	x	x	x	x	x	x	x	x
0500F	500	1.3	0.4	1.7	3.0	0.0022	0.0177	0.0001	0.0136	95.45	23.16
0500_sum	500	11.8	5.3	17.1	35.0	0.0647	0.0994	0.0178	0.0442	385.62	265.86
0500_mean	500	2.4	1.1	3.4	7.0	0.0129	0.0199	0.0036	0.0088	77.12	53.17
0500_SD	500	0.7	0.4	1.0	2.4	0.0080	0.0055	0.0027	0.0033	11.69	21.32
1000A	1000	2.1	0.7	2.8	7.5	0.0207	0.0192	0.0055	0.0056	73.43	70.83
1000B	1000	x	x	x	x	x	x	x	x	x	x
1000C	1000	2.5	1.1	3.6	7.0	0.0182	0.0216	0.0052	0.0049	71.43	77.31
1000D	1000	0.9	0.4	1.3	2.5	0.0050	0.0173	0.0012	0.0100	76.00	42.20
1000E	1000	2.1	0.7	2.8	6.0	0.0133	0.0193	0.0035	0.0093	73.68	51.81
1000F	1000	2.1	0.9	3.0	6.5	0.0181	0.0189	0.0059	0.0056	67.40	70.37
1000_sum	1000	9.7	3.8	13.5	29.5	0.0753	0.0963	0.0213	0.0354	361.95	312.53
1000_mean	1000	1.9	0.8	2.7	5.9	0.0151	0.0193	0.0043	0.0071	72.39	62.51
1000_SD	1000	0.6	0.3	0.8	2.0	0.0062	0.0015	0.0019	0.0024	3.22	14.81
2500A	2500	1.9	0.8	2.7	5.0	0.0125	0.0242	0.0033	0.0105	73.60	56.61
2500B	2500	1.8	0.9	2.7	4.0	0.0071	0.0235	0.0028	0.0117	60.56	50.21
2500C	2500	1.4	0.6	2.0	2.5	0.0062	0.0200	0.0018	0.0112	70.97	44.00
2500D	2500	2.0	1.0	3.0	4.5	0.0087	0.0265	0.0024	0.0111	72.41	58.11
2500E	2500	2.6	1.3	3.9	7.5	0.0213	0.0168	0.0074	0.0045	65.26	73.21
2500F	2500	2.9	0.6	3.5	2.5	0.0065	0.0198	0.0016	0.0094	75.38	52.53
2500_sum	2500	12.6	5.2	17.8	26.0	0.0623	0.1308	0.0193	0.0584	418.19	334.68
2500_mean	2500	2.1	0.9	3.0	4.3	0.0104	0.0218	0.0032	0.0097	69.70	55.78
2500_SD	2500	0.6	0.3	0.7	1.9	0.0058	0.0035	0.0021	0.0027	5.65	9.90

Table A.12.: A2 plant growth data for Na₂SeO₃ II (Planting Date: 29.05.2013, Experiment Repetition Alexandra Nothstein)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	2.4	0.9	3.3	4.5	0.0122	0.0314	0.0017	0.0136	86.07	56.69
0000B	0	3.7	1.7	5.4	16.0	0.0453	0.0439	0.0088	0.0090	80.57	79.50
0000C	0	3.5	1.5	5.0	14.5	0.0394	0.0342	0.0068	0.0073	82.74	78.65
0000D	0	2.0	0.7	2.7	7.0	0.0099	0.0248	0.0022	0.0103	77.78	58.47
0000E	0	1.1	0.8	1.9	2.5	0.0016	0.0215	0.0001	0.0143	93.75	33.49
0000F	0	x	x	x	x	x	x	x	x	x	x
<i>0000_sum</i>	<i>0</i>	<i>12.7</i>	<i>5.6</i>	<i>18.3</i>	<i>44.5</i>	<i>0.1084</i>	<i>0.1558</i>	<i>0.0196</i>	<i>0.0545</i>	<i>420.91</i>	<i>306.80</i>
<i>0000_mean</i>	<i>0</i>	<i>2.5</i>	<i>1.1</i>	<i>3.7</i>	<i>8.9</i>	<i>0.0217</i>	<i>0.0312</i>	<i>0.0039</i>	<i>0.0109</i>	<i>84.18</i>	<i>61.36</i>
<i>0000_SD</i>	<i>0</i>	<i>1.1</i>	<i>0.4</i>	<i>1.5</i>	<i>6.0</i>	<i>0.0194</i>	<i>0.0087</i>	<i>0.0037</i>	<i>0.0030</i>	<i>6.15</i>	<i>18.94</i>
0005A	5	2.2	1.1	3.3	8.5	0.0327	0.0319	0.0073	0.0076	77.68	76.18
0005B	5	3.2	1.7	4.9	11.5	0.0260	0.0161	0.0050	0.0056	80.77	65.22
0005C	5	3.5	1.6	5.1	14.5	0.0392	0.0172	0.0089	0.0073	77.30	57.56
0005D	5	3.5	1.7	5.2	13.0	0.0328	0.0196	0.0069	0.0070	78.96	64.29
0005E	5	2.8	1.4	4.2	8.5	0.0171	0.0221	0.0036	0.0068	78.95	69.23
0005F	5	3.6	1.8	5.4	11.5	0.0275	0.0122	0.0076	0.0072	72.36	40.98
<i>0005_sum</i>	<i>5</i>	<i>18.8</i>	<i>9.3</i>	<i>28.1</i>	<i>67.5</i>	<i>0.1753</i>	<i>0.1191</i>	<i>0.0393</i>	<i>0.0415</i>	<i>466.02</i>	<i>373.45</i>
<i>0005_mean</i>	<i>5</i>	<i>3.1</i>	<i>1.6</i>	<i>4.7</i>	<i>11.3</i>	<i>0.0292</i>	<i>0.0199</i>	<i>0.0066</i>	<i>0.0069</i>	<i>77.67</i>	<i>62.24</i>
<i>0005_SD</i>	<i>5</i>	<i>0.5</i>	<i>0.3</i>	<i>0.8</i>	<i>2.4</i>	<i>0.0075</i>	<i>0.0068</i>	<i>0.0019</i>	<i>0.0007</i>	<i>2.87</i>	<i>12.08</i>
0010A	10	3.8	1.5	5.3	13.0	0.0443	0.0374	0.0082	0.0068	81.49	81.82
0010B	10	x	x	x	x	x	x	x	x	x	x
0010C	10	x	x	x	x	x	x	x	x	x	x
0010D	10	3.2	1.5	4.7	12.0	0.0356	0.0367	0.0058	0.0071	83.71	80.65
0010E	10	3.7	1.5	5.2	13.5	0.0436	0.0459	0.0084	0.0088	80.73	80.83
0010F	10	2.8	1.0	3.8	10.0	0.0346	0.0427	0.0056	0.0073	83.82	82.90
<i>0010_sum</i>	<i>10</i>	<i>13.5</i>	<i>5.5</i>	<i>19.0</i>	<i>48.5</i>	<i>0.1581</i>	<i>0.1627</i>	<i>0.0280</i>	<i>0.0300</i>	<i>329.75</i>	<i>326.20</i>
<i>0010_mean</i>	<i>10</i>	<i>3.4</i>	<i>1.4</i>	<i>4.8</i>	<i>12.1</i>	<i>0.0395</i>	<i>0.0407</i>	<i>0.0070</i>	<i>0.0075</i>	<i>82.44</i>	<i>81.55</i>
<i>0010_SD</i>	<i>10</i>	<i>0.5</i>	<i>0.3</i>	<i>0.7</i>	<i>1.5</i>	<i>0.0051</i>	<i>0.0044</i>	<i>0.0015</i>	<i>0.0009</i>	<i>1.56</i>	<i>1.04</i>
0025A	25	2.7	1.1	3.8	10.5	0.0256	0.0349	0.0049	0.0072	80.86	79.37
0025B	25	3.7	1.6	5.3	16.0	0.0490	0.0392	0.0103	0.0096	78.98	75.51
0025C	25	1.8	0.6	2.4	5.5	0.0095	0.0295	0.0012	0.0111	87.37	62.37
0025D	25	1.3	0.7	2.0	5.5	0.0103	0.0182	0.0019	0.0036	81.55	80.22
0025E	25	x	x	x	x	x	x	x	x	x	x
0025F	25	x	x	x	x	x	x	x	x	x	x
<i>0025_sum</i>	<i>25</i>	<i>9.5</i>	<i>4.0</i>	<i>13.5</i>	<i>37.5</i>	<i>0.0944</i>	<i>0.1218</i>	<i>0.0183</i>	<i>0.0315</i>	<i>328.76</i>	<i>297.47</i>
<i>0025_mean</i>	<i>25</i>	<i>2.4</i>	<i>1.0</i>	<i>3.4</i>	<i>9.4</i>	<i>0.0236</i>	<i>0.0305</i>	<i>0.0046</i>	<i>0.0079</i>	<i>82.19</i>	<i>74.37</i>
<i>0025_SD</i>	<i>25</i>	<i>1.1</i>	<i>0.5</i>	<i>1.5</i>	<i>5.0</i>	<i>0.0185</i>	<i>0.0091</i>	<i>0.0041</i>	<i>0.0033</i>	<i>3.62</i>	<i>8.26</i>
0050A	50	x	x	x	x	x	x	x	x	x	x
0050B	50	x	x	x	x	x	x	x	x	x	x
0050C	50	3.7	1.5	5.2	12.0	0.0413	0.0348	0.0080	0.0079	80.63	77.30
0050D	50	3.5	1.6	5.1	12.5	0.0386	0.0324	0.0085	0.0072	77.98	77.78
0050E	50	3.5	1.5	5.0	12.5	0.0337	0.0284	0.0066	0.0064	80.42	77.46
0050F	50	3.6	1.5	5.1	13.5	0.0425	0.0330	0.0082	0.0074	80.71	77.58
<i>0050_sum</i>	<i>50</i>	<i>14.3</i>	<i>6.1</i>	<i>20.4</i>	<i>50.5</i>	<i>0.1561</i>	<i>0.1286</i>	<i>0.0313</i>	<i>0.0289</i>	<i>319.73</i>	<i>310.12</i>
<i>0050_mean</i>	<i>50</i>	<i>3.6</i>	<i>1.5</i>	<i>5.1</i>	<i>12.6</i>	<i>0.0390</i>	<i>0.0322</i>	<i>0.0078</i>	<i>0.0072</i>	<i>79.93</i>	<i>77.53</i>
<i>0050_SD</i>	<i>50</i>	<i>0.1</i>	<i>0.1</i>	<i>0.1</i>	<i>0.6</i>	<i>0.0039</i>	<i>0.0027</i>	<i>0.0008</i>	<i>0.0006</i>	<i>1.31</i>	<i>0.20</i>
0100A	100	x	x	x	x	x	x	x	x	x	x
0100B	100	3.7	1.6	5.3	11.5	0.0386	0.0207	0.0083	0.0098	78.50	52.66
0100C	100	3.6	1.5	5.1	10.5	0.0212	0.0186	0.0047	0.0065	77.83	65.05
0100D	100	x	x	x	3.5	0.0044	0.0209	0.0013	0.0137	70.45	34.45
0100E	100	3.6	1.6	5.2	13.5	0.0293	0.0113	0.0065	0.0084	77.82	25.66
0100F	100	x	x	x	x	x	x	x	x	x	x
<i>0100_sum</i>	<i>100</i>	<i>10.9</i>	<i>4.7</i>	<i>15.6</i>	<i>39.0</i>	<i>0.0935</i>	<i>0.0715</i>	<i>0.0208</i>	<i>0.0384</i>	<i>304.60</i>	<i>177.82</i>
<i>0100_mean</i>	<i>100</i>	<i>3.6</i>	<i>1.6</i>	<i>5.2</i>	<i>9.8</i>	<i>0.0234</i>	<i>0.0179</i>	<i>0.0052</i>	<i>0.0096</i>	<i>76.15</i>	<i>44.46</i>
<i>0100_SD</i>	<i>100</i>	<i>0.1</i>	<i>0.1</i>	<i>0.1</i>	<i>4.3</i>	<i>0.0145</i>	<i>0.0045</i>	<i>0.0030</i>	<i>0.0030</i>	<i>3.81</i>	<i>17.75</i>
0250A	250	2.3	0.9	3.2	8.0	0.0208	0.0197	0.0047	0.0068	77.40	65.48
0250B	250	3.5	1.5	5.0	12.0	0.0387	0.0285	0.0094	0.0080	75.71	71.93
0250C	250	1.8	0.8	2.6	3.0	0.0072	0.0220	0.0012	0.0110	83.33	50.00
0250D	250	1.9	1.1	3.0	6.0	0.0157	0.0215	0.0035	0.0056	77.71	73.95
0250E	250	x	x	x	x	x	x	x	x	x	x
0250F	250	2.4	0.9	3.3	9.0	0.0253	0.0270	0.0054	0.0071	78.66	73.70

Table A.13.: A2 plant growth data for Na_2SeO_3 II (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250_sum	250	11.9	5.2	17.1	38.0	0.1077	0.1187	0.0242	0.0385	392.81	335.07
0250_mean	250	2.4	1.0	3.4	7.6	0.0215	0.0237	0.0048	0.0077	78.56	67.01
0250_SD	250	0.7	0.3	0.9	3.4	0.0117	0.0038	0.0030	0.0020	2.87	10.11
0500A	500	2.2	1.1	3.3	5.5	0.0136	0.0189	0.0033	0.0064	75.74	66.14
0500B	500	3.4	1.5	4.9	9.5	0.0221	0.0097	0.0012	0.0057	94.57	41.24
0500C	500	2.0	1.1	3.1	4.5	0.0056	0.0241	0.0020	0.0082	64.29	65.98
0500D	500	1.9	0.4	2.3	6.0	0.0082	0.0202	0.0066	0.0071	19.51	64.85
0500E	500	3.5	1.4	4.9	11.0	0.0266	0.0205	0.0063	0.0113	76.32	44.88
0500F	500	x	x	x	x	x	x	x	x	x	x
0500_sum	500	13.0	5.5	18.5	36.5	0.0761	0.0934	0.0194	0.0387	330.42	283.08
0500_mean	500	2.6	1.1	3.7	7.3	0.0152	0.0187	0.0039	0.0077	66.08	56.62
0500_SD	500	0.8	0.4	1.2	2.8	0.0090	0.0054	0.0025	0.0022	28.20	12.45
1000A	1000	3.1	1.8	4.9	10.5	0.0250	0.0196	0.0088	0.0071	64.80	63.78
1000B	1000	3.0	1.7	4.7	10.0	0.0252	0.0107	0.0080	0.0066	68.25	38.32
1000C	1000	2.4	1.5	3.9	7.0	0.0116	0.0236	0.0039	0.0081	66.38	65.68
1000D	1000	3.2	1.4	4.6	9.5	0.0256	0.0168	0.0075	0.0067	70.70	60.12
1000E	1000	3.2	1.5	4.7	10.0	0.0239	0.0265	0.0084	0.0074	64.85	72.08
1000F	1000	1.5	0.7	2.2	3.5	0.0049	0.0084	0.0017	0.0029	65.31	65.48
1000_sum	1000	16.4	8.6	25.0	50.5	0.1162	0.1056	0.0383	0.0388	400.30	365.44
1000_mean	1000	2.7	1.4	4.2	8.4	0.0194	0.0176	0.0064	0.0065	66.72	60.91
1000_SD	1000	0.7	0.4	1.0	2.7	0.0089	0.0071	0.0029	0.0018	2.35	11.73
2500A	2500	x	x	x	x	x	x	x	x	x	x
2500B	2500	x	x	x	x	x	x	x	x	x	x
2500C	2500	2.6	1.2	3.8	8.0	0.0203	0.0224	0.0083	0.0082	59.11	63.39
2500D	2500	1.7	0.9	2.6	3.5	0.0066	0.0232	0.0024	0.0104	63.64	55.17
2500E	2500	2.7	1.3	4.0	8.5	0.0222	0.0108	0.0080	0.0058	63.96	46.30
2500F	2500	2.4	0.8	3.2	6.0	0.0191	0.0219	0.0070	0.0072	63.35	67.12
2500_sum	2500	9.4	4.2	13.6	26.0	0.0682	0.0783	0.0257	0.0316	250.06	231.98
2500_mean	2500	2.4	1.1	3.4	6.5	0.0171	0.0196	0.0064	0.0079	62.52	58.00
2500_SD	2500	0.5	0.2	0.6	2.3	0.0071	0.0059	0.0027	0.0019	2.28	9.26

Table A.14.: A2 plant growth data for Na₂SeO₃ III (Planting Date: 10.07.2013, Experiment Repetition Alexandra Nothstein)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	2.5	1.2	3.7	8.0	0.0207	0.0240	0.0054	0.0060	73.91	75.00
0000B	0	3.4	1.3	4.7	13.0	0.0354	0.0183	0.0084	0.0038	76.27	79.23
0000C	0	1.9	1.2	3.1	5.0	0.0109	0.0194	0.0027	0.0066	75.23	65.98
0000D	0	2.6	0.9	3.5	8.0	0.0171	0.0141	0.0042	0.0056	75.44	60.28
0000E	0	x	x	x	x	x	x	x	x	x	x
0000F	0	3.3	1.3	4.6	8.0	0.0153	0.0099	0.0033	0.0047	78.43	52.53
0000_sum	0	13.7	5.9	19.6	42.0	0.0994	0.0857	0.0240	0.0267	379.28	333.02
0000_mean	0	2.7	1.2	3.9	8.4	0.0199	0.0171	0.0048	0.0053	75.86	66.60
0000_SD	0	0.6	0.2	0.7	2.9	0.0094	0.0054	0.0023	0.0011	1.67	10.82
0005A	5	x	x	x	x	x	x	x	x	x	x
0005B	5	2.4	1.2	3.6	5.0	0.0071	0.0258	0.0012	0.0143	83.10	44.57
0005C	5	3.6	1.6	5.2	12.0	0.0348	0.0318	0.0065	0.0071	81.32	77.67
0005D	5	3.5	1.5	5.0	12.5	0.0368	0.0370	0.0074	0.0079	79.89	78.65
0005E	5	3.6	1.7	5.3	13.0	0.0382	0.0302	0.0077	0.0066	79.84	78.15
0005F	5	3.6	1.6	5.2	14.0	0.0395	0.0342	0.0081	0.0086	79.49	74.85
0005_sum	5	16.7	7.6	24.3	56.5	0.1564	0.1590	0.0309	0.0445	403.65	353.89
0005_mean	5	3.3	1.5	4.9	11.3	0.0313	0.0318	0.0062	0.0089	80.73	70.78
0005_SD	5	0.5	0.2	0.7	3.6	0.0136	0.0042	0.0028	0.0031	1.50	14.72
0010A	10	3.5	1.8	5.3	10.0	0.0270	0.0283	0.0057	0.0066	78.89	76.68
0010B	10	3.1	1.6	4.7	10.5	0.0291	0.0388	0.0052	0.0080	82.13	79.38
0010C	10	3.1	1.6	4.7	8.5	0.0160	0.0192	0.0028	0.0036	82.50	81.25
0010D	10	3.5	1.7	5.2	13.0	0.0436	0.0347	0.0083	0.0081	80.96	76.66
0010E	10	3.6	1.7	5.3	13.5	0.0383	0.0315	0.0076	0.0084	80.16	73.33
0010F	10	3.0	1.3	4.3	10.0	0.0226	0.0198	0.0048	0.0073	78.76	63.13
0010_sum	10	19.8	9.7	29.5	65.5	0.1766	0.1723	0.0344	0.0420	483.40	450.43
0010_mean	10	3.3	1.6	4.9	10.9	0.0294	0.0287	0.0057	0.0070	80.57	75.07
0010_SD	10	0.3	0.2	0.4	1.9	0.0101	0.0079	0.0020	0.0018	1.59	6.44
0025A	25	2.8	1.8	4.6	7.0	0.0123	0.0261	0.0046	0.0126	62.60	51.72
0025B	25	3.2	1.4	4.6	10.0	0.0198	0.0138	0.0029	0.0046	85.35	66.67
0025C	25	3.5	1.8	5.3	11.0	0.0255	0.0220	0.0057	0.0063	77.65	71.36
0025D	25	3.4	1.6	5.0	11.0	0.0285	0.0265	0.0070	0.0075	75.44	71.70
0025E	25	3.3	0.8	4.1	7.0	0.0172	0.0175	0.0043	0.0052	75.00	70.29
0025F	25	3.2	1.7	4.9	10.5	0.0274	0.0215	0.0060	0.0059	78.10	72.56
0025_sum	25	19.4	9.1	28.5	56.5	0.1307	0.1274	0.0305	0.0421	454.14	404.30
0025_mean	25	3.2	1.5	4.8	9.4	0.0218	0.0212	0.0051	0.0070	75.69	67.38
0025_SD	25	0.2	0.4	0.4	1.9	0.0064	0.0049	0.0014	0.0029	7.41	7.94
0050A	50	2.8	1.2	4.0	7.5	0.0104	0.0200	0.0022	0.0117	78.85	41.50
0050B	50	2.2	0.9	3.1	7.0	0.0091	0.0152	0.0018	0.0065	80.22	57.24
0050C	50	1.9	0.5	2.4	4.0	0.0039	0.0243	0.0007	0.0156	82.05	35.80
0050D	50	2.4	0.9	3.3	9.0	0.0221	0.0238	0.0046	0.0061	79.19	74.37
0050E	50	3.4	1.6	5.0	12.0	0.0301	0.0277	0.0066	0.0074	78.07	73.29
0050F	50	2.2	0.9	3.1	5.0	0.0075	0.0248	0.0014	0.0149	81.33	39.92
0050_sum	50	14.9	6.0	20.9	44.5	0.0831	0.1358	0.0173	0.0622	479.71	322.11
0050_mean	50	2.5	1.0	3.5	7.4	0.0139	0.0226	0.0029	0.0104	79.95	53.69
0050_SD	50	0.5	0.4	0.9	2.9	0.0101	0.0044	0.0023	0.0043	1.53	17.22
0100A	100	3.6	1.2	4.8	6.0	0.0131	0.0235	0.0033	0.0092	74.81	60.85
0100B	100	1.4	0.5	1.9	5.5	0.0099	0.0175	0.0019	0.0078	80.81	55.43
0100C	100	3.6	1.5	5.1	14.5	0.0375	0.0268	0.0075	0.0082	80.00	69.40
0100D	100	2.7	1.1	3.8	8.5	0.0189	0.0230	0.0049	0.0094	74.07	59.13
0100E	100	3.0	1.5	4.5	10.0	0.0179	0.0224	0.0044	0.0063	75.42	71.88
0100F	100	2.6	1.3	3.9	10.0	0.0230	0.0241	0.0053	0.0073	76.96	69.71
0100_sum	100	16.9	7.1	24.0	54.5	0.1203	0.1373	0.0273	0.0482	462.07	386.40
0100_mean	100	2.8	1.2	4.0	9.1	0.0201	0.0229	0.0046	0.0080	77.01	64.40
0100_SD	100	0.8	0.4	1.1	3.3	0.0097	0.0030	0.0019	0.0012	2.81	6.78
0250A	250	2.7	1.3	4.0	10.5	0.0251	0.0203	0.0049	0.0068	80.48	66.50
0250B	250	1.6	0.7	2.3	5.5	0.0099	0.0177	0.0015	0.0071	84.85	59.89
0250C	250	x	x	x	x	x	x	x	x	x	x
0250D	250	3.0	1.4	4.4	10.5	0.0240	0.0252	0.0046	0.0121	80.83	51.98
0250E	250	x	x	x	x	x	x	x	x	x	x
0250F	250	1.2	0.4	1.6	3.0	0.0069	0.0192	0.0011	0.0117	x	x

Table A.15.: A2 plant growth data for Na_2SeO_3 III (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
<i>0250_sum</i>	<i>250</i>	<i>8.5</i>	<i>3.8</i>	<i>12.3</i>	<i>29.5</i>	<i>0.0659</i>	<i>0.0824</i>	<i>0.0121</i>	<i>0.0377</i>	<i>246.16</i>	<i>178.37</i>
<i>0250_mean</i>	<i>250</i>	<i>2.1</i>	<i>1.0</i>	<i>3.1</i>	<i>7.4</i>	<i>0.0165</i>	<i>0.0206</i>	<i>0.0030</i>	<i>0.0094</i>	<i>82.05</i>	<i>59.46</i>
<i>0250_SD</i>	<i>250</i>	<i>0.9</i>	<i>0.5</i>	<i>1.3</i>	<i>3.8</i>	<i>0.0094</i>	<i>0.0032</i>	<i>0.0020</i>	<i>0.0029</i>	<i>2.43</i>	<i>7.27</i>
0500A	500	3.1	0.8	3.9	5.5	0.0141	0.0248	0.0036	0.0073	74.47	70.56
0500B	500	2.6	1.3	3.9	5.5	0.0209	0.0219	0.0052	0.0062	75.12	71.69
0500C	500	1.9	0.8	2.7	8.5	0.0165	0.0331	0.0071	0.0141	56.97	57.40
0500D	500	2.7	1.3	4.0	9.5	0.0255	0.0214	0.0039	0.0067	84.71	68.69
0500E	500	2.3	1.1	3.4	7.5	0.0220	0.0218	0.0044	0.0059	80.00	72.94
0500F	500	2.7	1.0	3.7	7.5	0.0144	0.0211	0.0041	0.0091	71.53	56.87
<i>0500_sum</i>	<i>500</i>	<i>15.3</i>	<i>6.3</i>	<i>21.6</i>	<i>44.0</i>	<i>0.1134</i>	<i>0.1441</i>	<i>0.0283</i>	<i>0.0493</i>	<i>442.79</i>	<i>398.16</i>
<i>0500_mean</i>	<i>500</i>	<i>2.6</i>	<i>1.1</i>	<i>3.6</i>	<i>7.3</i>	<i>0.0189</i>	<i>0.0240</i>	<i>0.0047</i>	<i>0.0082</i>	<i>73.80</i>	<i>66.36</i>
<i>0500_SD</i>	<i>500</i>	<i>0.4</i>	<i>0.2</i>	<i>0.5</i>	<i>1.6</i>	<i>0.0046</i>	<i>0.0046</i>	<i>0.0013</i>	<i>0.0031</i>	<i>9.47</i>	<i>7.28</i>
1000A	1000	2.0	1.1	3.1	6.5	0.0159	0.0187	0.0046	0.0051	71.07	72.73
1000B	1000	2.7	0.8	3.5	4.5	0.0081	0.0114	0.0022	0.0034	72.84	70.18
1000C	1000	1.7	0.9	2.6	4.5	0.0101	0.0182	0.0031	0.0117	69.31	35.71
1000D	1000	1.7	0.9	2.6	4.0	0.0062	0.0204	0.0017	0.0074	72.58	63.73
1000E	1000	x	x	x	x	x	x	x	x	x	x
1000F	1000	2.4	1.1	3.5	7.0	0.0158	0.0186	0.0043	0.0060	72.78	67.74
<i>1000_sum</i>	<i>1000</i>	<i>10.5</i>	<i>4.8</i>	<i>15.3</i>	<i>26.5</i>	<i>0.0561</i>	<i>0.0873</i>	<i>0.0159</i>	<i>0.0336</i>	<i>358.58</i>	<i>310.08</i>
<i>1000_mean</i>	<i>1000</i>	<i>2.1</i>	<i>1.0</i>	<i>3.1</i>	<i>5.3</i>	<i>0.0112</i>	<i>0.0175</i>	<i>0.0032</i>	<i>0.0067</i>	<i>71.72</i>	<i>62.02</i>
<i>1000_SD</i>	<i>1000</i>	<i>0.4</i>	<i>0.1</i>	<i>0.5</i>	<i>1.4</i>	<i>0.0044</i>	<i>0.0035</i>	<i>0.0013</i>	<i>0.0031</i>	<i>1.53</i>	<i>15.07</i>
2500A	2500	2.1	1.0	3.1	4.5	0.0123	0.0182	0.0039	0.0060	68.29	67.03
2500B	2500	1.7	1.0	2.7	5.0	0.0145	0.0217	0.0043	0.0088	70.34	59.45
2500C	2500	x	x	x	x	x	x	x	x	x	x
2500D	2500	1.7	0.6	2.3	3.0	0.0072	0.0166	0.0021	0.0105	70.83	36.75
2500E	2500	1.6	0.7	2.3	3.0	0.0070	0.0184	0.0021	0.0073	70.00	60.33
2500F	2500	x	x	x	x	x	x	x	x	x	x
<i>2500_sum</i>	<i>2500</i>	<i>7.1</i>	<i>3.3</i>	<i>10.4</i>	<i>15.5</i>	<i>0.0410</i>	<i>0.0749</i>	<i>0.0124</i>	<i>0.0326</i>	<i>279.47</i>	<i>223.55</i>
<i>2500_mean</i>	<i>2500</i>	<i>1.8</i>	<i>0.8</i>	<i>2.6</i>	<i>3.9</i>	<i>0.0103</i>	<i>0.0187</i>	<i>0.0031</i>	<i>0.0082</i>	<i>69.87</i>	<i>55.89</i>
<i>2500_SD</i>	<i>2500</i>	<i>0.2</i>	<i>0.2</i>	<i>0.4</i>	<i>1.0</i>	<i>0.0037</i>	<i>0.0021</i>	<i>0.0012</i>	<i>0.0019</i>	<i>1.10</i>	<i>13.20</i>

Table A.16.: A2 plant growth data for Na_2SeO_4 I (Planting Date: 28.11.2012, Bachelor Thesis Matthias von Brasch)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	2.8	1.2	4.0	7.0	0.0182	0.0286	0.0047	0.0113	74.18	60.49
0000B	0	3.0	1.3	4.3	9.0	0.0175	0.0255	0.0042	0.0104	76.00	59.22
0000C	0	2.2	0.9	3.1	9.0	0.0112	0.0301	0.0023	0.0125	79.46	58.47
0000D	0	1.9	0.7	2.6	5.5	0.0076	0.0209	0.0019	0.0131	75.00	37.32
0000E	0	3.1	1.3	4.4	10.5	0.0198	0.0297	0.0055	0.0112	72.22	62.29
0000F	0	3.1	1.2	4.3	10.0	0.0231	0.0224	0.0060	0.0077	74.03	65.63
0000_sum	0	16.1	6.6	22.7	51.0	0.0974	0.1572	0.0246	0.0662	450.89	343.41
0000_mean	0	2.7	1.1	3.8	8.5	0.0162	0.0262	0.0041	0.0110	75.15	57.24
0000_SD	0	0.5	0.2	0.8	1.9	0.0057	0.0039	0.0017	0.0019	2.46	10.09
0005A	5	3.5	1.3	4.8	12.5	0.0353	0.0420	0.0092	0.0101	73.94	75.95
0005B	5	2.9	1.1	4.0	8.0	0.0136	0.0265	0.0033	0.0130	75.74	50.94
0005C	5	2.1	0.9	3.0	4.0	0.0064	0.0208	0.0012	0.0090	81.25	56.73
0005D	5	3.3	1.2	4.5	10.5	0.0285	0.0313	0.0070	0.0085	75.44	72.84
0005E	5	2.1	0.8	2.9	6.0	0.0086	0.0216	0.0024	0.0116	72.09	46.30
0005F	5	3.2	1.2	4.4	10.0	0.0228	0.0201	0.0060	0.0069	73.68	65.67
0005_sum	5	17.1	6.5	23.6	51.0	0.1152	0.1623	0.0291	0.0591	452.14	368.44
0005_mean	5	2.9	1.1	3.9	8.5	0.0192	0.0271	0.0049	0.0099	75.36	61.41
0005_SD	5	0.6	0.2	0.8	3.1	0.0115	0.0085	0.0031	0.0022	3.17	12.00
0010A	10	2.8	1.1	3.9	8.5	0.0155	0.0255	0.0036	0.0110	76.77	56.86
0010B	10	3	1.2	4.2	9.0	0.0217	0.0266	0.0056	0.0095	74.19	64.29
0010C	10	3.3	1.2	4.5	10.5	0.0251	0.0254	0.0064	0.0070	74.50	72.44
0010D	10	2.7	0.9	3.6	8.0	0.0204	0.0262	0.0050	0.0100	75.49	61.83
0010E	10	3.1	1.2	4.3	11.0	0.0236	0.0297	0.0069	0.0088	70.76	70.37
0010F	10	3.2	1.3	4.5	10.5	0.0222	0.0321	0.0074	0.0086	66.67	73.21
0010_sum	10	18.1	6.9	25.0	57.5	0.1285	0.1655	0.0349	0.0549	438.39	399.00
0010_mean	10	3.0	1.2	4.2	9.6	0.0214	0.0276	0.0058	0.0092	73.06	66.50
0010_SD	10	0.2	0.1	0.4	1.2	0.0033	0.0027	0.0014	0.0014	3.72	6.56
0025A	25	1.6	0.5	2.1	4.5	0.0114	0.0223	0.0026	0.0112	77.19	49.78
0025B	25	2.0	0.7	2.7	4.5	0.0050	0.0191	0.0007	0.0134	86.00	29.84
0025C	25	3.1	1.1	4.2	9.5	0.0207	0.0265	0.0043	0.0122	79.23	53.96
0025D	25	1.7	0.6	2.3	5.0	0.0080	0.0192	0.0018	0.0141	77.50	26.56
0025E	25	2.1	0.6	2.7	8.5	0.0242	0.0278	0.0057	0.0086	76.45	69.06
0025F	25	2.9	1.1	4.0	10.0	0.0201	0.0245	0.0053	0.0079	73.63	67.76
0025_sum	25	13.4	4.6	18.0	42.0	0.0894	0.1394	0.0204	0.0674	470.00	296.96
0025_mean	25	2.2	0.8	3.0	7.0	0.0149	0.0232	0.0034	0.0112	78.33	49.49
0025_SD	25	0.6	0.3	0.9	2.6	0.0078	0.0037	0.0020	0.0025	4.18	18.16
0050A	50	2.8	1.1	3.9	9.0	0.0168	0.0205	0.0041	0.0102	75.60	50.24
0050B	50	x	x	x	x	x	x	x	x	x	x
0050C	50	2.3	0.9	3.2	3.5	0.0058	0.0254	0.0010	0.0164	82.76	35.43
0050D	50	3.1	1.1	4.2	12.0	0.0286	0.0293	0.0082	0.0121	71.33	58.70
0050E	50	2.1	0.6	2.7	8.5	0.0153	0.0206	0.0031	0.0051	79.74	75.24
0050F	50	2.8	1.0	3.8	7.0	0.0177	0.0285	0.0048	0.0119	72.88	58.25
0050_sum	50	13.1	4.7	17.8	40.0	0.0842	0.1243	0.0212	0.0557	382.30	277.87
0050_mean	50	2.6	0.9	3.6	8.0	0.0168	0.0249	0.0042	0.0111	76.46	55.57
0050_SD	50	0.4	0.2	0.6	3.1	0.0081	0.0042	0.0026	0.0041	4.75	14.47
0100A	100	2.0	0.9	2.9	6.5	0.0093	0.0237	0.0020	0.0141	78.49	40.51
0100B	100	1.4	0.4	1.8	4.0	0.0044	0.0216	0.0010	0.0162	77.27	25.00
0100C	100	x	x	x	x	x	x	x	x	x	x
0100D	100	3.1	1.2	4.3	11.0	0.0238	0.0131	0.0056	0.0083	76.47	36.64
0100E	100	3.3	1.6	4.9	12.0	0.0273	0.0158	0.0069	0.0073	74.73	53.80
0100F	100	2.4	1.0	3.4	7.0	0.0105	0.0218	0.0030	0.0116	71.43	46.79
0100_sum	100	12.2	5.1	17.3	40.5	0.0753	0.0960	0.0185	0.0575	378.39	202.73
0100_mean	100	2.4	1.0	3.5	8.1	0.0151	0.0192	0.0037	0.0115	75.68	40.55
0100_SD	100	0.8	0.4	1.2	3.3	0.0099	0.0045	0.0025	0.0038	2.74	10.86
0250A	250	1.7	0.6	2.3	2.5	0.0060	0.0230	0.0014	0.0116	76.67	49.57
0250B	250	2.3	0.9	3.2	3.5	0.0163	0.0306	0.0031	0.0113	80.98	63.07
0250C	250	2.2	1.2	3.4	6.5	0.0237	0.0264	0.0052	0.0071	78.06	73.11
0250D	250	0.9	0.5	1.4	3.0	0.0071	0.0215	0.0019	0.0070	73.24	67.44
0250E	250	2.0	1.1	3.1	6.5	0.0073	0.0213	0.0023	0.0071	68.49	66.67
0250F	250	1.7	0.6	2.3	8.0	0.0185	0.0263	0.0038	0.0118	79.46	55.13

Table A.17.: A2 plant growth data for Na_2SeO_4 I (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%] [± 0.0001]	root water [%] [± 0.0001]
<i>0250_sum</i>	<i>250</i>	<i>10.8</i>	<i>4.9</i>	<i>15.7</i>	<i>30.0</i>	<i>0.0789</i>	<i>0.1491</i>	<i>0.0177</i>	<i>0.0559</i>	<i>456.90</i>	<i>374.98</i>
<i>0250_mean</i>	<i>250</i>	<i>1.8</i>	<i>0.8</i>	<i>2.6</i>	<i>5.0</i>	<i>0.0132</i>	<i>0.0249</i>	<i>0.0030</i>	<i>0.0093</i>	<i>76.15</i>	<i>62.50</i>
<i>0250_SD</i>	<i>250</i>	<i>0.5</i>	<i>0.3</i>	<i>0.8</i>	<i>2.3</i>	<i>0.0074</i>	<i>0.0036</i>	<i>0.0014</i>	<i>0.0025</i>	<i>4.59</i>	<i>8.67</i>
0500A	500	x	x	x	x	x	x	x	x	x	x
0500B	500	1.4	0.6	2.0	4.0	0.0115	0.0164	0.0036	0.0045	68.70	72.56
0500C	500	1.2	0.8	2.0	3.0	0.0066	0.0225	0.0014	0.0151	78.79	32.89
0500D	500	1.9	0.9	2.8	5.0	0.0131	0.0119	0.0041	0.0027	68.70	77.31
0500E	500	2.1	1.2	3.3	3.5	0.0077	0.0211	0.0022	0.0126	71.43	40.28
0500F	500	2.0	0.9	2.9	5.0	0.0120	0.0190	0.0039	0.0108	67.50	43.16
<i>0500_sum</i>	<i>500</i>	<i>8.6</i>	<i>4.4</i>	<i>13.0</i>	<i>20.5</i>	<i>0.0509</i>	<i>0.0909</i>	<i>0.0152</i>	<i>0.0457</i>	<i>355.11</i>	<i>266.20</i>
<i>0500_mean</i>	<i>500</i>	<i>1.7</i>	<i>0.9</i>	<i>2.6</i>	<i>4.1</i>	<i>0.0102</i>	<i>0.0182</i>	<i>0.0030</i>	<i>0.0091</i>	<i>71.02</i>	<i>53.24</i>
<i>0500_SD</i>	<i>500</i>	<i>0.4</i>	<i>0.2</i>	<i>0.6</i>	<i>0.9</i>	<i>0.0029</i>	<i>0.0042</i>	<i>0.0012</i>	<i>0.0053</i>	<i>4.57</i>	<i>20.23</i>
1000A	1000	2.0	0.9	2.9	3.5	0.0077	0.0189	0.0029	0.0127	62.34	32.80
1000B	1000	1.6	0.8	2.4	4.5	0.0125	0.0191	0.0048	0.0085	61.60	55.50
1000C	1000	1.9	0.9	2.8	4.0	0.0092	0.0168	0.0029	0.0130	68.48	22.62
1000D	1000	1.8	0.7	2.5	4.0	0.0105	0.0163	0.0041	0.0089	60.95	45.40
1000E	1000	2.6	1.2	3.8	6.0	0.0172	0.0240	0.0072	0.0090	58.14	62.50
1000F	1000	2.8	0.8	3.6	4.5	0.0115	0.0161	0.0049	0.0107	57.39	33.54
<i>1000_sum</i>	<i>1000</i>	<i>12.7</i>	<i>5.3</i>	<i>18.0</i>	<i>26.5</i>	<i>0.0686</i>	<i>0.1112</i>	<i>0.0268</i>	<i>0.0628</i>	<i>368.90</i>	<i>252.36</i>
<i>1000_mean</i>	<i>1000</i>	<i>2.1</i>	<i>0.9</i>	<i>3.0</i>	<i>4.4</i>	<i>0.0114</i>	<i>0.0185</i>	<i>0.0045</i>	<i>0.0105</i>	<i>61.48</i>	<i>42.06</i>
<i>1000_SD</i>	<i>1000</i>	<i>0.5</i>	<i>0.2</i>	<i>0.6</i>	<i>0.9</i>	<i>0.0033</i>	<i>0.0030</i>	<i>0.0016</i>	<i>0.0020</i>	<i>3.95</i>	<i>15.14</i>
2500A	2500	1.7	1.0	2.7	3.5	0.0072	0.0202	0.0023	0.0134	68.06	33.66
2500B	2500	1.7	0.9	2.6	3.5	0.0086	0.0169	0.0031	0.0086	63.95	49.11
2500C	2500	1.6	0.9	2.5	2.5	0.0064	0.0234	0.0016	0.0166	75.00	29.06
2500D	2500	0.8	0.3	1.1	2.0	0.0039	0.0147	0.0006	0.0115	84.62	21.77
2500E	2500	1.5	0.5	2.0	2.0	0.0046	0.0140	0.0010	0.0099	78.26	29.29
2500F	2500	0.7	0.4	1.1	1.5	0.0023	0.0185	0.0001	0.0133	95.65	28.11
<i>2500_sum</i>	<i>2500</i>	<i>8.0</i>	<i>4.0</i>	<i>12.0</i>	<i>15.0</i>	<i>0.0330</i>	<i>0.1077</i>	<i>0.0087</i>	<i>0.0733</i>	<i>465.54</i>	<i>191.00</i>
<i>2500_mean</i>	<i>2500</i>	<i>1.3</i>	<i>0.7</i>	<i>2.0</i>	<i>2.5</i>	<i>0.0055</i>	<i>0.0180</i>	<i>0.0015</i>	<i>0.0122</i>	<i>77.59</i>	<i>31.83</i>
<i>2500_SD</i>	<i>2500</i>	<i>0.5</i>	<i>0.3</i>	<i>0.7</i>	<i>0.8</i>	<i>0.0023</i>	<i>0.0035</i>	<i>0.0011</i>	<i>0.0029</i>	<i>11.49</i>	<i>9.29</i>

Table A.18.: A2 plant growth data for Na_2SeO_4 II (Planting Date: 08.05.2013, Experiment Repetition Alexandra Nothstein)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	3.5	1.6	5.1	10.0	0.0178	0.0198	0.0048	0.0066	73.03	66.67
0000B	0	3.4	1.8	5.2	9.0	0.0247	0.0370	0.0067	0.0075	72.87	79.73
0000C	0	2.9	1.9	4.8	10.0	0.0147	0.0203	0.0047	0.0064	68.03	68.47
0000D	0	x	x	x	x	x	x	x	x	x	x
0000E	0	3.1	1.3	4.4	10.5	0.0224	0.0248	0.0071	0.0076	68.30	69.35
0000F	0	3.7	1.8	5.5	11.0	0.0231	0.0309	0.0074	0.0086	67.97	72.17
0000_sum	0	16.6	8.4	25.0	50.5	0.1027	0.1328	0.0307	0.0367	350.20	356.39
0000_mean	0	3.3	1.7	5.0	10.1	0.0205	0.0266	0.0061	0.0073	70.04	71.28
0000_SD	0	0.3	0.2	0.4	0.7	0.0042	0.0073	0.0013	0.0009	2.66	5.12
0005A	5	3.6	1.8	5.4	8.0	0.0163	0.0204	0.0035	0.0062	78.53	69.61
0005B	5	1.8	0.3	2.1	5.0	0.0287	0.0297	0.0085	0.0090	70.38	69.70
0005C	5	3.9	1.6	5.5	12.0	0.0181	0.0268	0.0034	0.0067	81.22	75.00
0005D	5	3.6	1.8	5.4	8.5	0.0201	0.0263	0.0068	0.0067	66.17	74.52
0005E	5	4.5	2.3	6.8	9.5	0.0164	0.0267	0.0061	0.0074	62.80	72.28
0005F	5	3.6	1.7	5.3	9.5	0.0189	0.0243	0.0058	0.0072	69.31	70.37
0005_sum	5	21.0	9.5	30.5	52.5	0.1185	0.1542	0.0341	0.0432	428.41	431.48
0005_mean	5	3.5	1.6	5.1	8.8	0.0198	0.0257	0.0057	0.0072	71.40	71.91
0005_SD	5	0.9	0.7	1.6	2.3	0.0046	0.0031	0.0020	0.0010	7.12	2.41
0010A	10	3.5	1.7	5.2	9.0	0.0205	0.0298	0.0061	0.0077	70.24	74.16
0010B	10	3.3	1.7	5.0	8.5	0.0213	0.0267	0.0050	0.0073	76.53	72.66
0010C	10	3.6	1.8	5.4	9.5	0.0192	0.0278	0.0070	0.0081	63.54	70.86
0010D	10	3.4	1.7	5.1	9.0	0.0171	0.0305	0.0063	0.0082	63.16	73.11
0010E	10	3.8	1.7	5.5	11.5	0.0219	0.0338	0.0088	0.0097	59.82	71.30
0010F	10	3.5	1.6	5.1	10.5	0.0176	0.0322	0.0076	0.0090	56.82	72.05
0010_sum	10	21.1	10.2	31.3	58.0	0.1176	0.1808	0.0408	0.0500	390.10	434.15
0010_mean	10	3.5	1.7	5.2	9.7	0.0196	0.0301	0.0068	0.0083	65.02	72.36
0010_SD	10	0.2	0.1	0.2	1.1	0.0020	0.0027	0.0013	0.0009	7.21	1.21
0025A	25	3.3	1.5	4.8	6.5	0.0088	0.0208	0.0066	0.0073	25.00	64.90
0025B	25	3.6	1.9	5.5	9.5	0.0191	0.0288	0.0020	0.0068	89.53	76.39
0025C	25	3.9	1.8	5.7	10.5	0.0221	0.0273	0.0081	0.0073	63.35	73.26
0025D	25	3.7	1.7	5.4	11.5	0.0170	0.0250	0.0083	0.0088	51.18	64.80
0025E	25	2.7	1.4	4.1	7.5	0.0166	0.0255	0.0038	0.0074	77.11	70.98
0025F	25	3.7	1.7	5.4	11.0	0.0203	0.0292	0.0070	0.0078	65.52	73.29
0025_sum	25	20.9	10.0	30.9	56.5	0.1039	0.1566	0.0358	0.0454	371.68	423.62
0025_mean	25	3.5	1.7	5.2	9.4	0.0173	0.0261	0.0060	0.0076	61.95	70.60
0025_SD	25	0.4	0.2	0.6	2.0	0.0046	0.0031	0.0025	0.0007	22.30	4.78
0050A	50	3.5	1.4	4.9	10.0	0.0211	0.0264	0.0079	0.0084	62.56	68.18
0050B	50	3.9	1.8	x	10.5	0.0257	0.0344	0.0082	0.0097	68.09	71.80
0050C	50	4.0	1.7	5.7	11.0	0.0198	0.0176	0.0071	0.0057	64.14	67.61
0050D	50	3.9	1.8	5.7	11.0	0.0251	0.0358	0.0088	0.0111	64.94	68.99
0050E	50	3.5	1.7	5.2	8.0	0.0110	0.0130	0.0044	0.0047	60.00	63.85
0050F	50	4.1	2.1	6.2	11.0	0.0194	0.0340	0.0081	0.0113	58.25	66.76
0050_sum	50	22.9	10.5	27.7	61.5	0.1221	0.1612	0.0445	0.0509	377.98	407.20
0050_mean	50	3.8	1.8	5.5	10.3	0.0204	0.0269	0.0074	0.0085	63.00	67.87
0050_SD	50	0.3	0.2	0.5	1.2	0.0053	0.0097	0.0016	0.0028	3.54	2.62
0100A	100	4.2	1.9	6.1	11.5	0.0223	0.0235	0.0079	0.0072	64.57	69.36
0100B	100	3.9	1.7	5.6	10.5	0.0190	0.0261	0.0078	0.0079	58.95	69.73
0100C	100	4.1	1.9	0.0	11.0	0.0220	0.0306	0.0084	0.0089	61.82	70.92
0100D	100	x	x	x	x	x	x	x	x	x	x
0100E	100	2.4	1.2	3.6	8.5	0.0162	0.0191	0.0051	0.0057	68.52	70.16
0100F	100	3.6	1.2	4.8	13.0	0.0231	0.0371	0.0097	0.0108	58.01	70.89
0100_sum	100	18.2	7.9	20.1	54.5	0.1026	0.1364	0.0389	0.0405	311.87	351.06
0100_mean	100	3.6	1.6	4.0	10.9	0.0205	0.0273	0.0078	0.0081	62.37	70.21
0100_SD	100	0.7	0.4	2.4	1.6	0.0029	0.0069	0.0017	0.0019	4.29	0.69
0250A	250	3.8	2.0	5.8	10.5	0.0223	0.0358	0.0090	0.0095	59.64	73.46
0250B	250	1.7	1.4	3.1	3.0	0.0048	0.0083	0.0020	0.0028	58.33	66.27
0250C	250	1.7	0.2	1.9	3.0	0.0102	0.0188	0.0025	0.0063	75.49	66.49
0250D	250	3.5	1.7	5.2	8.5	0.0188	0.0321	0.0072	0.0094	61.70	70.72
0250E	250	3.5	1.6	5.1	9.5	0.0209	0.0309	0.0073	0.0084	65.07	72.82
0250F	250	3.3	1.7	5.0	9.0	0.0142	0.0193	0.0058	0.0064	59.15	66.84

Table A.19.: A2 plant growth data for Na_2SeO_4 II (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250_sum	250	17.5	8.6	26.1	43.5	0.0912	0.1452	0.0338	0.0428	379.39	416.59
0250_mean	250	2.9	1.4	4.4	7.3	0.0152	0.0242	0.0056	0.0071	63.23	69.43
0250_SD	250	1.0	0.6	1.5	3.4	0.0068	0.0105	0.0028	0.0025	6.47	3.31
0500A	500	2.1	1.8	x	4.5	0.0118	0.0298	0.0046	0.0134	61.02	55.03
0500B	500	2.1	1.4	3.5	5.0	0.0127	0.0211	0.0046	0.0084	63.78	60.19
0500C	500	2.4	1.9	4.3	6.0	0.0182	0.0268	0.0070	0.0103	61.54	61.57
0500D	500	1.8	0.7	2.5	3.5	0.0075	0.0151	0.0024	0.0053	68.00	64.90
0500E	500	2.3	1.1	3.4	4.5	0.0140	0.0193	0.0063	0.0067	55.00	65.28
0500F	500	x	x	x	x	x	x	x	x	x	x
0500_sum	500	10.7	6.9	13.7	23.5	0.0642	0.1121	0.0249	0.0441	309.33	306.98
0500_mean	500	2.1	1.4	3.4	4.7	0.0128	0.0224	0.0050	0.0088	61.87	61.40
0500_SD	500	0.2	0.5	0.7	0.9	0.0039	0.0059	0.0018	0.0032	4.72	4.16
1000A	1000	2.4	1.4	3.8	5.0	0.0150	0.0201	0.0059	0.0049	60.67	75.62
1000B	1000	2.4	1.0	3.4	4.5	0.0131	0.0176	0.0050	0.0131	61.83	25.57
1000C	1000	2.5	1.0	3.5	4.5	0.0168	0.0114	0.0055	0.0035	67.26	69.30
1000D	1000	2.6	1.5	4.1	6.5	0.0174	0.0205	0.0070	0.0086	59.77	58.05
1000E	1000	2.7	1.6	4.3	6.0	0.0164	0.0242	0.0068	0.0112	58.54	53.72
1000F	1000	2.5	0.9	3.4	5.5	0.0141	0.0205	0.0051	0.0081	63.83	60.49
1000_sum	1000	15.1	7.4	22.5	32.0	0.0928	0.1143	0.0353	0.0494	371.90	342.74
1000_mean	1000	2.5	1.2	3.8	5.3	0.0155	0.0191	0.0059	0.0082	61.98	57.12
1000_SD	1000	0.1	0.3	0.4	0.8	0.0017	0.0043	0.0009	0.0036	3.16	17.38
2500A	2500	2.4	1.3	3.7	5.0	0.0127	0.0182	0.0051	0.0105	59.84	42.31
2500B	2500	2.2	1.3	3.5	3.5	0.0105	0.0103	0.0036	0.0025	65.71	75.73
2500C	2500	x	x	x	x	x	x	x	x	x	x
2500D	2500	2.5	1.2	3.7	6.0	0.0152	0.0252	0.0063	0.0101	58.55	59.92
2500E	2500	2.0	0.9	2.9	3.0	0.0039	0.0165	0.0019	0.0135	51.28	18.18
2500F	2500	2.1	1.1	3.2	5.0	0.0121	0.0155	0.0051	0.0077	57.85	50.32
2500_sum	2500	11.2	5.8	17.0	22.5	0.0544	0.0857	0.0220	0.0443	293.24	246.46
2500_mean	2500	2.2	1.2	3.4	4.5	0.0109	0.0171	0.0044	0.0089	58.65	49.29
2500_SD	2500	0.2	0.2	0.3	1.2	0.0043	0.0054	0.0017	0.0041	5.15	21.39

Table A.20.: A2 plant growth data for Na₂SeO₃ III (Planting Date: 29.05.2013, Experiment Repetition Alexandra Nothstein)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	x	x	x	x	x	x	x	x	x	x
0000B	0	5.5	1.6	7.1	20.0	0.0425	0.0202	0.0083	0.0062	80.47	69.31
0000C	0	2.0	1.0	3.0	3.5	0.0058	0.0183	0.0009	0.0110	84.48	39.89
0000D	0	3.6	1.4	5.0	13.0	0.0237	0.0157	0.0042	0.0036	82.28	77.07
0000E	0	3.3	1.7	5.0	7.0	0.0127	0.0117	0.0026	0.0027	79.53	76.92
0000F	0	3.4	1.6	5.0	16.5	0.0487	0.0162	0.0092	0.0073	81.11	54.94
<i>0000_sum</i>	<i>0</i>	<i>17.8</i>	<i>7.3</i>	<i>25.1</i>	<i>60.0</i>	<i>0.1334</i>	<i>0.0821</i>	<i>0.0252</i>	<i>0.0308</i>	<i>407.87</i>	<i>318.13</i>
<i>0000_mean</i>	<i>0</i>	<i>3.6</i>	<i>1.5</i>	<i>5.0</i>	<i>12.0</i>	<i>0.0267</i>	<i>0.0164</i>	<i>0.0050</i>	<i>0.0062</i>	<i>81.57</i>	<i>63.63</i>
<i>0000_SD</i>	<i>0</i>	<i>1.3</i>	<i>0.3</i>	<i>1.4</i>	<i>6.8</i>	<i>0.0185</i>	<i>0.0032</i>	<i>0.0036</i>	<i>0.0033</i>	<i>1.91</i>	<i>16.04</i>
0005A	5	3.9	1.2	5.1	15.0	0.0417	0.0144	0.0077	0.0051	81.53	64.58
0005B	5	3.8	1.4	5.2	14.5	0.0268	0.0184	0.0051	0.0039	80.97	78.80
0005C	5	4.0	1.5	5.5	15.0	0.0353	0.0208	0.0066	0.0057	98.30	72.60
0005D	5	2.7	0.5	3.2	2.5	0.0026	0.0201	0.0007	0.0013	73.08	93.54
0005E	5	4.4	1.8	6.2	16.5	0.0419	0.0185	0.0085	0.0063	79.71	65.95
0005F	5	x	x	x	x	x	x	x	x	x	x
<i>0005_sum</i>	<i>5</i>	<i>18.8</i>	<i>6.4</i>	<i>25.2</i>	<i>63.5</i>	<i>0.1483</i>	<i>0.0922</i>	<i>0.0226</i>	<i>0.0223</i>	<i>413.60</i>	<i>375.47</i>
<i>0005_mean</i>	<i>5</i>	<i>3.8</i>	<i>1.3</i>	<i>5.0</i>	<i>12.7</i>	<i>0.0297</i>	<i>0.0184</i>	<i>0.0045</i>	<i>0.0045</i>	<i>82.72</i>	<i>75.09</i>
<i>0005_SD</i>	<i>5</i>	<i>0.6</i>	<i>0.5</i>	<i>1.1</i>	<i>5.8</i>	<i>0.0163</i>	<i>0.0025</i>	<i>0.0037</i>	<i>0.0020</i>	<i>9.34</i>	<i>11.77</i>
0010A	10	4.3	1.5	5.8	15.0	0.0384	0.0242	0.0073	0.0071	80.99	70.66
0010B	10	3.0	1.2	4.2	11.0	0.0330	0.0175	0.0058	0.0062	82.42	64.57
0010C	10	3.6	0.6	4.2	9.0	0.0333	0.0277	0.0057	0.0069	82.88	75.09
0010D	10	1.8	0.5	2.3	5.5	0.0055	0.0234	0.0009	0.0130	83.64	44.44
0010E	10	4.4	1.7	6.1	16.0	0.0423	0.0197	0.0078	0.0066	81.56	97.01
0010F	10	3.1	1.3	4.4	13.0	0.0439	0.0323	0.0084	0.0084	80.87	73.99
<i>0010_sum</i>	<i>10</i>	<i>20.2</i>	<i>6.8</i>	<i>27.0</i>	<i>69.5</i>	<i>0.1964</i>	<i>0.1448</i>	<i>0.0359</i>	<i>0.0422</i>	<i>492.36</i>	<i>425.77</i>
<i>0010_mean</i>	<i>10</i>	<i>3.4</i>	<i>1.1</i>	<i>4.5</i>	<i>11.6</i>	<i>0.0327</i>	<i>0.0241</i>	<i>0.0060</i>	<i>0.0070</i>	<i>82.72</i>	<i>70.96</i>
<i>0010_SD</i>	<i>10</i>	<i>1.0</i>	<i>0.5</i>	<i>1.4</i>	<i>3.9</i>	<i>0.0141</i>	<i>0.0054</i>	<i>0.0027</i>	<i>0.0040</i>	<i>1.11</i>	<i>17.02</i>
0025A	25	2.8	0.9	3.7	8.5	0.0120	0.0286	0.0025	0.0130	79.17	54.55
0025B	25	4.4	1.6	6.0	17.5	0.0509	0.0307	0.0101	0.0076	80.16	75.24
0025C	25	2.6	0.9	3.5	7.5	0.0104	0.0264	0.0019	0.0117	81.73	55.68
0025D	25	2.3	0.4	2.7	5.5	0.0065	0.0172	0.0015	0.0093	76.92	45.93
0025E	25	4.3	1.8	6.1	17.0	0.0469	0.0215	0.0094	0.0074	79.96	65.58
0025F	25	3.1	1.3	4.4	12.5	0.0090	0.0099	0.0026	0.0046	71.11	53.54
<i>0025_sum</i>	<i>25</i>	<i>19.5</i>	<i>6.9</i>	<i>26.4</i>	<i>68.5</i>	<i>0.1357</i>	<i>0.1343</i>	<i>0.0280</i>	<i>0.0536</i>	<i>469.05</i>	<i>350.52</i>
<i>0025_mean</i>	<i>25</i>	<i>3.3</i>	<i>1.2</i>	<i>4.4</i>	<i>11.4</i>	<i>0.0226</i>	<i>0.0224</i>	<i>0.0047</i>	<i>0.0089</i>	<i>78.17</i>	<i>58.42</i>
<i>0025_SD</i>	<i>25</i>	<i>0.9</i>	<i>0.5</i>	<i>1.4</i>	<i>5.1</i>	<i>0.0205</i>	<i>0.0078</i>	<i>0.0040</i>	<i>0.0031</i>	<i>3.80</i>	<i>10.36</i>
0050A	50	x	x	x	x	x	x	x	x	x	x
0050B	50	2.7	1.1	3.8	6.0	0.0101	0.0243	0.0015	0.0110	85.15	54.73
0050C	50	x	x	x	x	x	x	x	x	x	x
0050D	50	3.7	1.6	5.3	15.0	0.0342	0.0217	0.0066	0.0058	80.70	73.27
0050E	50	4.2	1.4	5.6	17.0	0.0487	0.0302	0.0097	0.0072	80.08	76.16
0050F	50	x	x	x	x	x	x	x	x	x	x
<i>0050_sum</i>	<i>50</i>	<i>10.6</i>	<i>4.1</i>	<i>14.7</i>	<i>38.0</i>	<i>0.0930</i>	<i>0.0762</i>	<i>0.0178</i>	<i>0.0240</i>	<i>245.93</i>	<i>204.16</i>
<i>0050_mean</i>	<i>50</i>	<i>3.5</i>	<i>1.4</i>	<i>4.9</i>	<i>12.7</i>	<i>0.0310</i>	<i>0.0254</i>	<i>0.0059</i>	<i>0.0080</i>	<i>81.98</i>	<i>68.05</i>
<i>0050_SD</i>	<i>50</i>	<i>0.8</i>	<i>0.3</i>	<i>1.0</i>	<i>5.9</i>	<i>0.0195</i>	<i>0.0044</i>	<i>0.0041</i>	<i>0.0027</i>	<i>2.76</i>	<i>11.63</i>
0100A	100	2.2	1.0	3.2	7.0	0.0093	0.0202	0.0027	0.0102	70.97	49.50
0100B	100	x	x	x	x	x	x	x	x	x	x
0100C	100	4.6	1.6	6.2	15.5	0.0369	0.0167	0.0064	0.0050	82.66	70.06
0100D	100	x	x	x	x	x	x	x	x	x	x
0100E	100	4.1	1.4	5.5	16.5	0.0553	0.0165	0.0109	0.0068	80.29	58.79
0100F	100	2.5	1.0	3.5	11.0	0.0293	0.0201	0.0054	0.0052	81.57	74.13
<i>0100_sum</i>	<i>100</i>	<i>13.4</i>	<i>5.0</i>	<i>18.4</i>	<i>50.0</i>	<i>0.1308</i>	<i>0.0735</i>	<i>0.0254</i>	<i>0.0272</i>	<i>315.48</i>	<i>252.48</i>
<i>0100_mean</i>	<i>100</i>	<i>3.4</i>	<i>1.3</i>	<i>4.6</i>	<i>12.5</i>	<i>0.0327</i>	<i>0.0184</i>	<i>0.0064</i>	<i>0.0068</i>	<i>78.87</i>	<i>63.12</i>
<i>0100_SD</i>	<i>100</i>	<i>1.2</i>	<i>0.3</i>	<i>1.5</i>	<i>4.4</i>	<i>0.0190</i>	<i>0.0021</i>	<i>0.0034</i>	<i>0.0024</i>	<i>5.36</i>	<i>11.16</i>
0250A	250	2.7	1.6	4.3	11.0	0.0314	0.0232	0.0059	0.0057	81.21	75.43
0250B	250	1.7	0.9	2.6	6.0	0.0122	0.0173	0.0024	0.0074	80.33	57.23
0250C	250	1.6	1.1	2.7	5.0	0.0120	0.0242	0.0025	0.0109	79.17	54.96
0250D	250	x	x	x	x	x	x	x	x	x	x
0250E	250	1.2	0.3	1.5	3.0	0.0074	0.0261	0.0011	0.0117	85.14	55.17
0250F	250	x	x	x	x	x	x	x	x	x	x

Table A.21.: A2 plant growth data for Na_2SeO_3 III (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	shoot height (Day 16) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250_sum	250	7.2	3.9	11.1	25.0	0.0630	0.0908	0.0119	0.0357	325.84	242.79
0250_mean	250	1.8	1.0	2.8	6.3	0.0158	0.0227	0.0030	0.0089	81.46	60.70
0250_SD	250	0.6	0.5	1.2	3.4	0.0107	0.0038	0.0021	0.0028	2.59	9.88
0500A	500	0.7	0.2	0.0	2.0	0.0056	0.0239	0.0013	0.0154	76.79	35.56
0500B	500	2.7	1.5	4.2	4.5	0.0225	0.0229	0.0071	0.0095	68.44	58.52
0500C	500	1.7	1.7	3.4	6.5	0.0127	0.0198	0.0032	0.0055	74.80	72.22
0500D	500	1.4	0.7	2.1	2.5	0.0042	0.0242	0.0008	0.0142	80.95	41.32
0500E	500	2.6	1.2	3.8	7.0	0.0238	0.0189	0.0080	0.0043	66.39	77.25
0500F	500	x	x	x	x	x	x	x	x	x	x
0500_sum	500	9.1	5.3	13.5	22.5	0.0688	0.1097	0.0204	0.0189	367.37	284.87
0500_mean	500	1.8	1.1	2.7	4.5	0.0138	0.0219	0.0041	0.0098	73.47	56.97
0500_SD	500	0.8	0.6	1.7	2.3	0.0092	0.0024	0.0033	0.0050	6.00	18.37
1000A	1000	2.3	1.2	3.5	5.0	0.0160	0.0223	0.0060	0.0076	62.50	65.92
1000B	1000	x	x	x	1.5	0.0020	0.0239	0.0006	0.0157	70.00	34.31
1000C	1000	1.2	1.1	2.3	2.0	0.0051	0.0282	0.0012	0.0148	76.47	47.52
1000D	1000	2.0	0.7	2.7	3.0	0.0083	0.0233	0.0022	0.0094	73.49	59.66
1000E	1000	2.3	1.1	3.4	4.5	0.0141	0.0202	0.0048	0.0094	65.96	53.47
1000F	1000	1.5	1.1	2.6	2.5	0.0079	0.0201	0.0021	0.0073	73.42	63.68
1000_sum	1000	9.3	5.2	14.5	18.5	0.0534	0.1380	0.0169	0.0642	421.84	324.55
1000_mean	1000	1.9	1.0	2.9	3.1	0.0089	0.0230	0.0028	0.0107	70.31	54.09
1000_SD	1000	0.5	0.2	0.5	1.4	0.0053	0.0030	0.0021	0.0036	5.25	11.81
2500A	2500	1.1	0.9	2.0	1.5	0.0030	0.0218	0.0006	0.0144	80.00	33.94
2500B	2500	2.5	1.3	3.8	4.5	0.0165	0.0142	0.0059	0.0029	64.24	79.58
2500C	2500	x	x	x	x	x	x	x	x	x	x
2500D	2500	2.3	1.6	3.9	4.5	0.0151	0.0122	0.0052	0.0034	65.56	72.13
2500E	2500	x	x	x	x	x	x	x	x	x	x
2500F	2500	2.0	1.0	3.0	4.0	0.0125	0.0223	0.0044	0.0095	64.80	57.40
2500_sum	2500	7.9	4.8	12.7	14.5	0.0471	0.0705	0.0161	0.0302	274.61	243.05
2500_mean	2500	2.0	1.2	3.2	3.6	0.0118	0.0176	0.0040	0.0076	68.65	60.76
2500_SD	2500	0.6	0.3	0.9	1.4	0.0061	0.0052	0.0024	0.0055	7.59	20.11

A.2.2. A2 Plant Se content data

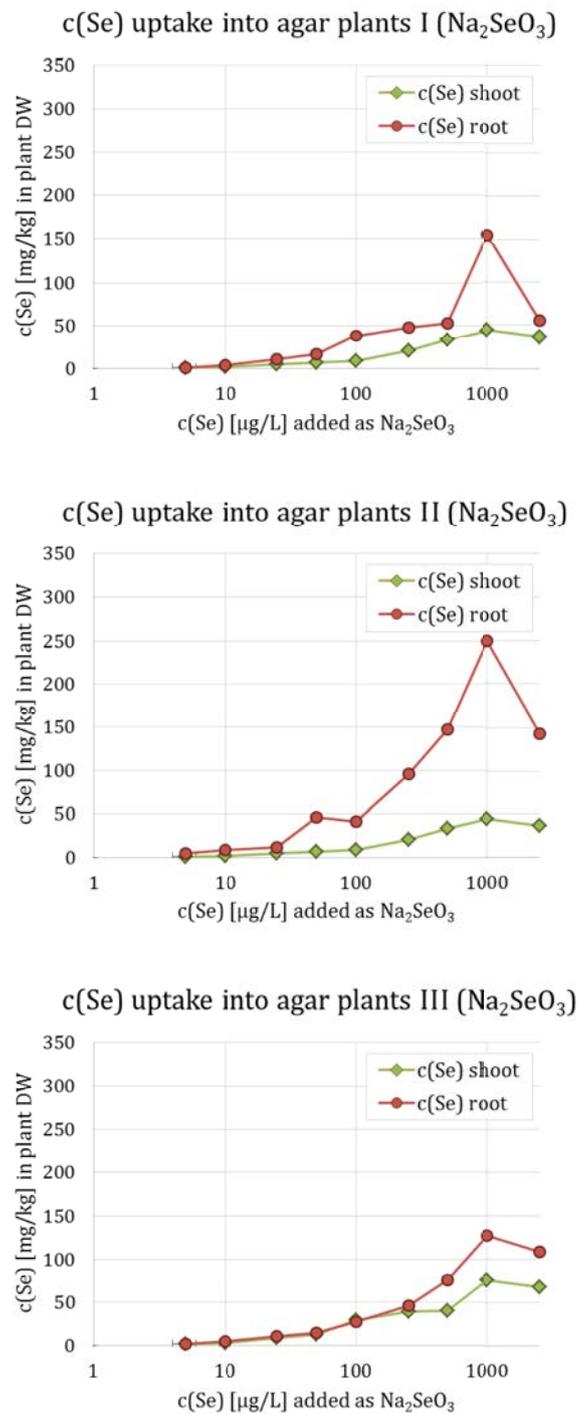


Figure A.7.: A2 plots of Se content in each of the three experimental runs for selenite

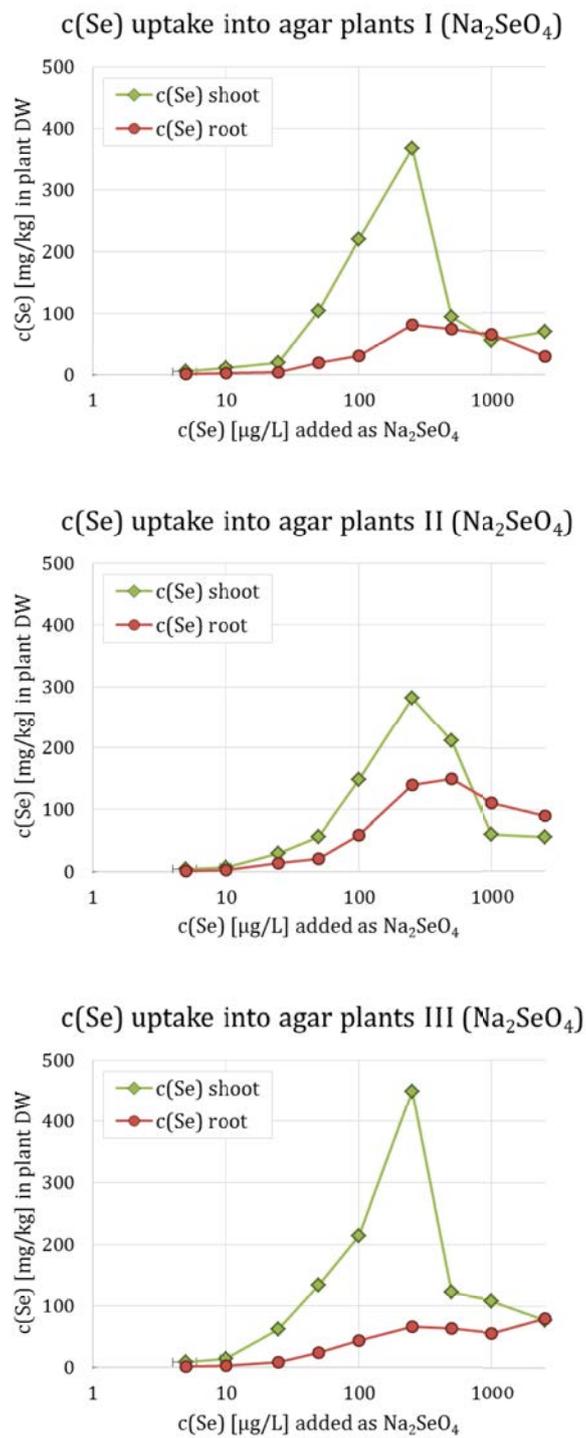


Figure A.8.: A2 plots of Se content in each of the three experimental runs for selenate

Table A.22.: A2 Se content of all three experimental runs for Na_2SeO_3

c(Se) [µg/L]				FIAS-Results				c(Se) dry weight (DW)			
	dig. weight shoot [g] [± 0.0001]	dig. weight root [g] [± 0.0001]	dig. volume [L] [± 0.0001]	c(Se) shoot [µg/L]	c(Se) shoot SD	c(Se) root [µg/L]	c(Se) root SD	c(Se) shoot [mg/kg]	c(Se) shoot SD	c(Se) root [mg/kg]	c(Se) root SD
Agar-Se (Na_2SeO_3) Planting Date: 09.01.2013 (Bachelor Thesis Matthias von Brasch)											
0	0.03464	0.04674	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.02971	0.05905	0.010	2.83	0.51	8.23	0.68	0.95	0.17	1.39	0.12
10	0.02393	0.03212	0.010	3.99	0.38	12.28	1.11	1.67	0.16	3.82	0.35
25	0.03055	0.04052	0.010	13.87	0.98	43.25	0.88	4.54	0.32	10.67	0.22
50	0.02704	0.04044	0.010	19.86	1.09	69.04	1.74	7.34	0.40	17.07	0.43
100	0.03997	0.05629	0.010	37.21	1.75	216.87	3.32	9.31	0.44	38.53	0.59
250	0.03144	0.05733	0.010	66.07	0.57	275.23	6.29	21.01	0.18	48.01	1.10
500	0.01823	0.04435	0.010	60.64	1.08	236.66	6.56	33.27	0.59	53.36	1.48
1000	0.02103	0.03533	0.010	92.80	1.54	546.36	14.46	44.13	0.73	154.64	4.09
2500	0.01735	0.05945	0.010	63.69	2.72	328.44	4.58	36.71	1.57	55.25	0.77
Agar-Se (Na_2SeO_3) Planting Date: 29.05.2013 (Experiment Repetition Alexandra Nothstein)											
0	0.02063	0.05857	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.03988	0.04313	0.010	9.17	0.63	20.94	1.58	2.30	0.16	4.85	0.37
10	0.02925	0.03222	0.010	10.04	0.61	29.38	0.38	3.43	0.21	9.12	0.12
25	0.01899	0.03192	0.010	13.52	0.52	38.74	0.53	7.12	0.27	12.14	0.17
50	0.03179	0.03008	0.010	54.05	0.81	140.55	2.26	17.00	0.25	46.72	0.75
100	0.02148	0.03594	0.010	60.48	7.00	147.43	9.36	28.15	3.26	41.02	2.60
250	0.01829	0.03248	0.011	90.69	3.11	282.03	7.21	54.54	1.87	95.50	2.44
500	0.02788	0.04805	0.010	198.07	5.33	705.40	63.67	71.05	1.91	146.82	13.25
1000	0.03711	0.03980	0.010	392.50	7.88	994.92	19.77	105.77	2.12	249.99	4.97
2500	0.02552	0.03122	0.010	152.97	7.80	447.02	14.26	59.94	3.05	143.19	4.57
Agar-Se (Na_2SeO_3) Planting Date: 10.07.2013 (Experiment Repetition Alexandra Nothstein)											
0	0.02237	0.02590	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.02933	0.04148	0.010	6.05	0.51	9.69	0.44	2.06	0.17	2.34	0.11
10	0.03245	0.03866	0.010	10.85	0.51	18.77	0.39	3.34	0.16	4.86	0.10
25	0.02806	0.04957	0.011	21.67	1.53	50.88	1.77	8.49	0.60	11.29	0.39
50	0.01673	0.03952	0.010	21.50	1.77	59.31	1.52	12.85	1.06	15.01	0.38
100	0.02598	0.04596	0.010	76.67	4.35	129.30	1.94	29.51	1.67	28.13	0.42
250	0.01411	0.03492	0.010	56.18	20.16	160.50	17.32	39.81	14.29	45.96	4.96
500	0.02565	0.04519	0.010	102.86	5.62	345.35	23.59	40.10	2.19	76.42	5.22
1000	0.01504	0.03153	0.010	114.70	21.58	401.40	12.27	76.24	14.34	127.30	3.89
2500	0.01525	0.03276	0.010	103.92	4.81	356.63	5.71	68.13	3.15	108.87	1.74
Digestion standards											
Standard Sample	dig. weight [g]	dig. volume [L]	c(Se) [µg/L]	c(Se) SD	c(Se) [mg/kg]	c(Se) SD					
dig_Std 2013_01_30 (0-5ppb)	0.10106	0.010	7.86	0.48	0.78	0.05					
dig_Std 2013_01_31 (10-100ppb)	0.10087	0.010	7.92	0.58	0.79	0.06					
dig_Std 2013_02_01 (250-2500ppb)	0.10348	0.010	8.77	0.54	0.85	0.05					
dig_Std 2013_09_17 (0-5ppb)	0.09988	0.010	8.59	0.32	0.86	0.03					
dig_Std 2013_09_18 (10-100ppb)	0.10022	0.010	9.60	0.57	0.96	0.06					
dig_Std 2013_09_19 (250-2500ppb)	0.09908	0.010	9.66	0.35	0.97	0.04					
dig_Std 2013_09_24 (0-5ppb)	0.10004	0.010	9.36	0.69	0.94	0.07					
dig_Std 2013_09_25 (10-100ppb)	0.09958	0.010	9.78	0.41	0.98	0.04					
dig_Std 2013_09_26 (250-2500ppb)	0.10027	0.010	10.85	0.98	1.08	0.10					

Table A.23.: A2 Se content of all three experimental runs for Na₂SeO₄

c(Se) [µg/L]	FIAS-Results			c(Se) dry weight (DW)							
	dig. weight shoot [g] [± 0.0001]	dig. weight root [g] [± 0.0001]	dig. volume [L] [± 0.0001]	c(Se) shoot [µg/L]	c(Se) shoot SD	c(Se) root [µg/L]	c(Se) root SD	c(Se) shoot [mg/kg]	c(Se) shoot SD	c(Se) root [mg/kg]	c(Se) root SD
Agar-Se (Na ₂ SeO ₄) Planting Date: 28.11.2012 (Bachelor Thesis Matthias von Brasch)											
0	0.02440	0.06680	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.02860	0.05860	0.010	14.80	1.41	8.25	0.90	5.17	0.49	1.41	0.15
10	0.03310	0.05370	0.010	36.59	4.62	16.20	0.59	11.06	1.40	3.02	0.11
25	0.02000	0.06750	0.010	39.20	10.50	29.28	1.45	19.60	5.25	4.34	0.21
50	0.02040	0.05440	0.010	213.84	8.85	108.63	1.34	104.82	4.34	19.97	0.25
100	0.01810	0.05580	0.010	397.15	14.73	174.92	5.50	219.42	8.14	31.35	0.99
250	0.01690	0.05510	0.010	622.11	21.32	448.54	17.86	368.11	12.61	81.41	3.24
500	0.01520	0.04560	0.010	144.08	11.35	338.20	18.11	94.79	7.46	74.17	3.97
1000	0.02300	0.05940	0.010	125.03	0.88	382.82	56.16	54.36	0.38	64.45	9.46
2500	0.00960	0.07420	0.010	65.80	2.07	223.96	9.92	68.54	2.16	30.18	1.34
Agar-Se (Na ₂ SeO ₄) Planting Date: 08.05.2013 (Experiment Repetition Alexandra Nothstein)											
0	0.03168	0.03861	0.010	0.63	0.27	0.34	0.28	0.20	0.08	0.09	0.07
5	0.03619	0.04379	0.010	16.68	1.32	8.90	0.47	4.61	0.37	2.03	0.11
10	0.04195	0.05178	0.010	28.83	0.51	18.38	1.49	6.87	0.12	3.55	0.29
25	0.03638	0.04797	0.010	108.59	1.21	69.20	3.16	29.85	0.33	14.43	0.66
50	0.04483	0.05231	0.010	252.47	5.78	109.38	1.36	56.32	1.29	20.91	0.26
100	0.03889	0.04004	0.010	574.27	24.75	239.89	10.96	147.67	6.36	59.91	2.74
250	0.03305	0.04304	0.010	931.19	29.75	599.88	14.86	281.75	9.00	139.38	3.45
500	0.02448	0.04561	0.010	519.22	16.35	684.84	19.58	212.10	6.68	150.15	4.29
1000	0.03683	0.05029	0.010	218.65	19.59	563.15	29.90	59.37	5.32	111.98	5.95
2500	0.02266	0.04677	0.010	125.61	6.05	422.38	32.74	55.43	2.67	90.31	7.00
Agar-Se (Na ₂ SeO ₄) Planting Date: 29.05.2013 (Experiment Repetition Alexandra Nothstein)											
0	0.02518	0.03092	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.02931	0.03603	0.010	25.68	1.11	7.40	0.44	8.76	0.38	2.05	0.12
10	0.03691	0.04516	0.010	51.67	1.27	15.28	0.77	14.00	0.34	3.38	0.17
25	0.02714	0.05227	0.010	169.76	4.87	41.78	3.34	62.55	1.79	7.99	0.64
50	0.01795	0.02341	0.010	241.75	3.80	55.87	2.07	134.68	2.12	23.86	0.88
100	0.02427	0.02665	0.010	518.51	7.36	116.21	6.96	213.64	3.03	43.60	2.61
250	0.01215	0.03522	0.010	546.81	10.56	232.00	10.04	450.05	8.69	65.87	2.85
500	0.01999	0.05012	0.010	245.16	10.59	315.47	17.22	122.64	5.30	62.94	3.44
1000	0.01631	0.06493	0.010	176.17	17.27	362.93	18.65	108.02	10.59	55.90	2.87
2500	0.01607	0.02163	0.010	125.33	12.89	175.29	8.96	77.99	8.02	81.04	4.14
Digestion standards											
Standard Sample	dig. weight [g]	dig. volume [L]	c(Se) [µg/L]	c(Se) SD	c(Se) [mg/kg]	c(Se) SD					
dig_Std 2012_12_19 (0-25ppb)	0.10417	0.010	10.20	0.32	0.98	0.03					
dig_Std 2012_12_20 (50-500ppb)	0.10446	0.010	6.39	0.26	0.61	0.02					
dig_Std 2012_12_21 (1000-2500ppb)	0.101	0.010	7.60	0.45	0.75	0.04					
dig_Std 2013_09_13 (0-25ppb)	0.10035	0.010	9.92	0.31	0.99	0.03					
dig_Std 2013_09_16 (50-500ppb)	0.10004	0.010	9.85	0.72	0.98	0.07					
dig_Std 2013_09_17 (1000-2500ppb)	0.09988	0.010	9.25	0.40	0.93	0.04					
dig_Std 2013_09_20 (0-25ppb)	0.09945	0.010	10.13	0.41	1.02	0.04					
dig_Std 2013_09_23 (50-500ppb)	0.09932	0.010	13.42	0.55	1.35	0.06					
dig_Std 2013_09_24 (1000-2500ppb)	0.10004	0.010	7.67	0.32	0.77	0.03					

A.2.3. Complete A2 results overview

Table A.24.: A2 results overview for Na_2SeO_3

ϕ (Se) [kg/L]	plants per box		2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		shoot height (Day 9)		shoot height (Day 16)		mean shoot DW		mean root DW		shoot water		root water		shoot FW		shoot water		root water		shoot FW		shoot water		root water					
	SD	SD	[mg/kg]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[%]			
0	5.3	0.6	2.74	0.21	1.19	0.08	3.94	0.29	3.47	0.79	8.85	0.43	0.0049	0.0010	0.0081	0.0028	80.29	4.19	70.39	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
5	5.7	0.6	3.11	0.24	1.42	0.19	4.54	0.42	3.51	0.30	10.38	1.55	0.0059	0.0009	0.0086	0.0015	78.43	2.03	66.77	0.38	0.16	2.85	1.78	75.35	29.57	198.12	147.63	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
10	5.0	1.0	3.19	0.26	1.38	0.23	4.58	0.45	3.62	0.18	10.71	1.52	0.0058	0.0011	0.0070	0.0005	80.84	1.48	75.59	0.54	0.19	5.90	2.79	53.15	16.58	134.48	29.44	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
25	5.0	1.0	2.93	0.48	1.31	0.27	4.24	0.75	3.44	0.51	9.60	0.35	0.0053	0.0009	0.0076	0.0005	77.79	3.81	71.47	1.49	0.45	11.20	0.72	59.27	20.44	129.49	15.91	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
50	5.0	1.0	2.91	0.58	1.30	0.27	4.21	0.82	3.46	1.32	9.58	2.71	0.0054	0.0025	0.0086	0.0016	79.51	0.74	68.56	2.54	0.99	25.60	17.29	50.37	18.47	145.38	61.64	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
100	4.3	1.5	3.11	0.45	1.35	0.20	4.46	0.65	3.17	0.96	9.36	0.35	0.0054	0.0009	0.0089	0.0008	75.90	1.25	59.93	8.72	2.72	33.96	6.47	52.89	25.28	146.66	70.55	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
250	5.0	1.0	2.35	0.21	0.97	0.06	3.32	0.21	2.50	0.87	7.71	0.41	0.0043	0.0012	0.0090	0.0012	77.32	5.46	62.19	0.00	0.00	57.65	25.59	33.14	12.01	92.40	29.13	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
500	5.3	0.6	2.50	0.13	1.07	0.03	3.57	0.14	2.21	0.54	7.21	0.18	0.0041	0.0006	0.0083	0.0006	72.34	5.66	58.72	13.32	3.81	79.92	42.20	28.14	17.60	76.26	44.29	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1000	5.3	0.6	2.26	0.42	1.05	0.35	3.31	0.76	1.93	0.57	6.54	1.65	0.0046	0.0016	0.0068	0.0003	70.27	3.10	61.81	22.41	5.57	49.98	22.98	17.60	76.02	44.29	26.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2500	4.7	1.2	2.08	0.29	0.91	0.12	2.99	0.40	1.33	0.58	4.90	1.40	0.0042	0.0019	0.0086	0.0010	67.36	4.20	56.55	17.93	5.32	84.07	36.38	7.22	11.57	17.68	7.26	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table A.25.: *A2 results overview for Na₂SeO₄*

c(Se) [µg/L]	plants per box		2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		shoot height (Day 9)		shoot height (Day 16)		mean shoot DW		mean root DW		shoot water		root water		c(Se) shoot FW		c(Se) root FW		shoot acc. factor		root acc. factor				
	[-]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD			
0	5.3	0.6	3.19	0.45	1.41	0.29	4.60	0.71	3.38	0.77	10.20	1.75	0.0051	0.0010	0.0082	0.0025	75.59	64.05	0.00	1.45	0.00	0.00	0.00	1.80	0.00	0.00	0.00	0.00	0.00		
5	5.7	0.6	3.37	0.47	1.32	0.25	4.69	0.65	3.65	0.80	9.98	2.36	0.0050	0.0006	0.0072	0.0027	76.49	69.47	2.83	1.45	0.53	0.95	1.80	0.36	0.00	273.80	25.53	0.00	108.36	5.92	
10	5.7	0.6	3.30	0.26	1.33	0.32	4.63	0.54	5.38	2.65	10.28	1.13	0.0062	0.0005	0.0082	0.0011	73.38	69.94	2.83	1.45	0.95	0.95	3.22	0.26	0.00	263.10	30.51	0.00	99.13	1.67	
25	5.7	0.6	2.99	0.66	1.19	0.45	4.18	1.09	2.58	0.23	9.28	2.21	0.0047	0.0013	0.0092	0.0019	72.82	63.83	6.01	10.15	6.10	6.10	8.01	4.59	0.00	196.17	130.07	41.08	154.76	21.62	
50	4.7	1.5	3.32	0.63	1.35	0.41	4.67	1.01	3.33	1.18	10.31	2.33	0.0059	0.0016	0.0092	0.0017	73.81	63.83	7.15	10.36	10.36	11.04	16.01	1.51	0.00	465.25	42.16	154.76	21.62	154.76	21.62
100	5.0	1.0	3.14	0.63	1.28	0.28	4.03	0.57	3.36	0.80	10.50	2.23	0.0059	0.0021	0.0088	0.0024	72.31	64.21	3.11	53.61	11.04	3.11	20.86	1.26	0.00	366.44	42.42	175.22	13.09	175.22	13.09
250	5.3	1.2	2.17	0.64	1.08	0.32	3.25	0.96	1.82	0.10	6.17	1.13	0.0039	0.0015	0.0085	0.0012	73.61	64.21	44.69	19.13	19.13	22.21	31.11	1.26	0.00	262.24	58.97	79.82	32.18	79.82	32.18
500	5.0	0.0	1.89	0.22	1.11	0.25	2.91	0.45	1.70	0.01	4.43	0.31	0.0040	0.0010	0.0092	0.0005	68.79	61.12	26.17	10.49	10.49	26.17	57.17	22.31	0.00	22.31	6.01	37.00	11.18	37.00	11.18
1000	5.3	0.6	2.16	0.33	1.05	0.18	3.22	0.46	1.63	0.53	4.28	1.13	0.0044	0.0015	0.0098	0.0014	64.59	51.09	47.30	21.34	21.34	47.30	26.17	22.31	0.00	22.31	6.01	37.00	11.18	37.00	11.18
2500	5.0	1.0	1.85	0.47	1.01	0.30	2.86	0.75	1.36	0.16	3.54	1.00	0.0033	0.0016	0.0095	0.0024	68.30	47.30	21.34	21.34	21.34	47.30	26.17	22.31	0.00	22.31	6.01	37.00	11.18	37.00	11.18

A.2.4. A2 analytical data

Table A.26.: A2 analytical data - HG-FIAS measurement I

Technique	AA FIAS-MHS	
Spectrometer Model	Aanalyst 200 S/N 200S6110908	
Autosampler Model	AS-90plus	
Batch ID	Pflanzenaufschlüsse	
Results Data Set	Brasch_Se_2013_01_17	
Date Measured	17.01.2013	
Method Name	Se Nothstein	
correl. coeff.	PQL (= lowest calib-10 %)	0.450
0.995303	LOQ (= 7-wash)	0.266
calib. slope	LOD (= 3-wash)	0.114
0.02535	analytical quality [%]	104.276

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0013	0.0	0.00	0.00
2	0.5 ppb	0.0099	0.0011	0.5	0.39	0.04
3	1.0 ppb	0.0226	0.0011	1.0	0.89	0.04
4	2.0 ppb	0.0437	0.0010	2.0	1.72	0.04
5	5.0 ppb	0.1298	0.0057	5.0	5.12	0.22

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.004	0.021	-0.004	0.021	1	0.00	0.02
2	wash	-0.013	0.033	-0.013	0.033	1	-0.01	0.03
3	HCl Blank	-0.018	0.051	-0.018	0.051	6	-0.11	0.31
4	Trace Metal 252 µg/L	4.534	0.057	4.602	0.058	60	276.10	3.47
5	Na2SeO4 reduced 10 µg/L	0.033	0.100	0.033	0.101	6	< PQL	< PQL
6	Na2SeO4 unreduced 10µg/L	0.045	0.076	0.046	0.077	6	< PQL	< PQL
7	Na2SeO3 reduced 10 µg/L	0.010	0.036	0.010	0.037	6	< PQL	< PQL
8	Na2SeO3 unreduced 10µg/L	1.643	0.070	1.667	0.071	6	10.00	0.43
9	wash	0.057	0.090	0.057	0.090	1	0.06	0.09
10	wash	-0.001	0.056	-0.001	0.056	1	0.00	0.06
11	Se_Std_0	0.030	0.057	0.030	0.057	1	0.03	0.06
12	Se_Std_0.5	0.374	0.030	0.374	0.030	1	0.37	0.03
13	Se_Std_1	0.785	0.017	0.785	0.017	1	0.78	0.02
14	Se_Std_2	1.698	0.060	1.698	0.060	1	1.70	0.06
15	Se_Std_5	5.149	0.103	5.149	0.103	1	5.15	0.10
16	wash	0.230	0.507	0.230	0.507	1	0.23	0.51
17	wash	0.021	0.020	0.021	0.020	1	0.02	0.02
18	2012-12-19 digest blank	-0.012	0.025	-0.014	0.031	12	< PQL	< PQL
19	2012-12-19 digest Stnd	0.683	0.021	0.837	0.026	12	10.04	0.31
20	2012-12-19 0 µg/L Se Shoot	0.013	0.036	0.015	0.044	12	< PQL	< PQL
21	2012-12-19 0 µg/L Se Root	-0.014	0.027	-0.017	0.033	12	< PQL	< PQL
22	2012-12-19 5 µg/L Se Shoot	1.006	0.096	1.233	0.117	12	14.80	1.41
23	2012-12-19 5 µg/L Se Root	0.561	0.061	0.687	0.075	12	8.25	0.90
24	2012-12-19 10 µg/L Se Shoot	2.489	0.314	3.049	0.385	12	36.59	4.62
25	2012-12-19 10 µg/L Se Root	1.102	0.040	1.350	0.049	12	16.20	0.59
26	2012-12-19 25 µg/L Se Shoot	1.777	0.476	2.178	0.583	18	39.20	10.50
27	2012-12-19 25 µg/L Se Root	1.525	0.055	1.899	0.069	12	22.79	0.82
28	wash	0.073	0.143	0.073	0.143	1	0.07	0.14
29	Se_Std_0	0.014	0.036	0.014	0.036	1	0.01	0.04
30	Se_Std_0.5	0.304	0.021	0.304	0.021	1	0.30	0.02
31	Se_Std_1	0.673	0.035	0.673	0.035	1	0.67	0.04
32	Se_Std_2	1.336	0.147	1.336	0.147	1	1.34	0.15
33	Se_Std_5	3.901	0.184	3.901	0.184	1	3.90	0.18
34	wash	0.136	0.209	0.136	0.209	1	0.14	0.21
28	wash	0.005	0.047	0.005	0.047	1	0.01	0.05
29	Se_Std_0	0.001	0.025	0.001	0.025	1	0.00	0.03
30	Se_Std_0.5	0.641	0.044	0.641	0.044	1	0.64	0.04
31	Se_Std_1	1.155	0.041	1.155	0.041	1	1.16	0.04
32	Se_Std_2	2.227	0.116	2.227	0.116	1	2.23	0.12
33	Se_Std_5	6.292	0.099	6.292	0.099	1	6.29	0.10
34	wash	-0.017	0.020	-0.017	0.020	1	-0.02	0.02
35	wash	-0.017	0.037	-0.017	0.037	1	-0.02	0.04
36	2012-12-20 digest blank	0.003	0.029	0.002	0.021	12	< PQL	< PQL
37	2012-12-20 digest Stnd	1.005	0.041	0.742	0.030	12	8.90	0.36
38	2012-12-20 50 µg/L Se Shoot	10.715	0.381	7.909	0.281	18	> calib	< calib
39	2012-12-20 50 µg/L Se Root	5.361	0.343	3.957	0.253	18	> calib	< calib
40	2012-12-20 100 µg/L Se Shoot	14.506	0.197	10.707	0.145	24	> calib	< calib
41	2012-12-20 100 µg/L Se Root	9.224	0.327	6.808	0.241	18	> calib	< calib
42	2012-12-20 250 µg/L Se Shoot	12.109	0.706	8.937	0.521	36	> calib	< calib
43	2012-12-20 250 µg/L Se Root	11.715	0.247	8.647	0.182	36	> calib	< calib
44	2012-12-20 500 µg/L Se Shoot	5.564	0.162	4.107	0.120	36	> calib	< calib
45	2012-12-20 500 µg/L Se Root	10.284	0.090	7.590	0.066	36	> calib	< calib
46	wash	-0.014	0.013	-0.014	0.013	1	-0.01	0.01
47	Se_Std_0	0.000	0.037	0.000	0.037	1	0.00	0.04
48	Se_Std_0.5	0.631	0.048	0.631	0.048	1	0.63	0.05
49	Se_Std_1	1.310	0.027	1.310	0.027	1	1.31	0.03
50	Se_Std_2	2.442	0.063	2.442	0.063	1	2.44	0.06
51	Se_Std_5	6.630	0.172	6.630	0.172	1	6.63	0.17
52	wash	-0.009	0.028	-0.009	0.028	1	-0.01	0.03
53	wash	-0.005	0.050	-0.005	0.050	1	-0.01	0.05
54	2012-12-21 digest blank	-0.019	0.026	-0.011	0.015	12	< PQL	< PQL
55	2012-12-21 digest Stnd	0.957	0.057	0.570	0.034	12	6.84	0.41
56	2012-12-21 1000 µg/L Se Shoot	4.711	0.033	3.473	0.025	36	125.03	0.88
57	2012-12-21 1000 µg/L Se Root	11.195	0.271	8.253	0.200	36	> calib	< calib
58	2012-12-21 2500 µg/L Se Shoot	3.719	0.117	2.742	0.086	24	65.80	2.07
59	2012-12-21 2500 µg/L Se Root	9.963	0.117	7.345	0.086	24	> calib	< calib
60	2012-12-21 0 µg/L Se AgarII	-0.013	0.037	-0.007	0.019	12	< PQL	< PQL
61	2012-12-21 5 µg/L Se AgarII	0.001	0.020	0.001	0.011	12	< PQL	< PQL
62	2012-12-21 10 µg/L Se AgarII	0.004	0.035	0.002	0.018	12	< PQL	< PQL
63	2012-12-21 25 µg/L Se AgarII	0.148	0.022	0.078	0.012	12	< PQL	< PQL
64	wash	-0.014	0.015	-0.014	0.015	1	-0.01	0.02

Table A.27.: A2 analytical data - HG-FIAS measurement I (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
65	Se_Std_0	0.018	0.034	0.018	0.034	1	0.02	0.03
66	Se_Std_0.5	0.522	0.046	0.522	0.046	1	0.52	0.05
67	Se_Std_1	1.192	0.048	1.192	0.048	1	1.19	0.05
68	Se_Std_2	2.272	0.058	2.272	0.058	1	2.27	0.06
69	Se_Std_5	6.301	0.115	6.301	0.115	1	6.30	0.12
70	wash	0.264	0.546	0.264	0.546	1	0.26	0.55
71	wash	-0.005	0.056	-0.005	0.056	1	-0.01	0.06
72	Trace Metal 252 µg/L	5.404	0.106	4.157	0.082	60	249.45	4.89
73	wash	-0.003	0.036	-0.003	0.036	1	0.00	0.04
correl. coeff. 0.995303	PQL (= lowest calib-10 %)	0.450						
calib. slope 0.02535	LOQ (= 7·wash)	0.266						
	LOD (= 3·wash)	0.114						
	analytical quality [%]	104.276						
Calibration	Sample ID	Mean signal [-]	SD [-]			entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0012			0.0	0.00	0.00
2	0.5 ppb	0.0115	0.0019			0.5	0.38	0.06
3	1.0 ppb	0.0257	0.0019			1.0	0.85	0.06
4	2.0 ppb	0.0541	0.0011			2.0	1.80	0.04
5	5.0 ppb	0.1532	0.0039			5.0	5.10	0.13
Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.070	0.037	-0.070	0.037	1	-0.07	0.04
2	wash	-0.010	0.043	-0.010	0.043	1	-0.01	0.04
3	Trace Metal 252 µg/L VF 60	4.501	0.144	4.501	0.144	60	270.06	8.64
4	wash	0.035	0.100	0.035	0.100	1	0.04	0.10
5	2012-12-19 25 µg/L Se Root	2.225	0.110	2.440	0.121	12	29.28	1.45
6	2012-12-20 50 µg/L Se Shoot	1.323	0.055	1.188	0.049	180	213.84	8.85
7	2012-12-20 50 µg/L Se Root	2.752	0.034	3.018	0.037	36	108.63	1.34
8	2012-12-20 100 µg/L Se Shoot	0.921	0.034	0.827	0.031	480	397.15	14.73
9	2012-12-20 100 µg/L Se Root	1.082	0.034	0.972	0.031	180	174.92	5.50
10	2012-12-20 250 µg/L Se Shoot	1.576	0.054	1.728	0.059	360	622.11	21.32
11	2012-12-20 250 µg/L Se Root	0.678	0.027	0.623	0.025	720	448.54	17.86
12	2012-12-20 500 µg/L Se Shoot	0.891	0.070	0.800	0.063	180	144.08	11.35
13	2012-12-20 500 µg/L Se Root	1.046	0.056	0.939	0.050	360	338.20	18.11
14	2012-12-21 1000 µg/L Se Root	1.184	0.174	1.063	0.156	360	382.82	56.16
15	2012-12-21 2500 µg/L Se Root	1.039	0.046	0.933	0.041	240	223.96	9.92
16	wash	0.007	0.041	0.007	0.041	1	0.01	0.04
17	wash	0.001	0.029	0.001	0.029	1	0.00	0.03
18	Se_Std_0	-0.011	0.034	-0.011	0.034	1	-0.01	0.03
19	Se_Std_0.5	0.413	0.040	0.413	0.040	1	0.41	0.04
20	Se_Std_1	0.941	0.034	0.941	0.034	1	0.94	0.03
21	Se_Std_2	1.629	0.210	1.629	0.210	1	1.63	0.21
22	Se_Std_5	4.679	0.097	4.679	0.097	1	4.68	0.10
23	wash	0.083	0.225	0.083	0.225	1	0.08	0.23

Table A.28.: A2 analytical data - HG-FIAS measurement II

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Pflanzenaufschlüsse		
Results Data Set	Brasch_Se_2013_02_05		
Date Measured	05.02.2013		
Method Name	Se Nothstein 5repl		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.999225	LOQ (= 7-wash)	0.236	
calib. slope	LOD (= 3-wash)	0.101	
0.02967	analytical quality [%]	96.786	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0014	0.0	0.00	0.00
2	0.5 ppb	0.0131	0.0008	0.5	0.44	0.03
3	1.0 ppb	0.0268	0.0008	1.0	0.90	0.03
4	2.0 ppb	0.0575	0.0022	2.0	1.94	0.07
5	5.0 ppb	0.1497	0.0042	5.0	5.05	0.14

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.022	0.024	-0.022	0.024	1	-0.02	0.02
2	wash	0.048	0.026	0.048	0.026	1	0.05	0.03
3	HCl Blank VF 6	-0.001	0.031	-0.001	0.026	6	-0.01	0.16
4	Trace Metal 252 µg/L	4.043	0.122	3.880	0.117	60	232.81	7.02
5	Na2SeO4 reduced 10 µg/L	0.413	0.036	0.347	0.031	6	2.08	0.18
6	Na2SeO4 unreduced 10 µg/L	0.067	0.029	0.056	0.024	6	< PQL	< PQL
7	Na2SeO3 reduced 10 µg/L	0.102	0.025	0.086	0.021	6	< PQL	< PQL
8	Na2SeO3 unreduced 10 µg/L	1.215	0.033	0.986	0.026	6	5.92	0.16
9	wash	0.030	0.018	0.030	0.018	1	0.03	0.02
10	wash	0.003	0.024	0.003	0.024	1	0.00	0.02
11	Se_Std_0	0.007	0.033	0.007	0.033	1	0.01	0.03
12	Se_Std_0.5	0.511	0.039	0.511	0.039	1	0.51	0.04
13	Se_Std_1	1.073	0.065	1.073	0.065	1	1.07	0.07
14	Se_Std_2	2.145	0.041	2.145	0.041	1	2.15	0.04
15	Se_Std_5	5.249	0.178	5.249	0.178	1	5.25	0.18
16	wash	0.026	0.038	0.026	0.038	1	0.03	0.04
17	wash	0.021	0.030	0.021	0.030	1	0.02	0.03
18	2013-01-30 dig. blank	0.012	0.034	0.011	0.029	12	< PQL	< PQL
19	2013-01-30 dig. Std WheatFlour 1567a	0.733	0.044	0.621	0.038	12	7.45	0.45
20	2013-01-30 250 µg/L Se Agar II	1.748	0.110	1.592	0.100	12	19.10	1.20
21	2013-01-30 500 µg/L Se Agar II	3.624	0.129	3.597	0.128	18	64.75	2.30
22	2013-01-30 1000 µg/L Se Agar II	3.038	0.092	2.766	0.084	48	132.78	4.02
23	2013-01-30 2500 µg/L Se Agar II	3.024	0.075	2.753	0.069	144	396.48	9.86
24	2013-01-30 0 µg/L Se Shoot	0.055	0.076	0.048	0.066	12	< PQL	< PQL
25	2013-01-30 0 µg/L Se Root	0.044	0.015	0.038	0.013	12	< PQL	< PQL
26	2013-01-30 5 µg/L Se Shoot	0.272	0.049	0.235	0.043	12	2.83	0.51
27	2013-01-30 5 µg/L Se Root	0.809	0.067	0.686	0.057	12	8.23	0.68
28	wash	0.033	0.042	0.033	0.042	1	0.03	0.04
29	Se_Std_0	0.022	0.025	0.022	0.025	1	0.02	0.03
30	Se_Std_0.5	0.489	0.046	0.489	0.046	1	0.49	0.05
31	Se_Std_1	1.008	0.064	1.008	0.064	1	1.01	0.06
32	Se_Std_2	2.078	0.041	2.078	0.041	1	2.08	0.04
33	Se_Std_5	4.917	0.292	4.917	0.292	1	4.92	0.29
34	wash	0.013	0.019	0.013	0.019	1	0.01	0.02
35	wash	-0.001	0.027	-0.001	0.027	1	0.00	0.03
36	2013-01-31 dig. blank	0.001	0.050	0.001	0.042	12	< PQL	< PQL
37	2013-01-31 dig. Std WheatFlour 1567a	0.667	0.077	0.564	0.065	12	6.77	0.78
38	2013-01-31 dig. Std WheatFlour 1567a	0.811	0.059	0.686	0.050	12	8.23	0.60
39	2013-01-31 10 µg/L Shoot	0.394	0.038	0.333	0.032	12	3.99	0.38
40	2013-01-31 10 µg/L Root	1.227	0.111	1.024	0.093	12	12.28	1.11
41	2013-01-31 25 µg/L Shoot	1.386	0.098	1.156	0.082	12	13.87	0.98
42	2013-01-31 25 µg/L Root	4.134	0.105	3.986	0.101	12	47.83	1.21
43	2013-01-31 50 µg/L Shoot	1.758	0.077	1.655	0.074	12	19.86	1.09
44	2013-01-31 50 µg/L Root	5.644	0.142	5.753	0.145	12	69.04	1.74
45	2013-01-31 100 µg/L Shoot	3.142	0.148	3.101	0.146	12	37.21	1.75
46	2013-01-31 100 µg/L Root	9.984	0.107	9.628	0.103	12	> calib	> calib
47	wash	0.062	0.040	0.062	0.040	1	0.06	0.04
48	Se_Std_0	0.000	0.022	0.000	0.022	1	0.00	0.02
49	Se_Std_0.5	0.530	0.028	0.530	0.028	1	0.53	0.03
50	Se_Std_1	1.098	0.063	1.098	0.063	1	1.10	0.06
51	Se_Std_2	2.256	0.072	2.256	0.072	1	2.26	0.07
52	Se_Std_5	5.535	0.139	5.535	0.139	1	5.54	0.14
53	wash	0.028	0.029	0.028	0.029	1	0.03	0.03
54	wash	0.029	0.033	0.029	0.033	1	0.03	0.03
55	2013-02-01 dig. blank	0.034	0.030	0.029	0.026	12	< PQL	< PQL
56	2013-02-01 dig. Std. WheatFlour 1567a	0.687	0.287	0.577	0.241	12	6.92	2.90
57	2013-02-01 250 µg/L Shoot	2.024	0.017	1.835	0.016	36	66.07	0.57
58	2013-02-01 250 µg/L Root	7.941	0.313	7.515	0.296	36	> calib	> calib
59	2013-02-01 500 µg/L Shoot	1.858	0.033	1.685	0.030	36	60.64	1.08
60	2013-02-01 500 µg/L Root	7.040	0.191	6.662	0.181	36	> calib	> calib
61	2013-02-01 1000 µg/L Shoot	3.992	0.066	3.867	0.064	24	92.80	1.54
62	2013-02-01 1000 µg/L Root	14.951	0.528	14.148	0.500	24	> calib	> calib
63	2013-02-01 2500 µg/L Shoot	2.926	0.125	2.654	0.113	24	63.69	2.72
64	2013-02-01 2500 µg/L Root	10.731	0.189	10.155	0.179	24	> calib	> calib
65	wash	0.025	0.033	0.025	0.033	1	0.02	0.03

Table A.29.: A2 analytical data - HG-FIAS measurement II (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
65	Se_Std_0	0.021	0.022	0.021	0.022	1	0.02	0.02
66	Se_Std_0.5	0.494	0.049	0.494	0.049	1	0.49	0.05
67	Se_Std_1	1.036	0.026	1.036	0.026	1	1.04	0.03
68	Se_Std_2	2.111	0.049	2.111	0.049	1	2.11	0.05
69	Se_Std_5	5.099	0.121	5.099	0.121	1	5.10	0.12
70	wash	0.184	0.411	0.184	0.411	1	0.18	0.41
71	wash	0.024	0.041	0.024	0.041	1	0.02	0.04
72	HCl Blank	0.039	0.067	0.038	0.064	6	0.23	0.39
73	Trace Metal 252 µg/L	4.031	0.130	4.250	0.137	60	254.99	8.25
74	Na2SeO4 reduced 10 µg/L	0.414	0.050	0.400	0.048	6	2.40	0.29
75	Na2SeO4 unreduced 10 µg/L	0.051	0.063	0.049	0.060	6	< PQL	< PQL
76	Na2SeO3 reduced 10 µg/L	0.099	0.020	0.096	0.019	6	< PQL	< PQL
77	Na2SeO3 unreduced 10 µg/L	1.123	0.055	1.057	0.052	6	6.34	0.31
78	wash	0.015	0.018	0.015	0.018	1	0.02	0.02
79	Se_Std_0	0.010	0.016	0.010	0.016	1	0.01	0.02
80	Se_Std_0.5	0.419	0.066	0.419	0.066	1	0.42	0.07
81	Se_Std_1	0.876	0.074	0.876	0.074	1	0.88	0.07
82	Se_Std_2	1.889	0.047	1.889	0.047	1	1.89	0.05
83	Se_Std_5	4.445	0.147	4.445	0.147	1	4.45	0.15
84	wash	0.058	0.086	0.058	0.086	1	0.06	0.09
85	wash	0.031	0.042	0.031	0.042	1	0.03	0.04

Table A.30.: A2 analytical data - HG-FIAS measurement III

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Agaraufschlüsse		
Results Data Set	Brasch_Se_2013_02_06II		
Date Measured	25.02.2013		
Method Name	Se Nothstein 5repl		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.999665	LOQ (= 7-wash)	-0.237	
calib. slope	LOD (= 3-wash)	-0.102	
0.0252	analytical quality [%]	92.321	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0027	0.0	0.00	0.00
2	0.5 ppb	0.0109	0.0008	0.5	0.44	0.03
3	1.0 ppb	0.0249	0.0008	1.0	0.99	0.03
4	2.0 ppb	0.0519	0.0021	2.0	2.06	0.08
5	5.0 ppb	0.1256	0.0042	5.0	4.98	0.17

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.015	0.058	-0.015	0.058	1	-0.02	0.06
2	wash	-0.023	0.032	-0.023	0.032	1	-0.02	0.03
3	HCl Blank	-0.033	0.073	-0.029	0.065	6	-0.17	0.39
4	Trace Metal 252 µg/L	4.584	0.100	4.081	0.089	60	244.84	5.33
5	wash	-0.029	0.026	-0.029	0.026	1	-0.03	0.03
6	wash	-0.037	0.047	-0.037	0.047	1	-0.04	0.05
7	Se_Std_0	-0.051	0.024	-0.051	0.024	1	-0.05	0.02
8	Se_Std_0.5	0.483	0.040	0.483	0.040	1	0.48	0.04
9	Se_Std_1	1.150	0.051	1.150	0.051	1	1.15	0.05
10	Se_Std_2	2.444	0.100	2.444	0.100	1	2.44	0.10
11	Se_Std_5	5.830	0.059	5.830	0.059	1	5.83	0.06
12	wash	-0.016	0.048	-0.016	0.048	1	-0.02	0.05
13	wash	-0.043	0.043	-0.043	0.043	1	-0.04	0.04
14	2013-01-16 dig. blank	-0.060	0.019	-0.048	0.015	12	< PQL	< PQL
15	2013-01-30 dig. Std WheatFlour 1567a	0.856	0.071	0.667	0.055	12	8.00	0.66
16	2013-01-16 0 µg/L Agar I	0.010	0.045	0.008	0.037	12	< PQL	< PQL
17	2013-01-16 5 µg/L Agar I	0.004	0.019	0.003	0.016	12	< PQL	< PQL
18	2013-01-16 10 µg/L Agar I	0.095	0.027	0.076	0.021	12	< PQL	< PQL
19	2013-01-16 25 µg/L Agar I	0.359	0.049	0.288	0.039	12	< PQL	< PQL
20	2013-01-16 50 µg/L Agar I	0.780	0.034	0.607	0.027	12	7.29	0.32
21	2013-01-16 100 µg/L Agar I	1.750	0.075	1.329	0.057	12	15.95	0.69
22	2013-01-16 250 µg/L Agar I	4.615	0.139	3.584	0.108	12	43.01	1.29
23	2013-01-16 500 µg/L Agar I	2.327	0.076	1.768	0.058	18	31.82	1.04
24	wash	-0.056	0.028	-0.056	0.028	1	-0.06	0.03
25	Se_Std_0	-0.037	0.033	-0.037	0.033	1	-0.04	0.03
26	Se_Std_0.5	0.558	0.039	0.558	0.039	1	0.56	0.04
27	Se_Std_1	1.267	0.048	1.267	0.048	1	1.27	0.05
28	Se_Std_2	2.663	0.095	2.663	0.095	1	2.66	0.09
29	Se_Std_5	6.363	0.181	6.363	0.181	1	6.36	0.18
30	wash	0.006	0.031	0.006	0.031	1	0.01	0.03
31	wash	-0.034	0.029	-0.034	0.029	1	-0.03	0.03
32	2013-01-29 dig. Blank	-0.063	0.029	-0.039	0.017	12	< PQL	< PQL
33	2013-01-29 dig. Std Wheat Flour 1567a	0.896	0.043	0.593	0.029	12	7.11	0.34
34	2013-01-29 1000 µg/L Agar I	10.334	0.332	7.186	0.231	48	344.93	11.08
35	2013-01-29 2500 µg/L Agar I	1.411	0.037	0.933	0.024	144	134.39	3.52
36	2013-01-29 0 µg/L Agar II	-0.030	0.031	-0.018	0.019	12	< PQL	< PQL
37	2013-01-29 5 µg/L Agar II	0.016	0.011	0.010	0.007	12	< PQL	< PQL
38	2013-01-29 10 µg/L Agar II	0.028	0.035	0.017	0.021	12	< PQL	< PQL
39	2013-01-29 25 µg/L Agar II	0.160	0.055	0.098	0.033	12	< PQL	< PQL
40	2013-01-29 50 µg/L Agar II	0.553	0.041	0.338	0.025	12	4.06	0.30
41	2013-01-29 100 µg/L Agar II	0.980	0.061	0.648	0.040	12	7.78	0.48
42	wash	-0.032	0.023	-0.032	0.023	1	-0.03	0.02
43	Se_Std_0	-0.036	0.033	-0.036	0.033	1	-0.04	0.03
44	Se_Std_0.5	0.650	0.027	0.650	0.027	1	0.65	0.03
45	Se_Std_1	1.383	0.022	1.383	0.022	1	1.38	0.02
46	Se_Std_2	2.915	0.056	2.915	0.056	1	2.92	0.06
47	Se_Std_5	6.639	0.125	6.639	0.125	1	6.64	0.13
48	wash	-0.025	0.051	-0.025	0.051	1	-0.02	0.05
49	wash	-0.039	0.020	-0.039	0.020	1	-0.04	0.02
50	2012-12-19 10 µg/L Shoot	4.306	0.103	2.753	0.066	18	49.55	1.19
51	2012-12-19 25 µg/L Shoot	3.759	0.077	2.403	0.049	18	43.25	0.88
52	2013-01-13 50 µg/L Agar II	0.134	0.029	0.064	0.014	12	< PQL	< PQL
53	2013-01-31 100 µg/L Root	3.770	0.058	2.410	0.037	90	216.87	3.32
54	2013-02-01 250 µg/L Root	2.686	0.061	1.529	0.035	180	275.23	6.29
55	2013-02-01 500 µg/L Root	2.309	0.064	1.315	0.036	180	236.66	6.56
56	2013-02-01 1000 µg/L Root	3.561	0.094	2.276	0.060	240	546.36	14.46
57	2013-02-01 2500 µg/L Root	4.282	0.060	2.737	0.038	120	328.44	4.58
58	wash	-0.063	0.056	-0.063	0.056	1	-0.06	0.06
59	wash	-0.049	0.049	-0.049	0.049	1	-0.05	0.05
60	HCl Blank	-0.033	0.035	-0.016	0.017	6	-0.10	0.10
61	Trace Metal 252 µg/L	5.748	0.075	3.674	0.048	60	220.46	2.86
62	wash	-0.038	0.055	-0.038	0.055	1	-0.04	0.06
63	Se_Std_0	-0.031	0.040	-0.031	0.040	1	-0.03	0.04
64	Se_Std_0.5	0.672	0.033	0.672	0.033	1	0.67	0.03
65	Se_Std_1	1.420	0.065	1.420	0.065	1	1.42	0.07
66	Se_Std_2	2.976	0.059	2.976	0.059	1	2.98	0.06
67	Se_Std_5	6.923	0.088	6.923	0.088	1	6.92	0.09
68	wash	-0.050	0.023	-0.050	0.023	1	-0.05	0.02
69	wash	0.005	0.072	0.005	0.072	1	0.00	0.07

Table A.31.: A2 analytical data - HG-FIAS measurement IV

Technique	AA FIAS-MHS							
Spectrometer Model	Aanalyst 200 S/N 200S6110908							
Autosampler Model	AS-90plus							
Batch ID	Pflanzenaufschlüsse							
Results Data Set	Se_Nothingstein_2013_09_30							
Date Measured	30.09.2013							
Method Name	Se Nothstein calib 6							
correl. coeff.	PQL (= lowest calib-10 %)	0.450						
0.999352	LOQ (= 7-wash)	0.282						
calib. slope	LOD (= 3-wash)	0.121						
0.02803	analytical quality [%]	108.905						
Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]		
1	Blank	0.0000	0.0008	0.0	0.00	0.00		
2	0.5 ppb	0.0127	0.0014	0.5	0.45	0.05		
3	0.75 ppb	0.0203	0.0014	0.75	0.72	0.05		
4	1.0 ppb	0.0245	0.0018	1.0	0.88	0.06		
5	2.0 ppb	0.0562	0.0006	2.0	2.00	0.02		
6	4.0 ppb	0.1156	0.0020	4.0	4.12	0.07		
7	5.0 ppb	0.1404	0.0016	5.0	5.01	0.06		
8	6.0 ppb	0.1662	0.0038	6.0	5.93	0.14		
Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.059	0.037	-0.059	0.037	1	-0.06	0.04
2	wash	0.062	0.029	0.062	0.029	1	0.06	0.03
3	HCl Blank	0.033	0.050	0.030	0.046	6	0.18	0.28
4	Trace Metal 252 µg/L	3.480	0.071	3.430	0.070	80	274.39	5.63
5	wash	0.025	0.050	0.025	0.050	1	0.02	0.05
6	Se_Std_0	0.024	0.026	0.024	0.026	1	0.02	0.03
7	Se_Std_0.5	0.495	0.055	0.495	0.055	1	0.49	0.06
8	Se_Std_0.75	0.773	0.062	0.773	0.062	1	0.77	0.06
9	Se_Std_1	1.024	0.043	1.024	0.043	1	1.02	0.04
10	Se_Std_2	2.080	0.030	2.080	0.030	1	2.08	0.03
11	Se_Std_4	4.184	0.110	4.184	0.110	1	4.18	0.11
12	Se_Std_5	5.080	0.054	5.080	0.054	1	5.08	0.05
13	Se_Std_6	6.145	0.112	6.145	0.112	1	6.15	0.11
14	wash	0.054	0.037	0.054	0.037	1	0.05	0.04
15	wash	0.038	0.025	0.038	0.025	1	0.04	0.02
16	2013-09-13 dig blind	0.048	0.047	0.043	0.042	8	< PQL	< PQL
17	2013-09-13 dig Std	1.222	0.052	1.132	0.048	8	9.06	0.38
18	2013-09-13 0ppb Shoot	0.089	0.038	0.079	0.034	8	< PQL	< PQL
19	2013-09-13 0ppb Root	0.048	0.040	0.042	0.036	8	< PQL	< PQL
20	2013-09-13 5 ppb Shoot	2.143	0.170	2.085	0.165	8	16.68	1.32
21	2013-09-13 5 ppb Root	1.200	0.064	1.112	0.059	8	8.90	0.47
22	2013-09-13 10 ppb Shoot	3.606	0.064	3.603	0.064	8	28.83	0.51
23	2013-09-13 10 ppb Root	2.362	0.192	2.297	0.187	8	18.38	1.49
24	2013-09-13 25 ppb Shoot	5.505	0.062	5.429	0.061	20	108.59	1.21
25	2013-09-13 25 ppb Root	3.463	0.158	3.460	0.158	20	69.20	3.16
26	wash	0.025	0.020	0.025	0.020	1	0.03	0.02
27	Se_Std_0.5	0.520	0.061	0.520	0.061	1	0.52	0.06
28	Se_Std_0.75	0.781	0.035	0.781	0.035	1	0.78	0.03
29	Se_Std_2	2.038	0.048	2.038	0.048	1	2.04	0.05
30	Se_Std_4	4.070	0.076	4.070	0.076	1	4.07	0.08
31	Se_Std_6	5.876	0.053	5.876	0.053	1	5.88	0.05
32	wash	0.018	0.028	0.018	0.028	1	0.02	0.03
33	wash	-0.007	0.038	-0.007	0.038	1	-0.01	0.04
34	2013-09-16 dig blind	0.042	0.079	0.036	0.068	8	< PQL	< PQL
35	2013-09-16 dig Std	1.152	0.088	1.056	0.080	8	8.44	0.64
36	2013-09-16 50 ppb Shoot	10.243	0.204	10.137	0.202	20	> calib	> calib
37	2013-09-16 50 ppb Root	5.526	0.069	5.469	0.068	20	109.38	1.36
38	2013-09-16 100 ppb Shoot	2.961	0.128	2.871	0.124	200	574.27	24.75
39	2013-09-16 100 ppb Root	1.309	0.060	1.199	0.055	200	239.89	10.96
40	2013-09-16 250 ppb Shoot	4.661	0.149	4.656	0.149	200	931.19	29.75
41	2013-09-16 250 ppb Root	3.002	0.074	2.999	0.074	200	599.88	14.86
42	2013-09-16 500 ppb Shoot	2.677	0.084	2.596	0.082	200	519.22	16.35
43	2013-09-16 500 ppb Root	3.428	0.098	3.424	0.098	200	684.84	19.58
44	wash	0.050	0.029	0.050	0.029	1	0.05	0.03
45	Se_Std_0.5	0.518	0.057	0.518	0.057	1	0.52	0.06
46	Se_Std_0.75	0.789	0.046	0.789	0.046	1	0.79	0.05
47	Se_Std_2	2.091	0.039	2.091	0.039	1	2.09	0.04
48	Se_Std_4	4.186	0.040	4.186	0.040	1	4.19	0.04
49	Se_Std_6	6.104	0.089	6.104	0.089	1	6.10	0.09
50	wash	0.001	0.045	0.001	0.045	1	0.00	0.05
51	wash	0.015	0.028	0.015	0.028	1	0.02	0.03
52	2013-09-17 dig blind	0.052	0.056	0.045	0.048	8	< PQL	< PQL
53	2013-09-17 dig Std	1.257	0.047	1.074	0.040	8	8.59	0.32
54	2013-09-17 1000ppb Shoot	1.121	0.100	1.093	0.098	200	218.65	19.59
55	2013-09-17 1000ppb Root	2.960	0.157	2.816	0.150	200	563.15	29.90
56	2013-09-17 2500 ppb Shoot	0.660	0.032	0.628	0.030	200	125.61	6.05
57	2013-09-17 2500 ppb Root	2.220	0.172	2.112	0.164	200	422.38	32.74
58	2013-09-17 0 ppb Shoot	0.027	0.022	0.023	0.019	8	< PQL	< PQL
59	2013-09-17 0 ppb Root	0.060	0.040	0.051	0.034	8	< PQL	< PQL
60	2013-09-17 5 ppb Shoot	1.203	0.083	1.146	0.079	8	9.17	0.63
61	2013-09-17 5 ppb Root	2.751	0.208	2.617	0.198	8	20.94	1.58
62	wash	0.000	0.026	0.000	0.026	1	0.00	0.03

Table A.32.: A2 analytical data - HG-FIAS measurement IV (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
63	Se_Std_0.5	0.522	0.043	0.522	0.043	1	0.52	0.04
64	Se_Std_0.75	0.728	0.029	0.728	0.029	1	0.73	0.03
65	Se_Std_2	2.112	0.054	2.112	0.054	1	2.11	0.05
66	Se_Std_4	4.138	0.094	4.138	0.094	1	4.14	0.09
67	Se_Std_6	5.377	0.347	5.377	0.347	1	5.38	0.35
68	wash	0.051	0.025	0.051	0.025	1	0.05	0.02
69	wash	0.017	0.024	0.017	0.024	1	0.02	0.02
70	2013-09-18 dig. Blind	-0.006	0.043	-0.005	0.038	8	< PQL	< PQL
71	2013-09-18 dig. Std.	1.223	0.072	1.200	0.071	8	9.60	0.57
72	2013-09-18 10 ppb Shoot	1.279	0.078	1.254	0.077	8	10.04	0.61
73	2013-09-18 10 ppb Root	3.600	0.046	3.672	0.047	8	29.38	0.38
74	2013-09-18 25 ppb Shoot	0.689	0.026	0.676	0.026	20	13.52	0.52
75	2013-09-18 25 ppb Root	2.044	0.028	1.937	0.027	20	38.74	0.53
76	2013-09-18 50 ppb Shoot	2.851	0.043	2.702	0.040	20	54.05	0.81
77	2013-09-18 50 ppb Root	6.696	0.108	7.028	0.113	20	140.55	2.26
78	2013-09-18 100 ppb Root	0.347	0.040	0.302	0.035	200	60.48	7.00
79	2013-09-18 100 ppb Root	0.752	0.048	0.737	0.047	200	147.43	9.36
80	wash	0.006	0.024	0.006	0.024	1	0.01	0.02
81	Se_Std_0.5	0.502	0.056	0.502	0.056	1	0.50	0.06
82	Se_Std_0.75	0.747	0.023	0.747	0.023	1	0.75	0.02
83	Se_Std_2	2.106	0.103	2.106	0.103	1	2.11	0.10
84	Se_Std_4	3.945	0.058	3.945	0.058	1	3.95	0.06
85	Se_Std_6	5.893	0.156	5.893	0.156	1	5.89	0.16
86	wash	0.021	0.015	0.021	0.015	1	0.02	0.01
87	wash	0.049	0.022	0.049	0.022	1	0.05	0.02
88	2013-09-19 dig. Blind	0.047	0.024	0.041	0.022	8	< PQL	< PQL
89	2013-09-19 dig. Std.	1.251	0.045	1.207	0.044	8	9.66	0.35
90	2013-09-19 250 ppb Shoot	0.513	0.018	0.453	0.016	200	90.69	3.11
91	2013-09-19 250 ppb Root	1.447	0.037	1.410	0.036	200	282.03	7.21
92	2013-09-19 500 ppb Shoot	1.027	0.028	0.990	0.027	200	198.07	5.33
93	2013-09-19 500 ppb Root	3.439	0.310	3.527	0.318	200	705.40	63.67
94	2013-09-19 1000 ppb Shoot	2.014	0.040	1.962	0.039	200	392.50	7.88
95	2013-09-19 1000 ppb Root	4.851	0.096	4.975	0.099	200	994.92	19.77
96	2013-09-19 2500 ppb Shoot	0.793	0.040	0.765	0.039	200	152.97	7.80
97	2013-09-19 2500 ppb Root	2.293	0.073	2.235	0.071	200	447.02	14.26
98	wash	0.023	0.020	0.023	0.020	1	0.02	0.02
99	HCl Blank	0.045	0.085	0.039	0.075	6	0.23	0.45
100	Trace Metal 252 µg/L	3.405	0.049	3.431	0.049	80	274.49	3.91
101	wash	0.014	0.010	0.014	0.010	1	0.01	0.01
102	2013-09-16 50 ppb Shoot	2.625	0.060	2.525	0.058	100	252.47	5.78
103	2013-09-18 50 ppb Root	1.712	0.052	1.757	0.054	80	140.59	4.29
104	Se_Std_0	-0.005	0.055	-0.005	0.055	1	-0.01	0.06
105	Se_Std_0.5	0.512	0.081	0.512	0.081	1	0.51	0.08
106	Se_Std_0.75	0.752	0.028	0.752	0.028	1	0.75	0.03
107	Se_Std_1	1.059	0.034	1.059	0.034	1	1.06	0.03
108	Se_Std_2	2.004	0.070	2.004	0.070	1	2.00	0.07
109	Se_Std_4	4.092	0.142	4.092	0.142	1	4.09	0.14
110	Se_Std_5	4.878	0.034	4.878	0.034	1	4.88	0.03
111	Se_Std_6	5.596	0.220	5.596	0.220	1	5.60	0.22
112	wash	0.006	0.053	0.006	0.053	1	0.01	0.05
113	wash	0.440	0.447	0.440	0.447	1	0.44	0.45

Table A.33.: A2 analytical data - HG-FIAS measurement V

Technique	AA FIAS-MHS							
Spectrometer Model	Aanalyst 200 S/N 200S6110908							
Autosampler Model	AS-90plus							
Batch ID	Pflanzenaufschlüsse							
Results Data Set	Se_Nothingstein_2013_10_09							
Date Measured	09.10.2013							
Method Name	Se Nothstein calib 6							
correl. coeff.	PQL (= lowest calib-10 %)	0.450						
0.999884	LOQ (= 7-wash)	0.108						
calib. slope	LOD (= 3-wash)	0.046						
0.02593	analytical quality [%]	108.413						
Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]		
1	Blank	0.0000	0.0010	0.0	0.00	0.00		
2	0.5 ppb	0.0119	0.0011	0.5	0.46	0.04		
3	0.75 ppb	0.0184	0.0011	0.75	0.71	0.04		
4	1.0 ppb	0.0247	0.0017	1.0	0.95	0.07		
5	2.0 ppb	0.0523	0.0016	2.0	2.02	0.06		
6	4.0 ppb	0.1043	0.0025	4.0	4.02	0.10		
7	5.0 ppb	0.1303	0.0016	5.0	5.02	0.06		
8	6.0 ppb	0.1552	0.0040	6.0	5.98	0.15		
Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.015	0.041	0.015	0.041	1	0.01	0.04
2	wash	0.016	0.040	0.016	0.040	1	0.02	0.04
3	HCl Blank	0.086	0.065	0.081	0.061	6	0.49	0.37
4	Trace Metal 252 µg/L	2.279	0.107	2.220	0.105	120	266.39	12.57
5	wash	0.042	0.070	0.042	0.070	1	0.04	0.07
6	Se_Std_0	-0.001	0.030	-0.001	0.030	1	0.00	0.03
7	Se_Std_0.5	0.484	0.037	0.484	0.037	1	0.48	0.04
8	Se_Std_0.75	0.733	0.113	0.733	0.113	1	0.73	0.11
9	Se_Std_1	1.018	0.056	1.018	0.056	1	1.02	0.06
10	Se_Std_2	2.085	0.084	2.085	0.084	1	2.08	0.08
11	Se_Std_4	4.127	0.112	4.127	0.112	1	4.13	0.11
12	Se_Std_5	5.061	0.148	5.061	0.148	1	5.06	0.15
13	Se_Std_6	6.021	0.090	6.021	0.090	1	6.02	0.09
14	wash	0.005	0.015	0.005	0.015	1	0.00	0.01
15	wash	-0.001	0.054	-0.001	0.054	1	0.00	0.05
16	2013-09-20 dig blind	-0.031	0.033	-0.030	0.032	8	< PQL	< PQL
17	2013-09-20 dig Std	1.240	0.042	1.215	0.041	8	9.72	0.33
18	2013-09-20 0ppb Shoot	-0.010	0.040	-0.009	0.039	8	< PQL	< PQL
19	2013-09-20 0ppb Root	-0.031	0.026	-0.029	0.025	8	< PQL	< PQL
20	2013-09-20 5 ppb Shoot	3.275	0.142	3.211	0.139	8	25.68	1.11
21	2013-09-20 5 ppb Root	0.944	0.056	0.925	0.055	8	7.40	0.44
22	2013-09-20 10 ppb Shoot	6.478	0.159	6.459	0.159	8	51.67	1.27
23	2013-09-20 10 ppb Root	1.991	0.101	1.909	0.097	8	15.28	0.77
24	2013-09-20 25 ppb Shoot	7.881	0.162	7.857	0.161	20	> calib	> calib
25	2013-09-20 25 ppb Root	2.178	0.174	2.089	0.167	20	41.78	3.34
26	wash	-0.013	0.041	-0.013	0.041	1	-0.01	0.04
27	Se_Std_0.5	0.473	0.018	0.473	0.018	1	0.47	0.02
28	Se_Std_0.75	0.711	0.064	0.711	0.064	1	0.71	0.06
29	Se_Std_2	2.110	0.048	2.110	0.048	1	2.11	0.05
30	Se_Std_4	4.078	0.065	4.078	0.065	1	4.08	0.07
31	Se_Std_6	5.980	0.076	5.980	0.076	1	5.98	0.08
32	wash	-0.029	0.026	-0.029	0.026	1	-0.03	0.03
33	wash	0.011	0.046	0.011	0.046	1	0.01	0.05
34	2013-09-23 dig blind	0.057	0.018	0.058	0.018	8	< PQL	< PQL
35	2013-09-23 dig Std	1.712	0.115	1.690	0.113	8	13.52	0.91
36	2013-09-23 50 ppb Shoot	10.150	0.275	10.274	0.279	20	> calib	> calib
37	2013-09-23 50 ppb Root	2.830	0.105	2.793	0.103	20	55.87	2.07
38	2013-09-23 100 ppb Shoot	19.090	0.643	19.325	0.651	20	> calib	> calib
39	2013-09-23 100 ppb Root	5.740	0.344	5.810	0.348	20	116.21	6.96
40	2013-09-23 250 ppb Shoot	2.812	0.054	2.734	0.053	200	546.81	10.56
41	2013-09-16 250 ppb Root	1.150	0.050	1.160	0.050	200	232.00	10.04
42	2013-09-16 500 ppb Shoot	1.215	0.052	1.226	0.053	200	245.16	10.59
43	2013-09-23 500 ppb Root	1.598	0.087	1.577	0.086	200	315.47	17.22
44	wash	0.008	0.027	0.008	0.027	1	0.01	0.03
45	Se_Std_0.5	0.422	0.063	0.422	0.063	1	0.42	0.06
46	Se_Std_0.75	0.692	0.053	0.692	0.053	1	0.69	0.05
47	Se_Std_2	1.972	0.181	1.972	0.181	1	1.97	0.18
48	Se_Std_4	4.056	0.024	4.056	0.024	1	4.06	0.02
49	Se_Std_6	5.839	0.049	5.839	0.049	1	5.84	0.05
50	wash	0.031	0.056	0.031	0.056	1	0.03	0.06
51	wash	0.000	0.040	0.000	0.040	1	0.00	0.04
52	2013-09-24 dig blind	0.005	0.039	0.005	0.041	8	< PQL	< PQL
53	2013-09-24 dig Std	1.168	0.086	1.170	0.086	8	9.36	0.69
54	2013-09-24 1000ppb Shoot	0.879	0.086	0.881	0.086	200	176.17	17.27
55	2013-09-24 1000ppb Root	1.811	0.093	1.815	0.093	200	362.93	18.65
56	2013-09-24 2500 ppb Shoot	0.601	0.062	0.627	0.064	200	125.33	12.89
57	2013-09-24 2500 ppb Root	0.875	0.045	0.876	0.045	200	175.29	8.96
58	2013-09-24 0 ppb Shoot	0.081	0.064	0.084	0.067	8	< PQL	< PQL
59	2013-09-24 0 ppb Root	0.052	0.027	0.054	0.028	8	< PQL	< PQL
60	2013-09-24 5 ppb Shoot	0.754	0.063	0.756	0.063	8	6.05	0.51
61	2013-09-24 5 ppb Root	1.209	0.055	1.212	0.055	8	9.69	0.44
62	wash	-0.017	0.047	-0.017	0.047	1	-0.02	0.05

Table A.34.: A2 analytical data - HG-FIAS measurement V (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
63	Se_Std_0.5	0.455	0.014	0.455	0.014	1	0.46	0.01
64	Se_Std_0.75	0.721	0.087	0.721	0.087	1	0.72	0.09
65	Se_Std_2	2.031	0.034	2.031	0.034	1	2.03	0.03
66	Se_Std_4	4.093	0.069	4.093	0.069	1	4.09	0.07
67	Se_Std_6	5.886	0.057	5.886	0.057	1	5.89	0.06
68	wash	-0.003	0.042	-0.003	0.042	1	0.00	0.04
69	wash	0.065	0.237	0.065	0.237	1	0.06	0.24
70	2013-09-25 dig. Blind	-0.021	0.022	-0.022	0.022	8	< PQL	< PQL
71	2013-09-25 dig. Std.	1.209	0.051	1.223	0.051	8	9.78	0.41
72	2013-09-25 10 ppb Shoot	1.342	0.063	1.357	0.064	8	10.85	0.51
73	2013-09-25 10 ppb Root	2.350	0.049	2.347	0.049	8	18.77	0.39
74	2013-09-25 25 ppb Shoot	1.071	0.075	1.083	0.076	20	21.67	1.53
75	2013-09-25 25 ppb Root	2.599	0.090	2.544	0.088	20	50.88	1.77
76	2013-09-25 50 ppb Shoot	1.063	0.087	1.075	0.088	20	21.50	1.77
77	2013-09-25 50 ppb Root	2.969	0.076	2.965	0.076	20	59.31	1.52
78	2013-09-25 100 ppb Root	3.916	0.222	3.833	0.217	20	76.67	4.35
79	2013-09-25 100 ppb Root	7.947	0.321	8.062	0.326	20	> calib	> calib
80	wash	-0.012	0.014	-0.012	0.014	1	-0.01	0.01
81	Se_Std_0.5	0.443	0.021	0.443	0.021	1	0.44	0.02
82	Se_Std_0.75	0.679	0.035	0.679	0.035	1	0.68	0.03
83	Se_Std_2	2.004	0.077	2.004	0.077	1	2.00	0.08
84	Se_Std_4	4.122	0.102	4.122	0.102	1	4.12	0.10
85	Se_Std_6	5.908	0.136	5.908	0.136	1	5.91	0.14
86	wash	-0.016	0.048	-0.016	0.048	1	-0.02	0.05
87	wash	-0.040	0.023	-0.040	0.023	1	-0.04	0.02
88	2013-09-26 dig. Blind	-0.041	0.050	-0.043	0.052	8	< PQL	< PQL
89	2013-09-26 dig. Std.	1.315	0.119	1.357	0.123	8	10.85	0.98
90	2013-09-26 250 ppb Shoot	0.267	0.096	0.281	0.101	200	< PQL	< PQL
91	2013-09-26 250 ppb Root	0.778	0.084	0.803	0.087	200	160.50	17.32
92	2013-09-26 500 ppb Shoot	0.489	0.027	0.514	0.028	200	102.86	5.62
93	2013-09-26 500 ppb Root	1.728	0.118	1.727	0.118	200	345.35	23.59
94	2013-09-26 1000 ppb Shoot	0.546	0.103	0.573	0.108	200	114.70	21.58
95	2013-09-26 1000 ppb Root	2.015	0.062	2.007	0.061	200	401.40	12.27
96	2013-09-26 2500 ppb Shoot	0.755	0.226	0.779	0.233	200	155.80	46.54
97	2013-09-26 2500 ppb Root	1.845	0.030	1.783	0.029	200	356.63	5.71
98	wash	-0.046	0.042	-0.046	0.042	1	-0.05	0.04
99	HCl Blank	0.040	0.190	0.042	0.203	6	0.25	1.22
100	Trace Metal 252 µg/L	2.356	0.300	2.333	0.297	120	280.01	35.65
101	wash	0.013	0.031	0.013	0.031	1	0.01	0.03
102	Se_Std_0	-0.025	0.043	-0.025	0.043	1	-0.02	0.04
103	Se_Std_0.5	0.426	0.060	0.426	0.060	1	0.43	0.06
104	Se_Std_0.75	0.692	0.078	0.692	0.078	1	0.69	0.08
105	Se_Std_1	0.993	0.022	0.993	0.022	1	0.99	0.02
106	Se_Std_2	2.042	0.043	2.042	0.043	1	2.04	0.04
107	Se_Std_4	4.062	0.074	4.062	0.074	1	4.06	0.07
108	Se_Std_5	5.109	0.114	5.109	0.114	1	5.11	0.11
109	Se_Std_6	6.582	1.296	6.582	1.296	1	6.58	1.30
110	2013-09-20 25 ppb Shoot	2.868	0.082	2.829	0.081	60	169.76	4.87
111	2013-09-23 50 ppb Shoot	3.052	0.048	3.022	0.048	80	241.75	3.80
112	2013-09-23 100 ppb Shoot	3.468	0.049	5.185	0.074	100	518.51	7.36
113	2013-09-25 100 ppb Root	2.886	0.043	4.310	0.065	30	129.30	1.94
114	wash	0.173	0.473	0.173	0.473	1	0.17	0.47
115	wash	0.123	0.030	0.123	0.030	1	0.12	0.03

A.3. Datasheets experiment A3

A.3.1. A3 Plant Growth Data

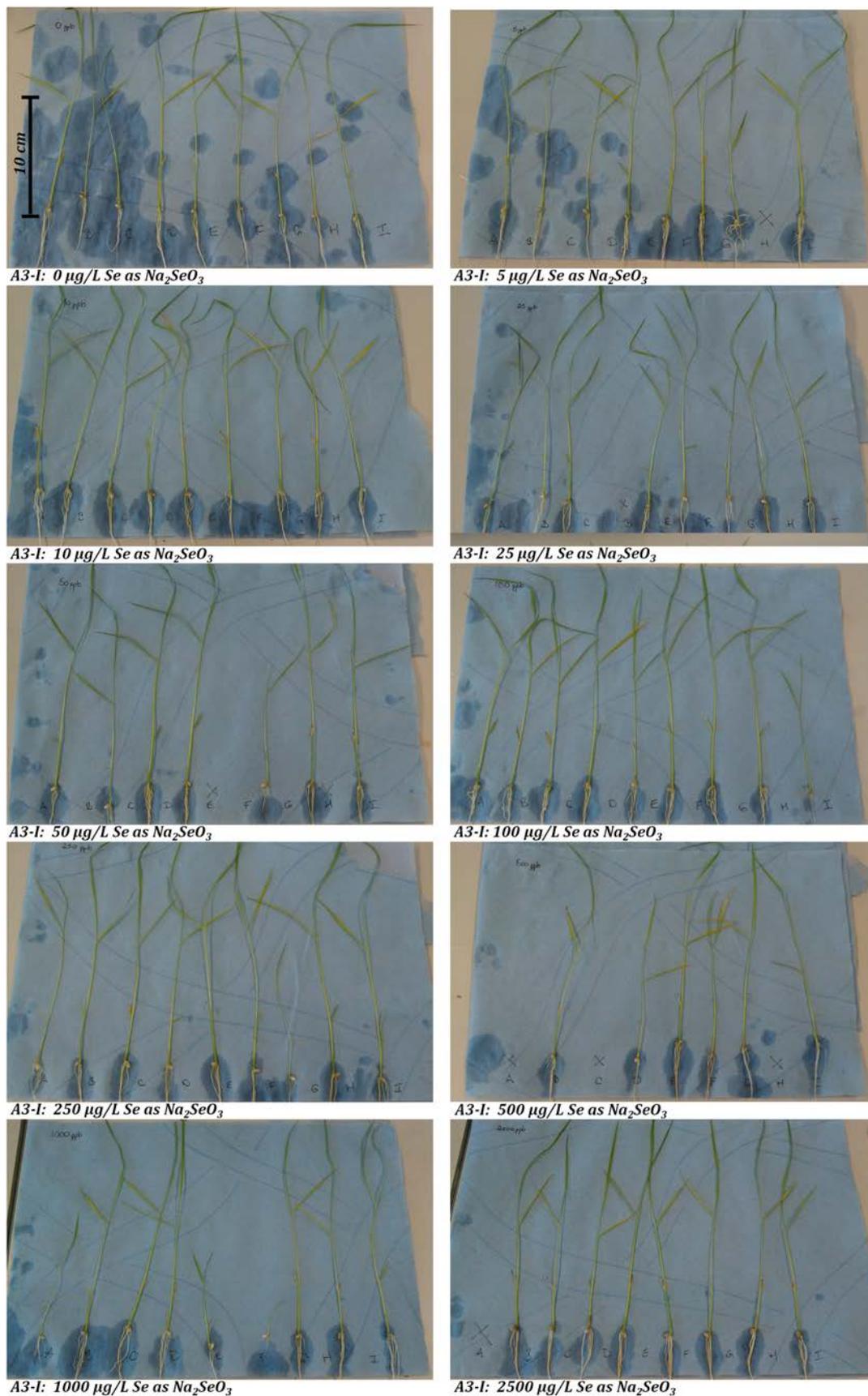


Figure A.9.: A3 photos of harvested plants treated with Na_2SeO_3

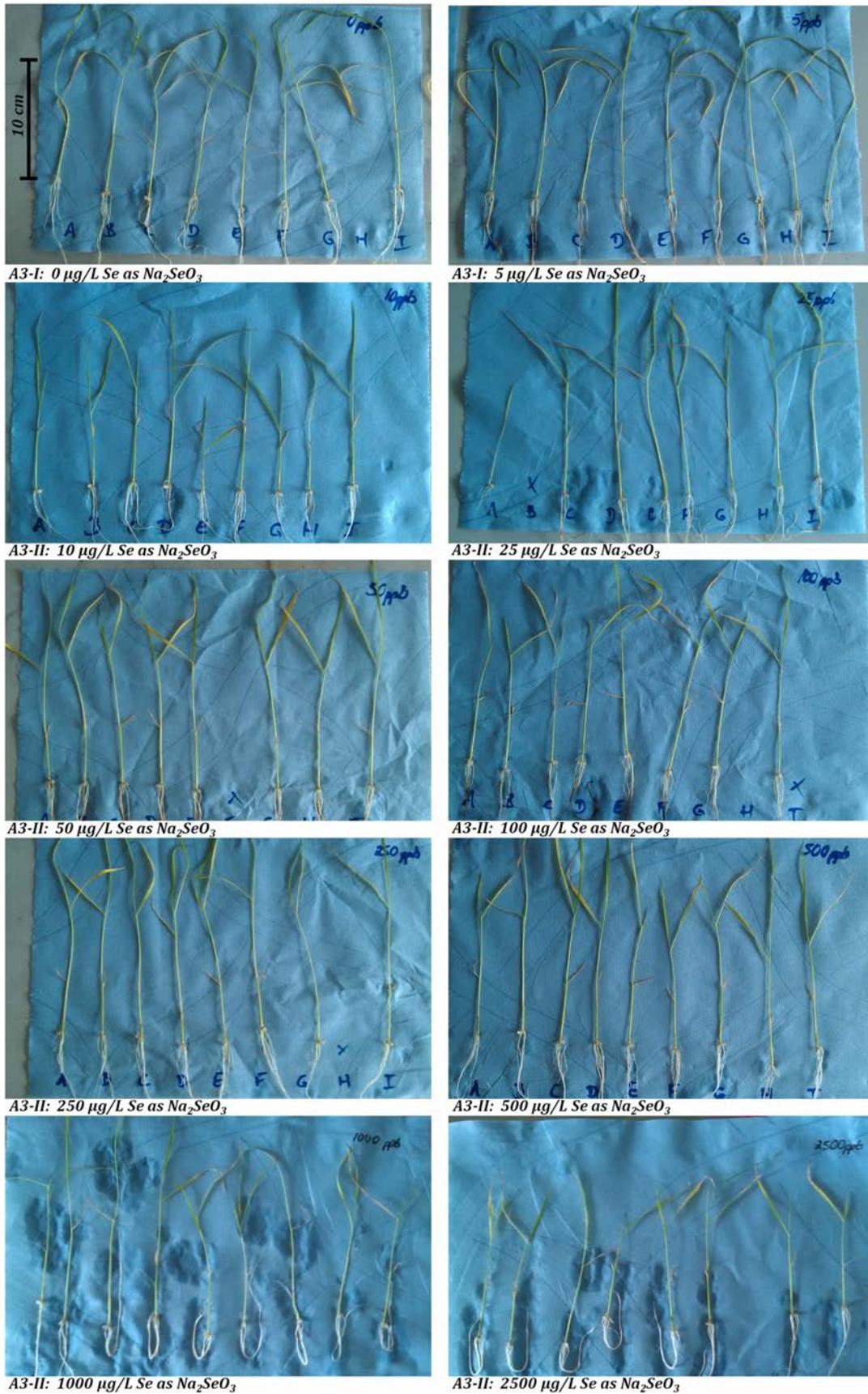


Figure A.10.: A3 photos of harvested plants treated with Na_2SeO_3

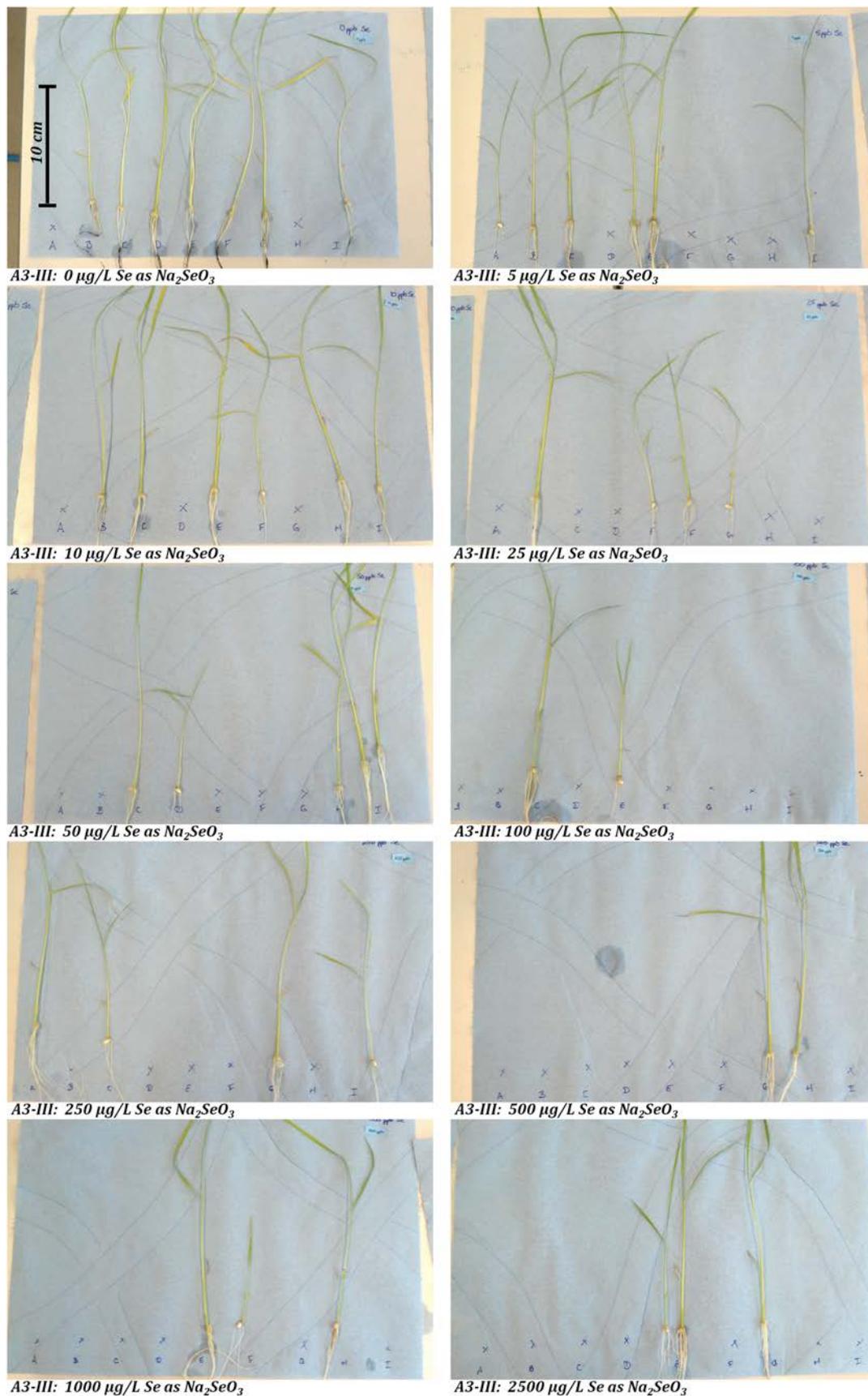


Figure A.11.: A3 photos of harvested plants treated with Na_2SeO_3

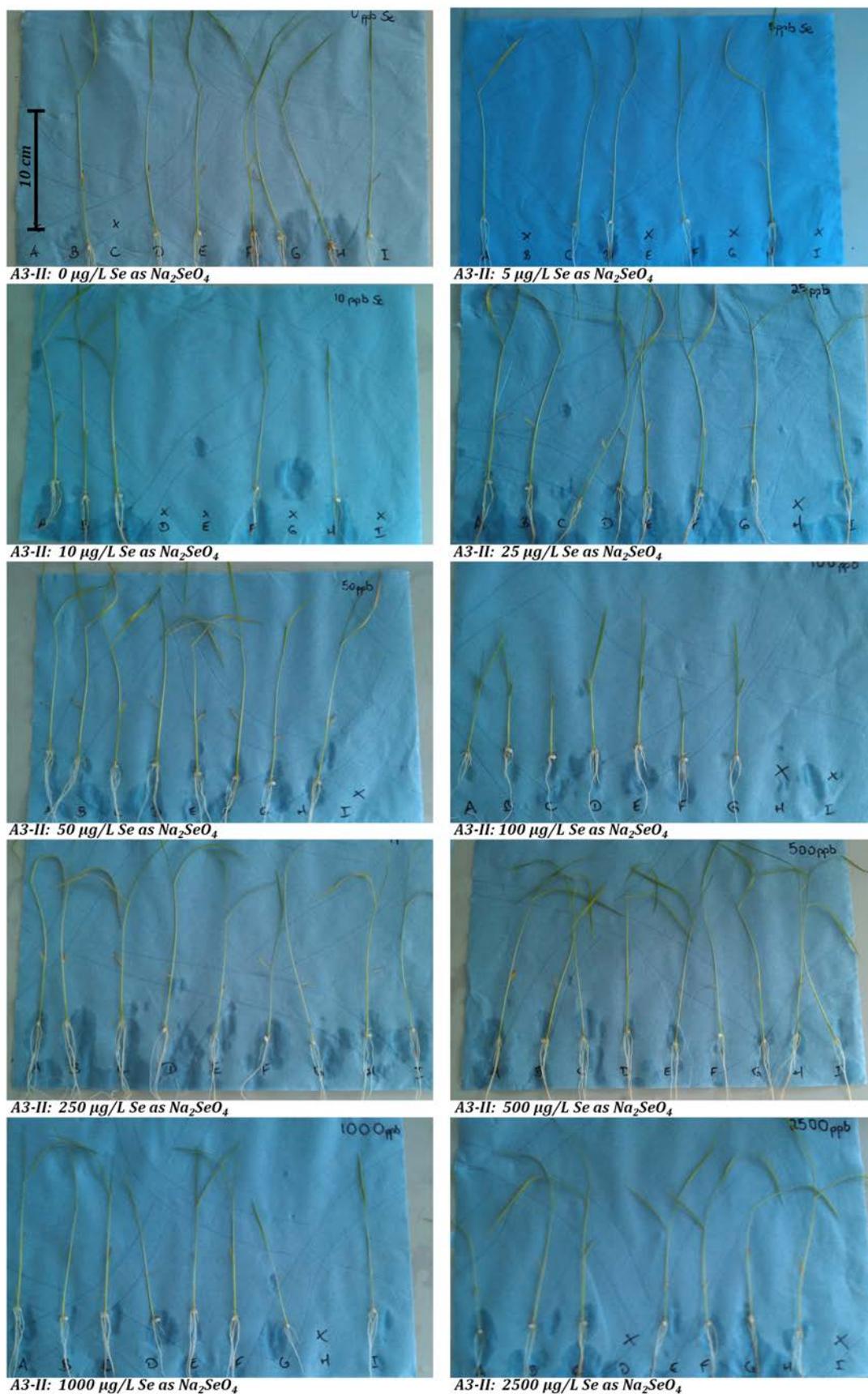


Figure A.12.: A3 photos of harvested plants treated with Na_2SeO_4



Figure A.13.: A3 photos of harvested plants treated with Na_2SeO_4

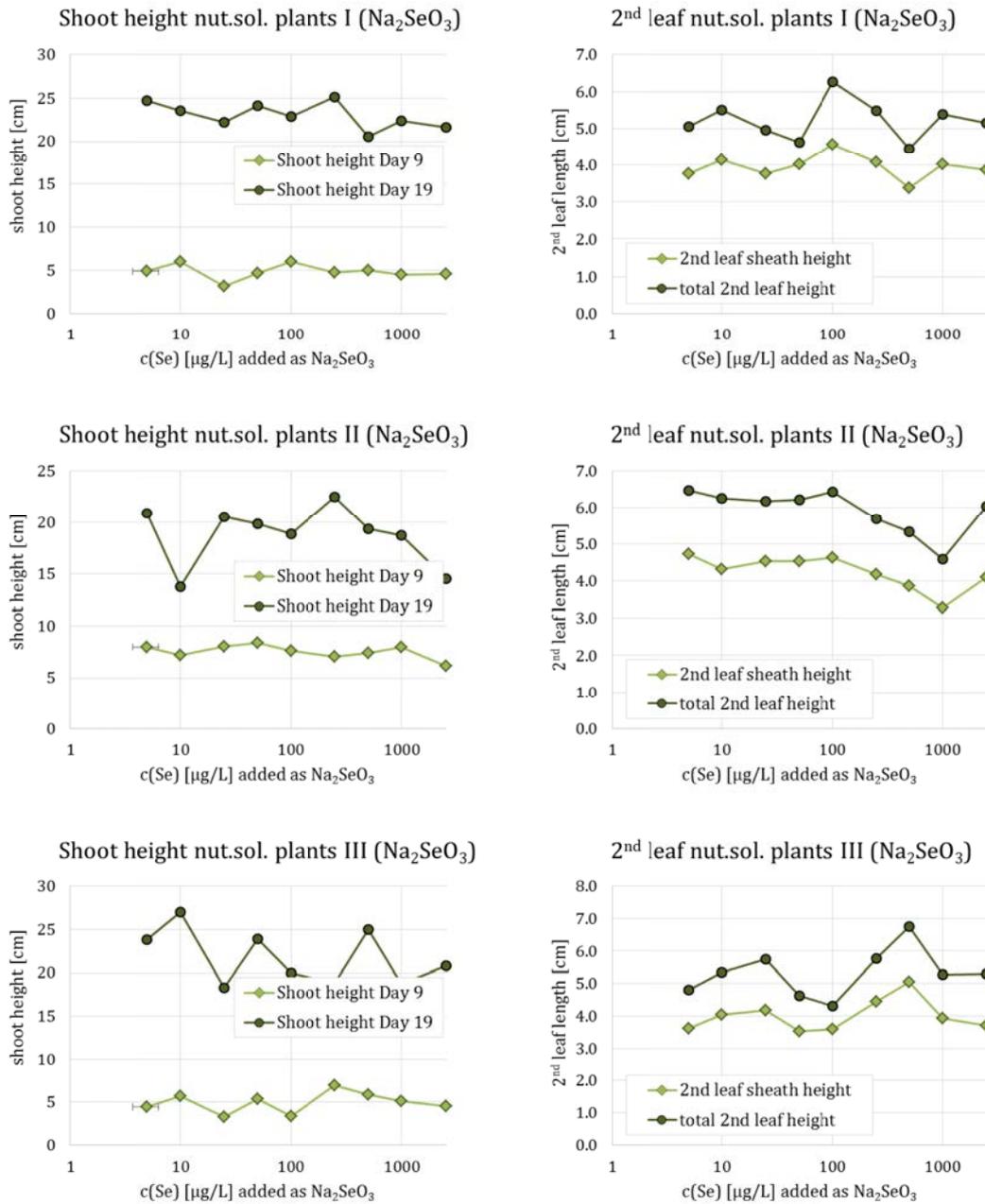


Figure A.14.: A3 shoot heights and 2nd leaf length for Na₂SeO₃ experiments

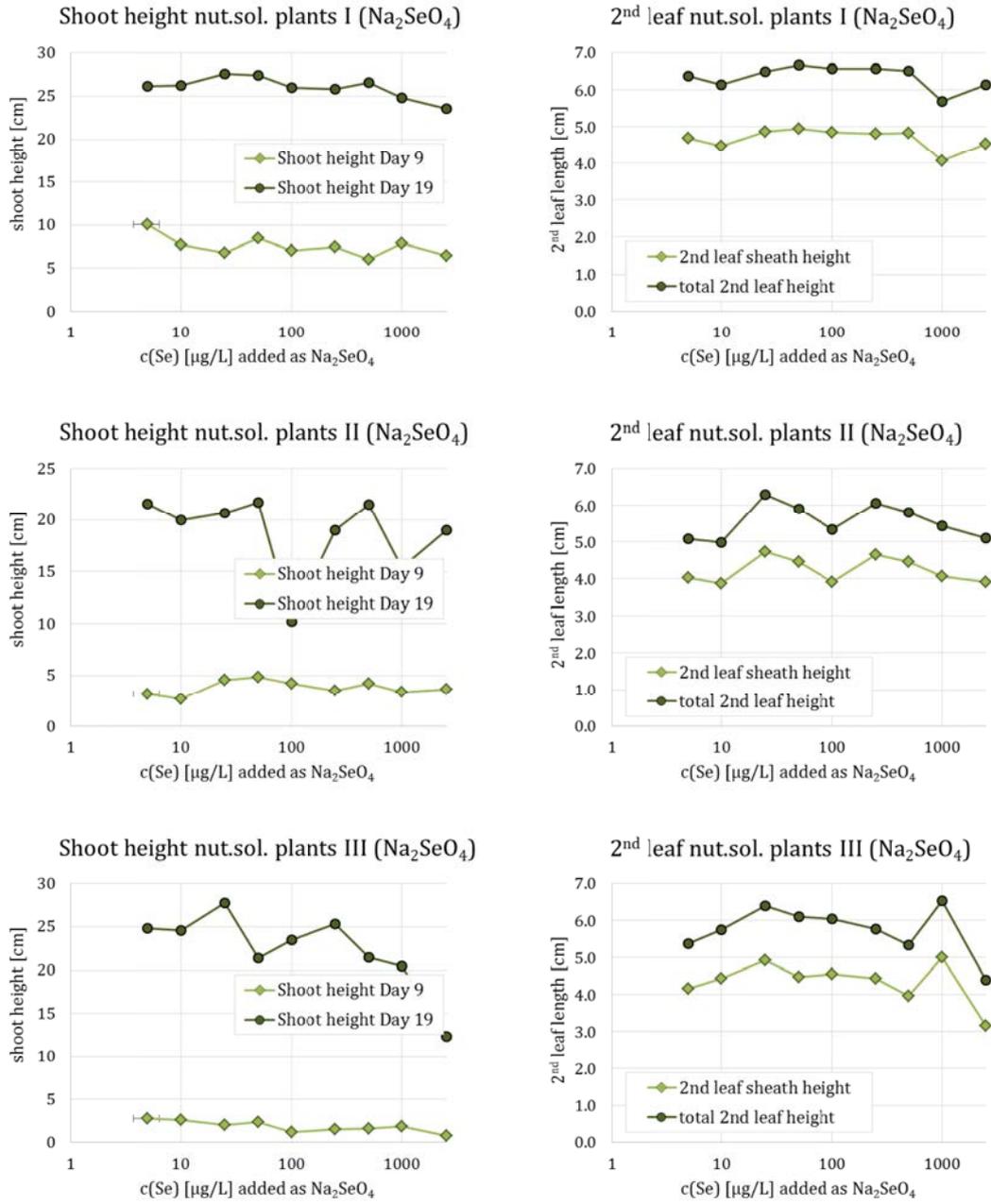


Figure A.15.: A3 shoot heights and 2nd leaf length for Na₂SeO₄ experiments

Table A.35.: A3 plant growth data for Na₂SeO₃ I (Planting Date: 10.01.2013)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	3.6	1.4	5.0	15	25.5	0.0481	0.0125	0.0157	0.0055	67.36	56.00
0000B	0	x	x	x	x	x	x	x	x	x	x	x
0000C	0	x	x	x	x	x	x	x	x	x	x	x
0000D	0	3.9	1.3	5.2	13	24.5	0.0485	0.0131	0.0111	0.0061	77.11	53.44
0000E	0	3.6	0.9	4.5	13	22.5	0.0296	0.0081	0.0073	0.0042	75.34	48.15
0000F	0	x	x	x	x	x	x	x	x	x	x	x
0000G	0	3.2	1.2	4.4	13	22.0	0.0236	0.0078	0.0064	0.0043	72.88	44.87
0000H	0	2.7	0.7	3.4	13	20.0	0.0266	0.0087	0.0067	0.0037	74.81	57.47
0000I	0	3.4	1.1	4.5	13	25.0	0.0401	0.0098	0.0109	0.0059	72.82	39.80
0000_sum	0	20.4	6.6	27.0	80.0	139.5	0.2165	0.0600	0.0581	0.0297	440.32	299.72
0000_mean	0	3.4	1.1	4.5	13.3	23.3	0.0361	0.0100	0.0097	0.0050	73.39	49.95
0000_SD	0	0.4	0.3	0.6	0.8	2.1	0.0110	0.0023	0.0036	0.0010	3.37	6.89
0005A	5	4.1	1.2	5.3	15	25.5	0.0510	0.0103	0.0109	0.0056	78.63	45.63
0005B	5	2.6	0.7	3.3	13	23.0	0.0320	0.0154	0.0072	0.0044	77.50	71.43
0005C	5	x	x	x	x	x	x	x	x	x	x	x
0005D	5	3.8	1.6	5.4	13	24.5	0.0466	0.0150	0.0099	0.0057	78.76	62.00
0005E	5	3.7	1.4	5.1	12	24.0	0.0367	0.0148	0.0091	0.0061	75.20	58.78
0005F	5	4.5	1.7	6.2	15	26.0	0.0546	0.0134	0.0155	0.0059	71.61	55.97
0005G	5	x	x	x	x	x	x	x	x	x	x	x
0005H	5	x	x	x	x	x	x	x	x	x	x	x
0005I	5	3.9	1.2	5.1	13	25.5	0.0466	0.0120	0.0116	0.0066	75.11	45.00
0005_sum	5	22.6	7.8	30.4	81.0	148.5	0.2675	0.0809	0.0642	0.0343	456.81	338.81
0005_mean	5	3.8	1.3	5.1	13.5	24.8	0.0446	0.0135	0.0107	0.0057	76.13	56.47
0005_SD	5	0.6	0.4	1.0	1.2	1.1	0.0086	0.0020	0.0028	0.0007	2.73	10.09
0010A	10	4.3	1.7	6.0	15	25.0	0.0430	0.0106	0.0103	0.0052	76.05	50.94
0010B	10	3.8	1.3	5.1	13	22.5	0.0272	0.0124	0.0077	0.0046	71.69	62.90
0010C	10	3.4	0.7	4.1	13	25.0	0.0267	0.0147	0.0086	0.0074	67.79	49.66
0010D	10	3.8	1.5	5.3	13	24.0	0.0456	0.0107	0.0098	0.0050	78.51	53.27
0010E	10	4.4	1.3	5.7	13	19.5	0.0279	0.0110	0.0068	0.0045	75.63	59.09
0010F	10	4.6	1.7	6.3	13	22.5	0.0413	0.0086	0.0086	0.0049	79.18	43.02
0010G	10	4.4	1.3	5.7	13	22.5	0.0397	0.0149	0.0090	0.0058	77.33	61.07
0010H	10	4.3	1.4	5.7	13	24.5	0.0422	0.0103	0.0104	0.0055	75.36	46.60
0010I	10	4.3	1.4	5.7	13	26.5	0.0400	0.0080	0.0116	0.0048	71.00	40.00
0010_sum	10	37.3	12.3	49.6	119.0	212.0	0.3336	0.1012	0.0828	0.0477	672.53	466.57
0010_mean	10	4.1	1.4	5.5	13.2	23.6	0.0371	0.0112	0.0092	0.0053	74.73	51.84
0010_SD	10	0.4	0.3	0.6	0.7	2.1	0.0076	0.0024	0.0015	0.0009	3.79	8.01
0025A	25	4.6	1.7	6.3	12	18.0	0.0298	0.0135	0.0078	0.0048	73.83	64.44
0025B	25	x	x	x	x	x	x	x	x	x	x	x
0025C	25	3.5	1.0	4.5	12	24.5	0.0327	0.0117	0.0092	0.0047	71.87	59.83
0025D	25	x	x	x	x	x	x	x	x	x	x	x
0025E	25	3.1	1.3	4.4	13	20.5	0.0250	0.0094	0.0057	0.0038	77.20	59.57
0025F	25	4.5	1.3	5.8	13	23.5	0.0300	0.0170	0.0077	0.0078	74.33	54.12
0025G	25	x	x	x	x	x	x	x	x	x	x	x
0025H	25	3.7	1.0	4.7	13	21.5	0.0232	0.0109	0.0066	0.0081	71.55	25.69
0025I	25	3.2	0.9	4.1	13	25.5	0.0363	0.0085	0.0112	0.0050	69.15	41.18
0025_sum	25	22.6	7.2	29.8	76.0	133.5	0.1770	0.0710	0.0482	0.0342	437.92	304.83
0025_mean	25	3.8	1.2	5.0	12.7	22.3	0.0295	0.0118	0.0080	0.0057	72.99	50.81
0025_SD	25	0.6	0.3	0.9	0.5	2.8	0.0048	0.0031	0.0020	0.0018	2.77	14.69
0050A	50	3.9	1.2	5.1	12	26.0	0.0384	0.0071	0.0102	0.0048	73.44	32.39
0050B	50	x	x	x	x	x	x	x	x	x	x	x
0050C	50	4.1	1.6	5.7	13	26.5	0.0533	0.0075	0.0142	0.0063	73.36	16.00
0050D	50	4.7	2.0	6.7	13	27.5	0.0467	0.0111	0.0144	0.0055	69.16	50.45
0050E	50	x	x	0.0	x	x	x	x	x	x	x	x
0050F	50	3.8	0.4	4.2	13	10.0	0.0114	0.0059	0.0034	0.0045	70.18	23.73
0050G	50	4.1	1.7	5.8	15	27.5	0.0435	0.0088	0.0117	0.0052	73.10	40.91
0050H	50	x	x	x	x	x	x	x	x	x	x	x
0050I	50	3.5	1.4	4.9	15	27.5	0.0477	0.0115	0.0143	0.0053	70.02	53.91
0050_sum	50	24.1	8.3	32.4	81.0	145.0	0.2410	0.0519	0.0682	0.0316	429.26	217.40
0050_mean	50	4.0	1.4	4.6	13.5	24.2	0.0402	0.0087	0.0114	0.0053	71.54	36.23
0050_SD	50	0.4	0.6	2.2	1.2	7.0	0.0149	0.0023	0.0043	0.0006	1.96	14.95
0100A	100	4.7	1.7	6.4	13	24.0	0.0455	0.0162	0.0123	0.0054	72.97	66.67
0100B	100	4.3	1.4	5.7	15	20.5	0.0360	0.0087	0.0085	0.0042	76.39	51.72
0100C	100	3.9	1.8	5.7	13	21.5	0.0366	0.0056	0.0089	0.0039	75.68	30.36
0100D	100	4.5	1.6	6.1	15	23.0	0.0360	0.0077	0.0108	0.0052	70.00	32.47
0100E	100	x	x	x	x	x	x	x	x	x	x	x
0100F	100	4.8	1.9	6.7	15	23.5	0.0416	0.0094	0.0112	0.0052	73.08	44.68
0100G	100	5.0	1.8	6.8	15	23.0	0.0376	0.0102	0.0105	0.0057	72.07	44.12
0100H	100	4.8	1.7	6.5	15	25.0	0.0374	0.0112	0.0119	0.0057	68.18	49.11
0100I	100	x	x	x	x	x	x	x	x	x	x	x
0100_sum	100	32.0	11.9	43.9	101.0	160.5	0.2707	0.0690	0.0741	0.0353	508.37	319.12
0100_mean	100	4.6	1.7	6.3	14.4	22.9	0.0387	0.0099	0.0106	0.0050	72.62	45.59
0100_SD	100	0.4	0.2	0.4	1.0	1.5	0.0036	0.0033	0.0014	0.0007	2.91	12.26

Table A.36.: A3 plant growth data for Na_2SeO_3 I (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	x	x	x	x	x	x	x	x	x	x	x
0250B	250	4.0	1.6	5.6	13	25.5	0.0335	0.0066	0.0097	0.0044	71.04	33.33
0250C	250	3.6	1.5	5.1	13	23.5	0.0290	0.0065	0.0088	0.0048	69.66	26.15
0250D	250	3.7	1.2	4.9	13	24.0	0.0267	0.0057	0.0083	0.0050	68.91	12.28
0250E	250	4.3	1.3	5.6	15	28.5	0.0431	0.0084	0.0140	0.0058	67.52	30.95
0250F	250	4.2	1.0	5.2	12	23.0	0.0267	0.0122	0.0088	0.0044	67.04	63.93
0250G	250	x	x	x	x	x	x	x	x	x	x	x
0250H	250	4.5	1.7	6.2	15	26.0	0.0451	0.0131	0.0131	0.0052	70.95	60.31
0250I	250	4.3	1.6	5.9	15	25.5	0.0380	0.0090	0.0131	0.0054	65.53	40.00
0250_sum	250	28.6	9.9	38.5	96.0	176.0	0.2421	0.0615	0.0758	0.0350	480.65	266.96
0250_mean	250	4.1	1.4	5.5	13.7	25.1	0.0346	0.0088	0.0108	0.0050	68.66	38.14
0250_SD	250	0.3	0.3	0.5	1.3	1.9	0.0077	0.0029	0.0025	0.0005	2.07	18.47
0500A	500	x	x	x	x	x	x	x	x	x	x	x
0500B	500	3.9	1.2	5.1	15	23.5	0.0267	0.0083	0.0107	0.0053	59.93	36.14
0500C	500	x	x	x	x	x	x	x	x	x	x	x
0500D	500	2.9	0.8	3.7	13	16.0	0.0101	0.0080	0.0048	0.0072	52.48	10.00
0500E	500	3.4	1.4	4.8	15	23.5	0.0388	0.0122	0.0116	0.0058	70.10	52.46
0500F	500	3.7	1.3	5.0	15	15.0	0.0222	0.0066	0.0078	0.0044	64.86	33.33
0500G	500	3.9	1.1	5.0	13	22.0	0.0290	0.0065	0.0094	0.0045	67.59	30.77
0500H	500	x	x	x	x	x	x	x	x	x	x	x
0500I	500	2.5	0.7	3.2	13	23.5	0.0404	0.0113	0.0085	0.0045	78.96	60.18
0500_sum	500	20.3	6.5	26.8	84.0	123.5	0.1672	0.0529	0.0528	0.0317	393.91	222.88
0500_mean	500	3.4	1.1	4.5	14.0	20.6	0.0279	0.0088	0.0088	0.0053	65.65	37.15
0500_SD	500	0.6	0.3	0.8	1.1	4.0	0.0112	0.0024	0.0024	0.0011	9.03	17.65
1000A	1000	x	x	x	x	x	x	x	x	x	x	x
1000B	1000	3.5	1.2	4.7	12	23.0	0.0281	0.0093	0.0080	0.0053	71.53	43.01
1000C	1000	4.1	1.3	5.4	13	25.0	0.0304	0.0092	0.0110	0.0059	63.82	35.87
1000D	1000	3.6	1.3	4.9	15	22.5	0.0220	0.0093	0.0090	0.0076	59.09	18.28
1000E	1000	x	x	x	x	x	x	x	x	x	x	x
1000F	1000	x	x	x	x	x	x	x	x	x	x	x
1000G	1000	4.4	1.4	5.8	15	21.0	0.0263	0.0112	0.0088	0.0059	66.54	47.32
1000H	1000	3.5	1.2	4.7	13	22.0	0.0250	0.0088	0.0080	0.0058	68.00	34.09
1000I	1000	5.1	1.8	6.9	12	21.0	0.0319	0.0081	0.0103	0.0068	67.71	16.05
1000_sum	1000	24.2	8.2	32.4	80.0	134.5	0.1637	0.0559	0.0551	0.0373	396.69	194.62
1000_mean	1000	4.0	1.4	5.4	13.3	22.4	0.0273	0.0093	0.0092	0.0062	66.11	32.44
1000_SD	1000	0.6	0.2	0.9	1.4	1.5	0.0036	0.0010	0.0012	0.0008	4.25	12.78
2500A	2500	x	x	x	x	x	x	x	x	x	x	x
2500B	2500	4.3	1.2	5.5	15	22.0	0.0277	0.0076	0.0091	0.0051	67.15	32.89
2500C	2500	3.7	1.4	5.1	13	18.5	0.0211	0.0060	0.0065	0.0040	69.19	33.33
2500D	2500	3.6	1.1	4.7	15	20.0	0.0206	0.0082	0.0076	0.0048	63.11	41.46
2500E	2500	4.1	1.4	5.5	15	23.0	0.0293	0.0072	0.0104	0.0055	64.51	23.61
2500F	2500	4.1	1.4	5.5	15	23.5	0.0289	0.0108	0.0096	0.0064	66.78	40.74
2500G	2500	x	x	x	x	x	x	x	x	x	x	x
2500H	2500	3.6	1.4	5.0	13	23.0	0.0270	0.0140	0.0092	0.0056	65.93	60.00
2500I	2500	3.7	1.1	4.8	13	21.5	0.0234	0.0089	0.0085	0.0055	63.68	38.20
2500_sum	2500	27.1	9.0	36.1	99.0	151.5	0.1780	0.0627	0.0609	0.0369	460.34	270.25
2500_mean	2500	3.9	1.3	5.2	14.1	21.6	0.0254	0.0090	0.0087	0.0053	65.76	38.61
2500_SD	2500	0.3	0.1	0.3	1.1	1.8	0.0037	0.0027	0.0013	0.0007	2.15	11.22

Table A.37.: A3 plant growth data for Na₂SeO₃ II (Planting Date: 02.10.2013)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	3.2	0.4	3.6	14	23.0	0.0338	0.0123	0.0076	0.0031	77.51	74.80
0000B	0	5.5	2.3	7.8	14	21.0	0.0357	0.0122	0.0084	0.0039	76.47	68.03
0000C	0	5.3	2.1	7.4	14	19.0	0.0313	0.0090	0.0069	0.0037	77.96	58.89
0000D	0	5.5	2.1	7.6	14	20.0	0.0339	0.0115	0.0083	0.0039	75.52	66.09
0000E	0	6.1	2.3	8.4	14	19.0	0.0378	0.0066	0.0084	0.0031	77.78	53.03
0000F	0	5.3	1.7	7.0	14	19.5	0.0269	0.0086	0.0082	0.0041	69.52	52.33
0000G	0	6.0	2.1	8.1	14	23.0	0.0420	0.0128	0.0105	0.0046	75.00	64.06
0000H	0	5.6	2.2	7.8	14	23.5	0.0360	0.0105	0.0106	0.0052	70.56	50.48
0000I	0	x	x	x	x	x	x	x	x	x	x	x
0000_sum	0	42.5	15.2	57.7	112.0	168.0	0.2774	0.0835	0.0689	0.0316	600.31	487.70
0000_mean	0	5.3	1.9	7.2	14.0	21.0	0.0347	0.0104	0.0086	0.0040	75.04	60.96
0000_SD	0	0.9	0.6	1.5	0.0	1.9	0.0045	0.0022	0.0013	0.0007	3.27	8.69
0005A	5	4.7	1.9	6.6	14	20.0	0.0258	0.0120	0.0073	0.0039	71.71	67.50
0005B	5	4.7	1.5	6.2	14	22.5	0.0336	0.0170	0.0090	0.0045	73.21	73.53
0005C	5	5.1	2.3	7.4	14	20.0	0.0265	0.0107	0.0060	0.0032	77.36	70.09
0005D	5	4.7	1.9	6.6	14	19.0	0.0293	0.0106	0.0087	0.0035	70.31	66.98
0005E	5	4.9	1.8	6.7	14	20.0	0.0259	0.0125	0.0079	0.0033	69.50	73.60
0005F	5	4.6	1.7	6.3	15	25.0	0.0337	0.0104	0.0102	0.0042	69.73	59.62
0005G	5	4.5	2.1	6.6	14	24.5	0.0420	0.0194	0.0089	0.0048	78.81	75.26
0005H	5	4.3	1.8	6.1	12	18.0	0.0235	0.0079	0.0056	0.0029	76.17	63.29
0005I	5	5.0	0.8	5.8	14	19.0	0.0155	0.0083	0.0051	0.0026	67.10	68.67
0005_sum	5	42.5	15.8	58.3	125.0	188.0	0.2558	0.1088	0.0687	0.0329	653.89	618.54
0005_mean	5	4.7	1.8	6.5	13.9	20.9	0.0284	0.0121	0.0076	0.0037	72.65	68.73
0005_SD	5	0.2	0.4	0.5	0.8	2.5	0.0075	0.0038	0.0018	0.0007	4.01	5.10
0010A	10	4.8	1.4	6.2	14	15.0	0.0184	0.0163	0.0054	0.0069	70.65	57.67
0010B	10	4.3	1.5	5.8	13	13.0	0.0251	0.0141	0.0067	0.0046	73.31	67.38
0010C	10	4.7	2.0	6.7	14	17.0	0.0268	0.0167	0.0075	0.0051	72.01	69.46
0010D	10	5.3	2.1	7.4	14	15.0	0.0268	0.0142	0.0083	0.0035	69.03	75.35
0010E	10	3.1	4.3	7.4	14	8.0	0.0175	0.0136	0.0052	0.0042	70.29	69.12
0010F	10	4.8	1.4	6.2	15	14.5	0.0286	0.0132	0.0091	0.0046	68.18	65.15
0010G	10	3.7	1.7	5.4	14	12.5	0.0222	0.0085	0.0075	0.0031	66.22	63.53
0010H	10	3.4	1.0	4.4	12	13.0	0.0126	0.0143	0.0039	0.0034	69.05	76.22
0010I	10	4.7	2.1	6.8	14	16.0	0.0356	0.0095	0.0097	0.0051	72.75	46.32
0010_sum	10	38.8	17.5	56.3	124.0	124.0	0.2136	0.1204	0.0633	0.0405	631.49	590.20
0010_mean	10	4.3	1.9	6.3	13.8	13.8	0.0237	0.0134	0.0070	0.0045	70.17	65.58
0010_SD	10	0.7	1.0	1.0	0.8	2.6	0.0069	0.0028	0.0019	0.0012	2.30	9.20
0025A	25	x	x	x	x	x	x	x	x	x	x	x
0025B	25	x	x	x	x	x	x	x	x	x	x	x
0025C	25	4.8	1.9	6.7	15	10.0	0.0218	0.0138	0.0082	0.0052	62.39	62.32
0025D	25	5.0	1.7	6.7	14	21.5	0.0403	0.0127	0.0101	0.0043	74.94	66.14
0025E	25	2.7	0.7	3.4	14	31.0	0.0511	0.0100	0.0124	0.0044	75.73	56.00
0025F	25	5.8	1.9	7.7	14	19.5	0.0256	0.0118	0.0087	0.0039	66.02	66.95
0025G	25	4.6	1.6	6.2	14	18.0	0.0250	0.0063	0.0068	0.0030	72.80	52.38
0025H	25	4.5	1.8	6.3	13	21.0	0.0267	0.0115	0.0090	0.0041	66.29	64.35
0025I	25	4.4	1.8	6.2	15	23.0	0.0310	0.0121	0.0092	0.0041	70.32	66.12
0025_sum	25	31.8	11.4	43.2	99.0	144.0	0.2215	0.0782	0.0644	0.0290	488.49	434.25
0025_mean	25	4.5	1.6	6.2	14.1	20.6	0.0316	0.0112	0.0092	0.0041	69.78	62.04
0025_SD	25	0.9	0.4	1.3	0.7	6.3	0.0105	0.0024	0.0017	0.0007	5.04	5.67
0050A	50	3.9	1.5	5.4	12	20.0	0.0290	0.0179	0.0084	0.0050	71.03	72.07
0050B	50	4.6	1.8	6.4	14	19.0	0.0377	0.0060	0.0096	0.0041	74.54	31.67
0050C	50	5.0	2.1	7.1	14	20.5	0.0309	0.0147	0.0074	0.0043	76.05	70.75
0050D	50	4.9	2.1	7.0	14	19.0	0.0330	0.0086	0.0084	0.0044	74.55	48.84
0050E	50	4.9	1.9	6.8	14	20.0	0.0366	0.0118	0.0093	0.0043	74.59	63.56
0050F	50	x	x	x	x	x	x	x	x	x	x	x
0050G	50	3.7	0.7	4.4	14	21.0	0.0356	0.0100	0.0110	0.0049	69.10	51.00
0050H	50	4.7	1.4	6.1	14	18.0	0.0247	0.0096	0.0082	0.0042	66.80	56.25
0050I	50	4.6	1.9	6.5	15	21.5	0.0312	0.0112	0.0101	0.0044	67.63	60.71
0050_sum	50	36.3	13.4	49.7	111.0	159.0	0.2587	0.0898	0.0724	0.0356	574.29	454.84
0050_mean	50	4.5	1.7	6.2	13.9	19.9	0.0323	0.0112	0.0091	0.0045	71.79	56.86
0050_SD	50	0.5	0.5	0.9	0.8	1.2	0.0043	0.0037	0.0012	0.0003	3.61	13.19
0100A	100	4.9	1.9	6.8	14	18.0	0.0177	0.0124	0.0069	0.0047	61.02	62.10
0100B	100	4.5	1.8	6.3	14	18.5	0.0170	0.0088	0.0066	0.0032	61.18	63.64
0100C	100	4.4	1.7	6.1	13	17.0	0.0138	0.0094	0.0058	0.0034	57.97	63.83
0100D	100	4.9	2.2	7.1	14	19.0	0.0265	0.0177	0.0084	0.0049	68.30	72.32
0100E	100	4.6	1.9	6.5	14	20.5	0.0275	0.0101	0.0111	0.0050	59.64	50.50
0100F	100	5.0	1.9	6.9	14	21.0	0.0302	0.0160	0.0087	0.0060	71.19	62.50
0100G	100	5.2	2.2	7.4	14	19.0	0.0301	0.0128	0.0081	0.0037	73.09	71.09
0100H	100	3.6	0.8	4.4	13	18.0	0.0178	0.0740	0.0075	0.0034	57.87	95.41
0100I	100	x	x	x	x	x	x	x	x	x	x	x
0100_sum	100	37.1	14.4	51.5	110.0	151.0	0.1806	0.1612	0.0631	0.0343	510.25	541.37
0100_mean	100	4.6	1.8	6.4	13.8	18.9	0.0226	0.0202	0.0079	0.0043	63.78	67.67
0100_SD	100	0.5	0.4	0.9	0.5	1.3	0.0066	0.0220	0.0016	0.0010	6.12	13.02

Table A.38.: A3 plant growth data for Na_2SeO_3 II (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	4.4	2.4	6.8	13	20.0	0.0311	0.0093	0.0076	0.0037	75.56	60.22
0250B	250	4.2	1.6	5.8	14	23.0	0.0388	0.0159	0.0085	0.0040	78.09	74.84
0250C	250	3.9	1.5	5.4	12	21.0	0.0408	0.0313	0.0084	0.0038	79.41	87.86
0250D	250	3.2	0.8	4.0	14	28.0	0.0628	0.0203	0.0110	0.0049	82.48	75.86
0250E	250	5.1	1.7	6.8	14	22.0	0.0420	0.0247	0.0105	0.0045	75.00	81.78
0250F	250	4.3	1.5	5.8	14	24.0	0.0462	0.0229	0.0107	0.0046	76.84	79.91
0250G	250	3.9	1.2	5.1	12	19.0	0.0247	0.0221	0.0057	0.0036	76.92	83.71
0250H	250	x	x	x	x	x	x	x	x	x	x	x
0250I	250	4.5	1.3	5.8	14	23.0	0.0285	0.0108	0.0086	0.0042	69.82	61.11
<i>0250_sum</i>	<i>250</i>	<i>33.5</i>	<i>12.0</i>	<i>45.5</i>	<i>107.0</i>	<i>180.0</i>	<i>0.3149</i>	<i>0.1573</i>	<i>0.0710</i>	<i>0.0333</i>	<i>614.14</i>	<i>605.29</i>
<i>0250_mean</i>	<i>250</i>	<i>4.2</i>	<i>1.5</i>	<i>5.7</i>	<i>13.4</i>	<i>22.5</i>	<i>0.0394</i>	<i>0.0197</i>	<i>0.0089</i>	<i>0.0042</i>	<i>76.77</i>	<i>75.66</i>
<i>0250_SD</i>	<i>250</i>	<i>0.6</i>	<i>0.5</i>	<i>0.9</i>	<i>0.9</i>	<i>2.8</i>	<i>0.0120</i>	<i>0.0073</i>	<i>0.0018</i>	<i>0.0005</i>	<i>3.67</i>	<i>10.14</i>
0500A	500	4.2	1.5	5.7	14	18.0	0.0387	0.0208	0.0078	0.0044	79.84	78.85
0500B	500	4.0	1.4	5.4	14	26.5	0.0451	0.0195	0.0084	0.0045	81.37	76.92
0500C	500	3.6	1.3	4.9	14	20.0	0.0435	0.0295	0.0104	0.0052	76.09	82.37
0500D	500	1.9	0.8	2.7	13	18.0	0.0459	0.0273	0.0092	0.0048	79.96	82.42
0500E	500	5.0	2.6	7.6	14	19.0	0.0406	0.0164	0.0071	0.0035	82.51	78.66
0500F	500	4.1	1.5	5.6	12	16.5	0.0276	0.0177	0.0056	0.0059	79.71	66.67
0500G	500	3.8	1.2	5.0	14	18.0	0.0418	0.0150	0.0078	0.0048	81.34	68.00
0500H	500	3.8	1.3	5.1	12	20.5	0.0271	0.0089	0.0079	0.0047	70.85	47.19
0500I	500	4.4	1.6	6.0	14	17.5	0.0268	0.0111	0.0071	0.0043	73.51	61.26
<i>0500_sum</i>	<i>500</i>	<i>34.8</i>	<i>13.2</i>	<i>48.0</i>	<i>121.0</i>	<i>174.0</i>	<i>0.3371</i>	<i>0.1662</i>	<i>0.0713</i>	<i>0.0421</i>	<i>705.19</i>	<i>642.34</i>
<i>0500_mean</i>	<i>500</i>	<i>3.9</i>	<i>1.5</i>	<i>5.3</i>	<i>13.4</i>	<i>19.3</i>	<i>0.0375</i>	<i>0.0185</i>	<i>0.0079</i>	<i>0.0047</i>	<i>78.35</i>	<i>71.37</i>
<i>0500_SD</i>	<i>500</i>	<i>0.8</i>	<i>0.5</i>	<i>1.3</i>	<i>0.9</i>	<i>3.0</i>	<i>0.0080</i>	<i>0.0068</i>	<i>0.0014</i>	<i>0.0007</i>	<i>3.98</i>	<i>11.74</i>
1000A	1000	4.2	1.7	5.9	13	18.0	0.0368	0.0192	0.0068	0.0049	81.52	74.48
1000B	1000	2.3	0.8	3.1	14	21.5	0.0342	0.0191	0.0095	0.0042	72.22	78.01
1000C	1000	2.1	0.9	3.0	14	24.0	0.0524	0.0164	0.0087	0.0048	83.40	70.73
1000D	1000	4.4	1.7	6.1	14	17.0	0.0452	0.0279	0.0080	0.0059	82.30	78.85
1000E	1000	4.6	1.6	6.2	14	18.0	0.0389	0.0174	0.0055	0.0051	85.86	70.69
1000F	1000	4.1	1.0	5.1	13	15.5	0.0214	0.0160	0.0091	0.0040	57.48	75.00
1000G	1000	2.1	0.9	3.0	14	21.5	0.0321	0.0089	0.0086	0.0037	73.21	58.43
1000H	1000	1.5	1.3	2.8	12	16.5	0.0281	0.0098	0.0060	0.0034	78.65	65.31
1000I	1000	4.2	1.9	6.1	14	16.5	0.0316	0.0153	0.0075	0.0042	76.27	72.55
<i>1000_sum</i>	<i>1000</i>	<i>29.5</i>	<i>11.8</i>	<i>41.3</i>	<i>122.0</i>	<i>168.5</i>	<i>0.3207</i>	<i>0.1500</i>	<i>0.0697</i>	<i>0.0402</i>	<i>690.90</i>	<i>644.05</i>
<i>1000_mean</i>	<i>1000</i>	<i>3.3</i>	<i>1.3</i>	<i>4.6</i>	<i>13.6</i>	<i>18.7</i>	<i>0.0356</i>	<i>0.0167</i>	<i>0.0077</i>	<i>0.0045</i>	<i>76.77</i>	<i>71.56</i>
<i>1000_SD</i>	<i>1000</i>	<i>1.2</i>	<i>0.4</i>	<i>1.6</i>	<i>0.7</i>	<i>2.9</i>	<i>0.0092</i>	<i>0.0056</i>	<i>0.0014</i>	<i>0.0008</i>	<i>8.58</i>	<i>6.41</i>
2500A	2500	3.9	1.4	5.3	14	14.0	0.0313	0.0153	0.0079	0.0053	74.76	65.36
2500B	2500	3.7	1.6	5.3	14	14.0	0.0313	0.0166	0.0077	0.0056	75.40	66.27
2500C	2500	6.5	3.7	10.2	15	16.5	0.0281	0.0123	0.0076	0.0047	72.95	61.79
2500D	2500	3.9	2.1	6.0	13	13.5	0.0258	0.0148	0.0088	0.0046	65.89	68.92
2500E	2500	4.0	1.6	5.6	14	15.5	0.0268	0.0128	0.0064	0.0049	76.12	61.72
2500F	2500	3.6	1.9	5.5	14	17.0	0.0336	0.0138	0.0099	0.0062	70.54	55.07
2500G	2500	x	x	x	x	x	x	x	x	x	x	x
2500H	2500	3.9	1.6	5.5	14	13.0	0.0259	0.0145	0.0070	0.0050	72.97	65.52
2500I	2500	3.4	1.6	5.0	14	13.0	0.0168	0.0148	0.0052	0.0048	69.05	67.57
<i>2500_sum</i>	<i>2500</i>	<i>32.9</i>	<i>15.5</i>	<i>48.4</i>	<i>112.0</i>	<i>116.5</i>	<i>0.2196</i>	<i>0.1149</i>	<i>0.0605</i>	<i>0.0411</i>	<i>577.68</i>	<i>512.21</i>
<i>2500_mean</i>	<i>2500</i>	<i>4.1</i>	<i>1.9</i>	<i>6.1</i>	<i>14.0</i>	<i>14.6</i>	<i>0.0275</i>	<i>0.0144</i>	<i>0.0076</i>	<i>0.0051</i>	<i>72.21</i>	<i>64.03</i>
<i>2500_SD</i>	<i>2500</i>	<i>1.0</i>	<i>0.7</i>	<i>1.7</i>	<i>0.5</i>	<i>1.6</i>	<i>0.0052</i>	<i>0.0014</i>	<i>0.0014</i>	<i>0.0005</i>	<i>3.50</i>	<i>4.41</i>

Table A.39.: A3 plant growth data for Na_2SeO_3 III (Planting Date: 21.11.2013)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	x	x	x	x	x	x	x	x	x	x	x
0000B	0	4.5	1.7	6.2	10	27.0	0.0342	0.0247	0.0085	0.0102	75.15	58.70
0000C	0	2.2	0.9	3.1	13	30.0	0.0561	0.0142	0.0123	0.0044	78.07	69.01
0000D	0	4.5	1.3	5.8	9	31.0	0.0966	0.0278	0.0171	0.0069	82.30	75.18
0000E	0	2.5	0.9	3.4	13	32.0	0.0827	0.0276	0.0171	0.0058	79.32	78.99
0000F	0	5.0	1.6	6.6	13	26.0	0.0438	0.0177	0.0095	0.0042	78.31	76.27
0000G	0	5.1	1.9	7.0	11	28.0	0.0472	0.0192	0.0120	0.0056	74.58	70.83
0000H	0	x	x	x	x	x	x	x	x	x	x	x
0000I	0	3.3	0.9	4.2	8	22.0	0.0133	0.0054	0.0052	0.0035	60.90	35.19
0000_sum	0	27.1	9.2	36.3	77.0	196.0	0.3739	0.1366	0.0817	0.0406	528.63	464.17
0000_mean	0	3.9	1.3	5.2	11.0	28.0	0.0534	0.0195	0.0117	0.0058	75.52	66.31
0000_SD	0	1.2	0.4	1.6	2.1	3.4	0.0284	0.0081	0.0044	0.0023	6.95	15.24
0005A	5	2.1	0.9	3.0	4	14.0	0.0101	0.0163	0.0027	0.0092	73.27	43.56
0005B	5	3.9	1.2	5.1	8	24.0	0.0294	0.0207	0.0077	0.0043	73.81	79.23
0005C	5	3.8	1.0	4.8	8	26.0	0.0424	0.0305	0.0109	0.0115	74.29	62.30
0005D	5	x	x	x	x	x	x	x	x	x	x	x
0005E	5	3.1	1.1	4.2	13	32.0	0.0769	0.0332	0.0185	0.0074	75.94	77.71
0005F	5	5.5	2.1	7.6	10	27.0	0.0354	0.0120	0.0093	0.0033	73.73	72.50
0005G	5	x	x	x	x	x	x	x	x	x	x	x
0005H	5	x	x	x	x	x	x	x	x	x	x	x
0005I	5	3.3	0.8	4.1	6	20.0	0.0190	0.0118	0.0062	0.0039	67.37	66.95
0005_sum	5	21.7	7.1	28.8	49.0	143.0	0.2132	0.1245	0.0553	0.0396	438.41	402.24
0005_mean	5	3.6	1.2	4.8	8.2	23.8	0.0355	0.0208	0.0092	0.0066	73.07	67.04
0005_SD	5	1.1	0.5	1.6	3.1	6.2	0.0233	0.0092	0.0053	0.0033	2.94	13.16
0010A	10	x	x	x	x	x	x	x	x	x	x	x
0010B	10	3.6	1.1	4.7	8	26.0	0.0307	0.0296	0.0097	0.0174	68.40	41.22
0010C	10	5.4	2.0	7.4	11	25.0	0.0522	0.0274	0.0174	0.0058	66.67	78.83
0010D	10	x	x	x	x	x	x	x	x	x	x	x
0010E	10	4.0	1.4	5.4	11	29.0	0.0678	0.0352	0.0154	0.0077	77.29	78.13
0010F	10	2.4	0.7	3.1	13	27.0	0.0172	0.0233	0.0038	0.0095	77.91	59.23
0010G	10	x	x	x	x	x	x	x	x	x	x	x
0010H	10	5.2	1.4	6.6	13	31.0	0.0658	0.0153	0.0178	0.0066	72.95	56.86
0010I	10	3.6	1.2	4.8	8	24.0	0.0216	0.0127	0.0075	0.0073	65.28	42.52
0010_sum	10	24.2	7.8	32.0	64.0	162.0	0.2553	0.1435	0.0716	0.0543	428.49	356.78
0010_mean	10	4.0	1.3	5.3	10.7	27.0	0.0426	0.0239	0.0119	0.0091	71.41	59.46
0010_SD	10	1.1	0.4	1.5	2.3	2.6	0.0223	0.0086	0.0058	0.0043	5.45	16.43
0025A	25	x	x	x	x	x	x	x	x	x	x	x
0025B	25	4.7	1.3	6.0	13	30.0	0.1001	0.0238	0.0240	0.0092	76.02	61.34
0025C	25	x	x	x	x	x	x	x	x	x	x	x
0025D	25	x	x	x	x	x	x	x	x	x	x	x
0025E	25	5.2	2.4	7.6	4	14.5	0.0089	0.0181	0.0031	0.0097	65.17	46.41
0025F	25	4.1	1.8	5.9	6	17.0	0.0235	0.0259	0.0064	0.0163	72.77	37.07
0025G	25	2.7	0.8	3.5	3	11.5	0.0128	0.0199	0.0028	0.0125	78.13	37.19
0025H	25	x	x	x	x	x	x	x	x	x	x	x
0025I	25	x	x	x	x	x	x	x	x	x	x	x
0025_sum	25	16.7	6.3	23.0	26.0	73.0	0.1453	0.0877	0.0363	0.0477	292.08	182.00
0025_mean	25	4.2	1.6	5.8	6.5	18.3	0.0363	0.0219	0.0091	0.0119	73.02	45.50
0025_SD	25	1.1	0.7	1.7	4.5	8.1	0.0430	0.0036	0.0101	0.0033	5.68	11.43
0050A	50	x	x	x	x	x	x	x	x	x	x	x
0050B	50	x	x	x	x	x	x	x	x	x	x	x
0050C	50	2.9	1.2	4.1	8	25.5	0.0263	0.0085	0.0025	0.0038	90.49	55.29
0050D	50	2.7	0.7	3.4	3	11.5	0.0127	0.0278	0.0067	0.0190	47.24	31.65
0050E	50	x	x	x	x	x	x	x	x	x	x	x
0050F	50	x	x	x	x	x	x	x	x	x	x	x
0050G	50	3.2	0.7	3.9	8	25.5	0.0323	0.0223	0.0087	0.0082	73.07	63.23
0050H	50	4.9	1.4	6.3	12	30.0	0.0896	0.0273	0.0219	0.0100	75.56	63.37
0050I	50	3.9	1.5	5.4	11	27.0	0.0489	0.0096	0.0137	0.0061	71.98	36.46
0050_sum	50	17.6	5.5	23.1	42.0	119.5	0.2098	0.0955	0.0535	0.0471	358.35	250.01
0050_mean	50	3.5	1.1	4.6	8.4	23.9	0.0420	0.0191	0.0107	0.0094	71.67	50.00
0050_SD	50	0.9	0.4	1.2	3.5	7.2	0.0296	0.0094	0.0074	0.0058	15.56	15.01
0100A	100	x	x	x	x	x	x	x	x	x	x	x
0100B	100	x	x	x	x	x	x	x	x	x	x	x
0100C	100	4.6	1.4	6.0	10	29.0	0.0732	0.0361	0.0194	0.0125	73.50	65.37
0100D	100	x	0.8	x	x	x	x	x	x	x	x	x
0100E	100	2.6	x	2.6	4	11.0	0.0183	0.0275	0.0032	0.0101	82.51	63.27
0100F	100	x	x	x	x	x	x	x	x	x	x	x
0100G	100	x	x	x	x	x	x	x	x	x	x	x
0100H	100	x	x	x	x	x	x	x	x	x	x	x
0100I	100	x	x	x	x	x	x	x	x	x	x	x
0100_sum	100	7.2	2.2	8.6	14.0	40.0	0.0915	0.0636	0.0226	0.0226	156.01	128.65
0100_mean	100	3.6	1.1	4.3	7.0	20.0	0.0458	0.0318	0.0113	0.0113	78.01	64.32
0100_SD	100	1.4	0.4	2.4	4.2	12.7	0.0388	0.0061	0.0115	0.0017	6.38	1.49

Table A.40.: A3 plant growth data for Na_2SeO_3 III (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	5.1	1.5	6.6	13	23.0	0.0688	0.0271	0.0158	0.0081	77.03	70.11
0250B	250	x	x	x	x	x	x	x	x	x	x	x
0250C	250	3.2	1.0	4.2	6	15.0	0.0238	0.0323	0.0052	0.0196	78.15	39.32
0250D	250	x	x	x	x	x	x	x	x	x	x	x
0250E	250	x	x	x	x	x	x	x	x	x	x	x
0250F	250	x	x	x	x	x	x	x	x	x	x	x
0250G	250	5.8	1.7	7.5	13	22.0	0.0413	0.0253	0.0102	0.0053	75.30	79.05
0250H	250	x	x	x	x	x	x	x	x	x	x	x
0250I	250	3.7	1.1	4.8	7	15.0	0.0151	0.0243	0.0035	0.0147	76.82	39.51
<i>0250_sum</i>	<i>250</i>	<i>17.8</i>	<i>5.3</i>	<i>23.1</i>	<i>39.0</i>	<i>75.0</i>	<i>0.1490</i>	<i>0.1090</i>	<i>0.0317</i>	<i>0.0477</i>	<i>307.31</i>	<i>227.99</i>
<i>0250_mean</i>	<i>250</i>	<i>4.5</i>	<i>1.3</i>	<i>5.8</i>	<i>9.8</i>	<i>18.8</i>	<i>0.0373</i>	<i>0.0273</i>	<i>0.0087</i>	<i>0.0119</i>	<i>76.83</i>	<i>57.00</i>
<i>0250_SD</i>	<i>250</i>	<i>1.2</i>	<i>0.3</i>	<i>1.5</i>	<i>3.8</i>	<i>4.3</i>	<i>0.0237</i>	<i>0.0036</i>	<i>0.0055</i>	<i>0.0065</i>	<i>1.17</i>	<i>20.63</i>
0500A	500	x	x	x	x	x	x	x	x	x	x	x
0500B	500	x	x	x	x	x	x	x	x	x	x	x
0500C	500	x	x	x	x	x	x	x	x	x	x	x
0500D	500	x	x	x	x	x	x	x	x	x	x	x
0500E	500	x	x	x	x	x	x	x	x	x	x	x
0500F	500	x	x	x	x	x	x	x	x	x	x	x
0500G	500	4.6	1.6	6.2	12	24.5	0.0662	0.0384	0.0169	0.0072	74.47	81.25
0500H	500	5.5	1.8	7.3	10	25.5	0.0521	0.0306	0.0149	0.0078	71.40	74.51
0500I	500	x	x	x	x	x	x	x	x	x	x	x
<i>0500_sum</i>	<i>500</i>	<i>10.1</i>	<i>3.4</i>	<i>13.5</i>	<i>22.0</i>	<i>50.0</i>	<i>0.1183</i>	<i>0.0690</i>	<i>0.0318</i>	<i>0.0150</i>	<i>145.87</i>	<i>155.76</i>
<i>0500_mean</i>	<i>500</i>	<i>5.1</i>	<i>1.7</i>	<i>6.8</i>	<i>11.0</i>	<i>25.0</i>	<i>0.0592</i>	<i>0.0345</i>	<i>0.0159</i>	<i>0.0075</i>	<i>72.94</i>	<i>77.88</i>
<i>0500_SD</i>	<i>500</i>	<i>0.6</i>	<i>0.1</i>	<i>0.8</i>	<i>1.4</i>	<i>0.7</i>	<i>0.0100</i>	<i>0.0055</i>	<i>0.0014</i>	<i>0.0004</i>	<i>2.17</i>	<i>4.77</i>
1000A	1000	x	x	x	x	x	x	x	x	x	x	x
1000B	1000	x	x	x	x	x	x	x	x	x	x	x
1000C	1000	x	x	x	x	x	x	x	x	x	x	x
1000D	1000	x	x	x	x	x	x	x	x	x	x	x
1000E	1000	5.3	2.0	7.3	12	25.0	0.0397	0.0196	0.0143	0.0074	63.98	62.24
1000F	1000	2.2	0.8	3.0	4	9.0	0.0120	0.0283	0.0036	0.0198	70.00	30.04
1000G	1000	x	x	x	x	x	x	x	x	x	x	x
1000H	1000	4.3	1.2	5.5	11	22.0	0.0441	0.0314	0.0127	0.0073	71.20	76.75
1000I	1000	x	x	x	x	x	x	x	x	x	x	x
<i>1000_sum</i>	<i>1000</i>	<i>11.8</i>	<i>4.0</i>	<i>15.8</i>	<i>27.0</i>	<i>56.0</i>	<i>0.0958</i>	<i>0.0793</i>	<i>0.0306</i>	<i>0.0345</i>	<i>205.18</i>	<i>169.03</i>
<i>1000_mean</i>	<i>1000</i>	<i>3.9</i>	<i>1.3</i>	<i>5.3</i>	<i>9.0</i>	<i>18.7</i>	<i>0.0319</i>	<i>0.0264</i>	<i>0.0102</i>	<i>0.0115</i>	<i>68.39</i>	<i>56.34</i>
<i>1000_SD</i>	<i>1000</i>	<i>1.6</i>	<i>0.6</i>	<i>2.2</i>	<i>4.4</i>	<i>8.5</i>	<i>0.0174</i>	<i>0.0061</i>	<i>0.0058</i>	<i>0.0072</i>	<i>3.87</i>	<i>23.91</i>
2500A	2500	x	x	x	x	x	x	x	x	x	x	x
2500B	2500	x	x	x	x	x	x	x	x	x	x	x
2500C	2500	x	x	x	x	x	x	x	x	x	x	x
2500D	2500	x	x	x	x	x	x	x	x	x	x	x
2500E	2500	2.4	0.9	3.3	13	15.5	0.0115	0.0158	0.0054	0.0079	53.04	50.00
2500F	2500	4.1	1.8	5.9	11	22.0	0.0365	0.0224	0.0129	0.0079	64.66	64.73
2500G	2500	4.6	2.1	6.7	13	25.0	0.0425	0.0191	0.0166	0.0081	60.94	57.59
2500H	2500	x	x	x	x	x	x	x	x	x	x	x
2500I	2500	x	x	x	x	x	x	x	x	x	x	x
<i>2500_sum</i>	<i>2500</i>	<i>11.1</i>	<i>4.8</i>	<i>15.9</i>	<i>37.0</i>	<i>62.5</i>	<i>0.0905</i>	<i>0.0573</i>	<i>0.0349</i>	<i>0.0239</i>	<i>178.64</i>	<i>172.32</i>
<i>2500_mean</i>	<i>2500</i>	<i>3.7</i>	<i>1.6</i>	<i>5.3</i>	<i>12.3</i>	<i>20.8</i>	<i>0.0302</i>	<i>0.0191</i>	<i>0.0116</i>	<i>0.0080</i>	<i>59.55</i>	<i>57.44</i>
<i>2500_SD</i>	<i>2500</i>	<i>1.2</i>	<i>0.6</i>	<i>1.8</i>	<i>1.2</i>	<i>4.9</i>	<i>0.0164</i>	<i>0.0033</i>	<i>0.0057</i>	<i>0.0001</i>	<i>5.93</i>	<i>7.37</i>

Table A.41.: A3 plant growth data for Na_2SeO_4 I (Planting Date: 22.11.2012)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	4.9	1.6	6.5	15	28.0	0.0591	0.0151	0.0128	0.0057	78.34	62.25
0000B	0	5.1	1.7	6.8	15	25.0	0.0507	0.0214	0.0152	0.0064	70.02	70.09
0000C	0	3.6	0.7	4.3	14	17.0	0.0251	0.0182	0.0056	0.0102	77.69	43.96
0000D	0	4.2	1.8	6	16	25.0	0.0604	0.0323	0.0152	0.0056	74.83	82.66
0000E	0	4.7	1.7	6.4	15	23.0	0.0437	0.0160	0.0094	0.0042	78.49	73.75
0000F	0	4.7	1.7	6.4	15	26.0	0.0679	0.0193	0.0119	0.0052	82.47	73.06
0000G	0	4.2	0.8	5	15	26.0	0.0648	0.0152	0.0197	0.0059	69.60	61.18
0000H	0	x	x	x	x	x	x	x	x	x	x	x
0000I	0	x	x	x	x	x	x	x	x	x	x	x
<i>0000_sum</i>	<i>0</i>	<i>31.4</i>	<i>10.0</i>	<i>41.4</i>	<i>105.0</i>	<i>170.0</i>	<i>0.3717</i>	<i>0.1375</i>	<i>0.0898</i>	<i>0.0432</i>	<i>531.45</i>	<i>466.95</i>
<i>0000_mean</i>	<i>0</i>	<i>4.5</i>	<i>1.4</i>	<i>5.9</i>	<i>15.0</i>	<i>24.3</i>	<i>0.0531</i>	<i>0.0196</i>	<i>0.0128</i>	<i>0.0062</i>	<i>75.92</i>	<i>66.71</i>
<i>0000_SD</i>	<i>0</i>	<i>0.5</i>	<i>0.5</i>	<i>0.9</i>	<i>0.6</i>	<i>3.5</i>	<i>0.0149</i>	<i>0.0060</i>	<i>0.0045</i>	<i>0.0019</i>	<i>4.73</i>	<i>12.41</i>
0005A	5	4.9	1.8	6.7	13	24.0	0.0417	0.0214	0.0102	0.0044	75.54	79.44
0005B	5	5.1	1.4	6.5	16	29.0	0.0750	0.0228	0.0170	0.0052	77.33	77.19
0005C	5	5.9	1.8	7.7	15	30.0	0.0648	0.0218	0.0125	0.0055	80.71	74.77
0005D	5	5.7	1.8	7.5	15	30.0	0.0703	0.0158	0.0158	0.0049	77.52	68.99
0005E	5	4.8	1.6	6.4	16	28.0	0.0760	0.0172	0.0139	0.0049	81.71	71.51
0005F	5	4.2	1.8	6	15	27.0	0.0492	0.0222	0.0088	0.0055	82.11	75.23
0005G	5	2.9	1.3	4.2	14	15.0	0.0169	0.0129	0.0033	0.0065	80.47	49.61
0005H	5	4.1	1.9	6	16	26.0	0.0296	0.0149	0.0096	0.0034	67.57	77.18
0005I	5	x	x	x	x	x	x	x	x	x	x	x
<i>0005_sum</i>	<i>5</i>	<i>37.6</i>	<i>13.4</i>	<i>51.0</i>	<i>120.0</i>	<i>209.0</i>	<i>0.4235</i>	<i>0.1490</i>	<i>0.0911</i>	<i>0.0403</i>	<i>622.97</i>	<i>573.92</i>
<i>0005_mean</i>	<i>5</i>	<i>4.7</i>	<i>1.7</i>	<i>6.4</i>	<i>15.0</i>	<i>26.1</i>	<i>0.0529</i>	<i>0.0186</i>	<i>0.0114</i>	<i>0.0050</i>	<i>77.87</i>	<i>71.74</i>
<i>0005_SD</i>	<i>5</i>	<i>1.0</i>	<i>0.2</i>	<i>1.1</i>	<i>1.1</i>	<i>4.9</i>	<i>0.0222</i>	<i>0.0039</i>	<i>0.0044</i>	<i>0.0009</i>	<i>4.77</i>	<i>9.54</i>
0010A	10	x	x	x	x	x	x	x	x	x	x	x
0010B	10	5.0	1.7	6.7	15	29.0	0.0747	0.0163	0.0135	0.0054	81.93	66.87
0010C	10	4.7	2.1	6.8	16	32.0	0.0730	0.0111	0.0148	0.0048	79.73	56.76
0010D	10	4.6	2	6.6	16	29.0	0.0815	0.0162	0.0159	0.0054	80.49	66.67
0010E	10	4.2	1.2	5.4	13	21.0	0.0254	0.0137	0.0062	0.0062	75.59	54.74
0010F	10	4.8	1.7	6.5	14	25.0	0.0616	0.0181	0.0143	0.0050	76.79	72.38
0010G	10	3.5	0.8	4.3	13	19.0	0.0188	0.0149	0.0049	0.0028	73.94	81.21
0010H	10	4.6	2.1	6.7	16	29.0	0.0669	0.0112	0.0149	0.0051	77.73	54.46
0010I	10	x	x	x	x	x	x	x	x	x	x	x
<i>0010_sum</i>	<i>10</i>	<i>31.4</i>	<i>11.6</i>	<i>43.0</i>	<i>103.0</i>	<i>184.0</i>	<i>0.4019</i>	<i>0.1015</i>	<i>0.0845</i>	<i>0.0347</i>	<i>546.18</i>	<i>453.09</i>
<i>0010_mean</i>	<i>10</i>	<i>4.5</i>	<i>1.7</i>	<i>6.1</i>	<i>14.7</i>	<i>26.3</i>	<i>0.0574</i>	<i>0.0145</i>	<i>0.0121</i>	<i>0.0050</i>	<i>78.03</i>	<i>64.73</i>
<i>0010_SD</i>	<i>10</i>	<i>0.5</i>	<i>0.5</i>	<i>0.9</i>	<i>1.4</i>	<i>4.8</i>	<i>0.0250</i>	<i>0.0027</i>	<i>0.0045</i>	<i>0.0011</i>	<i>2.84</i>	<i>10.06</i>
0025A	25	4.8	1.6	6.4	14	28.0	0.0610	0.0247	0.0124	0.0056	79.67	77.33
0025B	25	x	x	x	x	x	x	x	x	x	x	x
0025C	25	4.7	1.5	6.2	13	26.0	0.0436	0.0155	0.0129	0.0046	70.41	70.32
0025D	25	5.1	1.7	6.8	16	29.0	0.0852	0.0220	0.0189	0.0050	77.82	77.27
0025E	25	4.9	1.8	6.7	15	27.0	0.0506	0.0134	0.0151	0.0043	70.16	67.91
0025F	25	4.8	1.6	6.4	15	28.0	0.0718	0.0136	0.0159	0.0057	77.86	58.09
0025G	25	x	x	x	x	x	x	x	x	x	x	x
0025H	25	x	x	x	x	x	x	x	x	x	x	x
0025I	25	x	x	x	x	x	x	x	x	x	x	x
<i>0025_sum</i>	<i>25</i>	<i>24.3</i>	<i>8.2</i>	<i>32.5</i>	<i>73.0</i>	<i>138.0</i>	<i>0.3122</i>	<i>0.0892</i>	<i>0.0752</i>	<i>0.0252</i>	<i>375.92</i>	<i>350.92</i>
<i>0025_mean</i>	<i>25</i>	<i>4.9</i>	<i>1.6</i>	<i>6.5</i>	<i>14.6</i>	<i>27.6</i>	<i>0.0624</i>	<i>0.0178</i>	<i>0.0150</i>	<i>0.0050</i>	<i>75.18</i>	<i>70.18</i>
<i>0025_SD</i>	<i>25</i>	<i>0.2</i>	<i>0.1</i>	<i>0.2</i>	<i>1.1</i>	<i>1.1</i>	<i>0.0166</i>	<i>0.0052</i>	<i>0.0026</i>	<i>0.0006</i>	<i>4.53</i>	<i>7.95</i>
0050A	50	5.2	1.9	7.1	14	29.0	0.0587	0.0129	0.0203	0.0048	65.42	62.79
0050B	50	x	x	x	13	x	x	x	x	x	x	x
0050C	50	4.7	1.7	6.4	15	24.0	0.0376	0.0181	0.0092	0.0036	75.53	80.11
0050D	50	4.1	1.4	5.5	16	26.0	0.0689	0.0140	0.0145	0.0048	78.96	65.71
0050E	50	x	x	x	x	x	x	x	x	x	x	x
0050F	50	5.9	2.0	7.9	15	30.0	0.0731	0.0212	0.0201	0.0046	72.50	78.30
0050G	50	4.8	1.6	6.4	14	28.0	0.0477	0.0145	0.0097	0.0038	79.66	73.79
0050H	50	x	x	x	x	x	x	x	x	x	x	x
0050I	50	x	x	x	x	x	x	x	x	x	x	x
<i>0050_sum</i>	<i>50</i>	<i>24.7</i>	<i>8.6</i>	<i>33.3</i>	<i>87.0</i>	<i>137.0</i>	<i>0.2860</i>	<i>0.0807</i>	<i>0.0738</i>	<i>0.0216</i>	<i>372.07</i>	<i>360.71</i>
<i>0050_mean</i>	<i>50</i>	<i>4.9</i>	<i>1.7</i>	<i>6.7</i>	<i>14.5</i>	<i>27.4</i>	<i>0.0572</i>	<i>0.0161</i>	<i>0.0148</i>	<i>0.0043</i>	<i>74.41</i>	<i>72.14</i>
<i>0050_SD</i>	<i>50</i>	<i>0.7</i>	<i>0.2</i>	<i>0.9</i>	<i>1.0</i>	<i>2.4</i>	<i>0.0147</i>	<i>0.0034</i>	<i>0.0054</i>	<i>0.0006</i>	<i>5.79</i>	<i>7.63</i>
0100A	100	5	1.9	6.9	14	26.0	0.0540	0.0184	0.0104	0.0054	80.74	70.65
0100B	100	x	x	x	x	x	x	x	x	x	x	x
0100C	100	4.7	1.7	6.4	16	25.0	0.0671	0.0195	0.0130	0.0083	80.63	57.44
0100D	100	4.7	1.8	6.5	14	26.0	0.0650	0.0189	0.0109	0.0060	83.23	68.25
0100E	100	5.2	1.8	7	15	29.0	0.0868	0.0248	0.0152	0.0072	82.49	70.97
0100F	100	x	x	x	x	x	x	x	x	x	x	x
0100G	100	4.6	1.5	6.1	15	24.0	0.0627	0.0229	0.0124	0.0062	80.22	72.93
0100H	100	x	x	x	x	x	x	x	x	x	x	x
0100I	100	x	x	x	x	x	x	x	x	x	x	x
<i>0100_sum</i>	<i>100</i>	<i>24.2</i>	<i>8.7</i>	<i>32.9</i>	<i>74.0</i>	<i>130.0</i>	<i>0.3356</i>	<i>0.1045</i>	<i>0.0619</i>	<i>0.0331</i>	<i>407.31</i>	<i>340.24</i>
<i>0100_mean</i>	<i>100</i>	<i>4.8</i>	<i>1.7</i>	<i>6.6</i>	<i>14.8</i>	<i>26.0</i>	<i>0.0671</i>	<i>0.0209</i>	<i>0.0124</i>	<i>0.0066</i>	<i>81.46</i>	<i>68.05</i>
<i>0100_SD</i>	<i>100</i>	<i>0.3</i>	<i>0.2</i>	<i>0.4</i>	<i>0.8</i>	<i>1.9</i>	<i>0.0121</i>	<i>0.0028</i>	<i>0.0019</i>	<i>0.0011</i>	<i>1.32</i>	<i>6.16</i>

Table A.42.: A3 plant growth data for Na_2SeO_4 I (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	4.7	1.7	6.4	13	23.0	0.0384	0.0192	0.0068	0.0070	82.29	63.54
0250B	250	4.8	1.9	6.7	15	24.0	0.0444	0.0217	0.0112	0.0035	74.77	83.87
0250C	250	4.6	2.1	6.7	16	28.0	0.0683	0.0205	0.0155	0.0058	77.31	71.71
0250D	250	x	x	x	x	x	x	x	x	x	x	x
0250E	250	4.7	1.7	6.4	15	26.0	0.0548	0.0157	0.0108	0.0047	80.29	70.06
0250F	250	x	x	x	x	x	x	x	x	x	x	x
0250G	250	4.8	1.6	6.4	15	28.0	0.0523	0.0172	0.0167	0.0046	68.07	73.26
0250H	250	5.2	1.6	6.8	13	26.0	0.0539	0.0187	0.0104	0.0048	80.71	74.33
0250I	250	x	x	x	x	x	x	x	x	x	x	x
<i>0250_sum</i>	<i>250</i>	<i>28.8</i>	<i>10.6</i>	<i>39.4</i>	<i>87.0</i>	<i>155.0</i>	<i>0.3121</i>	<i>0.1130</i>	<i>0.0714</i>	<i>0.0304</i>	<i>463.44</i>	<i>436.77</i>
<i>0250_mean</i>	<i>250</i>	<i>4.8</i>	<i>1.8</i>	<i>6.6</i>	<i>14.5</i>	<i>25.8</i>	<i>0.0520</i>	<i>0.0188</i>	<i>0.0119</i>	<i>0.0051</i>	<i>77.24</i>	<i>72.80</i>
<i>0250_SD</i>	<i>250</i>	<i>0.2</i>	<i>0.2</i>	<i>0.2</i>	<i>1.2</i>	<i>2.0</i>	<i>0.0102</i>	<i>0.0022</i>	<i>0.0036</i>	<i>0.0012</i>	<i>5.24</i>	<i>6.63</i>
0500A	500	5.2	1.8	7	15	28.0	0.0547	0.0106	0.0154	0.0040	71.85	62.26
0500B	500	4.6	1.5	6.1	14	23.0	0.0488	0.0179	0.0094	0.0055	80.74	69.27
0500C	500	4.8	1.7	6.5	14	27.0	0.0617	0.0157	0.0120	0.0051	80.55	67.52
0500D	500	4.8	1.9	6.7	15	28.0	0.0638	0.0145	0.0127	0.0045	80.09	68.97
0500E	500	x	x	x	x	x	x	x	x	x	x	x
0500F	500	4.7	1.6	6.3	14	27.0	0.0469	0.0129	0.0158	0.0036	66.31	72.09
0500G	500	x	x	x	x	x	x	x	x	x	x	x
0500H	500	x	x	x	x	x	x	x	x	x	x	x
0500I	500	x	x	x	x	x	x	x	x	x	x	x
<i>0500_sum</i>	<i>500</i>	<i>24.1</i>	<i>8.5</i>	<i>32.6</i>	<i>72.0</i>	<i>133.0</i>	<i>0.2759</i>	<i>0.0716</i>	<i>0.0653</i>	<i>0.0227</i>	<i>379.54</i>	<i>340.11</i>
<i>0500_mean</i>	<i>500</i>	<i>4.8</i>	<i>1.7</i>	<i>6.5</i>	<i>14.4</i>	<i>26.6</i>	<i>0.0552</i>	<i>0.0143</i>	<i>0.0131</i>	<i>0.0045</i>	<i>75.91</i>	<i>68.02</i>
<i>0500_SD</i>	<i>500</i>	<i>0.2</i>	<i>0.2</i>	<i>0.3</i>	<i>0.5</i>	<i>2.1</i>	<i>0.0075</i>	<i>0.0028</i>	<i>0.0026</i>	<i>0.0008</i>	<i>6.54</i>	<i>3.62</i>
1000A	1000	5.1	1.8	6.9	15	28.0	0.0738	0.0278	0.0153	0.0069	79.27	75.18
1000B	1000	x	x	x	x	x	x	x	x	x	x	x
1000C	1000	x	x	x	x	x	x	x	x	x	x	x
1000D	1000	2.9	1.4	4.3	13	19.0	0.0183	0.0184	0.0050	0.0103	72.68	44.02
1000E	1000	3.9	1.5	5.4	14	25.0	0.0556	0.0224	0.0116	0.0058	79.14	74.11
1000F	1000	x	x	x	x	x	x	x	x	x	x	x
1000G	1000	4.2	1.8	6	14	25.0	0.0680	0.0231	0.0134	0.0059	80.29	74.46
1000H	1000	4.2	1.7	5.9	15	27.0	0.0576	0.0192	0.0131	0.0056	77.26	70.83
1000I	1000	x	x	x	x	x	x	x	x	x	x	x
<i>1000_sum</i>	<i>1000</i>	<i>20.3</i>	<i>8.2</i>	<i>28.5</i>	<i>71.0</i>	<i>124.0</i>	<i>0.2733</i>	<i>0.1109</i>	<i>0.0584</i>	<i>0.0345</i>	<i>388.63</i>	<i>338.60</i>
<i>1000_mean</i>	<i>1000</i>	<i>4.1</i>	<i>1.6</i>	<i>5.7</i>	<i>14.2</i>	<i>24.8</i>	<i>0.0547</i>	<i>0.0222</i>	<i>0.0117</i>	<i>0.0069</i>	<i>77.73</i>	<i>67.72</i>
<i>1000_SD</i>	<i>1000</i>	<i>0.8</i>	<i>0.2</i>	<i>1.0</i>	<i>0.8</i>	<i>3.5</i>	<i>0.0217</i>	<i>0.0037</i>	<i>0.0040</i>	<i>0.0020</i>	<i>3.03</i>	<i>13.35</i>
2500A	2500	x	x	x	x	x	x	x	x	x	x	x
2500B	2500	4.8	1.7	6.5	15	24.0	0.0525	0.0192	0.0136	0.0047	74.10	75.52
2500C	2500	3.9	1.6	5.5	14	21.0	0.0342	0.0122	0.0093	0.0039	72.81	68.03
2500D	2500	4.7	1.6	6.3	16	26.0	0.0687	0.0235	0.0231	0.0059	66.38	74.89
2500E	2500	4.6	1.5	6.1	15	24.0	0.0600	0.0185	0.0115	0.0055	80.83	70.27
2500F	2500	x	x	x	x	x	x	x	x	x	x	x
2500G	2500	x	x	x	x	x	x	x	x	x	x	x
2500H	2500	4.7	1.6	6.3	15	23.0	0.0331	0.0118	0.0108	0.0043	67.37	63.56
2500I	2500	x	x	x	x	x	x	x	x	x	x	x
<i>2500_sum</i>	<i>2500</i>	<i>22.7</i>	<i>8.0</i>	<i>30.7</i>	<i>75.0</i>	<i>118.0</i>	<i>0.2485</i>	<i>0.0852</i>	<i>0.0683</i>	<i>0.0243</i>	<i>361.48</i>	<i>352.28</i>
<i>2500_mean</i>	<i>2500</i>	<i>4.5</i>	<i>1.6</i>	<i>6.1</i>	<i>15.0</i>	<i>23.6</i>	<i>0.0497</i>	<i>0.0170</i>	<i>0.0137</i>	<i>0.0049</i>	<i>72.30</i>	<i>70.46</i>
<i>2500_SD</i>	<i>2500</i>	<i>0.4</i>	<i>0.1</i>	<i>0.4</i>	<i>0.7</i>	<i>1.8</i>	<i>0.0157</i>	<i>0.0050</i>	<i>0.0055</i>	<i>0.0008</i>	<i>5.82</i>	<i>4.97</i>

Table A.43.: A3 plant growth data for Na₂SeO₄ II (Planting Date: 12.09.2013)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	x	x	x	x	x	x	x	x	x	x	x
0000B	0	4.7	1.7	6.4	14	23.0	0.0406	0.0106	0.0104	0.0065	74.38	38.68
0000C	0	x	x	x	x	x	x	x	x	x	x	x
0000D	0	4.8	1.6	6.4	13	18.5	0.0155	0.0119	0.0043	0.0082	72.26	31.09
0000E	0	4.5	1.7	6.2	14	20.5	0.0253	0.0145	0.0067	0.0097	73.52	33.10
0000F	0	5.0	1.8	6.8	x	21.0	0.0580	0.0148	0.0123	0.0065	78.79	56.08
0000G	0	4.9	1.5	6.4	14	21.0	0.0219	0.0157	0.0062	0.0083	71.69	47.13
0000H	0	4.3	1.4	5.7	14	20.0	0.0348	0.0138	0.0086	0.0070	75.29	49.28
0000I	0	4.2	1.3	5.5	12	18.5	0.0120	0.0141	0.0038	0.0101	x	x
<i>0000_sum</i>	<i>0</i>	<i>32.4</i>	<i>11.0</i>	<i>43.4</i>	<i>81.0</i>	<i>142.5</i>	<i>0.2081</i>	<i>0.0954</i>	<i>0.0523</i>	<i>0.0563</i>	<i>445.93</i>	<i>255.37</i>
<i>0000_mean</i>	<i>0</i>	<i>4.6</i>	<i>1.6</i>	<i>6.2</i>	<i>13.5</i>	<i>20.4</i>	<i>0.0297</i>	<i>0.0136</i>	<i>0.0075</i>	<i>0.0080</i>	<i>74.32</i>	<i>42.56</i>
<i>0000_SD</i>	<i>0</i>	<i>0.3</i>	<i>0.2</i>	<i>0.5</i>	<i>0.8</i>	<i>1.6</i>	<i>0.0160</i>	<i>0.0018</i>	<i>0.0031</i>	<i>0.0015</i>	<i>2.56</i>	<i>9.85</i>
0005A	5	4.2	0.8	5.0	14	26.0	0.0522	0.0192	0.0113	0.0061	78.35	68.23
0005B	5	x	x	x	x	x	x	x	x	x	x	x
0005C	5	4.0	1.1	5.1	8	20.0	0.0228	0.0125	0.0050	0.0035	78.07	72.00
0005D	5	4.1	1.2	5.3	12	20.5	0.0231	0.0198	0.0070	0.0102	69.70	48.48
0005E	5	x	x	x	x	x	x	x	x	x	x	x
0005F	5	3.2	0.6	3.8	8	17.5	0.0178	0.0179	0.0047	0.0115	73.60	35.75
0005G	5	x	x	x	x	x	x	x	x	x	x	x
0005H	5	4.6	1.6	6.2	14	24.0	0.0390	0.0131	0.0108	0.0056	72.31	57.25
0005I	5	x	x	x	8	x	x	x	x	x	x	x
<i>0005_sum</i>	<i>5</i>	<i>20.1</i>	<i>5.3</i>	<i>25.4</i>	<i>64.0</i>	<i>108.0</i>	<i>0.1549</i>	<i>0.0825</i>	<i>0.0388</i>	<i>0.0369</i>	<i>372.02</i>	<i>281.72</i>
<i>0005_mean</i>	<i>5</i>	<i>4.0</i>	<i>1.1</i>	<i>5.1</i>	<i>10.7</i>	<i>21.6</i>	<i>0.0310</i>	<i>0.0165</i>	<i>0.0078</i>	<i>0.0074</i>	<i>74.40</i>	<i>56.34</i>
<i>0005_SD</i>	<i>5</i>	<i>0.5</i>	<i>0.4</i>	<i>0.9</i>	<i>3.0</i>	<i>3.4</i>	<i>0.0143</i>	<i>0.0035</i>	<i>0.0031</i>	<i>0.0033</i>	<i>3.75</i>	<i>14.77</i>
0010A	10	4.6	1.6	6.2	14	22.5	0.0642	0.0180	0.0118	0.0056	81.62	68.89
0010B	10	4.6	1.6	6.2	12	22.5	0.0490	0.0278	0.0088	0.0067	82.04	75.90
0010C	10	3.5	0.9	4.4	8	25.5	0.0618	0.0201	0.0121	0.0056	80.42	72.14
0010D	10	x	x	x	x	x	x	x	x	x	x	x
0010E	10	x	x	x	x	x	x	x	x	x	x	x
0010F	10	3.4	0.7	4.1	8	15.5	0.0120	0.0149	0.0036	0.0083	70.00	44.30
0010G	10	x	x	x	x	x	x	x	x	x	x	x
0010H	10	3.2	0.8	4.0	8	14.0	0.0089	0.0132	0.0023	0.0094	74.16	28.79
0010I	10	x	x	x	x	x	x	x	x	x	x	x
<i>0010_sum</i>	<i>10</i>	<i>19.3</i>	<i>5.6</i>	<i>24.9</i>	<i>50.0</i>	<i>100.0</i>	<i>0.1959</i>	<i>0.0940</i>	<i>0.0386</i>	<i>0.0356</i>	<i>388.24</i>	<i>290.01</i>
<i>0010_mean</i>	<i>10</i>	<i>3.9</i>	<i>1.1</i>	<i>5.0</i>	<i>10.0</i>	<i>20.0</i>	<i>0.0392</i>	<i>0.0188</i>	<i>0.0077</i>	<i>0.0071</i>	<i>77.65</i>	<i>58.00</i>
<i>0010_SD</i>	<i>10</i>	<i>0.7</i>	<i>0.4</i>	<i>1.1</i>	<i>2.8</i>	<i>5.0</i>	<i>0.0269</i>	<i>0.0057</i>	<i>0.0046</i>	<i>0.0017</i>	<i>5.33</i>	<i>20.49</i>
0025A	25	5.1	1.8	6.9	14	21.0	0.0790	0.0312	0.0114	0.0061	85.57	80.45
0025B	25	5.0	1.7	6.7	14	20.5	0.0581	0.0246	0.0101	0.0047	82.62	80.89
0025C	25	4.8	1.5	6.3	13	20.0	0.0551	0.0196	0.0105	0.0053	80.94	72.96
0025D	25	4.3	1.5	5.8	12	18.0	0.0246	0.0213	0.0055	0.0092	77.64	56.81
0025E	25	4.8	1.7	6.5	12	20.5	0.0336	0.0139	0.0099	0.0058	70.54	58.27
0025F	25	4.7	1.1	5.8	14	22.5	0.0364	0.0260	0.0108	0.0067	70.33	74.23
0025G	25	4.6	1.7	6.3	11	20.5	0.0209	0.0095	0.0075	0.0042	64.11	55.79
0025H	25	x	x	x	x	x	x	x	x	x	x	x
0025I	25	4.6	1.4	6.0	14	22.5	0.0296	0.0165	0.0099	0.0059	66.55	64.24
<i>0025_sum</i>	<i>25</i>	<i>37.9</i>	<i>12.4</i>	<i>50.3</i>	<i>104.0</i>	<i>165.5</i>	<i>0.3373</i>	<i>0.1626</i>	<i>0.0756</i>	<i>0.0479</i>	<i>598.31</i>	<i>543.65</i>
<i>0025_mean</i>	<i>25</i>	<i>4.7</i>	<i>1.6</i>	<i>6.3</i>	<i>13.0</i>	<i>20.7</i>	<i>0.0422</i>	<i>0.0203</i>	<i>0.0095</i>	<i>0.0060</i>	<i>74.79</i>	<i>67.96</i>
<i>0025_SD</i>	<i>25</i>	<i>0.3</i>	<i>0.2</i>	<i>0.4</i>	<i>1.2</i>	<i>1.4</i>	<i>0.0200</i>	<i>0.0070</i>	<i>0.0020</i>	<i>0.0015</i>	<i>7.96</i>	<i>10.47</i>
0050A	50	3.9	1.5	5.4	11	21.5	0.0499	0.0246	0.0083	0.0071	83.37	71.14
0050B	50	4.5	1.6	6.1	14	22.0	0.0672	0.0255	0.0108	0.0050	83.93	80.39
0050C	50	4.5	1.2	5.7	14	23.5	0.0626	0.0304	0.0123	0.0058	80.35	80.92
0050D	50	4.7	1.8	6.5	14	24.5	0.0559	0.0265	0.0106	0.0055	81.04	79.25
0050E	50	4.5	1.3	5.8	13	21.5	0.0427	0.0231	0.0094	0.0048	77.99	79.22
0050F	50	4.9	1.7	6.6	14	22.5	0.0456	0.0234	0.0114	0.0051	75.00	78.21
0050G	50	3.9	1.1	5.0	x	17.5	0.0157	0.0196	0.0048	0.0104	69.43	46.94
0050H	50	4.7	1.5	6.2	14	21.0	0.0370	0.0194	0.0098	0.0045	73.51	76.80
0050I	50	x	x	x	x	x	x	x	x	x	x	x
<i>0050_sum</i>	<i>50</i>	<i>35.6</i>	<i>11.7</i>	<i>47.3</i>	<i>94.0</i>	<i>174.0</i>	<i>0.3766</i>	<i>0.1925</i>	<i>0.0774</i>	<i>0.0482</i>	<i>624.61</i>	<i>592.87</i>
<i>0050_mean</i>	<i>50</i>	<i>4.5</i>	<i>1.5</i>	<i>5.9</i>	<i>13.4</i>	<i>21.8</i>	<i>0.0471</i>	<i>0.0241</i>	<i>0.0097</i>	<i>0.0060</i>	<i>78.08</i>	<i>74.11</i>
<i>0050_SD</i>	<i>50</i>	<i>0.4</i>	<i>0.2</i>	<i>0.5</i>	<i>1.1</i>	<i>2.1</i>	<i>0.0162</i>	<i>0.0036</i>	<i>0.0023</i>	<i>0.0019</i>	<i>5.09</i>	<i>11.40</i>
0100A	100	4.1	2.1	6.2	14	11.0	0.0418	0.0209	0.0090	0.0043	78.47	79.43
0100B	100	4.0	1.3	5.3	14	10.5	0.0293	0.0335	0.0065	0.0107	77.82	68.06
0100C	100	3.5	1.2	4.7	11	8.0	0.0262	0.0210	0.0062	0.0085	76.34	59.52
0100D	100	4.2	1.4	5.6	14	12.0	0.0192	0.0224	0.0061	0.0044	68.23	80.36
0100E	100	4.3	1.3	5.6	14	12.0	0.0359	0.0201	0.0111	0.0054	69.08	73.13
0100F	100	2.8	0.9	3.7	x	7.0	0.0127	0.0194	0.0032	0.0032	74.80	83.51
0100G	100	4.5	1.7	6.2	13	11.0	0.0121	0.0203	0.0048	0.0085	60.33	58.13
0100H	100	x	x	x	x	x	x	x	x	x	x	x
0100I	100	x	x	x	x	x	x	x	x	x	x	x
<i>0100_sum</i>	<i>100</i>	<i>27.4</i>	<i>9.9</i>	<i>37.3</i>	<i>80.0</i>	<i>71.5</i>	<i>0.1772</i>	<i>0.1576</i>	<i>0.0469</i>	<i>0.0450</i>	<i>505.06</i>	<i>502.13</i>
<i>0100_mean</i>	<i>100</i>	<i>3.9</i>	<i>1.4</i>	<i>5.3</i>	<i>13.3</i>	<i>10.2</i>	<i>0.0253</i>	<i>0.0225</i>	<i>0.0067</i>	<i>0.0064</i>	<i>72.15</i>	<i>71.73</i>
<i>0100_SD</i>	<i>100</i>	<i>0.6</i>	<i>0.4</i>	<i>0.9</i>	<i>1.2</i>	<i>2.0</i>	<i>0.0113</i>	<i>0.0049</i>	<i>0.0026</i>	<i>0.0028</i>	<i>6.60</i>	<i>10.18</i>

Table A.44.: A3 plant growth data for Na_2SeO_4 II (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	5.3	1.4	6.7	13	18.0	0.0605	0.0290	0.0089	0.0054	85.29	81.38
0250B	250	4.9	1.5	6.4	14	21.5	0.0647	0.0331	0.0114	0.0056	82.38	83.08
0250C	250	4.7	1.6	6.3	14	22.0	0.0504	0.0324	0.0115	0.0058	77.18	82.10
0250D	250	4.3	1.1	5.4	11	20.5	0.0341	0.0274	0.0074	0.0041	78.30	85.04
0250E	250	3.2	0.8	4.0	10	17.5	0.0256	0.0169	0.0059	0.0030	76.95	82.25
0250F	250	5.5	2.2	7.7	9	14.5	0.0132	0.0226	0.0032	0.0119	75.76	47.35
0250G	250	5.6	1.5	7.1	11	21.5	0.0180	0.0140	0.0060	0.0084	66.67	40.00
0250H	250	5.0	1.9	6.9	12	18.5	0.0210	0.0125	0.0074	0.0039	64.76	68.80
0250I	250	3.3	0.8	4.1	9	17.0	0.0122	0.0084	0.0060	0.0029	50.82	65.48
0250_sum	250	41.8	12.8	54.6	103.0	171.0	0.2997	0.1963	0.0677	0.0510	658.11	635.47
0250_mean	250	4.6	1.4	6.1	11.4	19.0	0.0333	0.0218	0.0075	0.0057	73.12	70.61
0250_SD	250	0.9	0.5	1.3	1.9	2.5	0.0203	0.0092	0.0027	0.0029	10.65	16.79
0500A	500	5.4	1.9	7.3	13	21.0	0.0504	0.0326	0.0105	0.0056	79.17	82.82
0500B	500	4.5	1.7	6.2	1	23.5	0.0392	0.0361	0.0110	0.0059	71.94	83.66
0500C	500	3.2	0.4	3.6	10	22.5	0.0356	0.0342	0.0086	0.0058	75.84	83.04
0500D	500	4.5	1.3	5.8	14	21.5	0.0382	0.0325	0.0100	0.0049	73.82	84.92
0500E	500	4.1	1.1	5.2	10	19.0	0.0267	0.0265	0.0068	0.0056	74.53	78.87
0500F	500	4.5	1.6	6.1	13	20.0	0.0190	0.0232	0.0048	0.0118	74.74	49.14
0500G	500	4.8	1.2	6.0	13	20.0	0.2400	0.0187	0.0091	0.0049	96.21	73.80
0500H	500	4.4	1.2	5.6	12	23.0	0.0223	0.0115	0.0108	0.0057	51.57	50.43
0500I	500	4.7	1.8	6.5	13	23.0	0.0206	0.0068	0.0096	0.0048	53.40	29.41
0500_sum	500	40.1	12.2	52.3	99.0	193.5	0.4920	0.2221	0.0812	0.0550	651.21	616.09
0500_mean	500	4.5	1.4	5.8	11.0	21.5	0.0547	0.0247	0.0090	0.0061	72.36	68.45
0500_SD	500	0.6	0.5	1.0	4.0	1.6	0.0703	0.0105	0.0020	0.0022	13.38	20.25
1000A	1000	4.9	1.6	6.5	13	16.0	0.0647	0.0419	0.0070	0.0083	89.18	80.19
1000B	1000	4.7	1.6	6.3	12	17.5	0.0347	0.0360	0.0025	0.0043	92.80	88.06
1000C	1000	4.5	1.4	5.9	12	18.0	0.0465	0.0388	0.0091	0.0068	80.43	82.47
1000D	1000	3.6	1.2	4.8	9	13.5	0.0149	0.0305	0.0099	0.0076	33.56	75.08
1000E	1000	4.1	1.3	5.4	10	15.5	0.0380	0.0302	0.0035	0.0135	90.79	55.30
1000F	1000	4.5	1.6	6.1	13	18.0	0.0333	0.0225	0.0105	0.0076	68.47	66.22
1000G	1000	3.5	1.2	4.7	11	11.0	0.0081	0.0056	0.0078	0.0099	3.70	-76.79
1000H	1000	x	x	x	x	x	x	x	x	x	x	x
1000I	1000	2.8	1.0	3.8	10	13.5	0.0186	0.0127	0.0119	0.0068	36.02	46.46
1000_sum	1000	32.6	10.9	43.5	90.0	123.0	0.2588	0.2182	0.0622	0.0648	494.95	416.99
1000_mean	1000	4.1	1.4	5.4	11.3	15.4	0.0324	0.0273	0.0078	0.0081	61.87	52.12
1000_SD	1000	0.7	0.2	0.9	1.5	2.5	0.0184	0.0128	0.0033	0.0027	33.34	53.97
2500A	2500	2.9	0.8	3.7	8	12.0	0.0157	0.0231	0.0029	0.0113	81.53	51.08
2500B	2500	4.6	1.4	6.0	11	18.5	0.0384	0.0105	0.0063	0.0034	83.59	67.62
2500C	2500	5.3	1.8	7.1	14	22.0	0.0544	0.0332	0.0129	0.0072	76.29	78.31
2500D	2500	x	x	x	x	x	x	x	x	x	x	x
2500E	2500	2.7	0.7	3.4	14	18.0	0.0261	0.0265	0.0069	0.0115	73.56	56.60
2500F	2500	2.7	0.8	3.5	10	21.5	0.0376	0.0184	0.0097	0.0047	74.20	74.46
2500G	2500	4.4	1.4	5.8	13	19.0	0.0221	0.0261	0.0060	0.0130	72.85	50.19
2500H	2500	4.7	1.5	6.2	14	22.0	0.0363	0.0086	0.0124	0.0065	65.84	24.42
2500I	2500	x	x	x	x	x	x	x	x	x	x	x
2500_sum	2500	27.3	8.4	35.7	84.0	133.0	0.2306	0.1464	0.0571	0.0576	527.87	402.69
2500_mean	2500	3.9	1.2	5.1	12.0	19.0	0.0329	0.0209	0.0082	0.0082	75.41	57.53
2500_SD	2500	1.1	0.4	1.5	2.4	3.5	0.0128	0.0089	0.0037	0.0037	5.89	18.32

Table A.45.: A3 plant growth data for Na_2SeO_4 III (Planting Date: 16.01.2014)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0000A	0	4.2	1.3	5.5	14	19.5	0.0224	0.0196	0.0049	0.0048	78.13	75.51
0000B	0	x	x	x	x	x	x	x	x	x	x	x
0000C	0	x	x	x	x	x	x	x	x	x	x	x
0000D	0	x	x	x	x	x	x	x	x	x	x	x
0000E	0	x	x	x	x	x	x	x	x	x	x	x
0000F	0	x	x	x	x	x	x	x	x	x	x	x
0000G	0	3.9	0.9	4.8	12	23.0	0.0488	0.0183	0.0136	0.0057	72.13	68.85
0000H	0	4.1	1.1	5.2	12	26.5	0.0429	0.0318	0.0096	0.0110	77.62	65.41
0000I	0	5.4	1.9	7.3	7	30.0	0.0883	0.0226	0.0198	0.0082	77.58	63.72
<i>0000_sum</i>	<i>0</i>	<i>17.6</i>	<i>5.2</i>	<i>22.8</i>	<i>45.0</i>	<i>99.0</i>	<i>0.2024</i>	<i>0.0923</i>	<i>0.0479</i>	<i>0.0297</i>	<i>305.45</i>	<i>273.49</i>
<i>0000_mean</i>	<i>0</i>	<i>4.4</i>	<i>1.3</i>	<i>5.7</i>	<i>11.3</i>	<i>24.8</i>	<i>0.0506</i>	<i>0.0231</i>	<i>0.0120</i>	<i>0.0074</i>	<i>76.36</i>	<i>68.37</i>
<i>0000_SD</i>	<i>0</i>	<i>0.7</i>	<i>0.4</i>	<i>1.1</i>	<i>3.0</i>	<i>4.5</i>	<i>0.0276</i>	<i>0.0061</i>	<i>0.0063</i>	<i>0.0028</i>	<i>2.83</i>	<i>5.22</i>
0005A	5	4.5	1.5	6.0	12	29.0	0.0691	0.0235	0.0133	0.0070	80.75	70.21
0005B	5	3.6	0.8	4.4	7	22.0	0.0254	0.0211	0.0081	0.0044	68.11	79.15
0005C	5	4.9	1.4	6.3	7	28.0	0.0782	0.0328	0.0167	0.0087	78.64	73.48
0005D	5	x	x	x	x	x	x	x	x	x	x	x
0005E	5	3.5	1.1	4.6	12	27.0	0.0783	0.0325	0.0191	0.0110	75.61	66.15
0005F	5	x	x	x	x	x	x	x	x	x	x	x
0005G	5	5.0	1.3	6.3	7	29.0	0.0692	0.0284	0.0142	0.0062	79.48	78.17
0005H	5	4.1	1.4	5.5	12	20.0	0.0324	0.0161	0.0081	0.0045	75.00	72.05
0005I	5	3.6	1.0	4.6	14	19.0	0.0260	0.0274	0.0050	0.0139	80.77	49.27
<i>0005_sum</i>	<i>5</i>	<i>29.2</i>	<i>8.5</i>	<i>37.7</i>	<i>71.0</i>	<i>174.0</i>	<i>0.3786</i>	<i>0.1818</i>	<i>0.0845</i>	<i>0.0557</i>	<i>538.36</i>	<i>488.48</i>
<i>0005_mean</i>	<i>5</i>	<i>4.2</i>	<i>1.2</i>	<i>5.4</i>	<i>10.1</i>	<i>24.9</i>	<i>0.0541</i>	<i>0.0260</i>	<i>0.0121</i>	<i>0.0080</i>	<i>76.91</i>	<i>69.78</i>
<i>0005_SD</i>	<i>5</i>	<i>0.6</i>	<i>0.3</i>	<i>0.8</i>	<i>3.0</i>	<i>4.4</i>	<i>0.0248</i>	<i>0.0061</i>	<i>0.0051</i>	<i>0.0035</i>	<i>4.51</i>	<i>10.09</i>
0010A	10	4.9	1.6	6.5	7	28.0	0.0687	0.0246	0.0139	0.0069	79.77	71.95
0010B	10	x	x	x	x	x	x	x	x	x	x	x
0010C	10	3.8	1.1	4.9	12	19.0	0.0387	0.0343	0.0069	0.0116	82.17	66.18
0010D	10	x	x	x	x	x	x	x	x	x	x	x
0010E	10	5.1	1.5	6.6	7	28.0	0.0801	0.0401	0.0171	0.0079	78.65	80.30
0010F	10	2.5	0.7	3.2	12	26.0	0.0580	0.0324	0.0111	0.0068	80.86	79.01
0010G	10	x	x	x	x	x	x	x	x	x	x	x
0010H	10	5.9	1.6	7.5	9	22.0	0.0494	0.0208	0.0120	0.0063	75.71	69.71
0010I	10	x	x	x	14	x	x	x	x	x	x	x
<i>0010_sum</i>	<i>10</i>	<i>22.2</i>	<i>6.5</i>	<i>28.7</i>	<i>61.0</i>	<i>123.0</i>	<i>0.2949</i>	<i>0.1522</i>	<i>0.0610</i>	<i>0.0395</i>	<i>397.16</i>	<i>367.16</i>
<i>0010_mean</i>	<i>10</i>	<i>4.4</i>	<i>1.3</i>	<i>5.7</i>	<i>10.2</i>	<i>24.6</i>	<i>0.0590</i>	<i>0.0304</i>	<i>0.0122</i>	<i>0.0079</i>	<i>79.43</i>	<i>73.43</i>
<i>0010_SD</i>	<i>10</i>	<i>1.3</i>	<i>0.4</i>	<i>1.7</i>	<i>2.9</i>	<i>4.0</i>	<i>0.0162</i>	<i>0.0077</i>	<i>0.0037</i>	<i>0.0021</i>	<i>2.46</i>	<i>6.06</i>
0025A	25	x	x	x	x	x	x	x	x	x	x	x
0025B	25	x	x	x	x	x	x	x	x	x	x	x
0025C	25	x	x	x	x	x	x	x	x	x	x	x
0025D	25	x	x	x	x	x	x	x	x	x	x	x
0025E	25	3.8	0.9	4.7	7	30.0	0.0991	0.0355	0.0163	0.0079	83.55	77.75
0025F	25	5.1	1.4	6.5	9	29.0	0.0589	0.0190	0.0152	0.0064	74.19	66.32
0025G	25	x	x	x	x	x	x	x	x	x	x	x
0025H	25	5.9	1.8	7.7	9	30.5	0.0917	0.0314	0.0159	0.0064	82.66	79.62
0025I	25	4.9	1.8	6.7	7	21.5	0.0312	0.0318	0.0084	0.0154	73.08	51.57
<i>0025_sum</i>	<i>25</i>	<i>19.7</i>	<i>5.9</i>	<i>25.6</i>	<i>32.0</i>	<i>111.0</i>	<i>0.2809</i>	<i>0.1177</i>	<i>0.0558</i>	<i>0.0361</i>	<i>313.48</i>	<i>275.25</i>
<i>0025_mean</i>	<i>25</i>	<i>4.9</i>	<i>1.5</i>	<i>6.4</i>	<i>8.0</i>	<i>27.8</i>	<i>0.0702</i>	<i>0.0294</i>	<i>0.0140</i>	<i>0.0090</i>	<i>78.37</i>	<i>68.81</i>
<i>0025_SD</i>	<i>25</i>	<i>0.9</i>	<i>0.4</i>	<i>1.2</i>	<i>1.2</i>	<i>4.2</i>	<i>0.0313</i>	<i>0.0072</i>	<i>0.0037</i>	<i>0.0043</i>	<i>5.50</i>	<i>12.91</i>
0050A	50	3.9	1.4	5.3	12	27.0	0.0719	0.0301	0.0173	0.0065	75.94	78.41
0050B	50	x	x	x	x	x	x	x	x	x	x	x
0050C	50	4.8	1.7	6.5	12	23.0	0.0514	0.0226	0.0088	0.0043	82.88	80.97
0050D	50	4.6	1.6	6.2	12	19.5	0.0329	0.0261	0.0063	0.0037	80.85	85.82
0050E	50	3.7	1.4	5.1	12	16.0	0.0175	0.0133	0.0041	0.0026	76.57	80.45
0050F	50	5.4	2.0	7.4	7	21.5	0.0496	0.0184	0.0108	0.0056	78.23	69.57
0050G	50	x	x	x	x	x	x	x	x	x	x	x
0050H	50	x	x	x	x	x	x	x	x	x	x	x
0050I	50	x	x	x	x	x	x	x	x	x	x	x
<i>0050_sum</i>	<i>50</i>	<i>22.4</i>	<i>8.1</i>	<i>30.5</i>	<i>55.0</i>	<i>107.0</i>	<i>0.2233</i>	<i>0.1105</i>	<i>0.0473</i>	<i>0.0227</i>	<i>394.47</i>	<i>395.22</i>
<i>0050_mean</i>	<i>50</i>	<i>4.5</i>	<i>1.6</i>	<i>6.1</i>	<i>11.0</i>	<i>21.4</i>	<i>0.0447</i>	<i>0.0221</i>	<i>0.0095</i>	<i>0.0045</i>	<i>78.89</i>	<i>79.04</i>
<i>0050_SD</i>	<i>50</i>	<i>0.7</i>	<i>0.2</i>	<i>0.9</i>	<i>2.2</i>	<i>4.1</i>	<i>0.0205</i>	<i>0.0065</i>	<i>0.0051</i>	<i>0.0015</i>	<i>2.93</i>	<i>5.96</i>
0100A	100	x	x	x	x	x	x	x	x	x	x	x
0100B	100	x	x	x	x	x	x	x	x	x	x	x
0100C	100	x	x	x	x	x	x	x	x	x	x	x
0100D	100	x	x	x	x	x	x	x	x	x	x	x
0100E	100	x	x	x	x	x	x	x	x	x	x	x
0100F	100	x	x	x	x	x	x	x	x	x	x	x
0100G	100	4.8	1.4	6.2	12	19.0	0.0287	0.0195	0.0059	0.0065	79.44	66.67
0100H	100	x	x	x	x	x	x	x	x	x	x	x
0100I	100	4.3	1.6	5.9	7	28.0	0.0555	0.0191	0.0127	0.0056	77.12	70.68
<i>0100_sum</i>	<i>100</i>	<i>9.1</i>	<i>3.0</i>	<i>12.1</i>	<i>19.0</i>	<i>47.0</i>	<i>0.0842</i>	<i>0.0386</i>	<i>0.0186</i>	<i>0.0121</i>	<i>156.56</i>	<i>137.35</i>
<i>0100_mean</i>	<i>100</i>	<i>4.6</i>	<i>1.5</i>	<i>6.1</i>	<i>9.5</i>	<i>23.5</i>	<i>0.0421</i>	<i>0.0193</i>	<i>0.0093</i>	<i>0.0061</i>	<i>78.28</i>	<i>68.67</i>
<i>0100_SD</i>	<i>100</i>	<i>0.4</i>	<i>0.1</i>	<i>0.2</i>	<i>3.5</i>	<i>6.4</i>	<i>0.0190</i>	<i>0.0003</i>	<i>0.0048</i>	<i>0.0006</i>	<i>1.64</i>	<i>2.84</i>

Table A.46.: A3 plant growth data for Na_2SeO_4 III (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	x	x	x	x	x	x	x	x	x	x	x
0250B	250	3.6	1.1	4.7	12	20.5	0.0389	0.0217	0.0113	0.0067	70.95	69.12
0250C	250	x	x	x	x	x	x	x	x	x	x	x
0250D	250	x	x	x	x	x	x	x	x	x	x	x
0250E	250	4.5	1.3	5.8	12	29.0	0.0548	0.0275	0.0135	0.0066	75.36	76.00
0250F	250	x	x	x	x	x	x	x	x	x	x	x
0250G	250	x	x	x	x	x	x	x	x	x	x	x
0250H	250	x	x	x	x	x	x	x	x	x	x	x
0250I	250	5.2	1.6	6.8	9	26.5	0.0686	0.0285	0.0165	0.0094	75.95	67.02
<i>0250_sum</i>	<i>250</i>	<i>13.3</i>	<i>4.0</i>	<i>17.3</i>	<i>33.0</i>	<i>76.0</i>	<i>0.1623</i>	<i>0.0777</i>	<i>0.0413</i>	<i>0.0227</i>	<i>222.26</i>	<i>212.14</i>
<i>0250_mean</i>	<i>250</i>	<i>4.4</i>	<i>1.3</i>	<i>5.8</i>	<i>11.0</i>	<i>25.3</i>	<i>0.0541</i>	<i>0.0259</i>	<i>0.0138</i>	<i>0.0076</i>	<i>74.09</i>	<i>70.71</i>
<i>0250_SD</i>	<i>250</i>	<i>0.8</i>	<i>0.3</i>	<i>1.1</i>	<i>1.7</i>	<i>4.4</i>	<i>0.0149</i>	<i>0.0037</i>	<i>0.0026</i>	<i>0.0016</i>	<i>2.73</i>	<i>4.70</i>
0500A	500	4.1	1.3	5.4	12	17.0	0.0204	0.0241	0.0044	0.0168	78.43	30.29
0500B	500	x	x	x	x	x	x	x	x	x	x	x
0500C	500	x	x	x	x	x	x	x	x	x	x	x
0500D	500	2.3	0.7	3.0	12	19.0	0.0471	0.0165	0.0085	0.0059	81.95	64.24
0500E	500	x	x	x	x	x	x	x	x	x	x	x
0500F	500	x	x	x	x	x	x	x	x	x	x	x
0500G	500	x	x	x	x	x	x	x	x	x	x	x
0500H	500	5.5	2.1	7.6	7	28.5	0.0674	0.0144	0.0160	0.0061	76.26	57.64
0500I	500	x	x	x	x	x	x	x	x	x	x	x
<i>0500_sum</i>	<i>500</i>	<i>11.9</i>	<i>4.1</i>	<i>16.0</i>	<i>31.0</i>	<i>64.5</i>	<i>0.1349</i>	<i>0.0550</i>	<i>0.0289</i>	<i>0.0288</i>	<i>236.65</i>	<i>152.17</i>
<i>0500_mean</i>	<i>500</i>	<i>4.0</i>	<i>1.4</i>	<i>5.3</i>	<i>10.3</i>	<i>21.5</i>	<i>0.0450</i>	<i>0.0183</i>	<i>0.0096</i>	<i>0.0096</i>	<i>78.88</i>	<i>50.72</i>
<i>0500_SD</i>	<i>500</i>	<i>1.6</i>	<i>0.7</i>	<i>2.3</i>	<i>2.9</i>	<i>6.1</i>	<i>0.0236</i>	<i>0.0051</i>	<i>0.0059</i>	<i>0.0062</i>	<i>2.87</i>	<i>18.00</i>
1000A	1000	5.4	2.1	7.5	7	21.0	0.0513	0.0204	0.0129	0.0063	74.85	69.12
1000B	1000	x	x	x	x	x	x	x	x	x	x	x
1000C	1000	x	x	x	x	x	x	x	x	x	x	x
1000D	1000	x	x	x	x	x	x	x	x	x	x	x
1000E	1000	6.1	1.9	8.0	7	26.0	0.0766	0.0212	0.0198	0.0090	74.15	57.55
1000F	1000	3.1	1.0	4.1	12	13.5	0.0188	0.0299	0.0043	0.0076	77.13	74.58
1000G	1000	x	x	x	x	x	x	x	x	x	x	x
1000H	1000	5.4	1.1	6.5	9	21.5	0.0644	0.0108	0.0113	0.0048	82.45	55.56
1000I	1000	x	x	x	x	x	x	x	x	x	x	x
<i>1000_sum</i>	<i>1000</i>	<i>20.0</i>	<i>6.1</i>	<i>26.1</i>	<i>35.0</i>	<i>82.0</i>	<i>0.2111</i>	<i>0.0823</i>	<i>0.0483</i>	<i>0.0277</i>	<i>308.59</i>	<i>256.80</i>
<i>1000_mean</i>	<i>1000</i>	<i>5.0</i>	<i>1.5</i>	<i>6.5</i>	<i>8.8</i>	<i>20.5</i>	<i>0.0528</i>	<i>0.0206</i>	<i>0.0121</i>	<i>0.0069</i>	<i>77.15</i>	<i>64.20</i>
<i>1000_SD</i>	<i>1000</i>	<i>1.3</i>	<i>0.6</i>	<i>1.7</i>	<i>2.4</i>	<i>5.2</i>	<i>0.0249</i>	<i>0.0078</i>	<i>0.0064</i>	<i>0.0018</i>	<i>3.76</i>	<i>9.15</i>
2500A	2500	3.0	1.2	4.2	12	10.5	0.0133	0.0227	0.0033	0.0102	75.19	55.07
2500B	2500	x	x	x	x	x	x	x	x	x	x	x
2500C	2500	x	x	x	x	x	x	x	x	x	x	x
2500D	2500	x	x	x	x	x	x	x	x	x	x	x
2500E	2500	3.2	1.3	4.5	14	13.5	0.0257	0.0358	0.0053	0.0233	79.38	34.92
2500F	2500	x	x	x	x	x	x	x	x	x	x	x
2500G	2500	x	x	x	x	x	x	x	x	x	x	x
2500H	2500	x	x	x	x	x	x	x	x	x	x	x
2500I	2500	3.3	1.2	4.5	14	13.0	0.0275	0.0195	0.0064	0.0050	76.73	74.36
<i>2500_sum</i>	<i>2500</i>	<i>9.5</i>	<i>3.7</i>	<i>13.2</i>	<i>40.0</i>	<i>37.0</i>	<i>0.0665</i>	<i>0.0780</i>	<i>0.0150</i>	<i>0.0385</i>	<i>231.29</i>	<i>164.34</i>
<i>2500_mean</i>	<i>2500</i>	<i>3.2</i>	<i>1.2</i>	<i>4.4</i>	<i>13.3</i>	<i>12.3</i>	<i>0.0222</i>	<i>0.0260</i>	<i>0.0050</i>	<i>0.0128</i>	<i>77.10</i>	<i>54.78</i>
<i>2500_SD</i>	<i>2500</i>	<i>0.2</i>	<i>0.1</i>	<i>0.2</i>	<i>1.2</i>	<i>1.6</i>	<i>0.0077</i>	<i>0.0086</i>	<i>0.0016</i>	<i>0.0094</i>	<i>2.12</i>	<i>19.72</i>

A.3.2. A3 Plant Se content data

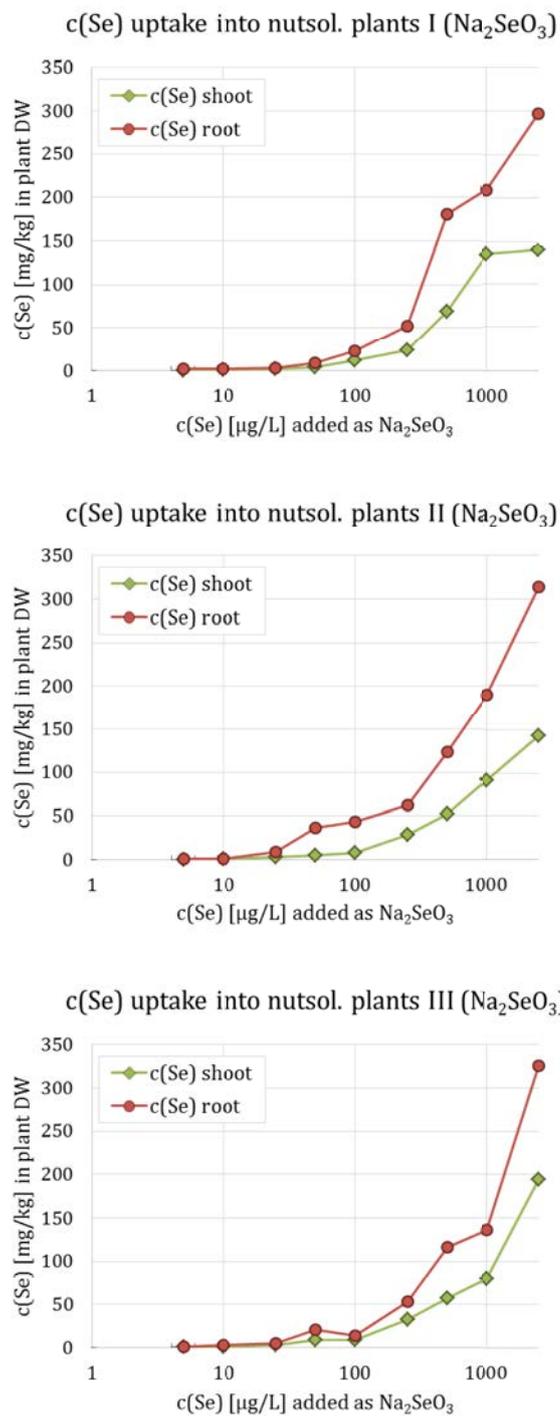


Figure A.16.: A3 plots of Se content in each of the three experimental runs for selenite and selenate

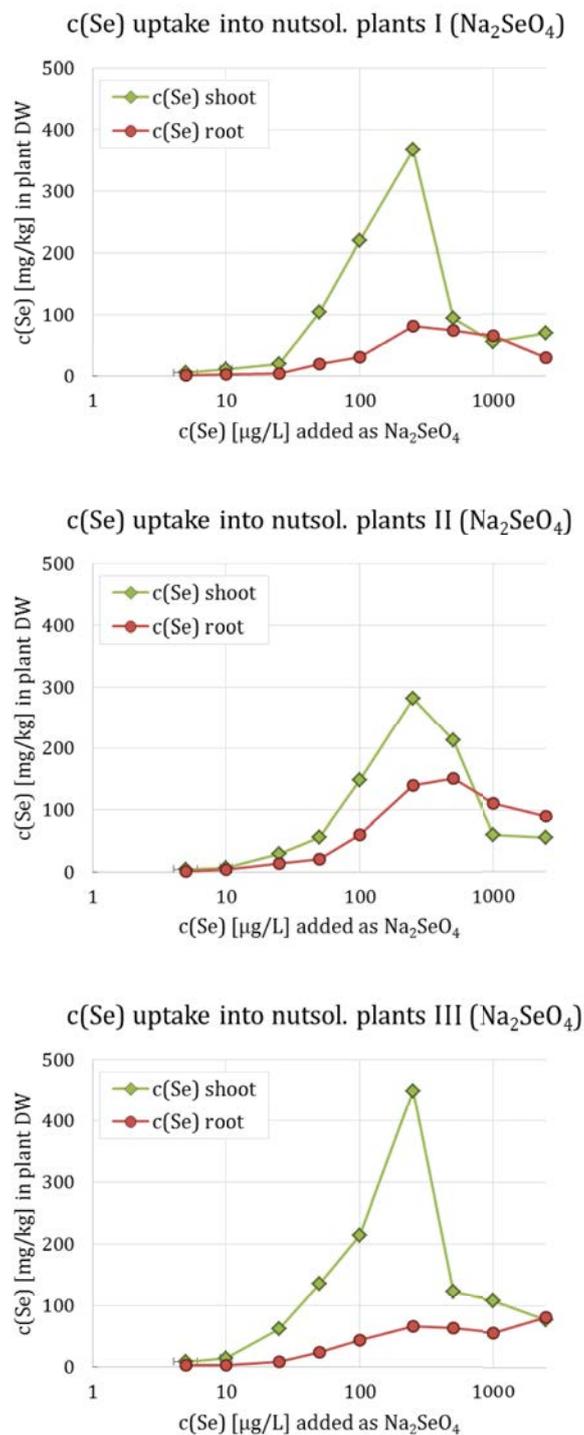


Figure A.17.: A3 plots of Se content in each of the three experimental runs for selenate

Table A.47.: A3 Se content of all three experimental runs for Na₂SeO₃

c(Se) [µg/L]				FIAS-Results				c(Se) dry weight (DW)			
	dig. weight shoot [g]	dig. weight root [g]	dig. volume [L]	c(Se) shoot [µg/L]	c(Se) shoot SD	c(Se) root [µg/L]	c(Se) root SD	c(Se) shoot [mg/kg]	c(Se) shoot SD	c(Se) root [mg/kg]	c(Se) root SD
	[± 0.0001]	[± 0.0001]	[± 0.0001]								
Nutrient-Solution-Se (Na ₂ SeO ₃) Planting Date: 10.01.2013											
0	0.05588	0.02962	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.05979	0.03284	0.014	2.34	0.29	3.42	0.12	0.39	0.07	1.46	0.05
10	0.08288	0.04893	0.010	8.84	0.53	10.00	1.12	1.07	0.06	2.04	0.23
25	0.04770	0.03413	0.010	8.15	0.49	11.41	0.34	1.71	0.10	3.34	0.10
50	0.06559	0.02905	0.010	25.74	4.59	25.94	3.67	3.92	0.70	8.93	1.26
100	0.07303	0.03477	0.010	84.39	8.66	78.94	7.89	11.56	1.19	22.70	2.27
250	0.07122	0.03289	0.010	171.11	13.23	171.59	6.37	24.03	1.86	52.17	1.94
500	0.04119	0.02289	0.010	285.50	7.79	414.17	6.71	69.31	1.89	180.94	2.93
1000	0.04491	0.03586	0.010	604.29	2.92	749.31	13.96	134.55	0.65	208.96	3.89
2500	0.06041	0.04224	0.010	843.03	19.01	1253.52	8.03	139.55	3.15	296.76	1.90
Nutrient-Solution-Se (Na ₂ SeO ₃) Planting Date: 02.10.2013											
0	0.07159	0.03234	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.07445	0.03922	0.010	1.86	0.57	17.67	0.79	0.25	0.08	0.45	0.20
10	0.06496	0.04158	0.010	3.24	0.69	3.98	0.45	0.50	0.11	0.96	0.11
25	0.06426	0.02975	0.010	16.12	0.89	25.18	0.82	2.51	0.14	8.47	0.27
50	0.07151	0.03656	0.010	31.43	1.27	131.80	7.99	4.40	0.18	36.05	2.19
100	0.06312	0.07376	0.010	51.02	1.53	320.67	7.87	8.08	0.24	43.47	1.07
250	0.07122	0.03398	0.010	206.26	8.71	212.37	5.47	28.96	1.22	62.50	1.61
500	0.07233	0.03486	0.010	376.11	22.92	428.72	9.72	52.00	3.17	122.98	2.79
1000	0.05963	0.03967	0.010	545.33	14.54	751.82	14.30	91.45	2.44	189.52	3.60
2500	0.06806	0.04118	0.010	976.07	31.11	1290.56	41.65	143.41	4.57	313.40	10.11
Nutrient-Solution-Se (Na ₂ SeO ₃) Planting Date: 21.11.2013											
0	0.08172	0.03466	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.05351	0.03598	0.010	3.20	0.25	4.68	1.00	0.60	0.05	1.30	0.28
10	0.06683	0.03935	0.010	8.93	0.67	11.01	0.63	1.34	0.10	2.80	0.16
25	0.03582	0.02748	0.010	10.16	0.61	13.00	1.35	2.84	0.17	4.73	0.49
50	0.05250	0.03453	0.010	44.13	1.43	72.75	0.95	8.41	0.27	21.07	0.28
100	0.02268	0.02051	0.010	20.63	0.76	28.59	0.71	9.10	0.33	13.94	0.35
250	0.03487	0.03664	0.010	112.51	4.34	196.77	3.26	32.27	1.25	53.70	0.89
500	0.03078	0.01614	0.010	174.53	2.95	188.00	6.30	56.70	0.96	116.48	3.90
1000	0.02947	0.02439	0.010	234.90	11.46	331.57	11.53	79.71	3.89	135.95	4.73
2500	0.03315	0.02330	0.010	643.07	14.84	759.52	18.98	193.99	4.48	325.98	8.15
Digestion standards											
Standard Sample		dig. weight [g]	dig. volume [L]	c(Se) [µg/L]	c(Se) SD			c(Se) [mg/kg]	c(Se) SD		
dig_Std 2013_02_21 (0-5ppb)		0.10046	0.010	8.91	0.50			0.89	0.05		
dig_Std 2013_02_22 (10-100ppb)		0.10134	0.010	9.14	0.66			0.90	0.06		
dig_Std 2013_02_25 (250-2500ppb)		0.10036	0.010	8.07	0.31			0.80	0.03		
dig_Std 2013_10_29 (0-5ppb)		0.09821	0.010	8.82	1.16			0.90	0.12		
dig_Std 2013_10_30 (10-100ppb)		0.10197	0.010	10.81	0.56			1.06	0.06		
dig_Std 2013_11_04 (250-2500ppb)		0.10064	0.010	10.74	0.68			1.07	0.07		
dig_Std 2014_02_11 (0-25ppb)		0.09940	0.010	12.29	0.43			1.24	0.04		
dig_Std 2014_02_12 (50-500ppb)		0.10321	0.010	10.64	0.94			1.03	0.09		
dig_Std 2014_02_13 (1000-2500ppb)		0.09961	0.010	7.97	0.79			0.80	0.08		

Table A.48.: A3 Se content of all three experimental runs for Na_2SeO_4

c(Se) [µg/L]	FIAS-Results			c(Se) dry weight (DW)							
	dig. weight shoot [g] [± 0.0001]	dig. weight root [g] [± 0.0001]	dig. volume [L] [± 0.0001]	c(Se) shoot [µg/L]	c(Se) shoot SD	c(Se) root [µg/L]	c(Se) root SD	c(Se) shoot [mg/kg]	c(Se) shoot SD	c(Se) root [mg/kg]	c(Se) root SD
Nutrient-Solution-Se (Na_2SeO_4) Planting Date: 22.11.2012											
0	0.06908	0.04384	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.07658	0.04168	0.010	2.21	0.38	0.00	0.00	0.29	0.05	0.00	0.00
10	0.07901	0.03544	0.010	6.23	0.98	1.74	0.22	0.79	0.12	0.49	0.06
25	0.05878	0.02645	0.010	11.33	0.80	3.08	0.45	1.93	0.14	1.17	0.17
50	0.05503	0.01964	0.010	40.56	3.62	6.56	1.42	7.37	0.66	3.34	0.73
100	0.06148	0.03329	0.010	81.74	2.00	15.35	2.17	13.30	0.33	4.61	0.65
250	0.05767	0.03392	0.010	190.48	6.68	61.26	7.92	33.03	1.16	18.06	2.34
500	0.05409	0.02408	0.010	364.47	6.63	94.46	7.40	67.38	1.23	39.23	3.07
1000	0.05849	0.03693	0.010	1121.66	31.43	150.15	10.31	191.77	5.37	40.66	2.79
2500	0.05310	0.02540	0.010	2255.29	70.08	399.43	7.22	424.73	13.20	157.26	2.84
Nutrient-Solution-Se (Na_2SeO_4) Planting Date: 12.09.2013											
0	0.05459	0.05883	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.03958	0.03816	0.010	1.35	0.24	0.00	0.00	0.34	0.06	0.00	0.00
10	0.03896	0.03605	0.010	2.16	0.26	0.58	0.32	0.55	0.07	0.16	0.09
25	0.07574	0.04858	0.010	16.69	2.14	5.74	0.66	2.20	0.28	1.18	0.14
50	0.07963	0.04864	0.010	36.83	0.85	9.94	0.76	4.62	0.11	2.04	0.16
100	0.04805	0.04704	0.010	16.47	0.59	9.21	0.86	3.43	0.12	1.96	0.18
250	0.06877	0.05381	0.010	246.66	7.80	40.82	1.16	35.87	1.13	7.59	0.22
500	0.08231	0.05698	0.010	790.32	22.69	164.93	3.38	96.02	2.76	28.95	0.59
1000	0.06055	0.06360	0.010	1196.31	23.70	541.78	13.38	197.57	3.91	85.19	2.10
2500	0.06576	0.05732	0.010	2969.86	40.86	570.65	23.01	451.62	6.21	99.56	4.01
Nutrient-Solution-Se (Na_2SeO_4) Planting Date: 16.01.2014											
0	0.04609	0.02926	0.010	0.87	0.75	0.14	0.43	0.19	0.16	0.05	0.15
5	0.08144	0.05390	0.010	9.06	0.98	5.81	0.62	1.11	0.12	1.08	0.11
10	0.06141	0.03437	0.010	5.65	0.96	0.00	0.68	0.92	0.16	0.00	0.20
25	0.05407	0.03328	0.010	13.31	0.64	0.00	0.47	2.46	0.12	0.00	0.14
50	0.04453	0.02274	0.010	23.45	2.34	4.81	0.44	5.27	0.53	2.11	0.19
100	0.01834	0.01145	0.010	19.25	2.40	3.78	0.54	10.50	1.31	3.30	0.47
250	0.03929	0.02274	0.010	207.61	8.83	60.20	2.96	52.84	2.25	26.47	1.30
500	0.02867	0.02525	0.010	233.68	3.52	55.41	6.78	81.51	1.23	21.94	2.68
1000	0.04695	0.02835	0.010	862.86	30.62	179.65	15.71	183.78	6.52	63.37	5.54
2500	0.00766	0.04340	0.010	260.19	4.63	768.53	38.47	339.67	6.04	177.08	8.86
Digestion standards											
Standard Sample	dig. weight [g]	dig. volume [L]	c(Se) [µg/L]	c(Se) SD	c(Se) [mg/kg]	c(Se) SD					
dig_Std 2013_02_19 (0-25ppb)	0.09599	0.010	8.90	0.60	0.93	0.06					
dig_Std 2013_02_20 (50-500ppb)	0.10316	0.010	9.64	0.68	0.93	0.07					
dig_Std 2013_02_21 (1000-2500ppb)	0.10046	0.010	8.91	0.50	0.89	0.05					
dig_Std 2013_10_25 (0-25ppb)	0.09944	0.010	8.60	1.07	0.86	0.11					
dig_Std 2013_10_28 (50-500ppb)	0.09948	0.010	10.45	0.89	1.05	0.09					
dig_Std 2013_10_29 (1000-2500ppb)	0.09821	0.010	8.82	1.16	0.90	0.12					
dig_Std 2014_02_14 (0-5ppb)	0.09961	0.010	7.97	0.79	0.80	0.08					
dig_Std 2014_02_17 (10-100ppb)	0.10055	0.010	9.19	0.63	0.91	0.06					
dig_Std 2014_02_18 (250-2500ppb)	0.10035	0.010	9.82	0.77	0.98	0.08					

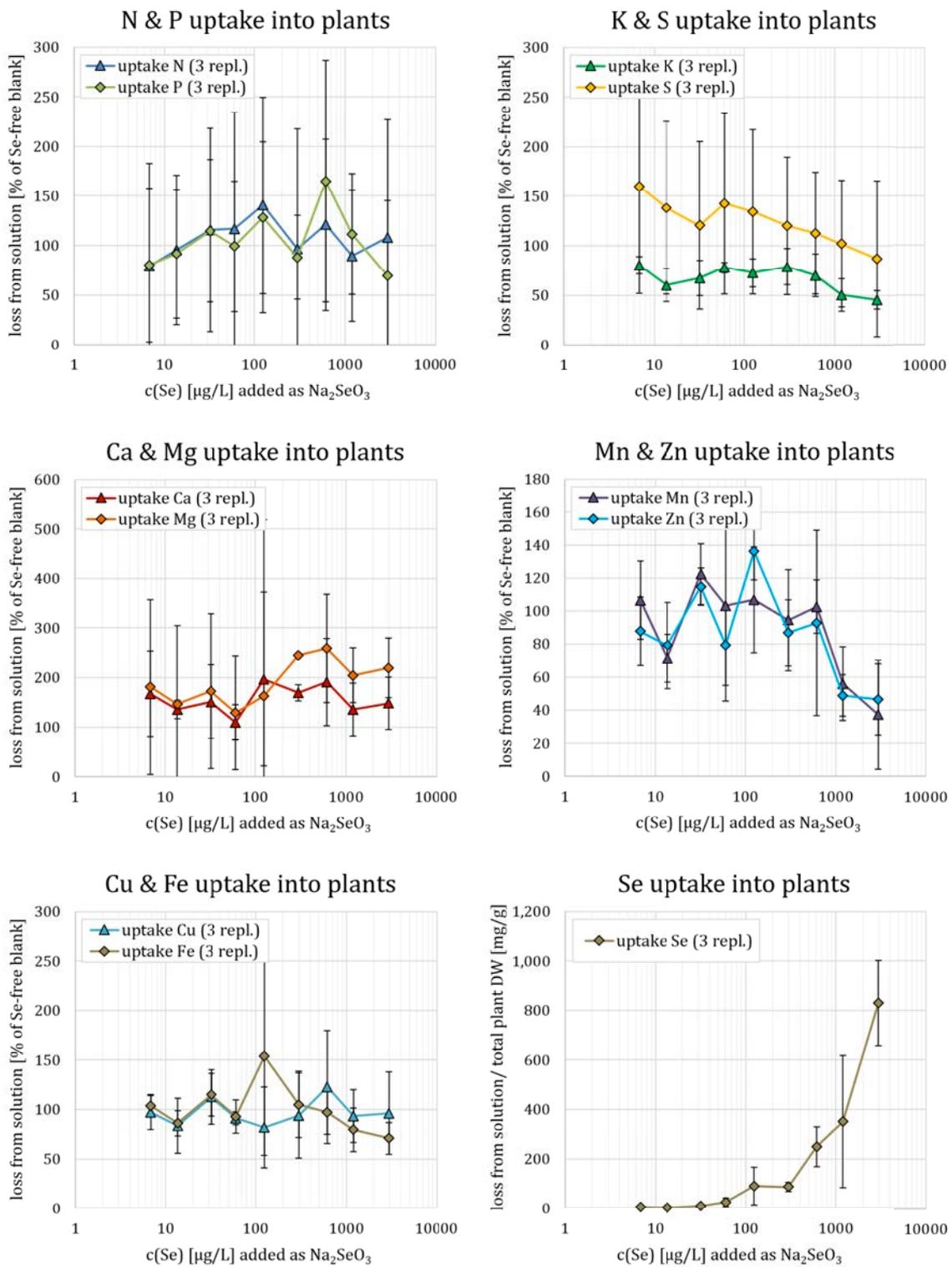
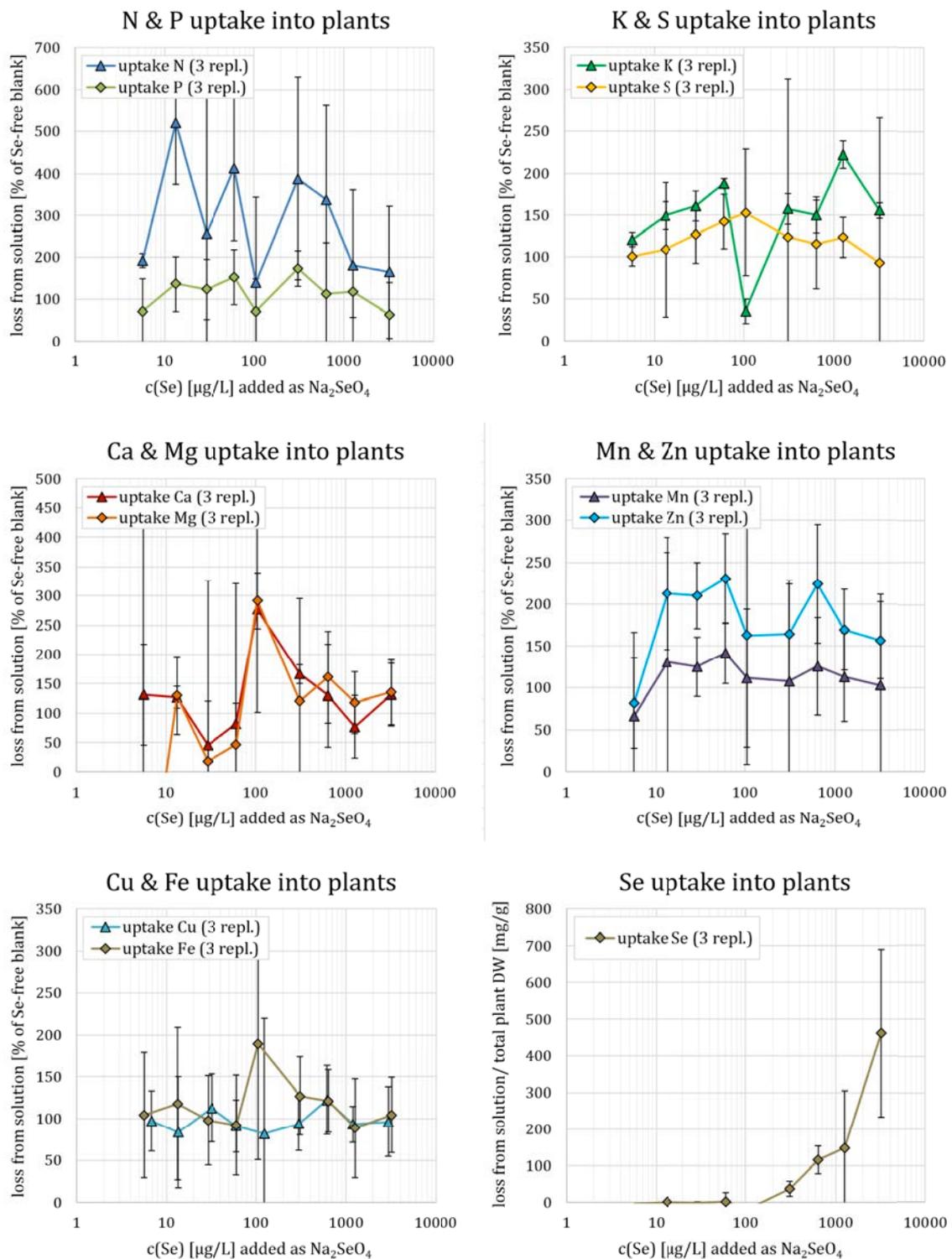


Figure A.18.: A3 results for nutrient uptake from solution (3 runs) Na_2SeO_3

Figure A.19.: A3 results for nutrient uptake from solution (3 runs) Na_2SeO_4

A.3.3. Complete A3 results overview

Table A.49.: *A3 plant nutrient element uptake data (calculated from loss of solution)*

Sample	from IC data												from ICP-NIS data													
	c(S _e) added [mg/L]	c(N)	SD	c(P)	SD	c(S)	SD	c(Mg)	SD	c(P)	SD	c(K)	SD	c(Ca)	SD	c(Mn)	SD	c(Fe)	SD	c(Cu)	SD	c(Zn)	SD	c(Se)	SD	
	[mg N/g DW]	[mg P/g DW]	[mg S/g DW]	[mg Mg/g DW]	[mg P/g DW]	[mg K/g DW]	[mg Ca/g DW]	[mg Mn/g DW]	[mg Fe/g DW]	[mg Cu/g DW]	[mg Zn/g DW]	[mg Se/g DW]														
all Nut-Sol-Se (Na₂SeO₄)																										
0000_summ	0.61	25.99	46.87	4.95	5.20	3.22	2.38	0.53	1.89	7.38	1.64	40.66	2.38	12.52	17.16	103.54	2.55	2932.22	384.78	26.34	7.86	73.87	8.22	0.28	0.85	
0005_summ	6.61	20.65	26.86	3.97	3.84	5.15	3.47	0.96	0.94	5.56	1.96	32.68	3.54	20.92	10.75	110.38	10.69	3050.23	294.62	25.67	4.66	64.79	17.63	3.97	4.33	
0010_summ	13.16	24.85	19.57	4.55	3.22	4.46	2.81	0.78	0.84	4.15	0.89	24.50	6.76	16.98	2.32	74.07	13.44	2526.31	378.45	22.04	7.37	58.49	10.65	2.49	1.28	
0025_summ	31.18	30.13	26.66	5.68	3.55	3.88	2.73	0.92	0.83	6.28	1.85	27.35	7.21	18.92	9.35	126.75	5.79	3371.66	635.41	29.72	7.22	84.81	13.73	9.52	3.69	
0050_summ	59.82	30.35	30.53	4.91	3.25	4.59	2.94	0.69	0.61	6.39	0.56	31.72	2.13	13.72	4.43	106.91	12.63	2719.15	500.36	24.06	1.73	58.62	42.55	23.88	18.20	
0100_summ	121.78	36.59	28.21	6.35	3.80	4.33	2.68	0.87	1.89	7.64	1.04	29.50	5.83	24.63	21.92	110.64	9.01	4514.51	2950.07	21.54	10.80	100.78	23.78	89.36	76.81	
0250_summ	295.32	25.13	31.45	4.37	2.09	3.87	2.23	1.30	0.02	6.28	1.49	32.01	7.46	21.17	2.03	97.93	10.36	3081.11	990.90	24.73	11.30	64.14	22.55	86.63	17.70	
0500_summ	602.90	31.50	22.49	8.16	6.04	3.63	1.98	1.38	0.58	5.85	1.50	28.48	8.81	23.89	10.96	106.23	29.09	2855.05	654.29	32.32	15.06	68.54	11.94	248.61	80.91	
1000_summ	1184.54	23.29	17.24	5.52	3.02	3.28	2.06	1.09	0.29	5.39	2.05	20.41	6.58	16.98	6.67	58.02	6.49	2331.58	653.88	24.58	7.07	36.17	16.51	350.99	267.31	
2500_summ	2936.46	28.17	30.80	3.43	3.75	2.80	2.54	1.17	0.32	6.12	1.15	18.46	3.80	18.54	6.65	38.59	11.18	2077.12	475.47	25.37	10.98	34.40	24.37	829.20	172.76	
all Nut-Sol-Se (Na₂SeO₄)																										
0000_summ	0.10	15.91	16.48	5.82	4.09	3.66	0.57	0.96	0.28	6.09	2.98	17.85	11.59	19.03	1.90	87.29	30.04	2354.56	1163.03	22.40	3.47	78.87	30.28	0.00	0.00	
0005_summ	5.72	30.62	23.07	4.15	2.79	3.69	0.54	0.80	0.07	4.88	1.52	21.56	14.38	10.96	1.24	57.99	47.14	2463.94	1759.20	13.08	8.03	49.67	8.87	1.23	0.31	
0010_summ	12.90	82.72	62.75	7.96	3.13	3.99	0.89	0.80	0.41	6.16	1.79	26.68	6.16	15.64	14.07	114.21	58.31	2783.43	2140.78	31.14	14.85	76.25	47.04	2.78	0.62	
0025_summ	29.11	40.75	27.53	7.20	4.13	4.65	0.50	1.21	0.14	8.22	5.57	28.75	5.84	15.93	1.38	109.26	34.56	2309.60	1253.68	26.40	9.03	75.40	12.68	5.35	1.22	
0050_summ	59.54	65.70	32.66	8.86	3.71	5.22	1.69	1.27	0.03	7.92	3.53	33.62	13.50	10.10	10.51	123.62	46.63	2175.92	1402.99	25.88	6.98	82.73	13.08	11.61	2.58	
0100_summ	107.01	44.32	3.47	9.19	2.67	5.60	2.87	1.81	0.30	6.51	2.69	24.73	15.39	25.44	36.54	168.68	74.70	4456.30	3252.91	44.45	23.59	58.40	29.52	13.48	5.66	
0250_summ	304.27	61.74	35.92	10.09	5.56	4.54	0.95	1.36	0.25	9.20	7.45	28.12	9.49	20.53	17.46	94.08	52.11	2996.11	1092.06	22.21	7.20	58.93	43.11	37.66	32.16	
0500_summ	623.00	53.75	28.92	6.54	6.01	4.22	1.91	1.00	0.48	5.16	2.96	26.83	4.29	16.00	8.09	109.82	61.73	2856.32	879.88	26.34	9.21	80.30	20.83	115.68	42.65	
1000_summ	1233.28	28.69	25.11	6.88	2.59	4.52	0.25	0.73	0.32	4.54	0.25	39.63	30.95	16.56	4.49	98.41	42.26	2089.13	1389.69	23.52	4.82	60.77	18.97	148.03	110.08	
2500_summ	3114.83	26.21	41.12	3.71	7.58	3.40	1.49	0.84	0.34	9.08	2.43	43.12	19.61	16.24	8.76	89.86	40.22	2458.17	1060.19	28.45	9.33	56.27	39.17	461.68	354.76	

Table A.50.: A3 results overview for Na_2SeO_3

c(Se) [µg/L]	plants per box		2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water	
	[-]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD
0	7.00	1.00	4.19	0.84	1.44	0.44	5.63	1.28	12.78	0.97	8.39	3.38	24.08	2.48	0.0100	0.0031	0.0049	0.0013	74.65	4.53	59.08	10.27
5	7.00	1.73	4.04	0.67	1.41	0.42	5.45	1.09	11.85	1.71	5.79	2.78	23.16	3.28	0.0092	0.0033	0.0053	0.0016	73.95	3.23	64.08	9.45
10	8.00	1.73	4.16	0.75	1.54	0.56	5.70	1.31	12.56	1.25	6.34	2.98	21.44	2.43	0.0094	0.0031	0.0063	0.0021	72.10	3.85	58.96	11.22
25	5.67	1.53	4.16	0.89	1.47	0.47	5.63	1.36	11.10	1.91	4.83	3.89	20.36	5.73	0.0088	0.0046	0.0073	0.0019	71.93	4.50	52.78	10.60
50	6.33	1.53	4.02	0.59	1.39	0.47	5.15	1.06	11.93	1.86	6.15	3.33	22.65	5.10	0.0104	0.0043	0.0064	0.0023	71.67	7.04	47.70	14.38
100	5.67	3.21	4.27	0.76	1.53	0.34	5.67	1.10	11.73	1.89	5.68	2.24	20.60	5.19	0.0099	0.0048	0.0069	0.0011	71.47	5.14	59.19	8.92
250	6.33	2.08	4.24	0.70	1.41	0.35	5.65	1.05	12.28	1.98	6.28	3.87	22.13	3.00	0.0095	0.0033	0.0070	0.0025	74.09	2.30	56.93	16.41
500	5.67	3.51	4.10	0.68	1.42	0.30	5.52	0.99	12.81	1.13	6.11	3.02	21.64	2.55	0.0109	0.0017	0.0058	0.0007	72.31	5.06	62.13	11.39
1000	6.00	3.00	3.75	1.15	1.34	0.42	5.09	1.57	11.96	2.15	5.86	2.48	19.94	4.30	0.0090	0.0028	0.0074	0.0029	70.43	5.57	53.45	14.37
2500	6.00	2.65	3.89	0.81	1.61	0.51	5.50	1.31	13.49	0.92	5.11	2.16	19.01	2.75	0.0093	0.0028	0.0061	0.0005	65.84	3.86	53.36	7.67

c(Se) [µg/L]	c(Se) shoot DW		c(Se) root DW		ratio root/shoot		ratio shoot/root		shoot-Se share		root-Se share		shoot water		root water		c(Se) shoot FW		c(Se) root FW		shoot water		root water	
	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD
0	0.00	0.00	0.00	0.00	x	x	x	x	x	x	x	x	74.65	59.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.41	0.18	1.07	0.54	2.59	0.45	0.39	0.21	27.9	7.5	72.1	7.5	73.95	64.08	0.11	0.05	1.07	0.54	21.54	9.59	80.31	49.66	42.81	
10	0.97	0.43	1.93	0.93	2.00	0.85	0.50	0.46	33.4	1.1	66.6	1.1	72.10	58.96	0.27	0.12	1.93	0.92	26.67	11.66	81.57	42.81	31.57	
25	2.35	0.58	5.51	2.65	2.34	1.36	0.43	1.13	29.9	7.6	70.1	7.6	71.93	52.78	0.66	0.16	5.48	2.63	26.47	6.93	99.16	31.57	211.88	
50	5.58	2.46	13.59	3.95	3.95	9.72	0.25	3.44	20.2	10.8	79.8	10.8	71.67	47.70	1.58	0.70	21.67	13.37	31.59	13.94	211.88	98.61	104.61	
100	9.58	1.79	26.71	15.17	2.79	4.98	0.36	5.44	26.4	12.4	73.6	12.4	71.47	59.19	2.73	0.51	25.98	14.75	26.97	6.15	104.61	48.27	54.16	
250	28.42	4.15	56.12	5.57	1.97	8.19	0.51	2.82	33.6	3.4	66.4	3.4	74.09	56.93	7.36	1.07	51.99	5.16	28.98	1.79	94.10	34.16	96.58	
500	59.34	8.95	140.13	35.49	2.36	21.14	0.42	15.03	29.7	2.5	70.3	2.5	72.31	62.13	16.43	2.48	117.11	29.66	33.61	12.80	116.47	48.89	84.81	
1000	101.91	28.88	178.14	37.81	1.75	50.48	0.57	21.63	36.4	3.4	63.6	3.4	70.43	53.45	30.14	8.54	124.45	26.42	30.68	13.07	84.81	48.89	14.04	
2500	158.98	30.38	312.04	14.65	1.96	59.62	0.51	7.47	33.8	3.3	66.2	3.3	65.84	53.36	54.31	10.38	142.58	6.70	22.15	8.16	57.82	14.04	14.04	

A.3.4. A3 analytical data

Table A.52.: A3 analytical data - HG-FIAS measurement I

Technique	AA FIAS-MHS	
Spectrometer Model	Aanalyst 200 S/N 200S6110908	
Autosampler Model	AS-90plus	
Batch ID	Pflanzenaufschlüsse	
Results Data Set	Nothstein_2013_08_30	
Date Measured	30.08.2013	
Method Name	Se Nothstein calib 6	
correl. coeff.	PQL (= lowest calib-10 %)	0.450
0.99964	LOQ (= 7-wash)	-0.057
calib. slope	LOD (= 3-wash)	-0.025
0.02014	analytical quality [%]	102.835

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0008	0.0	0.00	0.00
2	0.5 ppb	0.0079	0.0023	0.5	0.39	0.11
3	0.75 ppb	0.0136	0.0023	0.75	0.68	0.11
4	1.0 ppb	0.0192	0.0018	1.0	0.96	0.09
5	2.0 ppb	0.0396	0.0011	2.0	1.97	0.05
6	4.0 ppb	0.0807	0.0009	4.0	4.01	0.04
7	5.0 ppb	0.1015	0.0024	5.0	5.04	0.12
8	6.0 ppb	0.1207	0.0030	6.0	5.99	0.15

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.018	0.057	0.018	0.057	1	0.02	0.06
2	wash	-0.005	0.062	-0.005	0.062	1	-0.01	0.06
3	HCl Blank	0.043	0.117	0.041	0.112	6	0.25	0.67
4	Trace Metal 252 µg/L	4.421	0.071	4.202	0.068	60	252.14	4.06
5	wash	-0.071	0.041	-0.071	0.041	1	-0.07	0.04
6	Se_Std_0	-0.055	0.060	-0.055	0.060	1	-0.06	0.06
7	Se_Std_0.5	0.411	0.042	0.411	0.042	1	0.41	0.04
8	Se_Std_0.75	0.738	0.066	0.738	0.066	1	0.74	0.07
9	Se_Std_1	0.972	0.070	0.972	0.070	1	0.97	0.07
10	Se_Std_2	1.973	0.078	1.973	0.078	1	1.97	0.08
11	Se_Std_4	4.207	0.144	4.207	0.144	1	4.21	0.14
12	Se_Std_5	5.103	0.208	5.103	0.208	1	5.10	0.21
13	Se_Std_6	5.922	0.142	5.922	0.142	1	5.92	0.14
14	wash	-0.032	0.052	-0.032	0.052	1	-0.03	0.05
15	wash	0.045	0.129	0.045	0.129	1	0.05	0.13
16	2013-02-19 dig blind	0.074	0.094	0.068	0.087	8	< PQL	< PQL
17	2013-02-19 dig Std	1.145	0.077	1.113	0.075	8	8.90	0.60
18	2013-02-19 0ppb Shoot	-0.007	0.032	-0.007	0.029	8	< PQL	< PQL
19	2013-02-19 0ppb Root	-0.011	0.038	-0.010	0.035	8	< PQL	< PQL
20	2013-02-19 5 ppb Shoot	0.300	0.051	0.276	0.047	8	2.21	0.38
21	2013-02-19 5 ppb Root	0.056	0.101	0.052	0.093	8	< PQL	< PQL
22	2013-02-19 10 ppb Shoot	0.801	0.126	0.778	0.122	8	6.23	0.98
23	2013-02-19 10 ppb Root	0.237	0.030	0.218	0.028	8	1.74	0.22
24	2013-02-19 25 ppb Shoot	1.435	0.102	1.416	0.100	8	11.33	0.80
25	2013-02-19 25 ppb Root	0.419	0.062	0.386	0.057	8	3.08	0.45
26	wash	-0.084	0.060	-0.084	0.060	1	-0.08	0.06
27	Se_Std_0.5	0.438	0.036	0.438	0.036	1	0.44	0.04
28	Se_Std_0.75	0.654	0.045	0.654	0.045	1	0.65	0.05
29	Se_Std_2	2.018	0.057	2.018	0.057	1	2.02	0.06
30	Se_Std_4	4.155	0.064	4.155	0.064	1	4.16	0.06
31	Se_Std_6	5.898	0.135	5.898	0.135	1	5.90	0.13
32	wash	-0.004	0.040	-0.004	0.040	1	0.00	0.04
33	wash	0.000	0.138	0.000	0.138	1	0.00	0.14
34	2013-02-20 dig blind	0.020	0.090	0.019	0.084	8	< PQL	< PQL
35	2013-02-20 dig Std	1.205	0.085	1.205	0.085	8	9.64	0.68
36	2013-02-20 50ppb Shoot	1.014	0.090	1.014	0.090	40	40.56	3.62
37	2013-02-20 50ppb Root	0.176	0.038	0.164	0.036	40	6.56	1.42
38	2013-02-20 100 ppb Shoot	2.103	0.052	2.043	0.050	40	81.74	2.00
39	2013-02-20 100 ppb Root	0.412	0.058	0.384	0.054	40	15.35	2.17
40	2013-02-20 250 ppb Shoot	2.451	0.086	2.381	0.084	80	190.48	6.68
41	2013-02-20 250 ppb Root	0.766	0.099	0.766	0.099	80	61.26	7.92
42	2013-02-20 500 ppb Shoot	4.711	0.086	4.556	0.083	80	364.47	6.63
43	2013-02-20 500 ppb Root	1.181	0.093	1.181	0.093	80	94.46	7.40
44	wash	-0.030	0.053	-0.030	0.053	1	-0.03	0.05
45	Se_Std_0.5	0.401	0.076	0.401	0.076	1	0.40	0.08
46	Se_Std_0.75	0.700	0.103	0.700	0.103	1	0.70	0.10
47	Se_Std_2	2.032	0.108	2.032	0.108	1	2.03	0.11
48	Se_Std_4	4.124	0.104	4.124	0.104	1	4.12	0.10
49	Se_Std_6	6.176	0.122	6.176	0.122	1	6.18	0.12
50	wash	0.014	0.109	0.014	0.109	1	0.01	0.11
51	wash	0.062	0.074	0.062	0.074	1	0.06	0.07
52	2013-02-21 dig. Blind	-0.002	0.076	-0.002	0.069	8	< PQL	< PQL
53	2013-02-21 dig. Std	1.140	0.063	1.114	0.062	8	8.91	0.50
54	2013-02-21 1000 ppb Shoot	7.009	0.196	7.010	0.196	160	1121.66	31.43
55	2013-02-21 1000 ppb Root	0.960	0.066	0.938	0.064	160	150.15	10.31
56	2013-02-21 2500 ppb Shoot	12.350	0.384	12.353	0.384	160	> calib	> calib
57	2013-02-21 2500 ppb Root	2.673	0.048	2.496	0.045	160	399.43	7.22
58	2013-02-21 0 ppb Shoot	0.033	0.118	0.030	0.107	8	< PQL	< PQL
59	2013-02-21 0 ppb Root	0.006	0.063	0.005	0.057	8	< PQL	< PQL
60	2013-02-21 5 ppb Shoot	0.324	0.040	0.293	0.037	8	2.34	0.29
61	2013-02-21 5 ppb Root	0.472	0.016	0.428	0.014	8	3.42	0.12
62	wash	0.048	0.055	0.048	0.055	1	0.05	0.06
63	Se_Std_0.5	0.459	0.056	0.459	0.056	1	0.46	0.06
64	Se_Std_0.75	0.685	0.090	0.685	0.090	1	0.69	0.09
65	Se_Std_2	2.166	0.064	2.166	0.064	1	2.17	0.06
66	Se_Std_4	4.161	0.089	4.161	0.089	1	4.16	0.09
67	Se_Std_6	5.807	0.173	5.807	0.173	1	5.81	0.17

Table A.53.: A3 analytical data - HG-FIAS measurement I (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
68	wash	-0.036	0.059	-0.036	0.059	1	-0.04	0.06
69	wash	0.029	0.062	0.029	0.062	1	0.03	0.06
70	2013-02-22 dig. Blind	-0.017	0.074	-0.016	0.069	8	< PQL	< PQL
71	2013-02-22 dig. Std.	1.253	0.090	1.142	0.082	8	9.14	0.66
72	2013-02-22 10 ppb Root	1.213	0.072	1.105	0.066	8	8.84	0.53
73	2013-02-22 10 ppb Root	1.324	0.149	1.249	0.140	8	10.00	1.12
74	2013-02-22 25 ppb Root	1.118	0.068	1.019	0.062	8	8.15	0.49
75	2013-02-22 25 ppb Root	1.511	0.045	1.426	0.042	8	11.41	0.34
76	2013-02-22 50 ppb Root	0.706	0.126	0.644	0.115	40	25.74	4.59
77	2013-02-22 50 ppb Root	0.711	0.101	0.648	0.092	40	25.94	3.67
78	2013-02-22 100 ppb Shoot	2.235	0.229	2.110	0.217	40	84.39	8.66
79	2013-02-22 100 ppb Root	2.091	0.209	1.974	0.197	40	78.94	7.89
80	wash	-0.070	0.069	-0.070	0.069	1	-0.07	0.07
81	Se_Std_0.5	0.388	0.039	0.388	0.039	1	0.39	0.04
82	Se_Std_0.75	0.789	0.065	0.789	0.065	1	0.79	0.07
83	Se_Std_2	1.993	0.064	1.993	0.064	1	1.99	0.06
84	Se_Std_4	4.052	0.109	4.052	0.109	1	4.05	0.11
85	Se_Std_6	5.926	0.086	5.926	0.086	1	5.93	0.09
86	wash	0.005	0.109	0.005	0.109	1	0.01	0.11
87	wash	-0.036	0.049	-0.036	0.049	1	-0.04	0.05
88	2013-02-25 dig. Std	1.080	0.041	1.008	0.039	8	8.07	0.31
89	2013-02-25 250 ppb Shoot	2.238	0.173	2.139	0.165	80	171.11	13.23
90	2013-02-25 250 ppb Root	2.244	0.083	2.145	0.080	80	171.59	6.37
91	2013-02-25 500 ppb Shoot	3.637	0.099	3.569	0.097	80	285.50	7.79
92	2013-02-25 500 ppb Root	5.210	0.084	5.177	0.084	80	414.17	6.71
93	2013-02-25 1000 ppb Shoot	3.849	0.019	3.777	0.018	160	604.29	2.92
94	2013-02-25 1000 ppb Root	4.773	0.089	4.683	0.087	160	749.31	13.96
95	2013-02-25 2500 ppb Shoot	5.302	0.120	5.269	0.119	160	843.03	19.01
96	2013-02-25 2500 ppb Root	7.884	0.050	7.835	0.050	160	1253.52	8.03
97	wash	-0.037	0.044	-0.037	0.044	1	-0.04	0.04
98	HCl Blank	0.000	0.112	0.000	0.116	6	0.00	0.69
99	Trace Metal 252 µg/L	4.557	0.127	4.436	0.124	60	266.15	7.43
100	wash	0.018	0.092	0.018	0.092	1	0.02	0.09
101	Se_Std_0	-0.035	0.053	-0.035	0.053	1	-0.03	0.05
102	Se_Std_0.5	0.380	0.047	0.380	0.047	1	0.38	0.05
103	Se_Std_0.75	0.681	0.038	0.681	0.038	1	0.68	0.04
104	Se_Std_1	0.924	0.029	0.924	0.029	1	0.92	0.03
105	Se_Std_2	2.119	0.068	2.119	0.068	1	2.12	0.07
106	Se_Std_4	4.114	0.067	4.114	0.067	1	4.11	0.07
107	Se_Std_5	5.314	0.084	5.314	0.084	1	5.31	0.08
108	Se_Std_6	6.136	0.135	6.136	0.135	1	6.14	0.13
109	2013-02-21 2500 ppb Shoot	4.967	0.154	4.699	0.146	480	2255.29	70.08
110	wash	-0.043	0.062	-0.043	0.062	1	-0.04	0.06
111	wash	0.036	0.167	0.364	1.668	1	0.36	1.67

Table A.54.: A3 analytical data - HG-FIAS measurement II

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Plant Digestions		
Results Data Set	Nothstein_2014_03_19		
Date Measured	19.03.2014		
Method Name	Se Nothstein calib 6c		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.99891	LOQ (= 7-wash)	0.604	
calib. slope	LOD (= 3-wash)	0.259	
0.01252	analytical quality [%]	100.489	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0015	0.0	0.00	0.00
2	0.5 ppb	0.0033	0.0012	0.5	0.37	0.13
3	0.75 ppb	0.0068	0.0012	0.75	0.58	0.10
4	1.0 ppb	0.0080	0.0030	1.0	0.93	3.48
5	2.0 ppb	0.0203	0.0024	2.0	1.92	2.27
6	4.0 ppb	0.0408	0.0022	4.0	3.95	0.21
7	5.0 ppb	0.0527	0.0016	5.0	5.02	0.15
8	6.0 ppb	0.0657	0.0020	6.0	6.08	0.18

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.085	0.103	-0.085	0.103	1	-0.08	0.10
2	wash	0.121	0.113	0.121	0.113	1	0.12	0.11
3	6M HCl Blank	0.101	0.142	0.056	0.078	4	0.22	0.31
4	Trace Metal 252 µg/L	2.373	0.151	2.026	0.129	120	243.09	15.46
5	wash	0.126	0.086	0.126	0.086	1	0.13	0.09
6	Se_Std_0	0.113	0.118	0.113	0.118	1	0.11	0.12
7	Se_Std_0.5	0.536	0.090	0.536	0.090	1	0.54	0.09
8	Se_Std_0.75	0.681	0.105	0.681	0.105	1	0.68	0.10
9	Se_Std_1	1.140	0.088	1.140	0.088	1	1.14	0.09
10	Se_Std_2	2.202	0.130	2.202	0.130	1	2.20	0.13
11	Se_Std_4	4.294	0.162	4.294	0.162	1	4.29	0.16
12	Se_Std_5	5.548	0.112	5.548	0.112	1	5.55	0.11
13	Se_Std_6	6.667	0.174	6.667	0.174	1	6.67	0.17
14	wash	0.119	0.190	0.119	0.190	1	0.12	0.19
15	wash	0.073	0.142	0.073	0.142	1	0.07	0.14
16	2013-10-28 digestion blank	0.114	0.170	0.057	0.085	8	< PQL	< PQL
17	2013-10-28 digestion Std Wheat 1567a	1.448	0.180	1.074	0.134	8	8.60	1.07
18	2013-10-28 0 µg/L Shoot	0.161	0.132	0.081	0.066	8	< PQL	< PQL
19	2013-10-28 0 µg/L Root	0.091	0.135	0.046	0.068	8	< PQL	< PQL
20	2013-10-28 5 µg/L Shoot	0.337	0.060	0.169	0.030	8	1.35	0.24
21	2013-10-28 5 µg/L Root	0.040	0.105	0.020	0.053	8	< PQL	< PQL
22	2013-10-28 10 µg/L Shoot	0.538	0.064	0.270	0.032	8	2.16	0.26
23	2013-10-28 10 µg/L Root	0.145	0.080	0.073	0.040	8	< PQL	< PQL
24	2013-10-28 25 µg/L Shoot	2.579	0.331	2.086	0.267	8	16.69	2.14
25	2013-10-28 25 µg/L Root	0.966	0.112	0.717	0.083	8	5.74	0.66
26	wash	0.076	0.045	0.076	0.045	1	0.08	0.04
27	Se_Std_0	-0.019	0.056	-0.019	0.056	1	-0.02	0.06
28	Se_Std_0.5	0.573	0.199	0.573	0.199	1	0.57	0.20
29	Se_Std_0.75	0.888	0.181	0.888	0.181	1	0.89	0.18
30	Se_Std_1	1.195	0.119	1.195	0.119	1	1.19	0.12
31	Se_Std_2	2.375	0.134	2.375	0.134	1	2.37	0.13
32	Se_Std_4	4.660	0.152	4.660	0.152	1	4.66	0.15
33	Se_Std_5	5.618	0.115	5.618	0.115	1	5.62	0.12
34	Se_Std_6	6.742	0.158	6.742	0.158	1	6.74	0.16
35	wash	0.192	0.393	0.192	0.393	1	0.19	0.39
36	wash	0.086	0.059	0.086	0.059	1	0.09	0.06
37	2013-10-29 digestion blank	0.019	0.085	0.009	0.041	8	< PQL	< PQL
38	2013-10-29 digestion Std Wheat 1567a	1.667	0.142	1.307	0.112	8	10.45	0.89
39	2013-10-29 50 µg/L Shoot	5.252	0.122	4.604	0.107	8	36.83	0.85
40	2013-10-29 50 µg/L Root	1.584	0.121	1.242	0.095	8	9.94	0.76
41	2013-10-29 100 µg/L Shoot	2.626	0.095	2.059	0.074	8	16.47	0.59
42	2013-10-29 100 µg/L Root	1.428	0.134	1.151	0.108	8	9.21	0.86
43	2013-10-29 250 µg/L Shoot	5.705	0.180	5.139	0.163	48	246.66	7.80
44	2013-10-29 250 µg/L Root	5.665	0.161	5.103	0.145	8	40.82	1.16
45	2013-10-29 500 µg/L Shoot	7.312	0.210	6.586	0.189	120	790.32	22.69
46	2013-10-29 500 µg/L Root	4.138	0.085	3.436	0.070	48	164.93	3.38
47	wash	0.102	0.059	0.102	0.059	1	0.10	0.06
48	Se_Std_0	0.082	0.034	0.082	0.034	1	0.08	0.03
49	Se_Std_0.5	0.553	0.072	0.553	0.072	1	0.55	0.07
50	Se_Std_0.75	0.862	0.104	0.862	0.104	1	0.86	0.10
51	Se_Std_1	1.021	0.082	1.021	0.082	1	1.02	0.08
52	Se_Std_2	2.298	0.093	2.298	0.093	1	2.30	0.09
53	Se_Std_4	4.587	0.070	4.587	0.070	1	4.59	0.07
54	Se_Std_5	5.654	0.136	5.654	0.136	1	5.65	0.14
55	Se_Std_6	6.616	0.101	6.616	0.101	1	6.62	0.10
56	wash	0.126	0.162	0.126	0.162	1	0.13	0.16
57	wash	0.023	0.060	0.023	0.060	1	0.02	0.06
58	2013-10-30 digestion blank	0.054	0.125	0.024	0.057	8	< PQL	< PQL
59	2013-10-30 digestion Std Wheat 1567a	1.300	0.170	1.103	0.145	8	8.82	1.16
60	2013-10-30 1000 µg/L Shoot	5.512	0.109	4.985	0.099	240	1196.31	23.70
61	2013-10-30 1000 µg/L Root	4.992	0.123	4.515	0.111	120	541.78	13.38
62	2013-10-30 2500 µg/L Shoot	6.841	0.094	6.187	0.085	480	2969.86	40.86
63	2013-10-30 2500 µg/L Root	5.258	0.212	4.755	0.192	120	570.65	23.01
64	2013-10-30 0 µg/L Shoot	0.205	0.069	0.093	0.032	8	< PQL	< PQL
65	2013-10-30 0 µg/L Root	0.198	0.246	0.091	0.112	8	< PQL	< PQL
66	2013-10-30 5 µg/L Shoot	0.509	0.156	0.233	0.071	8	1.86	0.57
67	2013-10-30 5 µg/L Root	2.633	0.118	2.209	0.099	8	17.67	0.79

Table A.55.: A3 analytical data - HG-FIAS measurement II (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
68	wash	0.070	0.147	0.070	0.147	1	0.07	0.15
69	Se_Std_0	0.048	0.088	0.048	0.088	1	0.05	0.09
70	Se_Std_0.5	0.589	0.142	0.589	0.142	1	0.59	0.14
71	Se_Std_0.75	0.831	0.114	0.831	0.114	1	0.83	0.11
72	Se_Std_1	1.116	0.026	1.116	0.026	1	1.12	0.03
73	Se_Std_2	2.163	0.105	2.163	0.105	1	2.16	0.10
74	Se_Std_4	4.246	0.359	4.246	0.359	1	4.25	0.36
75	Se_Std_5	5.339	0.274	5.339	0.274	1	5.34	0.27
76	Se_Std_6	6.359	0.167	6.359	0.167	1	6.36	0.17
77	wash	0.147	0.165	0.147	0.165	1	0.15	0.16
78	wash	0.054	0.154	0.054	0.154	1	0.05	0.15
79	2013-11-04 digestion blank	0.082	0.083	0.045	0.046	8	< PQL	< PQL
80	2013-11-04 digestion Std Wheat 1567a	1.600	0.083	1.351	0.070	8	10.81	0.56
81	2013-11-04 10 µg/L Shoot	0.640	0.136	0.404	0.086	8	3.24	0.69
82	2013-11-04 10 µg/L Root	0.786	0.089	0.497	0.056	8	3.98	0.45
83	2013-11-04 25 µg/L Shoot	2.370	0.131	2.016	0.111	8	16.12	0.89
84	2013-11-04 25 µg/L Root	3.444	0.112	3.148	0.102	8	25.18	0.82
85	2013-11-04 50 µg/L Shoot	4.298	0.174	3.929	0.159	8	31.43	1.27
86	2013-11-04 50 µg/L Root	3.004	0.182	2.746	0.166	48	131.80	7.99
87	2013-11-04 100 µg/L Shoot	6.949	0.209	6.377	0.191	8	51.02	1.53
88	2013-11-04 100 µg/L Root	7.280	0.179	6.681	0.164	48	320.67	7.87
89	wash	0.112	0.145	0.112	0.145	1	0.11	0.14
90	Se_Std_0	0.089	0.108	0.089	0.108	1	0.09	0.11
91	Se_Std_0.5	0.483	0.075	0.483	0.075	1	0.48	0.08
92	Se_Std_0.75	0.761	0.125	0.761	0.125	1	0.76	0.13
93	Se_Std_1	1.028	0.106	1.028	0.106	1	1.03	0.11
94	Se_Std_2	2.253	0.153	2.253	0.153	1	2.25	0.15
95	Se_Std_4	4.338	0.114	4.338	0.114	1	4.34	0.11
96	Se_Std_5	5.519	0.137	5.519	0.137	1	5.52	0.14
97	Se_Std_6	6.794	0.147	6.794	0.147	1	6.79	0.15
98	wash	0.070	0.083	0.070	0.083	1	0.07	0.08
99	wash	0.129	0.127	0.129	0.127	1	0.13	0.13
100	2013-11-05 digestion blank	0.071	0.104	0.046	0.067	8	< PQL	< PQL
101	2013-11-05 digestion Std Wheat 1567a	1.602	0.101	1.343	0.084	8	10.74	0.68
102	2013-11-05 250 µg/L Shoot	4.822	0.204	4.297	0.181	48	206.26	8.71
103	2013-11-05 250 µg/L Root	4.965	0.128	4.424	0.114	48	212.37	5.47
104	2013-11-05 500 µg/L Shoot	3.603	0.220	3.134	0.191	120	376.11	22.92
105	2013-11-05 500 µg/L Root	4.107	0.093	3.573	0.081	120	428.72	9.72
106	2013-11-05 1000 µg/L Shoot	5.100	0.136	4.544	0.121	120	545.33	14.54
107	2013-11-05 1000 µg/L Root	7.032	0.134	6.265	0.119	120	751.82	14.30
108	2013-11-05 2500 µg/L Shoot	4.564	0.145	4.067	0.130	240	976.07	31.11
109	2013-11-05 2500 µg/L Root	6.035	0.195	5.377	0.174	240	1290.56	41.65
110	wash	0.034	0.053	0.034	0.053	1	0.03	0.05
111	6M HCl Blank	0.126	0.078	0.074	0.046	4	0.30	0.18
112	Trace Metal 252 µg/L	2.582	0.054	2.195	0.046	120	263.37	5.51
113	wash	0.028	0.115	0.028	0.115	1	0.03	0.12
114	Se_Std_0	0.084	0.087	0.084	0.087	1	0.08	0.09
115	Se_Std_0.5	0.523	0.080	0.523	0.080	1	0.52	0.08
116	Se_Std_0.75	0.857	0.107	0.857	0.107	1	0.86	0.11
117	Se_Std_1	1.158	0.156	1.158	0.156	1	1.16	0.16
118	Se_Std_2	2.209	0.124	2.209	0.124	1	2.21	0.12
119	Se_Std_4	4.597	0.231	4.597	0.231	1	4.60	0.23
120	Se_Std_5	5.607	0.208	5.607	0.208	1	5.61	0.21
120	Se_Std_6	6.683	0.089	6.683	0.089	1	6.68	0.09
121	wash	0.062	0.085	0.062	0.085	1	0.06	0.08
122	wash	0.145	0.087	0.145	0.087	1	0.15	0.09

Table A.56.: A3 analytical data - HG-FIAS measurement III

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Plant Digestions		
Results Data Set	Nothstein_2014_03_20		
Date Measured	20.03.2014		
Method Name	Se Nothstein calib 6c		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.999627	LOQ (= 7-wash)	-0.111	
calib. slope	LOD (= 3-wash)	-0.047	
0.01259	analytical quality [%]	109.825	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0003	0.0	0.00	0.00
2	0.5 ppb	0.0057	0.0014	0.5	0.45	0.11
3	0.75 ppb	0.0083	0.0014	0.8	0.66	0.11
4	1.0 ppb	0.0118	0.0016	1.0	0.94	0.13
5	2.0 ppb	0.0250	0.0017	2.0	1.99	0.14
6	4.0 ppb	0.0511	0.0025	4.0	4.06	0.20
7	5.0 ppb	0.0635	0.0012	5.0	5.05	0.10
8	6.0 ppb	0.0749	0.0029	6.0	5.95	0.23

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.019	0.097	0.019	0.097	1	0.02	0.10
2	wash	-0.004	0.108	-0.004	0.108	1	0.00	0.11
3	6M HCl Blank	0.017	0.109	0.019	0.118	4	0.07	0.47
4	Trace Metal 252 µg/L	2.359	0.109	2.309	0.107	120	277.04	12.78
5	wash	-0.040	0.060	-0.040	0.060	1	-0.04	0.06
6	Se_Std_0	0.002	0.097	0.002	0.097	1	0.00	0.10
7	Se_Std_0.5	0.417	0.101	0.417	0.101	1	0.42	0.10
8	Se_Std_0.75	0.701	0.095	0.701	0.095	1	0.70	0.10
9	Se_Std_1	0.920	0.088	0.920	0.088	1	0.92	0.09
10	Se_Std_2	2.029	0.145	2.029	0.145	1	2.03	0.15
11	Se_Std_4	4.172	0.192	4.172	0.192	1	4.17	0.19
12	Se_Std_5	5.045	0.141	5.045	0.141	1	5.05	0.14
13	Se_Std_6	6.061	0.203	6.061	0.203	1	6.06	0.20
14	wash	-0.032	0.103	-0.032	0.103	1	-0.03	0.10
15	wash	0.024	0.128	0.024	0.128	1	0.02	0.13
16	2014-02-12 digestion blank	-0.061	0.074	-0.069	0.084	8	< PQL	< PQL
17	2014-02-12 digestion Std Wheat 1567a	1.378	0.048	1.536	0.054	8	12.29	0.43
18	2014-02-12 0 µg/L Shoot	0.090	0.061	0.103	0.070	8	< PQL	< PQL
19	2014-02-12 0 µg/L Root	-0.025	0.038	-0.029	0.044	8	< PQL	< PQL
20	2014-02-12 5 µg/L Shoot	0.350	0.027	0.400	0.031	8	3.20	0.25
21	2014-02-12 5 µg/L Root	0.512	0.109	0.585	0.125	8	4.68	1.00
22	2014-02-12 10 µg/L Shoot	1.001	0.076	1.116	0.084	8	8.93	0.67
23	2014-02-12 10 µg/L Root	1.235	0.070	1.376	0.078	8	11.01	0.63
24	2014-02-12 25 µg/L Shoot	1.261	0.076	1.270	0.076	8	10.16	0.61
25	2014-02-12 25 µg/L Root	1.458	0.151	1.625	0.169	8	13.00	1.35
26	wash	-0.053	0.148	-0.053	0.148	1	-0.05	0.15
27	Se_Std_0	-0.003	0.064	-0.003	0.064	1	0.00	0.06
28	Se_Std_0.5	0.359	0.085	0.359	0.085	1	0.36	0.09
29	Se_Std_0.75	0.586	0.116	0.586	0.116	1	0.59	0.12
30	Se_Std_1	0.744	0.062	0.744	0.062	1	0.74	0.06
31	Se_Std_2	1.917	0.188	1.917	0.188	1	1.92	0.19
32	Se_Std_4	3.662	0.050	3.662	0.050	1	3.66	0.05
33	Se_Std_5	4.796	0.179	4.796	0.179	1	4.80	0.18
34	Se_Std_6	5.824	0.125	5.824	0.125	1	5.82	0.12
35	wash	-0.057	0.042	-0.057	0.042	1	-0.06	0.04
36	wash	-0.037	0.059	-0.037	0.059	1	-0.04	0.06
37	2014-02-13 digestion blank VF 8	0.018	0.064	0.022	0.077	8	< PQL	< PQL
38	2014-02-13 digestion Std Wheat 1567a	1.171	0.104	1.331	0.118	8	10.64	0.94
39	2014-02-13 50 µg/L Shoot	5.575	0.181	5.516	0.179	8	44.13	1.43
40	2014-02-13 50 µg/L Root	9.190	0.120	9.093	0.119	8	72.75	0.95
41	2014-02-13 100 µg/L Shoot	2.625	0.096	2.579	0.095	8	20.63	0.76
42	2014-02-13 100 µg/L Root	3.440	0.086	3.574	0.089	8	28.59	0.71
43	2014-02-13 250 µg/L Shoot	4.512	0.174	4.688	0.181	24	112.51	4.34
44	2014-02-13 250 µg/L Root	8.286	0.137	8.199	0.136	24	196.77	3.26
45	2014-02-13 500 µg/L Shoot	7.349	0.124	7.272	0.123	24	174.53	2.95
46	2014-02-13 500 µg/L Root	8.302	0.278	7.833	0.262	24	188.00	6.30
47	wash	0.052	0.092	0.052	0.092	1	0.05	0.09
48	Se_Std_0	0.063	0.128	0.063	0.128	1	0.06	0.13
49	Se_Std_0.5	0.354	0.135	0.354	0.135	1	0.35	0.14
50	Se_Std_0.75	0.797	0.024	0.797	0.024	1	0.80	0.02
51	Se_Std_1	0.881	0.083	0.881	0.083	1	0.88	0.08
52	Se_Std_2	2.127	0.098	2.127	0.098	1	2.13	0.10
53	Se_Std_4	4.134	0.039	4.134	0.039	1	4.13	0.04
54	Se_Std_5	5.128	0.157	5.128	0.157	1	5.13	0.16
55	Se_Std_6	6.203	0.168	6.203	0.168	1	6.20	0.17
56	wash	0.008	0.063	0.008	0.063	1	0.01	0.06
57	wash	0.023	0.089	0.023	0.089	1	0.02	0.09
58	2014-02-14 digestion blank	0.133	0.133	0.159	0.159	8	< PQL	< PQL
59	2014-02-14 digestion Std Wheat 1567a	0.988	0.098	0.996	0.099	8	7.97	0.79
60	2014-02-14 1000 µg/L Shoot	2.153	0.105	1.958	0.096	120	234.90	11.46
61	2014-02-14 1000 µg/L Root	3.039	0.106	2.763	0.096	120	331.57	11.53
62	2014-02-14 2500 µg/L Shoot	5.442	0.126	5.359	0.124	120	643.07	14.84
63	2014-02-14 2500 µg/L Root	6.647	0.166	6.329	0.158	120	759.52	18.98
64	2014-02-14 0 µg/L Shoot	0.091	0.078	0.109	0.093	8	< PQL	< PQL
65	2014-02-14 0 µg/L Root	0.015	0.044	0.018	0.053	8	< PQL	< PQL
66	2014-02-14 5 µg/L Shoot	1.124	0.122	1.133	0.123	8	9.06	0.98
67	2014-02-14 5 µg/L Root	0.848	0.090	0.726	0.077	8	5.81	0.62

Table A.57.: A3 analytical data - HG-FIAS measurement III (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
68	wash	-0.043	0.087	-0.043	0.087	1	-0.04	0.09
69	Se_Std_0	0.006	0.046	0.006	0.046	1	0.01	0.05
70	Se_Std_0.5	0.375	0.115	0.375	0.115	1	0.38	0.12
71	Se_Std_0.75	0.708	0.080	0.708	0.080	1	0.71	0.08
72	Se_Std_1	0.984	0.085	0.984	0.085	1	0.98	0.09
73	Se_Std_2	2.208	0.049	2.208	0.049	1	2.21	0.05
74	Se_Std_4	4.342	0.063	4.342	0.063	1	4.34	0.06
75	Se_Std_5	5.117	0.167	5.117	0.167	1	5.12	0.17
76	Se_Std_6	6.267	0.036	6.267	0.036	1	6.27	0.04
77	wash	-0.050	0.061	-0.050	0.061	1	-0.05	0.06
78	wash	-0.072	0.053	-0.072	0.053	1	-0.07	0.05
79	2014-02-17 digestion blank	0.075	0.164	0.085	0.186	8	< PQL	< PQL
80	2014-02-17 digestion Std Wheat 1567a	1.202	0.082	1.149	0.078	8	9.19	0.63
81	2014-02-17 10 µg/L Shoot	0.779	0.133	0.706	0.120	8	5.65	0.96
82	2014-02-17 10 µg/L Root	0.186	0.060	0.210	0.068	8	< PQL	< PQL
83	2014-02-17 25 µg/L Shoot	1.820	0.088	1.664	0.080	8	13.31	0.64
84	2014-02-17 25 µg/L Root	0.222	0.051	0.251	0.058	8	< PQL	< PQL
85	2014-02-17 50 µg/L Shoot	3.099	0.309	2.931	0.293	8	23.45	2.34
86	2014-02-17 50 µg/L Root	0.530	0.049	0.601	0.055	8	4.81	0.44
87	2014-02-17 100 µg/L Shoot	2.106	0.263	1.925	0.240	10	19.25	2.40
88	2014-02-17 100 µg/L Root	0.417	0.059	0.472	0.067	8	3.78	0.54
89	wash	0.013	0.105	0.013	0.105	1	0.01	0.11
90	Se_Std_0	0.033	0.076	0.033	0.076	1	0.03	0.08
91	Se_Std_0.5	0.410	0.084	0.410	0.084	1	0.41	0.08
92	Se_Std_0.75	0.732	0.029	0.732	0.029	1	0.73	0.03
93	Se_Std_1	0.978	0.113	0.978	0.113	1	0.98	0.11
94	Se_Std_2	2.107	0.116	2.107	0.116	1	2.11	0.12
95	Se_Std_4	4.211	0.083	4.211	0.083	1	4.21	0.08
96	Se_Std_5	5.155	0.102	5.155	0.102	1	5.16	0.10
97	Se_Std_6	6.236	0.129	6.236	0.129	1	6.24	0.13
98	wash	-0.018	0.047	-0.018	0.047	1	-0.02	0.05
99	wash	0.012	0.122	0.012	0.122	1	0.01	0.12
100	2014-02-18 digestion blank	0.005	0.038	0.005	0.043	8	< PQL	< PQL
101	2014-02-18 digestion Std Wheat 1567a	1.342	0.106	1.227	0.097	8	9.82	0.77
102	2014-02-18 250 µg/L Shoot	7.494	0.319	8.650	0.368	24	207.61	8.83
103	2014-02-18 250 µg/L Root	1.289	0.063	1.254	0.062	48	60.20	2.96
104	2014-02-18 500 µg/L Shoot	10.709	0.161	9.737	0.147	24	233.68	3.52
105	2014-02-18 500 µg/L Root	2.372	0.290	2.309	0.282	24	55.41	6.78
106	2014-02-18 1000 µg/L Shoot	6.229	0.221	7.191	0.255	120	862.86	30.62
107	2014-02-18 1000 µg/L Root	1.559	0.136	1.497	0.131	120	179.65	15.71
108	2014-02-18 2500 µg/L Shoot	1.788	0.032	2.168	0.039	120	260.19	4.63
109	2014-02-18 2500 µg/L Root	7.343	0.368	6.404	0.321	120	768.53	38.47
110	wash	-0.029	0.056	-0.029	0.056	1	-0.03	0.06
111	6M HCl Blank	-0.057	0.032	-0.064	0.036	4	-0.26	0.14
112	Trace Metal 252 µg/L	2.590	0.118	2.304	0.105	120	276.47	12.63
113	wash	-0.050	0.073	-0.050	0.073	1	-0.05	0.07
114	Se_Std_0	-0.065	0.050	-0.065	0.050	1	-0.06	0.05
115	Se_Std_0.5	0.391	0.097	0.391	0.097	1	0.39	0.10
116	Se_Std_0.75	0.727	0.097	0.727	0.097	1	0.73	0.10
117	Se_Std_1	1.072	0.073	1.072	0.073	1	1.07	0.07
118	Se_Std_2	2.207	0.122	2.207	0.122	1	2.21	0.12
119	Se_Std_4	4.638	0.229	4.638	0.229	1	4.64	0.23
120	Se_Std_5	3.379	0.918	3.379	0.918	1	3.38	0.92
120	Se_Std_6	6.140	0.136	6.140	0.136	1	6.14	0.14
123	wash	-0.007	0.062	-0.007	0.062	1	-0.01	0.06
123	wash	0.011	0.137	0.011	0.137	1	0.01	0.14

Table A.58.: A3 analytical data - IC measurement I

Technique		Ion Chromatography							
System		ICS-1000							
Quantification:		AnionenAS14							
Injection volume		25 µL							
Run time [min]		14							
Date Measured		04.04.2013							
Calibration ID		Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]
Calib_1		4.23	Cl ⁻	XQOff	5	-0.004	0.158	0.001	99.9988
Calib_2		6.94	NO ₃ ⁻	XQOff	5	-0.008	0.084	0.000	99.9985
Calib_3		8.64	PO ₄ ³⁻	XQOff	5	0.016	0.044	0.000	99.9984
Calib_4		10.13	SO ₄ ²⁻	XQOff	5	-0.002	0.112	0.000	99.9990
mean:						-0.0053	0.0992	0.0005	99.9987
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.26	7.24	8.89	10.47	1.01	2.01	3.01	1.99
2	Standard_2	4.26	7.19	8.87	10.44	4.94	9.89	14.88	10.04
3	Standard_3	4.26	7.16	8.86	10.41	10.05	20.13	30.24	20.08
4	Standard_4	4.26	7.12	8.83	10.38	20.01	39.97	59.86	39.85
5	Standard_5	4.28	7.07	8.79	10.34	39.99	80.00	120.03	80.05
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Std.3-1	4.23	7.03	8.62	10.14	10.83	21.49	32.34	21.21
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	nut_sol_0000ppbSe_2013_01_10	4.23	6.94	8.64	10.13	5.04	323.50	38.22	73.70
10	nut_sol_0005ppbSe_2013_01_10	4.23	6.94	8.64	10.13	4.75	324.34	37.27	73.58
11	nut_sol_0010ppbSe_2013_01_10	4.23	6.94	8.64	10.13	4.74	328.65	39.08	72.97
12	nut_sol_0025ppbSe_2013_01_10	4.23	6.94	8.64	10.13	5.71	332.37	38.57	71.24
13	nut_sol_0050ppbSe_2013_01_10	4.23	6.94	8.64	10.12	4.53	333.83	37.86	71.37
14	nut_sol_0100ppbSe_2013_01_10	4.23	6.95	8.63	10.12	5.71	328.87	37.92	70.22
15	nut_sol_0250ppbSe_2013_01_10	4.23	6.95	8.64	10.12	5.82	323.69	39.01	70.34
16	nut_sol_0500ppbSe_2013_01_10	4.23	6.95	8.64	10.12	6.20	324.91	37.94	70.17
17	nut_sol_1000ppbSe_2013_01_10	4.23	6.95	8.64	10.12	6.24	320.10	38.74	69.54
18	nut_sol_2500ppbSe_2013_01_10	4.23	6.95	8.63	10.13	6.66	320.10	39.19	70.16
19	nut_sol_blind_0000ppbSe	4.23	6.95	8.64	10.13	3.75	312.45	37.20	70.65
20	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Std.3-2	4.23	7.03	8.61	10.12	10.65	21.19	32.07	21.20
22	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_2013_01_29	4.23	7.01	8.66	10.15	4.01	140.95	20.93	65.01
24	nut_sol_0005ppbSe_2013_01_29	4.23	6.99	8.65	10.14	3.65	192.15	22.35	64.36
25	nut_sol_0010ppbSe_2013_01_29	4.23	6.98	8.65	10.13	3.38	177.13	21.02	63.22
26	nut_sol_0025ppbSe_2013_01_29	4.23	6.97	8.64	10.13	10.36	205.27	24.70	62.79
27	nut_sol_0050ppbSe_2013_01_29	4.23	6.99	8.65	10.14	3.11	165.28	22.88	62.36
28	nut_sol_0100ppbSe_2013_01_29	4.23	6.97	8.65	10.13	4.15	200.52	21.52	62.02
29	nut_sol_0250ppbSe_2013_01_29	4.22	6.98	8.65	10.14	3.30	146.88	25.85	61.62
30	nut_sol_0500ppbSe_2013_01_29	4.22	6.96	8.66	10.16	5.04	211.17	25.60	62.03
31	nut_sol_1000ppbSe_2013_01_29	4.22	6.95	8.63	10.14	4.91	223.20	25.82	61.62
32	nut_sol_2500ppbSe_2013_01_29	4.22	6.97	8.63	10.14	3.26	159.08	25.67	61.33
33	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Std.3-3	4.22	7.01	8.61	10.12	10.55	21.09	31.94	21.08
35	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table A.59.: A3 analytical data - IC measurement II

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	17.01.2013								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.08	Cl ⁻	XQOff	5	-0.008	0.163	0.001	99.9804	
Calib_2	6.78	NO ₃ ⁻	XQOff	5	-0.019	0.090	0.000	99.9881	
Calib_3	8.41	PO ₄ ³⁻	XQOff	5	0.016	0.047	0.000	99.9974	
Calib_4	10.00	SO ₄ ²⁻	XQOff	5	-0.011	0.116	0.000	99.9931	
mean:					-0.0053	0.1040	0.0004	99.9898	
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.14	7.08	8.74	10.45	1.02	2.04	3.01	2.03
2	Standard_2	4.14	7.04	8.72	10.44	4.90	9.83	14.98	9.88
3	Standard_3	4.14	7.02	8.70	10.42	9.83	19.76	29.74	19.80
4	Standard_4	4.15	6.98	8.68	10.40	20.34	40.53	60.36	40.41
5	Standard_5	4.16	6.91	8.65	10.36	39.90	79.84	119.90	79.88
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Std.3-1	4.08	6.87	8.40	9.99	9.66	18.94	28.55	19.27
8	wash-2	n.a.	n.a.	n.a.	10.01	n.a.	n.a.	n.a.	n.a.
9	nut_sol_0000ppbSe_2012_11_22	4.08	6.78	8.41	10.00	10.83	301.53	37.59	67.25
10	nut_sol_0005ppbSe_2012_11_22	4.10	6.79	8.41	10.00	95.55	298.56	35.17	68.22
11	nut_sol_0010ppbSe_2012_11_22	4.09	6.79	8.41	10.00	3.44	302.58	37.31	67.71
12	nut_sol_0025ppbSe_2012_11_22	4.08	6.80	8.42	10.00	3.66	224.19	28.63	66.93
13	nut_sol_0050ppbSe_2012_11_22	4.08	6.78	8.41	10.00	4.05	288.06	36.18	67.47
14	nut_sol_0100ppbSe_2012_11_22	4.08	6.78	8.41	10.00	4.24	302.72	35.12	66.06
15	nut_sol_0250ppbSe_2012_11_22	4.08	6.78	8.41	10.00	5.22	306.83	36.78	67.78
16	nut_sol_0500ppbSe_2012_11_22	4.12	6.78	8.42	10.01	205.89	304.93	37.65	66.95
17	nut_sol_1000ppbSe_2012_11_22	4.08	6.77	8.41	10.00	4.62	306.10	36.12	66.00
18	nut_sol_2500ppbSe_2012_11_22	4.12	6.79	8.42	10.01	206.97	282.18	27.04	63.25
19	nut_sol_blind_2012_11_22	4.08	n.a.	n.a.	n.a.	3.58	300.62	37.90	65.83
20	wash-3	4.08	6.87	8.39	10.00	n.a.	n.a.	n.a.	n.a.
21	Std.3-2	4.08	n.a.	n.a.	n.a.	3.02	4.08	5.96	6.87
22	wash-4	4.08	6.80	8.43	10.01	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_2012_12_11	4.08	6.84	8.42	10.01	3.60	187.56	17.97	60.06
24	nut_sol_0005ppbSe_2012_12_11	4.08	6.91	8.42	10.00	2.24	102.65	17.80	58.76
25	nut_sol_0010ppbSe_2012_12_11	4.08	6.88	8.44	10.00	1.90	18.55	17.96	58.81
26	nut_sol_0025ppbSe_2012_12_11	4.09	6.89	8.42	10.01	3.02	50.39	7.42	57.72
27	nut_sol_0050ppbSe_2012_12_11	4.08	6.81	8.43	10.01	2.99	49.15	13.58	59.64
28	nut_sol_0100ppbSe_2012_12_11	4.08	6.87	8.44	10.01	3.20	187.01	16.14	59.57
29	nut_sol_0250ppbSe_2012_12_11	4.08	6.83	8.42	10.01	3.52	60.53	7.37	60.03
30	nut_sol_0500ppbSe_2012_12_11	4.08	6.81	8.42	10.01	2.87	137.71	18.39	57.61
31	nut_sol_1000ppbSe_2012_12_11	4.08	6.81	8.41	10.00	3.92	193.14	20.60	58.92
32	nut_sol_2500ppbSe_2012_12_11	n.a.	n.a.	n.a.	n.a.	4.42	178.16	14.29	57.47
33	wash-5	4.08	6.86	8.39	9.99	n.a.	n.a.	n.a.	n.a.
34	Std.3-3	n.a.	n.a.	n.a.	n.a.	3.02	4.08	5.95	6.86
35	wash-6	4.08	6.77	8.41	10.01	n.a.	n.a.	n.a.	n.a.

Table A.60.: A3 analytical data - IC measurement III

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	05.12.2013								
	Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]
	Calib_1	4.16	Cl ⁻	XQOff	5	-0.005	0.146	0.001	99.9999
	Calib_2	6.77	NO ₃ ⁻	XQOff	5	-0.019	0.078	0.000	99.9962
	Calib_3	8.44	PO ₄ ³⁻	XQOff	5	-0.008	0.040	0.000	100.0000
	Calib_4	10.03	SO ₄ ²⁻	XQOff	5	-0.008	0.103	0.000	99.9999
					mean:	-0.0101	0.0921	0.0004	99.9990
Seq. No.	Sample ID	Cl⁻ [min]	Retention time		Cl⁻ [mg/L]	Ion concentration			SO₄²⁻ [mg/L]
			NO₃⁻ [min]	PO₄³⁻ [min]		NO₃⁻ [mg/L]	PO₄³⁻ [mg/L]		
1	Standard_1	4.21	7.01	8.62	10.27	2.00	4.01	5.99	3.99
2	Standard_2	4.21	6.99	8.62	10.27	4.99	10.03	15.03	10.02
3	Standard_3	4.22	6.96	8.61	10.25	9.99	19.78	29.98	20.00
4	Standard_4	4.22	6.93	8.59	10.23	20.02	40.23	59.99	39.98
5	Standard_5	4.24	6.88	8.55	10.19	39.99	79.94	120.00	80.01
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Std.3-1	4.17	6.85	8.43	10.04	10.32	20.26	30.67	20.31
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	nut_sol_blind_0000ppbSe_nit	4.16	6.76	8.45	10.04	3.85	311.97	36.47	68.78
10	nut_sol_0000ppbSe_2013_10_02	4.16	6.77	8.44	10.03	9.57	290.07	35.08	75.98
11	nut_sol_0005ppbSe_2013_10_02	4.16	6.77	8.44	10.04	3.91	322.99	37.91	77.05
12	nut_sol_0010ppbSe_2013_10_02	4.16	6.77	8.43	10.03	3.78	316.52	37.05	76.84
13	nut_sol_0025ppbSe_2013_10_02	4.16	6.77	8.44	10.04	5.37	322.40	37.16	72.72
14	nut_sol_0050ppbSe_2013_10_02	4.16	6.77	8.43	10.03	3.77	317.45	37.18	76.11
15	nut_sol_0100ppbSe_2013_10_02	4.16	6.77	8.43	10.03	3.69	296.70	36.56	76.06
16	nut_sol_0250ppbSe_2013_10_02	4.16	6.76	8.44	10.03	4.98	345.27	40.27	75.74
17	nut_sol_0500ppbSe_2013_10_02	4.16	6.76	8.44	10.03	6.08	345.97	41.88	76.91
18	nut_sol_1000ppbSe_2013_10_02	4.16	6.76	8.43	10.03	6.11	346.54	42.07	76.25
19	nut_sol_2500ppbSe_2013_10_02	4.16	6.76	8.43	10.03	5.78	343.84	43.38	75.91
20	wash-3	4.11	n.a.	n.a.	n.a.	0.48	n.a.	n.a.	n.a.
21	Std.3-2	4.17	6.84	8.42	10.03	41.88	82.20	124.40	81.72
22	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_2013_10_21	4.16	6.78	8.44	10.03	4.35	251.35	24.77	69.95
24	nut_sol_0005ppbSe_2013_10_21	4.16	6.78	8.44	10.04	4.57	242.52	23.88	68.74
25	nut_sol_0010ppbSe_2013_10_21	4.16	6.78	8.43	10.02	4.98	257.48	27.75	69.26
26	nut_sol_0025ppbSe_2013_10_21	4.16	6.78	8.42	10.02	4.73	255.26	22.05	68.17
27	nut_sol_0050ppbSe_2013_10_21	4.16	6.79	8.44	10.04	4.55	240.58	22.86	68.45
28	nut_sol_0100ppbSe_2013_10_21	4.16	6.78	8.43	10.03	4.37	244.80	22.77	67.99
29	nut_sol_0250ppbSe_2013_10_21	4.16	6.79	8.42	10.03	4.43	235.76	21.96	67.34
30	nut_sol_0500ppbSe_2012_10_21	4.18	6.78	8.43	10.04	7.00	260.27	24.25	68.10
31	nut_sol_1000ppbSe_2012_10_21	4.16	6.78	8.43	10.03	5.34	280.11	25.50	69.70
32	nut_sol_2500ppbSe_2012_10_21	4.19	6.77	8.42	10.03	12.86	286.15	28.05	69.56
33	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Std.3-3	4.17	6.85	8.41	10.02	41.70	81.78	124.39	81.81
35	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
36	nut_sol_0000ppbSenat_2013_09_12 wdh	4.160167	6.770167	8.4235	10.0235	3.850973	315.3354	35.37117	73.44737

Table A.61.: A3 analytical data - IC measurement IV

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	12.04.2013								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.08	Cl ⁻	XQOff	5	-0.008	0.163	0.001	99.9804	
Calib_2	6.78	NO ₃ ⁻	XQOff	5	-0.019	0.090	0.000	99.9881	
Calib_3	8.41	PO ₄ ³⁻	XQOff	5	0.016	0.047	0.000	99.9974	
Calib_4	10.00	SO ₄ ²⁻	XQOff	5	-0.011	0.116	0.000	99.9931	
mean:					-0.0053	0.1040	0.0004	99.9898	
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.21	7.01	8.62	10.27	2.00	4.01	5.99	3.99
2	Standard_2	4.21	6.99	8.62	10.27	4.99	10.03	15.03	10.02
3	Standard_3	4.22	6.96	8.61	10.25	9.99	19.78	29.98	20.00
4	Standard_4	4.22	6.93	8.59	10.23	20.02	40.23	59.99	39.98
5	Standard_5	4.24	6.88	8.55	10.19	39.99	79.94	120.00	80.01
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Std.3-1	4.18	6.87	8.45	10.06	9.93	19.51	29.44	19.77
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	nut_sol_blind_0000ppbSe_nat	4.16	6.91	8.43	10.06	3.97	318.51	36.95	69.81
10	nut_sol_0000ppbSe_2013_09_12	4.17	6.80	8.48	10.07	3.95	286.70	34.63	71.12
11	nut_sol_0005ppbSe_2013_09_12	4.17	6.82	8.47	10.06	2.95	211.84	26.21	70.59
12	nut_sol_0010ppbSe_2013_09_12	4.17	6.80	8.47	10.06	3.80	313.97	37.63	71.78
13	nut_sol_0025ppbSe_2013_09_12	4.17	6.82	8.47	10.06	3.48	249.92	31.39	71.54
14	nut_sol_0050ppbSe_2013_09_12	4.17	6.81	8.47	10.06	3.87	260.61	30.09	71.89
15	nut_sol_0100ppbSe_2013_09_12	4.17	6.80	8.47	10.06	4.16	318.67	36.21	71.94
16	nut_sol_0250ppbSe_2013_09_12	4.17	6.80	8.46	10.05	3.97	323.69	36.65	71.90
17	nut_sol_0500ppbSe_2013_09_12	4.17	6.80	8.47	10.06	4.28	327.59	36.99	72.56
18	nut_sol_1000ppbSe_2013_09_12	4.17	6.80	8.47	10.06	4.59	323.14	37.74	71.98
19	nut_sol_2500ppbSe_2013_09_12	4.17	6.81	8.47	10.06	3.75	306.11	36.53	70.64
20	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Std.3-2	4.18	6.87	8.45	10.05	10.20	20.13	30.65	20.44
22	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_2013_10_01	4.18	n.a.	8.47	10.05	3.02	n.a.	18.59	63.05
24	nut_sol_0005ppbSe_2013_10_01	4.17	6.84	8.47	10.06	12.92	178.22	23.30	65.38
25	nut_sol_0010ppbSe_2013_10_01	4.18	6.91	8.46	10.06	3.79	42.28	23.66	65.60
26	nut_sol_0025ppbSe_2013_10_01	4.18	6.88	8.47	10.06	3.18	108.25	17.45	61.74
27	nut_sol_0050ppbSe_2013_10_01	4.18	6.92	8.49	10.06	3.09	32.63	14.44	63.28
28	nut_sol_0100ppbSe_2013_10_01	4.17	6.83	8.46	10.05	4.61	218.48	24.09	65.46
29	nut_sol_0250ppbSe_2013_10_01	4.17	6.88	8.45	10.05	9.69	107.81	16.77	64.14
30	nut_sol_0500ppbSe_2012_10_01	4.17	6.89	8.47	10.05	2.81	87.18	19.06	61.95
31	nut_sol_1000ppbSe_2012_10_01	4.17	n.a.	8.46	10.05	2.36	n.a.	21.14	62.04
32	nut_sol_2500ppbSe_2012_10_01	4.17	6.86	8.46	10.05	3.79	138.40	18.91	60.93
33	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Std.3-3	4.18	6.89	8.44	10.05	10.38	20.61	31.26	20.56
35	wash-6	4.18	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table A.62.: A3 analytical data - IC measurement V

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	23.04.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.13	Cl ⁻	XQOff	5	-0.004	0.153	0.001	99.9973	
Calib_2	6.69	NO ₃ ⁻	XQOff	5	-0.013	0.080	0.000	99.9992	
Calib_3	8.27	PO ₄ ³⁻	XQOff	5	0.001	0.042	0.000	99.9999	
Calib_4	9.76	SO ₄ ²⁻	XQOff	5	-0.020	0.107	0.000	99.9997	
mean:					-0.0094	0.0954	0.0004	99.9990	
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.09	6.70	8.10	9.46	2.02	3.99	6.00	4.00
2	Standard_2	4.09	6.68	8.09	9.46	4.92	9.99	15.00	9.98
3	Standard_3	4.09	6.66	8.07	9.44	10.01	20.10	30.05	20.07
4	Standard_4	4.10	6.62	8.06	9.43	20.06	39.89	59.95	39.94
5	Standard_5	4.11	6.57	8.03	9.40	39.98	80.03	120.01	80.01
6	wash-1	4.10	n.a.	8.27	n.a.	n.a.	n.a.	n.a.	n.a.
7	Std.3-1	4.11	6.68	8.18	9.63	9.85	19.95	30.02	20.09
8	wash-2	4.11	6.76	8.20	9.65	n.a.	n.a.	n.a.	n.a.
9	nut_sol_blind_0000ppbSe_nat	4.10	6.66	8.19	9.63	5.86	143.80	13.17	35.97
10	nut_sol_0000ppbSe_2014_01_16	4.10	6.63	8.19	9.62	3.58	272.01	27.66	67.75
11	nut_sol_0005ppbSe_2014_01_16	4.11	6.63	8.19	9.62	6.62	284.98	29.74	69.26
12	nut_sol_0010ppbSe_2014_01_16	4.10	6.63	8.19	9.62	3.64	303.06	29.87	69.60
13	nut_sol_0025ppbSe_2014_01_16	4.10	6.63	8.19	9.62	3.37	285.47	30.05	67.66
14	nut_sol_0050ppbSe_2014_01_16	4.11	6.63	8.19	9.62	4.05	302.73	29.59	67.99
15	nut_sol_0100ppbSe_2014_01_16	4.11	6.64	8.19	9.62	5.10	268.67	26.03	67.98
16	nut_sol_0250ppbSe_2014_01_16	4.11	6.63	8.19	9.62	4.23	310.85	31.31	66.90
17	nut_sol_0500ppbSe_2014_01_16	4.11	6.63	8.19	9.62	5.41	314.30	30.65	66.49
18	nut_sol_1000ppbSe_2014_01_16	4.11	6.63	8.19	9.62	5.16	318.73	32.36	66.93
19	nut_sol_2500ppbSe_2014_01_16	4.10	6.65	8.19	9.62	3.68	254.71	25.14	64.30
20	wash-3	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Std..3-2	4.11	6.70	8.17	9.61	10.06	20.37	30.79	20.54
22	wash-4	4.16	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_2014_02_04	4.10	6.65	8.19	9.62	5.17	242.10	26.12	62.69
24	nut_sol_0005ppbSe_2014_02_04	4.10	6.65	8.19	9.62	3.28	220.91	22.20	61.67
25	nut_sol_0010ppbSe_2014_02_04	4.11	6.64	8.19	9.62	4.68	261.09	21.81	64.28
26	nut_sol_0025ppbSe_2014_02_04	4.10	6.64	8.19	9.62	4.62	257.41	24.05	60.79
27	nut_sol_0050ppbSe_2014_02_04	4.10	6.64	8.19	9.62	4.36	245.82	21.35	59.21
28	nut_sol_0100ppbSe_2014_02_04	4.10	6.63	8.18	9.62	5.43	286.49	29.31	63.15
29	nut_sol_0250ppbSe_2014_02_04	4.10	6.64	8.19	9.61	5.17	273.44	25.57	60.60
30	nut_sol_0500ppbSe_2014_02_04	4.10	6.63	8.19	9.61	5.80	283.50	30.45	64.24
31	nut_sol_1000ppbSe_2014_02_04	4.10	6.64	8.19	9.62	3.38	240.83	26.70	60.50
32	nut_sol_2500ppbSe_2014_02_04	4.11	6.63	8.18	9.62	6.94	283.51	29.99	62.57
33	wash-5	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Std.3-3	4.11	6.70	8.17	9.61	10.24	20.75	31.29	20.85
35	wash-6	4.06	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table A.63.: A3 analytical data - IC measurement VI

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	22.04.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.10	Cl ⁻	XQOff	5	-0.004	0.153	0.001	99.9973	
Calib_2	6.63	NO ₃ ⁻	XQOff	5	-0.013	0.080	0.000	99.9992	
Calib_3	8.19	PO ₄ ³⁻	XQOff	5	-0.001	0.042	0.000	99.9999	
Calib_4	9.62	SO ₄ ²⁻	XQOff	5	-0.020	0.107	0.000	99.9990	
mean:					-0.0094	0.0954	0.0004	99.9990	
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.09	6.70	8.10	9.46	2.02	3.99	6.00	4.00
2	Standard_2	4.09	6.68	8.09	9.46	4.92	9.99	15.00	9.98
3	Standard_3	4.09	6.66	8.07	9.44	10.01	20.10	30.05	20.07
4	Standard_4	4.10	6.62	8.06	9.43	20.06	39.89	59.95	39.94
5	Standard_5	4.11	6.57	8.03	9.40	39.98	80.03	120.01	80.01
6	wash-1	4.18	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Std.3-1	4.13	6.72	8.27	9.77	10.20	20.69	30.95	20.71
8	wash-2	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	nut_sol_blind_0000ppbSe_nit	4.12	6.66	8.28	9.76	4.26	304.78	28.67	67.87
10	nut_sol_0000ppbSe_2013_11_21	4.13	6.69	8.27	9.76	8.28	204.98	20.90	70.32
11	nut_sol_0005ppbSe_2013_11_21	4.12	6.69	8.27	9.76	2.42	224.10	24.52	70.56
12	nut_sol_0010ppbSe_2013_11_21	4.12	6.67	8.27	9.75	4.69	314.39	31.44	72.34
13	nut_sol_0025ppbSe_2013_11_21	4.13	6.67	8.27	9.76	3.98	334.16	32.53	72.22
14	nut_sol_0050ppbSe_2013_11_21	4.12	6.66	8.27	9.76	4.13	327.50	30.64	71.07
15	nut_sol_0100ppbSe_2013_11_21	4.12	6.66	8.27	9.76	5.37	326.01	31.36	72.78
16	nut_sol_0250ppbSe_2013_11_21	4.12	6.68	8.27	9.75	3.45	282.02	26.84	70.16
17	nut_sol_0500ppbSe_2013_11_21	4.13	6.67	8.27	9.76	4.28	330.19	35.76	70.54
18	nut_sol_1000ppbSe_2013_11_21	4.12	6.67	8.27	9.76	4.10	324.30	33.24	69.77
19	nut_sol_2500ppbSe_2013_11_21	4.13	6.69	8.27	9.76	3.33	266.46	25.99	66.27
20	wash-3	4.12	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Std.3-2	4.13	6.75	8.25	9.75	10.27	20.89	31.67	21.00
22	wash-4	4.12	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_2013_12_12	4.13	6.70	8.27	9.76	3.90	222.72	15.38	63.44
24	nut_sol_0005ppbSe_2013_12_12	4.13	6.70	8.27	9.76	4.28	217.17	21.79	57.98
25	nut_sol_0010ppbSe_2013_12_12	4.12	6.69	8.27	9.76	4.03	234.08	20.68	63.31
26	nut_sol_0025ppbSe_2013_12_12	4.12	6.68	8.27	9.76	4.60	281.11	24.26	63.79
27	nut_sol_0050ppbSe_2013_12_12	4.13	6.68	8.26	9.75	6.02	276.75	22.32	60.70
28	nut_sol_0100ppbSe_2013_12_12	4.13	6.69	8.27	9.76	6.52	255.88	24.21	62.89
29	nut_sol_0250ppbSe_2013_12_12	4.12	6.68	8.26	9.75	4.58	273.37	20.77	63.00
30	nut_sol_0500ppbSe_2013_12_12	4.12	6.68	8.27	9.76	4.44	286.86	23.75	64.05
31	nut_sol_1000ppbSe_2013_12_12	4.13	6.68	8.26	9.75	5.83	283.96	25.35	64.07
32	nut_sol_2500ppbSe_2013_12_12	4.12	6.69	8.26	9.76	4.54	242.21	25.43	63.71
33	wash-5	4.11	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Std.3-3	4.13	6.75	8.25	9.75	10.28	21.05	31.84	21.16
35	wash-6	4.12	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table A.64.: *A3 ICP-MS analysis datasheet I for nutrient solution experiments with Na₂SeO₄ (planted 22.1.2012)*

Technique	ICP-MS Quadrupole																			
System	X-Series Thermo Fischer																			
Date measured	23.01.2013																			
Isotope	¹¹ B	²³ Na	²⁵ Mg	²⁶ Mg	³¹ P	³⁹ K	⁴² Ca	⁴³ Ca	⁵⁵ Mn	⁵⁶ Fe	⁶³ Cu	⁶⁵ Cu	⁶⁴ Zn	⁶⁶ Zn	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	⁹⁸ Mo	
	[µg/L]	[µg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[µg/L]											
Analytical Quality																				
wash-mean	0.65	3.56	0.000	0.000	0.004	0.02	0.17	0.001	0.005	0.32	0.07	0.06	0.18	0.18	0.18	0.09	0.13	0.19	0.01	
wash-SD	0.52	1.65	0.000	0.000	0.000	0.02	0.05	0.001	0.002	0.17	0.02	0.02	0.05	0.05	0.05	0.05	0.04	0.05	0.00	
LOD (= 3-wash)	1.6	5.0	0.000	0.000	0.004	0.05	0.14	0.002	0.006	0.50	0.06	0.06	0.15	0.14	0.15	0.15	0.12	0.15	0.01	
HighPurityStd ref. value	30.00	460.00	1.60	1.60	1.60	0.50	6.20	6.20	8.00	18.00	4.00	4.00	15.00	15.00	2.20	2.20	2.20	2.20	22.00	
Quality [%]	106.20	102.25	102.91	102.84	102.84	104.60	103.47	102.90	101.79	109.42	106.21	107.33	106.03	103.30	119.41	104.66	109.09	109.27	100.30	
Calibration																				
Std 0ppb	0.14	0.71	0.00	0.00	0.00	0.00	0.07	0.00	0.01	0.15	0.08	0.07	0.16	0.16	0.13	0.05	0.09	0.06	0.00	
Std 0.5ppb	4.83	0.10	0.00	0.00	0.01	0.00	0.11	0.05	0.51	5.08	0.56	0.55	5.04	4.95	5.15	5.03	4.96	5.04	0.50	
Std 1ppb	9.90	3.08	0.00	0.00	0.01	0.01	0.16	0.10	1.02	10.35	1.08	1.11	10.13	10.17	9.70	10.12	9.95	10.03	1.01	
Std 2.5ppb	25.02	2.79	0.00	0.00	0.03	0.01	0.29	0.25	2.54	25.14	2.55	2.57	24.90	24.92	25.12	24.92	24.26	25.32	2.51	
Std 5.0ppb	50.20	4.73	0.01	0.00	0.05	0.01	0.53	0.48	5.07	50.24	5.02	5.05	49.56	49.94	50.08	48.69	49.95	50.05	5.01	
Std 10ppb	99.92	9.56	0.01	0.01	0.11	0.01	1.01	0.97	10.08	99.93	9.89	9.88	99.04	99.11	98.94	97.95	98.67	99.90	9.92	
Std 25ppb	241.6	24.21	0.02	0.03	0.11	0.03	2.40	2.39	24.99	249.9	24.53	24.74	245.9	246.5	246.3	243.8	245.6	247.4	24.77	
Std 50ppb	493.5	49.81	0.05	0.05	0.50	0.05	4.86	4.91	50.23	494.8	49.51	50.14	498.9	498.5	501.6	498.10	498.3	501.0	50.13	
Std 100ppb	1000	101.4	0.10	0.10	1.00	0.11	9.64	9.78	101.3	981.7	100.0	100.4	1002	1002	999.3	1003	1001	1001	101.8	
Std 500ppb/5ppm P	9.76	505.8	0.48	0.48	5.00	0.49	0.07	0.32	510.9	489.6	0.09	0.30	0.46	0.59	0.76	0.66	0.64	0.87	0.08	
Std 1000ppb/10ppm P	4.58	993.7	0.98	0.98	10.00	1.01	0.08	0.65	999.9	973.2	0.12	0.54	0.69	1.04	0.28	0.26	0.26	0.27	0.03	
Std 5ppm Na,Mg,K,Fe /25ppm Ca	3.12	4995	4.97	4.98	0.01	4.97	24.64	24.52	0.20	5003	0.07	0.07	0.16	0.15	0.16	0.14	0.19	0.27	0.02	
Std 10ppm Na,Mg,K /50ppm Ca	2.13	10000	10.00	10.01	0.01	10.02	50.31	50.36	0.03	1.15	0.08	0.08	0.18	0.19	0.30	0.13	0.14	0.15	0.01	
Samples																				
wash 2	1.60	3.83	0.00	0.00	0.00	0.01	0.20	0.00	0.01	0.32	0.07	0.07	0.17	0.16	0.17	0.08	0.12	0.20	0.01	
HPS VF 5	33.20	463.7	1.65	1.66	0.01	0.51	6.50	6.44	8.15	19.43	4.20	4.26	15.79	15.41	2.77	2.38	2.35	2.46	22.59	
wash 3	1.07	3.06	0.00	0.00	0.00	0.01	0.19	0.00	0.01	0.32	0.07	0.07	0.18	0.17	0.15	0.06	0.11	0.17	0.02	
2500ppb_2012_11_22	113.2	1462	8.54	8.57	13.13	57.68	108.1	108.4	77.00	2160	27.32	27.32	61.02	61.36	2712	2836	2846	2838	8.04	
1000ppb_2012_11_22	104.1	642.4	8.81	8.78	13.17	75.46	109.3	110.1	75.50	2184	28.58	28.44	72.02	71.76	1100	1152	1159	1142	8.04	
0500ppb_2012_11_22	103.8	368.6	8.93	8.88	13.42	47.30	109.3	109.7	76.10	2180	29.84	29.80	74.38	74.38	547.6	586.6	584.2	570.0	7.91	
0250ppb_2012_11_22	104.1	234.0	9.03	9.04	13.34	47.24	108.0	108.4	76.00	2222	29.68	29.40	73.74	73.90	281.4	293.0	293.0	284.2	7.95	
0100ppb_2012_11_22	112.0	147.4	9.14	9.14	13.50	48.10	107.7	108.4	76.22	2288	30.06	29.92	63.24	62.96	109.8	112.4	114.3	111.9	8.06	
0050ppb_2012_11_22	113.2	112.5	9.17	9.16	13.49	47.52	106.4	107.6	75.42	2240	29.04	29.00	59.36	59.56	55.94	57.74	55.58	55.58	7.88	
0025ppb_2012_11_22	111.9	132.0	9.14	9.11	13.34	47.50	106.1	107.1	75.00	2220	29.24	28.78	59.36	58.60	28.24	27.74	28.54	28.58	7.79	
0010ppb_2012_11_22	103.2	53.48	9.19	9.15	13.54	48.14	109.7	110.3	75.30	2234	29.88	29.74	59.14	59.20	11.72	11.71	11.57	11.57	7.85	
0005ppb_2012_11_22	101.3	36.28	9.14	9.10	13.35	47.02	105.7	106.6	76.42	2196	29.10	28.92	58.46	58.30	5.74	6.15	6.43	7.81	7.81	
0000ppb_2012_11_22	101.3	50.54	9.11	9.11	13.58	48.02	108.0	108.6	76.42	2236	29.58	29.54	63.06	63.46	<0.14	<0.14	0.27	0.27	7.97	
wash 4	0.51	6.39	0.00	0.00	0.01	0.08	0.21	0.00	0.01	0.73	0.11	0.11	0.30	0.29	0.20	0.06	0.13	0.13	0.01	
test 5ppb	50.71	8.76	0.01	0.01	0.05	0.05	0.66	0.51	4.96	53.59	5.39	5.36	51.63	51.63	49.13	49.52	49.62	49.03	4.75	
wash 5	0.24	4.00	0.00	0.00	0.00	0.04	0.17	0.00	0.01	0.30	0.08	0.08	0.23	0.23	0.27	0.18	0.22	0.27	0.01	
2500ppb_2012_12_11	176.0	4140	7.89	7.87	7.25	26.64	98.28	98.84	6.51	294.4	7.39	7.34	21.52	21.64	2346	2462	2464	2434	6.71	
1000ppb_2012_12_11	151.0	171.9	8.59	8.56	10.74	34.28	112.2	112.9	31.42	218.6	18.76	18.61	35.72	36.22	988.0	1046	1046	1025	6.53	
0500ppb_2012_12_11	164.1	3486	8.19	8.11	10.45	32.84	104.5	104.7	10.63	300.4	18.30	18.30	23.02	23.14	476.8	504.6	504.4	485.6	7.20	
0250ppb_2012_12_11	162.1	3142	8.11	8.20	2.69	28.92	92.08	92.44	3.62	86.22	18.10	18.10	13.69	13.70	243.2	243.2	255.6	253.2	7.13	
0100ppb_2012_12_11	171.0	2932	8.25	8.24	8.80	28.20	108.30	108.3	11.48	275.8	14.49	14.45	18.27	18.02	96.06	100.9	100.9	97.36	7.06	
0050ppb_2012_12_11	171.0	3624	8.48	8.46	6.76	32.90	102.8	103.1	8.23	112.6	17.20	17.06	16.60	16.67	49.32	51.48	50.46	50.38	7.27	
0025ppb_2012_12_11	172.2	3992	8.33	8.38	4.69	31.20	97.64	97.86	7.86	102.0	13.62	13.58	13.61	13.45	25.74	24.78	25.18	25.00	7.06	
0010ppb_2012_12_11	160.0	3652	8.46	8.45	9.29	29.98	107.3	109.1	14.71	348.2	6.32	6.27	18.25	18.26	9.36	9.33	10.16	10.45	6.91	
0005ppb_2012_12_11	162.8	3366	8.56	8.52	8.74	30.96	107.2	107.3	15.50	209.6	16.88	16.83	24.84	24.82	5.04	4.78	5.16	6.31	7.24	
0000ppb_2012_12_11	158.9	3492	8.52	8.51	8.22	28.68	108.8	109.4	9.35	53.24	11.55	11.72	18.34	18.27	<0.14	<0.14	<0.14	<0.14	6.99	
wash 6	1.00	5.41	0.00	0.00	0.00	0.05	0.21	0.00	0.00	0.32	0.06	0.05	0.16	0.16	0.13	0.04	0.10	0.20	0.01	
test 5ppb	51.16	11.54	0.01	0.00	0.01	0.04	0.65	0.49	5.06	53.30	5.30	5.31	52.41	52.47	51.96	50.79	51.11	50.64	4.79	
wash 7	0.41	2.80	0.00	0.00	0.01	0.08	0.18	0.00	0.00	0.22	0.04	0.04	0.16	0.17	0.19	0.16	0.16	0.18	0.01	
blind_VF2	89.74	58.68	8.01	7.99	12.37	44.68	103.5	104.6	73.70	2080	26.34	26.48	65.30	66.48	<0.14	<0.14	<0.14	<0.14	7.41	
conc_A_VF500	18755	18150	2601	20.00	2495	3226	20535	114.5	114.5	2564	1549	1549	3371	2702	<0.14	<0.14	<0.14	<0.14	88.50	
conc_B_VF500	<1.6	14670	1601	1600	<0.004	5740	<0.004	6.00	6.00	426650	5525	5495	11015	11105	<0.14	<0.14	<0.14	<0.14	1403	
test 5ppb	30.52	477.00	1.64	1.64	0.00	0.04	0.17	0.00	0.00	0.35	0.04	0.04	0.15							

Table A.65.: A3 ICP-MS analysis datasheet II for nutrient solution experiments with Na₂SeO₃ (planted 10.01.2013)

Technique		ICP-MS Quadrupole																	
System		X-Series Thermo Fischer																	
Date measured		20.02.2013																	
Isotope	¹¹ B [µg/L]	²³ Na [µg/L]	²⁵ Mg [mg/L]	²⁶ Mg [mg/L]	³¹ P [mg/L]	³⁹ K [mg/L]	⁴² Ca [mg/L]	⁴³ Ca [mg/L]	⁵⁵ Mn [µg/L]	⁵⁶ Fe [µg/L]	⁶³ Cu [µg/L]	⁶⁵ Cu [µg/L]	⁶⁴ Zn [µg/L]	⁶⁶ Zn [µg/L]	⁷⁶ Se [µg/L]	⁷⁷ Se [µg/L]	⁷⁸ Se [µg/L]	⁸² Se [µg/L]	⁹⁸ Mo [µg/L]
HighPurityStd ref. value	30.00	460.00	1.60	1.60	0.02	0.50	6.20	6.20	8.00	18.00	4.00	4.00	15.00	15.00	2.20	2.20	2.20	2.20	22.00
Quality	1.06	1.05	1.01	1.01	1.04	1.04	1.06	1.06	1.03	1.05	1.05	1.06	1.09	1.06	1.18	0.99	1.11	1.11	0.99
Analytical Quality																			
wash-mean	0.79	3.07	0.0002	0.0002	0.001	0.02	0.05	0.002	0.006	0.30	0.06	0.06	0.19	0.19	0.13	0.07	0.14	0.11	0.01
wash-SD	0.36	1.83	0.0001	0.0001	0.001	0.01	0.03	0.001	0.003	0.10	0.02	0.02	0.07	0.08	0.06	0.03	0.04	0.05	0.01
LOD (= 3 wash)	1.08	5.48	0.0003	0.0003	0.002	0.04	0.08	0.003	0.010	0.29	0.05	0.05	0.22	0.23	0.17	0.09	0.11	0.16	0.02
Calibration																			
Std 0ppb	0.34	0.25	0.00	0.00	0.00	0.00	0.03	0.00	0.00	0.24	0.04	0.04	0.18	0.17	0.01	0.01	0.07	0.03	0.00
Std 0.5ppb	4.86	0.71	0.00	0.00	0.01	0.00	0.08	0.05	0.50	5.25	0.63	0.62	5.21	5.27	4.93	4.86	5.06	4.85	0.50
Std 1ppb	9.93	4.89	0.00	0.00	0.01	0.01	0.12	0.11	1.03	10.34	1.11	1.12	10.31	10.45	10.06	9.98	9.81	10.41	1.00
Std 2.5ppb	25.32	2.21	0.00	0.00	0.03	0.00	0.27	0.25	2.56	25.74	2.61	2.59	25.53	25.59	24.93	25.01	25.74	25.12	2.51
Std 5ppb	50.58	4.06	0.01	0.01	0.05	0.00	0.52	0.50	5.05	50.92	5.16	5.13	50.68	50.70	52.03	49.95	50.32	50.44	4.99
Std 10ppb	99.64	9.94	0.01	0.01	0.10	0.01	0.99	0.99	9.88	100.60	10.01	10.06	99.63	99.52	100.00	99.59	100.60	99.01	9.83
Std 25ppb	242.40	24.79	0.02	0.02	0.25	0.03	2.48	2.46	24.80	249.50	24.98	25.09	246.90	247.90	246.00	247.50	248.80	248.40	24.54
Std 50ppb	489.90	49.30	0.05	0.05	0.51	0.05	4.86	4.94	49.70	481.30	49.95	50.14	498.70	499.10	501.40	501.30	500.40	502.10	49.57
Std 100ppb	999.80	99.17	0.10	0.10	1.00	0.10	10.07	10.04	100.20	986.00	100.00	99.89	1001.00	1001.00	1000.00	996.20	996.70	999.40	100.30
Std 500ppb/5ppm P	11.36	502.20	0.48	0.48	4.95	0.51	-0.01	0.29	501.00	509.20	0.08	0.30	0.40	0.56	0.48	0.44	0.50	0.59	0.09
Std 1000ppb/10ppm P	8.31	1008.00	0.98	0.98	10.02	1.02	-0.01	0.61	1000.00	1043.00	0.11	0.53	0.72	1.04	0.30	0.18	0.26	0.26	0.04
Std 5ppm Na,Mg,K,Fe /25ppm Ca	3.11	4987.00	4.99	4.99	0.00	4.95	24.87	24.77	0.21	5002.00	0.07	0.07	0.18	0.17	0.07	0.10	0.16	0.16	0.03
Std 10ppm Na,Mg,K /50ppm Ca	2.17	10010.00	10.01	10.01	0.00	10.03	50.19	50.24	0.04	1.03	0.07	0.08	0.21	0.20	0.10	0.09	0.16	0.17	0.01
Samples																			
HPS VF 5	32.50	459.90	1.60	1.61	0.01	0.50	6.45	6.44	8.26	18.73	4.18	4.17	15.67	15.43	2.60	2.52	2.36	2.23	22.82
wash 3	0.85	1.07	0.00	0.00	0.00	0.00	0.07	0.00	0.00	0.18	0.04	0.04	0.08	0.09	0.10	0.05	0.11	0.08	0.02
2500ppb_2013_01_10	100.32	1524	7.80	7.82	13.08	44.04	101.7	101.6	73.32	1937	24.12	24.16	61.76	61.96	2768	2880	2890	2910	7.66
1000ppb_2013_01_10	98.36	652.4	7.93	7.92	13.16	45.10	104.7	104.6	73.56	1962	24.12	24.04	58.84	59.00	1107	1168	1161	1170	7.62
0500ppb_2013_01_10	99.06	378.8	8.10	8.09	13.21	45.38	108.0	107.7	73.22	2022	25.08	25.24	57.72	57.68	540.4	566.6	571.8	570.8	7.65
0250ppb_2013_01_10	100.6	242.6	8.32	8.29	13.60	46.46	112.2	112.0	74.70	2050	25.28	25.26	65.16	65.46	275.4	287.4	286.8	288.0	7.66
0100ppb_2013_01_10	100.8	508.4	8.34	8.34	13.64	46.30	112.9	112.9	74.72	2060	24.94	25.14	68.42	68.38	110.3	113.7	116.6	115.7	7.57
0050ppb_2013_01_10	100.8	110.1	8.44	8.42	13.85	46.14	114.9	114.9	74.88	2148	26.30	26.78	67.40	67.40	56.62	57.44	57.98	58.42	7.74
0025ppb_2013_01_10	100.7	101.0	8.44	8.42	13.81	46.54	115.8	115.1	75.06	2136	26.76	26.78	67.70	67.70	27.80	28.86	28.94	28.58	7.72
0100ppb_2013_01_10	99.70	102.6	8.64	8.63	13.45	46.82	114.6	114.5	75.96	2126	27.66	27.82	66.14	66.02	11.87	12.02	12.08	11.69	7.85
0005ppb_2013_01_10	97.80	144.6	8.78	8.78	13.22	47.04	113.5	113.6	76.82	2110	28.88	28.92	64.98	64.68	6.13	5.96	6.01	5.54	7.95
0000ppb_2013_01_10	98.16	83.80	8.65	8.66	13.44	46.98	111.8	111.8	77.22	2088	28.84	28.68	65.84	65.32	<0.13	<0.13	<0.13	<0.13	7.81
blind_2013_01_09	90.36	66.54	8.22	8.19	12.47	44.28	105.5	105.7	73.62	2110	27.06	27.20	59.82	59.98	<0.13	<0.13	<0.13	<0.13	7.51
wash 4	0.69	3.70	0.00	0.00	0.00	0.04	0.06	0.00	0.01	0.47	0.07	0.07	0.17	0.17	0.18	0.07	0.14	0.10	0.01
test 5ppb	51.52	10.57	0.01	0.01	0.05	0.03	0.60	0.55	5.05	54.55	5.40	5.37	53.10	53.26	50.35	49.29	50.09	49.13	4.95
wash 5	0.37	2.80	0.00	0.00	0.00	0.02	0.04	0.00	0.01	0.30	0.05	0.05	0.19	0.19	0.16	0.11	0.17	0.10	0.01
2500ppb_2013_01_29	143.02	4064	7.07	7.08	10.16	30.90	93.86	93.62	50.92	626.4	13.87	13.91	39.66	39.94	2434	2526	2532	2506	6.55
1000ppb_2013_01_29	142.7	3368	7.28	7.27	11.22	33.96	96.98	97.32	48.50	405.8	6.55	6.55	33.82	33.38	776.4	808.8	810.0	804.2	7.42
0500ppb_2013_01_29	140.6	3516	7.60	7.57	11.26	35.98	99.12	99.20	31.46	227.6	12.73	12.73	28.72	28.56	390.2	412.6	412.4	405.4	6.72
0250ppb_2013_01_29	143.6	2554	7.47	7.46	10.48	26.50	99.66	99.90	26.40	322.0	17.36	17.47	26.16	26.04	232.6	244.8	242.6	242.8	7.30
0100ppb_2013_01_29	148.4	2626	7.33	7.31	9.11	23.56	100.2	100.2	16.71	317.0	14.63	14.57	16.68	16.64	96.00	100.6	100.3	99.68	6.77
0050ppb_2013_01_29	153.2	2800	7.81	7.76	10.24	26.92	105.8	106.0	6.93	293.4	12.05	12.12	19.31	19.26	48.16	50.70	51.78	52.34	7.01
0025ppb_2013_01_29	154.5	3098	7.67	7.63	11.01	31.24	102.3	102.4	19.15	160.8	13.78	13.71	23.82	23.86	24.98	25.84	25.22	25.50	6.99
0010ppb_2013_01_29	140.6	2460	7.66	7.63	10.21	26.18	99.48	99.48	18.49	188.2	12.23	12.02	13.62	13.50	9.83	9.99	9.87	11.22	6.90
0005ppb_2013_01_29	146.8	3032	7.84	7.82	11.29	28.40	99.76	99.76	22.06	145.7	17.16	17.05	22.52	22.56	4.30	4.76	4.97	6.09	7.13
0000ppb_2013_01_29	152.6	2944	7.74	7.73	10.36	27.30	97.84	97.44	26.76	345.4	19.75	19.66	31.46	31.46	<0.13	<0.13	<0.13	1.74	7.05
wash 6	1.01	5.20	0.00	0.00	0.00	0.03	0.07	0.00	0.01	0.36	0.08	0.07	0.24	0.25	0.17	0.09	0.14	0.15	0.01
test 5ppb	51.46	20.78	0.01	0.01	0.05	0.05	0.57	0.54	5.00	54.65	5.36	5.35	53.41	53.01	48.98	49.29	49.08	49.32	4.90
HPS VF 5 wd	31.67	481.60	1.61	1.61	0.01	0.52	6.59	6.59	8.21	18.86	4.20	4.25	16.35	15.89	2.59	2.17	2.44	2.44	21.85
HPS VF 5 Ref.-Wert	30.00	460.00	1.60	1.60	0.00	0.50	6.20	6.20	8.00	18.00	4.00	4.00	15.00	15.00	2.20	2.20	2.20	2.20	22.00
wash 7	0.94	5.34	0.00	0.00	0.00	0.02	0.00	0.00	0.01	0.25	0.08	0.09	0.23	0.23	0.17	0.09	0.19	0.25	0.03

Table A.66.: *A3 ICP-MS analysis datasheet III for nutrient solution experiments with Na₂SeO₃ (planted 12.09.2013) (continued from previous page)*

Technique		ICP-MS Quadrupole																		
System		X-Series Thermo Fischer																		
Date measured		16.01.2014																		
Isotope	¹¹ B	²³ Na	²⁵ Mg	²⁶ Mg	³¹ P	³⁹ K	⁴² Ca	⁴³ Ca	⁵⁵ Mn	⁵⁶ Fe	⁶³ Cu	⁶⁵ Cu	⁶⁴ Zn	⁶⁶ Zn	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	⁹⁸ Mo	
	[µg/L]	[µg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[µg/L]											
Analytical Quality	wash-mean	1.59	1.81	0.000	0.000	0.01	0.02	0.14	0.00	0.01	0.14	0.00	0.01	0.56	0.03	0.03	0.38	0.07	0.07	0.08
	wash-SD	0.53	1.13	0.000	0.000	0.00	0.01	0.05	0.01	0.26	0.02	0.02	0.17	0.02	0.02	0.04	0.17	0.04	0.04	0.02
	LOD (= 3-wash)	1.59	3.39	0.001	0.001	0.01	0.03	0.15	0.02	0.77	0.06	0.06	0.51	0.06	0.11	0.51	0.05	0.05	0.11	0.04
HighPurityStd ref. value	Quality	32.44	460.50	1.64	1.65	1.03	1.02	6.88	8.16	18.47	4.09	4.11	15.27	14.98	2.88	2.26	2.39	2.34	22.52	
Calibration																				
Std 0ppb	0.44	0.50	0.00	0.00	0.00	0.01	0.01	0.01	0.00	0.32	0.00	0.00	0.08	0.08	0.06	0.08	0.07	0.38	0.00	
Std 0.5ppb	5.17	4.97	0.00	0.00	0.01	0.01	0.06	0.05	0.49	5.20	0.54	0.54	5.20	5.22	5.03	5.04	4.84	5.40	0.00	
Std 1ppb	10.11	10.11	0.00	0.00	0.01	0.01	0.10	0.10	1.02	10.30	1.05	1.02	10.24	10.33	10.16	10.48	9.89	10.20	0.51	
Std 2.5ppb	24.58	2.84	0.00	0.00	0.03	0.01	0.25	0.26	2.52	25.19	2.56	2.59	25.46	25.34	25.25	25.87	24.84	25.44	2.60	
Std 5ppb	48.85	5.30	0.01	0.01	0.05	0.01	0.50	0.51	4.97	50.22	5.12	5.15	50.73	51.02	49.39	50.47	49.90	51.25	5.14	
Std 10ppb	97.11	10.22	0.01	0.01	0.10	0.02	1.01	1.02	9.95	99.73	10.26	10.07	100.9	100.9	100.9	100.8	100.4	99.4	10.29	
Std 25ppb	241.4	25.04	0.03	0.03	0.25	0.03	2.51	2.52	24.71	251.7	25.30	25.21	250.0	250.0	250.0	249.7	249.9	250.1	25.42	
Std 50ppb	484.0	49.63	0.05	0.05	0.50	0.05	4.93	4.94	49.28	498.6	49.78	49.81	494.3	493.6	498.5	491.7	490.0	499.0	49.71	
Std 100ppb	1011	100.7	0.10	0.10	1.00	0.10	10.03	10.02	100.4	1007	100.6	100.0	1003	1003	1000	999.2	1000	1001	100.7	
Std 500ppb / 5ppm P	11.50	484.1	0.50	0.49	4.99	0.48	49.99	51.45	506.0	506.0	0.06	0.20	0.49	0.49	0.53	0.57	0.71	0.53	0.19	
Std 1000ppb / 10ppm P	5.47	985.9	1.00	1.00	10.00	0.97	0.00	0.48	1001	1031	0.07	0.37	0.88	0.92	0.32	0.32	0.32	0.27	0.08	
Std 5ppm Na,Mg,K,Fe	3.83	5077	4.81	4.84	4.84	4.97	0.25	0.21	0.21	5014	0.05	0.06	0.26	0.26	0.23	0.25	0.25	0.21	0.01	
Std 10ppm Na,Mg,K	3.00	10000	10.11	10.09	10.09	10.00	0.14	0.02	0.03	6.65	0.03	0.04	0.23	0.24	0.13	0.15	0.15	0.15	0.05	
Std 25ppm Ca	2.49	2.00	0.00	0.00	0.01	0.02	0.14	0.02	0.02	1.76	0.09	0.09	0.30	0.30	0.18	0.12	0.14	0.17	0.03	
Std 50ppm Ca	1.97	1.41	0.00	0.00	0.00	0.03	0.00	0.00	0.01	0.66	0.02	0.03	0.22	0.21	0.19	0.11	0.13	0.21	0.02	
Samples																				
wash 2	1.71	1.57	0.00	0.00	0.00	0.01	0.15	0.00	0.00	0.30	0.02	0.02	0.16	0.15	0.12	0.06	0.12	0.17	0.02	
HPS VF 5	32.44	460.50	1.64	1.65	1.03	1.02	6.88	6.72	8.16	18.47	4.09	4.11	15.27	14.98	2.88	2.26	2.39	2.34	22.52	
wash 3	1.57	0.80	0.00	0.00	0.01	0.01	0.13	0.00	0.00	0.25	0.01	0.01	0.32	0.31	0.12	0.06	0.12	0.26	0.05	
2013_09_12_SeV1_2500ppb	422.2	6311	33.56	33.30	33.30	181.4	412.7	415.4	314.9	8368	102.9	102.4	273.3	273.52	6395.30	6379.27	6383.28	6383.28	15.28	
2013_09_12_SeV1_1000ppb	425.0	2735	34.94	34.82	34.82	185.0	440.0	443.0	317.3	8640	106.5	105.4	253.3	254.08	2546.74	2554.36	2561.98	2580.03	15.45	
2013_09_12_SeV1_0500ppb	703.5	2586	35.46	35.40	35.40	193.1	449.8	45.7	324.5	102.9	103.3	295.8	297.84	1313.03	1319.86	1318.65	1318.65	15.48		
2013_09_12_SeV1_0250ppb	845.6	1476	32.19	31.92	32.19	174.6	412.6	413.0	296.3	65.2	65.2	302.2	303.8	646.9	656.9	655.7	661.3	14.32		
2013_09_12_SeV1_0100ppb	555.3	1477	20.61	20.51	20.51	119.0	287.4	279.4	197.0	50.04	65.2	65.74	201.2	202.8	254.7	256.8	256.0	260.4	9.26	
2013_09_12_SeV1_0050ppb	737.5	1846	27.87	27.66	27.66	173.2	377.4	367.8	257.0	62.34	83.6	83.76	271.7	272.3	352.7	358.0	352.0	360.4	12.56	
2013_09_12_SeV1_0025ppb	428.4	692.2	26.19	26.10	26.10	173.5	367.4	356.5	245.9	83.4	83.4	83.76	212.5	214.5	67.39	67.43	69.45	67.92	11.98	
2013_09_12_SeV1_0010ppb	418.6	342.4	35.24	35.01	35.01	193.8	456.1	460.2	319.9	91.68	108.7	109.2	28.82	28.74	29.09	29.32	28.74	29.32	15.38	
2013_09_12_SeV1_0005ppb	291.8	272.2	22.97	22.93	22.93	170.0	345.4	337.8	215.2	87.78	75.7	75.75	176.2	177.1	131.4	135.58	130.07	133.08	10.49	
2013_09_12_SeV1_0000ppb	396.7	396.3	33.50	33.42	33.42	191.2	438.8	441.9	304.5	88.96	103.3	103.3	280.1	281.9	<0.17	<0.17	<0.17	1.53	14.72	
Test 5ppb	393.0	301.3	34.7	34.5	34.5	186.3	445.4	449.5	309.4	85.84	108.6	108.6	246.0	248.1	<0.17	<0.17	<0.17	1.27	14.82	
wash 4	1.71	3.82	0.00	0.00	0.01	0.04	0.18	0.00	0.01	0.62	0.05	0.04	0.38	0.40	0.16	0.04	0.07	0.18	0.02	
wash 5	52.76	6.82	0.01	0.01	0.03	0.03	0.71	0.56	5.31	53.18	5.33	5.39	53.06	51.52	51.90	51.90	51.60	51.60	4.86	
Test 5ppb	1.45	1.12	0.00	0.00	0.01	0.02	0.14	0.00	0.00	0.36	0.05	0.05	0.28	0.27	0.16	0.16	0.17	0.24	0.02	
wash 5	750.6	17968	31.87	31.61	31.61	102.2	393.8	397.4	68.82	1283	20.45	20.58	45.13	45.76	57.35	57.39	57.43	56.70	13.12	
2013_10_01_SeV1_2500ppb	828.0	15264	32.78	32.62	32.62	122.1	401.1	402.0	114.3	3226	28.81	28.78	134.3	134.9	221.7	222.6	223.0	221.7	13.32	
2013_10_01_SeV1_1000ppb	1098	13928	34.02	33.93	33.93	122.4	407.0	407.9	191.6	1082	52.72	52.43	111.0	111.4	118.4	118.8	118.4	118.4	14.08	
2013_10_01_SeV1_0500ppb	1295	16616	33.32	33.32	33.32	125.5	408.8	412.0	201.2	1691	30.4	30.4	573.8	572.2	564.5	573.0	573.0	573.0	14.76	
2013_10_01_SeV1_0250ppb	1234	17712	35.21	35.07	35.07	185.0	471.8	471.8	295.9	1829	67.17	67.58	147.9	148.6	237.1	233.8	240.7	240.7	14.50	
2013_10_01_SeV1_0100ppb	1350	14384	32.78	32.63	32.63	188.3	470.8	471.8	323.34	1864	17.87	17.58	52.74	53.30	111.9	111.9	115.9	116.4	13.82	
2013_10_01_SeV1_0050ppb	947.2	13056	32.26	32.18	32.18	105.1	404.7	406.2	34.45	1482	32.50	32.22	33.14	33.14	58.06	58.30	58.51	58.85	13.54	
2013_10_01_SeV1_0025ppb	844.0	16408	34.66	34.42	34.42	157.4	404.9	406.2	3.50	491.4	31.10	30.91	30.05	30.11	25.89	25.65	25.25	25.25	14.20	
2013_10_01_SeV1_0005ppb	882.4	16872	34.88	34.74	34.74	156.5	410.6	412.0	207.8	1306	63.89	63.46	196.0	197.4	14.00	14.59	14.96	17.53	14.82	
2013_10_01_SeV1_0000ppb	807.2	15064	33.73	33.59	33.59	129.0	393.0	397.2	2.77	624.4	37.94	37.81	24.89	24.62	3.08	3.20	3.67	4.74	13.60	

Table A.67.: A3 ICP-MS analysis datasheet IV for nutrient solution experiments with Na₂SeO₄ (planted 02.10.2013) (continued from previous page)

Technique	ICP-MS Quadrupole																			
System	X-Series Thermo Fischer																			
Date measured	16.01.2014																			
Isotope	¹¹ B	²³ Na	²⁵ Mg	²⁶ Mg	³¹ P	³⁹ K	⁴² Ca	⁴³ Ca	⁵⁵ Mn	⁵⁶ Fe	⁶³ Cu	⁶⁵ Cu	⁶⁴ Zn	⁶⁶ Zn	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	⁹⁸ Mo	
	[µg/L]	[µg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[µg/L]											
Analytical Quality																				
wash-mean	1.59	1.81	0.000	0.000	0.01	0.02	0.14	0.00	0.01	0.56	0.03	0.03	0.38	0.37	0.07	0.07	0.06	0.08	0.02	
wash-SD	0.53	1.13	0.000	0.000	0.00	0.05	0.05	0.00	0.01	0.26	0.02	0.02	0.17	0.17	0.04	0.02	0.02	0.04	0.01	
LOD (= 3-wash)	1.59	3.39	0.001	0.001	0.01	0.15	0.02	0.02	0.02	0.77	0.06	0.06	0.51	0.51	0.11	0.05	0.05	0.11	0.04	
HighPurityStd	32.44	460.5	1.64	1.65	32.44	6.88	6.72	8.16	18.47	4.09	4.11	15.27	14.98	2.88	2.26	2.39	2.34	22.52		
Quality	1.08	1.00	1.03	1.03	1.02	1.11	1.08	1.02	1.03	1.03	1.02	1.03	1.02	1.00	1.31	1.03	1.09	1.06	1.02	
Calibration																				
Std 0ppb	0.44	0.50	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.32	0.00	0.00	0.08	0.08	0.06	0.08	0.07	0.38	0.00	
Std 0.5ppb	5.17	4.97	0.00	0.00	0.01	0.06	0.05	0.49	5.20	5.20	0.54	0.54	5.20	5.22	5.03	5.04	4.84	5.40	0.51	
Std 1ppb	10.11	1.62	0.00	0.00	0.01	0.10	0.10	1.02	10.30	10.30	1.05	1.02	10.24	10.33	10.16	10.48	9.89	10.20	1.03	
Std 2.5ppb	24.58	2.84	0.00	0.00	0.03	0.25	0.26	2.52	25.19	25.19	2.56	2.59	25.46	25.34	25.25	25.87	24.84	25.44	2.60	
Std 5ppb	48.85	5.30	0.01	0.01	0.05	0.50	0.51	4.97	50.22	50.22	5.12	5.15	50.73	51.02	49.39	50.47	49.90	51.25	5.14	
Std 10ppb	97.11	10.22	0.01	0.01	0.10	1.01	1.02	9.95	99.73	99.73	10.26	10.07	100.9	100.8	100.4	102.0	100.6	99.4	10.29	
Std 25ppb	241.4	25.04	0.03	0.03	0.25	2.51	2.52	24.71	253.0	253.0	25.30	25.21	250.0	249.7	250.0	252.3	249.9	250.1	25.42	
Std 50ppb	484.0	49.63	0.05	0.05	0.50	4.93	4.94	49.28	498.6	498.6	49.78	49.81	494.3	493.6	498.5	501.7	500.0	499.0	49.71	
Std 100ppb	1011	100.7	0.10	0.10	1.00	10.03	10.02	100.4	1007	1007	100.6	100.0	1003	1000	1000	999.2	1000	1001	100.7	
Std 500ppb / 5ppm P	11.50	484.1	0.50	0.49	4.99	0.48	0.00	0.24	514.5	506.0	0.06	0.20	0.49	0.53	0.57	0.71	0.53	0.53	0.19	
Std 1000ppb / 10ppm P	5.47	985.9	1.00	1.00	10.00	0.97	0.00	4.81	1031	1031	0.07	0.37	0.88	0.92	0.32	0.32	0.32	0.27	0.08	
Std 5ppm Na,Mg,K,Fe	3.83	5077	4.81	4.84	0.00	4.97	0.25	0.21	5014	5014	0.05	0.06	0.26	0.25	0.23	0.20	0.21	0.01	0.05	
Std 10ppm Na,Mg,K	3.00	10000	10.11	10.09	0.00	10.00	0.14	0.02	0.03	0.65	0.03	0.04	0.23	0.24	0.13	0.15	0.15	0.29	0.03	
Std 25ppm Ca	2.49	2.00	0.00	0.00	0.01	25.67	25.20	0.02	1.76	0.09	0.02	0.09	0.30	0.30	0.18	0.14	0.14	0.17	0.03	
Std 50ppm Ca	1.97	1.41	0.00	0.00	0.00	50.10	50.10	0.01	0.66	0.09	0.03	0.03	0.22	0.21	0.19	0.11	0.13	0.21	0.02	
Samples																				
wash 6	2.99	1.55	0.00	0.00	0.01	0.18	0.18	0.00	0.01	0.78	0.02	0.01	0.34	0.32	0.12	0.06	0.11	0.23	0.02	
Test 5ppb	53.03	7.58	0.01	0.01	0.06	0.69	0.69	0.55	5.30	53.00	5.38	5.38	52.74	52.82	51.52	51.24	51.36	51.94	4.97	
wash 7	1.67	1.38	0.00	0.00	0.01	0.01	0.00	0.00	0.01	0.45	0.02	0.02	0.42	0.43	0.16	0.05	0.13	0.19	0.01	
2013_10_02_SeIV_2500ppb	415.3	6368	34.99	34.85	57.20	439.9	433.9	443.9	345.8	8832	107.6	107.20	263.84	263.68	6005.23	6009.33	6054.42	6042.12	15.96	
2013_10_02_SeIV_1000ppb	424.5	2780	36.54	36.42	59.66	463.9	469.0	469.0	357.5	8872	111.9	111.68	273.12	274.96	2370.93	2387.75	2396.78	2390.22	16.41	
2013_10_02_SeIV_0500ppb	457.4	1626	35.90	35.74	59.18	210.2	210.2	210.2	354.3	8872	111.6	112.72	274.48	275.36	1256.50	1251.98	1256.50	1253.63	15.93	
2013_10_02_SeIV_0250ppb	526.2	1072	35.96	35.89	58.12	208.3	208.3	208.3	353.0	8040	111.1	110.96	288.72	289.20	620.16	617.28	620.16	629.20	15.96	
2013_10_02_SeIV_0100ppb	455.5	633.1	30.66	30.59	53.75	199.8	199.8	199.8	304.6	7769	97.12	97.12	269.60	271.68	243.84	244.66	246.18	245.28	13.77	
2013_10_02_SeIV_0050ppb	469.1	523.8	32.96	32.84	55.51	204.2	204.2	204.2	326.6	7871	102.6	103.04	263.76	265.92	118.77	118.36	119.14	117.86	14.69	
2013_10_02_SeIV_0025ppb	438.2	455.6	33.74	33.60	56.22	198.4	198.4	198.4	330.6	8240	105.9	106.48	261.60	264.72	64.40	62.30	63.99	62.51	14.95	
2013_10_02_SeIV_0010ppb	396.6	352.0	34.59	34.44	58.07	188.9	188.9	188.9	336.3	9864	110.3	110.88	258.48	261.28	26.76	27.09	27.47	27.35	15.60	
2013_10_02_SeIV_0005ppb	391.7	334.8	34.11	33.97	58.46	209.9	209.9	209.9	332.1	9680	108.2	107.68	256.88	257.92	14.76	15.16	15.16	16.16	15.19	
2013_10_02_SeIV_0000ppb	346.5	338.0	29.89	29.74	60.23	414.4	416.3	416.3	323.8	9344	95.92	96.16	226.88	228.08	3.01	<0.17	3.21	<0.17	13.48	
2013_10_02_SeIV_0000ppb	367.0	312.9	32.94	32.83	53.51	191.0	191.0	191.0	312.6	8656	105.2	104.8	244.5	246.9	1.14	<0.17	1.19	1.19	14.19	
test 5ppb	50.49	6.70	0.01	0.01	0.06	0.03	0.70	0.54	5.34	53.20	5.33	5.39	52.86	53.07	52.35	52.61	52.16	52.05	4.80	
wash 9	1.39	1.39	0.00	0.00	0.00	0.14	0.14	0.01	0.01	0.57	0.02	0.02	0.33	0.33	0.17	0.14	0.22	0.27	0.01	
2013_10_21_SeIV_2500ppb	790.0	18648	33.11	32.86	43.02	163.3	163.3	163.3	307.4	3050	58.94	58.70	243.4	244.5	4879	4945	4949	4949	12.80	
2013_10_21_SeIV_1000ppb	864.2	16008	34.58	34.46	40.02	149.4	149.4	149.4	171.7	2784	64.46	64.50	157.9	158.6	2036	2042	2029	2027	13.94	
2013_10_21_SeIV_0500ppb	877.2	13456	33.07	32.89	41.22	120.9	120.9	120.9	187.8	2197	52.47	52.86	100.3	100.3	1036	1042.6	1041	1045	13.34	
2013_10_21_SeIV_0250ppb	893.6	12344	32.85	32.65	39.06	110.0	110.0	110.0	79.1	2205	41.22	41.23	72.14	71.79	512.0	509.9	516.56	507.0	13.08	
2013_10_21_SeIV_0100ppb	865.6	13768	33.69	33.43	37.62	145.6	145.6	145.6	20.4	1086	64.14	63.97	53.14	52.54	46.00	45.50	46.59	48.12	13.65	
2013_10_21_SeIV_0050ppb	824.8	11544	32.98	32.88	37.66	119.9	119.9	119.9	4.94	696.3	46.18	46.42	49.68	50.28	60.78	61.49	61.49	63.40	13.74	
2013_10_21_SeIV_0025ppb	820.8	13824	33.79	33.65	37.91	129.3	129.3	129.3	26.24	2000	52.26	53.10	53.70	54.14	47.55	48.04	49.16	52.12	13.47	
2013_10_21_SeIV_0010ppb	799.9	13064	35.06	34.89	50.20	167.7	167.7	167.7	222.0	2767	72.22	72.48	144.1	145.0	21.55	23.35	23.06	24.73	14.70	
2013_10_21_SeIV_0005ppb	772.2	11296	34.41	34.18	41.70	122.8	122.8	122.8	10.1	2820	42.22	41.82	73.70	73.83	4.96	4.09	4.16	6.29	14.32	
2013_10_21_SeIV_0000ppb	735.7	10336	33.87	33.54	43.67	127.8	127.8	127.8	73.6	2837	27.77	27.96	54.97	54.78	2.00	1.45	1.49	3.83	14.02	
wash 10	2.67	1.53	0.00	0.00	0.01	0.02	0.17	0.00	0.00	0.81	0.01	0.01	0.58	0.57	0.25	0.15	0.16	0.18	0.02	
test 5ppb	51.80	7.10	0.01	0.01	0.05	0.69	0.54	0.54	5.38	53.50	5.33	5.34	53.55	53.56	52.26	51.31	51.39	51.78	4.83	
HPS VF 5 wdh	34.09	471.60	1.63	1.62	0.00	0.53	6.74	6.52	8.38	19.13	4.13	4.18	15.70	15.18	2.84	2.51	2.36	2.55	21.19	
wash 11	1.68	2.02	0.00	0.00	0.00	0.15	0.02	0.01	0.01	0.48	0.03	0.02	0.70	0.70	0.21	0.09	0.15			

Table A.68.: *A9 ICP-MS analysis datasheet IV for nutrient solution experiments with Na₂SeO₄ (planted 02.10.2013) (continued from previous page)*

Technique System Date measured		ICP-MS Quadrupole X-Series Thermo Fischer 16.01.2014																		
Isotope	¹¹ B	²³ Na	²⁵ Mg	²⁶ Mg	³¹ P	³⁹ K	⁴² Ca	⁴³ Ca	⁵⁵ Mn	⁵⁶ Fe	⁶³ Cu	⁶⁵ Cu	⁶⁴ Zn	⁶⁶ Zn	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	⁹⁸ Mo	
[µg/L]	[µg/L]	[µg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[mg/L]	[µg/L]											
Analytical Quality	wash-mean	1.59	1.81	0.000	0.000	0.01	0.02	0.14	0.01	0.56	0.03	0.03	0.38	0.37	0.07	0.07	0.06	0.08	0.02	
	wash-SD	0.53	1.13	0.000	0.000	0.00	0.01	0.05	0.01	0.26	0.02	0.02	0.17	0.17	0.04	0.02	0.02	0.04	0.01	
	LOD (= 3-wash)	1.59	3.39	0.001	0.001	0.01	0.03	0.15	0.02	0.77	0.06	0.06	0.51	0.51	0.11	0.05	0.05	0.11	0.04	
HighPurityStd ref value	32.44	460.50	1.64	1.65	1.03	1.02	6.88	6.72	8.16	18.47	4.09	4.11	15.27	14.98	2.88	2.26	2.39	2.34	22.52	
Quality	1.08	1.00	1.03	1.03	1.03	1.02	1.11	1.08	1.02	1.03	1.02	1.03	1.02	1.00	1.31	1.03	1.09	1.06	1.02	
Calibration																				
Std 0ppb	0.44	0.50	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.32	0.00	0.00	0.08	0.08	0.06	0.08	0.07	0.38	0.00	
Std 0.5ppb	5.17	4.97	0.00	0.00	0.01	0.01	0.06	0.05	0.49	5.20	0.54	0.54	5.20	5.22	5.03	5.04	4.84	5.40	0.51	
Std 1ppb	10.11	1.62	0.00	0.00	0.01	0.01	0.10	0.10	1.02	10.30	1.05	1.02	10.24	10.33	10.16	10.48	9.89	10.20	1.03	
Std 2.5ppb	24.58	2.84	0.00	0.00	0.03	0.01	0.25	0.26	2.52	25.19	2.56	2.59	25.46	25.34	25.25	25.87	24.84	25.44	2.60	
Std 5ppb	48.85	5.30	0.01	0.01	0.01	0.01	0.50	0.51	4.97	50.22	5.12	5.15	50.73	51.02	49.39	50.47	49.90	51.25	5.14	
Std 10ppb	97.11	10.22	0.01	0.01	0.10	0.02	1.01	1.02	9.95	99.73	10.26	10.07	100.9	100.8	100.4	102.0	100.6	99.4	10.29	
Std 25ppb	241.4	25.04	0.03	0.03	0.25	0.03	2.51	2.52	24.71	251.7	25.30	25.21	250.0	249.7	250.0	252.3	249.9	250.1	25.42	
Std 50ppb	484.0	49.63	0.05	0.05	0.50	0.05	4.93	4.94	49.28	498.6	49.78	49.81	494.3	493.6	498.5	501.7	500.0	499.0	49.71	
Std 100ppb	1011	100.7	0.10	0.10	1.00	0.10	10.03	10.02	100.4	1007	100.6	100.0	1003	1003	1000	999.2	1000	1001	100.7	
Std 500ppb / 10ppm P	11.50	484.1	0.50	0.49	4.99	0.48	0.00	0.24	514.5	506.0	0.06	0.20	0.49	0.49	0.53	0.57	0.71	0.53	0.19	
Std 1000ppb / 10ppm P	5.47	983.9	1.00	1.00	10.00	0.97	0.00	0.48	1001	1031	0.07	0.37	0.88	0.92	0.32	0.32	0.32	0.27	0.08	
Std 5ppm Na,Mg,K,Fe	3.83	5077	4.81	4.84	0.00	4.97	0.25	0.21	501.4	501.4	0.05	0.06	0.26	0.25	0.23	0.20	0.21	0.01	0.05	
Std 10ppm Na,Mg,K	3.00	10000	10.11	10.09	0.00	10.00	0.14	0.02	0.03	0.65	0.03	0.04	0.23	0.23	0.13	0.15	0.15	0.15	0.03	
Std 25ppm Ca	2.49	2.00	0.00	0.00	0.01	0.02	25.67	25.20	0.02	1.76	0.09	0.09	0.30	0.30	0.18	0.12	0.14	0.17	0.03	
Std 50ppm Ca	1.97	1.41	0.00	0.00	0.00	0.03	50.00	50.10	0.01	0.66	0.02	0.03	0.22	0.21	0.19	0.11	0.13	0.21	0.02	
Samples																				
Test 5ppb wash 6	2.99	1.55	0.00	0.00	0.01	0.02	0.18	0.00	0.01	0.78	0.02	0.01	0.34	0.32	0.12	0.06	0.11	0.23	0.02	
Test 5ppb wash 7	53.03	7.58	0.01	0.01	0.06	0.02	0.69	0.55	5.30	53.00	5.38	5.38	52.74	52.82	51.52	51.24	51.36	51.94	4.97	
2013_10_02 SetV_2500ppb wash 7	1.67	1.38	0.00	0.00	0.00	0.01	0.16	0.00	0.01	0.45	0.02	0.02	0.42	0.43	0.16	0.05	0.13	0.19	0.01	
2013_10_02 SetV_2500ppb	415.2	6368	34.99	34.85	57.20	202.5	439.9	443.9	345.8	883.2	107.6	107.2	263.8	263.7	6005	6054	6054	6042.1	15.86	
2013_10_02 SetV_0500ppb	424.5	2780	36.54	36.42	35.90	210.6	463.9	469.0	357.5	933.8	111.9	111.7	273.1	275.0	2371	2388	2397	2390.2	16.41	
2013_10_02 SetV_0500ppb	457.4	1625	35.90	35.74	35.90	210.6	460.8	465.5	354.3	887.2	111.6	112.7	274.5	275.4	1251	1252	1257	1253.6	15.93	
2013_10_02 SetV_0250ppb	526.2	1072	35.96	35.89	35.89	208.3	461.9	467.8	353.0	804.0	111.1	111.0	274.5	289.2	620.2	617.3	627.2	629.2	15.96	
2013_10_02 SetV_0100ppb	455.5	633.1	30.66	30.59	30.59	199.8	414.6	417.5	304.6	776.9	97.1	97.12	269.6	271.7	243.8	244.7	246.2	245.3	13.77	
2013_10_02 SetV_0050ppb	469.1	453.8	32.96	32.84	32.84	204.2	434.5	437.5	326.6	787.1	102.6	103.0	263.8	265.9	118.8	118.4	119.1	117.9	14.69	
2013_10_02 SetV_0025ppb	488.2	455.0	33.74	33.60	33.60	198.4	437.0	439.2	330.6	824.0	105.9	106.5	261.6	264.7	64.4	62.80	63.99	62.51	14.95	
2013_10_02 SetV_0010ppb	396.6	345.9	34.59	34.44	34.44	208.9	457.7	463.1	336.3	986.4	110.3	110.9	258.5	261.3	26.8	27.09	27.47	27.35	15.60	
2013_10_02 SetV_0005ppb	391.7	334.8	34.11	33.97	33.97	209.9	453.7	458.6	332.8	968.0	108.2	107.7	256.9	257.9	14.8	15.26	15.16	16.16	15.19	
2013_10_02 SetV_0000ppb	346.5	338.0	29.99	29.74	29.74	224.9	414.4	416.3	323.8	934.6	95.9	96.16	226.9	228.1	3.01	<0.17	3.21	<0.17	13.48	
2013_10_02 SetV_bhd	367.0	312.9	32.94	32.83	32.83	191.0	427.2	431.7	312.6	865.6	105.2	104.8	244.5	246.9	1.14	<0.17	<0.17	<0.17	14.19	
test 5ppb wash 8	1.64	4.09	0.00	0.00	0.01	0.04	0.18	0.01	0.02	1.11	0.07	0.07	0.50	0.49	0.13	0.12	0.13	0.14	0.02	
test 5ppb wash 9	50.49	6.70	0.01	0.01	0.01	0.03	0.70	0.54	5.34	53.20	5.33	5.39	52.86	53.07	52.61	52.16	52.16	52.05	4.80	
2013_10_21 SetV_2500ppb	1.39	1.39	0.00	0.00	0.00	0.02	0.14	0.01	0.01	0.57	0.02	0.02	0.33	0.34	0.17	0.14	0.22	0.27	0.01	
2013_10_21 SetV_1000ppb	790.0	18648	33.11	32.86	43.02	163.3	403.0	405.8	307.4	3050	58.94	58.70	243.4	244.5	4879	4945	4949	4949	12.80	
2013_10_21 SetV_1000ppb	784.2	16008	34.88	34.46	40.02	140.9	432.6	435.4	171.7	2784	64.46	64.50	157.9	158.6	2006	2027	2029	2027	13.94	
2013_10_21 SetV_0500ppb	867.2	13456	33.07	32.85	41.22	129.4	415.1	413.8	187.8	2197	52.47	52.47	100.3	100.3	1036	1043	1041	1044	13.34	
2013_10_21 SetV_0250ppb	893.6	12344	33.06	32.65	39.06	110.0	409.0	413.8	79.09	2205	41.22	41.23	72.14	71.79	512.0	509.9	516.6	507.0	13.08	
2013_10_21 SetV_0100ppb	885.6	13768	33.69	33.43	37.62	145.6	402.2	403.2	20.42	1086	64.14	63.97	53.14	52.54	46.00	45.50	44.59	48.12	13.55	
2013_10_21 SetV_0050ppb	824.8	11544	32.88	32.88	37.66	119.9	412.2	414.5	4.94	696.3	46.18	46.42	49.68	50.28	46.00	45.50	44.59	48.12	13.74	
2013_10_21 SetV_0025ppb	820.8	13824	33.79	33.65	37.91	129.3	417.4	420.8	26.24	2000	52.26	53.10	53.70	55.14	47.75	48.04	49.16	49.16	13.47	
2013_10_21 SetV_0010ppb	799.9	13064	34.81	34.89	50.20	167.7	420.8	423.3	22.0	2870	42.22	42.22	144.1	145.0	21.55	23.35	23.06	24.73	14.70	
2013_10_21 SetV_0005ppb	772.2	11296	34.41	34.18	41.70	122.8	431.3	437.6	10.07	2850	42.22	41.82	73.70	73.83	4.96	4.09	4.16	4.32	14.32	
2013_10_21 SetV_0000ppb	735.7	10336	33.87	33.54	43.67	127.8	432.7	433.7	73.63	2837	27.77	27.96	54.97	54.78	2.00	1.45	1.49	1.45	14.02	
test 5ppb wash 10	2.67	1.53	0.00	0.00	0.01	0.02	0.17	0.00	0.00	0.81	0.01	0.01	0.58	0.57	0.25	0.15	0.16	0.18	0.02	
HPS VF 5 wdh	51.80	7.10	0.01	0.01	0.05	0.03	0.69	0.54	5.38	53.50	5.33	5.34	53.55	53.56	52.26	51.31	51.39	51.78	4.83	
	34.09	471.60	1.63	1.62	0.00	0.53	6.74	6.52	8.38	19.13	4.13	4.18	13.70	13.18	2.84	2.51	2.56	2.55	21.19	

A.4. Datasheets experiment A4

A.4.1. A4 Plant Growth Data

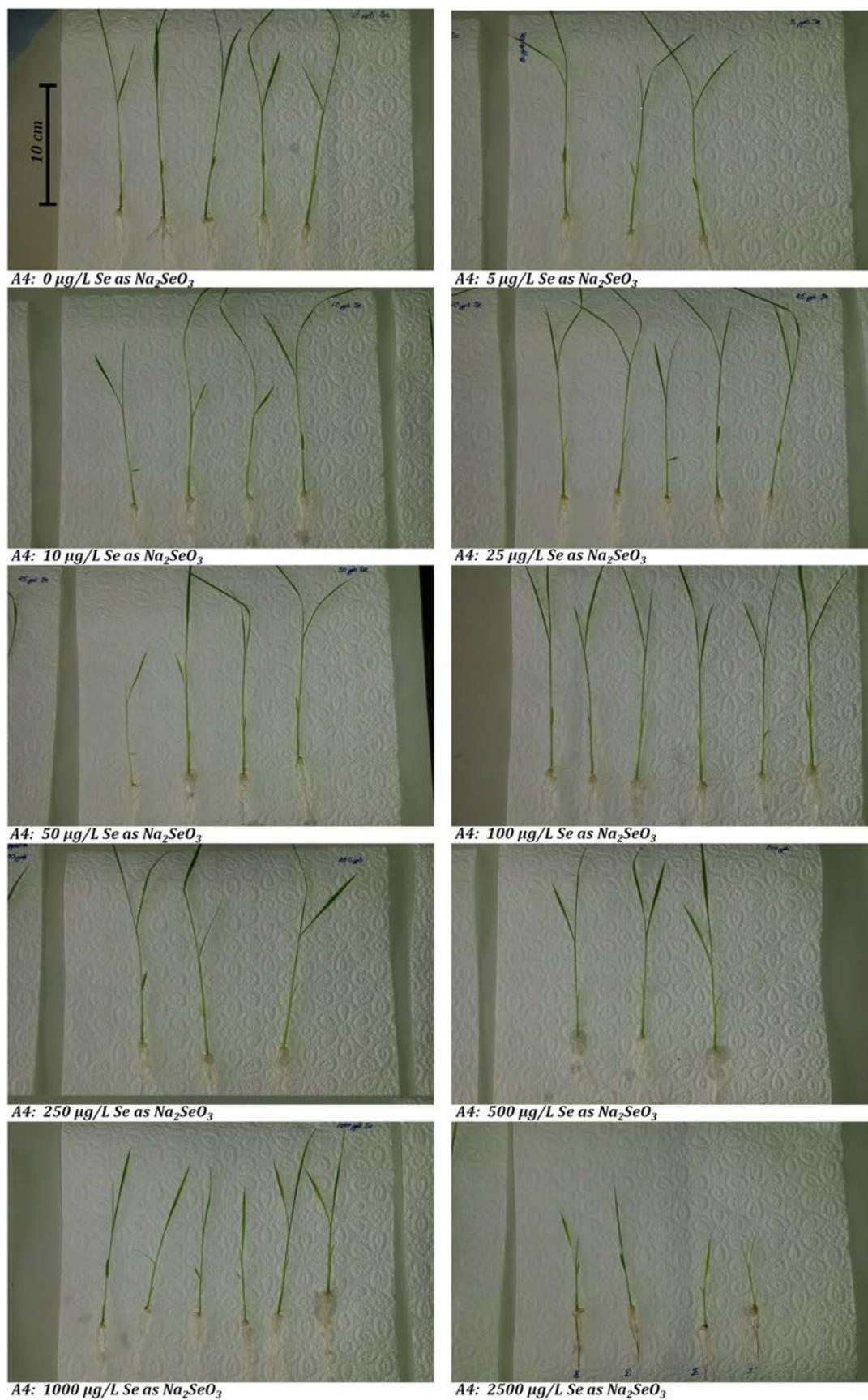


Figure A.20.: A_4 photos of harvested plants treated with Na_2SeO_3

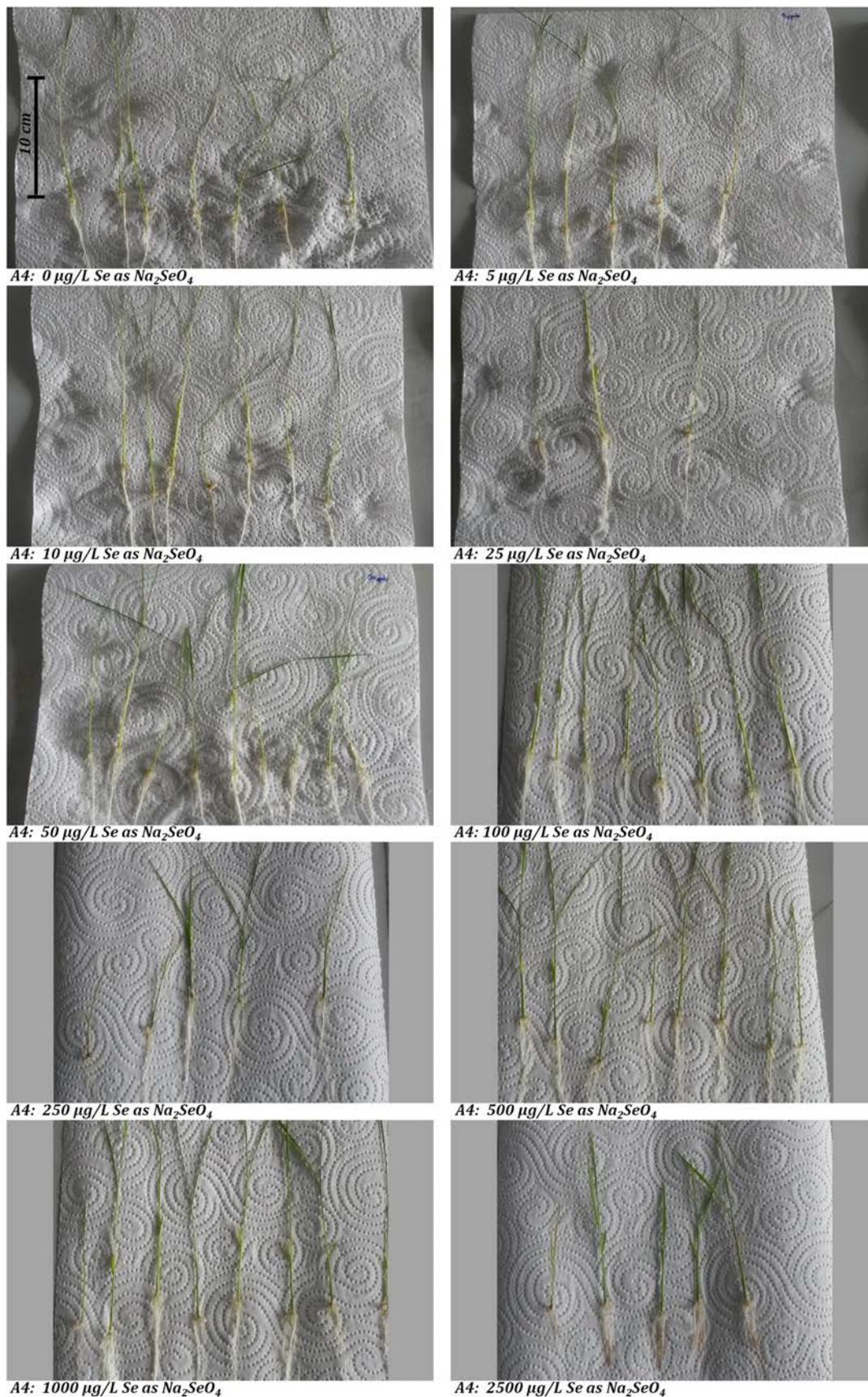
Figure A.21.: A₄ photos of harvested plants treated with Na_2SeO_4

Table A.69.: A_4 plant growth data $A_4 Na_2SeO_3$ (Planting Date: 12.09.2013)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	shoot FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	shoot water [%]	shoot water [%]
0000A	0	x	x	x	x	x	x	x	x	x	x	x
0000B	0	x	x	x	x	x	x	x	x	x	x	x
0000C	0	2.6	1.1	3.7	8	16.0	0.0282	0.0145	0.0067	0.0050	76.24	65.52
0000D	0	3.3	1.3	4.6	13	18.0	0.0301	0.0226	0.0101	0.0083	66.45	63.27
0000E	0	3.4	1.2	4.6	8	16.5	0.0353	0.0327	0.0089	0.0082	74.79	74.92
0000F	0	3.6	1.2	4.8	13	20.0	0.0402	0.0258	0.0103	0.0088	74.38	65.89
0000G	0	x	x	x	x	x	x	x	x	x	x	x
0000H	0	x	x	x	x	x	x	x	x	x	x	x
0000I	0	2.8	1.1	3.9	12	23.0	0.0395	0.0247	0.0119	0.0081	69.87	67.21
0000_sum	0	15.7	5.9	21.6	54.0	93.5	0.1733	0.1203	0.0479	0.0384	361.73	336.81
0000_mean	0	3.1	1.2	4.3	10.8	18.7	0.0347	0.0241	0.0096	0.0077	72.35	67.36
0000_SD	0	0.4	0.1	0.5	2.6	2.9	0.0054	0.0066	0.0019	0.0015	4.07	4.46
0005A	5	x	x	x	x	x	x	x	x	x	x	x
0005B	5	3.6	1.4	5	13	19.5	0.0309	0.0183	0.0115	0.0077	62.78	57.92
0005C	5	3.5	1.6	5.1	13	17.0	0.0239	0.0177	0.0078	0.0045	67.36	74.58
0005D	5	3.3	1.3	4.6	11	19.5	0.0275	0.0092	0.0097	0.0064	64.73	30.43
0005E	5	x	x	x	x	x	x	x	x	x	x	x
0005F	5	x	x	x	x	x	x	x	x	x	x	x
0005G	5	x	x	x	x	x	x	x	x	x	x	x
0005H	5	x	x	x	x	x	x	x	x	x	x	x
0005I	5	x	x	x	x	x	x	x	x	x	x	x
0005_sum	5	10.4	4.3	14.7	37.0	56.0	0.0823	0.0452	0.0290	0.0186	194.87	162.93
0005_mean	5	3.5	1.4	4.9	12.3	18.7	0.0274	0.0151	0.0097	0.0062	64.96	54.31
0005_SD	5	0.2	0.2	0.3	1.2	1.4	0.0035	0.0051	0.0019	0.0016	2.30	22.29
0010A	10	x	x	x	x	x	x	x	x	x	x	x
0010B	10	2.5	0.9	3.4	8	13.5	0.0182	0.0212	0.0053	0.0046	70.88	78.30
0010C	10	x	x	x	x	x	x	x	x	x	x	x
0010D	10	2.3	0	2.3	13	24.0	0.0523	0.0205	0.0116	0.0077	77.82	62.44
0010E	10	x	x	x	x	x	x	x	x	x	x	x
0010F	10	x	x	x	x	x	x	x	x	x	x	x
0010G	10	2.2	0.0	2.2	12	22.5	0.0397	0.0287	0.0079	0.0084	80.10	70.73
0010H	10	x	x	x	x	x	x	x	x	x	x	x
0010I	10	3.1	1.3	4.4	11	21.0	0.0301	0.0162	0.0114	0.0083	62.13	48.77
0010_sum	10	10.1	2.2	12.3	44.0	81.0	0.1403	0.0866	0.0362	0.0290	290.93	260.24
0010_mean	10	2.5	0.6	3.1	11.0	20.3	0.0351	0.0217	0.0091	0.0073	72.73	65.06
0010_SD	10	0.4	0.7	1.0	2.2	4.7	0.0145	0.0052	0.0030	0.0018	8.09	12.65
0025A	25	3.3	1.4	4.7	13	20.5	0.0219	0.0186	0.0091	0.0057	58.45	69.35
0025B	25	x	x	x	x	x	x	x	x	x	x	x
0025C	25	3.5	1.4	4.9	13	19.5	0.0248	0.0121	0.0094	0.0063	62.10	47.93
0025D	25	2.6	0.9	3.5	8	13.5	0.0142	0.0281	0.0047	0.0150	66.90	46.62
0025E	25	3.8	1.4	5.2	13	18.5	0.0232	0.0207	0.0095	0.0062	59.05	70.05
0025F	25	3.1	1.2	4.3	11	20.5	0.0254	0.0259	0.0099	0.0071	61.02	72.59
0025G	25	x	x	x	x	x	x	x	x	x	x	x
0025H	25	x	x	x	x	x	x	x	x	x	x	x
0025I	25	x	x	x	x	x	x	x	x	x	x	x
0025_sum	25	16.3	6.3	22.6	58.0	92.5	0.1095	0.1054	0.0426	0.0403	307.52	306.54
0025_mean	25	3.3	1.3	4.5	11.6	18.5	0.0219	0.0211	0.0085	0.0081	61.50	61.31
0025_SD	25	0.4	0.2	0.6	2.0	2.6	0.0040	0.0056	0.0019	0.0035	3.00	11.52
0050A	50	2.3	0.6	2.9	8	11.5	0.0103	0.0207	0.0019	0.0124	81.55	40.10
0050B	50	x	x	x	x	x	x	x	x	x	x	x
0050C	50	x	x	x	x	x	x	x	x	x	x	x
0050D	50	x	x	x	x	x	x	x	x	x	x	x
0050E	50	2.3	1.0	3.3	11	20.5	0.0352	0.0147	0.0104	0.0073	70.45	50.34
0050F	50	3.2	1.1	4.3	13	20.0	0.0285	0.0209	0.0113	0.0078	60.35	62.68
0050G	50	x	x	x	x	x	x	x	x	x	x	x
0050H	50	x	x	x	x	x	x	x	x	x	x	x
0050I	50	3.4	1.2	4.6	13	20.0	0.0299	0.0241	0.0118	0.0081	60.54	66.39
0050_sum	50	11.2	3.9	15.1	45.0	72.0	0.1039	0.0804	0.0354	0.0356	272.89	219.51
0050_mean	50	2.8	1.0	3.8	11.3	18.0	0.0260	0.0201	0.0089	0.0089	68.22	54.88
0050_SD	50	0.6	0.3	0.8	2.4	4.3	0.0108	0.0039	0.0047	0.0024	10.06	12.01
0100A	100	3.4	1.4	4.8	13	16.5	0.0265	0.0244	0.0090	0.0079	66.04	67.62
0100B	100	3.5	1.6	5.1	13	16.0	0.0196	0.0103	0.0070	0.0049	64.29	52.43
0100C	100	3.7	1.5	5.2	13	17.0	0.0302	0.0096	0.0097	0.0071	67.88	26.04
0100D	100	x	x	x	x	x	x	x	x	x	x	x
0100E	100	3.1	1.2	4.3	11	19.5	0.0259	0.0215	0.0106	0.0082	59.07	61.86
0100F	100	2.6	0.9	3.5	11	17.0	0.0174	0.0285	0.0070	0.0134	59.77	52.98
0100G	100	x	x	x	x	x	x	x	x	x	x	x
0100H	100	x	x	x	x	x	x	x	x	x	x	x
0100I	100	3.5	1.6	5.1	13	21.5	0.0332	0.0132	0.0154	0.0086	53.61	34.85
0100_sum	100	19.8	8.2	28.0	74.0	107.5	0.1528	0.1075	0.0587	0.0501	370.66	295.78
0100_mean	100	3.3	1.4	4.7	12.3	17.9	0.0255	0.0179	0.0098	0.0084	61.78	49.30
0100_SD	100	0.4	0.3	0.7	1.0	2.1	0.0060	0.0080	0.0031	0.0028	5.29	15.92

Table A.70.: A4 plant growth data A4 Na₂SeO₃ (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	x	x	x	x	x	x	x	x	x	x	x
0250B	250	x	x	x	x	x	x	x	x	x	x	x
0250C	250	3.9	1.6	5.5	13	17.0	0.0246	0.0251	0.0108	0.0087	56.10	65.34
0250D	250	x	x	x	x	x	x	x	x	x	x	x
0250E	250	2.8	0.9	3.7	11	19.0	0.0255	0.0176	0.0099	0.0076	61.18	56.82
0250F	250	x	x	x	x	x	x	x	x	x	x	x
0250G	250	3.6	1.4	5	13	18.0	0.0282	0.0253	0.0120	0.0087	57.45	65.61
0250H	250	x	x	x	x	x	x	x	x	x	x	x
0250I	250	x	x	x	x	x	x	x	x	x	x	x
<i>0250_sum</i>	<i>250</i>	<i>10.3</i>	<i>3.9</i>	<i>14.2</i>	<i>37.0</i>	<i>54.0</i>	<i>0.0783</i>	<i>0.0680</i>	<i>0.0327</i>	<i>0.0250</i>	<i>174.72</i>	<i>187.77</i>
<i>0250_mean</i>	<i>250</i>	<i>3.4</i>	<i>1.3</i>	<i>4.7</i>	<i>12.3</i>	<i>18.0</i>	<i>0.0261</i>	<i>0.0227</i>	<i>0.0109</i>	<i>0.0083</i>	<i>58.24</i>	<i>62.59</i>
<i>0250_SD</i>	<i>250</i>	<i>0.6</i>	<i>0.4</i>	<i>0.9</i>	<i>1.2</i>	<i>1.0</i>	<i>0.0019</i>	<i>0.0044</i>	<i>0.0011</i>	<i>0.0006</i>	<i>2.63</i>	<i>5.00</i>
0500A	500	x	x	x	x	x	x	x	x	x	x	x
0500B	500	x	x	x	x	x	x	x	x	x	x	x
0500C	500	x	x	x	x	x	x	x	x	x	x	x
0500D	500	2.5	1.2	3.7	8	15.5	0.0263	0.0323	0.0079	0.0124	69.96	61.61
0500E	500	3.1	1.4	4.5	13	16.5	0.0263	0.0317	0.0097	0.0101	63.12	68.14
0500F	500	x	x	x	x	x	x	x	x	x	x	x
0500G	500	3.3	1.4	4.7	13	18.0	0.0288	0.0207	0.0101	0.0076	64.93	63.29
0500H	500	x	x	x	x	x	x	x	x	x	x	x
0500I	500	x	x	x	x	x	x	x	x	x	x	x
<i>0500_sum</i>	<i>500</i>	<i>8.9</i>	<i>4.0</i>	<i>12.9</i>	<i>34.0</i>	<i>50.0</i>	<i>0.0814</i>	<i>0.0847</i>	<i>0.0277</i>	<i>0.0301</i>	<i>198.01</i>	<i>193.03</i>
<i>0500_mean</i>	<i>500</i>	<i>3.0</i>	<i>1.3</i>	<i>4.3</i>	<i>11.3</i>	<i>16.7</i>	<i>0.0271</i>	<i>0.0282</i>	<i>0.0092</i>	<i>0.0100</i>	<i>66.00</i>	<i>64.34</i>
<i>0500_SD</i>	<i>500</i>	<i>0.4</i>	<i>0.1</i>	<i>0.5</i>	<i>2.9</i>	<i>1.3</i>	<i>0.0014</i>	<i>0.0065</i>	<i>0.0012</i>	<i>0.0024</i>	<i>3.55</i>	<i>3.39</i>
1000A	1000	3.5	1.5	5	13	14.0	0.0234	0.0145	0.0083	0.0059	64.53	59.31
1000B	1000	3.4	2.1	5.5	6	12.0	0.0147	0.0316	0.0046	0.0201	68.71	36.39
1000C	1000	x	x	x	x	x	x	x	x	x	x	x
1000D	1000	2.6	1.1	3.7	7	11.5	0.0136	0.0300	0.0046	0.0172	66.18	42.67
1000E	1000	2.6	1.2	3.8	7	10.5	0.0164	0.0216	0.0047	0.0060	71.34	72.22
1000F	1000	x	x	x	x	x	x	x	x	x	x	x
1000G	1000	2.9	1.5	4.4	13	15.5	0.0326	0.0288	0.0104	0.0085	68.10	70.49
1000H	1000	2.5	1.3	3.8	11	14.0	0.0261	0.0144	0.0080	0.0081	69.35	43.75
1000I	1000	x	x	x	x	x	x	x	x	x	x	x
<i>1000_sum</i>	<i>1000</i>	<i>17.5</i>	<i>8.7</i>	<i>26.2</i>	<i>57.0</i>	<i>77.5</i>	<i>0.1268</i>	<i>0.1409</i>	<i>0.0406</i>	<i>0.0658</i>	<i>408.20</i>	<i>324.83</i>
<i>1000_mean</i>	<i>1000</i>	<i>2.9</i>	<i>1.5</i>	<i>4.4</i>	<i>9.5</i>	<i>12.9</i>	<i>0.0211</i>	<i>0.0235</i>	<i>0.0068</i>	<i>0.0110</i>	<i>68.03</i>	<i>54.14</i>
<i>1000_SD</i>	<i>1000</i>	<i>0.4</i>	<i>0.4</i>	<i>0.7</i>	<i>3.2</i>	<i>1.9</i>	<i>0.0075</i>	<i>0.0078</i>	<i>0.0025</i>	<i>0.0061</i>	<i>2.40</i>	<i>15.33</i>
2500A	2500	x	x	x	x	x	x	x	x	x	x	x
2500B	2500	2.4	1.3	3.7	11	8.0	0.0195	0.0154	0.0066	0.0067	66.15	56.49
2500C	2500	x	x	x	x	x	x	x	x	x	x	x
2500D	2500	2.7	1.4	4.1	13	10.0	0.0252	0.0245	0.0105	0.0102	58.33	58.37
2500E	2500	2.1	1.1	3.2	8	7.0	0.0085	0.0333	0.0031	0.0115	63.53	65.47
2500F	2500	x	x	x	x	x	x	x	x	x	x	x
2500G	2500	x	x	x	x	x	x	x	x	x	x	x
2500H	2500	x	x	x	x	x	x	x	x	x	x	x
2500I	2500	1.9	0.3	2.2	8	5.5	0.0145	0.0222	0.0051	0.0064	64.83	71.17
<i>2500_sum</i>	<i>2500</i>	<i>9.1</i>	<i>4.1</i>	<i>13.2</i>	<i>40.0</i>	<i>30.5</i>	<i>0.0677</i>	<i>0.0954</i>	<i>0.0253</i>	<i>0.0348</i>	<i>252.84</i>	<i>251.50</i>
<i>2500_mean</i>	<i>2500</i>	<i>2.3</i>	<i>1.0</i>	<i>3.3</i>	<i>10.0</i>	<i>7.6</i>	<i>0.0169</i>	<i>0.0239</i>	<i>0.0063</i>	<i>0.0087</i>	<i>63.21</i>	<i>62.87</i>
<i>2500_SD</i>	<i>2500</i>	<i>0.4</i>	<i>0.5</i>	<i>0.8</i>	<i>2.4</i>	<i>1.9</i>	<i>0.0071</i>	<i>0.0074</i>	<i>0.0031</i>	<i>0.0025</i>	<i>3.42</i>	<i>6.75</i>

Table A.71.: A_4 plant growth data $A_4 Na_2SeO_4$ (Planting Date: 06.02.2014)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%] [± 0.0001]	root water [%] [± 0.0001]
0000A	0	3.3	1.2	4.5	8	19.0	0.0150	0.0182	0.0069	0.0052	54.00	71.43
0000B	0	3.1	1.3	4.4	8	17.5	0.0166	0.0308	0.0059	0.0171	64.46	44.48
0000C	0	x	x	x	x	x	x	x	x	x	x	x
0000D	0	3.2	1.4	4.6	8	17.5	0.0193	0.0304	0.0060	0.0090	68.91	70.39
0000E	0	3.1	0.9	4	8	13.0	0.0116	0.0149	0.0036	0.0037	68.97	75.17
0000F	0	x	x	x	x	x	x	x	x	x	x	x
0000G	0	2.6	0.9	3.5	8	14.0	0.0107	0.0205	0.0041	0.0034	61.68	83.41
0000H	0	1.8	0.9	2.7	8	20.0	0.0139	0.0144	0.0060	0.0046	56.83	68.06
0000I	0	4	1.3	5.3	8	17.0	0.0165	0.0331	0.0062	0.0113	62.42	65.86
0000_sum	0	21.1	7.9	29.0	56.0	118.0	0.1036	0.1623	0.0387	0.0543	437.28	478.80
0000_mean	0	3.0	1.1	4.1	8.0	16.9	0.0148	0.0232	0.0055	0.0078	62.47	68.40
0000_SD	0	0.7	0.2	0.8	0.0	2.5	0.0030	0.0080	0.0012	0.0051	5.65	11.99
0005A	5	3.8	1.4	5.2	13	19.5	0.0213	0.0248	0.0113	0.0076	46.95	69.35
0005B	5	x	x	x	x	x	x	x	x	x	x	x
0005C	5	x	x	x	x	x	x	x	x	x	x	x
0005D	5	3.1	1.4	4.5	13	18.5	0.0178	0.0196	0.0083	0.0072	53.37	63.27
0005E	5	2.6	0.7	3.3	8	22.0	0.0184	0.0262	0.0091	0.0092	50.54	64.89
0005F	5	x	x	x	x	x	x	x	x	x	x	x
0005G	5	2.7	0.9	3.6	8	15.0	0.0093	0.0101	0.0047	0.0045	49.46	55.45
0005H	5	2.4	0.7	3.1	13	17.5	0.0103	0.0166	0.0061	0.0058	40.78	65.06
0005I	5	x	x	x	x	x	x	x	x	x	x	x
0005_sum	5	14.6	5.1	19.7	55.0	92.5	0.0771	0.0973	0.0395	0.0343	241.10	318.01
0005_mean	5	2.9	1.0	3.9	11.0	18.5	0.0154	0.0195	0.0079	0.0069	48.22	63.60
0005_SD	5	0.6	0.4	0.9	2.7	2.6	0.0053	0.0065	0.0026	0.0018	4.76	5.09
0010A	10	3.2	1.0	4.2	13	18.0	0.0184	0.0223	0.0077	0.0089	58.15	60.09
0010B	10	x	x	x	x	x	x	x	x	x	x	x
0010C	10	3	0.8	3.8	8	18.5	0.0177	0.0301	0.0074	0.0169	58.19	43.85
0010D	10	3.5	1.5	5	13	21.0	0.0237	0.0173	0.0121	0.0075	48.95	56.65
0010E	10	x	x	x	x	x	x	x	x	x	x	x
0010F	10	2.4	0.8	3.2	6	13.0	0.0076	0.0142	0.0036	0.0039	52.63	72.54
0010G	10	3.3	1.6	4.9	6	19.5	0.0196	0.0173	0.0088	0.0062	55.10	64.16
0010H	10	3.3	1.2	4.5	13	14.0	0.0146	0.0167	0.0061	0.0055	58.22	67.07
0010I	10	3.3	1.1	4.4	8	16.5	0.0146	0.0243	0.0069	0.0078	52.74	67.90
0010_sum	10	22.0	8.0	30.0	67.0	120.5	0.1162	0.1422	0.0526	0.0567	383.98	432.26
0010_mean	10	3.1	1.1	4.3	9.6	17.2	0.0166	0.0203	0.0075	0.0081	54.85	61.75
0010_SD	10	0.4	0.3	0.6	3.3	2.9	0.0050	0.0055	0.0026	0.0042	3.60	9.46
0025A	25	2.4	0.9	3.3	6	10.0	0.0091	0.0267	0.0033	0.0121	63.74	54.68
0025B	25	x	x	x	x	x	x	x	x	x	x	x
0025C	25	x	x	x	x	x	x	x	x	x	x	x
0025D	25	x	x	x	x	x	x	x	x	x	x	x
0025E	25	x	x	x	x	x	x	x	x	x	x	x
0025F	25	x	x	x	x	x	x	x	x	x	x	x
0025G	25	3.8	1.4	5.2	13	23.0	0.0380	0.0296	0.0169	0.0111	55.53	62.50
0025H	25	3.1	0.8	3.9	8	13.5	0.0107	0.0283	0.0041	0.0171	61.68	39.58
0025I	25	x	x	x	x	x	x	x	x	x	x	x
0025_sum	25	9.3	3.1	12.4	27.0	46.5	0.0578	0.0846	0.0243	0.0403	180.94	156.76
0025_mean	25	3.1	1.0	4.1	9.0	15.5	0.0193	0.0282	0.0081	0.0134	60.31	52.25
0025_SD	25	0.6	0.3	0.8	2.9	5.5	0.0133	0.0012	0.0062	0.0026	3.49	9.52
0050A	50	3.0	0.9	3.9	8	13.0	0.0123	0.0144	0.0051	0.0044	58.54	69.44
0050B	50	3.4	1.2	4.6	13	18.5	0.0201	0.0215	0.0100	0.0073	50.25	66.05
0050C	50	0.7	1.1	1.8	8	19.0	0.0142	0.0149	0.0057	0.0047	59.86	68.46
0050D	50	2.5	0.7	3.2	8	16.0	0.0175	0.0233	0.0056	0.0046	68.00	80.26
0050E	50	6.1	1.6	7.7	13	21.5	0.0340	0.0337	0.0143	0.0094	57.94	72.11
0050F	50	2.9	1.4	4.3	8	13.0	0.0092	0.0198	0.0032	0.0064	65.22	67.68
0050G	50	2.4	0.3	2.7	8	20.5	0.0193	0.0083	0.0081	0.0043	58.03	48.19
0050H	50	3.3	1.3	4.6	13	13.0	0.0106	0.0152	0.0053	0.0086	50.00	43.42
0050I	50	2.5	0.8	3.3	11	14.0	0.0109	0.0132	0.0049	0.0049	55.05	62.88
0050_sum	50	26.8	9.3	36.1	90.0	148.5	0.1481	0.1643	0.0622	0.0546	522.88	578.48
0050_mean	50	3.0	1.0	4.0	10.0	16.5	0.0165	0.0183	0.0069	0.0061	58.10	64.28
0050_SD	50	1.4	0.4	1.7	2.4	3.4	0.0077	0.0074	0.0034	0.0020	6.01	11.57
0100A	100	3.3	1.3	4.6	13	21.0	0.0277	0.0195	0.0120	0.0079	56.68	59.49
0100B	100	4.1	1.7	5.8	13	15.5	0.0165	0.0159	0.0083	0.0065	49.70	59.12
0100C	100	2.8	1.1	3.9	13	15.0	0.0181	0.0224	0.0059	0.0096	67.40	57.14
0100D	100	3.7	1.4	5.1	13	17.0	0.0212	0.0123	0.0081	0.0053	61.79	56.91
0100E	100	3.0	1.0	4	8	18.5	0.0168	0.0244	0.0075	0.0052	55.36	78.69
0100F	100	3.3	1.2	4.5	8	19.0	0.0167	0.0231	0.0080	0.0057	52.10	75.32
0100G	100	4.2	1.6	5.8	13	20.5	0.0243	0.0282	0.0109	0.0083	55.14	70.57
0100H	100	x	x	x	x	x	x	x	x	x	x	x
0100I	100	3.9	1.2	5.1	13	21.0	0.0232	0.0272	0.0113	0.0090	51.29	66.91
0100_sum	100	28.3	10.5	38.8	94.0	147.5	0.1645	0.1730	0.0720	0.0575	449.46	524.15
0100_mean	100	3.5	1.3	4.9	11.8	18.4	0.0206	0.0216	0.0090	0.0072	56.18	65.52
0100_SD	100	0.5	0.2	0.7	2.3	2.4	0.0042	0.0055	0.0021	0.0017	5.88	8.61

Table A.72.: A_4 plant growth data $A_4 Na_2SeO_4$ (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
0250A	250	2.8	1.1	3.9	7	10.0	0.0096	0.0323	0.0038	0.0216	60.42	33.13
0250B	250	4.2	1.6	5.8	13	21.5	0.0334	0.0305	0.0141	0.0095	57.78	68.85
0250C	250	4.3	1.6	5.9	13	17.5	0.0333	0.0303	0.0122	0.0089	63.36	70.63
0250D	250	3.5	1.1	4.6	8	16.0	0.0252	0.0332	0.0083	0.0178	67.06	46.39
0250E	250	3.7	1.8	5.5	13	16.5	0.0238	0.0201	0.0089	0.0064	62.61	68.16
0250F	250	x	x	x	x	x	x	x	x	x	x	x
0250G	250	3.8	1.6	5.4	13	19.0	0.0218	0.0114	0.0097	0.0070	55.50	38.60
0250H	250	3.5	1.2	4.7	8	17.0	0.0229	0.0234	0.0087	0.0066	62.01	71.79
0250I	250	2.5	0.9	3.4	8	18.0	0.0158	0.0251	0.0085	0.0069	46.20	72.51
0250_sum	250	28.3	10.9	39.2	83.0	135.5	0.1858	0.2063	0.0742	0.0847	474.95	470.05
0250_mean	250	3.5	1.4	4.9	10.4	16.9	0.0232	0.0258	0.0093	0.0106	59.37	58.76
0250_SD	250	0.6	0.3	0.9	2.8	3.3	0.0080	0.0074	0.0030	0.0058	6.38	16.50
0500A	500	3.3	1.3	4.6	11	17.5	0.0349	0.0240	0.0119	0.0081	65.90	66.25
0500B	500	4.2	1.7	5.9	13	17.0	0.0301	0.0123	0.0127	0.0072	57.81	41.46
0500C	500	3.2	1.1	4.3	13	17.0	0.0258	0.0268	0.0084	0.0058	67.44	78.36
0500D	500	2.5	0.7	3.2	13	10.0	0.0166	0.0148	0.0051	0.0058	69.28	60.81
0500E	500	3.8	1.7	5.5	13	15.0	0.0308	0.0241	0.0100	0.0058	67.53	75.93
0500F	500	x	x	x	x	x	x	x	x	x	x	x
0500G	500	3.6	1.5	5.1	13	17.5	0.0306	0.0165	0.0106	0.0058	65.36	64.85
0500H	500	3	1.2	4.2	8	12.0	0.0172	0.0354	0.0057	0.0195	66.86	44.92
0500I	500	3.3	1.4	4.7	13	11.0	0.0163	0.0138	0.0071	0.0069	56.44	50.00
0500_sum	500	26.9	10.6	37.5	97.0	117.0	0.2023	0.1677	0.0715	0.0649	516.62	482.58
0500_mean	500	3.4	1.3	4.7	12.1	14.6	0.0253	0.0210	0.0089	0.0081	64.58	60.32
0500_SD	500	0.5	0.3	0.8	1.8	3.1	0.0075	0.0080	0.0028	0.0047	4.76	13.76
1000A	1000	x	x	x	x	x	x	x	x	x	x	x
1000B	1000	x	x	x	x	x	x	x	x	x	x	x
1000C	1000	2.3	1.1	3.4	7	6.5	0.0102	0.0313	0.0031	0.0193	69.31	38.34
1000D	1000	2.7	0.7	3.4	13	7.5	0.0188	0.0241	0.0042	0.0064	77.61	73.44
1000E	1000	3.5	1.7	5.2	13	10.0	0.0301	0.0298	0.0298	0.0114	1.00	61.74
1000F	1000	x	x	x	x	x	x	x	x	x	x	x
1000G	1000	x	x	x	x	x	x	x	x	x	x	x
1000H	1000	3.8	1.8	5.6	13	12.5	0.0266	0.0141	0.0101	0.0073	62.03	48.23
1000I	1000	3.7	1.9	5.6	13	10.0	0.0222	0.0316	0.0088	0.0172	60.36	45.57
1000_sum	1000	16.0	7.2	23.2	59.0	46.5	0.1079	0.1309	0.0560	0.0616	270.31	267.32
1000_mean	1000	3.2	1.4	4.6	11.8	9.3	0.0216	0.0262	0.0112	0.0123	54.06	53.46
1000_SD	1000	0.7	0.5	1.1	2.7	2.4	0.0077	0.0074	0.0108	0.0058	30.44	14.02
2500A	2500	x	x	x	x	x	x	x	x	x	x	x
2500B	2500	x	x	x	x	x	x	x	x	x	x	x
2500C	2500	2.1	0.9	3	8	7.0	0.0137	0.0276	0.0047	0.0075	65.69	72.83
2500D	2500	x	x	x	x	x	x	x	x	x	x	x
2500E	2500	3.7	1.7	5.4	13	12.0	0.0376	0.0167	0.0117	0.0087	68.88	47.90
2500F	2500	3.4	1.5	4.9	11	9.0	0.0286	0.0186	0.0083	0.0066	70.98	64.52
2500G	2500	3.2	1.8	5	13	10.0	0.0324	0.0358	0.0104	0.0175	67.90	51.12
2500H	2500	x	x	x	x	x	x	x	x	x	x	x
2500I	2500	3.7	1.8	5.5	13	12.0	0.0362	0.0257	0.0131	0.0083	63.81	67.70
2500_sum	2500	16.1	7.7	23.8	58.0	50.0	0.1485	0.1244	0.0482	0.0486	337.27	304.07
2500_mean	2500	3.2	1.5	4.8	11.6	10.0	0.0297	0.0249	0.0096	0.0097	67.45	60.81
2500_SD	2500	0.7	0.4	1.0	2.2	2.1	0.0096	0.0076	0.0033	0.0044	2.79	10.80

A.4.2. A4 Plant Se content data

Table A.73.: A4 Se content of experimental runs for Na_2SeO_3 and Na_2SeO_4

c(Se) [$\mu\text{g}/\text{L}$]				FIAS-Results				c(Se) dry weight (DW)			
	dig. weight shoot [g] [\pm 0.0001]	dig. weight root [g] [\pm 0.0001]	dig. volume [L] [\pm 0.0001]	c(Se) shoot [$\mu\text{g}/\text{L}$]	c(Se) shoot SD	c(Se) root [$\mu\text{g}/\text{L}$]	c(Se) root SD	c(Se) shoot [mg/kg]	c(Se) shoot SD	c(Se) root [mg/kg]	c(Se) root SD
Nutrient-Solution-Se (Na_2SeO_3) Planting Date: 13.02.2014											
0	0.05029	0.04027	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.02825	0.02053	0.010	4.66	0.55	9.62	0.91	1.65	0.19	4.69	0.44
10	0.03643	0.02901	0.010	10.31	1.29	22.17	2.05	2.83	0.36	7.64	0.71
25	0.04497	0.03815	0.010	30.52	2.98	64.65	0.54	6.79	0.66	16.95	0.14
50	0.03703	0.03303	0.010	64.45	3.61	130.73	9.70	17.40	0.97	39.58	2.94
100	0.05829	0.04675	0.010	137.41	10.51	318.32	35.64	23.57	1.80	68.09	7.62
250	0.03504	0.02615	0.010	170.53	27.15	429.66	39.89	48.67	7.75	164.31	15.25
500	0.02993	0.02552	0.010	169.26	26.86	493.35	22.28	56.55	8.97	193.32	8.73
1000	0.04232	0.05273	0.010	393.42	31.94	1057.47	74.56	92.96	7.55	200.54	14.14
2500	0.02689	0.03311	0.010	180.66	19.46	889.17	34.92	67.19	7.24	268.55	10.55
Nutrient-Solution-Se (Na_2SeO_4) Planting Date: 06.02.2014											
0	0.03852	0.04554	0.010	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.03794	0.03138	0.010	13.78	0.55	2.73	0.17	3.63	0.14	0.87	0.05
10	0.05337	0.05095	0.010	39.23	2.39	10.80	1.19	7.35	0.45	2.12	0.23
25	0.02409	0.03495	0.010	45.11	1.22	13.90	1.19	18.73	0.51	3.98	0.34
50	0.06532	0.05938	0.010	501.92	17.82	125.22	3.02	76.84	2.73	21.09	0.51
100	0.07179	0.05716	0.010	1288.31	54.04	286.84	17.10	179.46	7.53	50.18	2.99
250	0.07410	0.05762	0.010	3550.38	161.32	717.19	28.80	479.13	21.77	124.47	5.00
500	0.07064	0.05822	0.010	6485.85	482.87	1439.86	50.17	918.16	68.36	247.31	8.62
1000	0.03991	0.03416	0.010	4149.12	227.24	1725.60	58.31	1039.62	56.94	505.15	17.07
2500	0.04646	0.04281	0.010	1775.57	213.92	1474.76	54.72	382.17	46.04	344.49	12.78
Digestion standards											
Standard Sample	dig. weight [g]	dig. volume [L]	c(Se) [$\mu\text{g}/\text{L}$]	c(Se) SD	c(Se) [mg/kg]	c(Se) SD					
dig_Std 2014_04_22 (0-5ppb)	0.10092	0.010	9.71	1.87	0.96	0.19					
dig_Std 2014_04_23 (10-100ppb)	0.10123	0.010	10.47	1.01	1.03	0.10					
dig_Std 2014_04_24 (250-2500ppb)	0.10021	0.010	11.02	0.90	1.10	0.09					
dig_Std 2014_04_24 (0-5ppb)	0.10021	0.010	11.02	0.90	1.10	0.09					
dig_Std 2014_04_25 (10-100ppb)	0.09996	0.010	10.63	1.25	1.06	0.13					
dig_Std 2014_04_28 (250-2500ppb)	0.10023	0.010	11.50	0.55	1.15	0.05					

A.4.3. Complete A4 results overview

Table A.74.: A4 results overview for Na_2SeO_3

c(Se) [µg/L]	plants per box	SD	2nd leaf sheath		2nd leaf blade		2nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water		c(Se) shoot FW		c(Se) root FW		shoot acc. factor		root acc. factor	
			[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[g]	SD	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD	[-]	SD
0	5	x	3.14	0.42	1.18	0.08	4.32	0.51	10.80	2.59	1.97	1.48	18.70	2.86	0.0096	0.0019	0.0077	0.0015	72.35	4.07	67.36	4.46								
5	3	x	3.47	0.15	1.43	0.15	4.90	0.31	12.33	1.15	2.29	2.08	18.67	1.44	0.0097	0.0019	0.0062	0.0016	64.96	2.30	54.31	22.29								
10	4	x	2.53	0.40	0.55	0.66	3.08	1.06	11.00	2.16	1.97	2.25	20.25	4.66	0.0091	0.0030	0.0073	0.0018	72.73	8.09	65.06	12.65								
25	5	x	3.26	0.40	1.26	0.20	4.52	0.60	11.60	1.96	2.71	2.12	18.50	2.61	0.0085	0.0019	0.0081	0.0035	61.50	3.00	61.31	11.52								
50	4	x	2.80	0.58	0.98	0.26	3.78	0.85	11.25	2.36	2.06	1.95	18.00	4.34	0.0089	0.0047	0.0089	0.0024	68.22	10.06	54.88	12.01								
100	6	x	3.30	0.39	1.37	0.27	4.67	0.67	12.33	1.03	2.94	1.70	17.92	2.13	0.0098	0.0031	0.0084	0.0028	61.78	5.29	49.30	15.92								
250	3	x	3.43	0.57	1.30	0.36	4.73	0.93	12.33	1.15	2.16	2.51	18.00	1.00	0.0109	0.0011	0.0083	0.0006	58.24	2.63	62.59	5.00								
500	3	x	2.97	0.42	1.33	0.12	4.30	0.53	11.33	2.89	1.56	1.48	16.67	1.26	0.0092	0.0012	0.0100	0.0024	66.00	3.55	64.34	3.39								
1000	6	x	2.92	0.44	1.45	0.36	4.37	0.79	9.50	3.21	1.94	1.57	12.92	1.88	0.0068	0.0025	0.0110	0.0061	68.03	2.40	54.14	15.33								
2500	4	x	2.28	0.35	1.03	0.50	3.30	0.85	10.00	2.45	1.38	1.06	7.63	1.89	0.0063	0.0031	0.0087	0.0025	63.21	3.42	62.87	6.75								

c(Se) [µg/L]	shoot DW	SD	root DW		ratio		ratio		shoot-Se share		root-Se share		shoot water		root water		c(Se) shoot FW		c(Se) root FW		shoot acc. factor		root acc. factor	
			[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[-]	SD	[-]	SD	[-]	SD
0	0.00	0.00	0.00	0.00	x	x	x	x	26.06	14.34	73.94	0.00	72.345	67.363	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	1.65	0.19	4.69	0.44	2.84	0.35	0.00	0.00	27.02	25.92	72.98	19.09	64.988	54.312	0.58	0.07	2.14	0.00	115.73	13.59	428.13	0.00		
10	2.83	0.36	7.64	0.71	2.70	0.37	0.26	0.26	27.02	25.92	72.98	19.09	72.732	65.060	0.77	0.10	2.67	0.25	77.17	9.68	267.07	24.68		
25	6.79	0.66	16.95	0.14	2.50	1.66	0.40	0.06	28.59	47.36	71.41	4.01	61.504	61.309	2.61	0.26	6.56	0.05	104.49	10.21	262.28	2.17		
50	17.40	0.97	39.58	2.27	2.27	0.44	1.29	0.35	30.54	67.72	69.46	89.66	68.223	54.877	5.53	0.31	17.86	1.32	110.61	6.20	357.18	26.49		
100	23.57	1.80	68.09	7.62	2.89	5.21	0.35	2.64	25.72	133.95	74.38	196.08	61.777	49.297	9.01	0.69	34.52	3.87	90.10	6.89	345.23	38.66		
250	48.67	7.75	164.31	15.25	3.38	26.16	0.30	4.52	22.85	597.86	77.15	348.55	58.240	62.590	20.32	3.24	61.47	5.71	81.29	12.94	245.87	22.82		
500	56.55	8.97	193.32	8.73	3.42	30.67	0.29	2.55	22.63	694.23	77.37	197.55	66.003	64.345	19.23	3.05	68.93	6.10	38.45	6.10	137.86	6.22		
1000	92.96	7.55	200.54	14.14	2.16	16.28	0.46	6.55	31.67	515.71	68.33	447.84	68.034	54.138	29.72	2.41	91.97	2.41	29.72	2.41	91.97	6.48		
2500	67.19	7.24	268.55	10.55	4.00	28.93	0.25	2.64	20.01	579.01	79.99	211.04	63.211	62.874	24.72	2.66	99.70	3.92	9.89	1.07	39.88	1.57		

Table A.75.: A4 results overview for Na_2SeO_4

c(Se) [$\mu\text{g}/\text{L}$]	plants per box		2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water	
	[-]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD
0	7	x	3.01	0.68	1.13	0.22	4.14	0.90	8.00	0.00	1.14	0.24	16.86	2.53	0.0055	0.0012	0.0078	0.0051	62.47	5.65	68.40	11.99
5	5	x	2.92	0.55	1.02	0.36	3.94	0.91	11.00	2.74	2.67	1.63	18.50	2.57	0.0079	0.0026	0.0069	0.0018	48.22	4.76	63.60	5.09
10	7	x	3.14	0.36	1.14	0.32	4.29	0.68	9.57	3.31	2.75	1.93	17.21	2.90	0.0075	0.0026	0.0081	0.0042	54.85	3.60	61.75	9.46
25	3	x	3.10	0.57	1.03	0.26	4.13	0.83	9.00	2.94	1.50	2.63	15.50	5.49	0.0081	0.0062	0.0134	0.0026	60.31	3.49	52.25	9.52
50	9	x	2.98	1.41	1.03	0.40	4.01	1.81	10.00	2.45	3.06	1.99	16.50	3.44	0.0069	0.0034	0.0061	0.0026	58.10	6.01	64.28	11.57
100	8	x	3.54	0.52	1.31	0.24	4.85	0.76	11.75	2.31	4.13	1.71	18.44	2.40	0.0090	0.0021	0.0072	0.0017	56.18	5.88	65.52	8.61
250	8	x	3.54	0.63	1.36	0.32	4.90	0.95	10.38	2.83	4.13	2.81	16.94	3.29	0.0093	0.0030	0.0106	0.0058	59.37	6.38	58.76	16.50
500	8	x	3.36	0.52	1.33	0.33	4.69	0.85	12.13	1.81	3.61	1.76	14.63	3.15	0.0089	0.0028	0.0081	0.0047	64.58	4.76	60.32	13.76
1000	5	x	3.20	0.66	1.44	0.52	4.64	1.18	11.80	2.68	2.19	1.86	9.30	2.36	0.0112	0.0108	0.0123	0.0058	54.06	30.44	53.46	14.02
2500	5	x	3.22	0.66	1.54	0.38	4.76	1.04	11.60	2.19	2.83	1.89	10.00	2.12	0.0096	0.0033	0.0097	0.0044	67.45	2.79	60.81	10.80

c(Se) [$\mu\text{g}/\text{L}$]	c(Se) shoot DW		ratio root/shoot		ratio shoot/root		shoot-Se share		root-Se share		shoot water		shoot water		c(Se) shoot FW		c(Se) root FW		shoot water		root water			
	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	[%]	SD	[%]	SD	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD	
0	0.00	0.00	x	x	x	x	x	x	x	x	62.47	11.99	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
5	3.63	0.14	0.87	0.05	0.24	0.03	0.29	0.13	3.47	0.81	48.22	5.09	1.88	0.08	0.83	0.05	376.22	15.01	331.87	20.21	192.00	10.41	165.03	
10	7.35	0.45	2.12	0.23	0.29	0.13	0.29	0.13	3.47	0.81	54.85	9.46	3.32	0.20	1.92	0.21	297.25	8.02	297.25	8.02	143.99	12.30	143.99	
25	18.73	0.51	3.98	0.34	0.21	0.11	0.21	0.11	4.71	1.60	60.31	9.52	7.43	0.20	3.60	0.31	643.95	22.87	643.95	22.87	372.96	9.01	372.96	
50	76.84	2.73	21.09	0.51	0.27	0.75	0.27	0.75	58.76	21.53	58.10	11.57	32.20	1.14	18.65	0.45	786.32	32.98	786.32	32.98	458.62	27.35	458.62	
100	179.46	7.53	50.18	2.99	0.28	2.10	3.58	10.70	78.15	164.49	21.85	233.83	56.18	78.63	3.30	45.86	2.73	786.32	32.98	786.32	32.98	458.62	27.35	458.62
250	479.13	21.77	124.47	5.00	0.26	5.66	19.24	79.38	448.94	20.62	396.81	59.37	16.50	194.68	8.85	103.93	4.17	778.71	35.38	778.71	35.38	415.70	16.70	415.70
500	918.16	68.36	247.31	8.62	0.27	18.41	31.99	78.78	1450.53	21.22	678.84	64.58	13.76	325.23	24.21	213.30	7.43	650.46	48.43	650.46	48.43	426.59	14.86	426.59
1000	1039.62	56.94	505.15	17.07	0.49	27.67	67.30	1861.88	32.70	1148.77	54.06	14.02	477.59	26.16	434.33	14.68	477.59	26.16	477.59	26.16	434.33	14.68	434.33	
2500	382.17	46.04	344.49	12.78	0.90	41.50	1.11	14.18	52.59	2182.77	67.45	10.80	124.38	14.99	307.30	11.40	49.75	5.99	49.75	5.99	122.92	4.56	122.92	

A.4.4. A4 analytical data

Table A.76.: A4 analytical data - HG-FIAS measurement I

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Plant Digestions		
Results Data Set	Nothstein_2014_05_13		
Date Measured	13.05.2014		
Method Name	Se Nothstein calib 6c		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.998648	LOQ (= 7-wash)	0.033	
calib. slope	LOD (= 3-wash)	0.014	
0.01287	analytical quality [%]	117.863	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0015	0.0	0.00	0.00
2	0.5 ppb	0.0041	0.0012	0.5	0.32	0.09
3	0.75 ppb	0.0077	0.0012	0.8	0.60	0.09
4	1.0 ppb	0.0124	0.0009	1.0	0.96	0.07
5	2.0 ppb	0.0256	0.0012	2.0	1.99	0.09
6	4.0 ppb	0.0528	0.0012	4.0	4.10	0.09
7	5.0 ppb	0.0631	0.0008	5.0	4.90	0.06
8	6.0 ppb	0.0778	0.0030	6.0	6.05	0.23

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.032	0.076	0.032	0.076	1	0.03	0.08
2	wash	0.073	0.143	0.073	0.143	1	0.07	0.14
3	6M HCl Blank	0.008	0.059	0.006	0.048	4	0.03	0.19
4	Trace Metal 252 µg/L	2.450	0.109	2.573	0.115	120	308.79	13.80
5	wash	0.000	0.146	0.000	0.146	1	0.00	0.15
6	Se_Std_0	-0.033	0.116	-0.033	0.116	1	-0.03	0.12
7	Se_Std_0.5	0.379	0.156	0.379	0.156	1	0.38	0.16
8	Se_Std_0.75	0.685	0.070	0.685	0.070	1	0.69	0.07
9	Se_Std_1	0.968	0.125	0.968	0.125	1	0.97	0.12
10	Se_Std_2	1.888	0.058	1.888	0.058	1	1.89	0.06
11	Se_Std_4	4.036	0.058	4.036	0.058	1	4.04	0.06
12	Se_Std_5	4.767	0.180	4.767	0.180	1	4.77	0.18
13	Se_Std_6	5.785	0.028	5.785	0.028	1	5.78	0.03
14	wash	-0.007	0.069	-0.007	0.069	1	-0.01	0.07
15	wash	-0.027	0.070	-0.027	0.070	1	-0.03	0.07
16	2014-04-23 digestion blank	0.004	0.044	0.004	0.038	8	< PQL	< PQL
17	2014-04-23 digestion Std Wheat 1567a	1.187	0.229	1.214	0.234	8	9.71	1.87
18	2014-04-23 0 µg/L Shoot	-0.039	0.060	-0.033	0.052	8	< PQL	< PQL
19	2014-04-23 0 µg/L Root	0.031	0.073	0.027	0.063	8	< PQL	< PQL
20	2014-04-23 5 µg/L Shoot	3.092	0.123	3.446	0.137	4	13.78	0.55
21	2014-04-23 5 µg/L Root	0.764	0.048	0.682	0.043	4	2.73	0.17
22	2014-04-23 10 µg/L Shoot	4.400	0.268	4.904	0.299	8	39.23	2.39
23	2014-04-23 10 µg/L Root	1.288	0.142	1.351	0.149	8	10.80	1.19
24	2014-04-23 25 µg/L Shoot	5.181	0.140	5.639	0.152	8	45.11	1.22
25	2014-04-23 25 µg/L Root	1.658	0.142	1.738	0.148	8	13.90	1.19
26	wash	0.003	0.068	0.003	0.068	1	0.00	0.07
27	Se_Std_0	0.002	0.103	0.002	0.103	1	0.00	0.10
28	Se_Std_0.5	0.345	0.036	0.345	0.036	1	0.34	0.04
29	Se_Std_0.75	0.642	0.026	0.642	0.026	1	0.64	0.03
30	Se_Std_1	0.911	0.036	0.911	0.036	1	0.91	0.04
31	Se_Std_2	1.896	0.076	1.896	0.076	1	1.90	0.08
32	Se_Std_4	3.232	0.169	3.232	0.169	1	3.23	0.17
33	Se_Std_5	4.166	0.069	4.166	0.069	1	4.17	0.07
34	Se_Std_6	5.360	0.089	5.360	0.089	1	5.36	0.09
35	wash	-0.059	0.091	-0.059	0.091	1	-0.06	0.09
36	wash	-0.040	0.085	-0.040	0.085	1	-0.04	0.08
37	2014-04-24 digestion blank	-0.019	0.041	-0.015	0.033	8	< PQL	< PQL
38	2014-04-24 digestion Std Wheat 1567a	1.211	0.117	1.309	0.126	8	10.47	1.01
39	2014-04-24 50 µg/L Shoot	3.679	0.131	4.183	0.149	120	501.92	17.82
40	2014-04-24 50 µg/L Root	1.978	0.048	2.087	0.050	60	125.22	3.02
41	2014-04-24 100 µg/L Shoot	4.880	0.205	5.368	0.225	240	1288.31	54.04
42	2014-04-24 100 µg/L Root	4.205	0.251	4.781	0.285	60	286.84	17.10
43	2014-04-24 250 µg/L Shoot	5.389	0.245	5.917	0.269	600	3550.38	161.32
44	2014-04-24 250 µg/L Root	5.443	0.219	5.977	0.240	120	717.19	28.80
45	2014-04-24 500 µg/L Shoot	2.562	0.191	2.702	0.201	2400	6485.85	482.87
46	2014-04-24 500 µg/L Root	5.464	0.190	5.999	0.209	240	1439.86	50.17
47	wash	0.034	0.214	0.034	0.214	1	0.03	0.21
48	Se_Std_0	-0.011	0.094	-0.011	0.094	1	-0.01	0.09
49	Se_Std_0.5	0.423	0.119	0.423	0.119	1	0.42	0.12
50	Se_Std_0.75	0.673	0.128	0.673	0.128	1	0.67	0.13
51	Se_Std_1	0.856	0.042	0.856	0.042	1	0.86	0.04
52	Se_Std_2	1.861	0.105	1.861	0.105	1	1.86	0.11
53	Se_Std_4	3.853	0.030	3.853	0.030	1	3.85	0.03
54	Se_Std_5	4.651	0.184	4.651	0.184	1	4.65	0.18
55	Se_Std_6	5.547	0.100	5.547	0.100	1	5.55	0.10
56	wash	0.016	0.120	0.016	0.120	1	0.02	0.12
57	wash	0.050	0.179	0.050	0.179	1	0.05	0.18
58	2014-04-25 digestion blank	-0.024	0.107	-0.015	0.069	8	< PQL	< PQL
59	2014-04-25 digestion Std Wheat 1567a	1.233	0.101	1.377	0.113	8	11.02	0.90
60	2014-04-25 1000 µg/L Shoot	7.075	0.315	7.612	0.339	600	> calib	> calib
61	2014-04-25 1000 µg/L Root	7.626	0.535	8.206	0.575	240	> calib	> calib
62	2014-04-25 2500 µg/L Shoot	2.808	0.338	2.959	0.357	600	1775.57	213.92
63	2014-04-25 2500 µg/L Root	5.711	0.212	6.145	0.228	240	1474.76	54.72
64	2014-04-25 0 µg/L Shoot	0.167	0.093	0.107	0.059	8	< PQL	< PQL
65	2014-04-25 0 µg/L Root	0.259	0.103	0.166	0.066	8	< PQL	< PQL
66	2014-04-25 5 µg/L Shoot	1.044	0.123	1.166	0.137	4	4.66	0.55
67	2014-04-25 5 µg/L Root	2.282	0.216	2.405	0.227	4	9.62	0.91

Table A.77.: A_4 analytical data - HG-FIAS measurement I (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]	c(Se) driftcorr. [$\mu\text{g/L}$]	SD driftcorr. [$\mu\text{g/L}$]	dilution factor [-]	c(Se) conc. [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]
68	wash	-0.037	0.087	-0.037	0.087	1	-0.04	0.09
69	Se_Std_0	-0.031	0.064	-0.031	0.064	1	-0.03	0.06
70	Se_Std_0.5	0.441	0.066	0.441	0.066	1	0.44	0.07
71	Se_Std_0.75	0.599	0.032	0.599	0.032	1	0.60	0.03
72	Se_Std_1	0.840	0.062	0.840	0.062	1	0.84	0.06
73	Se_Std_2	1.900	0.112	1.900	0.112	1	1.90	0.11
74	Se_Std_4	3.712	0.146	3.712	0.146	1	3.71	0.15
75	Se_Std_5	4.527	0.089	4.527	0.089	1	4.53	0.09
76	Se_Std_6	5.627	0.052	5.627	0.052	1	5.63	0.05
77	wash	0.047	0.061	0.047	0.061	1	0.05	0.06
78	wash	0.022	0.057	0.022	0.057	1	0.02	0.06
79	2014-04-28 digestion blank	-0.070	0.059	-0.049	0.042	8	< PQL	< PQL
80	2014-04-28 digestion Std Wheat 1567a	1.119	0.132	1.328	0.157	8	10.63	1.25
81	2014-04-28 10 $\mu\text{g/L}$ Shoot	1.086	0.136	1.289	0.162	8	10.31	1.29
82	2014-04-28 10 $\mu\text{g/L}$ Root	2.482	0.229	2.772	0.256	8	22.17	2.05
83	2014-04-28 25 $\mu\text{g/L}$ Shoot	3.395	0.332	3.814	0.373	8	30.52	2.98
84	2014-04-28 25 $\mu\text{g/L}$ Root	7.210	0.490	7.844	0.533	8	> calib	> calib
85	2014-04-28 50 $\mu\text{g/L}$ Shoot	0.905	0.051	1.074	0.060	60	64.45	3.61
86	2014-04-28 50 $\mu\text{g/L}$ Root	1.951	0.145	2.179	0.162	60	130.73	9.70
87	2014-04-28 100 $\mu\text{g/L}$ Shoot	2.050	0.157	2.290	0.175	60	137.41	10.51
88	2014-04-28 100 $\mu\text{g/L}$ Root	4.722	0.529	5.305	0.594	60	318.32	35.64
89	wash	-0.032	0.060	-0.032	0.060	1	-0.03	0.06
90	Se_Std_0	0.028	0.122	0.028	0.122	1	0.03	0.12
91	Se_Std_0.5	0.383	0.029	0.383	0.029	1	0.38	0.03
92	Se_Std_0.75	0.583	0.081	0.583	0.081	1	0.58	0.08
93	Se_Std_1	0.723	0.067	0.723	0.067	1	0.72	0.07
94	Se_Std_2	1.611	0.077	1.611	0.077	1	1.61	0.08
95	Se_Std_4	3.483	0.092	3.483	0.092	1	3.48	0.09
96	Se_Std_5	4.284	0.107	4.284	0.107	1	4.28	0.11
97	Se_Std_6	5.403	0.170	5.403	0.170	1	5.40	0.17
98	wash	-0.006	0.103	-0.006	0.103	1	-0.01	0.10
99	wash	0.002	0.067	0.002	0.067	1	0.00	0.07
100	2014-02-30 digestion blank	0.035	0.055	0.031	0.048	8	< PQL	< PQL
101	2014-02-30 digestion Std Wheat 1567a	1.197	0.057	1.437	0.069	8	11.50	0.55
102	2014-02-30 250 $\mu\text{g/L}$ Shoot	1.184	0.188	1.421	0.226	120	170.53	27.15
103	2014-02-30 250 $\mu\text{g/L}$ Root	3.179	0.295	3.580	0.332	120	429.66	39.89
104	2014-02-30 500 $\mu\text{g/L}$ Shoot	0.705	0.112	0.705	0.112	240	169.26	26.86
105	2014-02-30 500 $\mu\text{g/L}$ Root	1.876	0.085	2.056	0.093	240	493.35	22.28
106	2014-02-30 1000 $\mu\text{g/L}$ Shoot	1.365	0.111	1.639	0.133	240	393.42	31.94
107	2014-02-30 1000 $\mu\text{g/L}$ Root	3.912	0.276	4.406	0.311	240	1057.47	74.56
108	2014-02-30 2500 $\mu\text{g/L}$ Shoot	0.752	0.081	0.753	0.081	240	180.66	19.46
109	2014-02-30 2500 $\mu\text{g/L}$ Root	3.289	0.129	3.705	0.145	240	889.17	34.92
110	wash	0.049	0.060	0.049	0.060	1	0.05	0.06
111	6M HCl Blank	-0.010	0.121	-0.009	0.117	4	-0.04	0.47
112	Trace Metal 252 $\mu\text{g/L}$	2.304	0.100	2.377	0.103	120	285.24	12.38
113	wash	-0.014	0.042	-0.014	0.042	1	-0.01	0.04
114	Se_Std_0	0.064	0.052	0.064	0.052	1	0.06	0.05
115	Se_Std_0.5	0.330	0.066	0.330	0.066	1	0.33	0.07
116	Se_Std_0.75	0.614	0.068	0.614	0.068	1	0.61	0.07
117	Se_Std_1	0.813	0.021	0.813	0.021	1	0.81	0.02
118	Se_Std_2	1.925	0.063	1.925	0.063	1	1.93	0.06
119	Se_Std_4	3.688	0.082	3.688	0.082	1	3.69	0.08
120	Se_Std_5	4.577	0.098	4.577	0.098	1	4.58	0.10
120	Se_Std_6	5.613	0.069	5.613	0.069	1	5.61	0.07
121	2014-04-25 1000 $\mu\text{g/L}$ Shoot	3.458	0.189	3.458	0.189	1200	4149.12	227.24
122	2014-04-25 1000 $\mu\text{g/L}$ Root	3.595	0.121	3.595	0.121	480	1725.60	58.31
123	2014-04-28 25 $\mu\text{g/L}$ Root	3.669	0.030	4.041	0.033	16	64.65	0.54
124	wash	0.025	0.086	0.025	0.086	1	0.03	0.09
125	wash	-0.031	0.051	-0.031	0.051	1	-0.03	0.05

B. Adsorption-Desorption Experiments Se & Kaolinite, Goethite

B.1. Datasheets Material Characterization

B.1.1. WDX Analysis of Kaolinite and FeOOH

B.1.2. TG-DSC data

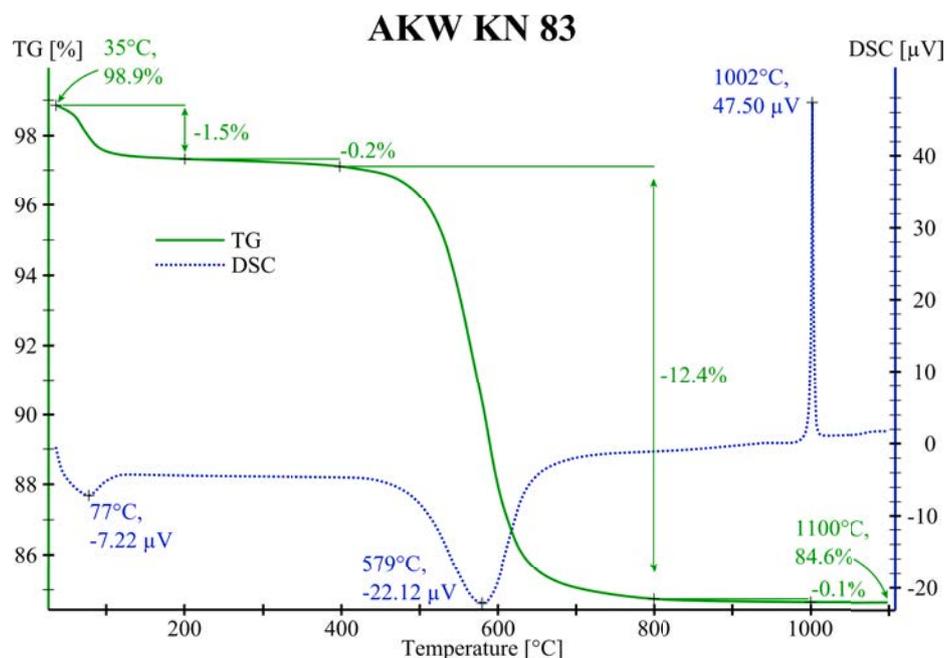


Figure B.1.: TG-DSC curve of Kaolin powder AKW KN 83 measured at CMM

Table B.1.: WDX datasheet

sample	Na ₂ O [%]	MgO [%]	Al ₂ O ₃ [%]	SiO ₂ [%]	P ₂ O ₅ [%]	K ₂ O [%]	CaO [%]	TiO ₂ [%]	MnO [%]	Fe ₂ O ₃ [%]	sum	ignition loss
Kaolin_AKW_KN_83	0.064	0.000	35.842	44.151	0.035	0.654	0.063	0.823	0.002	0.357	81.991	16.4589
Kaolin_KBS_0_alpha	0.092	0.243	34.526	45.968	0.104	2.095	0.078	0.035	0.009	0.821	83.972	13.6533
Kaolin_KBS_BT_GHB	0.210	0.000	39.024	45.027	0.028	0.153	0.037	0.818	0.000	0.526	85.823	12.9298
FeOOH_B_E216	0.081	0.116	0.043	0.322	0.000	0.016	0.299	0.000	0.244	81.393	98.635	16.3442
FeOOH_B_920Z	0.099	0.000	0.000	8.271	0.000	0.016	0.074	0.025	0.066	80.082	99.863	11.2459
SiO2_Dors_9S_1-1.6	0.037	0.000	0.486	98.415	0.000	0.119	0.026	0.193	0.000	0.229	99.505	n. a.

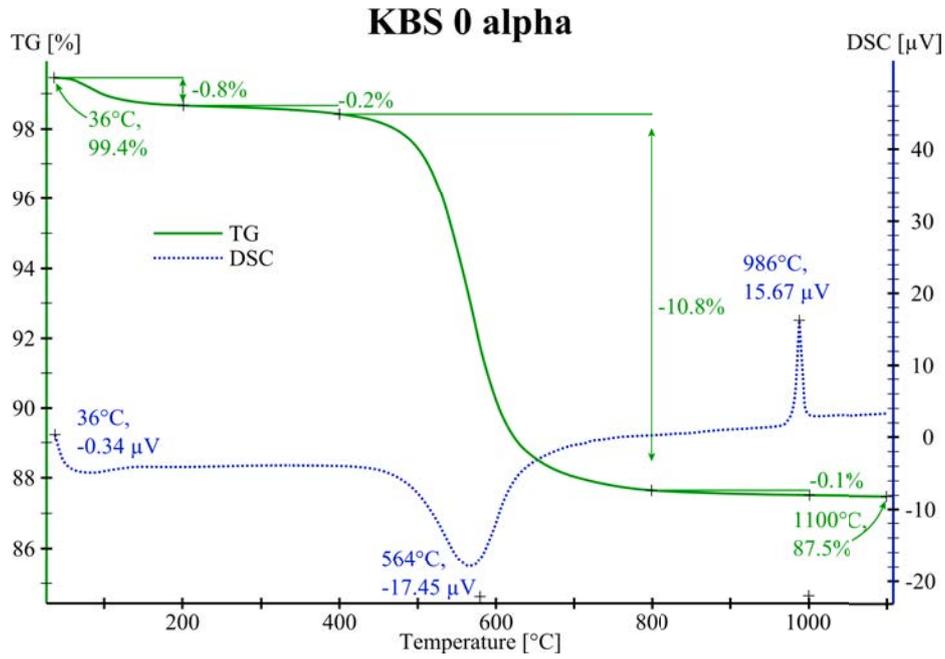


Figure B.2.: TG-DSC curve of Kaolin powder KBS 0 alpha measured at CMM

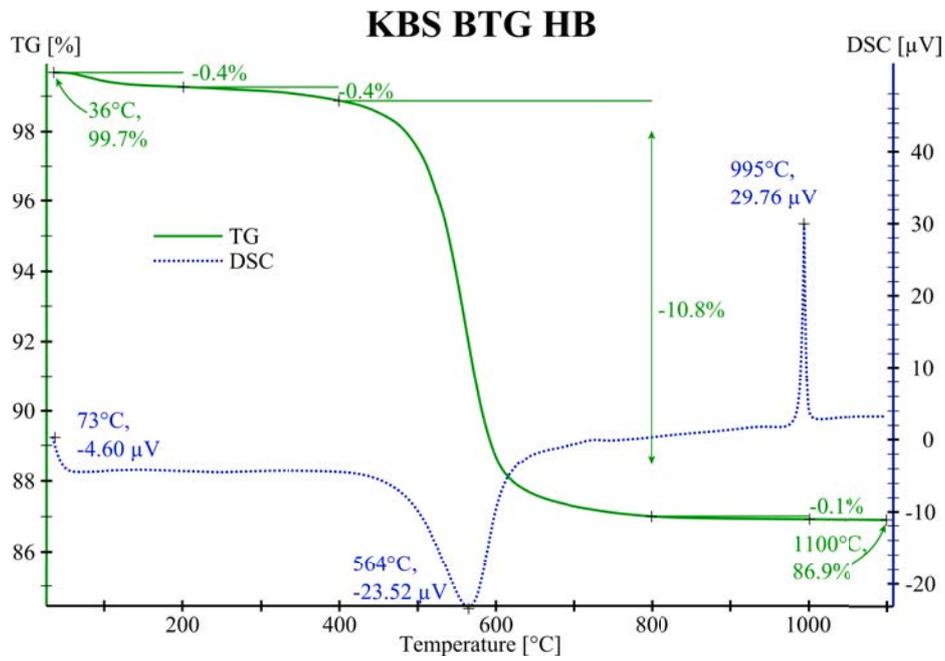


Figure B.3.: TG-DSC curve of Kaolin powder KBS BT GHB measured at CMM

B.1.3. STA-analysis

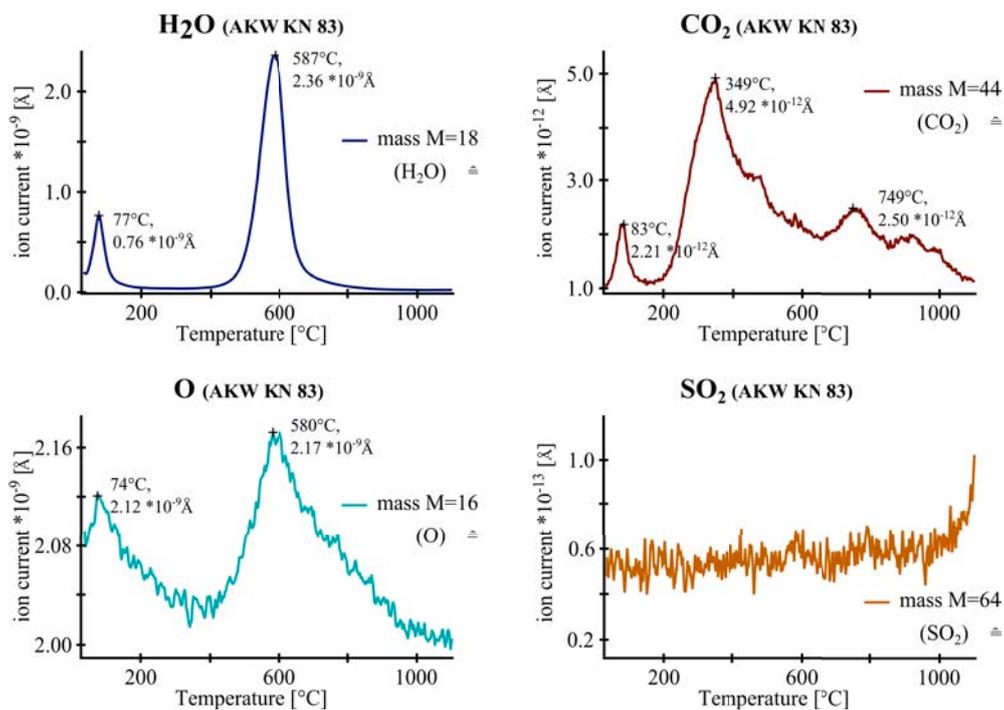


Figure B.4.: IR-MS measurements of TG-DSC analysis for AKW KN 83

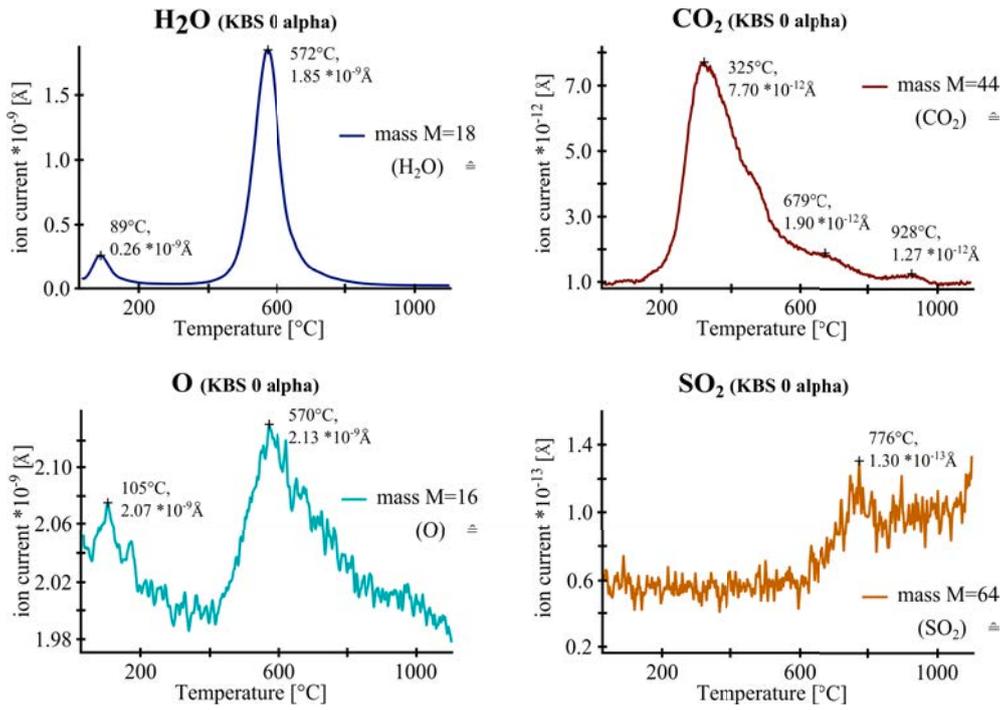


Figure B.5.: IR-MS measurements of TG-DSC analysis for KBS 0 alpha

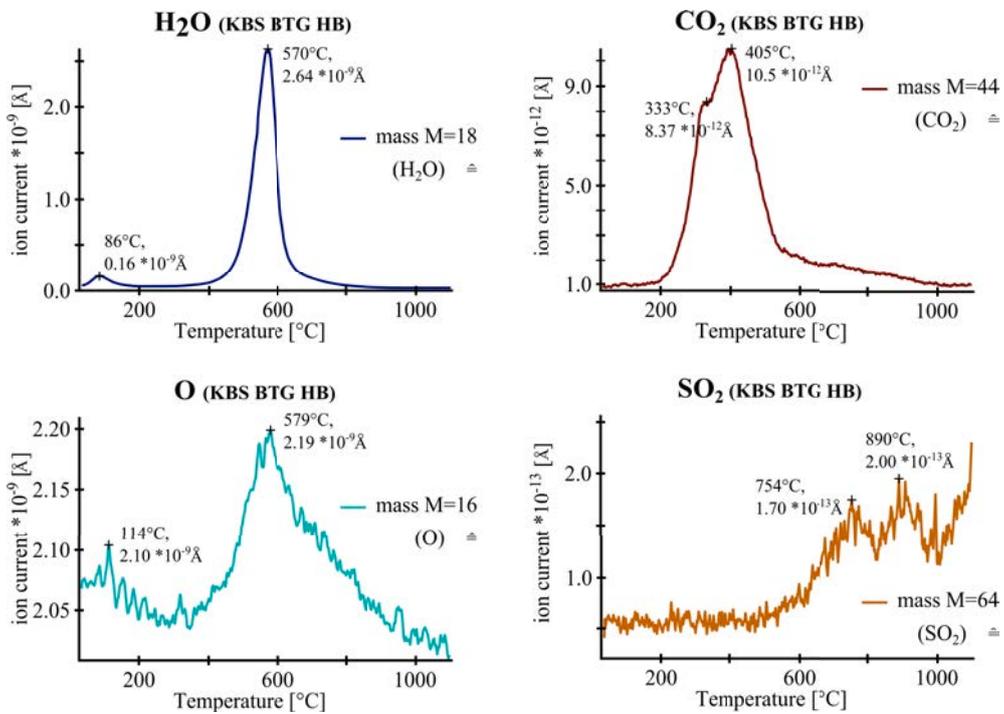


Figure B.6.: IR-MS measurements of TG-DSC analysis for KBS BT GHB

B.1.4. Texture XRD

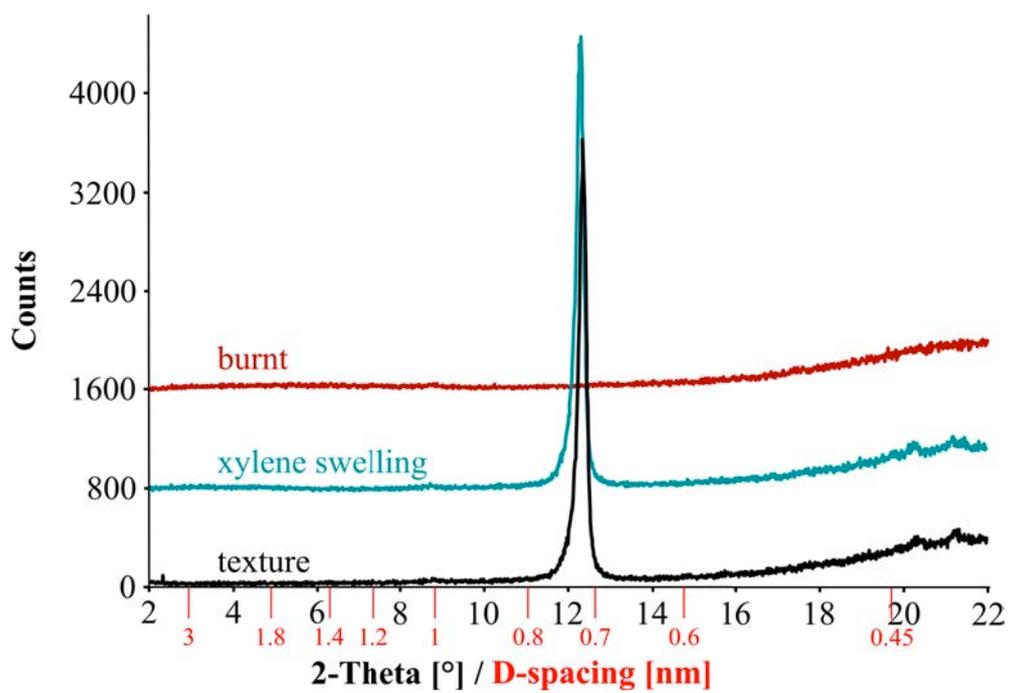
Texture XRD AKW KN 83

Figure B.7.: XRD analysis of AKW KN 83 texture samples

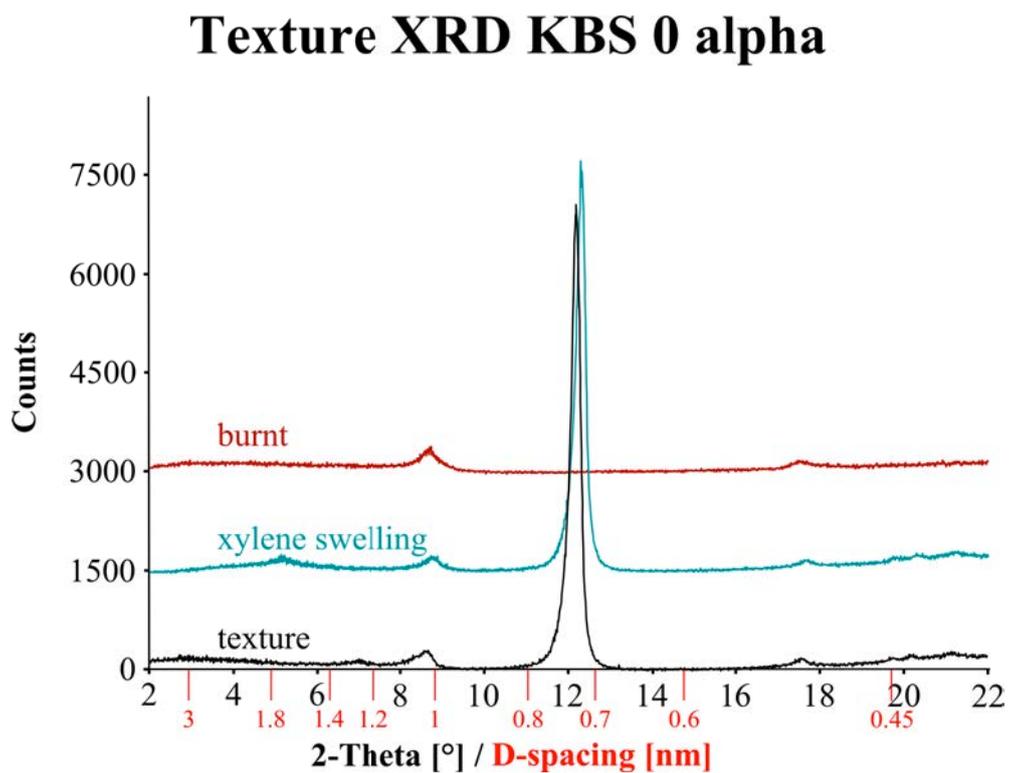


Figure B.8.: XRD analysis of KBS 0 alpha texture samples

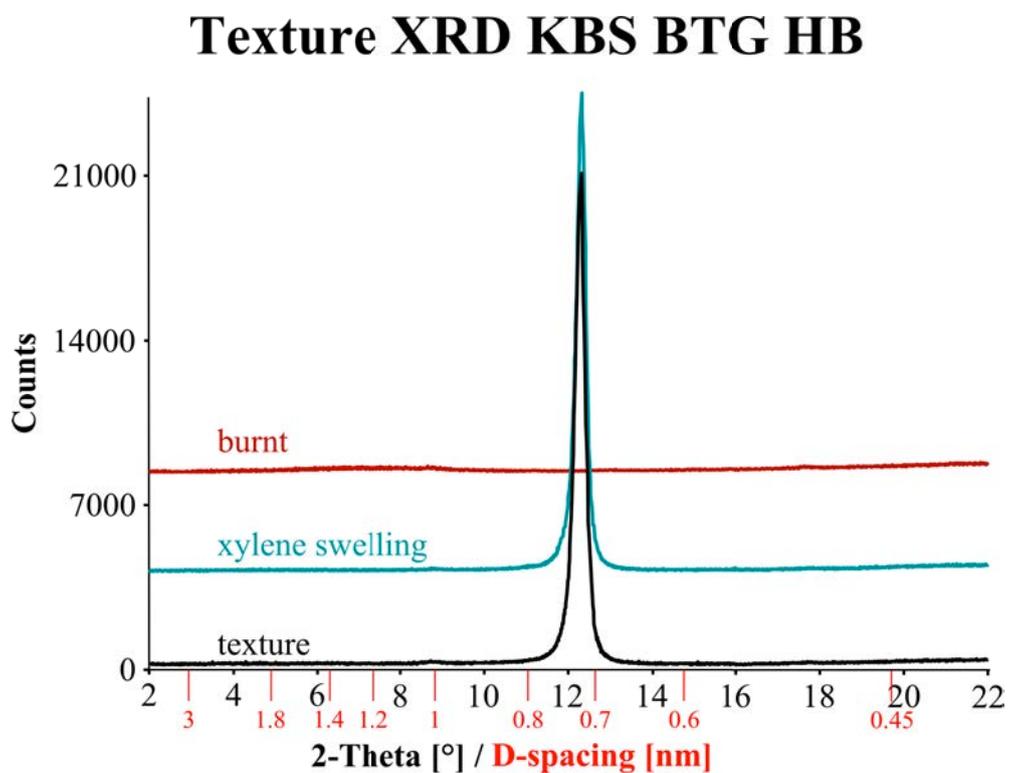


Figure B.9.: XRD analysis of KBS BT GHB texture samples

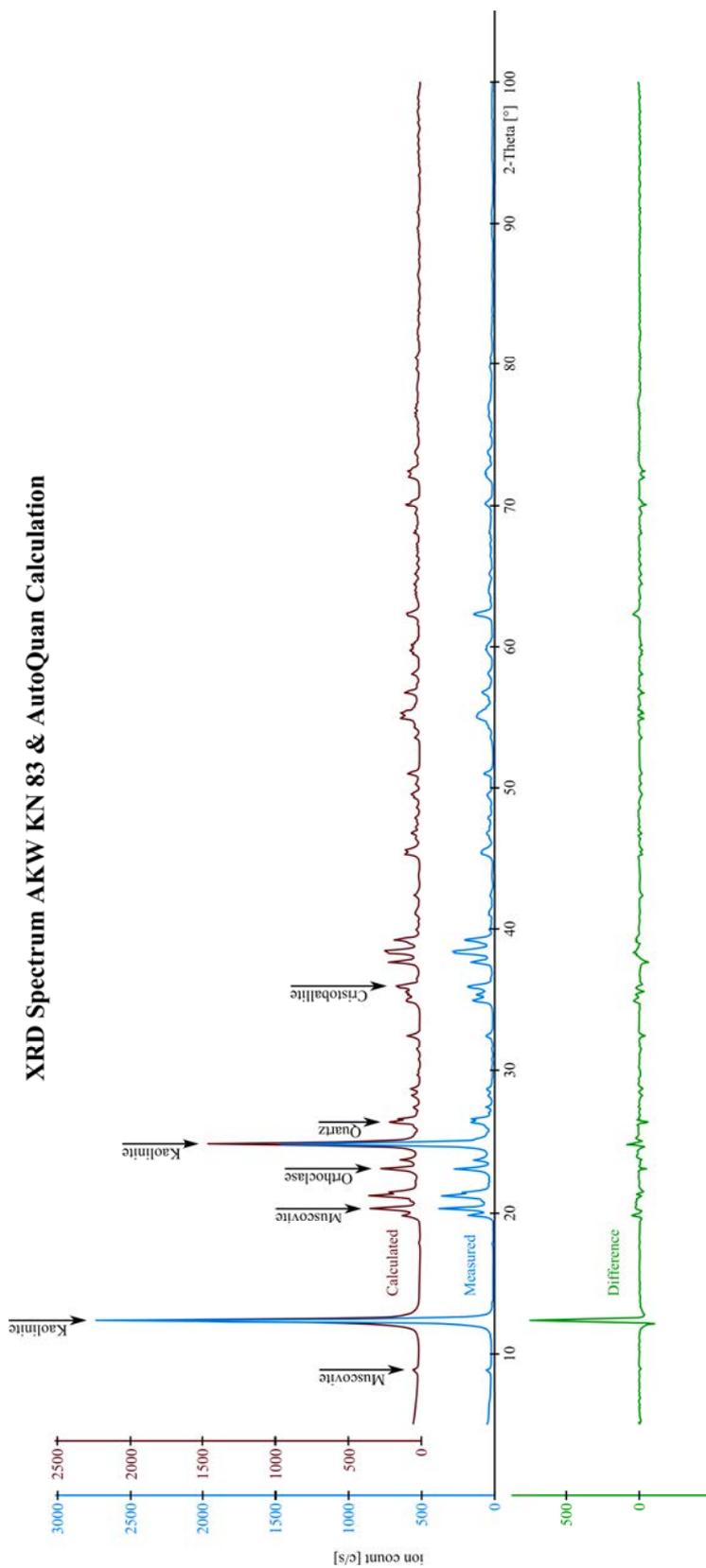


Figure B.10.: AutoQuan-calculated theoretical XRD spectrum of AKW KN 83 in comparison to the measured spectrum

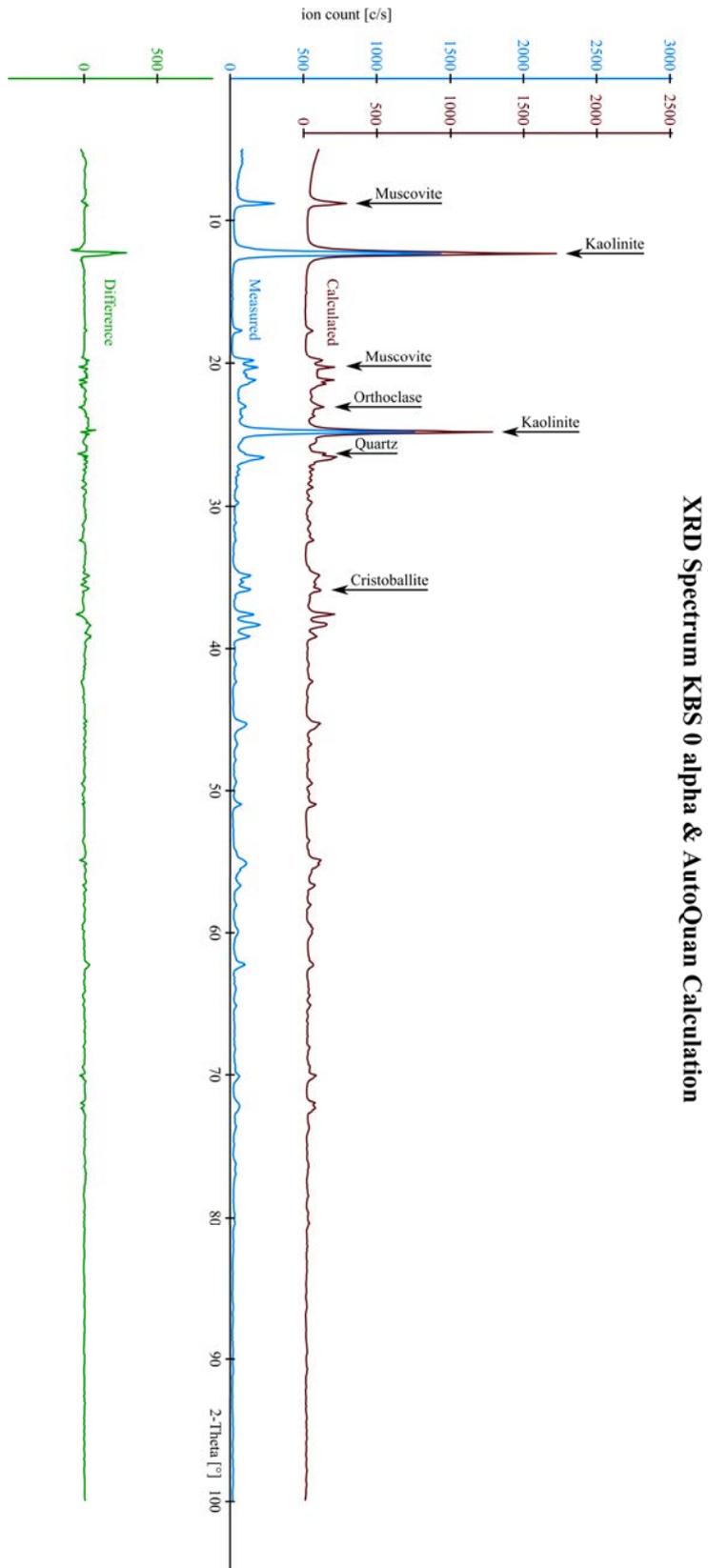


Figure B.11.: *AutoQuan-calculated theoretical XRD spectrum of KBS 0 alpha in comparison to the measured spectrum*

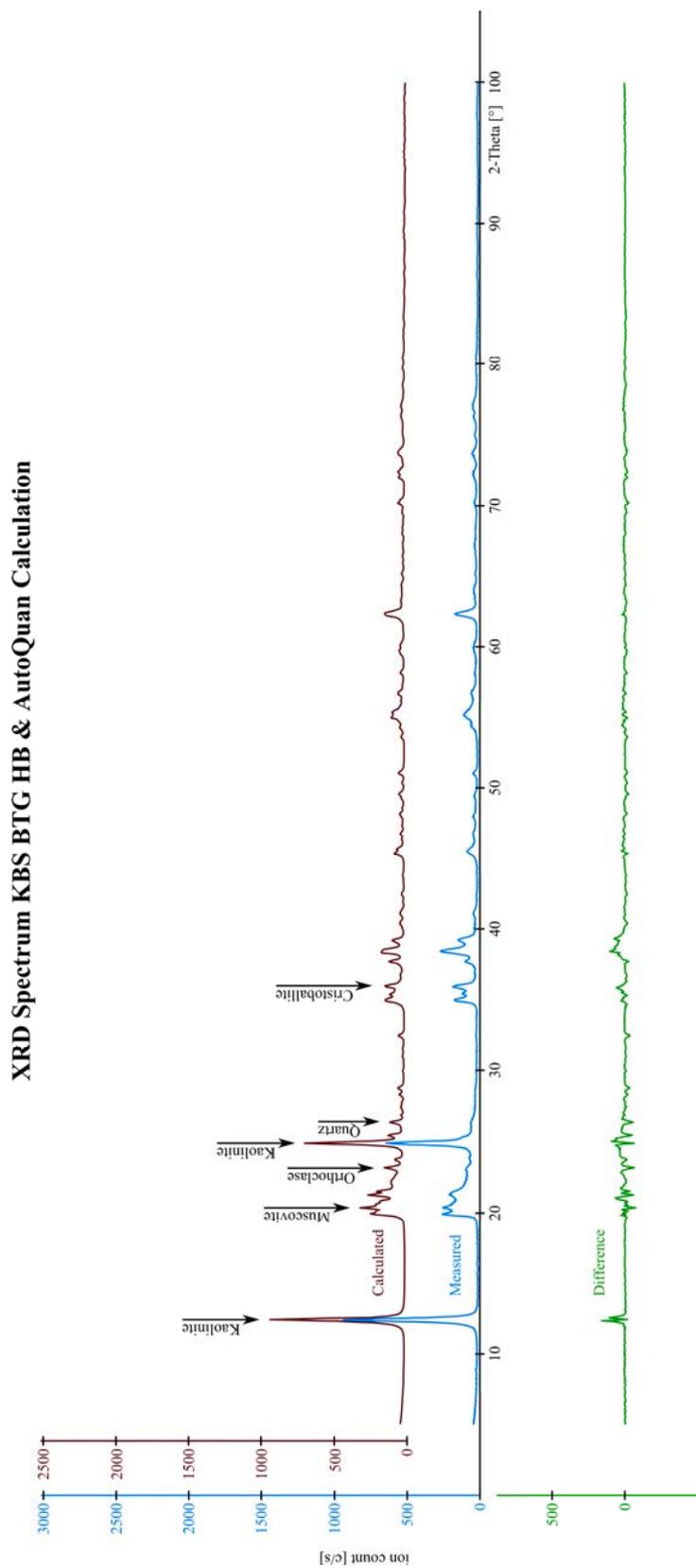


Figure B.12.: AutoQuan-calculated theoretical XRD spectrum of KBS BTGHB in comparison to the measured spectrum

sample	AKW KN 83		KBS 0 alpha		KBS BT GHB	
mineral phase	content [%]	std dev	content [%]	std dev	content [%]	std dev
anatase	x	x	x	x	2.88	0.42
calcite	x	x	0.78	0.19	x	x
crystalite	2.2	0.39	2.99	0.36	13.91	0.93
hematite	x	x	x	x	x	x
ilmenite	x	x	x	x	x	x
kaolinite (C1 ideal, BISH)	88.45	1.02	64.18	1.02	66.3	2.01
magnetite	x	x	0.88	0.22	x	x
muscovite (2M1 Fe)	5.61	1.02	21.06	1.08	12.81	1.11
orthoclase	1.69	0.42	5.28	0.6	2.46	0.6
quartz	1.23	0.28	1.58	0.36	x	x
rutile	x	x	x	x	0.84	0.26
tridymite, low	x	x	3.25	0.48	0.79	2.43

B.1.5. AutoQuan calculated mineral composition

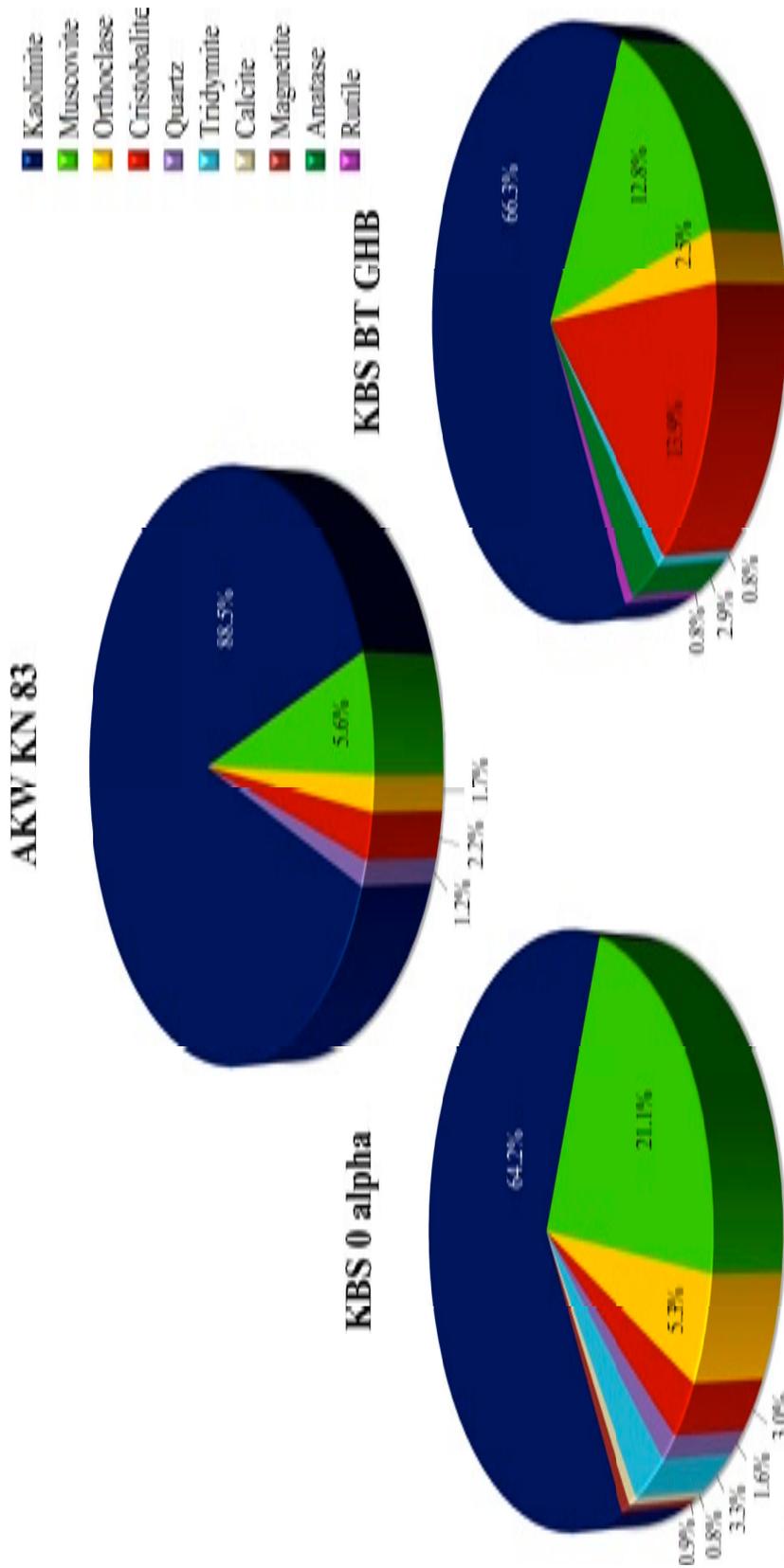


Figure B.13.: Mineral composition for kaolin samples AKW KN 83, KBS 0 alpha and KBS BTG HB as computed with AutoQuan

B.2. Datasheets experiment B0 - data overview

Table B.2.: B0 datasheet - sorption, wash and desorption data

Sample			Sorption				wash			desorption				
c(Se)	Substr.		c(Se) sol	SD	Se sorp	SD	c(Se) _{max} wash	c(Se) wash	c(Se) wash	c(Se) _{max} desorp.	c(Se) desorp.	SD	Se desorb	SD
[µg/L]	[mg]		(FIAS) [µg/L]	(FIAS) [µg/L]	[mg/kg]	[mg/kg]	(calc.) [µg/L]	(FIAS) [µg/L]	[%-calc.]	(calc.) [µg/L]	(FIAS) [µg/L]	[µg/L]	[%-sorb]	[%]
Kaolinite														
Se50-Blank	50	0.00	26.71	0.07	x	x	x	x	x	26.71	x	x	x	x
Se50-K0	50	0.00	26.30	0.11	x	x	1.32	-0.28	-20.99	26.58	x	x	x	x
Se50-K50	50	50.00	20.40	0.14	1.16	0.01	1.02	0.02	2.35	20.38	0.54	0.96	2.63	4.71
Se50-K100	50	100.00	17.18	0.06	0.91	0.00	0.86	-0.20	-23.74	17.39	0.71	0.11	4.10	0.62
Se50-K500	50	500.00	9.10	0.07	0.34	0.00	0.45	-0.05	-10.55	9.14	1.42	1.39	15.49	15.22
Se50-K1000	50	1000.00	6.84	0.08	0.19	0.00	0.34	0.00	0.00	6.84	1.28	1.13	18.77	16.49
Se500-Blank	500	0.00	459.12	0.11	x	x	x	x	x	459.12	x	x	x	x
Se500-K0	500	0.00	469.68	0.16	x	x	23.48	2.00	8.53	467.68	x	x	x	x
Se500-K50	500	50.00	383.52	0.11	16.93	0.00	19.18	0.88	4.57	382.64	34.92	2.04	9.13	0.53
Se500-K100	500	100.00	332.16	0.11	13.71	0.00	16.61	0.11	0.65	332.05	60.72	6.72	18.29	2.02
Se500-K500	500	500.00	186.24	0.08	5.67	0.00	9.31	0.34	3.61	185.90	114.60	14.52	61.64	7.81
Se500-K1000	500	1000.00	118.80	0.10	3.50	0.00	5.94	0.24	4.04	118.56	112.32	4.08	94.74	3.44
Se5000-Blank	5000	0.00	4550.40	0.14	x	x	x	x	x	4550.40	x	x	x	x
Se5000-K0	5000	0.00	4555.20	0.05	x	x	227.76	26.09	11.45	4529.11	x	x	x	x
Se5000-K50	5000	50.00	3782.40	0.13	153.94	0.01	189.12	15.55	8.22	3766.85	423.60	14.88	11.25	0.40
Se5000-K100	5000	100.00	3900.00	0.93	65.13	0.02	195.00	20.24	10.38	3879.76	198.00	90.00	5.10	2.32
Se5000-K500	5000	500.00	2683.20	0.21	37.29	0.00	134.16	12.13	9.04	2671.07	982.80	63.60	36.79	2.38
Se5000-K1000	5000	1000.00	1960.80	0.08	25.91	0.00	98.04	7.54	7.69	1953.26	1531.20	9.60	78.39	0.49
Goethite														
Se50-Blank	50	0.00	26.71	0.07	x	x	x	x	x	26.71	x	x	x	x
Se50-G0	50	0.00	26.30	0.11	x	x	1.98	-20.99	-1061.08	47.29	x	x	x	x
Se50-G50	50	50.00	9.58	0.19	3.31	0.07	0.72	0.02	3.33	9.55	1.50	0.44	15.74	4.65
Se50-G100	50	100.00	9.43	0.15	1.68	0.03	0.71	0.42	59.22	9.01	1.80	0.17	19.97	1.86
Se50-G500	50	500.00	8.28	0.07	0.36	0.00	0.62	0.48	77.10	7.80	1.22	0.23	15.69	2.92
Se50-G1000	50	1000.00	8.54	0.12	0.18	0.00	0.64	0.20	31.76	8.34	4.37	0.85	52.37	10.22
Se500-Blank	500	0.00	459.12	0.11	x	x	x	x	x	459.12	x	x	x	x
Se500-G0	500	0.00	469.68	0.16	x	x	35.31	8.53	24.16	461.15	x	x	x	x
Se500-G50	500	50.00	216.00	0.05	50.84	0.01	16.24	5.10	31.40	210.90	42.72	4.26	20.26	2.02
Se500-G100	500	100.00	184.08	0.15	28.42	0.02	13.84	4.38	31.65	179.70	55.68	1.44	30.98	0.80
Se500-G500	500	500.00	123.60	0.08	6.92	0.00	9.29	7.02	75.54	116.58	71.34	7.50	61.19	6.43
Se500-G1000	500	1000.00	119.52	0.13	3.50	0.00	8.99	5.16	57.42	114.36	83.58	2.22	73.08	1.94
Se5000-Blank	5000	0.00	4550.40	0.14	x	x	x	x	x	4550.40	x	x	x	x
Se5000-G0	5000	0.00	4555.20	0.05	x	x	342.50	11.45	3.34	4543.75	x	x	x	x
Se5000-G50	5000	50.00	2025.60	0.11	503.90	0.03	152.30	51.85	34.05	1973.75	405.60	25.80	20.55	1.31
Se5000-G100	5000	100.00	1759.20	0.10	277.66	0.02	132.27	56.20	42.49	1703.00	564.00	96.00	33.12	5.64
Se5000-G500	5000	500.00	1137.60	0.15	68.30	0.01	85.53	66.84	78.14	1070.76	894.00	3.18	83.49	0.30
Se5000-G1000	5000	1000.00	1089.60	0.14	34.63	0.00	81.92	54.26	66.24	1035.34	1057.20	36.00	102.11	3.48

Table B.3.: B0 datasheet II

volume [mL]	measured by	kaolinite [mg]	c(Se) (FIAS) [$\mu\text{g/L}$]	SD (FIAS) [$\mu\text{g/L}$]	Se sorb [%]	SD sorb [%]
10	pipette	0	795.98	14.95		
10	pipette	0.99	408.34	6.41	48.6998562	0.76425355
50	100mL cylinder	5.04	406.74	10.36	48.9007269	1.24550094
100	100mL cylinder	9.98	370.23	6.14	53.4872745	0.88659272
500	1000mL cylinder	49.90	308.91	19.47	61.191415	3.85658738
1000	1000mL cylinder	99.80	430.41	5.22	45.9267247	0.55732429
volume [mL]	measured by	goethite [mg]	c(Se) (FIAS) [$\mu\text{g/L}$]	SD (FIAS) [$\mu\text{g/L}$]	Se sorb [%]	SD sorb [%]
10	pipette	0	766.28	12.71		
10	pipette	0.99	115.56	7.37	84.9194349	5.41831715
50	100mL cylinder	5.00	110.79	5.95	85.5421699	4.59206338
100	100mL cylinder	10.00	116.31	7.35	84.8208352	5.35885527
500	1000mL cylinder	50.47	122.08	4.65	84.0683638	3.20080567
1000	1000mL cylinder	100.49	107.77	2.93	85.9365687	2.33296204

B.3. B0 analytical data

Table B.4.: *B0 analytical data - HG-FIAS measurement I*

Technique	AA FIAS-MHS							
Spectrometer Model	Aanalyst 200 S/N 200S6110908							
Autosampler Model	AS-90plus							
Batch ID	Sorp-Desorp-2012-06-13							
Results Data Set	Se_Nothingstein_2012_06_21							
Date Measured	27.06.2012							
Method Name	Se Nothingstein							
correl. coeff.	PQL (= lowest calib-10 %)	0.450						
0.998892	LOQ (= 7-wash)	0.008						
calib. slope	LOD (= 3-wash)	0.004						
0.01167	analytical quality [%]	118.762						
Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [$\mu\text{g/L}$]	calc. c(Se) [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]		
1	Blank	0.0000	0.0001	0.0	0.00	0.00		
2	0.5 ppb	0.0051	0.0020	0.5	0.43	0.00		
3	1.0 ppb	0.0106	0.0020	1.0	0.90	0.00		
4	2.0 ppb	0.0222	0.0008	2.0	1.90	0.00		
5	5.0 ppb	0.0591	0.0025	5.0	5.06	0.00		
Sequence No.	Sample ID	c(Se) diluted [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]	c(Se) driftcorr. [$\mu\text{g/L}$]	SD driftcorr. [$\mu\text{g/L}$]	dilution factor [-]	c(Se) conc. [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]
1	Wash Milli-Q	-0.146	0.069	-0.146	0.069	1	-0.15	0.07
2	Se_red_HCl_blank	0.067	0.109	0.067	0.109	12	0.80	0.11
3	TWStd_4.2 $\mu\text{g/L}$	4.988	0.094	4.988	0.094	12	59.86	0.09
4	no_sorp_Blank_50ppb	1.113	0.067	1.113	0.067	24	26.71	0.07
5	no_sorp_Blank_500ppb	1.913	0.108	1.913	0.108	240	459.12	0.11
6	no_sorp_Blank_5000ppb	1.896	0.139	1.896	0.139	2400	4550.40	0.14
7	sorp_blnd_0mg_50ppb	1.096	0.112	1.096	0.112	24	26.30	0.11
8	sorp_blnd_0mg_500ppb	1.957	0.162	1.957	0.162	240	469.68	0.16
9	sorp_blnd_0mg_5000ppb	1.898	0.054	1.898	0.054	2400	4555.20	0.05
10	wash	0.698	0.060	0.698	0.060	1	0.70	0.06
11	sorp_K-AKW_50mg_50ppb	0.850	0.137	0.850	0.137	24	20.40	0.14
12	sorp_K-AKW_50mg_500ppb	1.598	0.112	1.598	0.112	240	383.52	0.11
13	sorp_K-AKW_50mg_5000ppb	1.576	0.127	1.576	0.127	2400	3782.40	0.13
14	sorp_K-AKW_100mg_50ppb	0.716	0.059	0.716	0.059	24	17.18	0.06
15	sorp_K-AKW_100mg_500ppb	1.384	0.110	1.384	0.110	240	332.16	0.11
16	sorp_K-AKW_100mg_5000ppb	1.625	0.928	1.625	0.928	2400	3900.00	0.93
17	sorp_K-AKW_500mg_50ppb	0.379	0.067	0.379	0.067	24	9.10	0.07
18	sorp_K-AKW_500mg_500ppb	0.776	0.075	0.776	0.075	240	186.24	0.08
19	sorp_K-AKW_500mg_5000ppb	1.118	0.210	1.118	0.210	2400	2683.20	0.21
20	sorp_K-AKW_1000mg_50ppb	0.285	0.075	0.285	0.075	24	6.84	0.08
21	sorp_K-AKW_1000mg_500ppb	0.495	0.103	0.495	0.103	240	118.80	0.10
22	sorp_K-AKW_1000mg_5000ppb	0.817	0.077	0.817	0.077	2400	1960.80	0.08
23	wash	0.034	0.033	0.034	0.033	1	0.03	0.03
24	Std_0.0ppb	0.040	0.098	0.040	0.098	1	0.04	0.10
25	Std_0.5ppb	0.636	0.069	0.636	0.069	1	0.64	0.07
26	Std_1.0ppb	0.954	0.221	0.954	0.221	1	0.95	0.22
27	Std_2.0ppb	1.689	0.080	1.689	0.080	1	1.69	0.08
28	Std_5.0ppb	4.744	0.070	4.744	0.070	1	4.74	0.07
29	wash	0.029	0.043	0.029	0.043	1	0.03	0.04
30	sorp_F-E216_50mg_50ppb	0.399	0.191	0.399	0.191	24	9.58	0.19
31	sorp_F-E216_50mg_500ppb	0.900	0.050	0.900	0.050	240	216.00	0.05
32	sorp_F-E216_50mg_5000ppb	0.844	0.113	0.844	0.113	2400	2025.60	0.11
33	sorp_F-E216_100mg_50ppb	0.393	0.154	0.393	0.154	24	9.43	0.15
34	sorp_F-E216_100mg_500ppb	0.767	0.147	0.767	0.147	240	184.08	0.15
35	sorp_F-E216_100mg_5000ppb	0.733	0.096	0.733	0.096	2400	1759.20	0.10
36	sorp_F-E216_500mg_50ppb	0.345	0.070	0.345	0.070	24	8.28	0.07
37	sorp_F-E216_500mg_500ppb	0.515	0.077	0.515	0.077	240	123.60	0.08
38	sorp_F-E216_500mg_5000ppb	0.474	0.153	0.474	0.153	2400	1137.60	0.15
39	sorp_F-E216_1000mg_50ppb	0.356	0.120	0.356	0.120	24	8.54	0.12
40	sorp_F-E216_1000mg_500ppb	0.498	0.132	0.498	0.132	240	119.52	0.13
41	sorp_F-E216_1000mg_5000ppb	0.454	0.142	0.454	0.142	2400	1089.60	0.14
42	wash	0.013	0.086	0.013	0.086	1	0.01	0.09
43	Std_0.0ppb	0.233	0.062	0.233	0.062	1	0.23	0.06
44	Std_0.5ppb	1.210	0.134	1.210	0.134	1	1.21	0.13
45	Std_1.0ppb	2.318	0.100	2.318	0.100	1	2.32	0.10
46	Std_2.0ppb	4.250	0.282	4.250	0.282	1	4.25	0.28
47	Std_5.0ppb	10.827	0.231	10.827	0.231	1	10.83	0.23
48	wash	0.076	0.103	0.076	0.103	1	0.08	0.10

Table B.5.: B0 analytical data - HG-FIAS measurement II

Technique	AA FIAS-MHS		
Spectrometer Model	Aanalyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Sorp-Desorp-2012-06-13		
Results Data Set	Se_Notheinstein_T_2012_07_02		
Date Measured	03.07.2012		
Method Name	Se Notheinstein		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.997676	LOQ (= 7-wash)	-0.003	
calib. slope	LOD (= 3-wash)	-0.001	
0.03757	analytical quality [%]	97.286	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0000	0.0	0.00	0.00
2	0.5 ppb	0.0247	0.0000	0.5	0.55	0.00
3	1.0 ppb	0.0527	0.0000	1.0	1.17	0.00
4	2.0 ppb	0.0926	0.0001	2.0	2.06	0.00
5	5.0 ppb	0.2222	0.0002	5.0	4.93	0.00

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.008	0.006	-0.008	0.006	1	-0.01	0.01
2	Na2SeO3_ungekocht_1.6ppb	3.134	0.040	3.134	0.040	6	18.80	0.24
3	Na2SeO3_gekocht_1.6ppb	2.867	0.093	2.867	0.093	6	17.20	0.56
4	Na2SeO4_ungekocht_1.6ppb	0.197	0.034	0.197	0.034	6	1.18	0.20
5	Na2SeO4_gekocht_1.6ppb	2.932	0.102	2.932	0.102	6	17.59	0.61
6	Se_red_HCl_blank	0.012	0.031	0.012	0.031	6	0.07	0.19
7	TWStd_4.2µg/L	4.132	0.113	4.132	0.113	60	247.92	6.78
8	spül_blind_50ppb	-0.023	0.032	-0.023	0.032	12	-0.28	0.38
9	spül_blind_500ppb	0.167	0.019	0.167	0.019	12	2.00	0.23
10	spül_blind_5000ppb	2.174	0.058	2.174	0.058	12	26.09	0.70
11	wash	0.029	0.028	0.029	0.028	1	0.03	0.03
12	Std_0.0ppb	0.025	0.059	0.025	0.059	1	0.03	0.06
13	Std_0.5ppb	0.516	0.051	0.516	0.051	1	0.52	0.05
14	Std_1.0ppb	1.080	0.049	1.080	0.049	1	1.08	0.05
15	Std_2.0ppb	2.032	0.051	2.032	0.051	1	2.03	0.05
16	Std_5.0ppb	5.064	0.024	5.064	0.024	1	5.06	0.02
17	wash	0.004	0.024	0.004	0.024	1	0.00	0.02
18	spül_K-AKW_50mg_50ppb	0.002	0.017	0.002	0.017	12	0.02	0.20
19	spül_K-AKW_50mg_500ppb	0.073	0.016	0.073	0.016	12	0.88	0.19
20	spül_K-AKW_50mg_5000ppb	1.296	0.110	1.296	0.110	12	15.55	1.32
21	spül_K-AKW_100mg_50ppb	-0.017	0.033	-0.017	0.033	12	-0.20	0.40
22	spül_K-AKW_100mg_500ppb	0.009	0.016	0.009	0.016	12	0.11	0.19
23	spül_K-AKW_100mg_5000ppb	1.687	0.035	1.687	0.035	12	20.24	0.42
24	spül_K-AKW_500mg_50ppb	-0.004	0.015	-0.004	0.015	12	-0.05	0.18
25	spül_K-AKW_500mg_500ppb	0.028	0.026	0.028	0.026	12	0.34	0.31
26	spül_K-AKW_500mg_5000ppb	1.011	0.051	1.011	0.051	12	12.13	0.61
27	spül_K-AKW_1000mg_50ppb	0.000	0.026	0.000	0.026	12	0.00	0.31
28	spül_K-AKW_1000mg_500ppb	0.020	0.015	0.020	0.015	12	0.24	0.18
29	spül_K-AKW_1000mg_5000ppb	0.628	0.037	0.628	0.037	12	7.54	0.44
30	wash	0.020	0.044	0.020	0.044	1	0.02	0.04
31	Std_0.0ppb	0.002	0.048	0.002	0.048	1	0.00	0.05
32	Std_0.5ppb	0.480	0.061	0.480	0.061	1	0.48	0.06
33	Std_1.0ppb	1.042	0.039	1.042	0.039	1	1.04	0.04
34	Std_2.0ppb	1.991	0.030	1.991	0.030	1	1.99	0.03
35	Std_5.0ppb	4.832	0.078	4.832	0.078	1	4.83	0.08
36	wash	-0.036	0.015	-0.036	0.015	1	-0.04	0.02
37	spül_F-E216_50mg_50ppb	0.002	0.015	0.002	0.015	12	0.02	0.18
38	spül_F-E216_50mg_500ppb	0.425	0.030	0.425	0.030	12	5.10	0.36
39	spül_F-E216_50mg_5000ppb	4.321	0.187	4.321	0.187	12	51.85	2.24
40	spül_F-E216_100mg_50ppb	0.035	0.052	0.035	0.052	12	0.42	0.62
41	spül_F-E216_100mg_500ppb	0.365	0.034	0.365	0.034	12	4.38	0.41
42	spül_F-E216_100mg_5000ppb	4.683	0.143	4.683	0.143	12	56.20	1.72
43	spül_F-E216_500mg_50ppb	0.040	0.042	0.040	0.042	12	0.48	0.50
44	spül_F-E216_500mg_500ppb	0.585	0.038	0.585	0.038	12	7.02	0.46
45	spül_F-E216_500mg_5000ppb	5.570	0.076	5.570	0.076	12	66.84	0.91
46	spül_F-E216_1000mg_50ppb	0.017	0.037	0.017	0.037	12	0.20	0.44
47	spül_F-E216_1000mg_500ppb	0.430	0.071	0.430	0.071	12	5.16	0.85
48	spül_F-E216_1000mg_5000ppb	4.522	0.134	4.522	0.134	12	54.26	1.61
49	wash	0.005	0.005	0.005	0.005	12	0.06	0.06
50	Std_0.0ppb	0.028	0.014	0.028	0.014	1	0.03	0.01
51	Std_0.5ppb	0.496	0.047	0.496	0.047	1	0.50	0.05
52	Std_1.0ppb	1.024	0.071	1.024	0.071	1	1.02	0.07
53	Std_2.0ppb	1.882	0.045	1.882	0.045	1	1.88	0.05
54	Std_5.0ppb	4.628	0.085	4.628	0.085	1	4.63	0.09
55	wash	-0.016	0.012	-0.016	0.012	1	-0.02	0.01
56	Na2SeO3_ungekocht_1.6ppb	2.926	0.066	2.926	0.066	6	17.56	0.40
57	Na2SeO3_gekocht_1.6ppb	2.686	0.043	2.686	0.043	6	16.12	0.26
58	Na2SeO4_ungekocht_1.6ppb	0.169	0.007	0.169	0.007	6	1.01	0.04
59	Na2SeO4_gekocht_1.6ppb	2.795	0.066	2.795	0.066	6	16.77	0.40
60	HCL Blank	0.003	0.031	0.003	0.031	6	0.02	0.19
61	TWStd_4.2µg/L	4.040	0.156	4.040	0.156	60	242.40	9.36
62	wash	-0.032	0.017	-0.032	0.017	1	-0.03	0.02
63	wash	0.030	0.020	0.030	0.020	1	0.03	0.02

Table B.6.: B0 analytical data - HG-FIAS measurement III

Technique	AA FIAS-MHS	
Spectrometer Model	Analyst 200 S/N 200S6110908	
Autosampler Model	AS-90plus	
Batch ID	Sorp-Desorp-2012-06-13	
Results Data Set	Nothstein_2012_07_23_test	
Date Measured	23.07.2012	
Method Name	Se Nothstein	
correl. coeff.	PQL (= lowest calib-10 %)	0.450
0.999695	LOQ (= 7-wash)	0.039
calib. slope	LOD (= 3-wash)	0.017
0.02894	analytical quality [%]	97.798

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0000	0.0	0.00	0.00
2	0.5 ppb	0.0144	0.0000	0.5	0.50	0.00
3	1.0 ppb	0.0290	0.0000	1.0	1.000	0.00
4	2.0 ppb	0.0602	0.0001	2.0	2.08	0.00
5	5.0 ppb	0.1437	0.0002	5.0	4.97	0.00

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.000	0.066	0.000	0.066	1	0.00	0.07
2	Se_0.0ppb	-0.032	0.017	-0.032	0.017	1	-0.03	0.02
3	Se_0.5ppb	0.466	0.033	0.466	0.033	1	0.47	0.03
4	Se_1.0ppb	1.015	0.015	1.015	0.015	1	1.02	0.02
5	Se_2.0ppb	1.836	0.145	1.836	0.145	1	1.84	0.15
6	Se_5.0ppb	4.828	0.070	4.828	0.070	1	4.83	0.07
7	wash	-0.026	0.027	-0.026	0.027	1	-0.03	0.03
8	Na2SeO3_ungekocht_1.66ppb	-0.002	0.025	-0.002	0.025	12	-0.02	0.30
9	Na2SeO3_gekocht_1.66ppb	0.662	0.093	0.662	0.093	12	7.94	1.12
10	Na2SeO4_ungekocht_1.66ppb	0.198	0.033	0.198	0.033	12	2.38	0.40
11	Na2SeO4_gekocht_1.66ppb	0.597	0.055	0.597	0.055	12	7.16	0.66
12	HCl_blank	-0.038	0.043	-0.038	0.043	12	-0.46	0.52
13	TWStd_4.2µg/L	5.020	0.015	5.020	0.015	60	301.20	0.87
14	desorp_blind_50ppb	-0.038	0.014	-0.038	0.014	12	-0.46	0.17
15	desorp_blind_500ppb	-0.020	0.029	-0.020	0.029	120	-2.40	3.48
16	desorp_blind_5000ppb	-0.034	0.065	-0.034	0.065	1200	-40.80	78.00
17	wash	-0.016	0.038	-0.016	0.038	1	-0.02	0.04
18	Se_0.0ppb	-0.060	0.010	-0.060	0.010	1	-0.06	0.01
19	Se_0.5ppb	0.466	0.017	0.466	0.017	1	0.47	0.02
20	Se_1.0ppb	0.997	0.124	0.997	0.124	1	1.00	0.12
21	Se_2.0ppb	2.085	0.007	2.085	0.007	1	2.09	0.01
22	Se_5.0ppb	5.273	0.031	5.273	0.031	1	5.27	0.03
23	wash	-0.049	0.037	-0.049	0.037	1	-0.05	0.04
24	desorp_AKW_50mg_50ppb	0.045	0.080	0.045	0.080	12	0.54	0.96
25	desorp_AKW_50mg_500ppb	0.291	0.017	0.291	0.017	120	34.92	2.04
26	desorp_AKW_50mg_5000ppb	0.353	0.012	0.353	0.012	1200	423.60	14.88
27	desorp_AKW_100mg_50ppb	0.059	0.009	0.059	0.009	12	0.71	0.11
28	desorp_AKW_100mg_500ppb	0.506	0.056	0.506	0.056	120	60.72	6.72
29	desorp_AKW_100mg_5000ppb	0.165	0.075	0.165	0.075	1200	198.00	90.00
30	desorp_AKW_500mg_50ppb	0.118	0.116	0.118	0.116	12	1.42	1.39
31	desorp_AKW_500mg_500ppb	0.955	0.121	0.955	0.121	120	114.60	14.52
32	desorp_AKW_500mg_5000ppb	0.819	0.053	0.819	0.053	1200	982.80	63.60
33	desorp_AKW_1000mg_50ppb	0.207	0.094	0.207	0.094	12	2.48	1.13
34	desorp_AKW_1000mg_500ppb	0.936	0.034	0.936	0.034	120	112.32	4.08
35	desorp_AKW_1000mg_5000ppb	1.276	0.008	1.276	0.008	1200	1531.20	9.60
36	wash	0.000	0.091	0.000	0.091	1	0.00	0.09
37	Se_0.0ppb	-0.015	0.034	-0.015	0.034	1	-0.02	0.03
38	Se_0.5ppb	0.607	0.057	0.607	0.057	1	0.61	0.06
39	Se_1.0ppb	1.193	0.116	1.193	0.116	1	1.19	0.10
40	Se_2.0ppb	2.231	0.067	2.231	0.067	1	2.23	0.07
41	Se_5.0ppb	5.574	0.113	5.574	0.113	1	5.57	0.11
42	wash	-0.028	0.078	-0.028	0.078	1	-0.03	0.08
43	desorp_E216_50mg_50ppb	0.125	0.037	0.125	0.037	12	1.50	0.44
44	desorp_E216_50mg_500ppb	0.712	0.071	0.712	0.071	60	42.72	4.26
45	desorp_E216_50mg_5000ppb	0.676	0.043	0.676	0.043	600	405.60	25.80
46	desorp_F-E216_100mg_50ppb	0.150	0.014	0.150	0.014	12	1.80	0.17
47	desorp_F-E216_100mg_500ppb	0.928	0.024	0.928	0.024	60	55.68	1.44
48	desorp_F-E216_100mg_5000ppb	0.940	0.160	0.940	0.160	600	564.00	96.00
49	desorp_F-E216_500mg_50ppb	0.102	0.019	0.102	0.019	12	1.22	0.23
50	desorp_F-E216_500mg_500ppb	1.189	0.125	1.189	0.125	60	71.34	7.50
51	desorp_F-E216_500mg_5000ppb	1.490	0.005	1.490	0.005	600	894.00	3.18
52	desorp_F-E216_1000mg_50ppb	0.364	0.071	0.364	0.071	12	4.37	0.85
53	desorp_F-E216_1000mg_500ppb	1.393	0.037	1.393	0.037	60	83.58	2.22
54	desorp_F-E216_1000mg_5000ppb	1.762	0.060	1.762	0.060	600	1057.20	36.00
55	wash	-0.002	0.068	-0.002	0.068	1	0.00	0.07
56	Std_0.0ppb	-0.003	0.029	-0.003	0.029	1	0.00	0.03
57	Std_0.5ppb	0.561	0.055	0.561	0.055	1	0.56	0.06
58	Std_1.0ppb	1.156	0.023	1.156	0.023	1	1.16	0.10
59	Std_2.0ppb	2.289	0.076	2.289	0.076	1	2.29	0.08
60	Std_5.0ppb	5.494	0.041	5.494	0.041	1	5.49	0.04
61	wash	0.011	0.125	0.011	0.125	1	0.01	0.13
62	Na2SeO3_ungekocht_1.6ppb	0.002	0.048	0.002	0.048	6	0.01	0.29
63	Na2SeO3_gekocht_1.6ppb	0.700	0.028	0.700	0.028	6	4.20	0.17
64	Na2SeO4_ungekocht_1.6ppb	0.178	0.012	0.178	0.012	6	1.07	0.07
65	Na2SeO4_gekocht_1.6ppb	0.620	0.042	0.620	0.042	6	3.72	0.25
66	HCl_blank	-0.048	0.037	-0.048	0.037	6	-0.29	0.22
67	TWStd_4.2µg/L	3.195	2.589	3.195	2.589	60	191.70	155.34
68	wash	0.164	0.291	0.164	0.291	1	0.16	0.29
69	wash	0.002	0.045	0.002	0.045	1	0.00	0.05

Table B.7.: B0 analytical data - HG-FIAS measurement IV

Technique	AA FIAS-MHS							
Spectrometer Model	Aanalyst 200 S/N 200S6110908							
Autosampler Model	AS-90plus							
Batch ID	Sorp-Desorp-2012-06-13							
Results Data Set	Nothstein_Se_2013_03_06b							
Date Measured	06.03.2013							
Method Name	Se Nothstein 5repl							
correl. coeff.	PQL (= lowest calib-10 %)	0.450						
0.99096	LOQ (= 7-wash)	0.093						
calib. slope	LOD (= 3-wash)	0.040						
0.02658	analytical quality [%]	106.531						
Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [$\mu\text{g/L}$]	calc. c(Se) [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]		
1	Blank	0.0000	0.0000	0.0	0.00	0.00		
2	0.5 ppb	0.0129	0.0000	0.5	0.49	0.00		
3	1.0 ppb	0.0281	0.0000	1.0	1.06	0.00		
4	2.0 ppb	0.0563	0.0001	2.0	2.12	0.00		
5	5.0 ppb	0.1312	0.0002	5.0	4.94	0.00		
Sequence No.	Sample ID	c(Se) diluted [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]	c(Se) driftcorr. [$\mu\text{g/L}$]	SD driftcorr. [$\mu\text{g/L}$]	dilution factor [-]	c(Se) conc. [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]
1	Wash Milli-Q	-0.014	0.020	-0.014	0.020	1	-0.01	0.02
2	wash	0.010	0.011	0.010	0.011	1	0.01	0.01
3	HCl Blank	0.026	0.019	0.023	0.016	6	0.14	0.10
4	Trace Metal 252 $\mu\text{g/L}$	4.543	0.087	4.425	0.084	60	265.49	5.06
5	wash	0.030	0.030	0.030	0.030	1	0.03	0.03
6	Se_Std_0	0.026	0.020	0.026	0.020	1	0.03	0.02
7	Se_Std_0.5	0.546	0.022	0.546	0.022	1	0.55	0.02
8	Se_Std_1	1.096	0.047	1.096	0.047	1	1.10	0.05
9	Se_Std_2	2.213	0.041	2.213	0.041	1	2.21	0.04
10	Se_Std_5	5.065	0.050	5.065	0.050	1	5.07	0.05
11	wash	0.000	0.028	0.000	0.028	1	0.00	0.03
12	wash	-0.010	0.011	-0.010	0.011	1	-0.01	0.01
13	upscaling blank	3.409	0.103	3.225	0.097	240	774.00	23.30
14	upscaling Kaolinite 0 mg	3.506	0.066	3.317	0.062	240	795.98	14.95
15	upscaling FeOOH 0 mg	3.375	0.056	3.193	0.053	240	766.28	12.71
16	upscaling Kaolinite 1 mg	1.839	0.029	1.701	0.027	240	408.34	6.41
17	upscaling FeOOH 1 mg	0.581	0.037	0.481	0.031	240	115.56	7.37
18	upscaling Kaolinite 5 mg	1.832	0.047	1.695	0.043	240	406.74	10.36
19	upscaling FeOOH 5 mg	0.557	0.030	0.462	0.025	240	110.79	5.95
20	upscaling Kaolinite 10 mg	1.667	0.028	1.543	0.026	240	370.23	6.14
21	upscaling FeOOH 10 mg 0	0.585	0.037	0.485	0.031	240	116.31	7.35
22	upscaling Kaolinite 50 mg	1.443	0.091	1.287	0.081	240	308.91	19.47
23	upscaling FeOOH 50 mg	0.614	0.023	0.509	0.019	240	122.08	4.65
24	upscaling Kaolinite 100 mg	1.938	0.024	1.793	0.022	240	430.41	5.22
25	upscaling FeOOH 100 mg	0.542	0.015	0.449	0.012	240	107.77	2.93
26	wash	0.031	0.045	0.031	0.045	1	0.03	0.05
27	HCl Blank	0.006	0.010	0.005	0.008	6	0.03	0.05
28	Trace Metal 252 $\mu\text{g/L}$	4.927	0.091	4.524	0.084	60	271.43	5.02
29	wash	0.017	0.030	0.017	0.030	1	0.02	0.03
30	Se_Std_0	0.022	0.014	0.022	0.014	1	0.02	0.01
31	Se_Std_0.5	0.591	0.023	0.591	0.023	1	0.59	0.02
32	Se_Std_1	1.250	0.085	1.250	0.085	1	1.25	0.08
33	Se_Std_2	2.343	0.074	2.343	0.074	1	2.34	0.07
34	Se_Std_5	5.341	0.086	5.341	0.086	1	5.34	0.09
35	wash	0.022	0.020	0.022	0.020	1	0.02	0.02
36	wash	0.033	0.045	0.033	0.045	1	0.03	0.05

B.4. B1 Datasheets - sorption experiments

Table B.8.: PHREEQ-C calculation input file for initial sorption solution pH values after addition of selenite

```
1  DATABASE wateq4f.dat
2  TITLE KCl Selenite
3
4  SELECTED_OUTPUT
5  -reset false
6  -pH true
7  -molalities H2SeO3 HSe- H2Se HSeO3- SeO3-2 H2SeO3 SeO4-2 HSeO4-
8
9  SOLUTION 1 # KCl in water
10 units mol/L
11 temp 25
12 pH 7
13 REACTION 1
14 K 0.007735
15 Cl 0.007735
16
17 EQUILIBRIUM_PHASES 1
18 CO2(g) -3.3974 # log10 p(CO2) in bar; 400 ppm = log10 (0.0004)
19 SAVE SOLUTION 2 # KCl-solution in equilibrium with air-CO2
20 END
21
22 USE SOLUTION 2
23 REACTION 1
24 HCl 1 # set pH to measured value 5.21
25 0.0000055 in 1
26 SAVE SOLUTION 3 # KCl-solution CO2-eq and measured pH
27 END
28
29 USE SOLUTION 3 #1
30 REACTION 2
31 Na2SeO3 1
32 0.00000633 in 1
33 EQUILIBRIUM_PHASES 2
34 CO2(g) -3.3974
35 SAVE SOLUTION 4
36 END
37 USE SOLUTION 4 #2
38 REACTION 3
39 Na2SeO3 1
40 0.00000633 in 1
41 EQUILIBRIUM_PHASES 3
42 CO2(g) -3.3974
43 SAVE SOLUTION 5
44 END
45 USE SOLUTION 5 #3
46 REACTION 4
47 Na2SeO3 1
48 0.00000633 in 1
49 EQUILIBRIUM_PHASES 4
50 CO2(g) -3.3974
51 SAVE SOLUTION 6
52 END
53 USE SOLUTION 6 #4
54 REACTION 5
55 Na2SeO3 1
56 0.00000633 in 1
```

Table B.9.: PHREEQ-C calculation input file for initial sorption solution pH values after addition of selenite (continued from previous page)

```
57 EQUILIBRIUM_PHASES 5
58 CO2(g) -3.3974
59 SAVE SOLUTION 7
60 END
61 USE SOLUTION 7 #5
62 REACTION 6
63 Na2SeO3 1
64 0.00000633 in 1
65 EQUILIBRIUM_PHASES 6
66 CO2(g) -3.3974
67 SAVE SOLUTION 8
68 END
69 USE SOLUTION 8 #6
70 REACTION 7
71 Na2SeO3 1
72 0.00000633 in 1
73 EQUILIBRIUM_PHASES 7
74 CO2(g) -3.3974
75 SAVE SOLUTION 9
76 END
77 USE SOLUTION 9 #7
78 REACTION 8
79 Na2SeO3 1
80 0.00000633 in 1
81 EQUILIBRIUM_PHASES 8
82 CO2(g) -3.3974
83 SAVE SOLUTION 10
84 END
85 USE SOLUTION 10 #8
86 REACTION 9
87 Na2SeO3 1
88 0.00000633 in 1
89 EQUILIBRIUM_PHASES 9
90 CO2(g) -3.3974
91 SAVE SOLUTION 11
92 END
93 USE SOLUTION 11 #9
94 REACTION 10
95 Na2SeO3 1
96 0.00000633 in 1
97 EQUILIBRIUM_PHASES 10
98 CO2(g) -3.3974
99 SAVE SOLUTION 12
100 END
101 USE SOLUTION 12 #10
102 REACTION 11
103 Na2SeO3 1
104 0.00000633 in 1
105 EQUILIBRIUM_PHASES 11
106 CO2(g) -3.3974
107 SAVE SOLUTION 13
108 END
109 END
```

Table B.10.: PHREEQ-C calculation input file for initial sorption solution pH values after addition of selenate

```

1  DATABASE wateq4f.dat
2  TITLE KCl Selenate
3
4  SELECTED_OUTPUT
5  -reset false
6  -pH true
7  -molalities H2SeO3 HSe- H2Se HSeO3- SeO3-2 H2SeO3 SeO4-2 HSeO4-
8
9  SOLUTION 1 # KCl in water
10 units mol/L
11 temp 25
12 pH 7
13 REACTION 1
14 K 0.007735
15 Cl 0.007735
16
17 EQUILIBRIUM_PHASES 1
18 CO2(g) -3.3974 # log10 p(CO2) in bar; 400 ppm = log10 (0.0004)
19 SAVE SOLUTION 2 # KCl-solution in equilibrium with air-CO2
20 END
21
22 USE SOLUTION 2
23 REACTION 1
24 KOH 1 # set pH to measured value 5.75
25 0.00000158 in 1
26 SAVE SOLUTION 3 # KCl-solution CO2-eq and measured pH
27 END
28
29 USE SOLUTION 3 #1
30 REACTION 2
31 Na2SeO4 1
32 0.00000633 in 1
33 EQUILIBRIUM_PHASES 2
34 CO2(g) -3.3974
35 SAVE SOLUTION 4
36 END
37 USE SOLUTION 4 #2
38 REACTION 3
39 Na2SeO4 1
40 0.00000633 in 1
41 EQUILIBRIUM_PHASES 3
42 CO2(g) -3.3974
43 SAVE SOLUTION 5
44 END
45 USE SOLUTION 5 #3
46 REACTION 4
47 Na2SeO4 1
48 0.00000633 in 1
49 EQUILIBRIUM_PHASES 4
50 CO2(g) -3.3974
51 SAVE SOLUTION 6
52 END
53 USE SOLUTION 6 #4
54 REACTION 5
55 Na2SeO4 1
56 0.00000633 in 1

```

Table B.11.: PHREEQ-C calculation input file for initial sorption solution pH values after addition of selenate (continued from previous page)

```
57 EQUILIBRIUM_PHASES 5
58 CO2(g) -3.3974
59 SAVE SOLUTION 7
60 END
61 USE SOLUTION 7 #5
62 REACTION 6
63 Na2SeO4 1
64 0.00000633 in 1
65 EQUILIBRIUM_PHASES 6
66 CO2(g) -3.3974
67 SAVE SOLUTION 8
68 END
69 USE SOLUTION 8 #6
70 REACTION 7
71 Na2SeO4 1
72 0.00000633 in 1
73 EQUILIBRIUM_PHASES 7
74 CO2(g) -3.3974
75 SAVE SOLUTION 9
76 END
77 USE SOLUTION 9 #7
78 REACTION 8
79 Na2SeO4 1
80 0.00000633 in 1
81 EQUILIBRIUM_PHASES 8
82 CO2(g) -3.3974
83 SAVE SOLUTION 10
84 END
85 USE SOLUTION 10 #8
86 REACTION 9
87 Na2SeO4 1
88 0.00000633 in 1
89 EQUILIBRIUM_PHASES 9
90 CO2(g) -3.3974
91 SAVE SOLUTION 11
92 END
93 USE SOLUTION 11 #9
94 REACTION 10
95 Na2SeO4 1
96 0.00000633 in 1
97 EQUILIBRIUM_PHASES 10
98 CO2(g) -3.3974
99 SAVE SOLUTION 12
100 END
101 USE SOLUTION 12 #10
102 REACTION 11
103 Na2SeO4 1
104 0.00000633 in 1
105 EQUILIBRIUM_PHASES 11
106 CO2(g) -3.3974
107 SAVE SOLUTION 13
108 END
109 END
```

Table B.12.: B1 analytical data - ICP-MS measurement sorption samples Na_2SeO_3

Technique	ICP-MS Quadrupole						
System	X-Series Thermo Fischer						
Date measured	05.11.2014						
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean $^{76}Se, ^{77}Se, ^{78}Se$	SD
	[$\mu g/L$]	[$\mu g/L$]	[$\mu g/L$]	[$\mu g/L$]	[-]	[$\mu g/L$]	[$\mu g/L$]
Analytical Quality							
wash-mean	0.42	0.22	0.23	0.92	0.29		
wash-SD	0.16	0.15	0.13	1.59	0.15		
LOD (= 3-wash)	0.47	0.45	0.40	4.78	0.44		
HighPurityStd ref. value	5.50	5.50	5.50	5.50		5.50	
Quality [%]	132.81	101.78	103.16	104.15		102.47	
Calibration							
Std 0ppb	0.12	0.04	0.04	3.43	1	0.06	0.05
Std 5ppb Se	5.23	4.74	4.93	6.56	1	4.97	0.25
Std 10ppb Se	9.86	10.00	9.64	12.09	1	9.83	0.18
Std 25ppb Se	25.10	25.08	25.08	27.18	1	25.09	0.01
Std 50ppb Se	49.95	49.71	49.79	50.55	1	49.82	0.12
Std 100ppb Se	99.63	99.81	98.66	100.80	1	99.37	0.62
Std 250ppb Se	251.90	251.60	251.50	249.70	1	251.67	0.21
Std 500ppb Se	497.30	501.10	501.30	499.20	1	499.90	2.25
Std 1000ppb Se	1001.00	999.50	999.20	1000.00	1	999.90	0.96
Samples							
wash 3	0.79	0.58	0.59	2.03		0.65	
HPS	7.33	5.43	5.71	7.79		5.57	
wash 4	0.35	0.17	0.13	0.98		0.22	
initsol_SeO3_Se5000	1018.0	1029.0	1023.0	1020.0	5	5116.7	27.54
initsol_SeO3_Se3500	299.7	302.5	305.9	305.3	5	1513.5	15.52
initsol_SeO3_Se2500	504.0	504.9	497.9	503.5	5	2511.3	19.04
initsol_SeO3_Se2000	513.6	516.7	516.1	516.9	5	2577.3	8.22
initsol_SeO3_Se1500	302.8	307.9	307.6	308.2	5	1530.5	14.31
initsol_SeO3_Se1000	522.0	534.1	533.1	533.3	2	1059.5	13.43
initsol_SeO3_Se0750	502.6	509.0	507.2	507.5	2	1012.5	6.60
initsol_SeO3_Se0500	268.8	271.4	271.5	276.5	2	541.1	3.06
initsol_SeO3_Se0350	184.5	186.4	185.7	192.1	2	371.1	1.92
wash 4	1.42	1.09	1.01	1.28		1.17	
test 25ppb	26.45	26.06	25.66	27.23		26.06	
wash 5	0.75	0.56	0.49	1.74		0.60	
initsol_SeO3_Se0250	102.5	102.5	103.0	106.5	2	205.3	0.58
initsol_SeO3_Se0200	136.4	136.2	137.1	142.0	2	273.1	0.95
initsol_SeO3_Se0150	77.7	78.0	77.2	81.4	2	155.2	0.78
initsol_SeO3_Se0100	40.4	40.8	40.6	45.4	2	81.2	0.36
initsol_SeO3_Se0100wdh	41.4	41.1	40.6	46.6	2	82.1	0.75
initsol_SeO3_Se0075	52.3	53.9	54.0	59.4	2	106.7	1.86
initsol_SeO3_Se0050	22.9	24.2	23.7	30.6	2	47.2	1.35
initsol_SeO3_Se0025	13.4	13.2	13.2	18.3	2	26.5	0.22
initsol_SeO3_Se0010	5.31	5.31	5.72	11.79	2	10.9	0.47
initsol_SeO3_Se0000	0.67	0.63	0.60	12.45	1	0.64	0.04
wash 6	0.42	0.19	0.23	1.32		0.28	
test 25ppb	25.37	25.48	25.42	27.24		25.42	
wash 7	0.37	0.18	0.19	1.90		0.25	
sorp-K_SeO3_Se5000	1878.0	1901.0	1886.0	1891.0	2	3776.7	23.35
sorp-K_SeO3_Se3500	469.2	475.6	471.6	477.0	2	944.3	6.47
sorp-K_SeO3_Se2500	832.3	853.0	850.1	853.4	2	1690.3	22.42
sorp-K_SeO3_Se2000	876.4	888.0	885.7	883.7	2	1766.7	12.28
sorp-K_SeO3_Se1500	396.7	400.3	400.3	403.9	2	798.2	4.16
sorp-K_SeO3_Se1000	289.4	295.4	293.6	300.6	2	585.6	6.16
sorp-K_SeO3_Se0750	279.9	282.7	281.3	285.7	2	562.6	2.80
sorp-K_SeO3_Se0500	133.3	135.7	133.1	138.2	2	268.1	2.89
sorp-K_SeO3_Se0350	86.5	87.1	86.8	93.1	2	173.6	0.61
wash 7	0.76	0.61	0.64	1.36		0.67	
test 25ppb	25.25	25.84	25.97	26.47		25.69	
wash 8	0.57	0.39	0.28	1.14		0.42	
sorp-K_SeO3_Se0250	56.2	57.7	57.4	61.7	2	114.2	1.60
sorp-K_SeO3_Se0200	46.8	47.0	47.6	54.0	2	94.3	0.84
sorp-K_SeO3_Se0150	32.2	33.0	32.3	38.8	2	65.0	0.88
sorp-K_SeO3_Se0100	21.2	20.9	20.9	26.8	2	42.0	0.39
sorp-K_SeO3_Se0075	15.7	15.6	15.0	20.2	2	30.9	0.71
sorp-K_SeO3_Se0050	9.59	9.76	9.74	15.56	2	19.4	0.18
sorp-K_SeO3_Se0025	5.14	4.98	4.94	10.37	2	10.0	0.21
sorp-K_SeO3_Se0010	2.03	2.18	2.10	7.27	2	4.21	0.15
sorp-K_SeO3_Se0000	1.04	0.99	1.01	10.07	1	1.01	0.02
wash 9	0.39	0.15	0.19	0.20		0.24	
test 25ppb	25.72	26.33	26.01	26.77		26.02	
wash 10	0.46	0.19	0.18	0.81		0.28	

Table B.13.: *B1 analytical data - ICP-MS measurement sorption samples Na₂SeO₃ (continued from previous page)*

Isotope	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	dil. factor	Se mean	
						⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se	SD
sorp-G_SeO3_Se5000	15.00	14.90	14.69	27.06	1	14.86	0.16
sorp-G_SeO3_Se3500	4.38	4.37	4.81	16.33	1	4.38	0.01
sorp-G_SeO3_Se2500	7.37	7.36	7.64	19.54	1	7.37	0.01
sorp-G_SeO3_Se2000	7.20	7.04	7.44	18.18	1	7.12	0.11
sorp-G_SeO3_Se1500	4.53	4.42	5.22	14.98	1	4.47	0.08
sorp-G_SeO3_Se1000	3.17	2.99	3.64	14.65	1	3.08	0.13
sorp-G_SeO3_Se0750	3.20	3.25	3.60	13.71	1	3.23	0.04
sorp-G_SeO3_Se0500	1.70	1.60	2.23	12.96	1	1.65	0.07
sorp-G_SeO3_Se0350	1.48	1.50	1.92	13.21	1	1.49	0.01
wash 11	0.28	0.11	0.26	-0.40	1	0.22	0.13
test 25ppb	25.31	24.74	25.24	26.21	1	25.10	0.40
wash 12	0.57	0.40	0.41	0.24	1	0.46	0.12
sorp-G_SeO3_Se0250	1.10	1.24	1.58	8.72	1	1.17	0.09
sorp-G_SeO3_Se0200	1.11	0.93	1.54	12.75	1	1.02	0.13
sorp-G_SeO3_Se0150	0.91	0.72	1.27	10.03	1	0.82	0.14
sorp-G_SeO3_Se0100	0.64	0.63	1.23	10.38	1	0.63	0.01
sorp-G_SeO3_Se0075	0.69	0.47	1.26	9.72	1	0.58	0.15
sorp-G_SeO3_Se0050	0.58	0.37	1.27	11.02	1	0.48	0.15
sorp-G_SeO3_Se0025	0.52	0.35	1.16	11.50	1	0.43	0.12
sorp-G_SeO3_Se0010	0.59	0.28	1.17	10.71	1	0.43	0.22
sorp-G_SeO3_Se0000	0.92	0.74	1.72	12.47	1	0.83	0.13
wash 13	0.35	0.10	0.28	-2.06	1	0.24	0.13
test 25ppb	24.46	24.20	23.93	23.88	1	24.20	0.27
HPS wdh	7.28	5.77	5.64	3.67	(2)	5.70	0.09
wash 14	0.51	0.30	0.29	-0.98	1	0.37	0.13

Table B.14.: B1 analytical data - ICP-MS measurement sorption samples Na_2SeO_4

Technique	ICP-MS Quadrupole							
System	X-Series Thermo Fischer							
Date measured	14.04.2014							
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean	SD	
	[$\mu g/L$]	[$\mu g/L$]	[$\mu g/L$]	[$\mu g/L$]	[-]	$^{76}Se, ^{77}Se, ^{78}Se$	[$\mu g/L$]	
Analytical Quality								
wash-mean	0.13	0.09	0.11	0.12	1			
wash-SD	0.06	0.05	0.04	0.06	1			
LOD (= 3-wash)	0.17	0.14	0.11	0.18	1			
HighPurityStd ref. value	5.50	5.50	5.50	5.50		5.50		
Quality [%]	132.31	104.34	102.34	104.04				
Calibration								
Std Oppb	0.11	0.04	0.07	0.06	1	0.07	0.03	
Std 2.5ppb Se	2.60	2.60	2.62	2.58	1	2.61	0.01	
Std 5ppb Se	5.24	4.97	5.15	5.25	1	5.12	0.14	
Std 10ppb Se	10.22	10.20	10.01	10.10	1	10.14	0.12	
Std 25ppb Se	25.84	25.10	25.28	24.91	1	25.41	0.39	
Std 50ppb Se	49.81	48.94	50.05	49.61	1	49.60	0.58	
Std 100ppb Se	98.02	101.30	99.99	100.70	1	99.77	1.65	
Std 250ppb Se	249.90	248.70	250.70	249.10	1	249.77	1.01	
Std 500ppb Se	501.00	499.80	500.30	500.10	1	500.37	0.60	
Std 1000ppb Se	999.70	1000.00	999.70	1000.00	1	999.80	0.17	
Samples								
wash 2	0.25	0.23	0.21	0.21	1			
HPS wdh	7.36	5.77	5.73	5.72	(2)			
wash 3	0.14	0.10	0.12	0.11	1			
initsol_SeO4_Se5000	1127.0	1124.0	1118.0	1118.0	5	5615.0	22.91	
initsol_SeO4_Se3500	795.1	785.6	791.9	792.4	5	3954.3	24.17	
initsol_SeO4_Se2500	570.2	570.2	573.9	571.2	5	2857.2	10.68	
initsol_SeO4_Se2000	453.7	454.3	455.3	452.8	5	2272.2	4.04	
initsol_SeO4_Se1500	340.8	340.6	341.2	338.3	5	1704.3	1.53	
initsol_SeO4_Se1000	610.3	610.5	611.0	610.0	2	1221.2	0.72	
initsol_SeO4_Se0750	465.6	466.0	468.5	466.8	2	933.4	3.14	
initsol_SeO4_Se0500	310.2	308.4	307.9	305.1	2	617.7	2.42	
initsol_SeO4_Se0350	213.9	214.3	214.9	214.4	2	428.7	1.01	
wash 4	0.26	0.07	0.13	0.20	1			
test 25ppb	25.27	24.64	25.26	24.62	1			
wash 5	0.16	0.08	0.09	0.06	1			
initsol_SeO4_Se0250	152.5	153.9	153.7	154.6	2	306.7	1.51	
initsol_SeO4_Se0200	121.6	121.8	121.8	123.1	2	243.5	0.23	
initsol_SeO4_Se0150	90.9	91.3	91.1	91.6	2	182.2	0.35	
initsol_SeO4_Se0100	46.5	47.9	47.5	48.3	2	94.6	1.40	
initsol_SeO4_Se0075	45.1	45.4	45.8	46.0	2	90.9	0.68	
initsol_SeO4_Se0050	30.3	30.7	30.6	31.6	2	61.0	0.40	
initsol_SeO4_Se0025	16.2	16.4	16.0	17.6	2	32.4	0.48	
initsol_SeO4_Se0010	6.4	6.3	6.4	7.4	2	12.8	0.09	
initsol_SeO4_Se0000	0.30	0.30	0.28	0.37	1	0.29	0.01	
wash 6	0.09	0.05	0.08	0.16	1			
test 25ppb	25.14	24.59	24.44	24.46	1			
wash 7	0.09	0.06	0.08	0.06	1			
sorp-K_SeO4_Se5000	1667.0	1662.0	1655.0	1646.0	2	3322.7	12.06	
sorp-K_SeO4_Se3500	1049.0	1046.0	1047.0	1040.0	2	2094.7	3.06	
sorp-K_SeO4_Se2500	666.1	669.7	667.3	659.1	2	1335.4	3.67	
sorp-K_SeO4_Se2000	491.9	496.6	495.2	491.8	2	989.1	4.83	
sorp-K_SeO4_Se1500	357.6	359.8	359.7	359.9	2	718.1	2.48	
sorp-K_SeO4_Se1000	210.7	212.9	213.2	213.8	2	424.5	2.73	
sorp-K_SeO4_Se0750	157.2	157.3	156.6	155.7	2	314.1	0.76	
sorp-K_SeO4_Se0500	96.0	96.8	97.3	97.3	2	193.4	1.25	
sorp-K_SeO4_Se0350	66.3	64.7	65.5	66.9	2	131.1	1.64	
wash 7	0.08	0.08	0.11	0.18	1			
test 25ppb	24.88	24.91	25.49	25.19	1			
wash 8	0.15	0.06	0.08	0.07	1			
sorp-K_SeO4_Se0250	44.5	43.8	44.7	45.4	2	88.7	0.90	
sorp-K_SeO4_Se0200	35.7	35.5	35.4	36.4	2	71.0	0.29	
sorp-K_SeO4_Se0150	26.3	26.2	26.2	28.1	2	52.5	0.18	
sorp-K_SeO4_Se0100	16.0	15.6	15.9	17.6	2	31.7	0.36	
sorp-K_SeO4_Se0075	12.2	11.8	11.9	13.4	2	23.9	0.38	
sorp-K_SeO4_Se0050	9.0	8.2	8.2	9.8	2	16.9	0.88	
sorp-K_SeO4_Se0025	4.48	4.59	4.47	5.75	2	9.02	0.13	
sorp-K_SeO4_Se0010	1.82	1.66	1.66	3.25	2	3.32	0.18	
sorp-K_SeO4_Se0000	0.55	0.30	0.24	0.35	2	0.27	0.16	
wash 9	0.04	0.07	0.09	0.17	1			
test 25ppb	25.37	25.23	25.34	25.55	1			
wash 10	0.09	0.06	0.09	0.06	1			

Table B.15.: B1 analytical data - ICP-MS measurement sorption samples Na_2SeO_4 (continued from previous page)

Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean	SD
						$^{76}\text{Se}, ^{77}\text{Se}, ^{78}\text{Se}$	
sorp-G_SeO4_Se5000	1778.0	1782.0	1788.0	1766.0	2	3565.3	10.07
sorp-G_SeO4_Se3500	1250.0	1250.0	1251.0	1236.0	2	2500.7	1.15
sorp-G_SeO4_Se2500	885.0	882.1	882.4	880.9	2	1766.3	3.19
sorp-G_SeO4_Se2000	704.7	710.0	712.5	705.5	2	1418.1	7.97
sorp-G_SeO4_Se1500	513.0	514.0	512.0	511.6	2	1026.0	2.00
sorp-G_SeO4_Se1000	352.1	355.7	353.4	352.2	2	707.5	3.65
sorp-G_SeO4_Se0750	267.5	270.0	267.2	265.1	2	536.5	3.07
sorp-G_SeO4_Se0500	176.2	176.1	177.2	175.9	2	353.0	1.22
sorp-G_SeO4_Se0350	120.3	120.5	121.5	122.2	2	241.5	1.29
wash 11	0.15	0.11	0.13	0.11	1		
test 25ppb	24.93	24.73	24.69	24.67	1		
wash 12	0.21	0.20	0.20	0.17	1		
sorp-G_SeO4_Se0250	89.2	90.1	90.2	91.2	2	179.7	1.07
sorp-G_SeO4_Se0200	68.7	68.5	68.8	70.2	2	137.3	0.30
sorp-G_SeO4_Se0150	53.9	53.8	54.2	55.3	2	107.9	0.44
sorp-G_SeO4_Se0100	34.6	35.0	35.0	36.8	2	69.7	0.46
sorp-G_SeO4_Se0075	24.9	25.9	25.5	26.4	2	50.9	1.05
sorp-G_SeO4_Se0050	17.8	18.1	17.5	18.9	2	35.6	0.68
sorp-G_SeO4_Se0025	9.4	8.9	9.0	10.5	2	18.2	0.57
sorp-G_SeO4_Se0010	3.82	3.65	3.67	5.04	2	7.32	0.19
sorp-G_SeO4_Se0000	1.46	1.40	1.42	4.42	1	1.41	0.03
wash 13	0.11	0.05	0.07	0.10	1		
test 25ppb	24.52	24.71	24.48	24.01	1	24.57	0.12
HPS wdh	7.19	5.71	5.53	5.73	(2)		
wash 14	0.19	0.17	0.17	0.23	1		

B.5. B2 analytical data

Table B.16.: B2 analytical data - ICP-MS measurement desorption samples Na₂SeO₃

Technique	ICP-MS Quadrupole						
System	X-Series Thermo Fischer						
Date measured	06.11.2014						
Isotope	⁷⁶ Se [µg/L]	⁷⁷ Se [µg/L]	⁷⁸ Se [µg/L]	⁸² Se [µg/L]	dil. factor [-]	Se mean ⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se [µg/L]	SD [µg/L]
Analytical Quality							
wash-mean	0.46	0.13	0.25	1.907			
wash-SD	0.12	0.11	0.15	1.205			
LOD (= 3·wash)	0.35	0.33	0.45	3.614			
HighPurityStd ref. value	5.50	5.50	5.50	5.50		5.50	
Quality [%]	139.90	106.73	107.03	128.11			
Calibration							
Std 0ppb	0.15	0.03	0.09	2.373	1		0.06
Std 5ppb Se	4.96	4.72	4.99	5.874	1	4.89	0.15
Std 10ppb Se	9.95	10.04	9.82	11.76	1	9.94	0.11
Std 25ppb Se	25.18	24.95	24.78	25.52	1	24.97	0.20
Std 50ppb Se	49.84	50.71	50.10	49.56	1	50.22	0.45
Std 100ppb Se	100.10	97.95	99.64	98.77	1	99.23	1.13
Std 250ppb Se	249.70	253.10	251.30	248.8	1	251.37	1.70
Std 500ppb Se	500.10	498.90	498.40	498.6	1	499.13	0.87
Std 1000ppb Se	1000.00	1000.00	1001.00	1001	1	1000.33	0.58
Sample							
wash 3	1.44	1.25	1.22	1.921	1		
HPS	7.89	5.93	6.00	7.612	(2)		
wash 4	0.72	0.43	0.41	1.368	1		
desorp-K_Na2SeO3_5000ppb	128.80	130.10	130.20	127.3	10	1297.00	7.81
desorp-K_Na2SeO3_3500ppb	54.69	54.44	54.06	59.88	10	543.97	3.17
desorp-K_Na2SeO3_2500ppb	77.46	80.26	79.89	83.77	10	792.03	15.21
desorp-K_Na2SeO3_2000ppb	76.92	77.28	78.11	84.23	10	774.37	6.10
desorp-K_Na2SeO3_1500ppb	56.86	57.18	56.85	66.39	10	569.63	1.88
desorp-K_Na2SeO3_1000ppb	40.97	42.83	41.43	53.07	10	417.43	9.69
desorp-K_Na2SeO3_0750ppb	38.82	39.31	39.79	50.78	10	393.07	4.85
desorp-K_Na2SeO3_0500ppb	23.19	22.32	23.24	35.21	10	229.17	5.17
desorp-K_Na2SeO3_0350ppb	17.51	17.12	17.27	28.34	10	173.00	1.97
wash 4	0.40	0.10	0.20	1.404	1		
test 25ppb	25.72	25.18	25.30	26.13	1		
wash 5	0.52	0.18	0.20	1.813	1		
desorp-K_Na2SeO3_0250ppb	12.67	13.04	12.46	23.8	10	127.23	2.94
desorp-K_Na2SeO3_0200ppb	9.94	10.11	10.32	21.76	10	101.23	1.90
desorp-K_Na2SeO3_0150ppb	7.69	7.75	7.73	19.75	10	77.21	0.32
desorp-K_Na2SeO3_0100ppb	5.53	5.31	5.66	17.29	10	55.00	1.76
desorp-K_Na2SeO3_0075ppb	4.38	4.43	4.58	16.29	10	44.03	1.04
desorp-K_Na2SeO3_0050ppb	3.05	2.62	2.92	14.97	10	26.17	2.20
desorp-K_Na2SeO3_0025ppb	1.67	1.31	1.66	14.4	10	13.14	2.00
desorp-K_Na2SeO3_0010ppb	1.02	0.55	1.06	12.52	10	5.47	2.85
desorp-K_Na2SeO3_0000ppb	0.81	0.23	0.77	14.28	10	2.31	3.23
wash 6	0.39	0.05	0.25	3.213	1		
test 25ppb	25.48	25.23	25.70	26.67	1		
wash 7	0.50	0.18	0.39	2.844	1		
desorp-G_Na2SeO3_5000ppb	428.00	434.20	428.40	429.3	10	4302.00	34.70
desorp-G_Na2SeO3_3500ppb	126.80	129.50	126.00	133.6	10	1274.33	18.34
desorp-G_Na2SeO3_2500ppb	211.70	209.80	211.40	215.4	10	2109.67	10.21
desorp-G_Na2SeO3_2000ppb	216.80	218.40	216.60	222.3	10	2172.67	9.87
desorp-G_Na2SeO3_1500ppb	128.30	129.80	129.00	137.8	10	1290.33	7.51
desorp-G_Na2SeO3_1000ppb	88.47	87.56	88.23	96.15	10	880.87	4.72
desorp-G_Na2SeO3_0750ppb	83.12	82.51	81.39	90.04	10	823.40	8.77
desorp-G_Na2SeO3_0500ppb	43.44	43.61	43.63	53.29	10	435.60	1.04
desorp-G_Na2SeO3_0350ppb	31.33	30.39	30.98	41.42	10	309.00	4.75
wash 8	0.59	0.09	0.45	2.61	1		
test 25ppb	26.01	26.37	25.65	25.17	1		
wash 9	0.47	0.18	0.40	1.813	1		
desorp-G_Na2SeO3_0250ppb	22.69	22.72	22.19	31.72	10	225.33	2.98
desorp-G_Na2SeO3_0200ppb	17.66	17.56	18.01	27.28	10	177.43	2.36
desorp-G_Na2SeO3_0150ppb	13.14	12.73	13.51	24.25	10	131.27	3.90
desorp-G_Na2SeO3_0100ppb	8.95	8.98	9.34	19.64	10	89.63	2.17
desorp-G_Na2SeO3_0075ppb	6.70	6.56	6.95	17.42	10	66.31	1.94
desorp-G_Na2SeO3_0050ppb	5.06	4.14	4.87	15.51	10	41.37	4.85
desorp-G_Na2SeO3_0025ppb	2.84	2.37	2.90	12.86	10	23.72	2.88
desorp-G_Na2SeO3_0010ppb	1.53	0.93	1.62	13.23	10	9.26	3.78
desorp-G_Na2SeO3_0000ppb	0.89	0.29	1.00	10.65	10	2.91	3.82
wash 10	0.37	0.08	0.26	1.087	1		
test 25ppb	26.22	26.10	26.34	26.08	1		
HPS wdh	7.50	5.81	5.78	6.48	(2)		
wash 11	0.38	0.09	0.15	-0.868	1		

Table B.17.: B2 analytical data - ICP-MS measurement desorption samples Na_2SeO_4

Technique	ICP-MS Quadrupole							
System	X-Series Thermo Fischer							
Date measured	15.04.2014							
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean		
	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]		$^{76}\text{Se}, ^{77}\text{Se}, ^{78}\text{Se}$	SD	
					[-]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	
Analytical Quality								
wash-mean	0.15	0.06	0.10	0.15	1			
wash-SD	0.05	0.03	0.04	0.04	1			
LOD (= 3-wash)	0.15	0.08	0.12	0.12	1			
HighPurityStd ref. value	5.50	5.50	5.50	5.50		5.50		
Quality [%]	127.60	102.56	101.91	105.98				
Calibration								
Std 0ppb	0.07	0.06	0.07	0.16	1	0.07	0.01	
Std 2.5ppb Se	2.48	2.50	2.50	2.61	1	2.49	0.01	
Std 5ppb Se	4.96	5.01	4.98	5.27	1	4.98	0.02	
Std 10ppb Se	9.31	10.00	10.02	10.10	1	9.78	0.41	
Std 25ppb Se	24.50	24.21	25.11	25.12	1	24.61	0.46	
Std 50ppb Se	49.94	49.59	50.31	49.95	1	49.95	0.36	
Std 100ppb Se	100.10	99.29	100.30	99.46	1	99.90	0.53	
Std 250ppb Se	250.00	248.10	250.50	250.20	1	249.53	1.27	
Std 500ppb Se	503.30	501.20	499.70	502.20	1	501.40	1.81	
Sample								
wash 2	0.41	0.38	0.45	0.47	1			
HPS VF 2	8.05	6.02	6.10	6.07	2			
wash 3	0.22	0.12	0.19	0.24	1			
sorp-G_Na2SeO4_0000ppb	0.81	0.79	0.87	2.60	2	1.30	0.08	
initisol_Na2SeO4_0100ppb	51.60	51.41	51.17	53.58	2	102.8	0.43	
desorp-K_Na2SeO4_5000ppb	224.50	225.20	226.40	224.50	10	2253.7	9.61	
desorp-K_Na2SeO4_3500ppb	178.10	180.90	182.20	179.20	10	1804.0	20.95	
desorp-K_Na2SeO4_2500ppb	152.00	153.20	153.80	147.80	10	1530.0	9.17	
desorp-K_Na2SeO4_2000ppb	126.80	130.90	130.20	124.70	10	1293.0	21.93	
desorp-K_Na2SeO4_1500ppb	98.57	99.15	99.11	95.67	10	98.94	3.24	
desorp-K_Na2SeO4_1000ppb	69.86	70.77	70.42	68.02	10	703.5	4.59	
desorp-K_Na2SeO4_0750ppb	54.54	55.76	55.22	53.70	10	551.7	6.11	
desorp-K_Na2SeO4_0500ppb	38.22	38.26	38.12	37.38	10	382.0	0.72	
desorp-K_Na2SeO4_0350ppb	27.06	27.00	27.33	26.87	10	271.3	1.76	
wash 4	0.23	0.04	0.08	0.15	1			
test 25ppb	24.31	24.28	24.35	24.54	1			
wash 5	0.14	0.08	0.13	0.18	1			
desorp-K_Na2SeO4_0250ppb	20.23	19.51	20.25	20.01	10	200.0	4.22	
desorp-K_Na2SeO4_0200ppb	15.76	15.52	15.61	15.78	10	156.3	1.21	
desorp-K_Na2SeO4_0150ppb	11.64	11.60	12.04	11.82	10	117.6	2.43	
desorp-K_Na2SeO4_0100ppb	8.39	8.38	8.27	8.19	10	83.5	0.65	
desorp-K_Na2SeO4_0075ppb	6.39	6.23	6.21	5.96	10	62.8	1.01	
desorp-K_Na2SeO4_0050ppb	4.26	4.12	4.12	4.31	10	41.7	0.82	
desorp-K_Na2SeO4_0025ppb	2.26	2.36	2.21	2.37	10	22.8	0.78	
desorp-K_Na2SeO4_0010ppb	1.04	0.86	1.00	0.90	10	9.29	0.93	
desorp-K_Na2SeO4_0000ppb	0.27	0.15	0.16	0.29	10	1.56	0.64	
wash 6	0.16	0.04	0.08	0.12	1			
test 25ppb	24.43	24.48	24.72	24.19	1			
wash 7	0.10	0.06	0.11	0.13	1			
desorp-G_Na2SeO4_5000ppb	187.10	189.40	188.80	184.60	10	1884.3	11.93	
desorp-G_Na2SeO4_3500ppb	136.00	138.70	138.00	136.60	10	1375.7	14.01	
desorp-G_Na2SeO4_2500ppb	97.23	98.68	97.76	94.72	10	978.9	7.34	
desorp-G_Na2SeO4_2000ppb	80.16	81.08	80.14	78.05	10	804.6	5.37	
desorp-G_Na2SeO4_1500ppb	60.74	61.89	61.66	60.68	10	614.3	6.09	
desorp-G_Na2SeO4_1000ppb	38.94	39.30	39.07	38.39	10	391.0	1.82	
desorp-G_Na2SeO4_0750ppb	31.14	31.08	31.07	30.36	10	311.0	0.38	
desorp-G_Na2SeO4_0500ppb	19.77	19.49	20.11	19.57	10	197.9	3.10	
desorp-G_Na2SeO4_0350ppb	14.80	14.72	14.65	14.53	10	147.2	0.75	
wash 8	0.16	0.05	0.06	0.13	1			
test 25ppb	24.50	24.85	24.62	24.88	1			
wash 9	0.17	0.06	0.10	0.14	1			
desorp-G_Na2SeO4_0250ppb	10.35	10.13	10.14	9.93	10	102.1	1.24	
desorp-G_Na2SeO4_0200ppb	8.49	8.35	8.31	8.08	10	83.8	0.92	
desorp-G_Na2SeO4_0150ppb	6.56	6.05	6.24	6.04	10	61.5	2.56	
desorp-G_Na2SeO4_0100ppb	4.36	3.92	3.96	4.04	10	39.4	2.40	
desorp-G_Na2SeO4_0075ppb	3.59	3.24	3.18	3.31	10	32.1	2.23	
desorp-G_Na2SeO4_0050ppb	2.54	2.02	2.13	2.10	10	20.8	2.74	
desorp-G_Na2SeO4_0025ppb	1.42	1.02	1.12	1.07	10	10.7	2.09	
desorp-G_Na2SeO4_0010ppb	0.73	0.50	0.53	0.65	10	5.11	1.28	
desorp-G_Na2SeO4_0000ppb	0.35	0.16	0.23	0.38	10	1.97	0.96	
wash 10	0.15	0.03	0.06	0.12	1			
test 25ppb	24.69	25.00	24.75	24.91	1			
HPS VF 2 wdh	7.02	5.64	5.61	5.83	2			
wash 11	0.15	0.04	0.09	0.15	1			

B.6. B3 analytical data

Table B.18.: *B3 analytical data - IC measurement I (note: these solutions contained no sulphate, the peaks identified as sulphate are selenate from added selenite and were used to correct sulphate measurements in the presence of selenite)*

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	01.10.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.21	Cl ⁻	XQOff	5	-0.008	0.146	0.001	99.9985	
Calib_2	7.20	NO ₃ ⁻	XQOff	5	-0.021	0.077	0.000	99.9984	
Calib_3	10.33	PO ₄ ³⁻	XQOff	5	0.003	0.041	0.000	99.9997	
Calib_4	12.80	SO ₄ ²⁻	XQOff	5	0.011	0.103	0.000	99.9998	
mean:					-0.0069	0.1086	0.0006	99.9987	
standard repetition mean [mg/L]		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
		10.21	20.59	30.64	19.81				
standard repetition SD [mg/L]		0.19	0.48	0.46	0.52				
standard repetition RSD [%]		1.84	2.32	1.49	2.61				
analytical quality [%]		104.91							
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.19	7.28	10.22	12.52	2.01	4.02	6.01	4.00
2	Standard_2	4.20	7.24	10.21	12.51	5.00	9.97	14.99	10.00
3	Standard_3	4.20	7.20	10.20	12.51	9.93	19.88	29.96	19.95
4	Standard_4	4.21	7.15	10.17	12.49	20.09	40.18	60.06	40.06
5	Standard_5	4.24	7.10	10.13	12.46	39.98	79.95	119.98	79.98
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.19	7.16	10.17	12.57	10.22	20.81	30.59	20.53
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	sorp_NO3_initsol_SO3_0010ppb	4.31	7.23	n.a.	n.a.	98.33	47.32	n.a.	n.a.
10	sorp_NO3_initsol_SO3_0025ppb	4.27	7.23	n.a.	n.a.	66.74	46.47	n.a.	n.a.
11	sorp_NO3_initsol_SO3_0050ppb	4.27	7.23	n.a.	n.a.	65.95	46.87	n.a.	n.a.
12	sorp_NO3_initsol_SO3_0100ppb	4.27	7.23	n.a.	n.a.	65.54	47.36	n.a.	n.a.
13	sorp_NO3_initsol_SO3_0250ppb	4.27	7.22	n.a.	n.a.	64.83	47.05	n.a.	n.a.
14	sorp_NO3_initsol_SO3_0500ppb	4.26	7.21	n.a.	n.a.	65.56	46.82	n.a.	n.a.
15	sorp_NO3_initsol_SO3_1000ppb	4.26	7.21	n.a.	n.a.	65.26	46.90	n.a.	n.a.
16	sorp_NO3_initsol_SO3_2500ppb	4.26	7.21	n.a.	n.a.	64.90	46.47	n.a.	n.a.
17	sorp_NO3_initsol_SO3_5000ppb	4.26	7.21	n.a.	n.a.	64.19	45.93	n.a.	n.a.
18	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
19	Standard_3-2	4.20	7.17	10.16	12.54	10.26	20.80	30.87	81.87
20	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Test-Riverwater	4.24	7.30	n.a.	12.49	45.15	2.01	n.a.	153.94
22	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	sorp_NO3_Ksorp_SO3_0010ppb	4.30	7.21	n.a.	n.a.	97.00	46.05	n.a.	n.a.
24	sorp_NO3_Ksorp_SO3_0025ppb	4.26	7.21	n.a.	n.a.	66.14	46.91	n.a.	n.a.
25	sorp_NO3_Ksorp_SO3_0050ppb	4.26	7.21	n.a.	n.a.	65.28	46.63	n.a.	n.a.
26	sorp_NO3_Ksorp_SO3_0100ppb	4.26	7.21	n.a.	n.a.	64.57	46.55	n.a.	n.a.
27	sorp_NO3_Ksorp_SO3_0250ppb	4.26	7.21	n.a.	n.a.	63.92	46.04	n.a.	n.a.
28	sorp_NO3_Ksorp_SO3_0500ppb	4.26	7.21	n.a.	n.a.	64.25	46.50	n.a.	n.a.
29	sorp_NO3_Ksorp_SO3_1000ppb	4.26	7.21	n.a.	n.a.	64.47	46.23	n.a.	n.a.
30	sorp_NO3_Ksorp_SO3_2500ppb	4.26	7.21	n.a.	n.a.	65.22	46.96	n.a.	n.a.
31	sorp_NO3_Ksorp_SO3_5000ppb	4.26	7.21	9.70	12.57	64.63	46.25	0.92	2.67
32	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
33	Standard_3-3	4.20	7.19	10.16	12.54	10.29	20.86	30.77	19.51
34	wash-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
35	sorp_NO3_Gsorp_SO3_0010ppb	4.30	7.22	n.a.	12.55	97.21	47.60	n.a.	52.44
36	sorp_NO3_Gsorp_SO3_0025ppb	4.27	7.22	n.a.	12.55	65.89	47.04	n.a.	50.58
37	sorp_NO3_Gsorp_SO3_0050ppb	4.26	7.22	n.a.	12.55	64.02	46.46	n.a.	49.21
38	sorp_NO3_Gsorp_SO3_0100ppb	4.27	7.22	n.a.	12.55	64.58	47.03	n.a.	50.07
39	sorp_NO3_Gsorp_SO3_0250ppb	4.26	7.22	n.a.	12.56	63.19	47.14	n.a.	52.10
40	sorp_NO3_Gsorp_SO3_0500ppb	4.26	7.22	n.a.	12.55	64.15	47.36	n.a.	49.97
41	sorp_NO3_Gsorp_SO3_1000ppb	4.27	7.22	n.a.	12.55	64.46	47.69	n.a.	50.79
42	sorp_NO3_Gsorp_SO3_2500ppb	4.27	7.22	n.a.	12.56	64.54	47.17	n.a.	53.52
43	sorp_NO3_Gsorp_SO3_5000ppb	4.27	7.22	n.a.	12.55	64.30	47.45	n.a.	53.87
44	wash-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
45	Standard_3-4	4.2	7.19	10.15	12.55	10.34	20.84	30.94	19.31
46	wash-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
47	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table B.19.: *B3 analytical data - IC measurement II (note: these solutions contained no sulphate, the peaks identified as sulphate are selenate and were used to correct sulphate measurements in the presence of selenate)*

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	30.09.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.21	Cl ⁻	XQOff	5	-0.008	0.146	0.001	99.9985	
Calib_2	7.20	NO ₃ ⁻	XQOff	5	-0.021	0.077	0.000	99.9984	
Calib_3	10.33	PO ₄ ³⁻	XQOff	5	0.003	0.041	0.000	99.9997	
Calib_4	12.80	SO ₄ ²⁻	XQOff	5	0.011	0.103	0.000	99.9998	
mean:					-0.0069	0.1086	0.0006	99.9987	
standard repetition mean [mg/L]		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
standard repetition SD [mg/L]		10.05	20.22	30.30	20.20				
standard repetition RSD [%]		0.15	0.74	0.35	0.24				
		1.54	3.64	1.14	1.21				
analytical quality [%]		103.49							
Seq. No.	Sample ID	Cl ⁻ [min]	NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.19	7.28	10.22	12.52	2.01	4.02	6.01	4.01
2	Standard_2	4.20	7.24	10.21	12.51	4.99	9.97	14.99	10.00
3	Standard_3	4.20	7.20	10.20	12.51	9.93	19.87	29.96	19.95
4	Standard_4	4.21	7.15	10.17	12.49	20.10	40.18	60.06	40.06
5	Standard_5	4.24	7.10	10.13	12.46	39.97	79.95	119.98	79.98
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.19	7.15	10.13	12.43	9.89	19.09	29.89	19.97
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	sorp_NO3_initsol_SO4_0000ppb	4.25	7.19	n.a.	n.a.	68.02	45.42	n.a.	n.a.
10	sorp_NO3_initsol_SO4_0010ppb	4.25	7.19	n.a.	n.a.	65.98	44.88	n.a.	n.a.
11	sorp_NO3_initsol_SO4_0025ppb	4.25	7.20	n.a.	n.a.	65.52	45.92	n.a.	n.a.
12	sorp_NO3_initsol_SO4_0050ppb	4.25	7.20	n.a.	n.a.	65.77	44.75	n.a.	n.a.
13	sorp_NO3_initsol_SO4_0100ppb	4.25	7.20	n.a.	n.a.	69.99	45.97	n.a.	n.a.
14	sorp_NO3_initsol_SO4_0250ppb	4.25	7.19	n.a.	n.a.	65.48	45.07	n.a.	n.a.
15	sorp_NO3_initsol_SO4_0500ppb	4.25	7.19	n.a.	n.a.	66.44	45.46	n.a.	n.a.
16	sorp_NO3_initsol_SO4_1000ppb	4.25	7.19	n.a.	n.a.	67.61	45.75	n.a.	n.a.
17	sorp_NO3_initsol_SO4_2500ppb	4.25	7.19	n.a.	n.a.	66.70	45.09	n.a.	n.a.
18	sorp_NO3_initsol_SO4_5000ppb	4.25	7.19	n.a.	n.a.	66.01	44.41	n.a.	n.a.
19	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
20	Standard_3-2	4.19	7.16	10.13	12.43	10.02	20.52	30.46	20.17
21	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
22	Test-Riverwater	4.23	7.28	n.a.	12.38	44.58	1.48	n.a.	151.72
23	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
24	sorp_NO3_Ksorp_SO4_0000ppb	4.25	7.19	n.a.	12.48	69.63	45.92	n.a.	2.24
25	sorp_NO3_Ksorp_SO4_0010ppb	4.25	7.19	n.a.	12.46	66.48	45.89	n.a.	2.20
26	sorp_NO3_Ksorp_SO4_0025ppb	4.25	7.19	n.a.	12.48	66.29	47.07	n.a.	2.07
27	sorp_NO3_Ksorp_SO4_0050ppb	4.25	7.19	n.a.	12.38	66.98	45.79	n.a.	2.14
28	sorp_NO3_Ksorp_SO4_0100ppb	4.25	7.19	n.a.	12.46	71.00	46.42	n.a.	2.07
29	sorp_NO3_Ksorp_SO4_0250ppb	4.25	7.19	n.a.	12.44	66.78	46.46	n.a.	1.76
30	sorp_NO3_Ksorp_SO4_0500ppb	4.25	7.19	n.a.	12.48	68.05	46.11	n.a.	2.01
31	sorp_NO3_Ksorp_SO4_1000ppb	4.25	7.19	n.a.	12.48	67.79	45.95	n.a.	2.08
32	sorp_NO3_Ksorp_SO4_2500ppb	4.25	7.20	n.a.	12.43	66.95	45.44	n.a.	2.56
33	sorp_NO3_Ksorp_SO4_5000ppb	4.25	7.20	n.a.	12.44	67.41	45.89	n.a.	2.44
34	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
35	Standard_3-3	4.19	7.17	10.13	12.43	10.22	20.81	30.63	20.38
36	wash-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
37	sorp_NO3_Gsorp_SO4_0000ppb	4.31	7.20	n.a.	12.43	119.96	46.51	n.a.	57.38
38	sorp_NO3_Gsorp_SO4_0010ppb	4.25	7.20	n.a.	12.43	67.402	45.45	n.a.	56.44
39	sorp_NO3_Gsorp_SO4_0025ppb	4.25	7.20	n.a.	12.43	66.84	46.80	n.a.	57.11
40	sorp_NO3_Gsorp_SO4_0050ppb	4.25	7.20	n.a.	12.43	67.645	46.98	n.a.	57.039
41	sorp_NO3_Gsorp_SO4_0100ppb	4.26	7.20	n.a.	12.44	70.603	46.70	n.a.	56.41
42	sorp_NO3_Gsorp_SO4_0250ppb	4.25	7.20	n.a.	12.44	66.984	47.22	n.a.	57.56
43	sorp_NO3_Gsorp_SO4_0500ppb	4.25	7.20	n.a.	12.43	68.365	46.97	n.a.	57.12
44	sorp_NO3_Gsorp_SO4_1000ppb	4.25	7.20	n.a.	12.44	68.453	47.10	n.a.	56.16
45	sorp_NO3_Gsorp_SO4_2500ppb	4.25	7.20	n.a.	12.44	67.413	46.55	n.a.	56.84
46	sorp_NO3_Gsorp_SO4_5000ppb	4.25	7.20	n.a.	12.44	67.735	46.92	n.a.	56.76
47	wash-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
48	Standard_3-4	4.19	7.17	10.13	12.43	10.21	20.79	30.55	20.51
49	wash-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
50	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table B.20.: B3 analytical data - IC measurement III (note: these solutions contained no sulphate, the peaks identified as sulphate are selenate and were used to correct sulphate measurements in the presence of selenate)

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	30.09.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.21	Cl ⁻	XQOff	5	-0.008	0.146	0.001	99.9985	
Calib_2	7.20	NO ₃ ⁻	XQOff	5	-0.021	0.077	0.000	99.9984	
Calib_3	10.33	PO ₄ ³⁻	XQOff	5	0.003	0.041	0.000	99.9997	
Calib_4	12.80	SO ₄ ²⁻	XQOff	5	0.011	0.103	0.000	99.9998	
mean:					-0.0069	0.1086	0.0006	99.9987	
standard repetition mean [mg/L]	Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻	10.20	20.79	23.36	27.96	
standard repetition SD [mg/L]	0.10	0.11	5.04	5.31					
standard repetition RSD [%]	1.03	0.51	21.56	18.99					
analytical quality [%]		105.50							
Seq. No.	Sample ID	Cl ⁻ [min]	NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.19	7.28	10.22	12.52	2.01	4.02	6.01	4.01
2	Standard_2	4.20	7.24	10.21	12.51	5.00	9.97	15.00	10.00
3	Standard_3	4.20	7.20	10.20	12.51	9.93	19.89	29.95	19.95
4	Standard_4	4.21	7.15	10.17	12.49	20.09	40.17	60.06	40.06
5	Standard_5	4.24	7.10	10.13	12.46	39.98	79.95	119.98	79.98
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.21	7.21	10.29	12.78	10.18	20.66	30.91	19.99
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	sorp_PO4_initsol_SeO3_0010ppb	4.28	n.a.	10.29	n.a.	269.84	n.a.	73.00	n.a.
10	sorp_PO4_initsol_SeO3_0025ppb	4.28	n.a.	10.29	n.a.	265.37	n.a.	72.60	n.a.
11	sorp_PO4_initsol_SeO3_0050ppb	4.28	n.a.	10.29	n.a.	262.88	n.a.	71.47	n.a.
12	sorp_PO4_initsol_SeO3_0100ppb	4.28	n.a.	10.29	n.a.	263.12	n.a.	71.59	n.a.
13	sorp_PO4_initsol_SeO3_0250ppb	4.27	n.a.	10.29	n.a.	259.99	n.a.	72.99	n.a.
14	sorp_PO4_initsol_SeO3_0500ppb	4.28	n.a.	10.29	n.a.	267.46	n.a.	73.75	n.a.
15	sorp_PO4_initsol_SeO3_1000ppb	4.28	n.a.	10.29	n.a.	267.15	n.a.	73.55	n.a.
16	sorp_PO4_initsol_SeO3_2500ppb	4.28	n.a.	10.29	n.a.	260.63	n.a.	73.84	n.a.
17	sorp_PO4_initsol_SeO3_5000ppb	4.28	n.a.	10.29	n.a.	267.73	n.a.	79.47	n.a.
18	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
19	Standard_3-2	4.21	7.21	10.28	12.74	10.06	20.76	20.76	30.77
20	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Test-Riverwater	4.25	7.32	n.a.	12.69	44.73	n.a.	1.51	n.a.
22	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	sorp_PO4_Ksorp_SeO3_0010ppb	4.28	n.a.	10.30	12.72	278.50	n.a.	52.78	3.08
24	sorp_PO4_Ksorp_SeO3_0025ppb	4.28	n.a.	10.29	12.74	262.38	n.a.	53.22	3.84
25	sorp_PO4_Ksorp_SeO3_0050ppb	4.28	n.a.	10.30	12.76	267.19	n.a.	53.70	3.97
26	sorp_PO4_Ksorp_SeO3_0100ppb	4.28	n.a.	10.31	12.80	268.96	n.a.	53.54	3.06
27	sorp_PO4_Ksorp_SeO3_0250ppb	4.29	n.a.	10.31	12.78	261.73	n.a.	54.15	3.73
28	sorp_PO4_Ksorp_SeO3_0500ppb	4.28	n.a.	10.29	12.77	268.55	n.a.	56.35	4.00
29	sorp_PO4_Ksorp_SeO3_1000ppb	4.28	n.a.	10.30	12.77	265.65	n.a.	56.78	3.70
30	sorp_PO4_Ksorp_SeO3_2500ppb	4.28	n.a.	10.29	12.76	267.94	n.a.	58.59	3.18
31	sorp_PO4_Ksorp_SeO3_5000ppb	4.29	n.a.	10.31	12.75	266.51	n.a.	60.86	3.59
32	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
33	Standard_3-3	4.21	7.21	10.28	12.74	10.26	20.86	20.86	30.57
34	wash-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
35	sorp_PO4_Gsorp_SeO3_0010ppb	4.28	n.a.	n.a.	12.75	267.84	n.a.	n.a.	75.54
36	sorp_PO4_Gsorp_SeO3_0025ppb	4.28	n.a.	n.a.	12.74	266.71	n.a.	n.a.	75.86
37	sorp_PO4_Gsorp_SeO3_0050ppb	4.28	n.a.	n.a.	12.74	269.98	n.a.	n.a.	77.15
38	sorp_PO4_Gsorp_SeO3_0100ppb	4.28	n.a.	n.a.	12.74	264.97	n.a.	n.a.	75.79
39	sorp_PO4_Gsorp_SeO3_0250ppb	4.28	n.a.	n.a.	12.74	263.69	n.a.	n.a.	76.31
40	sorp_PO4_Gsorp_SeO3_0500ppb	4.28	n.a.	n.a.	12.75	270.15	n.a.	n.a.	76.53
41	sorp_PO4_Gsorp_SeO3_1000ppb	4.29	n.a.	n.a.	12.76	269.38	n.a.	n.a.	75.47
42	sorp_PO4_Gsorp_SeO3_2500ppb	4.29	7.40	n.a.	12.76	270.46	n.a.	n.a.	77.53
43	sorp_PO4_Gsorp_SeO3_5000ppb	4.28	n.a.	n.a.	12.75	266.49	n.a.	n.a.	77.24
44	wash-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
45	Standard_3-4	4.22	7.22	10.28	12.76	10.29	20.89	20.89	30.49
46	wash-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
47	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
48	Standard_3-4	4.19	7.17	10.13	12.43	10.2144	20.79	30.55	20.51
49	wash-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
50	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table B.21.: *B3 analytical data - IC measurement IV (note: these solutions contained no sulphate, the peaks identified as sulphate are selenate and were used to correct sulphate measurements in the presence of selenate)*

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	30.09.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.21	Cl ⁻	XQOff	5	-0.008	0.146	0.001	99.9985	
Calib_2	7.20	NO ₃ ⁻	XQOff	5	-0.021	0.077	0.000	99.9984	
Calib_3	10.33	PO ₄ ³⁻	XQOff	5	0.003	0.041	0.000	99.9997	
Calib_4	12.80	SO ₄ ²⁻	XQOff	5	0.011	0.103	0.000	99.9998	
mean:					-0.0069	0.1086	0.0006	99.9987	
standard repetition mean [mg/L]	10.45	Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻	19.88			
standard repetition SD [mg/L]	0.10	0.08	0.24	1.22					
standard repetition RSD [%]	0.99	0.36	0.78	6.12					
analytical quality [%]		105.80							
Seq. No.	Sample ID	Cl ⁻ [min]	NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.19	7.28	10.22	12.52	2.01	4.02	6.01	4.01
2	Standard_2	4.20	7.24	10.21	12.51	4.98	9.97	15.00	10.00
3	Standard_3	4.20	7.20	10.20	12.51	9.92	19.89	29.95	19.95
4	Standard_4	4.21	7.15	10.17	12.49	20.12	40.17	60.06	40.06
5	Standard_5	4.24	7.10	10.13	12.46	39.97	79.95	119.98	79.98
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.38	7.48	10.65	13.19	10.56	20.76	30.80	18.06
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	sorp_PO4_initsol_SeO4_0000ppb	4.39	n.a.	10.52	n.a.	269.08	n.a.	73.73	n.a.
10	sorp_PO4_initsol_SeO4_0010ppb	4.39	n.a.	10.53	n.a.	269.77	n.a.	73.27	n.a.
11	sorp_PO4_initsol_SeO4_0025ppb	4.36	n.a.	10.46	n.a.	269.17	n.a.	73.73	n.a.
12	sorp_PO4_initsol_SeO4_0050ppb	4.35	n.a.	10.46	n.a.	266.73	n.a.	73.66	n.a.
13	sorp_PO4_initsol_SeO4_0100ppb	4.34	n.a.	10.43	n.a.	264.75	n.a.	73.64	n.a.
14	sorp_PO4_initsol_SeO4_0250ppb	4.37	n.a.	10.39	n.a.	258.48	n.a.	72.02	n.a.
15	sorp_PO4_initsol_SeO4_0500ppb	4.28	n.a.	10.29	n.a.	265.45	n.a.	73.38	n.a.
16	sorp_PO4_initsol_SeO4_1000ppb	4.29	n.a.	10.31	n.a.	267.73	n.a.	71.95	n.a.
17	sorp_PO4_initsol_SeO4_2500ppb	4.28	n.a.	10.30	n.a.	264.20	n.a.	72.11	n.a.
18	sorp_PO4_initsol_SeO4_5000ppb	4.28	n.a.	10.30	n.a.	266.48	n.a.	72.72	n.a.
19	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
20	Standard_3-2	4.22	7.21	10.29	12.74	10.31	20.88	31.29	20.38
21	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
22	Test-Riverwater	4.26	7.36	n.a.	12.69	46.20	1.92	n.a.	152.92
23	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
24	sorp_PO4_Ksorp_SeO4_0000ppb	4.29	n.a.	10.29	12.74	271.60	n.a.	54.45	3.91
25	sorp_PO4_Ksorp_SeO4_0010ppb	4.29	n.a.	10.29	12.72	268.38	n.a.	55.16	3.66
26	sorp_PO4_Ksorp_SeO4_0025ppb	4.29	n.a.	10.30	12.72	272.30	n.a.	55.97	3.61
27	sorp_PO4_Ksorp_SeO4_0050ppb	4.29	n.a.	10.28	12.75	270.81	n.a.	56.15	3.72
28	sorp_PO4_Ksorp_SeO4_0100ppb	4.29	n.a.	10.29	12.74	270.14	n.a.	55.10	4.00
29	sorp_PO4_Ksorp_SeO4_0250ppb	4.29	n.a.	10.29	12.75	263.29	n.a.	54.66	4.14
30	sorp_PO4_Ksorp_SeO4_0500ppb	4.29	n.a.	10.29	12.78	272.35	n.a.	56.35	4.07
31	sorp_PO4_Ksorp_SeO4_1000ppb	4.29	n.a.	10.29	12.76	273.57	n.a.	55.84	3.84
32	sorp_PO4_Ksorp_SeO4_2500ppb	4.29	n.a.	10.29	12.75	268.62	n.a.	53.67	3.83
33	sorp_PO4_Ksorp_SeO4_5000ppb	4.29	n.a.	10.29	12.76	269.74	n.a.	56.54	3.38
34	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
35	Standard_3-3	4.22	7.23	10.28	12.73	10.48	20.87	30.85	20.49
36	wash-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
37	sorp_PO4_Gsorp_SeO4_0000ppb	4.29	7.37	n.a.	12.74	271.04	1.86	n.a.	79.13
38	sorp_PO4_Gsorp_SeO4_0010ppb	4.29	7.37	n.a.	12.74	270.19	1.53	n.a.	78.61
39	sorp_PO4_Gsorp_SeO4_0025ppb	4.29	7.37	n.a.	12.74	270.76	1.78	n.a.	80.17
40	sorp_PO4_Gsorp_SeO4_0050ppb	4.29	7.39	n.a.	12.74	268.71	1.78	n.a.	79.76
41	sorp_PO4_Gsorp_SeO4_0100ppb	4.29	7.38	n.a.	12.74	266.19	2.05	n.a.	78.80
42	sorp_PO4_Gsorp_SeO4_0250ppb	4.29	7.36	n.a.	12.74	260.97	1.76	n.a.	78.83
43	sorp_PO4_Gsorp_SeO4_0500ppb	4.29	7.38	n.a.	12.74	268.77	1.63	n.a.	78.93
44	sorp_PO4_Gsorp_SeO4_1000ppb	4.29	7.40	n.a.	12.74	271.89	1.4	n.a.	79.55
45	sorp_PO4_Gsorp_SeO4_2500ppb	4.29	7.41	n.a.	12.74	268.49	1.75	n.a.	79.31
46	sorp_PO4_Gsorp_SeO4_5000ppb	4.29	7.36	n.a.	12.75	265.50	2.00	n.a.	77.06
47	wash-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
48	Standard_3-4	4.22	7.24	10.28	12.75	10.45	20.94	30.77	20.59
49	wash-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
50	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table B.22.: B3 analytical data - IC measurement V

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	30.09.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.21	Cl ⁻	XQOff	5	-0.008	0.146	0.001	99.9985	
Calib_2	7.20	NO ₃ ⁻	XQOff	5	-0.021	0.077	0.000	99.9984	
Calib_3	10.33	PO ₄ ³⁻	XQOff	5	0.003	0.041	0.000	99:9997	
Calib_4	12.80	SO ₄ ²⁻	XQOff	5	0.011	0.103	0.000	99.9998	
mean:					-0.0069	0.1086	0.0006	99.9987	
		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
standard repetition mean [mg/L]		10.37	21.17	23.48	28.35				
standard repetition SD [mg/L]		0.04	0.19	4.50	5.47				
standard repetition RSD [%]		0.41	0.91	19.17	19.29				
analytical quality [%]		105.85							
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.19	7.28	10.22	12.52	2.00	4.04	6.01	4.02
2	Standard_2	4.20	7.24	10.21	12.51	5.00	9.93	15.00	9.96
3	Standard_3	4.20	7.20	10.20	12.51	9.94	19.77	29.95	19.95
4	Standard_4	4.21	7.15	10.17	12.49	20.06	40.35	60.06	40.11
5	Standard_5	4.24	7.10	10.13	12.46	39.98	79.90	119.98	79.97
6	Dest.Wasser-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.20	7.18	10.23	12.67	10.33	20.99	30.23	20.15
8	Dest.Wasser-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	sorp_SO4_initsol_SeO3_0010ppb	4.27	n.a.	n.a.	12.67	263.06	n.a.	n.a.	76.55
10	sorp_SO4_initsol_SeO3_0025ppb	4.27	n.a.	n.a.	12.67	263.10	n.a.	n.a.	76.33
11	sorp_SO4_initsol_SeO3_0050ppb	4.27	n.a.	n.a.	12.66	263.55	n.a.	n.a.	76.56
12	sorp_SO4_initsol_SeO3_0100ppb	4.27	n.a.	n.a.	12.67	260.25	n.a.	n.a.	76.71
13	sorp_SO4_initsol_SeO3_0250ppb	4.27	n.a.	n.a.	12.67	256.10	n.a.	n.a.	76.61
14	sorp_SO4_initsol_SeO3_0500ppb	4.27	n.a.	n.a.	12.67	262.62	n.a.	n.a.	76.54
15	sorp_SO4_initsol_SeO3_1000ppb	4.27	n.a.	9.78	12.67	264.45	n.a.	1.45	51.46
16	sorp_SO4_initsol_SeO3_2500ppb	4.27	n.a.	9.76	12.67	263.31	n.a.	2.95	76.19
17	sorp_SO4_initsol_SeO3_5000ppb	4.27	n.a.	9.78	12.68	262.51	n.a.	6.28	76.23
18	Dest.Wasser-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
19	Standard_3-2	4.21	7.19	10.23	12.67	10.39	21.20	21.20	30.86
20	Dest.Wasser-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Test-Riverwater	4.25	n.a.	n.a.	12.63	44.88	n.a.	n.a.	n.a.
22	Dest.Wasser-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	sorp_SO4_Ksorp_SeO3_0010ppb	4.27	n.a.	n.a.	12.67	264.20	n.a.	n.a.	74.92
24	sorp_SO4_Ksorp_SeO3_0025ppb	4.27	n.a.	n.a.	12.67	260.60	n.a.	n.a.	73.60
25	sorp_SO4_Ksorp_SeO3_0050ppb	4.27	n.a.	n.a.	12.68	264.96	n.a.	n.a.	74.18
26	sorp_SO4_Ksorp_SeO3_0100ppb	4.27	n.a.	n.a.	12.68	261.01	n.a.	n.a.	74.25
27	sorp_SO4_Ksorp_SeO3_0250ppb	4.27	n.a.	n.a.	12.68	254.00	n.a.	n.a.	73.98
28	sorp_SO4_Ksorp_SeO3_0500ppb	4.27	n.a.	n.a.	12.68	264.29	n.a.	n.a.	74.88
29	sorp_SO4_Ksorp_SeO3_1000ppb	4.27	n.a.	n.a.	12.68	260.79	n.a.	n.a.	49.77
30	sorp_SO4_Ksorp_SeO3_2500ppb	4.28	n.a.	9.78	12.69	263.82	n.a.	1.92	75.00
31	sorp_SO4_Ksorp_SeO3_5000ppb	4.27	n.a.	9.77	12.68	263.19	n.a.	5.05	74.85
32	Dest.Wasser-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
33	Standard_3-3	4.21	7.19	10.23	12.68	10.35	21.06	21.06	31.23
34	Dest.Wasser-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
35	sorp_SO4_Gsorp_SeO3_0010ppb	4.27	7.30	n.a.	12.67	256.74	2.25	n.a.	117.60
36	sorp_SO4_Gsorp_SeO3_0025ppb	4.27	7.34	n.a.	12.66	254.17	n.a.	n.a.	115.87
37	sorp_SO4_Gsorp_SeO3_0050ppb	4.27	7.35	n.a.	12.67	257.24	n.a.	n.a.	117.49
38	sorp_SO4_Gsorp_SeO3_0100ppb	4.27	7.32	n.a.	12.66	255.28	n.a.	n.a.	117.57
39	sorp_SO4_Gsorp_SeO3_0250ppb	4.27	7.36	n.a.	12.67	254.02	n.a.	n.a.	118.75
40	sorp_SO4_Gsorp_SeO3_0500ppb	4.27	7.35	n.a.	12.66	261.04	n.a.	n.a.	119.87
41	sorp_SO4_Gsorp_SeO3_1000ppb	4.27	7.37	n.a.	12.67	254.49	n.a.	n.a.	96.02
42	sorp_SO4_Gsorp_SeO3_2500ppb	4.27	7.32	n.a.	12.66	259.93	n.a.	n.a.	120.06
43	sorp_SO4_Gsorp_SeO3_5000ppb	4.27	7.31	n.a.	12.67	259.33	n.a.	n.a.	121.00
44	Dest.Wasser-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
45	Standard_3-4	4.21	7.20	10.21	12.67	10.42	21.43	21.43	31.17
46	Dest.Wasser-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
47	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table B.23.: B3 analytical data - IC measurement VI

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	30.09.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.21	Cl ⁻	XQOff	5	-0.008	0.146	0.001	99.9985	
Calib_2	7.20	NO ₃ ⁻	XQOff	5	-0.021	0.077	0.000	99.9984	
Calib_3	10.33	PO ₄ ³⁻	XQOff	5	0.003	0.041	0.000	99.9997	
Calib_4	12.80	SO ₄ ²⁻	XQOff	5	0.011	0.103	0.000	99.9998	
mean:					-0.0069	0.1086	0.0006	99.9987	
		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
standard repetition mean [mg/L]		10.28	20.88	30.47	19.49				
standard repetition SD [mg/L]		0.07	0.32	0.29	0.05				
standard repetition RSD [%]		0.64	1.52	0.96	0.24				
analytical quality [%]		101.45							
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.19	7.28	10.22	12.52	2.01	4.02	6.01	4.01
2	Standard_2	4.20	7.24	10.21	12.51	5.00	9.97	14.93	10.00
3	Standard_3	4.20	7.20	10.20	12.51	9.93	19.89	30.08	19.95
4	Standard_4	4.21	7.15	10.17	12.49	20.08	40.17	59.97	40.06
5	Standard_5	4.24	7.10	10.13	12.46	39.98	79.95	120.00	79.98
6	Dest.Wasser-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.21	7.20	10.33	12.80	10.19	20.50	30.28	19.42
8	Dest.Wasser-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	sorp_SO4_initsol_SeO4_0000ppb	4.28	n.a.	n.a.	12.80	267.79	n.a.	n.a.	73.39
10	sorp_SO4_initsol_SeO4_0010ppb	4.28	n.a.	n.a.	12.79	263.57	n.a.	n.a.	73.92
11	sorp_SO4_initsol_SeO4_0025ppb	4.28	n.a.	n.a.	12.79	261.87	n.a.	n.a.	74.44
12	sorp_SO4_initsol_SeO4_0050ppb	4.28	7.34	n.a.	12.79	259.04	3.54	n.a.	72.91
13	sorp_SO4_initsol_SeO4_0100ppb	4.28	n.a.	n.a.	12.80	261.86	n.a.	n.a.	73.86
14	sorp_SO4_initsol_SeO4_0250ppb	4.28	n.a.	n.a.	12.80	255.17	n.a.	n.a.	73.85
15	sorp_SO4_initsol_SeO4_0500ppb	4.28	n.a.	n.a.	12.80	258.84	n.a.	n.a.	72.79
16	sorp_SO4_initsol_SeO4_1000ppb	4.28	n.a.	n.a.	12.80	261.39	n.a.	n.a.	73.64
17	sorp_SO4_initsol_SeO4_2500ppb	4.28	n.a.	n.a.	12.80	261.32	n.a.	n.a.	73.44
18	sorp_SO4_initsol_SeO4_5000ppb	4.28	n.a.	n.a.	12.80	261.37	n.a.	n.a.	73.11
19	Dest.Wasser-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
20	Standard_3-2	4.22	7.21	10.32	12.80	10.35	20.94	30.64	19.51
21	Dest.Wasser-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
22	Test-Riverwater	4.26	n.a.	n.a.	12.75	44.72	n.a.	n.a.	145.16
23	Dest.Wasser-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
24	sorp_SO4_Ksorp_SeO4_0000ppb	4.28	n.a.	n.a.	12.80	267.22	n.a.	n.a.	71.72
25	sorp_SO4_Ksorp_SeO4_0010ppb	4.29	n.a.	n.a.	12.80	262.97	n.a.	n.a.	71.67
26	sorp_SO4_Ksorp_SeO4_0025ppb	4.28	n.a.	n.a.	12.80	262.03	n.a.	n.a.	72.24
27	sorp_SO4_Ksorp_SeO4_0050ppb	4.28	n.a.	n.a.	12.80	261.47	n.a.	n.a.	71.81
28	sorp_SO4_Ksorp_SeO4_0100ppb	4.28	n.a.	n.a.	12.80	261.97	n.a.	n.a.	72.39
29	sorp_SO4_Ksorp_SeO4_0250ppb	4.28	n.a.	n.a.	12.80	256.19	n.a.	n.a.	72.40
30	sorp_SO4_Ksorp_SeO4_0500ppb	4.28	n.a.	n.a.	12.80	262.27	n.a.	n.a.	72.16
31	sorp_SO4_Ksorp_SeO4_1000ppb	4.29	n.a.	n.a.	12.80	264.03	n.a.	n.a.	71.92
32	sorp_SO4_Ksorp_SeO4_2500ppb	4.28	7.36	n.a.	12.80	259.42	2.20	n.a.	70.90
33	sorp_SO4_Ksorp_SeO4_5000ppb	4.29	n.a.	n.a.	12.81	260.88	n.a.	n.a.	71.73
34	Dest.Wasser-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
35	Standard_3-3	4.22	7.23	10.32	12.80	10.28	20.81	30.79	19.51
36	Dest.Wasser-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
37	sorp_SO4_Gsorp_SeO4_0000ppb	4.29	7.37	n.a.	12.80	271.83	2.06	n.a.	113.07
38	sorp_SO4_Gsorp_SeO4_0010ppb	4.29	7.38	n.a.	12.80	260.65	1.83	n.a.	111.68
39	sorp_SO4_Gsorp_SeO4_0025ppb	4.29	7.37	n.a.	12.79	261.95	2.075	n.a.	114.34
40	sorp_SO4_Gsorp_SeO4_0050ppb	4.29	7.37	n.a.	12.80	259.19	2.019	n.a.	112.77
41	sorp_SO4_Gsorp_SeO4_0100ppb	4.29	7.34	n.a.	12.80	259.69	2.086	n.a.	112.91
42	sorp_SO4_Gsorp_SeO4_0250ppb	4.28	7.37	n.a.	12.80	256.04	2.44	n.a.	113.82
43	sorp_SO4_Gsorp_SeO4_0500ppb	4.29	7.34	n.a.	12.80	260.87	2.07	n.a.	113.31
44	sorp_SO4_Gsorp_SeO4_1000ppb	4.29	7.38	n.a.	12.80	266.65	2.07	n.a.	113.95
45	sorp_SO4_Gsorp_SeO4_2500ppb	4.29	7.36	n.a.	12.80	262.49	1.95	n.a.	114.02
46	sorp_SO4_Gsorp_SeO4_5000ppb	4.29	7.32	n.a.	12.95	258.71	1.87	n.a.	110.51
47	Dest.Wasser-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
48	Standard_3-4	4.22	7.23	10.31	12.81	10.28	21.268	30.17	19.52
49	Dest.Wasser-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
50	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table B.24.: B3 analytical data - ICP-MS measurement; Se sorption in the presence of NO_3^-

Technique	ICP-MS Quadrupole						
System	X-Series Thermo Fischer						
Date measured	07.10.2014						
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean $^{76}\text{Se}, ^{77}\text{Se}, ^{78}\text{Se}$	SD
	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[-]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]
Analytical Quality							
wash-mean	0.20	0.16	0.17	0.77			
wash-SD	0.08	0.10	0.09	0.26			
LOD (= 3·wash)	0.25	0.30	0.28	0.78			
HighPurityStd ref. value	5.50	5.50	5.50	5.50			
Quality [%]	132.45	103.41	102.80	111.06			
Calibration							
Std 0ppb	0.08	0.11	0.10	0.32	1	0.49	0.09
Std 5ppb Se	5.05	4.96	5.03	5.26	1	10.02	0.09
Std 10ppb Se	9.93	10.01	10.02	10.39	1	19.98	0.09
Std 25ppb Se	24.95	24.69	24.83	25.12	1	49.65	0.26
Std 50ppb Se	49.85	50.27	49.70	49.61	1	99.88	0.59
Std 100ppb Se	100.40	100.70	99.63	99.49	1	200.49	1.10
Std 250ppb Se	251.10	253.70	251.50	251.00	1	504.20	2.80
Std 500ppb Se	498.00	498.50	499.10	498.10	1	997.07	1.10
Std 1000ppb Se	1001.00	999.70	1000.00	1001.00	1	2000.47	0.42
Samples							
wash 2	0.38	0.37	0.39	0.57	1	0.38	
HPS	7.18	5.69	5.69	5.91	(2)	5.69	
wash 3	0.11	0.11	0.17	0.19	1	0.13	
N-sorp_initsol_SeO4_5000ppb	1095.0	1095.0	1103.0	1096.0	5	5488.3	
N-sorp_initsol_SeO4_2500ppb	547.1	545.7	547.1	547.8	5	2733.2	4.04
N-sorp_initsol_SeO4_1000ppb	740.0	742.1	735.7	745.3	2	1478.5	6.52
N-sorp_initsol_SeO4_0500ppb	292.3	292.3	291.7	297.9	2	584.2	0.69
N-sorp_initsol_SeO4_0250ppb	151.0	154.6	153.7	156.7	2	306.2	3.75
N-sorp_initsol_SeO4_0100ppb	62.0	62.0	61.2	64.6	2	123.5	0.97
N-sorp_initsol_SeO4_0050ppb	31.8	31.1	31.7	36.1	2	63.1	0.76
N-sorp_initsol_SeO4_0025ppb	15.2	15.1	15.8	20.0	2	30.7	0.73
N-sorp_initsol_SeO4_0010ppb	6.57	6.70	6.34	10.46	2	13.1	0.36
N-sorp_initsol_SeO4_0000ppb	0.23	0.18	0.19	4.12	2	0.37	0.01
wash 4	0.14	0.09	0.09	0.65	1	0.11	0.00
test 50ppb	52.81	51.78	52.08	54.52	1	52.22	0.00
wash 5	0.17	0.13	0.13	0.96	1	0.14	0.00
N-sorp_Ksorp_SeO4_5000ppb	772.9	772.6	768.2	779.2	5	3856.2	13.16
N-sorp_Ksorp_SeO4_2500ppb	338.9	338.3	340.1	343.8	5	1695.5	4.58
N-sorp_Ksorp_SeO4_1000ppb	415.3	417.0	419.4	423.6	2	834.5	4.12
N-sorp_Ksorp_SeO4_0500ppb	152.5	151.6	150.9	154.3	2	303.3	1.60
N-sorp_Ksorp_SeO4_0250ppb	76.9	75.4	75.9	79.1	2	152.1	1.50
N-sorp_Ksorp_SeO4_0100ppb	30.7	30.9	30.7	34.4	2	61.5	0.31
N-sorp_Ksorp_SeO4_0050ppb	15.2	14.3	14.9	19.4	2	29.6	0.88
N-sorp_Ksorp_SeO4_0025ppb	7.54	7.61	7.50	11.54	2	15.1	0.10
N-sorp_Ksorp_SeO4_0010ppb	3.22	3.22	3.24	7.05	2	6.45	0.02
N-sorp_Ksorp_SeO4_0000ppb	10.61	10.33	10.23	14.96	2	20.78	0.39
wash 6	0.14	0.08	0.05	0.68	1	0.09	0.00
test 50ppb	52.92	52.44	52.56	52.66	1	52.64	0.00
wash 7	0.16	0.11	0.12	0.55	1	0.13	0.00
N-sorp_Gsorp_SeO4_5000ppb	694.8	692.8	692.2	700.6	5	3466.3	6.81
N-sorp_Gsorp_SeO4_2500ppb	341.2	339.5	338.4	346.4	5	1698.5	7.05
N-sorp_Gsorp_SeO4_1000ppb	458.8	456.1	455.3	463.5	2	913.5	3.67
N-sorp_Gsorp_SeO4_0500ppb	176.1	177.4	177.3	181.9	2	353.9	1.45
N-sorp_Gsorp_SeO4_0250ppb	89.6	90.6	89.8	94.6	2	179.9	1.04
N-sorp_Gsorp_SeO4_0100ppb	36.9	36.9	36.7	41.4	2	73.7	0.23
N-sorp_Gsorp_SeO4_0050ppb	18.2	18.7	18.6	22.0	2	37.0	0.51
N-sorp_Gsorp_SeO4_0025ppb	9.33	9.53	9.49	13.55	2	18.9	0.21
N-sorp_Gsorp_SeO4_0010ppb	4.13	3.78	3.96	8.25	2	7.91	0.35
N-sorp_Gsorp_SeO4_0000ppb	0.96	0.68	1.08	5.80	2	1.81	0.41
wash 8	0.18	0.04	0.08	0.76	1	0.10	0.00
test 50ppb	51.62	51.51	51.48	52.41	1	51.54	0.00
wash 9	0.18	0.17	0.17	0.84	1	0.17	0.00
N-sorp_initsol_SeO3_5000ppb	1042.0	1039.0	1043.0	1065.0	5	5206.7	10.41
N-sorp_initsol_SeO3_2500ppb	539.4	533.0	533.2	544.3	5	2676.0	18.19
N-sorp_initsol_SeO3_1000ppb	724.0	724.6	724.1	737.0	2	1448.5	0.64
N-sorp_initsol_SeO3_0500ppb	279.3	275.0	275.1	285.7	2	552.9	4.91
N-sorp_initsol_SeO3_0250ppb	148.9	148.1	146.1	152.7	2	295.4	2.88
N-sorp_initsol_SeO3_0100ppb	59.4	58.2	59.3	63.4	2	117.9	1.31
N-sorp_initsol_SeO3_0050ppb	29.0	29.1	29.3	33.7	2	58.2	0.36
N-sorp_initsol_SeO3_0025ppb	15.3	14.9	15.0	19.5	2	30.2	0.35
N-sorp_initsol_SeO3_0010ppb	5.73	5.72	5.77	11.15	2	11.5	0.06
wash 10	0.31	0.36	0.36	1.06	1	0.34	0.00
test 50ppb	53.93	52.64	53.55	53.57	1	53.37	0.00
wash 11	0.45	0.32	0.49	1.18	1	0.42	0.00
N-sorp_Ksorp_SeO3_5000ppb	756.3	753.6	753.1	763.0	5	3771.7	8.61
N-sorp_Ksorp_SeO3_2500ppb	340.3	336.6	338.8	344.6	5	1692.8	9.31
N-sorp_Ksorp_SeO3_1000ppb	411.0	406.2	405.8	412.2	2	815.3	5.79
N-sorp_Ksorp_SeO3_0500ppb	124.1	122.8	123.4	128.5	2	246.9	1.30
N-sorp_Ksorp_SeO3_0250ppb	60.8	59.5	59.9	64.0	2	120.2	1.41
N-sorp_Ksorp_SeO3_0100ppb	21.8	21.1	21.1	25.4	2	42.6	0.84
N-sorp_Ksorp_SeO3_0050ppb	9.99	10.00	9.65	14.16	2	19.8	0.40
N-sorp_Ksorp_SeO3_0025ppb	4.77	4.70	4.76	8.61	2	9.48	0.07
N-sorp_Ksorp_SeO3_0010ppb	1.81	1.70	1.71	7.38	2	3.48	0.12

Table B.25.: *B3 analytical data - ICP-MS measurement; Se sorption in the presence of NO₃⁻ (continued from previous page)*

Isotope	⁷⁶ Se [µg/L]	⁷⁷ Se [µg/L]	⁷⁸ Se [µg/L]	⁸² Se [µg/L]	dil. factor [-]	⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se [µg/L]	SD [µg/L]
wash 12	0.29	0.28	0.26	1.20	1	0.27	0.00
test 50ppb	53.40	52.67	51.96	55.71	1	52.68	0.00
wash 13	0.33	0.29	0.23	1.06	1	0.28	0.00
N-sorp_Gsorp_SeO3_5000ppb	2.95	2.93	2.78	5.17	5	14.42	0.47
N-sorp_Gsorp_SeO3_2500ppb	1.57	1.57	1.55	3.65	5	7.80	0.05
N-sorp_Gsorp_SeO3_1000ppb	2.30	1.88	2.06	6.76	2	4.16	0.42
N-sorp_Gsorp_SeO3_0500ppb	0.92	1.03	0.99	4.96	2	1.96	0.11
N-sorp_Gsorp_SeO3_0250ppb	0.65	0.56	0.67	4.42	2	1.25	0.12
N-sorp_Gsorp_SeO3_0100ppb	0.33	0.33	0.39	4.00	2	0.70	0.07
N-sorp_Gsorp_SeO3_0050ppb	0.41	0.25	0.33	3.94	2	0.58	0.12
N-sorp_Gsorp_SeO3_0025ppb	0.35	0.24	0.27	4.28	2	0.51	0.03
N-sorp_Gsorp_SeO3_0010ppb	1.01	0.87	1.07	6.13	2	1.97	0.21
wash 14	0.18	0.11	0.16	1.00	1	0.15	0.00
HPS VF 2 wdh	7.39	5.69	5.62	6.31	1	5.65	0.00
test 50ppb	52.54	51.25	52.13	52.88	1	51.97	0.00
wash 15	0.24	0.21	0.24	0.69	1	0.23	0.00

Table B.26.: B3 analytical data - ICP-MS measurement; Se sorption in the presence of PO_4^{3-}

Technique System Date measured	ICP-MS Quadrupole X-Series Thermo Fischer 08.10.2014						
Isotope	^{76}Se [µg/L]	^{77}Se [µg/L]	^{78}Se [µg/L]	^{82}Se [µg/L]	dil. factor [-]	Se mean $^{76}\text{Se}, ^{77}\text{Se}, ^{78}\text{Se}$ [µg/L]	SD [µg/L]
Analytical Quality							
wash-mean	0.27	0.16	0.19	0.34		0.21	
wash-SD	0.10	0.09	0.08	0.21		0.09	
LOD (= 3-wash)	0.30	0.26	0.25	0.62		0.27	
HighPurityStd ref. value	5.50	5.50	5.50	5.50		5.50	
Quality [%]	123.25	99.93	100.25	96.35			
Calibration							
Std 0ppb	0.10	0.08	0.06	0.22	1	0.41	0.10
Std 5ppb Se	5.23	4.96	5.00	5.10	1	25.31	0.73
Std 10ppb Se	9.97	10.12	9.87	9.98	1	19.98	0.25
Std 25ppb Se	24.96	25.73	24.87	25.72	1	50.37	0.95
Std 50ppb Se	50.72	49.78	50.52	50.00	1	100.68	0.99
Std 100ppb Se	99.31	98.45	99.84	99.15	1	198.40	1.40
Std 250ppb Se	248.80	249.50	249.60	250.70	1	498.60	0.87
Std 500ppb Se	501.10	499.70	500.30	499.80	1	1000.73	1.40
Std 1000ppb Se	999.80	1000.00	1000.00	1000.00	1	1999.87	0.23
Samples							
wash 2	0.48	0.39	0.40	0.31	1	0.84	0.10
HPS	7.10	5.56	5.79	5.94	(2)	5.68	
wash 3	0.25	0.17	0.22	0.33	1	0.21	
P-sorp_initisol_SeO4_5000ppb	1200.0	1200.0	1201.0	1199.0	5	6001.7	2.89
P-sorp_initisol_SeO4_2500ppb	601.5	600.4	599.8	600.6	5	3002.8	4.31
P-sorp_initisol_SeO4_1000ppb	812.3	809.9	809.3	809.6	2	1621.0	3.17
P-sorp_initisol_SeO4_0500ppb	314.4	315.9	317.3	319.4	2	631.7	2.90
P-sorp_initisol_SeO4_0250ppb	153.0	152.1	152.4	155.7	2	305.0	0.92
P-sorp_initisol_SeO4_0100ppb	60.0	60.8	60.4	63.8	2	120.8	0.72
P-sorp_initisol_SeO4_0050ppb	31.0	30.9	31.0	34.1	2	61.9	0.18
P-sorp_initisol_SeO4_0025ppb	15.3	15.5	15.4	19.0	2	30.8	0.21
P-sorp_initisol_SeO4_0010ppb	6.42	6.35	6.50	9.94	2	12.8	0.15
P-sorp_initisol_SeO4_0000ppb	0.30	0.28	0.35	3.28	2	0.61	0.07
N-sorp_Ksorp_SeO4_0010ppb	3.15	3.15	3.18	6.58	2	6.31	0.03
N-sorp_Ksorp_SeO4_0000ppb	10.29	10.19	10.03	14.00	2	20.34	0.26
wash 4	0.20	0.10	0.10	0.37	1	0.13	0.00
test 50ppb	51.09	50.52	51.05	51.36	1	50.89	0.00
wash 5	0.14	0.12	0.14	0.24	1	0.13	0.00
P-sorp_Ksorp_SeO4_5000ppb	1158.0	1168.0	1161.0	1157.0	5	5811.7	25.66
P-sorp_Ksorp_SeO4_2500ppb	587.2	590.9	588.8	589.5	5	2944.8	9.28
P-sorp_Ksorp_SeO4_1000ppb	792.9	786.3	787.7	792.0	2	1577.9	6.96
P-sorp_Ksorp_SeO4_0500ppb	303.2	303.1	301.4	303.8	2	605.1	2.02
P-sorp_Ksorp_SeO4_0250ppb	146.3	146.9	145.6	150.8	2	292.5	1.30
P-sorp_Ksorp_SeO4_0100ppb	58.3	57.8	58.4	60.5	2	116.4	0.63
P-sorp_Ksorp_SeO4_0050ppb	29.3	29.9	29.2	32.2	2	58.9	0.70
P-sorp_Ksorp_SeO4_0025ppb	14.7	14.8	14.4	17.9	2	29.3	0.39
P-sorp_Ksorp_SeO4_0010ppb	6.38	6.19	6.36	9.86	2	12.6	0.21
P-sorp_Ksorp_SeO4_0000ppb	0.78	0.48	0.50	4.04	2	0.98	0.03
wash 6	0.15	0.05	0.10	0.51	1	0.10	0.00
test 50ppb	50.43	49.56	50.91	51.11	1	50.30	0.00
wash 7	0.23	0.09	0.12	0.26	1	0.14	0.00
P-sorp_Gsorp_SeO4_5000ppb	986.6	984.2	980.9	978.4	5	4919.5	14.31
P-sorp_Gsorp_SeO4_2500ppb	493.5	494.6	493.8	494.1	5	2469.8	2.84
P-sorp_Gsorp_SeO4_1000ppb	660.4	663.6	663.8	660.5	2	1325.2	3.82
P-sorp_Gsorp_SeO4_0500ppb	253.5	253.8	255.7	259.5	2	508.7	2.39
P-sorp_Gsorp_SeO4_0250ppb	121.3	121.9	122.9	125.0	2	244.1	1.62
P-sorp_Gsorp_SeO4_0100ppb	49.9	48.8	49.1	52.0	2	98.5	1.12
P-sorp_Gsorp_SeO4_0050ppb	24.7	25.0	24.9	27.6	2	49.7	0.22
P-sorp_Gsorp_SeO4_0025ppb	12.1	12.2	12.1	14.6	2	24.3	0.10
P-sorp_Gsorp_SeO4_0010ppb	5.27	5.07	5.25	8.46	2	10.4	0.22
P-sorp_Gsorp_SeO4_0000ppb	0.31	0.22	0.38	3.91	2	0.61	0.16
wash 8	0.18	0.07	0.09	0.27	1	0.11	0.00
test 50ppb	49.41	49.22	49.25	49.31	1	49.29	0.00
wash 9	0.30	0.27	0.26	0.49	1	0.28	0.00
P-sorp_initisol_SeO3_5000ppb	1054.0	1059.0	1057.0	1055.0	5	5283.3	12.58
P-sorp_initisol_SeO3_2500ppb	525.4	525.1	528.6	524.8	5	2631.8	9.70
P-sorp_initisol_SeO3_1000ppb	707.4	711.5	711.8	712.2	2	1420.5	4.92
P-sorp_initisol_SeO3_0500ppb	270.5	272.7	272.8	272.6	2	544.0	2.60
P-sorp_initisol_SeO3_0250ppb	144.2	142.5	144.0	147.8	2	287.1	1.86
P-sorp_initisol_SeO3_0100ppb	57.9	57.4	57.3	61.4	2	115.1	0.65
P-sorp_initisol_SeO3_0050ppb	29.2	30.1	29.8	32.4	2	59.4	0.92
P-sorp_initisol_SeO3_0025ppb	13.9	14.7	14.3	17.3	2	28.6	0.77
P-sorp_initisol_SeO3_0010ppb	6.28	6.04	5.82	9.60	2	12.1	0.47
wash 10	0.42	0.27	0.28	0.72	1	0.32	0.00
test 50ppb	51.35	49.71	50.77	51.28	1	50.61	0.00
wash 11	0.37	0.24	0.28	0.48	1	0.30	0.00
P-sorp_Ksorp_SeO3_5000ppb	1005.0	1010.0	1010.0	1011.0	5	5041.7	14.43
P-sorp_Ksorp_SeO3_2500ppb	505.4	500.4	506.4	507.4	5	2520.3	16.07
P-sorp_Ksorp_SeO3_1000ppb	663.7	671.9	667.5	667.0	2	1335.4	8.21
P-sorp_Ksorp_SeO3_0500ppb	252.8	252.9	252.6	255.6	2	505.5	0.31
P-sorp_Ksorp_SeO3_0250ppb	132.1	132.9	133.1	135.3	2	265.4	1.06
P-sorp_Ksorp_SeO3_0100ppb	52.1	52.1	51.3	54.2	2	103.6	0.91
P-sorp_Ksorp_SeO3_0050ppb	25.7	25.4	25.3	28.9	2	50.9	0.41
P-sorp_Ksorp_SeO3_0025ppb	12.3	12.5	12.3	15.9	2	24.7	0.22
P-sorp_Ksorp_SeO3_0010ppb	4.80	4.82	4.75	7.88	2	9.6	0.07

Table B.27.: B3 analytical data - ICP-MS measurement; Se sorption in the presence of PO_4^{3-} (continued from previous page)

Isotope	^{76}Se [$\mu\text{g/L}$]	^{77}Se [$\mu\text{g/L}$]	^{78}Se [$\mu\text{g/L}$]	^{82}Se [$\mu\text{g/L}$]	dil. factor [-]	$^{76}\text{Se}, ^{77}\text{Se}, ^{78}\text{Se}$ [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]
wash 12	0.40	0.23	0.25	0.51	1	0.30	0.00
test 50ppb	50.42	51.29	51.02	50.86	1	50.91	0.00
wash 13	0.38	0.27	0.30	0.11	1	0.32	0.00
P-sorp_Gsorp_SeO3_5000ppb	3.70	3.65	3.83	4.82	5	18.63	0.46
P-sorp_Gsorp_SeO3_2500ppb	1.79	1.81	1.97	3.33	5	9.28	0.49
P-sorp_Gsorp_SeO3_1000ppb	2.54	2.61	2.48	5.62	2	5.09	0.13
P-sorp_Gsorp_SeO3_0500ppb	1.16	1.19	1.21	4.28	2	2.38	0.05
P-sorp_Gsorp_SeO3_0250ppb	0.70	0.64	0.83	4.00	2	1.44	0.20
P-sorp_Gsorp_SeO3_0100ppb	0.45	0.45	0.54	3.99	2	0.96	0.10
P-sorp_Gsorp_SeO3_0050ppb	0.40	0.29	0.37	3.42	2	0.66	0.10
P-sorp_Gsorp_SeO3_0025ppb	0.40	0.24	0.36	3.93	2	0.60	0.17
P-sorp_Gsorp_SeO3_0010ppb	0.48	0.25	0.50	3.64	2	0.82	0.28
wash 14	0.22	0.11	0.14	0.11	1	0.15	0.00
HPS wdh	6.78	5.50	5.51	5.30	(2)	5.51	0.00
test 50ppb	50.39	50.62	50.17	49.65	1	50.39	0.00
wash 15	0.35	0.23	0.27	-0.09	1	0.28	0.00

Table B.28.: B3 analytical data - ICP-MS measurement; Se sorption in the presence of SO_4^{2-}

Technique	ICP-MS Quadrupole					Se mean	
System	X-Series Thermo Fischer					$^{76}Se, ^{77}Se, ^{78}Se$	SD
Date measured	09.10.2014					$^{76}Se, ^{77}Se, ^{78}Se$	[$\mu g/L$]
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	$^{76}Se, ^{77}Se, ^{78}Se$	SD
	[$\mu g/L$]	[$\mu g/L$]	[$\mu g/L$]	[$\mu g/L$]	[-]	[$\mu g/L$]	[$\mu g/L$]
Analytical Quality							
wash-mean	0.22	0.18	0.20	0.38		0.20	
wash-SD	0.10	0.09	0.10	0.21		0.09	
LOD (= 3-wash)	0.29	0.26	0.30	0.63		0.28	
HighPurityStd ref. value	5.50	5.50	5.50	5.50		5.50	
Quality [%]	121.56	103.02	98.82	104.91			
Calibration							
Std 0ppb	0.11	0.04	0.09	0.17	1	0.40	0.17
Std 5ppb Se	5.03	4.99	5.06	5.08	1	25.13	0.17
Std 10ppb Se	10.05	9.95	10.03	10.63	1	20.02	0.11
Std 25ppb Se	25.00	24.87	24.89	25.32	1	49.84	0.14
Std 50ppb Se	49.88	49.41	49.72	50.10	1	99.34	0.48
Std 100ppb Se	99.87	98.48	99.61	99.96	1	198.64	1.48
Std 250ppb Se	250.40	250.90	250.10	248.60	1	500.93	0.81
Std 500ppb Se	500.10	499.30	501.00	499.60	1	1000.27	1.70
Std 1000ppb Se	1000.00	1000.00	999.50	1001.00	1	1999.67	0.58
Samples							
wash 2	0.49	0.49	0.50	0.30	1	0.99	0.01
HPS	7.11	5.62	5.62	5.96	(2)	5.62	
wash 3	0.22	0.19	0.21	0.35	1	0.21	
S-sorp_initsol_SeO4_5000ppb	1088.0	1074.0	1081.0	1074.0	5	5405.0	35.00
S-sorp_initsol_SeO4_2500ppb	537.3	535.8	537.1	534.2	5	2683.7	4.07
S-sorp_initsol_SeO4_1000ppb	744.1	734.4	735.9	736.4	2	1476.3	10.44
S-sorp_initsol_SeO4_0500ppb	286.9	286.7	285.6	285.1	2	572.8	1.40
S-sorp_initsol_SeO4_0250ppb	147.9	148.1	148.0	149.0	2	296.0	0.20
S-sorp_initsol_SeO4_0100ppb	60.2	58.7	59.8	62.0	2	119.1	1.53
S-sorp_initsol_SeO4_0050ppb	29.1	29.0	29.4	31.2	2	58.4	0.43
S-sorp_initsol_SeO4_0025ppb	14.7	15.1	14.8	17.8	2	29.7	0.39
S-sorp_initsol_SeO4_0010ppb	5.94	5.82	5.92	8.58	2	11.8	0.12
S-sorp_initsol_SeO4_0000ppb	0.17	0.15	0.26	3.32	2	0.39	0.12
wash 4	0.12	0.10	0.07	0.17	1	0.10	0.00
test 50ppb	50.60	50.33	50.16	49.61	1	50.36	0.00
wash 5	0.17	0.18	0.18	0.10	1	0.18	0.00
S-sorp_Ksorp_SeO4_5000ppb	1056.0	1050.0	1049.0	1048.0	5	5258.3	18.93
S-sorp_Ksorp_SeO4_2500ppb	526.7	521.5	527.5	522.9	5	2626.2	16.29
S-sorp_Ksorp_SeO4_1000ppb	697.3	698.2	701.9	696.3	2	1398.3	4.88
S-sorp_Ksorp_SeO4_0500ppb	270.3	272.2	273.3	273.2	2	543.9	3.04
S-sorp_Ksorp_SeO4_0250ppb	141.5	141.1	141.8	143.3	2	282.9	0.70
S-sorp_Ksorp_SeO4_0100ppb	56.7	55.8	57.2	59.1	2	113.1	1.44
S-sorp_Ksorp_SeO4_0050ppb	28.7	28.5	28.9	31.9	2	57.4	0.36
S-sorp_Ksorp_SeO4_0025ppb	14.3	15.0	14.5	17.8	2	29.2	0.67
S-sorp_Ksorp_SeO4_0010ppb	5.88	5.70	5.74	8.79	2	11.5	0.19
S-sorp_Ksorp_SeO4_0000ppb	0.58	0.51	0.51	3.67	2	1.07	0.08
wash 6	0.15	0.07	0.09	0.10	1	0.10	0.00
test 50ppb	50.55	50.18	49.89	49.02	1	50.21	0.00
wash 7	0.19	0.18	0.18	0.31	1	0.18	0.00
S-sorp_Gsorp_SeO4_5000ppb	790.5	782.7	785.6	776.3	5	3931.3	19.71
S-sorp_Gsorp_SeO4_2500ppb	393.8	390.8	392.9	388.1	5	1962.5	7.70
S-sorp_Gsorp_SeO4_1000ppb	521.3	517.6	519.3	515.0	2	1038.8	3.70
S-sorp_Gsorp_SeO4_0500ppb	200.0	199.7	201.3	201.2	2	400.7	1.70
S-sorp_Gsorp_SeO4_0250ppb	104.7	103.9	104.9	106.1	2	209.0	1.06
S-sorp_Gsorp_SeO4_0100ppb	43.1	41.3	42.6	45.1	2	84.6	1.93
S-sorp_Gsorp_SeO4_0050ppb	21.6	21.8	21.6	24.7	2	43.3	0.15
S-sorp_Gsorp_SeO4_0025ppb	10.9	10.7	10.9	14.2	2	21.7	0.25
S-sorp_Gsorp_SeO4_0010ppb	4.15	4.06	4.19	7.58	2	8.26	0.13
S-sorp_Gsorp_SeO4_0000ppb	0.39	0.30	0.47	3.59	2	0.77	0.17
wash 8	0.09	0.07	0.07	0.20	1	0.08	0.00
test 50ppb	50.14	48.85	48.99	48.70	1	49.33	0.00
wash 9	0.29	0.28	0.26	0.22	1	0.28	0.00
S-sorp_initsol_SeO3_5000ppb	1049.0	1048.0	1053.0	1045.0	5	5250.0	13.23
S-sorp_initsol_SeO3_2500ppb	532.2	524.8	526.7	521.8	5	2639.5	19.22
S-sorp_initsol_SeO3_1000ppb	334.0	335.3	336.4	330.6	2	1676.2	6.01
S-sorp_initsol_SeO3_0500ppb	271.4	269.1	272.5	272.5	2	542.0	3.47
S-sorp_initsol_SeO3_0250ppb	142.7	143.0	144.1	145.1	2	286.5	1.47
S-sorp_initsol_SeO3_0100ppb	56.8	56.5	56.9	60.2	2	113.5	0.44
S-sorp_initsol_SeO3_0050ppb	29.0	28.8	29.3	31.7	2	58.1	0.48
S-sorp_initsol_SeO3_0025ppb	14.1	14.0	14.8	17.1	2	28.6	0.91
S-sorp_initsol_SeO3_0010ppb	6.31	6.07	6.28	9.29	2	12.4	0.26
wash 10	0.27	0.28	0.30	0.60	1	0.28	0.00
test 50ppb	49.69	49.53	50.24	49.56	1	49.82	0.00
wash 11	0.37	0.30	0.35	0.58	1	0.34	0.00
S-sorp_Ksorp_SeO3_5000ppb	818.9	815.2	815.7	809.4	5	4083.0	10.04
S-sorp_Ksorp_SeO3_2500ppb	362.4	361.3	366.9	361.6	5	1817.7	14.84
S-sorp_Ksorp_SeO3_1000ppb	632.6	627.3	628.2	629.1	2	1258.7	5.67
S-sorp_Ksorp_SeO3_0500ppb/5	114.8	114.7	114.6	116.5	0.4	229.4	0.20
S-sorp_Ksorp_SeO3_0250ppb	65.3	65.9	66.6	69.1	2	131.8	1.35
S-sorp_Ksorp_SeO3_0100ppb	23.1	23.5	23.1	25.7	2	46.5	0.47
S-sorp_Ksorp_SeO3_0050ppb	11.8	11.6	11.8	14.6	2	23.5	0.22
S-sorp_Ksorp_SeO3_0025ppb	5.71	5.68	5.63	9.20	2	11.3	0.08
S-sorp_Ksorp_SeO3_0010ppb	3.08	3.10	3.01	6.27	2	6.12	0.09

Table B.29.: B3 analytical data - ICP-MS measurement; Se sorption in the presence of SO_4^{2-} (continued from previous page)

Isotope	^{76}Se [$\mu\text{g/L}$]	^{77}Se [$\mu\text{g/L}$]	^{78}Se [$\mu\text{g/L}$]	^{82}Se [$\mu\text{g/L}$]	dil. factor [-]	$^{76}\text{Se}, ^{77}\text{Se}, ^{78}\text{Se}$ [$\mu\text{g/L}$]	SD [$\mu\text{g/L}$]
wash 12	0.32	0.26	0.28	0.69	1	0.29	0.00
test 50ppb	49.52	49.24	49.71	50.16	1	49.49	0.00
wash 13	0.37	0.28	0.34	0.46	1	0.33	0.00
S-sorp_Gsorp_SeO3_5000ppb	3.38	3.24	3.35	4.71	5	16.62	0.36
S-sorp_Gsorp_SeO3_2500ppb	1.83	1.80	1.80	4.00	5	9.05	0.11
S-sorp_Gsorp_SeO3_1000ppb	2.83	2.88	2.90	5.95	2	5.74	0.08
S-sorp_Gsorp_SeO3_0500ppb	1.05	1.07	1.20	4.45	2	2.21	0.16
S-sorp_Gsorp_SeO3_0250ppb	0.71	0.67	0.75	3.99	2	1.41	0.08
S-sorp_Gsorp_SeO3_0100ppb	0.44	0.43	0.62	3.73	2	0.99	0.22
S-sorp_Gsorp_SeO3_0050ppb	0.37	0.28	0.47	4.13	2	0.74	0.19
S-sorp_Gsorp_SeO3_0025ppb	0.33	0.17	0.45	3.97	2	0.63	0.28
S-sorp_Gsorp_SeO3_0010ppb	0.34	0.32	0.45	3.98	2	0.74	0.14
wash 14	0.18	0.11	0.12	0.57	1	0.14	0.00
HPS wdh	6.69	5.67	5.44	5.77	(2)	5.55	0.00
test 50ppb	50.12	48.80	49.13	49.10	1	49.35	0.00
wash 15	0.43	0.32	0.37	0.42	1	0.37	0.00

C. C Datasheets - plant-uptake sorption experiments

C.1. C Plant Growth Data

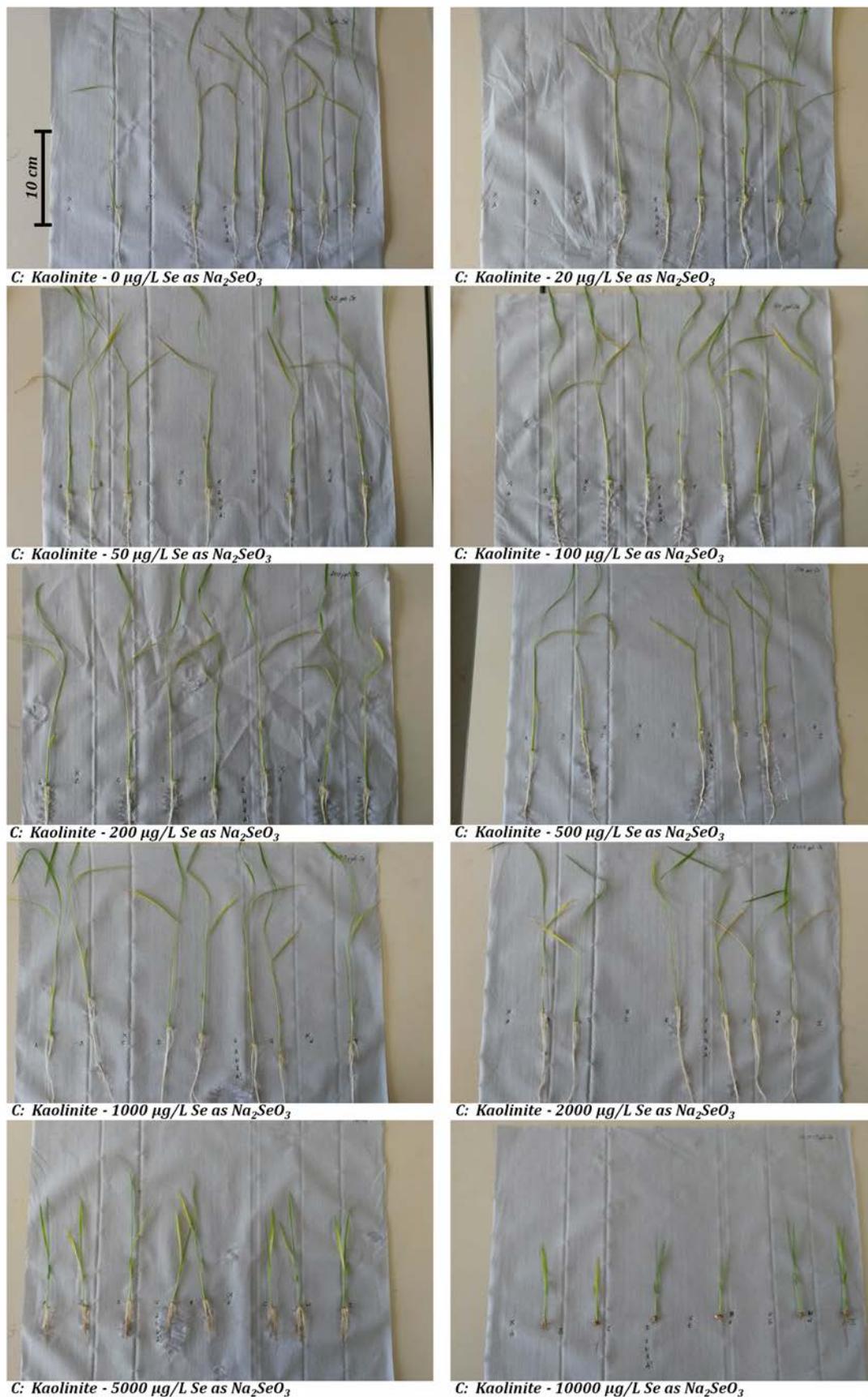


Figure C.1.: *C* photos of harvested plants treated with Na₂SeO₃ and kaolinite sorption competition

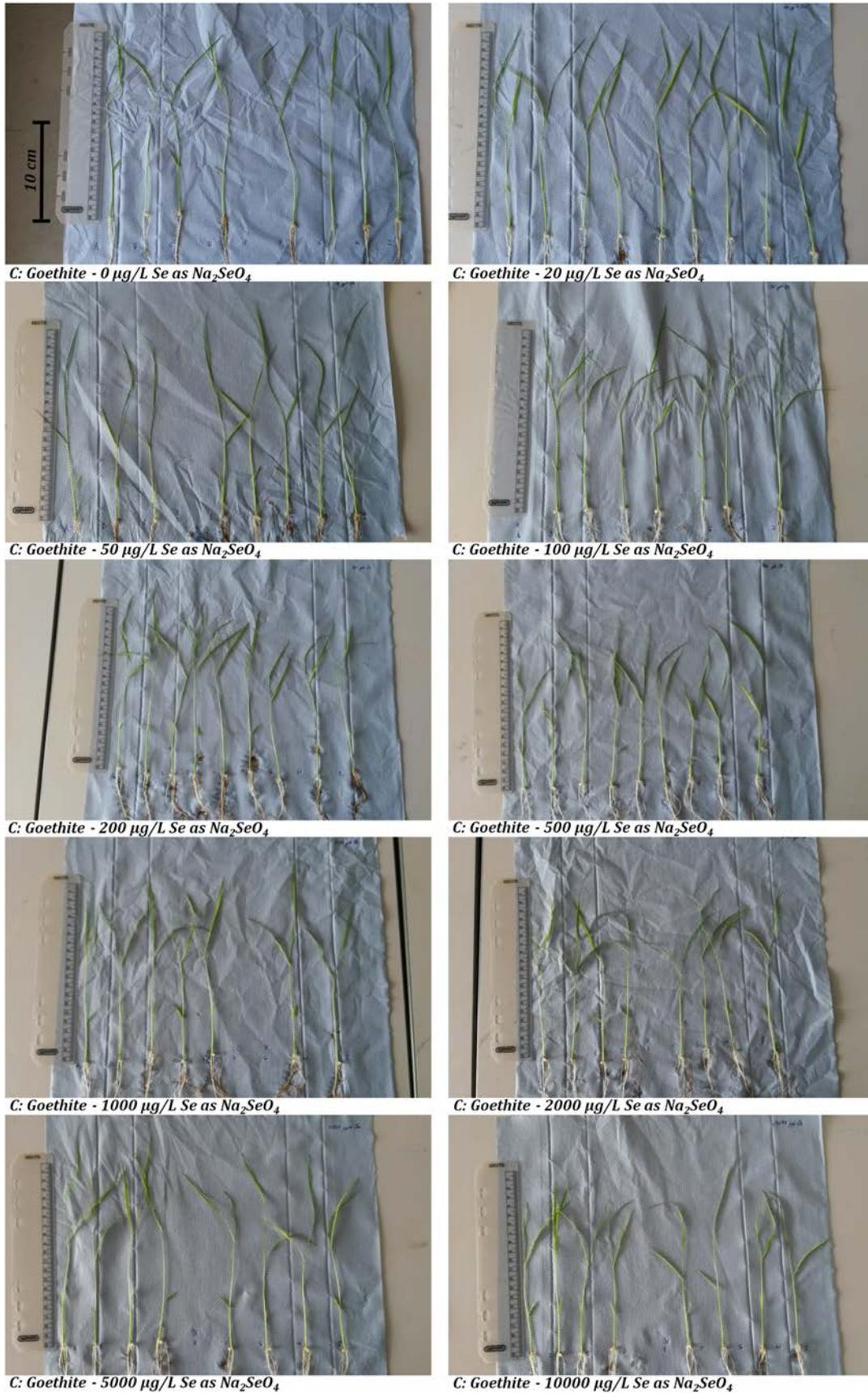


Figure C.2.: C photos of harvested plants treated with Na_2SeO_3 and goethite sorption competition

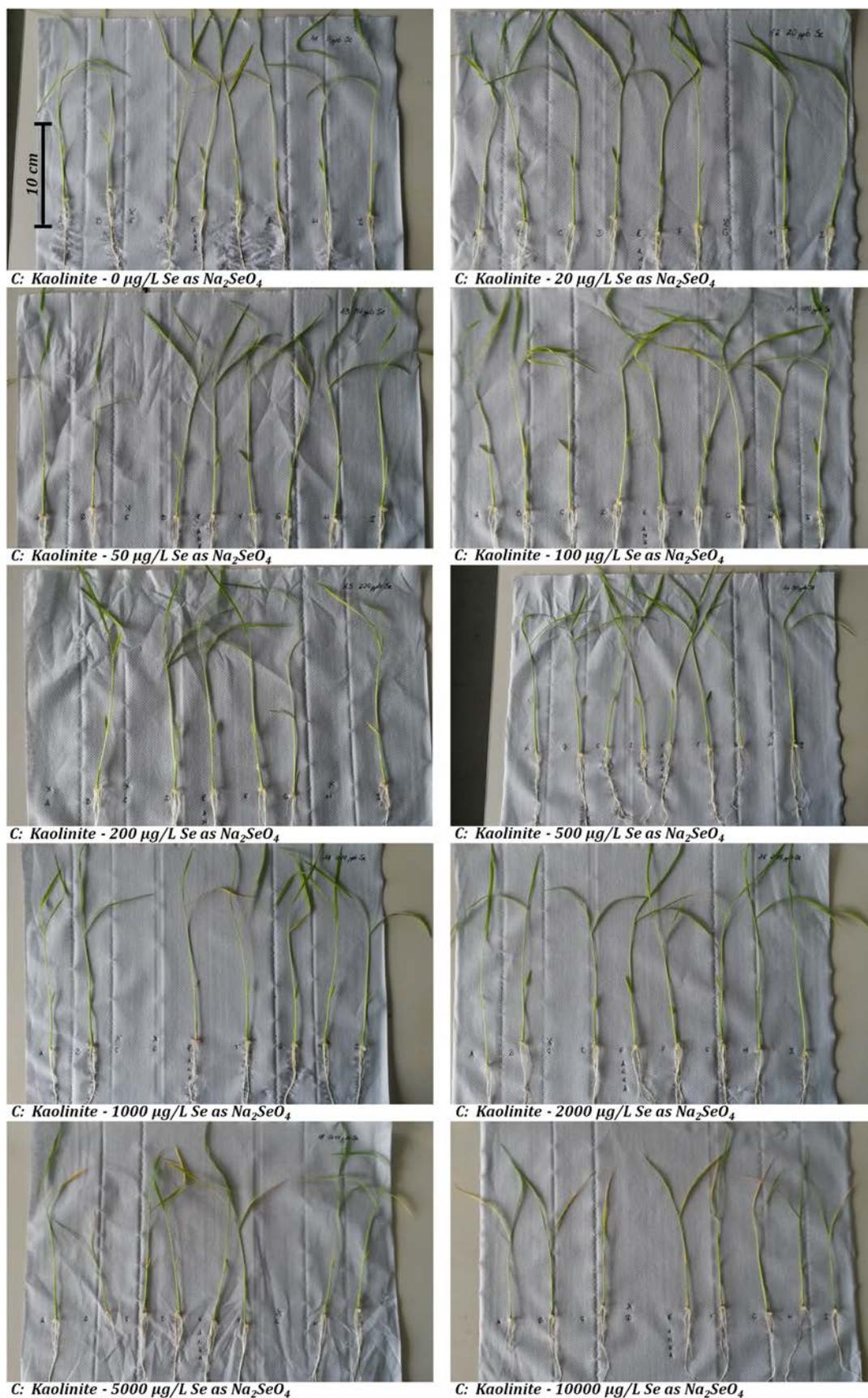


Figure C.3.: C photos of harvested plants treated with Na_2SeO_4 and kaolinite sorption competition

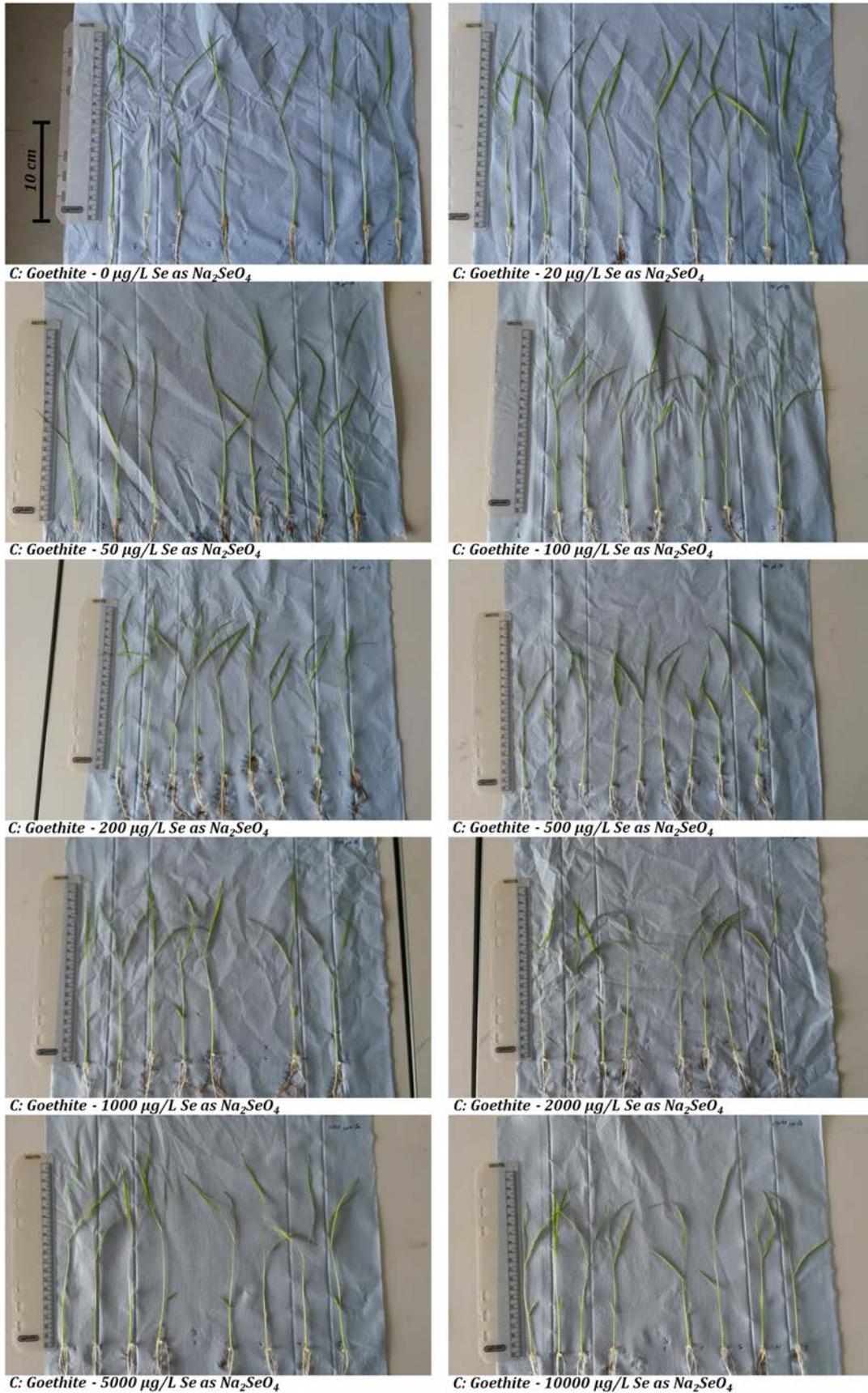


Figure C.4.: C photos of harvested plants treated with Na_2SeO_4 and goethite sorption competition

Table C.1.: C plant growth data Na_2SeO_3 , kaolinite (Planting Date: 27.03.2014)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
00000A	0	x	x	x	x	x	x	x	x	x	x	x
00000B	0	3.3	1.1	4.4	9	27.0	0.3120	0.0216	0.0048	0.0098	98.46	54.63
00000C	0	x	x	x	x	x	x	x	x	x	x	x
00000D	0	3.2	0.8	4	13	31.5	0.0525	0.0193	0.0162	0.0067	69.14	65.28
00000E	0	4.5	1.2	5.7	13	32.5	0.0497	0.0141	Synchrotron measurement			
00000F	0	3.8	1.2	5	13	29.5	0.0394	0.0111	0.0136	0.0057	65.48	48.65
00000G	0	2.8	0.9	3.7	12	30.5	0.0384	0.0071	0.0135	0.0053	64.84	25.35
00000H	0	3.7	0.9	4.6	13	28.0	0.0405	0.0087	0.0132	0.0050	67.41	42.53
00000I	0	2.4	0.7	3.1	10	26.0	0.0261	0.0286	0.0088	0.0063	66.28	77.97
00000_sum	0	23.7	6.8	30.5	83.0	205.0	0.5586	0.1105	0.0701	0.0388	431.62	314.42
00000_mean	0	3.4	1.0	4.4	11.9	29.3	0.0798	0.0158	0.0117	0.0065	71.94	52.40
00000_SD	0	0.7	0.2	0.9	1.7	2.4	0.1027	0.0078	0.0041	0.0017	13.08	18.26
00020A	20	x	x	x	x	x	x	x	x	x	x	x
00020B	20	x	x	x	x	x	x	x	x	x	x	x
00020C	20	x	x	x	x	x	x	x	x	x	x	x
00020D	20	4.1	1.6	5.7	13	28.0	0.0381	0.0125	0.0142	0.0063	62.73	49.60
00020E	20	3.9	1.3	5.2	13	32.0	0.0428	0.0109	Synchrotron measurement			
00020F	20	3.8	1.4	5.2	13	29.5	0.0433	0.0121	0.0150	0.0066	65.36	45.45
00020G	20	3.9	0.8	4.7	13	28.5	0.0408	0.0260	0.0145	0.0075	64.46	71.15
00020H	20	4.3	1.4	5.7	13	27.0	0.0325	0.0175	0.0119	0.0059	63.38	66.29
00020I	20	3.7	0.6	4.3	10	25.0	0.0234	0.0213	0.0104	0.0046	55.56	78.40
00020_sum	20	23.7	7.1	30.8	75.0	170.0	0.2209	0.1003	0.0660	0.0309	311.49	310.90
00020_mean	20	4.0	1.2	5.1	12.5	28.3	0.0368	0.0167	0.0132	0.0062	62.30	62.18
00020_SD	20	0.2	0.4	0.6	1.2	2.4	0.0077	0.0060	0.0020	0.0011	3.90	14.13
00050A	50	3.5	1.4	4.9	13	31.0	0.0344	0.0111	0.0126	0.0056	63.37	49.55
00050B	50	3.9	1.6	5.5	13	31.0	0.0393	0.0174	0.0134	0.0061	65.90	64.94
00050C	50	3.5	1.1	4.6	13	29.5	0.0388	0.0158	0.0124	0.0065	68.04	58.86
00050D	50	x	x	x	x	x	x	x	x	x	x	x
00050E	50	3.7	1.4	5.1	14	30.5	0.0385	0.0091	Synchrotron measurement			
00050F	50	x	x	x	x	x	x	x	x	x	x	x
00050G	50	3.7	1.3	5	13	28.0	0.0396	0.0167	0.0136	0.0054	65.66	67.66
00050H	50	x	x	x	x	x	x	x	x	x	x	x
00050I	50	3.8	1.3	5.1	13	29.0	0.0467	0.0164	0.0145	0.0071	68.95	56.71
00050_sum	50	22.1	8.1	30.2	79.0	179.0	0.2373	0.0865	0.0665	0.0307	331.92	297.72
00050_mean	50	3.7	1.4	5.0	13.2	29.8	0.0396	0.0144	0.0133	0.0061	66.38	59.54
00050_SD	50	0.2	0.2	0.3	0.4	1.2	0.0040	0.0034	0.0008	0.0007	2.19	7.13
00100A	100	x	x	x	x	x	x	x	x	x	x	x
00100B	100	2.9	1.3	4.2	12	26.0	0.0351	0.0159	0.0096	0.0061	72.65	61.64
00100C	100	x	x	x	x	x	x	x	x	x	x	x
00100D	100	3.6	1.3	4.9	14	26.5	0.0449	0.0171	0.0133	0.0063	70.38	63.16
00100E	100	3.9	1.6	5.5	13	26.0	0.0422	0.0176	Synchrotron measurement			
00100F	100	3.7	1.3	5	13	26.5	0.0328	0.0103	0.0129	0.0061	60.67	40.78
00100G	100	3.9	1.4	5.3	13	28.0	0.0439	0.0243	0.0141	0.0068	67.88	72.02
00100H	100	3.6	1.3	4.9	13	26.0	0.0415	0.0102	0.0129	0.0059	68.92	42.16
00100I	100	3.7	1.5	5.2	13	25.5	0.0408	0.0123	0.0126	0.0059	69.12	52.03
00100_sum	100	25.3	9.7	35.0	91.0	184.5	0.2812	0.1077	0.0754	0.0371	409.61	331.78
00100_mean	100	3.6	1.4	5.0	13.0	26.4	0.0402	0.0154	0.0126	0.0062	68.27	55.30
00100_SD	100	0.3	0.1	0.4	0.6	0.8	0.0045	0.0050	0.0015	0.0003	4.07	12.46
00200A	200	3.8	1.7	5.5	13	21.5	0.0271	0.0150	0.0097	0.0058	64.21	61.33
00200B	200	x	x	x	x	x	x	x	x	x	x	x
00200C	200	3.5	1.4	4.9	13	27.5	0.0376	0.0123	0.0122	0.0068	67.55	44.72
00200D	200	3.8	1.4	5.2	13	26.5	0.0359	0.0123	0.0125	0.0064	65.18	47.97
00200E	200	3.4	0.7	4.1	12	26.5	0.0276	0.0201	0.0109	0.0069	60.51	65.67
00200F	200	4	1.3	5.3	13	26.5	0.0449	0.0196	Synchrotron measurement			
00200G	200	x	x	x	x	x	x	x	x	x	x	x
00200H	200	3.3	1.1	4.4	12	26.0	0.0398	0.0167	0.0135	0.0080	66.08	52.10
00200I	200	3.5	1.4	4.9	13	25.0	0.0280	0.0102	0.0116	0.0062	58.57	39.22
00200_sum	200	25.3	9.0	34.3	89.0	179.5	0.2409	0.1062	0.0704	0.0401	382.10	311.00
00200_mean	200	3.6	1.3	4.9	12.7	25.6	0.0344	0.0152	0.0117	0.0067	63.68	51.83
00200_SD	200	0.3	0.3	0.5	0.5	2.0	0.0070	0.0038	0.0013	0.0008	3.45	10.07
00500A	500	3.6	1.4	5	13	31.5	0.0549	0.0172	0.0165	0.0070	69.95	59.30
00500B	500	3.4	1.6	5	13	30.5	0.0510	0.0166	0.0146	0.0070	71.37	57.83
00500C	500	x	x	x	x	x	x	x	x	x	x	x
00500D	500	x	x	x	x	x	x	x	x	x	x	x
00500E	500	x	x	x	x	x	x	x	x	x	x	x
00500F	500	3.5	1.3	4.8	13	31.5	0.0487	0.0139	Synchrotron measurement			
00500G	500	3.2	1.1	4.3	13	27.0	0.0379	0.0127	0.0125	0.0064	67.02	49.61
00500H	500	3.2	1.4	4.6	14	28.5	0.0588	0.0176	0.0153	0.0069	73.98	60.80
00500I	500	x	x	x	x	x	x	x	x	x	x	x
00500_sum	500	16.9	6.8	23.7	66.0	149.0	0.2513	0.0780	0.0589	0.0273	282.32	227.54
00500_mean	500	3.4	1.4	4.7	13.2	29.8	0.0503	0.0156	0.0147	0.0068	70.58	56.88
00500_SD	500	0.2	0.2	0.3	0.4	2.0	0.0079	0.0022	0.0017	0.0003	2.90	5.00

Table C.2.: C plant growth data Na_2SeO_3 , kaolinite (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
01000A	1000	3.7	1.5	5.2	13	24.5	0.0318	0.0176	0.0117	0.0065	63.21	63.07
01000B	1000	3.4	1.6	5	13	25.5	0.0366	0.0204	0.0115	0.0068	68.58	66.67
01000C	1000	x	x	x	x	x	x	x	x	x	x	x
01000D	1000	3.5	1.3	4.8	13	27.0	0.0349	0.0198	0.0123	0.0073	64.76	63.13
01000E	1000	2.9	1.3	4.2	12	25.5	0.0376	0.0191	0.0111	0.0074	70.48	61.26
01000F	1000	3.9	1.4	5.3	13	26.0	0.0326	0.0142	Synchrotron measurement			
01000G	1000	2.8	1	3.8	13	23.0	0.0249	0.0115	0.0101	0.0071	59.44	38.26
01000H	1000	x	x	x	x	x	x	x	x	x	x	x
01000I	1000	3.3	1.3	4.6	13	26.5	0.0335	0.0119	0.0120	0.0066	64.18	44.54
01000_sum	1000	23.5	9.4	32.9	90.0	178.0	0.2319	0.1145	0.0687	0.0417	390.64	336.92
01000_mean	1000	3.4	1.3	4.7	12.9	25.4	0.0331	0.0164	0.0115	0.0070	65.11	56.15
01000_SD	1000	0.4	0.2	0.5	0.4	1.3	0.0042	0.0038	0.0008	0.0004	3.94	11.73
02000A	2000	x	x	x	x	x	x	x	x	x	x	x
02000B	2000	3.2	1.3	4.5	13	23.5	0.0251	0.0132	0.0115	0.0088	54.18	33.33
02000C	2000	3.1	0.7	3.8	13	21.0	0.0221	0.0199	0.0101	0.0074	54.30	62.81
02000D	2000	x	x	x	x	x	x	x	x	x	x	x
02000E	2000	3.5	1.7	5.2	13	24.5	0.0292	0.0218	0.0123	0.0079	57.88	63.76
02000F	2000	3.1	1.2	4.3	13	21.5	0.0263	0.0136	Synchrotron measurement			
02000G	2000	2.9	1.3	4.2	14	20.0	0.0195	0.0118	0.0096	0.0074	50.77	37.29
02000H	2000	x	x	x	x	x	x	x	x	x	x	x
02000I	2000	2.8	0.9	3.7	12	21.5	0.0216	0.0116	0.0106	0.0075	50.93	35.34
02000_sum	2000	18.6	7.1	25.7	78.0	132.0	0.1438	0.0919	0.0541	0.0390	268.05	232.54
02000_mean	2000	3.1	1.2	4.3	13.0	22.0	0.0240	0.0153	0.0108	0.0078	53.61	46.51
02000_SD	2000	0.2	0.3	0.5	0.6	1.7	0.0036	0.0044	0.0011	0.0006	2.93	15.38
05000A	5000	2.6	1.5	4.1	13	11.0	0.0168	0.0090	0.0095	0.0060	43.45	33.33
05000B	5000	2.4	1.4	3.8	11	11.5	0.0186	0.0099	0.0083	0.0061	55.38	38.38
05000C	5000	2.8	1.2	4	13	15.5	0.0213	0.0149	0.0135	0.0074	36.62	50.34
05000D	5000	2.8	1.6	4.4	13	10.0	0.0196	0.0096	Synchrotron measurement			
05000E	5000	2.6	1.3	3.9	13	13.5	0.0209	0.0125	0.0104	0.0054	50.24	56.80
05000F	5000	x	x	x	13	x	x	x	x	x	x	x
05000G	5000	2.8	1.5	4.3	13	10.0	0.0190	0.0084	0.0078	0.0052	58.95	38.10
05000H	5000	2.3	0.7	3	12	12.0	0.0168	0.0149	0.0079	0.0061	52.98	59.06
05000I	5000	2.8	1.6	4.4	13	11.5	0.0242	0.0129	0.0098	0.0073	59.50	43.41
05000_sum	5000	21.1	10.8	31.9	114.0	95.0	0.1572	0.0921	0.0672	0.0435	357.12	319.42
05000_mean	5000	2.6	1.4	4.0	12.7	11.9	0.0197	0.0115	0.0096	0.0062	51.02	45.63
05000_SD	5000	0.2	0.3	0.5	0.7	1.8	0.0025	0.0026	0.0020	0.0009	8.40	9.94
10000A	10000	x	x	x	x	x	x	x	x	x	x	x
10000B	10000	2.5	1.2	3.7	12	8.0	0.0236	0.0273	0.0119	0.0112	49.58	58.97
10000C	10000	2.3	1.3	3.6	12	6.5	0.0199	0.0094	0.0090	0.0054	54.77	42.55
10000D	10000	1.3	1.1	2.4	10	8.5	0.0256	0.0178	Synchrotron measurement			
10000E	10000	x	x	x	x	x	x	x	x	x	x	x
10000F	10000	2	1.2	3.2	9	6.5	0.0154	0.0352	0.0071	0.0192	53.90	45.45
10000G	10000	x	x	x	x	x	x	x	x	x	x	x
10000H	10000	2.5	1.4	3.9	9	10.0	0.0325	0.0191	0.0135	0.0064	58.46	66.49
10000I	10000	2.6	1.3	3.9	10	9.0	0.0265	0.0102	0.0136	0.0067	48.68	34.31
10000_sum	10000	13.2	7.5	20.7	62.0	48.5	0.1435	0.1190	0.0551	0.0489	265.39	247.79
10000_mean	10000	2.2	1.3	3.5	10.3	8.1	0.0239	0.0198	0.0110	0.0098	53.08	49.56
10000_SD	10000	0.5	0.1	0.6	1.4	1.4	0.0059	0.0100	0.0029	0.0057	4.00	12.98

Table C.3.: C plant growth data Na_2SeO_3 , goethite (Planting Date: 15.05.2014)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
00000A	0	4.5	1.8	6.3	14	20.0	0.0398	0.0114	0.0094	0.0056	76.38	50.88
00000B	0	3.8	1.4	5.2	11	20.5	0.0359	0.0176	0.0102	0.0067	71.59	61.93
00000C	0	3.7	1.4	5.1	13	24.4	0.0436	0.0132	0.0110	0.0075	74.77	43.18
00000D	0	3.4	1.3	4.7	12	20.5	0.0311	0.0069	0.0076	0.0051	75.56	26.09
00000E	0	4.6	1.8	6.4	14	24.0	0.0480	0.0137	0.0122	0.0067	74.58	51.09
00000F	0	4.3	1.8	6.1	14	23.5	0.0463	0.0102	0.0119	0.0074	74.30	27.45
00000G	0	4.6	1.9	6.5	14	20.5	0.0398	0.0145	0.0103	0.0059	74.12	59.31
00000H	0	4.1	1.8	5.9	14	22.0	0.0328	0.0090	0.0094	0.0057	71.34	36.67
00000I	0	4.5	1.8	6.3	14	25.0	0.0395	0.0151	0.0123	0.0066	68.86	56.29
00000_sum	0	37.5	15.0	52.5	120.0	200.4	0.3568	0.1116	0.0943	0.0572	661.51	412.89
00000_mean	0	4.2	1.7	5.8	13.3	22.3	0.0396	0.0124	0.0105	0.0064	73.50	45.88
00000_SD	0	0.4	0.2	0.7	1.1	2.0	0.0057	0.0033	0.0016	0.0008	2.40	13.33
00020A	20	5.9	3.4	9.3	11	16.5	0.0267	0.0083	0.0065	0.0042	75.66	49.40
00020B	20	x	x	x	x	x	x	x	x	x	x	x
00020C	20	3.0	1.0	4.0	11	27.0	0.0516	0.0172	0.0118	0.0064	77.13	62.79
00020D	20	4.2	1.7	5.9	14	25.0	0.0411	0.0081	0.0091	0.0054	77.86	33.33
00020E	20	3.1	1.1	4.2	11	22.5	0.0242	0.0069	0.0084	0.0049	65.29	28.99
00020F	20	x	x	x	x	x	x	x	x	x	x	x
00020G	20	3.4	1.3	4.7	11	25.0	0.0518	0.0138	0.0113	0.0060	78.19	56.52
00020H	20	4.2	1.7	5.9	14	25.5	0.0472	0.0077	0.0151	0.0054	68.01	29.87
00020I	20	4.1	1.8	5.9	14	24.5	0.0479	0.0186	0.0127	0.0062	73.49	66.67
00020_sum	20	27.9	12.0	39.9	86.0	166.0	0.2905	0.0806	0.0749	0.0385	515.62	327.57
00020_mean	20	4.0	1.7	5.7	12.3	23.7	0.0415	0.0115	0.0107	0.0055	73.66	46.80
00020_SD	20	1.0	0.8	1.8	1.6	3.5	0.0115	0.0049	0.0029	0.0008	5.10	16.01
00050A	50	x	x	x	x	x	x	x	x	x	x	x
00050B	50	4.1	1.7	5.8	14	23.5	0.0467	0.0144	0.0131	0.0069	71.95	52.08
00050C	50	4.5	2.1	6.6	14	23.5	0.0537	0.0182	0.0127	0.0067	76.35	63.19
00050D	50	4.5	1.7	6.2	14	23.5	0.0565	0.0133	0.0128	0.0071	77.35	46.62
00050E	50	3.8	1.5	5.3	11	23.0	0.0410	0.0171	0.0110	0.0068	73.17	60.23
00050F	50	4.2	1.8	6.0	14	19.0	0.0324	0.0117	0.0096	0.0052	70.37	55.56
00050G	50	4.0	2.4	6.4	11	18.5	0.0268	0.0093	0.0072	0.0049	73.13	47.31
00050H	50	4.0	1.8	5.8	13	22.5	0.0498	0.0121	0.0117	0.0063	76.51	47.93
00050I	50	3.7	1.0	4.7	11	24.5	0.0324	0.0153	0.0093	0.0056	71.30	63.40
00050_sum	50	32.8	14.0	46.8	102.0	178.0	0.3393	0.1114	0.0874	0.0495	590.12	436.32
00050_mean	50	4.1	1.8	5.9	12.8	22.3	0.0424	0.0139	0.0109	0.0062	73.77	54.54
00050_SD	50	0.3	0.4	0.6	1.5	2.2	0.0110	0.0029	0.0021	0.0008	2.64	7.09
00100A	100	3.8	1.6	5.4	14	26.0	0.0317	0.0073	0.0107	0.0051	66.25	30.14
00100B	100	4.1	1.8	5.9	14	21.5	0.0336	0.0103	0.0100	0.0052	70.24	49.51
00100C	100	2.6	0.7	3.3	11	19.5	0.0144	0.0096	0.0046	0.0077	68.06	19.79
00100D	100	4.5	1.7	6.2	14	24.5	0.0371	0.0111	0.0107	0.0062	71.16	44.14
00100E	100	3.7	1.9	5.6	12	24.0	0.0418	0.0159	0.0115	0.0066	72.49	58.49
00100F	100	3.4	1.0	4.4	11	24.5	0.0345	0.0076	0.0097	0.0056	71.88	26.32
00100G	100	4.2	1.8	6.0	13	21.5	0.0338	0.0099	0.0099	0.0051	70.71	48.48
00100H	100	3.4	1.2	4.6	11	24.0	0.0332	0.0123	0.0093	0.0052	71.99	57.72
00100I	100	4.0	1.5	5.5	14	25.5	0.0454	0.0120	0.0126	0.0063	72.25	47.50
00100_sum	100	33.7	13.2	46.9	114.0	211.0	0.3055	0.0960	0.0890	0.0530	635.02	382.10
00100_mean	100	3.7	1.5	5.2	12.7	23.4	0.0339	0.0107	0.0099	0.0059	70.56	42.46
00100_SD	100	0.6	0.4	0.9	1.4	2.1	0.0086	0.0026	0.0022	0.0009	2.11	13.83
00200A	200	4.2	1.8	6.0	14	21.5	0.0414	0.0109	0.0114	0.0077	72.46	29.36
00200B	200	x	x	x	x	x	x	x	x	x	x	x
00200C	200	3.8	1.1	4.9	11	18.0	0.0288	0.0171	0.0098	0.0065	65.97	61.99
00200D	200	3.0	1.2	4.2	11	16.5	0.0154	0.0121	0.0056	0.0105	63.64	13.22
00200E	200	3.9	1.3	5.2	12	20.0	0.0433	0.0135	0.0102	0.0069	76.44	48.89
00200F	200	4.3	1.9	6.2	14	25.0	0.0389	0.0149	0.0113	0.0067	70.95	55.03
00200G	200	4.4	1.9	6.3	14	21.0	0.0421	0.0121	0.0116	0.0060	72.45	50.41
00200H	200	3.2	1.1	4.3	11	23.0	0.0365	0.0176	0.0101	0.0057	72.33	67.61
00200I	200	x	x	x	x	x	x	x	x	x	x	x
00200_sum	200	26.8	10.3	37.1	87.0	145.0	0.2464	0.0982	0.0700	0.0500	494.24	326.52
00200_mean	200	3.8	1.5	5.3	12.4	20.7	0.0352	0.0140	0.0100	0.0071	70.61	46.65
00200_SD	200	0.5	0.4	0.9	1.5	2.9	0.0100	0.0026	0.0021	0.0016	4.36	19.606
00500A	500	3.4	1.4	4.8	12	23.5	0.0405	0.0188	0.0099	0.0064	75.56	65.96
00500B	500	4.4	1.8	6.2	14	20.5	0.0447	0.0160	0.0113	0.0068	74.72	57.50
00500C	500	4.4	2.0	6.4	14	20.5	0.0296	0.0105	0.0091	0.0047	69.26	55.24
00500D	500	3.9	1.5	5.4	14	25.5	0.0571	0.0130	0.0139	0.0076	75.66	41.54
00500E	500	4.1	2.0	6.1	14	21.0	0.0358	0.0125	0.0105	0.0056	70.67	55.20
00500F	500	4.0	1.7	5.7	14	22.0	0.0389	0.0093	0.0098	0.0050	74.81	46.24
00500G	500	4.2	1.9	6.1	14	24.5	0.0465	0.0081	0.0109	0.0057	76.56	29.63
00500H	500	x	x	x	x	x	x	x	x	x	x	x
00500I	500	3.7	2.0	5.7	11	21.0	0.0306	0.0151	0.0083	0.0045	72.88	70.20
00500_sum	500	32.1	14.3	46.4	107.0	178.5	0.3237	0.1033	0.0837	0.0463	590.10	421.50
00500_mean	500	4.0	1.8	5.8	13.4	22.3	0.0405	0.0129	0.0105	0.0058	73.76	52.69
00500_SD	500	0.3	0.2	0.5	1.2	1.9	0.0090	0.0036	0.0017	0.0011	2.60	13.18

Table C.4.: C plant growth data Na_2SeO_3 , goethite (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
01000A	1000	3.4	1.0	4.4	11	21.0	0.0287	0.0136	0.0089	0.0057	68.99	58.09
01000B	1000	3.7	1.6	5.3	14	23.5	0.0349	0.0132	0.0118	0.0056	66.19	57.58
01000C	1000	3.9	1.7	5.6	14	25.0	0.0351	0.0161	0.0112	0.0065	68.09	59.63
01000D	1000	4.1	1.9	6.0	13	23.5	0.0460	0.0150	0.0124	0.0065	73.04	56.67
01000E	1000	3.4	1.3	4.7	11	19.5	0.0217	0.0121	0.0083	0.0055	61.75	54.55
01000F	1000	3.3	1.0	4.3	11	21.5	0.0271	0.0118	0.0095	0.0062	64.94	47.46
01000G	1000	4.5	2.1	6.6	14	22.5	0.0296	0.0083	0.0114	0.0064	61.49	22.89
01000H	1000	x	x	x	x	x	x	x	x	x	x	x
01000I	1000	3.2	1.1	4.3	13	23.5	0.0303	0.0085	0.0096	0.0053	68.32	37.65
01000_sum	1000	29.5	11.7	41.2	101.0	180.0	0.2534	0.0986	0.0831	0.0477	532.81	394.50
01000_mean	1000	3.7	1.5	5.2	12.6	22.5	0.0317	0.0123	0.0104	0.0060	66.60	49.31
01000_SD	1000	0.5	0.4	0.9	1.4	1.8	0.0072	0.0028	0.0015	0.0005	3.87	12.193
02000A	2000	4.3	2.0	6.3	13	28.0	0.0440	0.0161	0.0154	0.0078	65.00	51.55
02000B	2000	4.0	1.5	5.5	13	25.0	0.0472	0.0126	0.0137	0.0072	70.97	42.86
02000C	2000	4.8	2.1	6.9	14	24.5	0.0415	0.0111	0.0132	0.0074	68.19	33.33
02000D	2000	3.2	1.2	4.4	11	24.0	0.0314	0.0126	0.0097	0.0062	69.11	50.79
02000E	2000	2.0	3.6	5.6	11	23.0	0.0297	0.0093	0.0089	0.0054	70.03	41.94
02000F	2000	4.1	2.6	6.7	11	14.5	0.0115	0.0097	0.0540	0.0066	53.04	31.96
02000G	2000	x	x	x	x	x	x	x	x	x	x	x
02000H	2000	3.2	1.3	4.5	11	18.0	0.0278	0.0100	0.0093	0.0052	66.55	48.00
02000I	2000	4.2	1.8	6.0	14	20.5	0.0319	0.0128	0.0114	0.0072	64.26	43.75
02000_sum	2000	29.8	16.1	45.9	98.0	177.5	0.2650	0.0942	0.0870	0.0530	512.16	344.18
02000_mean	2000	3.7	2.0	5.7	12.3	22.2	0.0331	0.0128	0.0109	0.0066	65.90	43.02
02000_SD	2000	0.9	0.8	0.9	1.4	4.3	0.0113	0.0022	0.0032	0.0010	5.70	7.33
05000A	5000	4.3	1.9	6.2	13	20.0	0.0370	0.0138	0.0106	0.0060	71.35	56.52
05000B	5000	4.2	1.9	6.1	13	23.0	0.0394	0.0193	0.0126	0.0068	68.02	64.77
05000C	5000	2.5	1.2	3.7	11	24.5	0.0350	0.0083	0.0106	0.0058	69.71	30.12
05000D	5000	4.2	1.3	5.5	14	21.5	0.0404	0.0173	0.0108	0.0067	73.27	61.27
05000E	5000	4.4	2.0	6.4	13	20.0	0.0251	0.0122	0.0084	0.0044	66.53	63.93
05000F	5000	4.3	1.8	6.1	13	19.5	0.0298	0.0066	0.0103	0.0054	65.44	18.18
05000G	5000	4.1	1.9	6.0	13	20.5	0.0702	0.0137	0.0111	0.0063	84.19	54.01
05000H	5000	3.5	1.2	4.7	11	22.0	0.0286	0.0117	0.0095	0.0060	66.78	48.72
05000I	5000	4.0	1.8	5.8	13	19.5	0.0292	0.0124	0.0101	0.0053	65.41	57.26
05000_sum	5000	35.5	15.0	50.5	114.0	190.5	0.3347	0.1153	0.0940	0.0527	630.71	454.79
05000_mean	5000	3.9	1.7	5.6	12.7	21.2	0.0372	0.0128	0.0104	0.0059	70.08	50.53
05000_SD	5000	0.6	0.3	0.9	1.0	1.7	0.0135	0.0039	0.0011	0.0007	5.94	16.04
10000A	10000	4.3	1.9	6.2	14	24.0	0.0390	0.0174	0.0123	0.0068	68.46	60.92
10000B	10000	4.4	2.0	6.4	14	23.0	0.0493	0.0180	0.0132	0.0069	73.23	61.67
10000C	10000	4.1	1.9	6.0	14	19.5	0.0339	0.0097	0.0096	0.0051	71.68	47.42
10000D	10000	4.4	1.8	6.2	14	20.5	0.0311	0.0154	0.0099	0.0061	68.17	60.39
10000E	10000	4.1	2.0	6.1	14	21.5	0.0450	0.0148	0.0115	0.0064	74.44	56.76
10000F	10000	4.3	1.7	6.0	13	23.5	0.0467	0.0247	0.0132	0.0067	71.73	72.87
10000G	10000	4.4	1.8	6.2	13	21.5	0.0345	0.0127	0.0105	0.0057	69.57	55.12
10000H	10000	4.3	1.9	6.2	14	23.5	0.0465	0.0125	0.0128	0.0063	72.47	49.60
10000I	10000	4.0	1.6	5.6	14	24.5	0.0438	0.0122	0.0125	0.0063	71.46	48.36
10000_sum	10000	38.3	16.6	54.9	124.0	201.5	0.3698	0.1374	0.1055	0.0563	641.21	513.11
10000_mean	10000	4.3	1.8	6.1	13.8	22.4	0.0411	0.0153	0.0117	0.0063	71.25	57.01
10000_SD	10000	0.2	0.1	0.2	0.4	1.7	0.0066	0.0044	0.0014	0.0006	2.13	8.10

Table C.5.: C plant growth data Na_2SeO_4 , kaolinite (Planting Date: 25.03.2014)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
00000A	0	4.2	1.3	5.5	13	30.0	0.0557	0.0164	0.0154	0.0076	72.35	53.66
00000B	0	4.3	1.6	5.9	13	28.5	0.0451	0.0178	0.0132	0.0063	70.73	64.61
00000C	0	x	x	x	x	x	x	x	x	x	x	x
00000D	0	4.0	1.6	5.6	13	26.5	0.0356	0.0096	0.0118	0.0055	66.85	42.71
00000E	0	4.5	1.7	6.2	13	26.5	0.0448	0.0189	Synchrotron measurement			
00000F	0	3.0	1.0	4.0	12	28.5	0.0349	0.0074	0.0109	0.0064	68.77	13.51
00000G	0	4.1	1.4	5.5	13	25.5	0.0283	0.0073	0.0104	0.0058	63.25	20.55
00000H	0	3.8	1.4	5.2	12	27.5	0.0424	0.0139	0.0131	0.0073	69.10	47.48
00000I	0	3.9	1.3	5.2	13	28.5	0.0353	0.0119	0.0128	0.0066	63.74	44.54
00000_sum	0	31.8	11.3	43.1	102.0	221.5	0.3221	0.1032	0.0876	0.0455	474.80	287.05
00000_mean	0	4.0	1.4	5.4	12.8	27.7	0.0403	0.0129	0.0125	0.0065	67.83	41.01
00000_SD	0	0.5	0.2	0.7	0.5	1.5	0.0085	0.0046	0.0017	0.0008	3.42	18.02
00020A	20	3.3	1.2	4.5	11	20.0	0.0225	0.0134	0.0086	0.0056	61.78	58.21
00020B	20	5.2	1.6	6.8	13	27.0	0.0443	0.0194	0.0152	0.0061	65.69	68.56
00020C	20	5.1	1.8	6.9	13	24.0	0.0414	0.0144	0.0133	0.0057	67.87	60.42
00020D	20	5.2	1.8	7.0	12	21.5	0.0275	0.0111	0.0107	0.0050	61.09	54.95
00020E	20	4.5	1.5	6.0	13	25.0	0.0395	0.0100	Synchrotron measurement			
00020F	20	4.6	1.7	6.3	13	26.0	0.0359	0.0120	0.0133	0.0063	62.95	47.50
00020G	20	x	x	x	x	x	x	x	x	x	x	x
00020H	20	4.6	1.9	6.5	12	21.0	0.0293	0.0155	0.0107	0.0062	63.48	60.00
00020I	20	4.6	1.7	6.3	13	26.5	0.0394	0.0129	0.0138	0.0058	64.97	55.04
00020_sum	20	37.1	13.2	50.3	100.0	191.0	0.2798	0.1087	0.0856	0.0407	447.84	404.68
00020_mean	20	4.6	1.7	6.3	12.5	23.9	0.0350	0.0136	0.0122	0.0058	63.98	57.81
00020_SD	20	0.6	0.2	0.8	0.8	2.7	0.0077	0.0029	0.0023	0.0004	2.37	6.45
00050A	50	4.6	1.5	6.1	13	25.5	0.0434	0.0141	0.0135	0.0064	68.89	54.61
00050B	50	3.1	0.8	3.9	11	20.5	0.0321	0.0139	0.0107	0.0073	66.67	47.48
00050C	50	x	x	x	x	x	x	x	x	x	x	x
00050D	50	4.7	1.8	6.5	13	21.5	0.0336	0.0104	0.0131	0.0061	61.01	41.35
00050E	50	4.5	1.4	5.9	13	20.5	0.0296	0.0106	Synchrotron measurement			
00050F	50	4.7	1.6	6.3	13	20.5	0.0346	0.0107	0.0118	0.0051	65.90	52.34
00050G	50	4.5	1.9	6.4	13	21.5	0.0298	0.0096	0.0088	0.0054	70.47	43.75
00050H	50	4.8	1.5	6.3	13	23.5	0.0364	0.0105	0.0159	0.0062	56.32	40.95
00050I	50	4.9	1.8	6.7	13	26.0	0.0363	0.0179	0.0136	0.0071	62.53	60.34
00050_sum	50	35.8	12.3	48.1	102.0	179.5	0.2758	0.0977	0.0874	0.0436	451.79	340.81
00050_mean	50	4.5	1.5	6.0	12.8	22.4	0.0345	0.0122	0.0125	0.0062	64.54	48.69
00050_SD	50	0.6	0.3	0.9	0.7	2.3	0.0045	0.0028	0.0023	0.0008	4.91	7.34
00100A	100	5.1	1.4	6.5	13	24.0	0.0505	0.0120	0.0123	0.0055	75.64	54.17
00100B	100	5.2	1.7	6.9	13	26.5	0.0540	0.0146	0.0131	0.0058	75.74	60.27
00100C	100	5.4	1.8	7.2	13	22.5	0.0398	0.0134	0.0114	0.0062	71.36	53.73
00100D	100	5.4	1.8	7.2	13	23.0	0.0486	0.0130	0.0123	0.0062	74.69	52.31
00100E	100	5.0	1.6	6.6	13	25.5	0.0467	0.0132	Synchrotron measurement			
00100F	100	5.3	1.9	7.2	13	23.5	0.0409	0.0170	0.0127	0.0055	68.95	67.65
00100G	100	5.1	1.9	7.0	13	27.0	0.0425	0.0168	0.0136	0.0056	68.00	66.67
00100H	100	3.9	1.6	5.5	13	25.5	0.0364	0.0194	0.0107	0.0063	70.60	67.53
00100I	100	5.4	2.0	7.4	12	26.0	0.0412	0.0139	0.0133	0.0065	67.72	53.24
00100_sum	100	45.8	15.7	61.5	116.0	223.5	0.4006	0.1333	0.0994	0.0476	572.70	475.56
00100_mean	100	5.1	1.7	6.8	12.9	24.8	0.0445	0.0148	0.0124	0.0060	71.59	59.44
00100_SD	100	0.5	0.2	0.6	0.3	1.6	0.0057	0.0024	0.0010	0.0004	3.36	6.92
00200A	200	x	x	x	x	x	x	x	x	x	x	x
00200B	200	5.4	1.9	7.3	14	26.5	0.0479	0.0169	0.0149	0.0064	68.89	62.13
00200C	200	x	x	x	x	x	x	x	x	x	x	x
00200D	200	4.9	1.8	6.7	12	26.0	0.0439	0.0221	0.0140	0.0066	68.11	70.14
00200E	200	5.1	1.9	7.0	13	25.0	0.0510	0.0157	Synchrotron measurement			
00200F	200	4.9	1.7	6.6	13	26.0	0.0502	0.0136	0.0149	0.0066	70.32	51.47
00200G	200	7.1	2.6	9.7	11	25.0	0.0268	0.0248	0.0059	0.0066	77.99	73.39
00200H	200	x	x	x	x	x	x	x	x	x	x	x
00200I	200	4.7	1.6	6.3	14	21.5	0.0407	0.0208	0.0124	0.0057	69.53	72.60
00200_sum	200	32.1	11.5	43.6	77.0	150.0	0.2605	0.1139	0.0621	0.0319	354.84	329.72
00200_mean	200	5.4	1.9	7.3	12.8	25.0	0.0434	0.0190	0.0124	0.0064	70.97	65.94
00200_SD	200	0.9	0.4	1.2	1.2	1.8	0.0090	0.0043	0.0038	0.0004	4.01	9.24
00500A	500	3.9	1.4	5.3	13	21.0	0.0630	0.0199	0.0115	0.0061	81.75	69.35
00500B	500	4.5	1.7	6.2	13	23.0	0.0721	0.0151	0.0138	0.0059	80.86	60.93
00500C	500	4.2	1.6	5.8	13	23.5	0.0750	0.0224	0.0136	0.0055	81.87	75.45
00500D	500	4.1	1.3	5.4	13	23.0	0.0686	0.0154	0.0135	0.0062	80.32	59.74
00500E	500	4.3	1.2	5.5	13	22.0	0.0638	0.0138	Synchrotron measurement			
00500F	500	4.1	1.3	5.4	13	23.5	0.0736	0.0170	0.0134	0.0056	81.79	67.06
00500G	500	3.4	1.1	4.5	11	19.5	0.0312	0.0260	0.0066	0.0117	78.85	55.00
00500H	500	x	x	x	x	x	x	x	x	x	x	x
00500I	500	4.2	1.2	5.4	13	23.5	0.0706	0.0170	0.0134	0.0064	81.02	62.35
00500_sum	500	32.7	10.8	43.5	102.0	179.0	0.5179	0.1466	0.0858	0.0474	566.45	449.87
00500_mean	500	4.1	1.4	5.4	12.8	22.4	0.0647	0.0183	0.0123	0.0068	80.92	64.27
00500_SD	500	0.3	0.2	0.5	0.7	1.5	0.0142	0.0042	0.0026	0.0022	1.08	6.83

Table C.6.: C plant growth data Na_2SeO_4 , kaolinite (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
01000A	1000	4.1	1.7	5.8	12	20.5	0.0520	0.0196	0.0098	0.0052	81.15	73.47
01000B	1000	4.1	1.1	5.2	13	26.0	0.0518	0.0861	0.0145	0.0057	72.01	93.38
01000C	1000	x	x	x	x	x	x	x	x	x	x	x
01000D	1000	x	x	x	x	x	x	x	x	x	x	x
01000E	1000	5.1	0.9	6.0	13	21.5	0.0634	0.0167	Synchrotron measurement			
01000F	1000	4.3	1.7	6.0	13	22.0	0.0748	0.0247	0.0132	0.0057	82.35	76.92
01000G	1000	4.3	1.7	6.0	14	26.0	0.0709	0.0190	0.0136	0.0060	80.82	68.42
01000H	1000	4.2	1.6	5.8	13	24.5	0.0781	0.0127	0.0127	0.0054	83.74	57.48
01000I	1000	4.1	1.5	5.6	12	24.5	0.0695	0.0199	0.0128	0.0055	81.58	72.36
01000_sum	1000	30.2	10.2	40.4	90.0	165.0	0.4605	0.1987	0.0766	0.0335	481.65	442.04
01000_mean	1000	4.3	1.5	5.8	12.9	23.6	0.0658	0.0284	0.0128	0.0056	80.28	73.67
01000_SD	1000	0.4	0.3	0.3	0.7	2.2	0.0105	0.0257	0.0016	0.0003	4.18	11.75
02000A	2000	5.2	1.6	6.8	13	23.0	0.0511	0.0144	0.0111	0.0050	78.28	65.28
02000B	2000	5.2	1.9	7.1	14	24.0	0.0603	0.0195	0.0122	0.0057	79.77	70.77
02000C	2000	x	x	x	x	x	x	x	x	x	x	x
02000D	2000	3.5	1.2	4.7	10	19.0	0.0523	0.0179	0.0096	0.0053	81.64	70.39
02000E	2000	5.0	1.8	6.8	14	24.5	0.0782	0.0256	Synchrotron measurement			
02000F	2000	2.6	1.1	3.7	11	25.5	0.0712	0.0275	0.0126	0.0076	82.30	72.36
02000G	2000	4.8	1.9	6.7	13	27.5	0.0984	0.0279	0.0186	0.0073	81.10	73.84
02000H	2000	5.2	1.6	6.8	13	25.5	0.0788	0.0148	0.0145	0.0059	81.60	60.14
02000I	2000	5.0	1.6	6.6	13	21.5	0.0641	0.0145	0.0134	0.0059	79.10	59.31
02000_sum	2000	36.5	12.7	49.2	101.0	190.5	0.5544	0.1621	0.0920	0.0427	563.79	472.08
02000_mean	2000	4.6	1.6	6.2	12.6	23.8	0.0693	0.0203	0.0131	0.0061	80.54	67.44
02000_SD	2000	1.0	0.3	1.2	1.4	2.6	0.0158	0.0059	0.0029	0.0010	1.50	5.90
05000A	5000	3.6	1.6	5.2	11	24.5	0.0684	0.0297	0.0131	0.0074	80.85	75.08
05000B	5000	1.6	0.8	2.4	10	12.5	0.0213	0.0182	0.0047	0.0037	77.93	79.67
05000C	5000	4.2	1.6	5.8	13	18.5	0.0589	0.0165	0.0116	0.0062	80.31	62.42
05000D	5000	3.9	1.3	5.2	13	19.0	0.0531	0.0209	0.0117	0.0069	77.97	66.99
05000E	5000	4.4	2.0	6.4	13	22.5	0.0797	0.0210	Synchrotron measurement			
05000F	5000	3.5	1.4	4.9	13	17.5	0.0525	0.0222	0.0101	0.0066	80.76	70.27
05000G	5000	x	x	x	x	x	x	x	x	x	x	x
05000H	5000	4.1	1.5	5.6	13	21.5	0.0732	0.0214	0.0144	0.0064	80.33	70.09
05000I	5000	4.4	1.5	5.9	13	21.0	0.0552	0.0176	0.0127	0.0061	76.99	65.34
05000_sum	5000	29.7	11.7	41.4	99.0	157.0	0.4623	0.1675	0.0783	0.0433	555.14	489.87
05000_mean	5000	3.7	1.5	5.2	12.4	19.6	0.0578	0.0209	0.0112	0.0062	79.31	69.98
05000_SD	5000	0.9	0.3	1.2	1.2	3.7	0.0178	0.0041	0.0032	0.0012	1.61	5.88
10000A	10000	3.8	1.1	4.9	13	18.5	0.0498	0.0204	0.0116	0.0049	76.71	75.98
10000B	10000	3.7	1.1	4.8	13	16.0	0.0474	0.0189	0.0117	0.0057	75.32	69.84
10000C	10000	3.9	1.4	5.3	13	14.5	0.0339	0.0113	0.0084	0.0039	75.22	65.49
10000D	10000	x	x	x	x	x	x	x	x	x	x	x
10000E	10000	4.0	1.9	5.9	12	18.0	0.0584	0.0584	Synchrotron measurement			
10000F	10000	3.7	1.2	4.9	13	19.5	0.0525	0.0525	0.0131	0.0052	75.05	90.10
10000G	10000	3.5	1.4	4.9	12	16.0	0.0385	0.0385	0.0095	0.0042	75.32	89.09
10000H	10000	3.6	1.2	4.8	13	16.0	0.0425	0.0425	0.0122	0.0045	71.29	89.41
10000I	10000	3.6	1.5	5.1	12	13.0	0.0365	0.0365	0.0095	0.0045	73.97	87.67
10000_sum	10000	29.8	10.8	40.6	101.0	131.5	0.3595	0.2790	0.0760	0.0329	522.88	567.58
10000_mean	10000	3.7	1.4	5.1	12.6	16.4	0.0449	0.0349	0.0109	0.0047	74.70	81.08
10000_SD	10000	0.2	0.3	0.4	0.5	2.1	0.0085	0.0167	0.0017	0.0006	1.70	10.44

Table C.7.: C plant growth data Na_2SeO_4 , goethite (Planting Date: 25.03.2014)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	shoot FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
00000A	0	4.7	2.0	6.7	13	21.0	0.0483	0.0111	0.0114	0.0059	76.40	46.85
00000B	0	4.8	2.0	6.8	13	22.5	0.0451	0.0118	0.0105	0.0045	76.72	61.86
00000C	0	4.7	1.9	6.6	11	21.0	0.0573	0.0198	0.0122	0.0079	78.71	60.10
00000D	0	4.2	1.7	5.9	13	20.5	0.0431	0.0089	0.0102	0.0065	76.33	26.97
00000E	0	x	x	x	x	x	x	x	x	x	x	x
00000F	0	4.4	1.6	6.0	13	20.5	0.0472	0.0144	0.0129	0.0069	72.67	52.08
00000G	0	4.5	1.9	6.4	13	21.5	0.0316	0.0062	0.0076	0.0038	75.95	38.71
00000H	0	3.2	1.0	4.2	10	21.0	0.0350	0.0144	0.0098	0.0073	72.00	49.31
00000I	0	4.5	1.7	6.2	13	21.5	0.0475	0.0143	0.0102	0.0073	78.53	48.95
00000_sum	0	35.0	13.8	48.8	99.0	169.5	0.3551	0.1009	0.0848	0.0501	607.30	384.83
00000_mean	0	4.4	1.7	6.1	12.4	21.2	0.0444	0.0126	0.0106	0.0063	75.91	48.10
00000_SD	0	0.5	0.3	0.8	1.2	0.7	0.0080	0.0041	0.0016	0.0014	2.44	11.26
00020A	20	3.1	1.2	4.3	11	21.5	0.0375	0.0137	0.0099	0.0075	73.60	45.26
00020B	20	4.1	1.9	6.0	12	21.0	0.0413	0.0164	0.0110	0.0052	73.37	68.29
00020C	20	2.9	1.1	4.0	10	22.5	0.0352	0.0079	0.0098	0.0059	72.16	25.32
00020D	20	4.2	1.9	6.1	12	20.5	0.0430	0.0106	0.0101	0.0071	76.51	33.02
00020E	20	4.3	1.9	6.2	12	22.0	0.0407	0.0131	0.0120	0.0084	70.52	35.88
00020F	20	3.2	1.1	4.3	10	22.0	0.0269	0.0081	0.0082	0.0054	69.52	33.33
00020G	20	2.7	0.9	3.6	10	22.5	0.0352	0.0110	0.0106	0.0064	69.89	41.82
00020H	20	3.7	1.7	5.4	11	22.0	0.0339	0.0108	0.0109	0.0081	67.85	25.00
00020I	20	3.2	1.1	4.3	10	23.0	0.0410	0.0152	0.0109	0.0075	73.41	50.66
00020_sum	20	31.4	12.8	44.2	98.0	197.0	0.3347	0.1068	0.0934	0.0615	646.82	358.57
00020_mean	20	3.5	1.4	4.9	10.9	21.9	0.0372	0.0119	0.0104	0.0068	71.87	39.84
00020_SD	20	0.6	0.4	1.0	0.9	0.8	0.0050	0.0030	0.0011	0.0012	2.66	13.67
00050A	50	2.9	1.7	4.6	8	21.0	0.0390	0.0083	0.0083	0.0049	78.72	40.96
00050B	50	3.1	1.6	4.7	9	19.5	0.0375	0.0181	0.0079	0.0051	78.93	71.82
00050C	50	2.7	1.2	3.9	9	20.0	0.0317	0.0097	0.0069	0.0050	78.23	48.45
00050D	50	x	x	x	x	x	x	x	x	x	x	x
00050E	50	2.8	1.4	4.2	9	21.5	0.0432	0.0166	0.0088	0.0064	79.63	61.45
00050F	50	3.5	1.5	5.0	10	23.0	0.0592	0.0185	0.0136	0.0063	77.03	65.95
00050G	50	3.3	2.0	5.3	10	18.5	0.0387	0.0089	0.0074	0.0036	80.88	59.55
00050H	50	3.0	1.6	4.6	9	19.5	0.0398	0.0155	0.0087	0.0055	78.14	64.52
00050I	50	3.7	1.9	5.6	10	23.5	0.0397	0.0179	0.0107	0.0056	73.05	68.72
00050_sum	50	25.0	12.9	37.9	74.0	166.5	0.3288	0.1155	0.0723	0.0424	624.61	481.41
00050_mean	50	3.1	1.6	4.7	9.3	20.8	0.0411	0.0142	0.0090	0.0053	78.08	60.18
00050_SD	50	0.3	0.3	0.6	0.7	1.8	0.0080	0.0044	0.0022	0.0009	2.32	10.48
00100A	100	x	x	x	x	x	x	x	x	x	x	x
00100B	100	4.1	1.6	5.7	12	20.5	0.0474	0.0190	0.0104	0.0066	78.06	65.26
00100C	100	4.1	2.0	6.1	12	18.5	0.0396	0.0194	0.0092	0.0061	76.77	68.56
00100D	100	4.0	1.9	5.9	12	17.5	0.0370	0.0074	0.0075	0.0038	79.73	48.65
00100E	100	1.6	1.0	2.6	10	23.5	0.0449	0.0201	0.0095	0.0062	78.84	69.15
00100F	100	4.0	1.6	5.6	12	21.5	0.0457	0.0106	0.0103	0.0061	77.46	42.45
00100G	100	3.6	1.5	5.1	10	19.0	0.0385	0.0141	0.0081	0.0049	78.96	65.25
00100H	100	x	x	x	x	x	x	x	x	x	x	x
00100I	100	3.7	1.5	5.2	12	21.5	0.0404	0.0151	0.0091	0.0061	77.48	59.60
00100_sum	100	25.1	11.1	36.2	80.0	142.0	0.2935	0.1057	0.0641	0.0398	547.30	418.93
00100_mean	100	3.6	1.6	5.2	11.4	20.3	0.0419	0.0151	0.0092	0.0057	78.19	59.85
00100_SD	100	0.9	0.3	1.2	1.0	2.1	0.0040	0.0048	0.0011	0.0010	1.04	10.40
00200A	200	4.1	1.5	5.6	13	21.5	0.0571	0.0182	0.0101	0.0064	82.31	64.84
00200B	200	4.2	1.6	5.8	13	22.5	0.0625	0.0174	0.0117	0.0074	81.28	57.47
00200C	200	4.5	1.8	6.3	13	20.5	0.0575	0.0199	0.0108	0.0057	81.22	71.36
00200D	200	4.2	1.7	5.9	13	21.0	0.0697	0.0172	0.0109	0.0061	84.36	64.53
00200E	200	4.1	1.6	5.7	12	20.5	0.0528	0.0252	0.0104	0.0073	80.30	71.03
00200F	200	4.1	1.6	5.7	12	20.0	0.0428	0.0151	0.0090	0.0036	78.97	76.16
00200G	200	3.1	1.0	4.1	10	17.5	0.0350	0.0176	0.0086	0.0056	75.43	68.18
00200H	200	4.1	2.1	6.2	12	20.0	0.0318	0.0171	0.0084	0.0051	73.58	70.18
00200I	200	3.5	1.4	4.9	10	19.5	0.0342	0.0146	0.0089	0.0067	73.98	54.11
00200_sum	200	35.9	14.3	50.2	108.0	183.0	0.4434	0.1623	0.0888	0.0539	711.44	597.86
00200_mean	200	4.0	1.6	5.6	12.0	20.3	0.0493	0.0180	0.0099	0.0060	79.05	66.43
00200_SD	200	0.4	0.3	0.7	1.2	1.4	0.0137	0.0031	0.0012	0.0012	3.85	7.03
00500A	500	3.7	1.9	5.6	11	17.5	0.0392	0.0093	0.0084	0.0043	78.57	53.76
00500B	500	2.6	1.1	3.7	10	21.0	0.0391	0.0136	0.0078	0.0041	80.05	69.85
00500C	500	3.3	1.5	4.8	10	16.5	0.0342	0.0158	0.0058	0.0083	83.04	47.47
00500D	500	3.5	1.7	5.2	10	20.0	0.0543	0.0149	0.0094	0.0056	82.69	62.42
00500E	500	3.6	1.6	5.2	11	19.0	0.0389	0.0113	0.0074	0.0050	80.98	55.75
00500F	500	3.8	1.9	5.7	11	18.5	0.0377	0.0115	0.0091	0.0049	75.86	57.39
00500G	500	2.4	1.0	3.4	9	16.5	0.0340	0.0116	0.0078	0.0024	77.06	79.31
00500H	500	2.6	1.2	3.8	10	19.0	0.0324	0.0125	0.0075	0.0051	76.85	59.20
00500I	500	3.1	1.6	4.7	10	20.5	0.0488	0.0132	0.0102	0.0054	79.10	59.09
00500_sum	500	28.6	13.5	42.1	92.0	168.5	0.3586	0.1137	0.0734	0.0451	714.20	544.25
00500_mean	500	3.2	1.5	4.7	10.2	18.7	0.0398	0.0126	0.0082	0.0050	79.36	60.47
00500_SD	500	0.5	0.3	0.9	0.7	1.6	0.0072	0.0020	0.0013	0.0016	2.56	9.33

Table C.8.: C plant growth data Na_2SeO_4 , goethite (continued from previous page)

ID Seedling	c(Se) [ppb]	2 nd leaf sheath [cm] [± 0.1]	2 nd leaf blade leaf [cm] [± 0.1]	2 nd leaf total [cm] [± 0.1]	uptake time [days] [± 0.5]	shoot height (Day 19) [cm] [± 0.25]	shoot FW [g] [± 0.0001]	root FW [g] [± 0.0001]	shoot DW [g] [± 0.0001]	root DW [g] [± 0.0001]	shoot water [%]	root water [%]
01000A	1000	4.2	1.7	5.9	13	18.0	0.0481	0.0192	0.0093	0.0050	80.67	73.96
01000B	1000	4.3	1.6	5.9	13	18.5	0.0609	0.0221	0.0118	0.0072	80.62	67.42
01000C	1000	3.9	1.8	5.7	12	21.0	0.0371	0.0078	0.0075	0.0046	79.78	41.03
01000D	1000	4.4	2.1	6.5	13	20.0	0.0497	0.0213	0.0092	0.0059	81.49	72.30
01000E	1000	4.3	1.9	6.2	13	21.0	0.0423	0.0164	0.0083	0.0048	80.38	70.73
01000F	1000	x	x	x	x	x	x	x	x	x	x	x
01000G	1000	x	x	x	x	x	x	x	x	x	x	x
01000H	1000	3.7	1.5	5.2	11	22.5	0.0457	0.0191	0.0102	0.0046	77.68	75.92
01000I	1000	3.0	1.0	4.0	11	18.5	0.0335	0.0150	0.0073	0.0070	78.21	53.33
01000_sum	1000	27.8	11.6	39.4	86.0	139.5	0.3173	0.1209	0.0636	0.0391	558.83	451.69
01000_mean	1000	4.0	1.7	5.6	12.3	19.9	0.0453	0.0173	0.0091	0.0056	79.83	64.96
01000_SD	1000	0.5	0.4	0.8	1.0	1.7	0.0090	0.0049	0.0016	0.0011	1.39	12.92
02000A	2000	4.1	1.5	5.6	13	20.5	0.0532	0.0201	0.0109	0.0056	79.51	72.14
02000B	2000	3.1	1.2	4.3	13	20.0	0.0426	0.0115	0.0092	0.0042	78.40	63.48
02000C	2000	3.0	1.7	4.7	13	19.5	0.0407	0.0209	0.0070	0.0052	82.80	75.12
02000D	2000	4.3	1.7	6.0	13	23.0	0.0683	0.0154	0.0126	0.0065	81.55	57.79
02000E	2000	x	x	x	x	x	x	x	x	x	x	x
02000F	2000	3.0	1.1	4.1	10	18.5	0.0339	0.0133	0.0066	0.0040	80.53	69.92
02000G	2000	4.1	1.2	5.3	13	19.5	0.0418	0.0121	0.0099	0.0056	76.32	53.72
02000H	2000	4.0	1.8	5.8	13	20.5	0.0398	0.0162	0.0098	0.0061	75.38	62.35
02000I	2000	4.0	1.6	5.6	13	20.0	0.0492	0.0149	0.0141	0.0068	71.34	54.36
02000_sum	2000	29.6	11.8	41.4	101.0	161.5	0.3695	0.1244	0.0801	0.0440	625.83	508.88
02000_mean	2000	3.7	1.5	5.2	12.6	20.2	0.0462	0.0156	0.0100	0.0055	78.23	63.61
02000_SD	2000	0.6	0.3	0.7	1.1	1.3	0.0107	0.0035	0.0026	0.0010	3.74	8.14
05000A	5000	4.3	1.0	5.3	13	22.5	0.0606	0.0147	0.0124	0.0060	79.54	59.18
05000B	5000	3.0	1.2	4.2	10	20.0	0.0332	0.0086	0.0074	0.0035	77.71	59.30
05000C	5000	4.4	1.9	6.3	13	23.0	0.0568	0.0149	0.0110	0.0059	80.63	60.40
05000D	5000	4.2	1.7	5.9	13	21.5	0.0432	0.0199	0.0089	0.0098	79.40	50.75
05000E	5000	x	x	x	10	x	x	x	x	x	x	x
05000F	5000	4.2	2.1	6.3	12	21.5	0.0454	0.0107	0.0095	0.0066	79.07	38.32
05000G	5000	3.0	1.0	4.0	10	22.5	0.0381	0.0141	0.0094	0.0054	75.33	61.70
05000H	5000	3.1	1.0	4.1	10	22.0	0.0442	0.0195	0.0102	0.0061	76.92	68.72
05000I	5000	4.0	1.8	5.8	13	20.0	0.0434	0.0141	0.0096	0.0057	77.88	59.57
05000_sum	5000	30.2	11.7	41.9	104.0	173.0	0.3649	0.1165	0.0784	0.0490	626.49	457.95
05000_mean	5000	3.8	1.5	5.2	11.6	21.6	0.0456	0.0146	0.0098	0.0061	78.31	57.24
05000_SD	5000	0.6	0.5	1.0	1.5	1.1	0.0090	0.0039	0.0015	0.0017	1.69	9.07
10000A	10000	3.8	1.9	5.7	13	18.5	0.0411	0.0156	0.0086	0.0055	79.08	64.74
10000B	10000	4.0	1.8	5.8	12	19.5	0.0517	0.0153	0.0098	0.0052	81.04	66.01
10000C	10000	4.0	1.8	5.8	13	18.0	0.0480	0.0139	0.0092	0.0051	80.83	63.31
10000D	10000	3.5	1.5	5.0	12	18.0	0.0336	0.0175	0.0074	0.0049	77.98	72.00
10000E	10000	x	x	x	x	x	x	x	x	x	x	x
10000F	10000	2.9	1.5	4.4	11	18.5	0.0413	0.0265	0.0080	0.0039	80.63	85.28
10000G	10000	2.0	0.7	2.7	10	22.5	0.0419	0.0170	0.0065	0.0053	84.49	68.82
10000H	10000	4.1	1.9	6.0	12	18.0	0.0434	0.0177	0.0088	0.0059	79.72	66.67
10000I	10000	3.7	1.0	4.7	10	18.0	0.0305	0.0146	0.0073	0.0036	76.07	75.34
10000_sum	10000	28.0	12.1	40.1	93.0	151.0	0.3315	0.1381	0.0656	0.0394	639.83	562.18
10000_mean	10000	3.5	1.5	5.0	11.6	18.9	0.0414	0.0173	0.0082	0.0049	79.98	70.27
10000_SD	10000	0.7	0.4	1.1	1.2	1.6	0.0069	0.0040	0.0011	0.0008	2.47	7.23

C.2. C Plant Se content data

Table C.9.: C Se content of experimental runs for Na_2SeO_3 and Na_2SeO_4 with adsorption onto kaolinite and goethite

c(Se) [µg/L]	FIAS-Results			c(Se) dry weight (DW)							
	dig. weight shoot [g] [± 0.0001]	dig. weight root [g] [± 0.0001]	dig. volume [L] [± 0.0001]	c(Se) shoot [µg/L]	c(Se) shoot SD	c(Se) root [µg/L]	c(Se) root SD	c(Se) shoot [mg/kg]	c(Se) shoot SD	c(Se) root [mg/kg]	c(Se) root SD
Nutrient-Solution-Kaolinite-Se (Na_2SeO_3) Planting Date: 27.03.2014											
0	0.0768	0.0347	0.010	0.09	0.95	-0.85	0.49	0.01	0.12	-0.25	0.14
20	0.0662	0.0326	0.010	9.39	0.64	10.00	1.39	1.42	0.10	3.07	0.43
50	0.0676	0.0318	0.010	25.75	1.16	26.77	0.85	3.81	0.17	8.41	0.27
100	0.0373	0.0129	0.010	31.48	2.36	18.33	4.74	8.43	0.63	14.18	3.67
200	0.0729	0.0417	0.010	126.98	4.81	136.42	4.02	17.42	0.66	32.75	0.97
500	0.0610	0.0289	0.010	219.24	5.27	289.40	14.95	35.97	0.87	100.00	5.16
1000	0.0698	0.0427	0.010	451.86	25.65	647.14	20.63	64.71	3.67	151.56	4.83
2000	0.0557	0.0408	0.009	725.40	36.24	1091.88	103.97	117.27	5.86	240.62	22.91
5000	0.1070	0.0724	0.010	911.87	36.90	2129.21	64.33	85.20	3.45	294.05	8.88
10000	0.0572	0.0432	0.010	457.57	31.82	1916.89	70.92	79.94	5.56	443.62	16.41
Nutrient-Solution-Kaolinite-Se (Na_2SeO_4) Planting Date: 25.03.2014											
0	0.0930	0.0485	0.010	-0.26	0.70	0.04	0.66	-0.03	0.08	0.01	0.14
20	0.0882	0.0426	0.010	7.70	0.46	1.14	0.48	0.87	0.05	0.27	0.11
50	0.0869	0.0446	0.010	41.76	1.54	7.44	1.19	4.80	0.18	1.67	0.27
100	0.1010	0.0490	0.010	123.40	4.75	16.02	3.25	12.21	0.47	3.27	0.66
200	0.0633	0.0314	0.010	157.23	6.88	23.12	4.32	24.85	1.09	7.37	1.38
500	0.0873	0.0440	0.010	526.93	21.98	110.23	3.54	60.37	2.52	25.07	0.81
1000	0.0769	0.0348	0.010	972.45	38.55	172.04	8.33	126.52	5.02	49.38	2.39
2000	0.0917	0.0444	0.010	2480.51	168.82	379.99	23.92	270.41	18.40	85.55	5.38
5000	0.0782	0.0439	0.010	5307.36	166.85	934.41	43.07	678.52	21.33	213.09	9.82
10000	0.0775	0.0341	0.010	8362.85	182.62	1369.43	146.65	1079.64	23.58	401.59	43.00
Nutrient-Solution-Goethite-Se (Na_2SeO_3) Planting Date: 15.05.2014											
0	0.0893	0.0545	0.010	0.01	0.04	0.01	0.03	0.00	0.00	0.00	0.01
20	0.0734	0.0402	0.010	0.01	0.01	0.02	0.06	0.00	0.00	0.00	0.01
50	0.0857	0.0489	0.010	0.01	0.02	0.00	0.05	0.00	0.00	0.00	0.01
100	0.0878	0.0534	0.010	0.88	0.93	0.93	0.40	0.10	0.11	0.17	0.07
200	0.0652	0.0493	0.010	0.65	1.29	0.00	0.04	0.10	0.20	0.00	0.01
500	0.0817	0.0458	0.010	0.00	0.03	0.04	0.02	0.00	0.00	0.01	0.00
1000	0.0807	0.0466	0.010	0.03	0.04	8.17	1.11	0.00	0.00	1.75	0.24
2000	0.0815	0.0523	0.009	0.08	0.02	17.00	0.64	0.01	0.00	2.93	0.11
5000	0.0917	0.0513	0.010	8.13	0.87	38.26	0.77	0.89	0.10	7.46	0.15
10000	0.1019	0.0535	0.010	19.46	1.26	53.17	0.52	1.91	0.12	9.93	0.10
Nutrient-Solution-Goethite-Se (Na_2SeO_4) Planting Date: 16.05.2014											
0	0.0797	0.0494	0.010	0.20	0.40	-0.07	0.39	0.03	0.05	-0.01	0.08
20	0.0859	0.0572	0.010	6.24	0.54	0.83	0.48	0.73	0.06	0.14	0.08
50	0.0778	0.0491	0.010	8.89	3.76	3.57	1.24	1.14	0.48	0.73	0.25
100	0.0666	0.0442	0.010	34.56	7.44	4.87	2.72	5.19	1.12	1.10	0.61
200	0.0911	0.0573	0.010	125.76	6.39	9.27	4.44	13.81	0.70	1.62	0.77
500	0.0787	0.0523	0.010	258.68	13.94	41.23	3.88	32.88	1.77	7.88	0.74
1000	0.0642	0.0412	0.010	405.39	24.86	62.32	11.67	63.17	3.87	15.14	2.84
2000	0.0790	0.0473	0.010	1082.03	67.59	151.77	43.41	137.04	8.56	32.08	9.18
5000	0.0708	0.0500	0.010	1339.03	84.20	223.25	21.84	189.10	11.89	44.68	4.37
10000	0.0659	0.0432	0.010	2289.99	63.98	362.92	12.15	347.34	9.70	84.11	2.82
Digestion standards											
Standard Sample	dig. weight [g]	dig. volume [L]	c(Se) [µg/L]	c(Se) SD	c(Se) [mg/kg]	c(Se) SD					
dig_std_2014_06_20 (0-20ppb)	0.09925	0.010	11.37	1.56	1.15	0.16					
dig_std_2014_06_23 (50-500ppb)	0.10131	0.010	11.47	0.63	1.13	0.06					
dig_std_2014_06_24 (1000-10000ppb)	0.09967	0.010	10.32	1.21	1.04	0.12					
dig_std_2014_06_16 (0-100 ppb)	0.09959	0.010	12.40	1.36	1.24	0.14					
dig_std_2014_06_17 (200-2000ppb)	0.10002	0.010	10.98	0.79	1.10	0.08					
dig_std_2014_06_20 (5000-10000ppb)	0.09925	0.010	11.37	1.56	1.15	0.16					
dig_std_2014_06_27 (0-20 ppb)	0.10011	0.010	7.01	0.49	0.70	0.05					
dig_std_2014_06_30 (50-500 ppb)	0.09967	0.010	5.46	0.83	0.55	0.08					
dig_std_2014_07_01 (1000-10000 ppb)	0.09987	0.010	13.52	1.76	1.35	0.18					
dig_std_2014_06_25 (0-100 ppb)	0.09953	0.010	7.70	0.79	0.77	0.08					
dig_std_2014_06_26 (200-2000 ppb)	0.10049	0.010	6.79	0.18	0.68	0.02					
dig_std_2014_06_27 (5000-10000 ppb)	0.10011	0.010	7.01	0.49	0.70	0.05					

C.3. C results overview - plant growth & Se partitioning

Table C.10.: *C results overview of plant growth & Se partitioning for Na₂SeO₃ in the presence of kaolinite*

c(Se) [µg/L]	plants per box		2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water			
	[-]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[g]	SD	[g]	SD		
0	7.00	x	3.39	0.69	0.97	0.20	4.36	0.86	11.86	1.68	7.93	4.75	29.29	2.40	0.0117	0.0041	0.0065	0.0017	71.94	52.40	0.00	0.00		
20	6.00	x	3.95	0.22	1.18	0.39	5.13	0.55	12.50	1.22	6.56	5.32	28.33	2.36	0.0132	0.0020	0.0062	0.0011	62.30	62.18	0.04	0.00		
50	6.00	x	3.68	0.16	1.35	0.16	5.03	0.29	13.17	0.41	9.54	4.36	29.83	1.21	0.0133	0.0008	0.0061	0.0007	66.38	59.54	0.06	0.06		
100	7.00	x	3.61	0.34	1.39	0.12	5.00	0.42	13.00	0.80	8.53	4.31	26.36	0.80	0.0126	0.0015	0.0062	0.0003	68.27	55.30	1.28	0.20		
200	7.00	x	3.61	0.25	1.29	0.31	4.90	0.50	12.71	1.97	7.63	3.97	25.64	1.97	0.0117	0.0013	0.0067	0.0008	63.68	51.83	2.68	0.20		
500	5.00	x	3.38	0.18	1.36	0.18	4.74	0.30	13.20	1.99	5.67	4.74	29.80	1.99	0.0147	0.0017	0.0068	0.0003	63.68	56.88	6.33	0.24		
1000	7.00	x	3.36	0.40	1.34	0.19	4.70	0.30	12.86	1.34	7.28	3.42	25.43	1.34	0.0115	0.0008	0.0070	0.0004	65.11	56.15	10.58	0.25		
2000	6.00	x	3.10	1.18	1.18	0.35	4.28	0.54	13.00	1.67	5.69	2.96	22.00	1.67	0.0108	0.0011	0.0078	0.0006	53.61	46.51	2.72	2.72		
5000	8.00	x	2.64	0.20	1.35	0.30	3.99	0.46	12.67	1.85	4.22	1.15	11.88	1.85	0.0096	0.0020	0.0062	0.0009	51.02	45.63	41.73	2.72		
10000	6.00	x	2.20	0.49	1.25	0.10	3.45	0.58	10.33	1.39	2.94	1.10	8.08	1.39	0.0110	0.0029	0.0098	0.0057	53.08	49.56	37.51	2.61		
0	0.01	0.12	-0.25	0.14	x	x	x	x	x	x	x	x	71.94	52.40	0.00	0.00	0.00	0.00	62.30	62.18	0.53	0.00		
20	1.42	0.10	3.07	0.43	2.16	0.21	0.46	0.20	31.60	6.59	68.40	13.48	62.30	62.18	0.53	0.04	0.005	0.004	63.30	62.18	0.53	0.04		
50	3.81	0.17	8.41	0.27	2.21	0.38	0.45	0.12	31.19	11.79	68.81	8.29	66.38	59.54	1.28	0.06	0.006	0.007	66.38	59.54	1.28	0.06		
100	8.43	0.63	14.18	0.67	1.68	1.06	0.59	0.18	37.30	39.71	62.70	136.70	68.27	55.30	2.68	0.20	0.013	0.008	66.38	55.30	2.68	0.20		
200	17.42	0.66	32.75	0.97	1.88	1.24	0.53	0.51	34.72	43.03	65.28	136.62	63.68	51.83	6.33	0.24	0.024	0.024	63.68	56.88	6.33	0.24		
500	35.97	0.87	100.00	5.16	2.78	2.40	0.36	1.86	26.45	257.38	73.55	136.62	70.58	56.88	10.58	0.25	0.025	0.025	63.68	56.88	10.58	0.25		
1000	64.71	3.67	151.56	4.83	2.34	8.60	0.43	2.06	29.92	363.89	70.08	144.56	65.11	56.15	22.58	1.28	0.128	0.128	65.11	56.15	22.58	1.28		
2000	117.27	5.86	240.62	22.91	2.05	12.02	0.49	11.17	32.77	393.89	67.23	750.80	53.61	46.51	54.40	2.72	2.72	109.72	53.61	46.51	2.72			
5000	85.20	3.45	294.05	8.88	3.45	11.90	0.29	2.57	22.46	267.29	77.54	199.59	51.02	45.63	41.73	1.69	1.69	171.33	51.02	45.63	1.69			
10000	79.94	5.56	443.62	16.41	5.55	30.85	0.18	2.96	15.27	471.04	84.73	250.58	53.08	49.56	37.51	2.61	2.61	277.22	53.08	49.56	2.61			
availab. c(Se) [µg/L]	shoot DW [mg/kg]	SD	root DW [mg/kg]	SD	ratio shoot/shoot [-]	SD	ratio shoot/root [-]	SD	shoot-Se share [%]	SD	root-Se share [%]	SD	shoot water [%]	SD	root water [%]	SD	c(Se) shoot FW [mg/kg]	SD	c(Se) root FW [mg/kg]	SD	shoot acc. factor [-]	SD	root acc. factor [-]	SD
1	0.01	0.12	-0.25	0.14	x	x	x	x	x	x	x	x	71.94	52.40	0.00	0.00	0.00	0.00	63.30	62.18	0.53	0.00	0.00	
23	1.42	0.10	3.07	0.43	2.16	0.21	0.46	0.20	31.60	6.59	68.40	13.48	62.30	62.18	0.53	0.04	0.005	0.004	63.30	62.18	0.53	0.04		
60	3.81	0.17	8.41	0.27	2.21	0.38	0.45	0.12	31.19	11.79	68.81	8.29	66.38	59.54	1.28	0.06	0.006	0.007	66.38	59.54	1.28	0.06		
120	8.43	0.63	14.18	0.67	1.68	1.06	0.59	0.18	37.30	39.71	62.70	136.70	68.27	55.30	2.68	0.20	0.013	0.008	66.38	55.30	2.68	0.20		
233	17.42	0.66	32.75	0.97	1.88	1.24	0.53	0.51	34.72	43.03	65.28	136.62	63.68	51.83	6.33	0.24	0.024	0.024	63.68	56.88	6.33	0.24		
556	35.97	0.87	100.00	5.16	2.40	8.60	0.43	2.06	26.45	257.38	73.55	136.62	70.58	56.88	10.58	0.25	0.025	0.025	63.68	56.88	10.58	0.25		
1183	64.71	3.67	151.56	4.83	2.34	11.90	0.49	11.17	32.77	393.89	67.23	144.56	65.11	56.15	22.58	1.28	1.28	117.34	65.11	56.15	22.58	1.28		
2377	117.27	5.86	240.62	22.91	2.05	12.02	0.49	11.17	32.77	393.89	67.23	750.80	53.61	46.51	54.40	2.72	2.72	109.72	53.61	46.51	2.72			
5707	85.20	3.45	294.05	8.88	3.45	11.90	0.29	2.57	22.46	267.29	77.54	199.59	51.02	45.63	41.73	1.69	1.69	171.33	51.02	45.63	1.69			
1378	79.94	5.56	443.62	16.41	5.55	30.85	0.18	2.96	15.27	471.04	84.73	250.58	53.08	49.56	37.51	2.61	2.61	277.22	53.08	49.56	2.61			

Table C.11.: C results overview of plant growth & Se partitioning for Na_2SeO_3 in the presence of goethite

c(Se) [µg/L]	plants per box [-]	2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water			
		[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD		
0	9.00	x	4.17	0.44	1.67	0.23	5.83	0.66	13.33	1.12	7.93	4.75	22.27	1.97	0.0105	0.0016	0.0064	0.0008	73.50	2.40	45.88	13.33	
20	7.00	x	3.99	0.99	1.71	0.81	5.70	1.79	12.29	1.60	6.56	5.32	23.71	3.45	0.0107	0.0029	0.0055	0.0008	73.66	5.10	46.80	16.01	
50	8.00	x	4.10	0.29	1.75	0.41	5.85	0.61	12.75	2.24	9.54	4.36	22.25	2.24	0.0109	0.0021	0.0062	0.0008	73.77	2.64	54.54	7.09	
100	9.00	x	3.74	0.56	1.47	0.41	5.21	0.94	12.67	2.14	8.53	4.31	23.44	2.14	0.0099	0.0022	0.0059	0.0009	70.56	2.11	42.46	13.83	
200	7.00	x	3.83	0.54	1.47	0.38	5.30	0.88	12.43	2.88	7.63	3.97	20.71	2.88	0.0100	0.0021	0.0071	0.0016	70.61	4.36	46.65	19.06	
500	8.00	x	4.01	0.34	1.79	0.24	5.80	0.52	13.38	1.94	5.67	4.74	22.31	1.94	0.0105	0.0017	0.0058	0.0011	73.76	2.60	52.69	13.18	
1000	8.00	x	3.69	0.45	1.46	0.42	5.15	0.87	12.63	1.75	7.28	5.82	22.50	1.75	0.0104	0.0015	0.0060	0.0005	66.60	3.87	49.31	12.93	
2000	8.00	x	3.73	0.88	2.01	0.79	5.74	0.93	12.25	4.32	5.69	4.83	22.19	4.32	0.0109	0.0032	0.0066	0.0010	65.90	5.70	43.02	7.33	
5000	9.00	x	3.94	0.60	1.67	0.33	5.61	0.88	12.67	1.73	4.22	1.33	21.17	1.73	0.0104	0.0011	0.0059	0.0007	70.08	5.94	50.53	16.04	
10000	9.00	x	4.26	0.15	1.84	0.13	6.10	0.22	13.78	1.71	2.94	1.89	22.39	1.71	0.0117	0.0014	0.0063	0.0006	71.25	2.13	57.01	8.10	
appoint.																							
c(Se) [µg/L]	c(Se) shoot DW		ratio root/shoot		ratio shoot/root		shoot-Se share		root-Se share		shoot water		shoot water		c(Se) shoot FW		c(Se) root FW		shoot acc. factor		root acc. factor		
	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	[%]	SD	[%]	SD	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD
0	0.00	0.00	x	0.01	x	0.42	x	0.01	x	0.08	x	70.44	x	0.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	0.00	0.00	x	0.01	x	1.02	x	0.01	x	50.58	x	49.42	x	0.49	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
50	0.00	0.00	x	0.01	x	0.58	x	0.04	x	36.59	x	63.41	x	2.73	0.03	0.03	0.17	0.07	0.30	0.01	0.00	0.01	0.02
100	0.10	0.11	x	0.07	x	104.56	x	0.77	x	99.05	x	99.05	x	0.73	0.06	0.06	0.00	0.01	0.15	0.29	0.00	0.00	0.04
200	0.00	0.00	x	0.01	x	0.06	x	0.00	x	5.78	x	94.22	x	0.05	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
500	0.00	0.00	x	0.01	x	0.00	x	0.00	x	0.21	x	99.79	x	0.03	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
1000	0.00	0.00	x	0.24	x	478.54	x	2.33	x	0.49	x	99.70	x	0.03	0.00	0.00	1.75	0.24	0.00	0.00	0.00	0.00	0.24
2000	0.01	0.00	x	0.11	x	335.32	x	0.80	x	0.30	x	99.70	x	0.03	0.00	0.00	2.93	0.11	0.00	0.00	0.00	0.00	0.06
5000	0.89	0.10	x	7.46	x	8.41	x	0.80	x	10.62	x	89.38	x	1.60	0.03	0.27	7.44	0.15	0.05	0.01	0.05	0.01	1.49
10000	1.91	0.12	x	9.93	x	5.20	x	0.19	x	16.13	x	83.87	x	1.55	0.04	0.55	9.88	0.10	0.05	0.00	0.05	0.00	0.99
availab.																							
c(Se) [µg/L]	c(Se) shoot DW		ratio root/shoot		ratio shoot/root		shoot-Se share		root-Se share		shoot water		shoot water		c(Se) shoot FW		c(Se) root FW		shoot acc. factor		root acc. factor		
	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	[%]	SD	[%]	SD	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD
2	0.00	0.00	x	0.01	x	0.42	x	0.01	x	29.56	x	70.44	x	0.43	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
23	0.00	0.00	x	0.01	x	1.02	x	0.01	x	50.58	x	49.42	x	0.49	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
55	0.00	0.00	x	0.07	x	0.58	x	0.04	x	36.59	x	63.41	x	2.73	0.03	0.03	0.17	0.07	0.30	0.01	0.00	0.01	0.02
106	0.10	0.11	x	0.07	x	104.56	x	0.77	x	99.05	x	99.05	x	0.73	0.06	0.07	0.00	0.01	0.15	0.29	0.00	0.00	0.17
212	0.10	0.20	x	0.01	x	0.00	x	0.00	x	5.78	x	94.22	x	0.05	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.03
521	0.00	0.00	x	0.01	x	0.06	x	0.00	x	0.21	x	99.79	x	0.03	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00
1069	0.00	0.00	x	0.24	x	478.54	x	2.33	x	0.49	x	99.70	x	0.05	0.00	0.00	1.75	0.24	0.00	0.00	0.00	0.00	0.01
2111	0.01	0.00	x	2.93	x	335.32	x	0.80	x	0.30	x	99.70	x	0.03	0.00	0.00	2.93	0.11	0.00	0.00	0.00	0.00	0.22
5370	0.89	0.10	x	7.46	x	8.41	x	0.80	x	10.62	x	89.38	x	1.60	0.03	0.27	7.44	0.15	0.05	0.01	0.05	0.01	1.38
10135	1.91	0.12	x	9.93	x	5.20	x	0.19	x	16.13	x	83.87	x	1.55	0.04	0.55	9.88	0.10	0.05	0.00	0.05	0.00	0.97

Table C.12.: *C results overview of plant growth & Se partitioning for Na₂SeO₄ in the presence of kaolinite*

c(Se) [µg/L]	plants per box		2nd leaf sheath		2nd leaf blade		2nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water			
	-	SD	[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD		
0	8.00	x	3.98	0.45	1.41	0.22	5.39	0.65	12.75	0.46	4.22	1.44	27.69	1.46	0.0125	0.0017	0.0065	0.0008	67.83	41.01	0.00	0.00		
20	8.00	x	4.64	0.62	1.65	0.22	6.29	0.80	12.50	0.76	4.17	1.56	23.88	2.71	0.0122	0.0023	0.0058	0.0004	63.98	57.81	0.11	0.00		
50	8.00	x	4.48	0.57	1.54	0.35	6.01	0.89	12.75	0.71	4.28	1.56	22.44	2.27	0.0125	0.0023	0.0060	0.0008	64.54	48.69	0.86	0.14		
100	9.00	x	5.09	0.47	1.74	0.19	6.83	0.58	12.89	0.33	5.56	0.98	24.83	1.62	0.0124	0.0010	0.0060	0.0004	71.59	3.36	1.32	0.27		
200	6.00	x	5.35	0.89	1.92	0.35	7.27	1.24	12.83	1.17	3.59	2.52	25.00	1.82	0.0124	0.0038	0.0064	0.0004	70.97	4.01	2.51	0.32		
500	8.00	x	4.09	0.33	1.35	0.21	5.44	0.48	12.75	0.71	4.44	1.67	22.38	1.46	0.0123	0.0026	0.0068	0.0022	80.92	1.08	3.47	0.47		
1000	7.00	x	4.31	0.36	1.46	0.33	5.77	0.29	12.86	0.69	3.50	2.57	23.57	2.23	0.0128	0.0016	0.0056	0.0003	80.28	4.18	2.51	0.29		
2000	8.00	x	4.56	0.97	1.59	0.30	6.15	1.24	12.63	1.41	5.31	1.00	23.81	2.64	0.0131	0.0029	0.0061	0.0010	80.54	1.50	2.85	0.63		
5000	8.00	x	3.71	0.92	1.46	0.34	5.18	1.22	12.38	1.19	4.00	1.37	19.63	3.67	0.0112	0.0032	0.0062	0.0012	79.31	1.61	2.95	1.75		
10000	8.00	x	3.73	0.17	1.35	0.27	5.08	0.37	12.63	0.52	4.22	1.23	16.44	2.15	0.0109	0.0017	0.0047	0.0006	74.70	1.70	2.85	1.75		
appoint. c(Se) [µg/L]	shoot DW	c(Se) [mg/kg]	root DW	c(Se) [mg/kg]	ratio [-]	shoot/root SD	ratio [-]	shoot/root SD	shoot/Se share [%]	root/Se share [%]	shoot/Se share [%]	shoot/Se share [%]	shoot water [%]	root water [%]	shoot FW	c(Se) [mg/kg]	root FW	c(Se) [mg/kg]	shoot water [%]	root water [%]	shoot water [%]	root water [%]	shoot water [%]	root water [%]
0	0.87	0.08	0.01	0.14	x	x	x	x	1.23	x	8.65	x	67.83	41.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20	4.80	0.18	1.67	0.27	0.35	0.06	2.88	0.77	4.38	25.78	19.87	64.54	48.69	57.81	0.31	0.02	0.06	0.11	0.05	0.05	0.05	0.05	0.05	
50	12.21	0.47	3.27	0.66	0.27	0.13	3.74	2.48	9.92	21.10	52.24	71.59	59.44	71.59	1.70	0.06	0.13	0.86	0.14	0.14	0.14	0.14	0.14	
100	24.85	1.09	7.37	1.38	0.30	0.32	3.37	4.64	24.87	106.20	106.20	70.97	65.94	7.21	0.32	0.32	2.51	1.32	0.27	1.32	0.27	1.32	0.27	
200	60.37	2.52	25.07	0.81	0.42	1.05	2.41	1.94	70.65	29.35	56.93	80.92	73.86	11.52	0.48	0.38	8.96	0.29	0.29	0.29	0.29	0.29	0.29	
500	126.52	5.02	49.38	2.39	0.39	1.96	2.56	6.13	140.81	28.07	172.00	73.86	73.67	33.08	1.31	0.41	13.00	0.63	0.63	0.63	0.63	0.63	0.63	
1000	270.41	18.40	85.35	5.38	0.32	5.82	3.16	17.02	442.28	24.03	409.01	80.54	67.44	52.62	3.58	0.41	27.85	1.75	1.75	1.75	1.75	1.75	1.75	
2000	678.52	21.33	213.09	9.82	0.31	6.70	3.18	31.27	509.82	23.90	747.42	69.98	69.98	140.42	5.97	4.41	63.97	2.95	2.95	2.95	2.95	2.95	2.95	
5000	1079.64	23.58	401.59	43.00	0.37	8.77	2.69	115.61	639.20	27.11	3134.53	74.70	81.08	273.17	5.97	5.97	75.97	8.14	8.14	8.14	8.14	8.14	8.14	
available c(Se) [µg/L]	shoot DW	c(Se) [mg/kg]	root DW	c(Se) [mg/kg]	ratio [-]	shoot/root SD	ratio [-]	shoot/root SD	shoot/Se share [%]	root/Se share [%]	shoot/Se share [%]	shoot/Se share [%]	shoot water [%]	root water [%]	shoot FW	c(Se) [mg/kg]	root FW	c(Se) [mg/kg]	shoot water [%]	root water [%]	shoot water [%]	root water [%]	shoot water [%]	root water [%]
0	0.87	0.08	0.01	0.14	x	x	x	x	1.23	x	8.65	x	67.83	41.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
27	4.80	0.18	1.67	0.27	0.35	0.06	2.88	0.77	4.38	25.78	19.87	64.54	48.69	57.81	0.31	0.02	0.06	0.11	0.05	0.05	0.05	0.05		
66	12.21	0.47	3.27	0.66	0.27	0.13	3.74	2.48	9.92	21.10	52.24	71.59	59.44	71.59	1.70	0.06	0.13	0.86	0.14	0.14	0.14	0.14		
124	24.85	1.09	7.37	1.38	0.30	0.32	3.37	4.64	24.87	106.20	106.20	70.97	65.94	7.21	0.32	0.32	2.51	1.32	0.27	1.32	0.27	1.32		
265	60.37	2.52	25.07	0.81	0.42	1.05	2.41	1.94	70.65	29.35	56.93	80.92	73.86	11.52	0.48	0.38	8.96	0.29	0.29	0.29	0.29	0.29		
622	126.52	5.02	49.38	2.39	0.39	1.96	2.56	6.13	140.81	28.07	172.00	73.86	73.67	33.08	1.31	0.41	13.00	0.63	0.63	0.63	0.63	0.63		
1255	270.41	18.40	85.35	5.38	0.32	5.82	3.16	17.02	442.28	24.03	409.01	80.54	67.44	52.62	3.58	0.41	27.85	1.75	1.75	1.75	1.75	1.75		
2458	678.52	21.33	213.09	9.82	0.31	6.70	3.18	31.27	509.82	23.90	747.42	69.98	69.98	140.42	5.97	4.41	63.97	2.95	2.95	2.95	2.95	2.95		
6285	1079.64	23.58	401.59	43.00	0.37	8.77	2.69	115.61	639.20	27.11	3134.53	74.70	81.08	273.17	5.97	5.97	75.97	8.14	8.14	8.14	8.14	8.14		
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Table C.13.: C results overview of plant growth & Se partitioning for Na_2SeO_4 in the presence of goethite

c(Se) [µg/L]	plants per box		2 nd leaf sheath		2 nd leaf blade		2 nd leaf total length		root-Se uptake time		shoot height (Day 9)		shoot height (Day 19)		mean shoot DW		mean root DW		shoot water		root water			
	[-]	SD	[cm]	SD	[cm]	SD	[cm]	SD	[days]	SD	[cm]	SD	[cm]	SD	[g]	SD	[g]	SD	[%]	SD	[%]	SD		
0	8.00	x	4.38	0.51	1.73	0.33	6.10	0.83	12.38	1.19	3.75	0.96	21.19	0.65	0.0106	0.0016	0.0063	0.0014	75.91	2.44	48.10	11.26		
20	9.00	x	3.49	0.60	1.42	0.42	4.91	1.01	10.89	0.93	2.61	0.93	21.89	0.78	0.0104	0.0011	0.0068	0.0012	71.87	2.66	39.84	13.67		
50	8.00	x	3.13	0.35	1.61	0.26	4.74	0.56	9.25	0.71	1.51	0.81	20.81	1.77	0.0090	0.0022	0.0053	0.0009	78.08	4.91	60.18	10.48		
100	7.00	x	3.59	0.90	1.59	0.32	5.17	1.19	11.43	0.98	2.89	1.38	20.29	2.08	0.0092	0.0011	0.0057	0.0010	78.19	3.36	59.85	10.40		
200	9.00	x	3.99	0.42	1.59	0.30	5.58	0.68	12.00	1.22	3.94	1.04	20.33	1.39	0.0099	0.0012	0.0060	0.0012	79.05	4.01	66.43	7.03		
500	9.00	x	3.18	0.53	1.50	0.33	4.68	0.85	10.22	0.67	2.33	0.87	18.72	1.64	0.0082	0.0013	0.0050	0.0016	79.36	1.08	60.47	9.33		
1000	7.00	x	3.97	0.50	1.66	0.35	5.63	0.82	12.29	0.95	3.83	1.76	19.93	1.67	0.0091	0.0016	0.0056	0.0011	79.83	4.18	64.96	12.92		
2000	8.00	x	3.70	0.56	1.48	0.27	5.18	0.72	12.63	1.06	4.06	1.10	20.19	1.31	0.0100	0.0026	0.0055	0.0010	78.23	1.50	63.61	8.14		
5000	8.00	x	3.78	0.63	1.46	0.46	5.24	0.99	11.56	1.51	3.89	1.45	21.63	1.13	0.0098	0.0015	0.0061	0.0017	78.31	1.61	57.24	9.07		
10000	8.00	x	3.50	0.72	1.51	0.45	5.01	1.10	11.63	1.19	3.88	1.19	18.88	1.55	0.0082	0.0011	0.0049	0.0008	79.98	1.70	70.27	7.23		
appoint.	c(Se) shoot DW		c(Se) root DW		ratio root/shoot		ratio shoot/root		shoot-Se share		shoot-Se share		shoot water		shoot water		c(Se) root FW		shoot water		shoot water		root water	
c(Se) [µg/L]	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[mg/kg]	SD	[%]	SD	[%]	SD	acc. factor	acc. factor
0	0.03	0.05	-0.01	0.08	x	x	x	x	x	x	x	x	75.91	48.10	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00
20	0.73	0.06	0.14	0.08	0.20	0.01	5.02	0.42	83.39	1.05	16.61	6.96	71.87	39.84	0.20	0.02	0.09	0.10	10.22	0.89	4.35	2.51	2.00	
50	1.14	0.48	0.73	0.25	0.64	0.31	1.57	0.40	61.12	18.81	38.88	15.37	78.08	60.18	0.25	0.11	0.29	0.10	5.01	2.12	5.78	2.00	2.00	
100	5.19	1.12	1.10	0.61	0.21	0.24	4.71	2.90	82.49	19.57	17.51	50.70	78.19	59.85	1.13	0.24	0.44	0.25	11.32	2.44	4.42	2.47	2.47	
200	13.81	0.70	1.62	0.77	0.12	0.08	8.54	6.61	89.52	7.35	10.48	69.31	79.05	66.43	2.89	0.15	0.54	0.26	14.46	0.73	2.71	1.30	1.30	
500	32.88	1.77	7.88	0.74	0.24	0.42	4.17	3.09	80.67	34.26	19.33	59.75	79.36	60.47	6.79	0.37	3.11	0.29	13.57	0.73	6.23	0.59	0.59	
1000	63.17	3.87	15.14	2.84	0.24	0.93	4.17	11.83	80.67	74.89	19.33	228.73	79.83	64.96	12.74	0.78	5.31	0.99	12.74	0.78	5.31	0.99	0.99	
2000	137.04	8.56	32.08	9.18	0.23	2.00	4.27	39.20	81.03	162.38	18.97	743.52	78.23	63.61	29.83	1.86	11.67	3.34	14.92	0.93	5.84	1.67	1.67	
5000	189.10	11.89	44.68	4.37	0.24	2.81	4.23	18.50	80.89	227.23	19.11	353.49	78.31	57.24	41.01	2.58	19.10	1.87	8.20	0.52	3.82	0.37	0.37	
10000	347.34	9.70	84.11	2.82	0.24	2.35	4.13	11.63	80.51	189.16	19.49	226.65	79.98	70.27	69.54	1.94	25.00	0.84	6.95	0.19	2.50	0.08	0.08	
availab.	c(Se) shoot DW		c(Se) root DW		ratio root/shoot		ratio shoot/root		shoot-Se share		shoot-Se share		shoot water		shoot water		c(Se) root FW		shoot water		shoot water		root water	
c(Se) [µg/L]	[mg/kg]	SD	[mg/kg]	SD	[-]	SD	[-]	SD	[%]	SD	[%]	SD	[%]	SD	[%]	SD	[mg/kg]	SD	[%]	SD	[%]	SD	acc. factor	acc. factor
1	0.03	0.05	-0.01	0.08	x	x	x	x	x	x	x	x	75.91	48.10	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00
26	0.73	0.06	0.14	0.08	0.20	0.01	5.02	0.42	83.39	1.05	16.61	6.96	71.87	39.84	0.20	0.02	0.09	0.10	10.22	0.89	4.35	2.51	2.51	
60	1.14	0.48	0.73	0.25	0.64	0.31	1.57	0.40	61.12	18.81	38.88	15.37	78.08	60.18	0.25	0.11	0.29	0.10	5.01	2.12	5.78	2.00	2.00	
114	5.19	1.12	1.10	0.61	0.21	0.24	4.71	2.90	82.49	19.57	17.51	50.70	78.19	59.85	1.13	0.24	0.44	0.25	11.32	2.44	4.42	2.47	2.47	
234	13.81	0.70	1.62	0.77	0.12	0.08	8.54	6.61	89.52	7.35	10.48	69.31	79.05	66.43	2.89	0.15	0.54	0.26	14.46	0.73	2.71	1.30	1.30	
567	32.88	1.77	7.88	0.74	0.24	0.42	4.17	3.09	80.67	34.26	19.33	59.75	79.36	60.47	6.79	0.37	3.11	0.29	13.57	0.73	6.23	0.59	0.59	
1149	63.17	3.87	15.14	2.84	0.24	0.93	4.17	11.83	80.67	74.89	19.33	228.73	79.83	64.96	12.74	0.78	5.31	0.99	12.74	0.78	5.31	0.99	0.99	
2227	137.04	8.56	32.08	9.18	0.23	2.00	4.27	39.20	81.03	162.38	18.97	743.52	78.23	63.61	29.83	1.86	11.67	3.34	14.92	0.93	5.84	1.67	1.67	
2285	189.10	11.89	44.68	4.37	0.24	2.81	4.23	18.50	80.89	227.23	19.11	353.49	78.31	57.24	41.01	2.58	19.10	1.87	8.20	0.52	3.82	0.37	0.37	
4585	347.34	9.70	84.11	2.82	0.24	2.35	4.13	11.63	80.51	189.16	19.49	226.65	79.98	70.27	69.54	1.94	25.00	0.84	6.95	0.19	2.50	0.08	0.08	

C.4. C results overview - sorption data

Table C.14.: C results overview of sorption & plant uptake for Na_2SeO_3 in the presence of kaolinite

Nut-Sol-Kaolinite-Se (Na2SeO3) Planting Date: 27.03.2014												
initial solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	pH_init [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD			
blnd	4.76	67.35	0.44	11.12	0.10	22.14	0.20	1.14	0.11			
0	5.01	50.65	0.33	8.69	0.08	20.70	0.18	0.94	0.10			
20	4.94	61.01	0.40	10.30	0.10	22.22	0.20	23.19	0.80			
50	5.08	49.21	0.32	8.71	0.08	19.12	0.17	59.63	2.36			
100	5.23	43.36	0.29	7.54	0.07	17.59	0.16	120.15	3.99			
200	5.17	53.53	0.35	9.20	0.09	20.38	0.18	233.00	6.76			
500	5.19	60.49	0.40	10.35	0.10	22.36	0.20	555.53	15.90			
1000	5.16	67.25	0.44	11.70	0.11	22.84	0.20	1182.73	35.99			
2000	5.42	63.92	0.42	11.63	0.11	22.78	0.20	2376.67	73.66			
5000	5.96	51.81	0.34	10.37	0.10	20.08	0.18	5706.67	170.39			
10000	6.33	62.48	0.41	14.58	0.14	23.15	0.21	11378.33	332.92			
Kaolinite sorption solution				IC Measurement - Element Concentrations						ICP-MS Analysis		
c(Se)	in-weight [g] ± 0.0003	volume [mL] ± 10	pH_end [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD	
blnd				71.15	0.47	4.57	0.04	23.55	0.21	2.15	0.07	
0	8.5257	170	6.48	69.04	0.46	3.87	0.04	22.77	0.20	18.24	0.26	
20	8.4421	170	6.68	70.13	0.46	4.27	0.04	23.12	0.21	46.37	0.96	
50	8.4133	170	6.64	70.69	0.47	4.02	0.04	23.19	0.21	96.23	2.76	
100	8.6784	170	6.62	69.90	0.46	4.19	0.04	23.09	0.21	193.75	5.20	
200	8.4258	170	6.66	56.00	0.37	2.82	0.03	17.62	0.16	476.73	15.63	
500	8.4503	170	6.63	71.27	0.47	4.76	0.04	23.28	0.21	1019.27	29.00	
1000	8.4962	170	6.65	69.67	0.46	4.04	0.04	22.77	0.20	1944.20	59.08	
2000	8.5001	170	6.74	72.90	0.48	6.22	0.06	23.96	0.21	5178.33	134.29	
5000	8.4301	170	6.76	70.69	0.47	8.08	0.08	23.05	0.21	10466.67	319.47	
10000	8.5542	170	6.86									
Kaolinite sorption + plant uptake solution					IC Measurement - Element Concentrations						ICP-MS Analysis	
c(Se)	dry plant mass [g] ± 0.0003	in-weight [g] ± 0.0003	volume [mL] ± 10	pH_end [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD
blnd					54.81	0.36	1.36	0.01	21.08	0.19	2.36	0.09
0	0.1089	8.5980	170	7.15	49.92	0.33	1.35	0.01	20.24	0.18	15.77	0.59
20	0.0969	8.4769	170	7.23	44.20	0.29	1.69	0.02	20.56	0.18	40.62	1.55
50	0.0972	8.4955	170	7.35	53.87	0.36	1.69	0.02	21.38	0.19	81.66	1.94
100	0.1125	8.5183	170	7.30	54.35	0.36	1.38	0.01	20.78	0.19	165.95	4.96
200	0.1105	8.4941	170	7.24	46.78	0.31	1.54	0.01	20.24	0.18	361.87	11.27
500	0.0862	8.3966	170	7.37	55.78	0.37	2.49	0.02	21.05	0.19	908.13	24.38
1000	0.1104	8.5463	170	7.31	58.07	0.38	1.79	0.02	20.63	0.18	1621.67	47.17
2000	0.0931	8.4936	170	5.79	53.82	0.35	4.68	0.04	20.14	0.18	4480.17	133.33
5000	0.1107	8.5318	170	7.02	21.48	0.14	7.67	0.07	22.63	0.20	9738.33	267.32
10000	0.1040	8.6387	170	7.04								
c(Se)		c(N)		c(P)		Sorption Amount		c(S)		c(Se)		
		[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[µg/L]	[%]	
0		-20.51	-40.49	4.11	47.34	-2.86	-13.80	-1.21	-128.94			
20		-8.03	-13.16	6.43	62.45	-0.55	-2.49	4.95	21.34			
50		-20.92	-42.51	4.44	50.97	-3.99	-20.88	13.26	22.24			
200		-16.37	-30.58	5.01	54.47	-2.71	-13.27	39.25	16.85			
500		4.49	7.42	7.52	72.71	4.74	21.21	78.80	14.18			
1000		-4.01	-5.97	6.94	59.34	-0.43	-1.90	163.47	13.82			
2000		-5.75	-9.00	7.59	65.28	0.01	0.05	432.47	18.20			
5000		-21.09	-40.71	4.15	40.05	-3.88	-19.30	528.33	9.26			
10000		-8.21	-13.14	6.49	44.56	0.09	0.40	911.67	8.01			
c(Se)		c(N)		Plant Uptake + Sorption Amount		c(P)		c(S)		c(Se)		
		[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[µg/L]	[%]	
0		-4.16	-8.22	7.33	84.38	-0.39	-1.88	-1.42	-151.13			
20		11.09	18.18	8.94	86.84	1.98	8.89	7.42	32.01			
50		5.01	10.18	7.02	80.60	-1.44	-7.51	19.01	31.88			
100		-10.51	-24.25	5.85	77.57	-3.79	-21.56	38.49	32.03			
200		-0.82	-1.53	7.83	85.05	-0.40	-1.96	67.05	28.78			
500		13.71	22.66	8.81	85.13	2.12	9.49	193.67	34.86			
1000		11.47	17.06	9.21	78.70	1.79	7.83	274.60	23.22			
2000		5.85	9.15	9.84	84.64	2.15	9.45	755.00	31.77			
5000		-2.01	-3.88	5.69	54.88	-0.06	-0.30	1226.50	21.49			
10000		41.00	65.63	6.91	47.40	0.51	2.22	1640.00	14.41			

Table C.15.: C results overview of sorption & plant uptake for Na₂SeO₃ in the presence of goethite

Nut-Sol-Goethite-Se (Na ₂ SeO ₃) Planting Date: 27.03.2014												
initial solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	pH_init [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD			
blnd	5.33									1.78	0.06	
0	4.85	62.62	0.51	7.69	0.04	19.96	0.10			1.80	0.11	
20	4.85	34.67	0.28	5.21	0.03	12.19	0.06			23.01	0.56	
50	4.78	61.89	0.50	7.43	0.04	18.88	0.10			55.24	1.58	
100	4.81	55.22	0.45	8.18	0.04	19.41	0.10			105.83	2.60	
200	5.29	55.84	0.45	7.49	0.04	18.01	0.09			211.80	5.90	
500	4.85	66.55	0.54	8.58	0.04	20.70	0.11			521.40	16.00	
1000	5.01	65.35	0.53	8.61	0.04	20.06	0.10			1068.53	29.43	
2000	5.15	65.83	0.53	8.73	0.04	20.93	0.11			2110.67	70.04	
5000	5.61	67.33	0.54	10.13	0.05	20.65	0.11			5370.00	167.26	
10000	6.04	60.91	0.49	12.60	0.06	20.11	0.10			10135.00	368.07	
Goethite sorption solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	in-weight [g] ± 0.0003	volume [mL] ± 10	pH_end [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD	
blnd												
0	8.5004	170	7.61	63.31	0.51	0.00	0.00	19.63	0.10	1.06	0.14	
20	8.5253	170	8.05	52.53	0.42	0.00	0.00	16.86	0.09	1.34	0.13	
50	8.5011	170	8.16	65.49	0.53	0.00	0.00	19.03	0.10	2.85	0.08	
100	8.5038	170	7.97	62.28	0.50	0.00	0.00	18.30	0.09	2.34	0.17	
200	8.4964	170	8.05	63.94	0.52	0.00	0.00	19.08	0.10	2.11	0.21	
500	8.5027	170	8.25	64.38	0.52	0.00	0.00	19.30	0.10	2.43	0.15	
1000	8.5061	170	8.68	64.30	0.52	0.00	0.00	19.39	0.10	3.29	0.23	
2000	8.4979	170	7.93	65.23	0.53	0.00	0.00	19.23	0.10	6.56	0.44	
5000	8.5007	170	8.68	63.04	0.51	0.00	0.00	20.12	0.10	15.35	0.11	
10000	8.5096	170	8.43	62.67	0.51	0.00	0.00	19.86	0.10	31.90	0.53	
Goethite sorption + plant uptake solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	dry plant mass [g] ± 0.0003	in-weight [g] ± 0.0003	volume [mL] ± 10	pH_end [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD
blnd												
0	0.1515	8.5072	170	7.43	47.04	0.38	0.00	0.00	21.10	0.11	3.64	0.08
20	0.1134	8.4961	170	7.34	41.12	0.33	0.00	0.00	23.25	0.12	1.37	0.15
50	0.1369	8.5042	170	7.46	49.70	0.40	0.00	0.00	20.82	0.11	1.20	0.05
100	0.1420	8.5062	170	7.86	44.58	0.36	0.00	0.00	21.29	0.11	1.61	0.02
200	0.1200	8.5112	170	7.53	46.63	0.38	0.00	0.00	21.72	0.11	1.17	0.06
500	0.1300	8.4999	170	7.63	48.79	0.39	0.00	0.00	22.34	0.12	2.01	0.18
1000	0.1308	8.5047	170	7.36	47.89	0.39	0.00	0.00	21.53	0.11	3.28	0.11
2000	0.1917	8.5052	170	7.63	47.56	0.38	0.00	0.00	21.22	0.11	5.20	0.15
5000	0.1467	8.5066	170	7.77	49.69	0.40	0.00	0.00	22.68	0.12	12.13	0.67
10000	0.1618	8.5091	170	8.32	40.61	0.33	0.00	0.00	23.87	0.12	21.19	0.25
c(Se)		c(N)		Sorption Amount		c(P)		c(S)		c(Se)		
		[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[µg/L]	[%]	
0		-0.69	-1.11	7.69	100.00	0.33	1.66	0.74	40.99			
20		-17.86	-51.53	5.21	100.00	-4.67	-38.30	21.66	94.16			
50		-3.60	-5.82	7.43	100.00	-0.15	-0.78	52.39	94.84			
100		-7.06	-12.78	8.18	100.00	1.11	5.73	103.49	97.79			
200		-8.10	-14.52	7.49	100.00	-1.07	-5.92	209.69	99.00			
500		2.16	3.25	8.58	100.00	1.41	6.79	518.97	99.53			
1000		1.05	1.60	8.61	100.00	0.67	3.33	1065.24	99.69			
2000		0.59	0.90	8.73	100.00	1.70	8.14	2104.10	99.69			
5000		4.29	6.37	10.13	100.00	0.52	2.54	5354.65	99.71			
10000		-1.76	-2.89	12.60	100.00	0.25	1.25	10103.10	99.69			
c(Se)		c(N)		Plant Uptake + Sorption Amount		c(P)		c(S)		c(Se)		
		[mg/L]	[%]	[mg/L]	[%]	[mg/L]	[%]	[µg/L]	[%]			
0		15.58	24.88	7.69	100.00	-1.14	-5.70	-1.84	-101.96			
20		-6.45	-18.61	5.21	100.00	-11.06	-90.67	21.63	94.02			
50		12.19	19.70	7.43	100.00	-1.94	-10.27	54.04	97.83			
100		10.64	19.26	8.18	100.00	-1.89	-9.72	104.22	98.48			
200		9.21	16.49	7.49	100.00	-3.71	-20.59	210.63	99.45			
500		17.76	26.69	8.58	100.00	-1.63	-7.88	519.39	99.62			
1000		17.46	26.71	8.61	100.00	-1.48	-7.35	1065.25	99.69			
2000		18.27	27.76	8.73	100.00	-0.29	-1.39	2105.47	99.75			
5000		17.64	26.19	10.13	100.00	-2.04	-9.88	5357.87	99.77			
10000		20.30	33.33	12.60	100.00	-3.76	-18.72	10113.81	99.79			

Table C.16.: C results overview of sorption & plant uptake for Na_2SeO_4 in the presence of kaolinite

Nut-Sol-Kaolinite-Se (Na ₂ SeO ₄) Planting Date: 27.03.2014												
initial solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	pH_init	c(N)	SD	c(P)	SD	c(S)	SD	c(Se)	SD			
	[-] ± 0.05	[mg/L]		[mg/L]		[mg/L]		[µg/L]				
blnd	4.70	59.77	0.65	10.35	0.11	22.49	0.28					
0	4.72	68.17	0.74	10.91	0.12	22.64	0.28	0.23	0.08			
20	4.80	70.03	0.76	11.29	0.12	23.39	0.29	27.47	0.88			
50	5.04	69.90	0.76	11.16	0.12	23.74	0.30	66.38	2.32			
100	5.14	38.54	0.42	6.72	0.07	17.57	0.22	123.57	3.40			
200	4.88	70.83	0.77	11.06	0.12	23.60	0.29	265.47	7.60			
500	4.86	73.34	0.80	11.99	0.13	23.62	0.30	621.93	20.51			
1000	5.04	48.52	0.53	8.76	0.09	20.82	0.26	1254.60	42.12			
2000	5.07	32.31	0.35	5.79	0.06	14.57	0.18	2458.00	81.46			
5000	5.14	46.64	0.51	7.87	0.08	19.27	0.24	6285.00	199.44			
10000	4.94	56.94	0.62	9.77	0.10	21.22	0.27	12430.00	368.48			
Kaolinite sorption solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	in-weight	volume	pH_end	c(N)	SD	c(P)	SD	c(S)	SD	c(Se)	SD	
	[g] ± 0.0003	[mL] ± 10	[-] ± 0.05	[mg/L]		[mg/L]		[mg/L]		[µg/L]		
blnd				71.15	0.47	4.57	0.04	23.55	0.21	2.15	0.07	
0	8.5257	170	6.48	69.04	0.46	3.87	0.04	22.77	0.20	18.24	0.26	
20	8.4421	170	6.68	70.13	0.46	4.27	0.04	23.12	0.21	46.37	0.96	
50	8.4133	170	6.64	70.69	0.47	4.02	0.04	23.19	0.21	96.23	2.76	
100	8.6784	170	6.62	69.90	0.46	4.19	0.04	23.09	0.21	193.75	5.20	
200	8.4258	170	6.66	56.00	0.37	2.82	0.03	17.62	0.16	476.73	15.63	
500	8.4503	170	6.63	71.27	0.47	4.76	0.04	23.28	0.21	1019.27	29.00	
1000	8.4962	170	6.65	69.67	0.46	4.04	0.04	22.77	0.20	1944.20	59.08	
2000	8.5001	170	6.74	72.90	0.48	6.22	0.06	23.96	0.21	5178.33	134.29	
5000	8.4301	170	6.76	70.69	0.47	8.08	0.08	23.05	0.21	10466.67	319.47	
10000	8.5542	170	6.86									
Kaolinite sorption + plant uptake solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	dry plant mass	in-weight	volume	pH_end	c(N)	SD	c(P)	SD	c(S)	SD	c(Se)	SD
	[g] ± 0.0003	[g] ± 0.0003	[mL] ± 10	[-] ± 0.05	[mg/L]		[mg/L]		[mg/L]		[µg/L]	
blnd					65.72	0.72	2.73	0.03	22.10	0.28	1.03	0.31
0	8.4774	170	6.76	67.53	0.74	2.55	0.03	23.31	0.29	24.13	0.98	
20	8.5647	170	6.71	72.44	0.79	3.92	0.04	23.49	0.29	61.41	1.99	
50	8.5480	170	6.78	63.86	0.70	2.42	0.03	22.59	0.28	104.25	3.56	
100	8.5118	170	6.74	72.75	0.79	3.78	0.04	23.19	0.29	241.40	8.16	
200	8.5470	170	6.71	0.14	0.00	0.04	0.00	0.25	0.00	538.47	19.30	
500	8.4568	170	6.64	62.32	0.68	2.80	0.03	23.10	0.29	1102.93	38.88	
1000	8.5207	170	6.68	59.50	0.65	2.82	0.03	22.38	0.28	2303.33	68.71	
2000	8.4806	170	7.04	70.89	0.77	2.73	0.03	23.69	0.30	5790.00	191.57	
5000	8.5390	170	6.70	68.83	0.75	3.34	0.04	22.98	0.29	11331.67	371.16	
10000	8.4969	170	6.72									
c(Se)		Sorption Amount										
		c(N)	c(P)	c(S)	c(Se)							
		[mg/L]	[%]	[mg/L]	[%]	[µg/L]	[%]					
0		2.45	3.59	8.18	74.96	0.54	2.40	-0.80	-349.57			
20		2.49	3.56	8.74	77.42	0.08	0.33	3.34	12.16			
50		-2.53	-3.63	7.24	64.92	0.25	1.06	4.97	7.48			
100		-25.32	-65.71	4.30	64.02	-5.02	-28.60	19.31	15.63			
200		-1.92	-2.70	7.28	65.83	0.41	1.75	24.07	9.07			
500		73.20	99.80	11.95	99.70	23.37	98.94	83.47	13.42			
1000		-13.81	-28.46	5.96	67.99	-2.28	-10.93	151.67	12.09			
2000		-27.19	-84.17	2.97	51.32	-7.81	-53.61	154.67	6.29			
5000		-24.24	-51.98	5.14	65.27	-4.42	-22.92	495.00	7.88			
10000		-11.89	-20.88	6.44	65.84	-1.75	-8.26	1098.33	8.84			
c(Se)		Plant Uptake + Sorption Amount										
		c(N)	c(P)	c(S)	c(Se)							
		[mg/L]	[%]	[mg/L]	[%]	[µg/L]	[%]					
0		23.56	34.56	10.13	92.89	2.69	11.88	-1.21	-524.35			
20		26.00	37.14	10.85	96.14	2.31	9.90	4.47	16.29			
50		16.53	23.64	9.54	85.46	1.90	8.01	9.40	14.16			
100		-10.67	-27.69	5.28	78.58	-3.96	-22.52	20.93	16.94			
200		12.56	17.73	8.82	79.81	1.18	5.01	43.93	16.55			
500		23.16	31.58	10.85	90.53	2.16	9.13	105.33	16.94			
1000		-3.91	-8.06	7.15	81.66	-0.39	-1.89	212.60	16.95			
2000		-15.36	-47.56	4.64	80.04	-5.38	-36.92	453.53	18.45			
5000		-7.89	-16.92	6.34	80.61	-1.77	-9.18	1013.33	16.12			
10000		4.34	7.62	7.95	81.31	0.47	2.21	2075.00	16.69			

Table C.17.: C results overview of sorption & plant uptake for Na_2SeO_4 in the presence of goethite

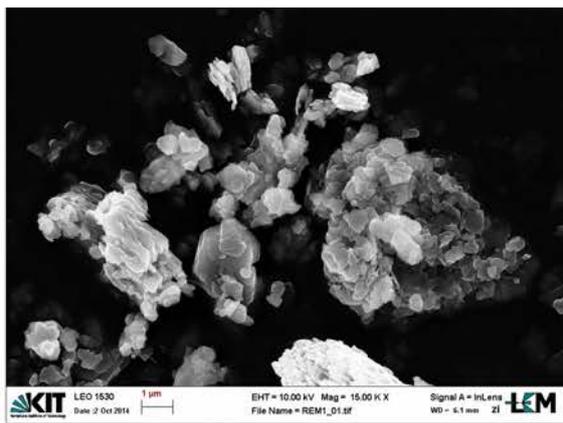
Nut-Sol-Goethite-Se (Na2SeO4) Planting Date: 27.03.2014												
initial solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	pH_init [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD			
blnd	5.35	1.41	0.04	0.00	0.00	0.00	0.00	0.91	0.08			
0	4.82	66.75	1.86	7.73	0.15	20.38	0.25	0.81	0.25			
20	4.84	67.14	1.87	7.67	0.15	20.79	0.26	25.63	0.53			
50	4.92	65.89	1.84	8.07	0.16	20.71	0.26	59.67	1.97			
100	4.66	65.60	1.83	7.51	0.15	20.26	0.25	114.25	3.65			
200	4.74	62.25	1.74	7.33	0.15	20.01	0.25	233.80	8.19			
500	4.69	66.71	1.86	7.30	0.15	20.83	0.26	566.53	18.38			
1000	4.51	69.48	1.94	8.23	0.16	21.12	0.26	1148.93	37.19			
2000	4.56	61.95	1.73	7.18	0.14	19.49	0.24	2284.67	66.58			
5000	4.65	57.30	1.60	7.77	0.16	20.57	0.25	2227.17	58.62			
10000	4.58	59.91	1.67	8.62	0.17	19.64	0.24	4585.33	124.65			
Goethite sorption solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	in-weight [g] ± 0.0003	volume [mL] ± 10	pH_end [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD	
blnd				66.11	1.84	0.00	0.00	18.27	0.23	0.72	0.13	
0	8.4641	170	7.04	66.50	1.85	0.00	0.00	18.93	0.23	11.86	0.32	
20	8.4774	170	7.11	65.43	1.82	0.00	0.00	18.64	0.23	29.95	1.00	
50	8.4268	170	6.89	65.06	1.81	0.00	0.00	20.13	0.25	49.30	1.42	
100	8.4529	170	6.94	54.67	1.52	0.00	0.00	18.63	0.23	98.02	1.41	
200	8.4351	170	6.91	65.90	1.84	0.00	0.00	18.04	0.22	266.40	7.45	
500	8.5028	170	7.15	64.76	1.81	0.00	0.00	20.16	0.25	488.13	13.86	
1000	8.4732	170	7.04	65.97	1.84	0.00	0.00	19.19	0.24	986.13	26.80	
2000	8.4878	170	6.89	51.28	1.43	0.00	0.00	19.23	0.24	708.67	25.36	
5000	8.4497	170	6.92	64.66	1.80	0.00	0.00	18.05	0.22	1826.17	55.10	
Goethite sorption + plant uptake solution		IC Measurement - Element Concentrations								ICP-MS Analysis		
c(Se)	dry plant mass [g] ± 0.0003	in-weight [g] ± 0.0003	volume [mL] ± 10	pH_end [-] ± 0.05	c(N) [mg/L]	SD	c(P) [mg/L]	SD	c(S) [mg/L]	SD	c(Se) [µg/L]	SD
blnd					44.38	1.24	0.00	0.00	21.85	0.27	1.32	0.06
0	0.1349	8.5086	170	7.11	30.41	0.85	0.00	0.00	22.15	0.27	10.25	0.21
20	0.1549	8.4970	170	7.24	34.29	0.96	0.00	0.00	24.74	0.31	21.62	0.71
50	0.1147	8.5413	170	7.93	48.07	1.34	0.00	0.00	21.76	0.27	44.62	1.49
100	0.1039	8.4930	170	7.28	44.69	1.25	0.00	0.00	21.68	0.27	82.28	2.58
200	0.1427	8.4701	170	7.25	35.80	1.00	0.00	0.00	21.91	0.27	195.68	5.98
500	0.1185	8.4978	170	7.89	51.25	1.43	0.00	0.00	22.24	0.27	422.27	11.14
1000	0.1027	8.4561	170	7.22	42.65	1.19	0.00	0.00	23.89	0.30	825.73	18.93
2000	0.1241	8.4901	170	6.93	39.96	1.11	0.00	0.00	18.18	0.22	816.17	26.27
5000	0.1274	8.4686	170	7.97	46.41	1.29	0.00	0.00	21.87	0.27	1692.00	45.89
10000	0.1050	8.5120	170	7.13								
c(Se)		Sorption Amount		c(Se)								
		c(N) [mg/L]	[%]	c(P) [mg/L]	[%]	c(S) [mg/L]	[%]	[µg/L]	[%]			
0		0.64	0.97	7.73	100.00	2.10	10.33	0.09	10.75			
20		0.64	0.95	7.67	100.00	1.85	8.91	13.76	53.70			
50		0.46	0.70	8.07	100.00	2.07	9.99	29.71	49.80			
100		0.55	0.83	7.51	100.00	0.13	0.63	64.95	56.85			
200		7.58	12.18	7.33	100.00	1.38	6.88	135.78	58.08			
500		0.80	1.21	7.30	100.00	2.79	13.38	300.13	52.98			
1000		4.72	6.79	8.23	100.00	0.97	4.57	660.80	57.51			
2000		-4.02	-6.50	7.18	100.00	0.30	1.54	1298.53	56.84			
5000		6.03	10.52	7.77	100.00	1.35	6.54	1518.50	68.18			
10000		-4.75	-7.94	8.62	100.00	1.59	8.09	2759.17	60.17			
c(Se)		Plant Uptake + Sorption Amount										
		c(N) [mg/L]	[%]	c(P) [mg/L]	[%]	c(S) [mg/L]	[%]	[µg/L]	[%]			
0		22.38	33.52	7.73	100.00	-1.47	-7.22	-0.51	-63.61			
20		36.73	54.70	7.67	100.00	-1.37	-6.58	15.38	60.00			
50		31.60	47.96	8.07	100.00	-4.03	-19.44	38.05	63.77			
100		17.53	26.72	7.51	100.00	-1.50	-7.43	69.63	60.95			
200		17.56	28.21	7.33	100.00	-1.67	-8.36	151.52	64.81			
500		30.91	46.33	7.30	100.00	-1.08	-5.19	370.85	65.46			
1000		18.22	26.23	8.23	100.00	-1.12	-5.29	726.67	63.25			
2000		19.30	31.15	7.18	100.00	-4.40	-22.59	1458.93	63.86			
5000		17.35	30.27	7.77	100.00	2.39	11.63	1411.00	63.35			
10000		13.50	22.53	8.62	100.00	-2.24	-11.39	2893.33	63.10			

C.5. C results overview - desorption data

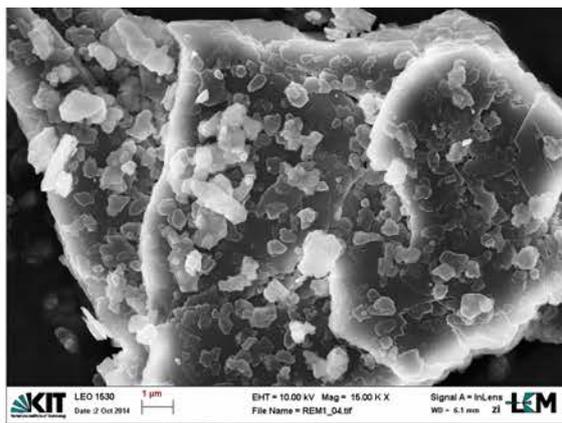
Table C.18: *C results for Na₂SeO₃ and Na₂SeO₄ desorption from kaolinite and goethite*

substrate sorption										substrate sorption + plant uptake									
added c(Se) [µg/L]	substrate weight [g]	(pH _{init} 7.99) pH _{fin} [-]	c(Se) sorp [µg/L]	SD [µg/L]	c(Se) desorp [µg/L]	SD [µg/L]	Se desorp [%]	added c(Se) [µg/L]	substrate weight [g]	(pH _{init} 7.99) pH _{fin} [-]	c(Se) sorp [µg/L]	SD [µg/L]	c(Se) desorp [µg/L]	SD [µg/L]	Se desorp [%]				
Nut-Sol-Kaolinite-Se (Na₂SeO₃) Planting Date: 27.03.2014																			
0	0.5011	8.02	-1.21	-128.94	1.13	0.51	-93.59	0	0.5052	8.03	-1.21	-128.94	1.72	0.46	-141.86				
20	0.5099	8.02	21.34	21.34	3.64	0.36	73.56	20	0.5003	8.03	4.95	21.34	3.96	0.42	79.96				
50	0.5065	8.02	13.26	22.24	7.70	0.48	58.11	50	0.5017	8.02	13.26	22.24	7.53	0.55	56.81				
100	0.4998	8.02	23.91	19.90	12.43	0.81	51.96	100	0.5059	8.03	23.91	19.90	14.04	2.06	58.71				
200	0.5020	8.02	39.25	16.85	21.18	0.94	53.95	200	0.5046	8.02	39.25	16.85	17.97	1.16	45.78				
500	0.5027	8.02	78.80	14.18	45.46	2.91	57.70	500	0.5000	8.02	78.80	14.18	39.17	0.79	49.71				
1000	0.5003	8.02	163.47	13.82	79.94	2.21	48.90	1000	0.5031	8.02	163.47	13.82	56.66	0.93	34.66				
2000	0.4982	8.02	432.47	18.20	136.21	6.19	31.50	2000	0.5047	8.01	432.47	18.20	113.83	4.70	26.32				
5000	0.5032	8.02	528.33	9.26	171.53	4.47	32.47	5000	0.5012	8.02	528.33	9.26	245.50	4.26	46.47				
10000	0.0502	8.02	911.67	8.01	470.42	2.69	51.60	10000	0.5023	8.02	911.67	8.01	364.88	10.55	40.02				
Nut-Sol-Goethite-Se (Na₂SeO₃) Planting Date: 15.05.2014																			
0	0.4979	9.48	0.74	40.99	26.55	0.95	3593.64	0	0.4981	9.55	0.74	40.99	7.11	0.72	962.55				
20	0.5026	9.47	21.66	94.16	16.87	2.30	77.88	20	0.5049	9.54	21.66	94.16	16.78	0.90	77.46				
50	0.5008	9.46	52.39	94.84	33.71	2.01	64.35	50	0.5018	9.49	52.39	94.84	38.46	2.06	73.41				
100	0.4981	9.46	103.49	97.79	80.23	1.99	70.72	100	0.5028	9.56	103.49	97.79	77.48	2.98	74.86				
200	0.4985	9.44	209.69	99.00	137.85	2.42	65.74	200	0.4981	9.51	209.69	99.00	154.05	3.80	73.47				
500	0.4993	9.46	518.97	99.53	328.80	4.63	63.36	500	0.4998	9.59	518.97	99.53	386.00	9.95	74.38				
1000	0.4981	9.52	1065.24	99.69	709.45	16.28	66.60	1000	0.5042	9.56	1065.24	99.69	738.60	10.60	69.34				
2000	0.4974	9.51	2104.10	99.69	1516.00	25.51	72.05	2000	0.4992	9.56	2104.10	99.69	1462.50	7.12	69.51				
5000	0.5047	9.49	5354.65	99.71	3744.50	30.84	69.93	5000	0.5007	9.55	5354.65	99.71	4348.50	24.76	81.21				
10000	0.5051	9.56	10103.10	99.69	7527.00	28.26	74.50	10000	0.5087	9.52	10103.10	99.69	7705.50	20.11	76.27				
Nut-Sol-Kaolinite-Se (Na₂SeO₄) Planting Date: 25.03.2014																			
0	0.5008	8.04	-0.80	-349.57	0.98	0.21	-121.93	0	0.5014	8.03	-0.80	-349.57	1.75	0.37	-217.65				
20	0.5025	8.04	3.34	12.16	2.30	0.10	68.82	20	0.5036	8.03	3.34	12.16	2.74	0.21	82.11				
50	0.4997	8.03	4.97	7.48	4.48	0.22	90.20	50	0.4996	8.03	4.97	7.48	3.47	0.82	69.90				
100	0.4988	8.03	19.31	15.63	8.74	1.05	45.23	100	0.5028	8.03	19.31	15.63	7.15	1.02	37.01				
200	0.5059	8.03	24.07	9.07	11.27	0.46	46.83	200	0.5036	8.03	24.07	9.07	9.57	0.46	39.77				
500	0.5021	8.03	83.47	13.42	35.49	2.07	42.52	500	0.4994	8.03	83.47	13.42	31.47	1.35	37.71				
1000	0.5034	8.03	151.67	12.09	78.31	1.70	51.63	1000	0.5031	8.03	151.67	12.09	61.19	2.79	40.34				
2000	0.5043	8.03	154.67	6.29	124.82	4.53	80.71	2000	0.5000	8.03	154.67	6.29	126.70	1.88	81.92				
5000	0.5072	8.03	495.00	7.88	361.95	4.20	73.12	5000	0.5002	8.03	495.00	7.88	281.24	6.50	56.82				
10000	0.5008	8.03	1098.33	8.84	594.95	7.49	54.17	10000	0.5023	8.03	1098.33	8.84	572.34	8.06	52.11				
Nut-Sol-Goethite-Se (Na₂SeO₄) Planting Date: 16.05.2014																			
0	0.5026	9.48	0.09	10.75	10.07	0.28	11619.23	0	0.5017	9.41	0.09	10.75	2.69	0.26	3098.08				
20	0.5050	9.47	13.76	53.70	12.24	1.06	88.94	20	0.5021	9.41	13.76	53.70	10.91	0.19	79.27				
50	0.5068	9.51	29.71	49.80	34.55	0.95	116.28	50	0.5005	9.47	29.71	49.80	19.18	0.91	64.53				
100	0.5016	9.44	64.95	56.85	56.51	2.30	86.99	100	0.5089	9.49	64.95	56.85	37.56	1.47	57.82				
200	0.5018	9.44	135.78	58.08	122.20	6.29	90.00	200	0.4985	9.49	135.78	58.08	70.87	3.22	52.19				
500	0.4982	9.48	300.13	52.98	312.70	8.47	104.19	500	0.5077	9.55	300.13	52.98	186.40	6.99	62.11				
1000	0.4987	9.52	660.80	57.51	620.80	6.58	97.35	1000	0.5025	9.45	660.80	57.51	365.15	7.89	55.26				
2000	0.4976	9.50	1298.53	56.84	1264.00	13.66	97.34	2000	0.5022	9.59	1298.53	56.84	649.65	13.52	50.03				
5000	0.4982	9.45	1518.50	68.18	1238.50	22.41	81.56	5000	0.5058	9.32	1518.50	68.18	1184.00	12.27	77.97				
10000	0.5023	9.48	2759.17	60.17	2623.50	13.52	95.08	10000	0.5086	9.45	2759.17	60.17	1387.50	23.62	50.29				

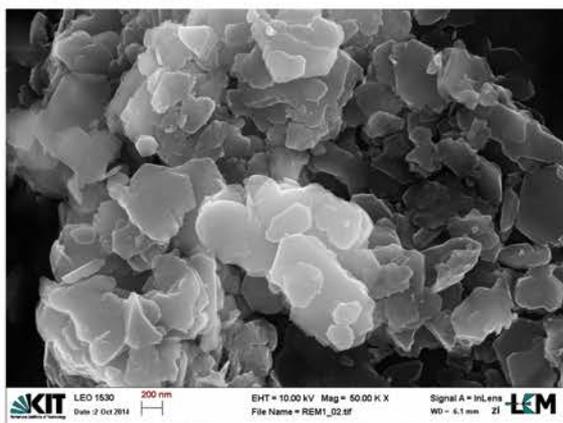
C.5.1. C SEM images



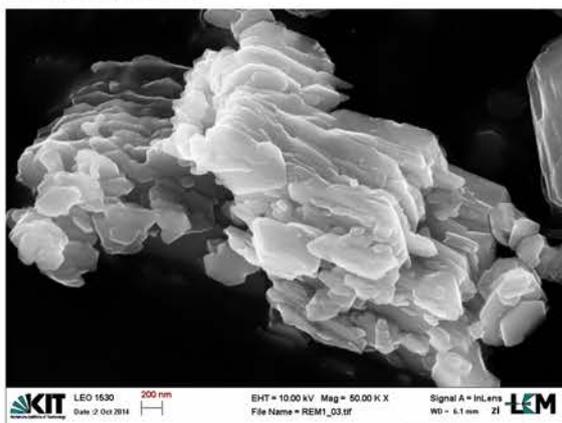
Kaolinite untreated



Kaolinite untreated

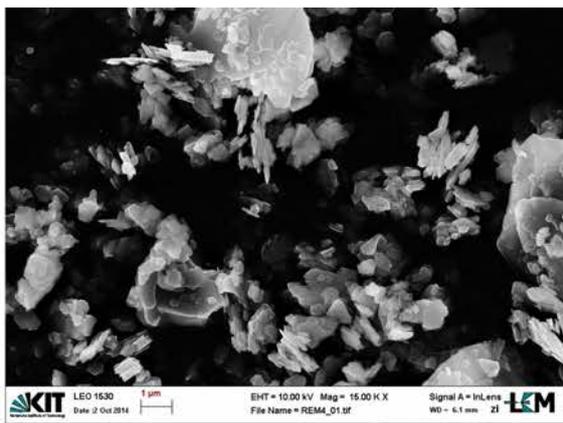


Kaolinite untreated

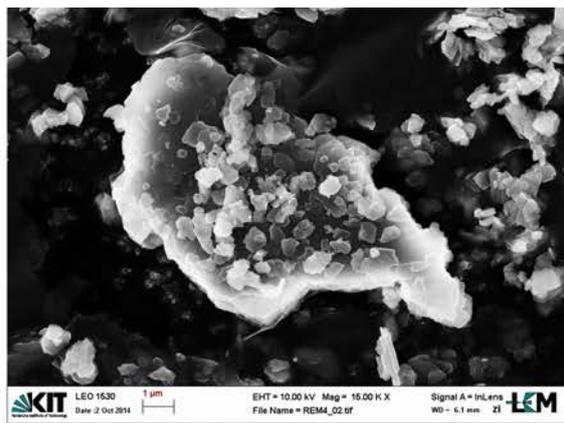


Kaolinite untreated

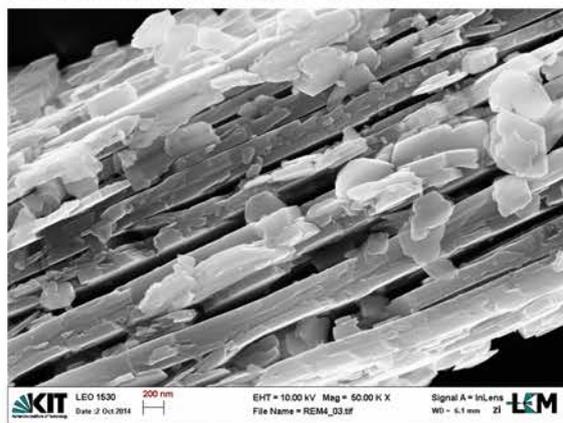
Figure C.5.: SEM images of untreated kaolinite (magnification 15 000 and 50 000)



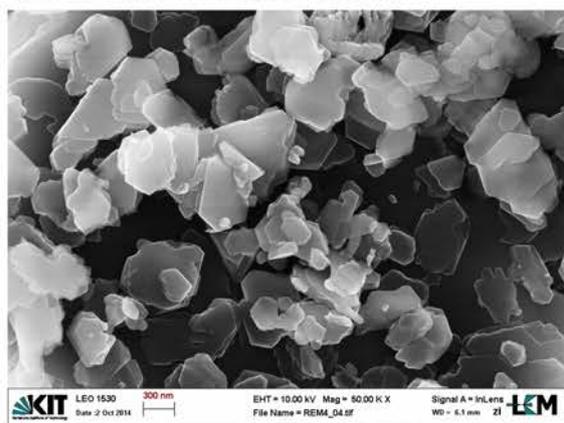
Kaolinite sorption 5000 µg/L Se as SeO_3^{2-}



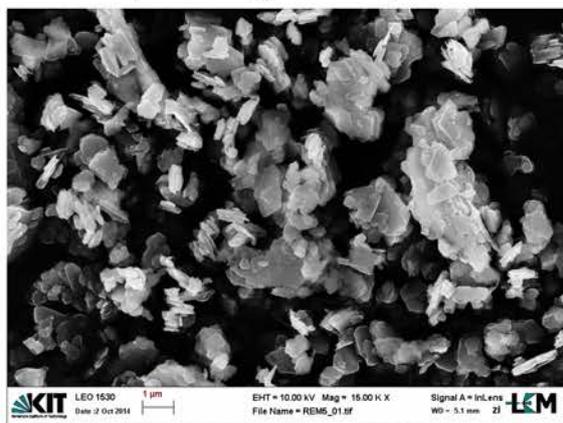
Kaolinite sorption 5000 µg/L Se as SeO_3^{2-}



Kaolinite sorption 5000 µg/L Se as SeO_3^{2-}



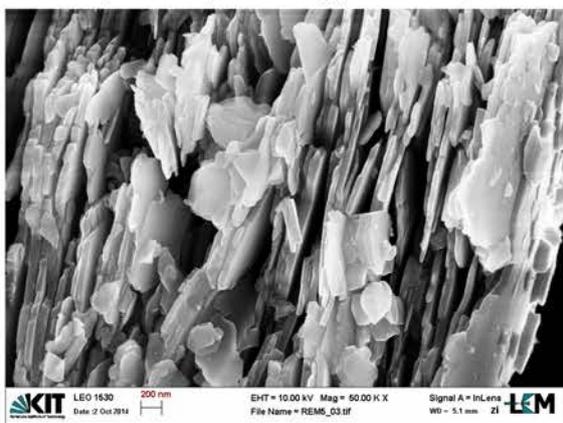
Kaolinite sorption 5000 µg/L Se as SeO_3^{2-}



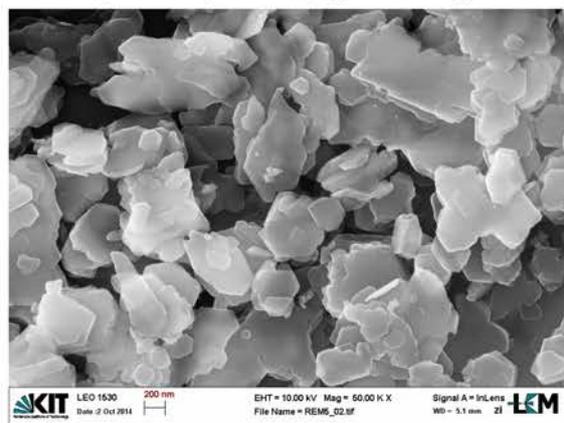
Kaolinite plant + sorption 5000 µg/L Se as SeO_3^{2-}



Kaolinite plant + sorption 5000 µg/L Se as SeO_3^{2-}

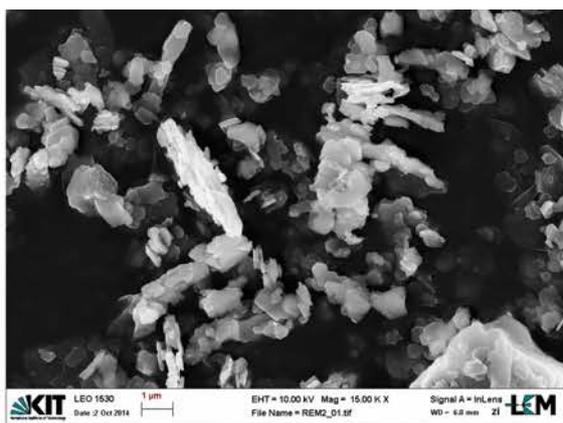


Kaolinite plant + sorption 5000 µg/L Se as SeO_3^{2-}

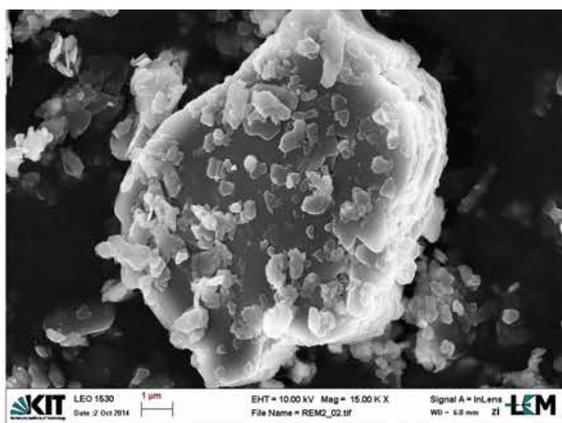


Kaolinite plant + sorption 5000 µg/L Se as SeO_3^{2-}

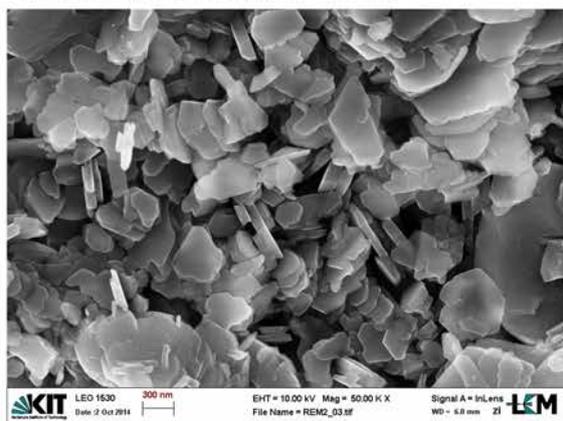
Figure C.6.: SEM images of kaolinite after sorption of 5000 µg/L Se as Na_2SeO_3 in Exp. C (magnification 15 000 and 50 000)



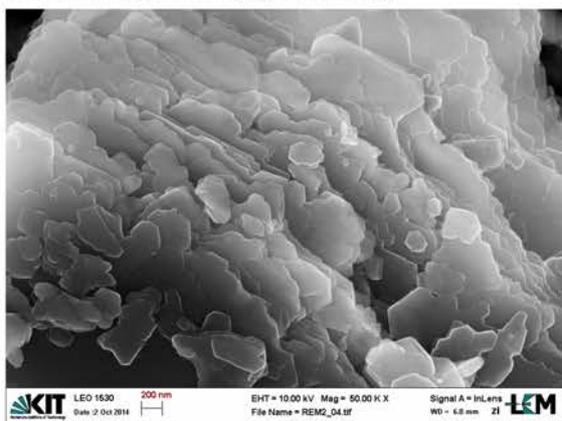
Kaolinite sorption 5000 µg/L Se as SeO_4^{2-}



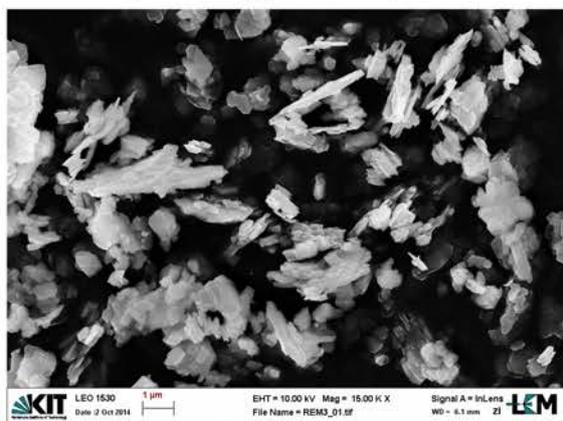
Kaolinite sorption 5000 µg/L Se as SeO_4^{2-}



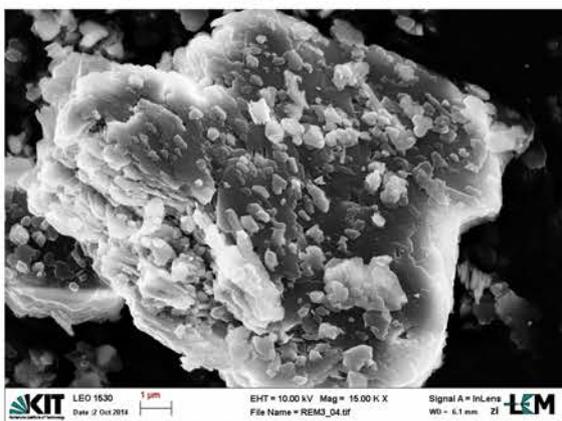
Kaolinite sorption 5000 µg/L Se as SeO_4^{2-}



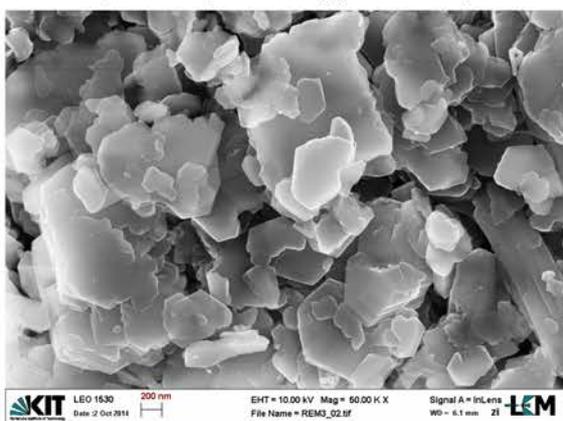
Kaolinite sorption 5000 µg/L Se as SeO_4^{2-}



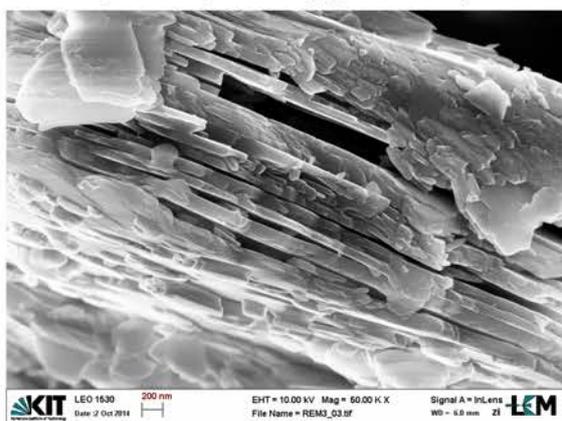
Kaolinite plant + sorption 5000 µg/L Se as SeO_4^{2-}



Kaolinite plant + sorption 5000 µg/L Se as SeO_4^{2-}

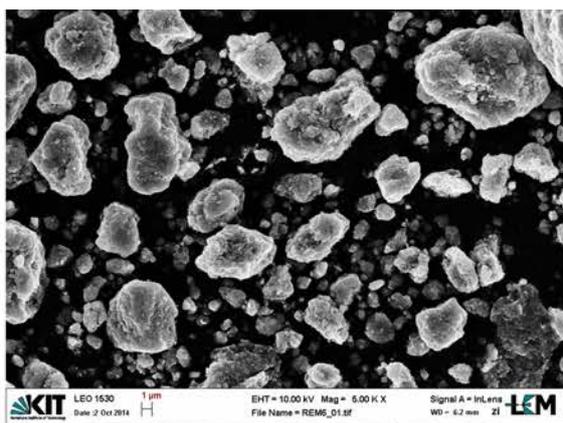


Kaolinite plant + sorption 5000 µg/L Se as SeO_4^{2-}

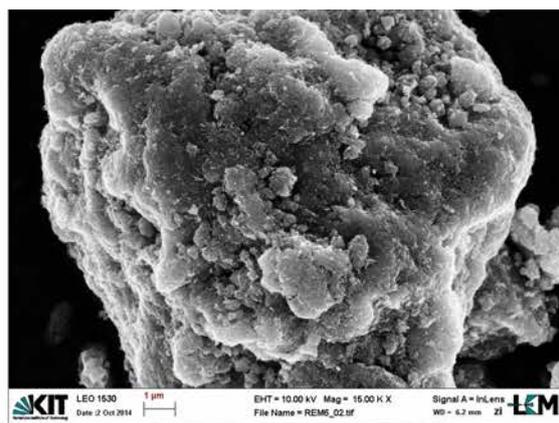


Kaolinite plant + sorption 5000 µg/L Se as SeO_4^{2-}

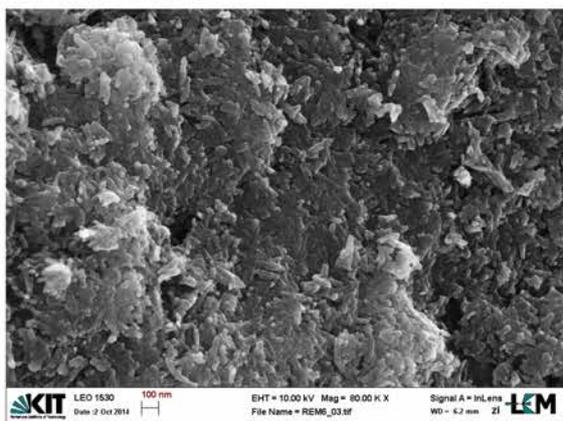
Figure C.7.: SEM images of kaolinite after sorption of 5000 µg/L Se as Na_2SeO_4 in Exp. C (magnification 15 000 and 50 000)



Goethite untreated

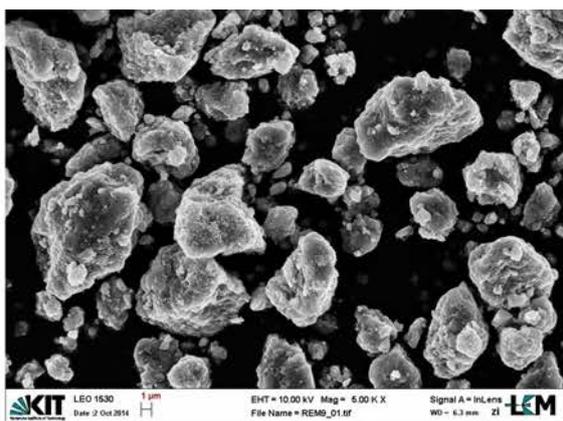


Goethite untreated

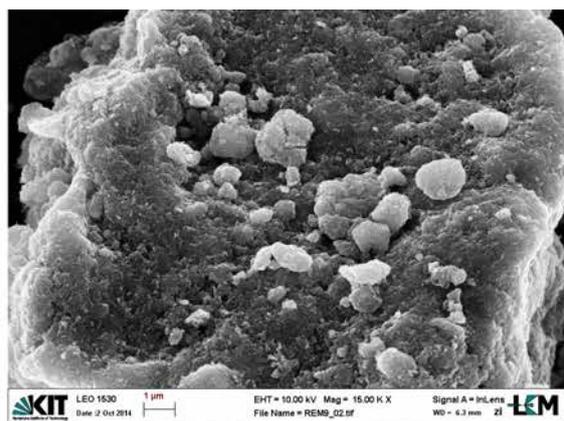


Goethite untreated

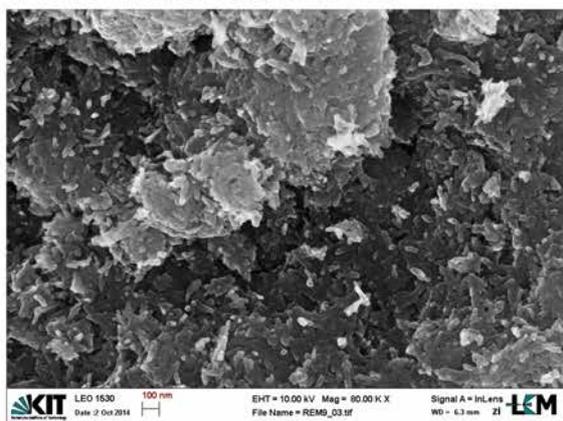
Figure C.8.: SEM images of untreated goethite (magnification 6 000, 15 000 and 50 000)



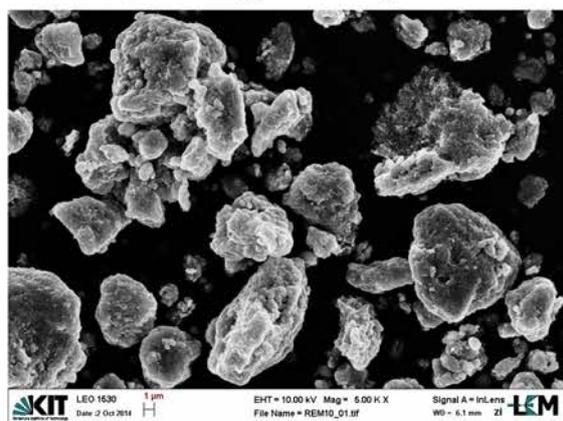
Goethite sorption 5000 µg/L Se as SeO_3^{2-}



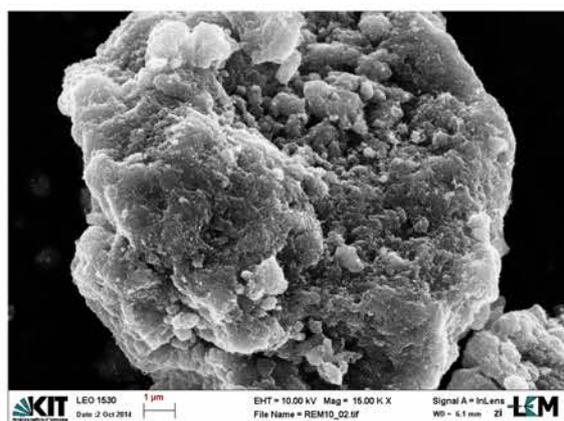
Goethite sorption 5000 µg/L Se as SeO_3^{2-}



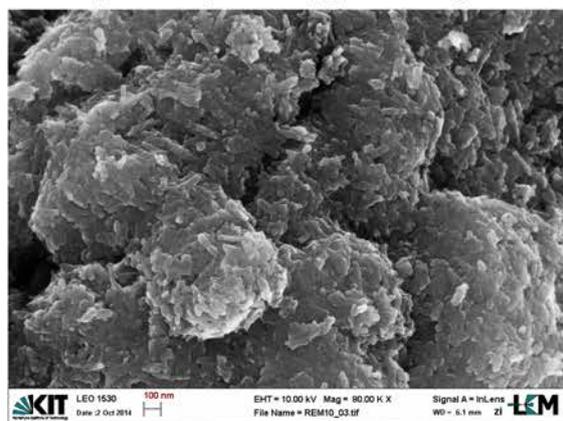
Goethite sorption 5000 µg/L Se as SeO_3^{2-}



Goethite plant + sorption 5000 µg/L Se as SeO_3^{2-}

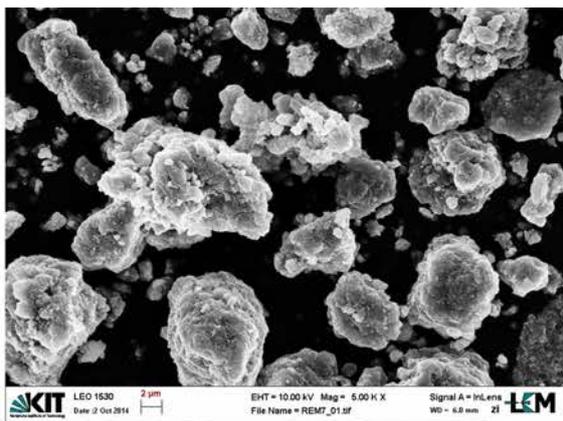


Goethite plant + sorption 5000 µg/L Se as SeO_3^{2-}

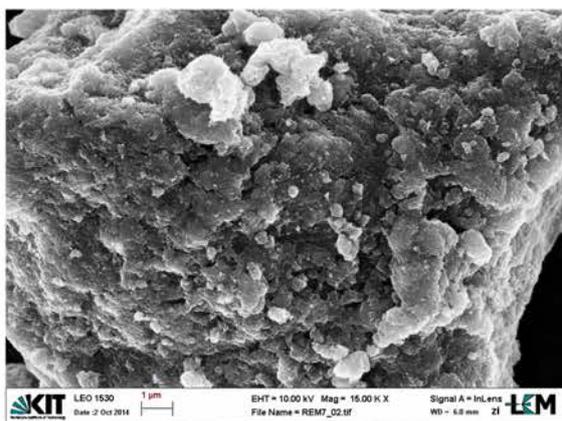


Goethite plant + sorption 5000 µg/L Se as SeO_3^{2-}

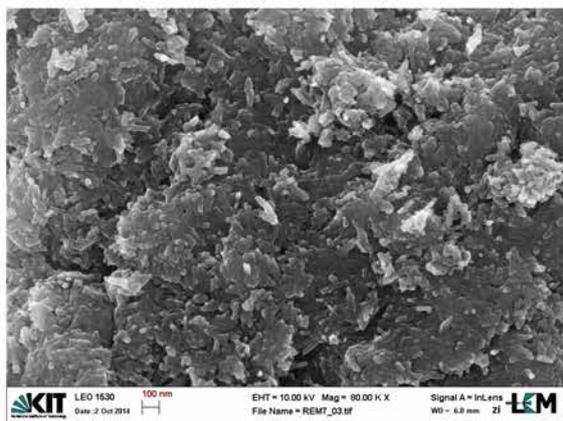
Figure C.9.: SEM images of goethite after sorption of 5000 µg/L Se as Na_2SeO_3 in Exp. C (magnification 6 000, 15 000 and 50 000)



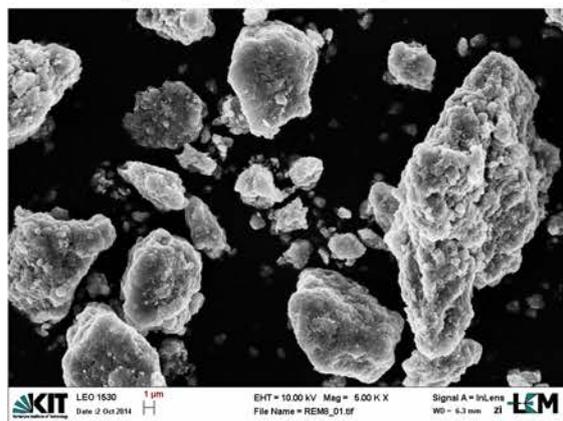
Goethite sorption 5000 µg/L Se as SeO_4^{2-}



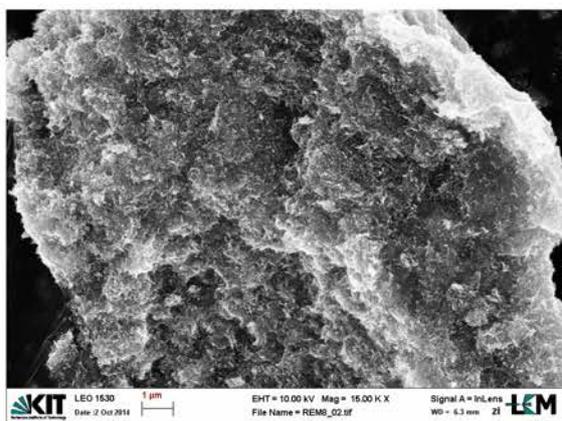
Goethite sorption 5000 µg/L Se as SeO_4^{2-}



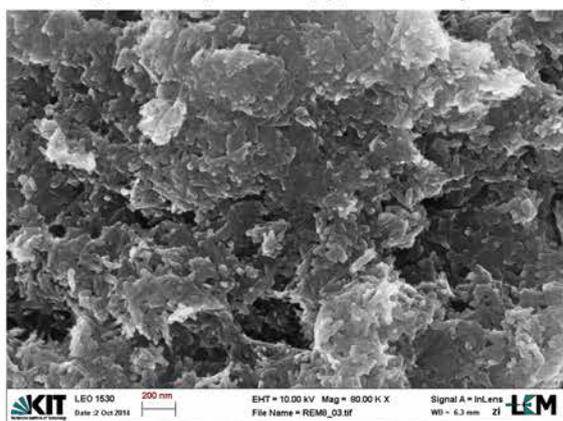
Goethite sorption 5000 µg/L Se as SeO_4^{2-}



Goethite plant + sorption 5000 µg/L Se as SeO_4^{2-}



Goethite plant + sorption 5000 µg/L Se as SeO_4^{2-}



Goethite plant + sorption 5000 µg/L Se as SeO_4^{2-}

Figure C.10.: SEM images of goethite after sorption of 5000 µg/L Se as Na_2SeO_4 in Exp. C (magnification 6 000, 15 000 and 50 000)

C.5.2. C XANES Spectra

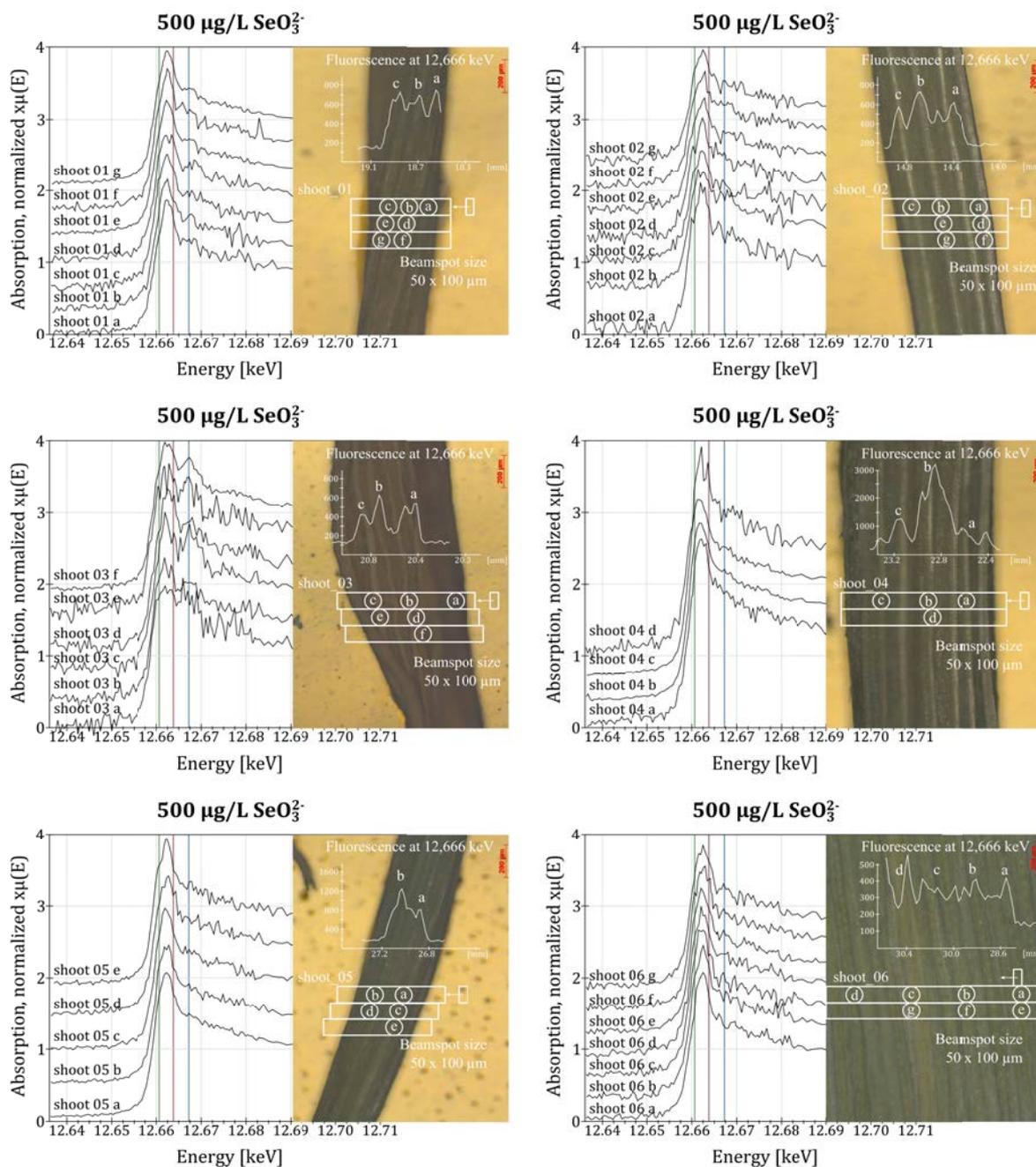


Figure C.11.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 500 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

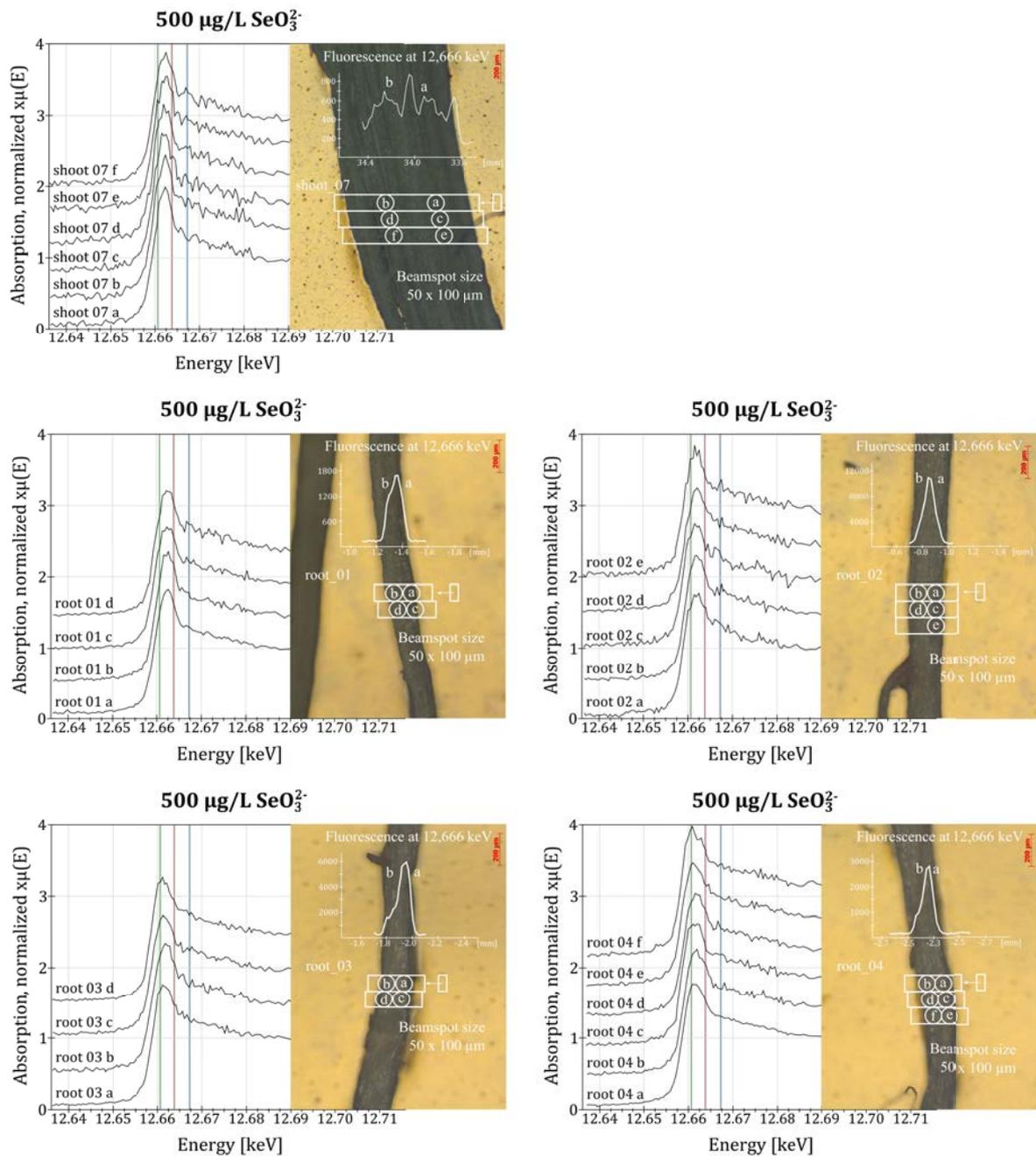


Figure C.12.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 500 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; superimposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

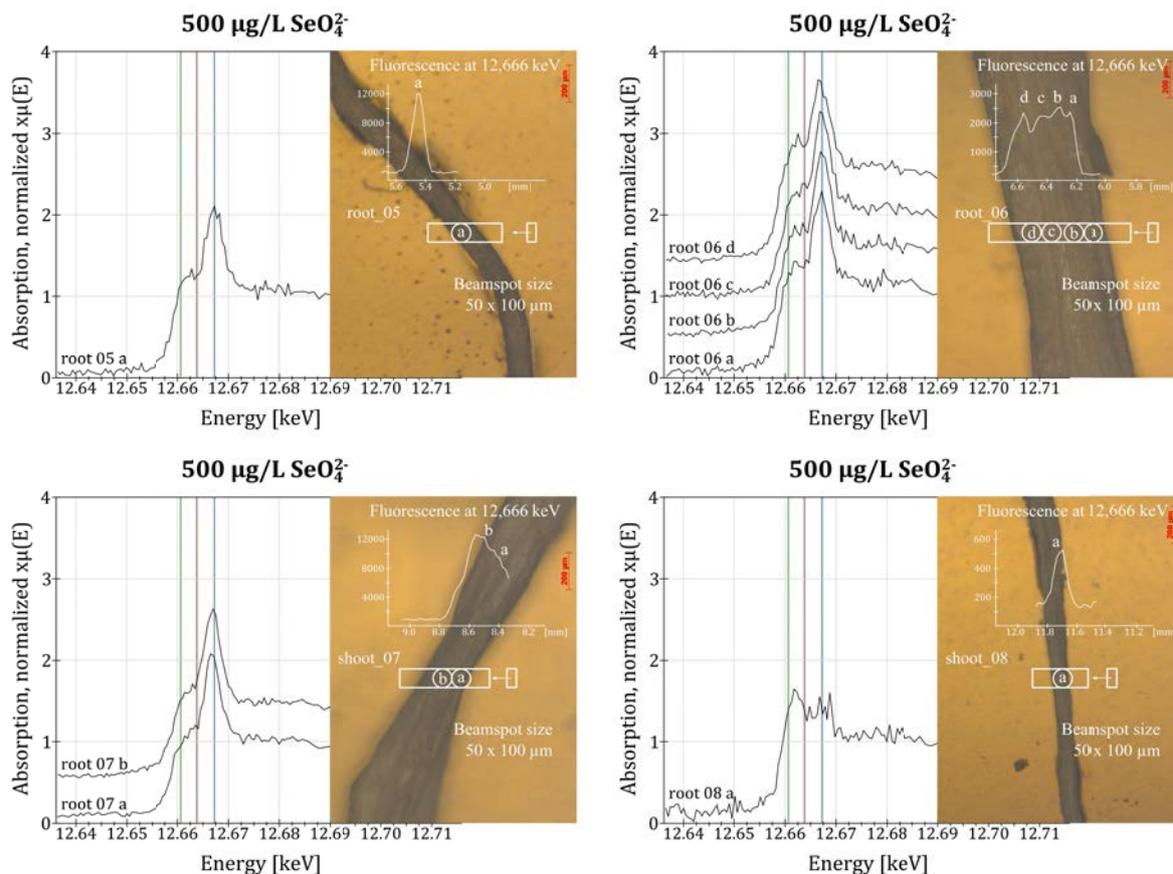


Figure C.13.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 500 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

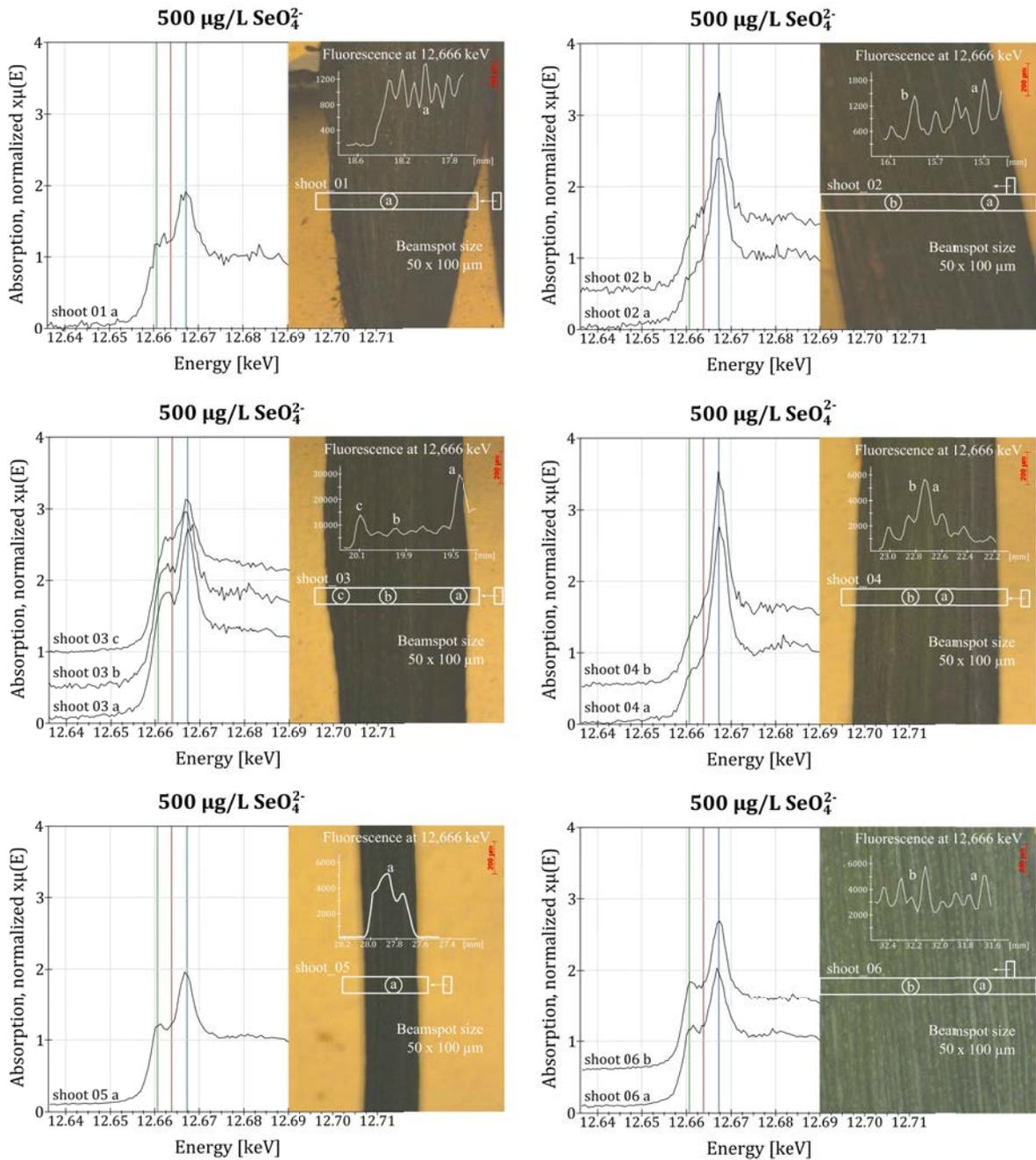


Figure C.14.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 500 µg/L Se as Na₂SeO₄; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

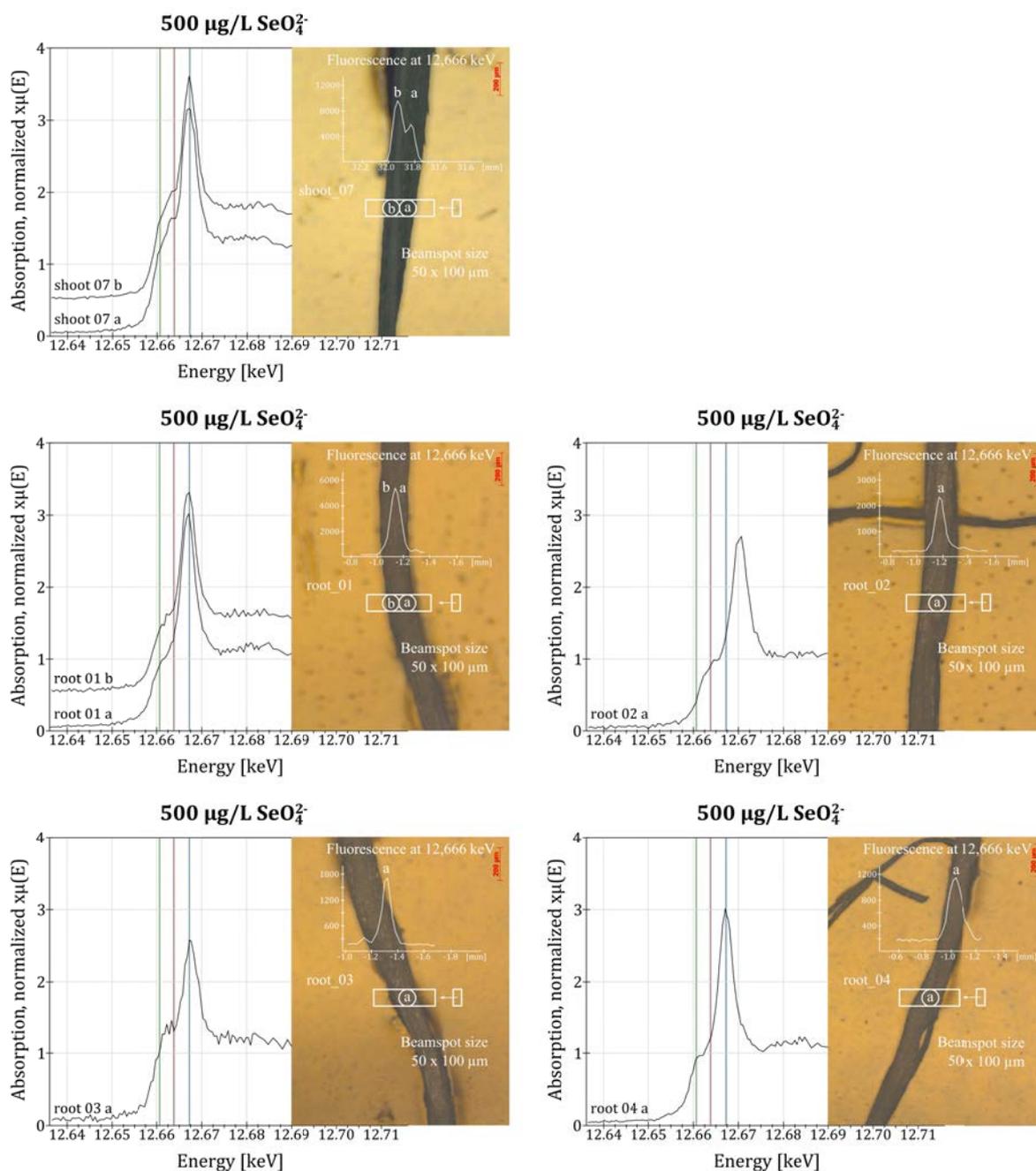


Figure C.15.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 500 µg/L Se as Na₂SeO₄; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

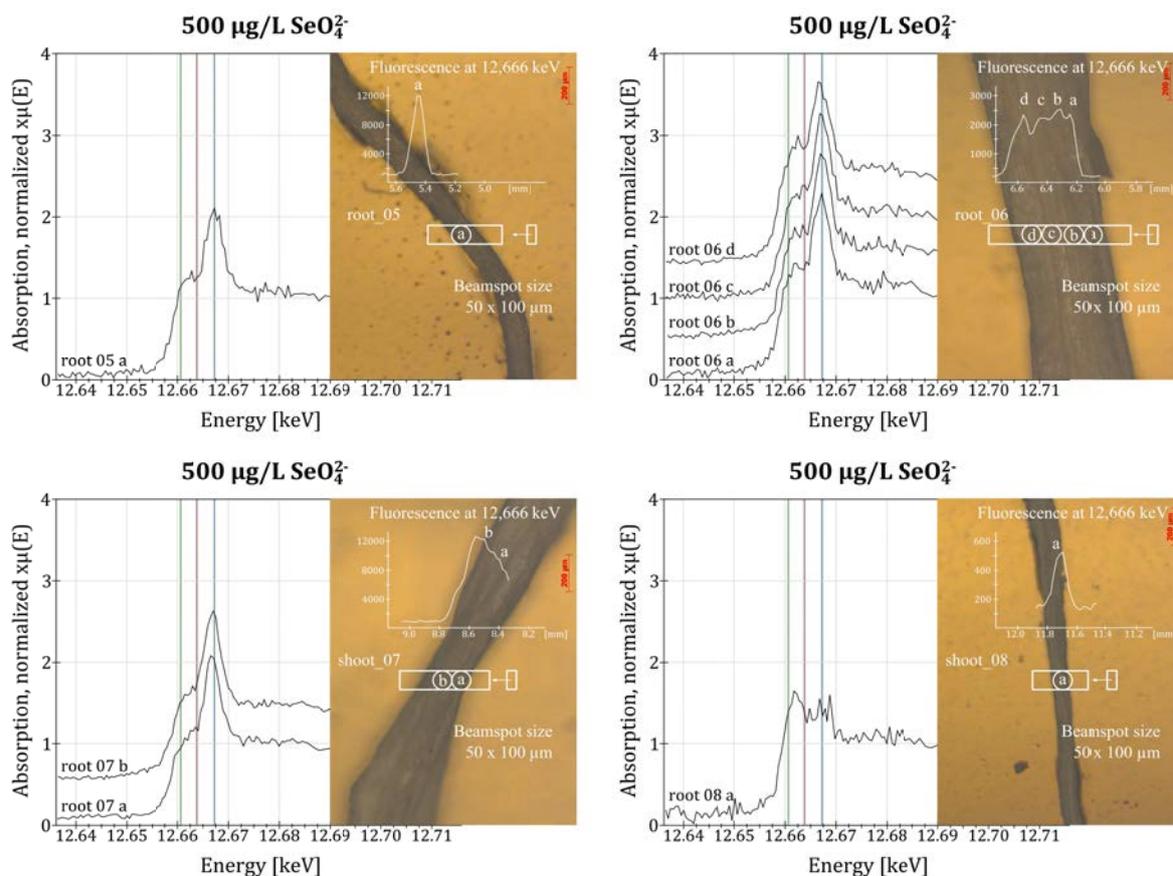


Figure C.16.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 500 µg/L Se as Na₂SeO₄; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

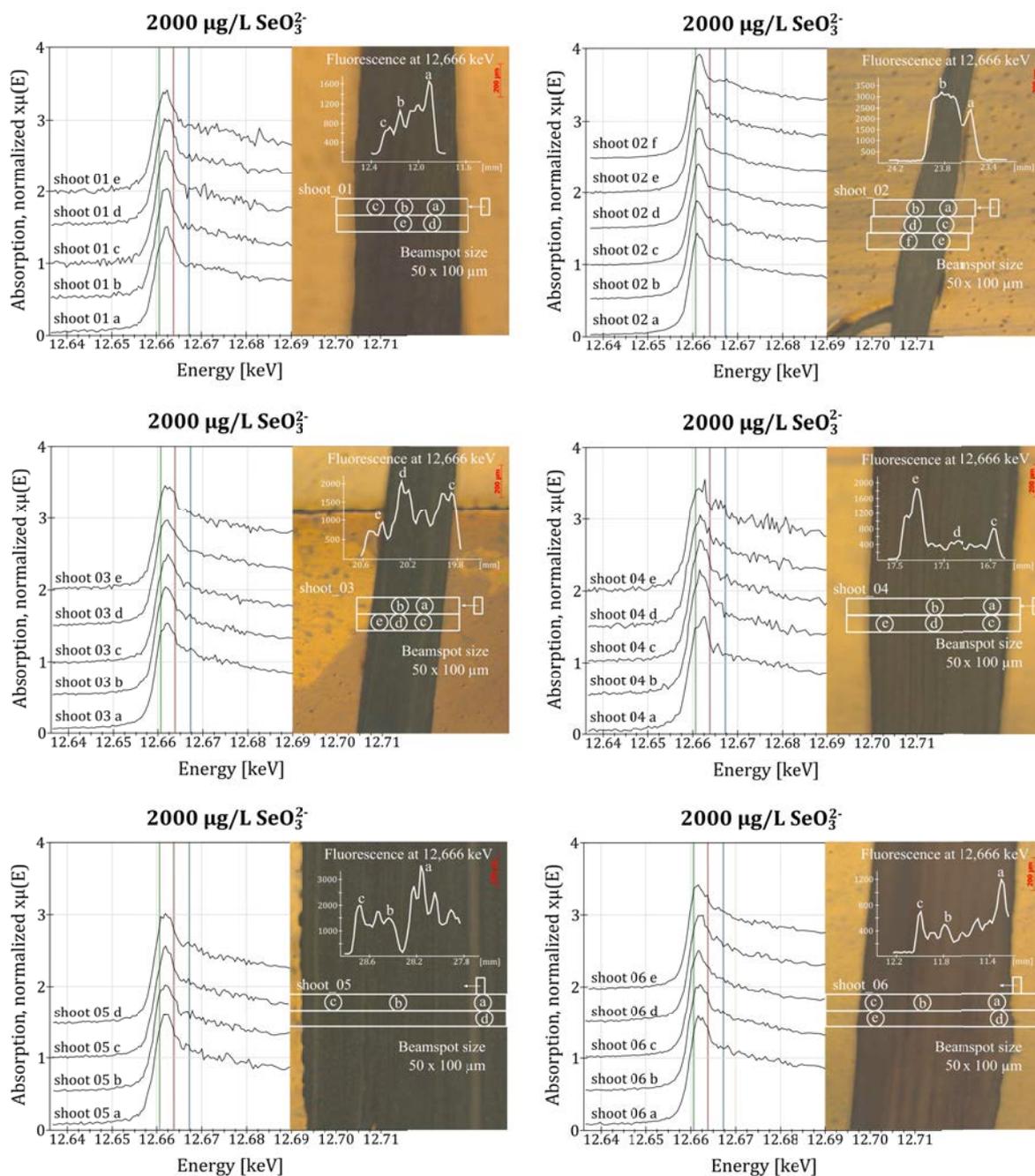


Figure C.17.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 2000 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

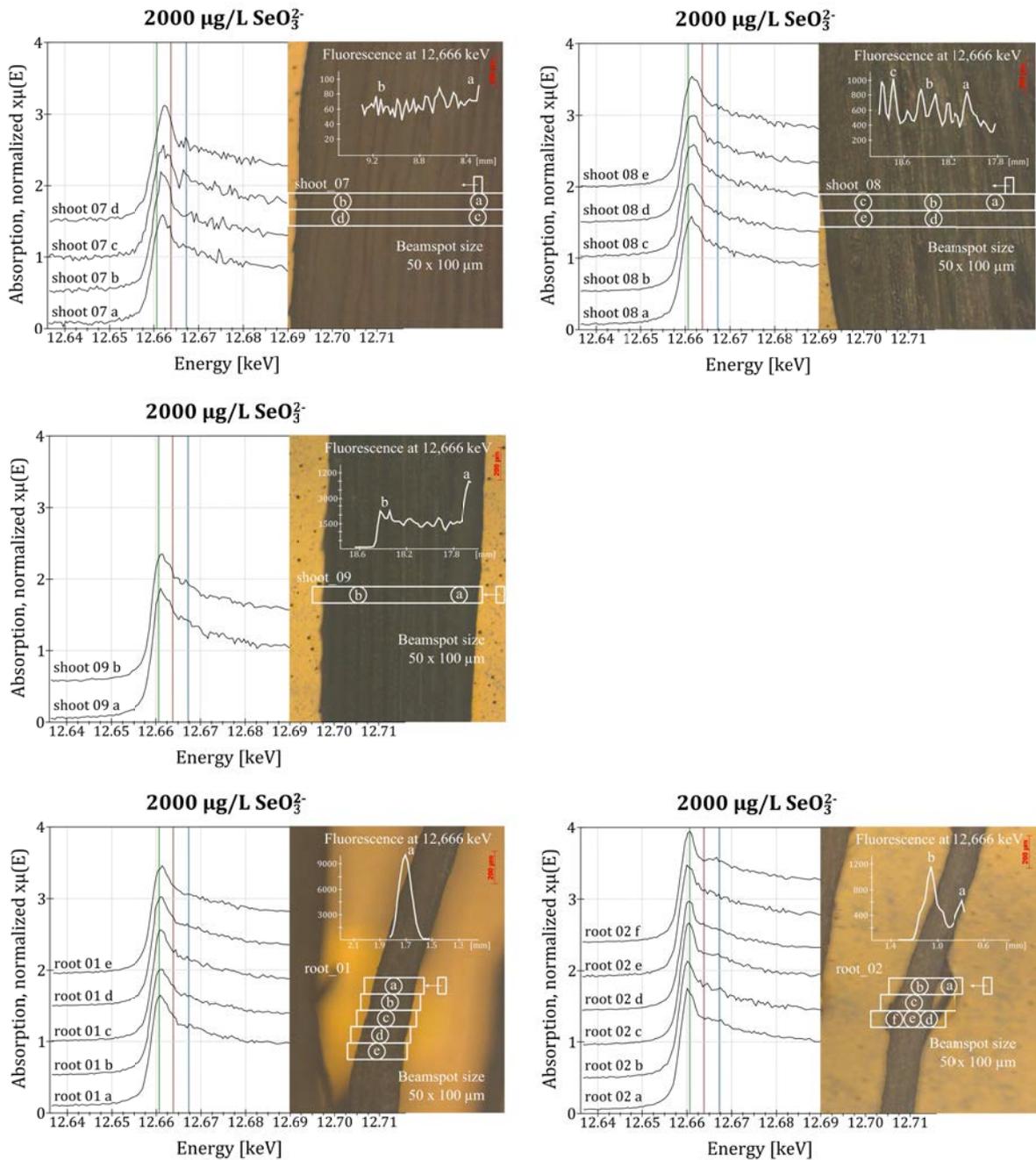


Figure C.18.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 2000 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

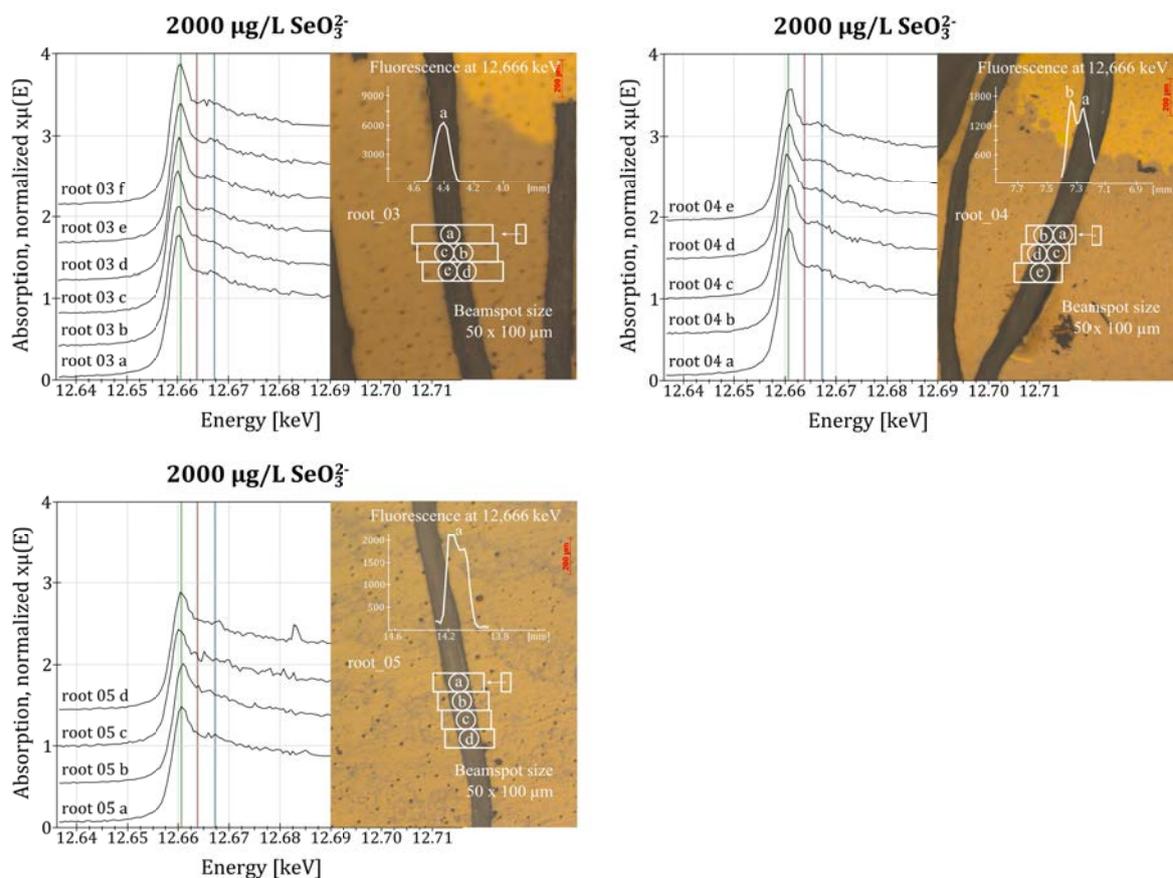


Figure C.19.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 2000 µg/L Se as Na_2SeO_3 ; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

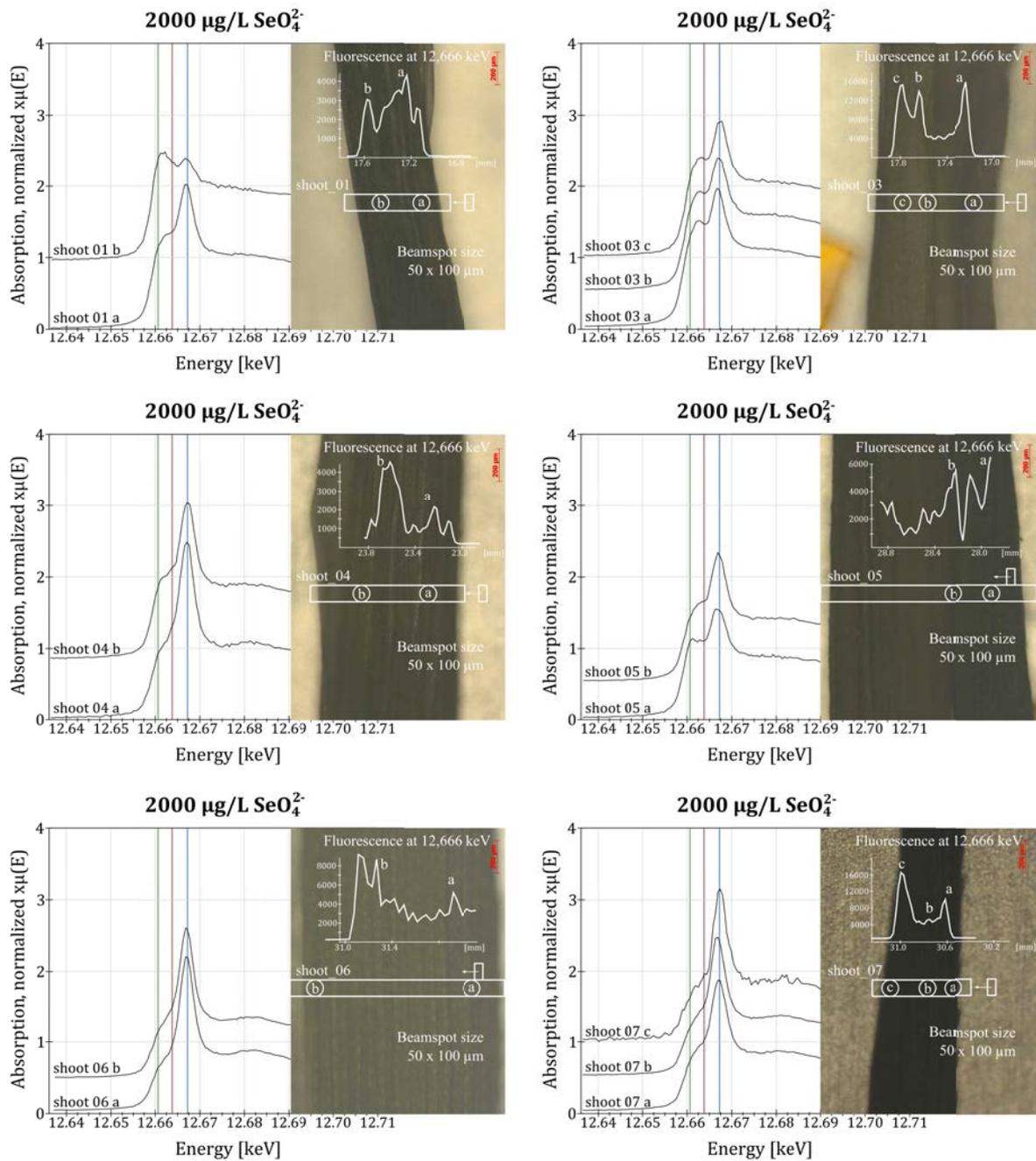


Figure C.20.: all XANES spectra of each region of interest (ROI) on a rice plant treated with 2000 µg/L Se as Na₂SeO₄; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)

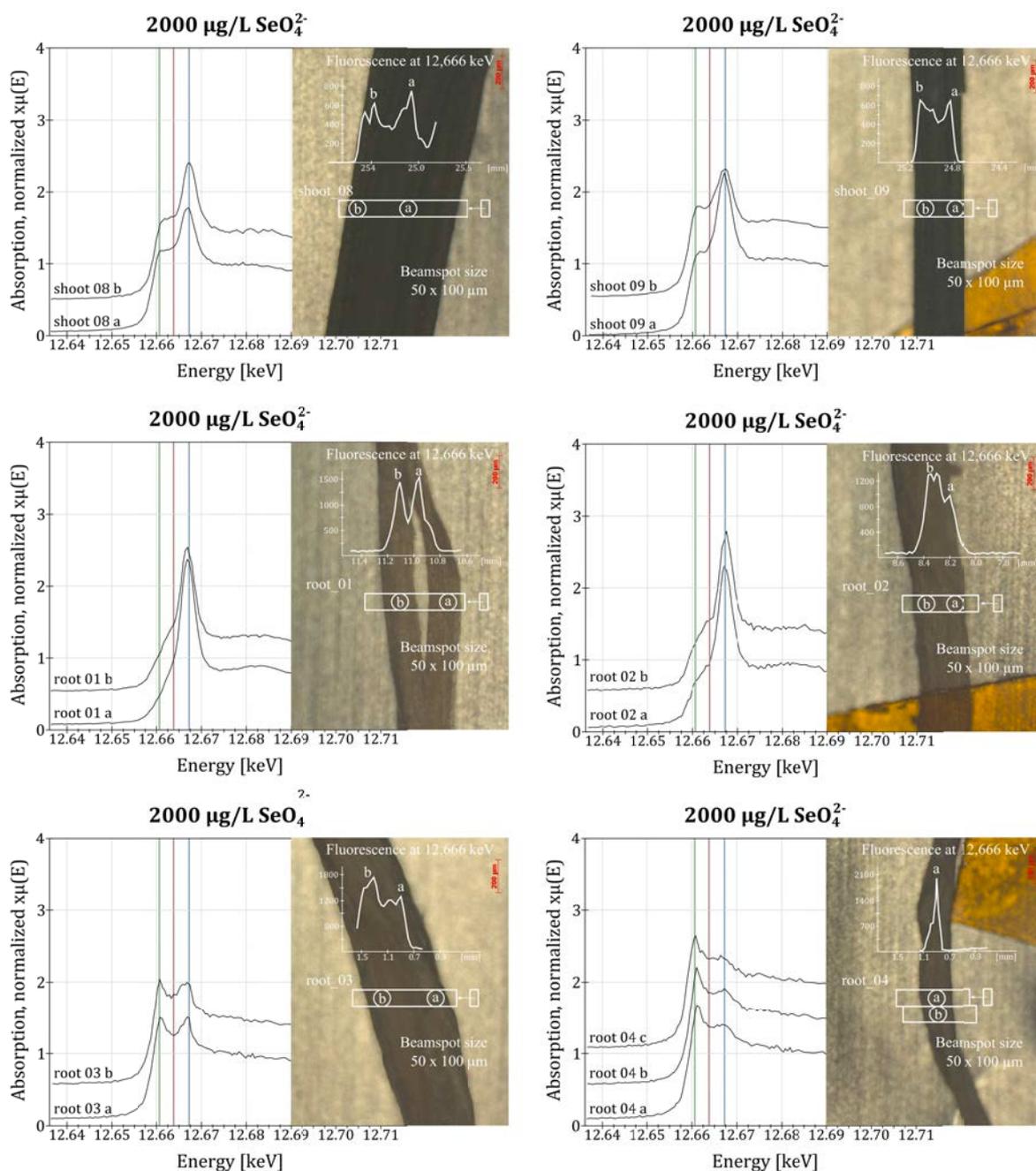


Figure C.21.: all XANES spectra of each region of interest (ROI) on a rice plant treated with 2000 µg/L Se as Na_2SeO_4 ; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)

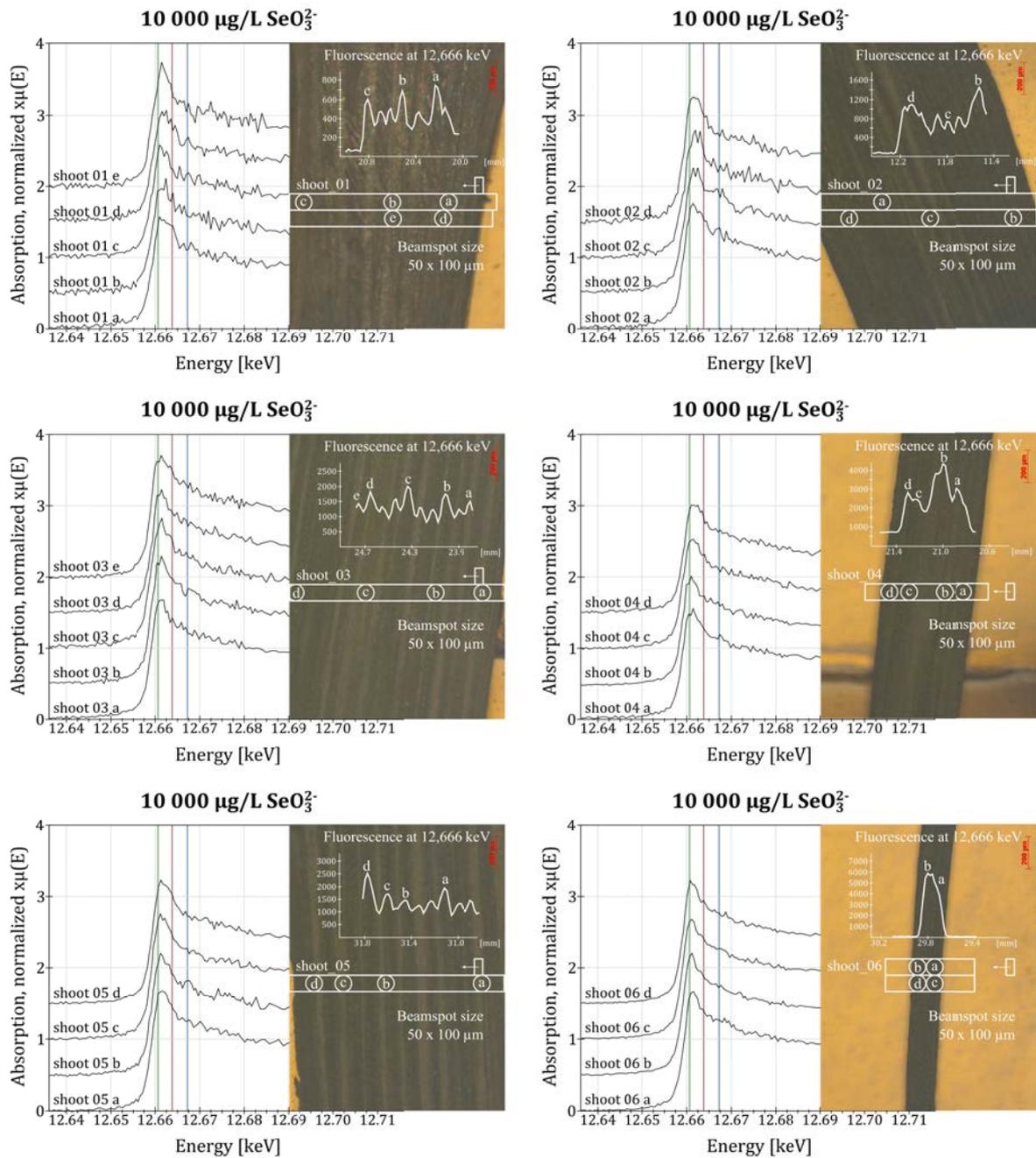


Figure C.22.: all XANES spectra of each region of interest (ROI) on a rice plant treated with 10000 μg/L Se as Na₂SeO₃; right: microscope image (200 μm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)

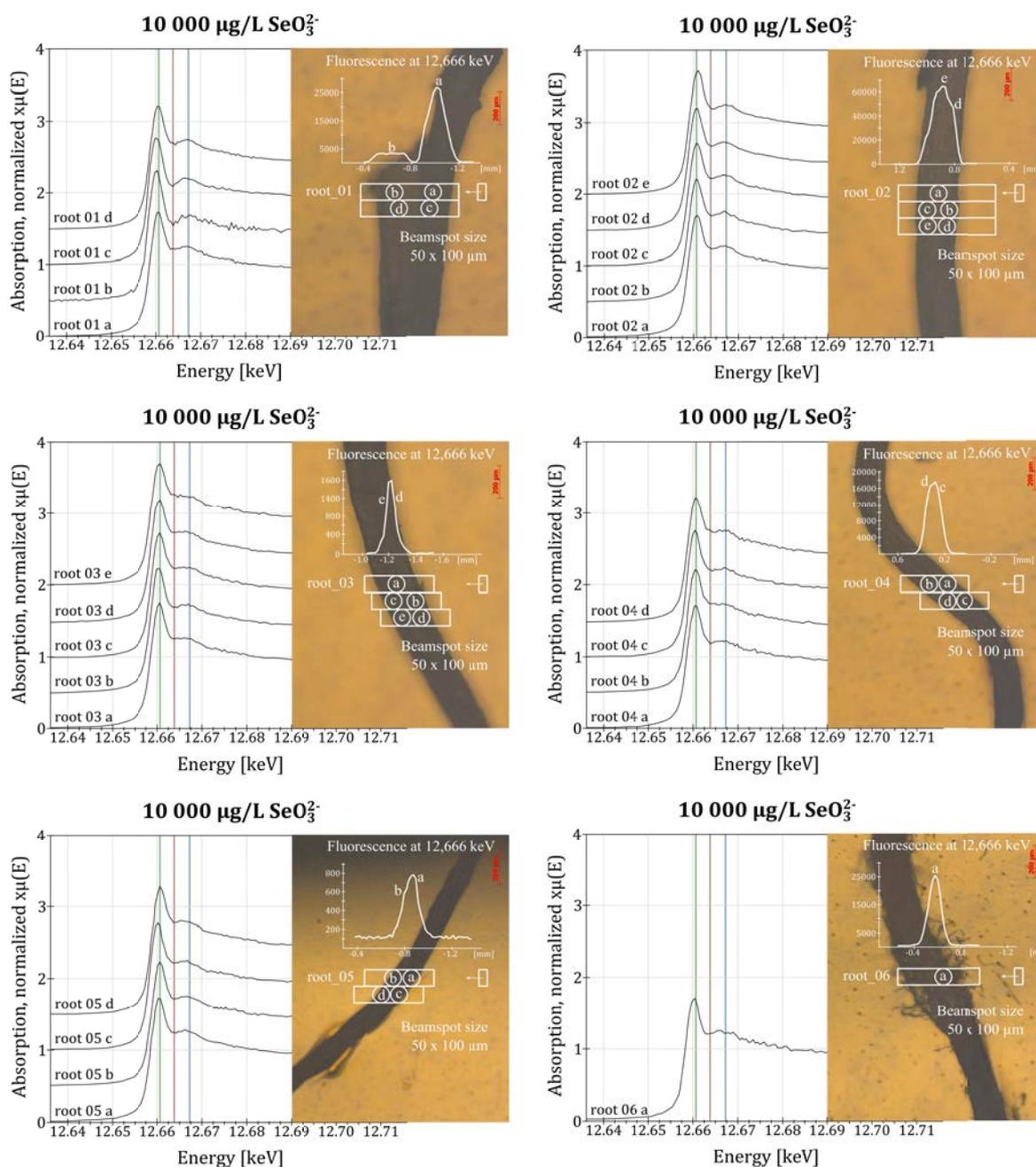


Figure C.23.: all XANES spectra of each region of interest (ROI) on a rice plant treated with 10000 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; superimposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)

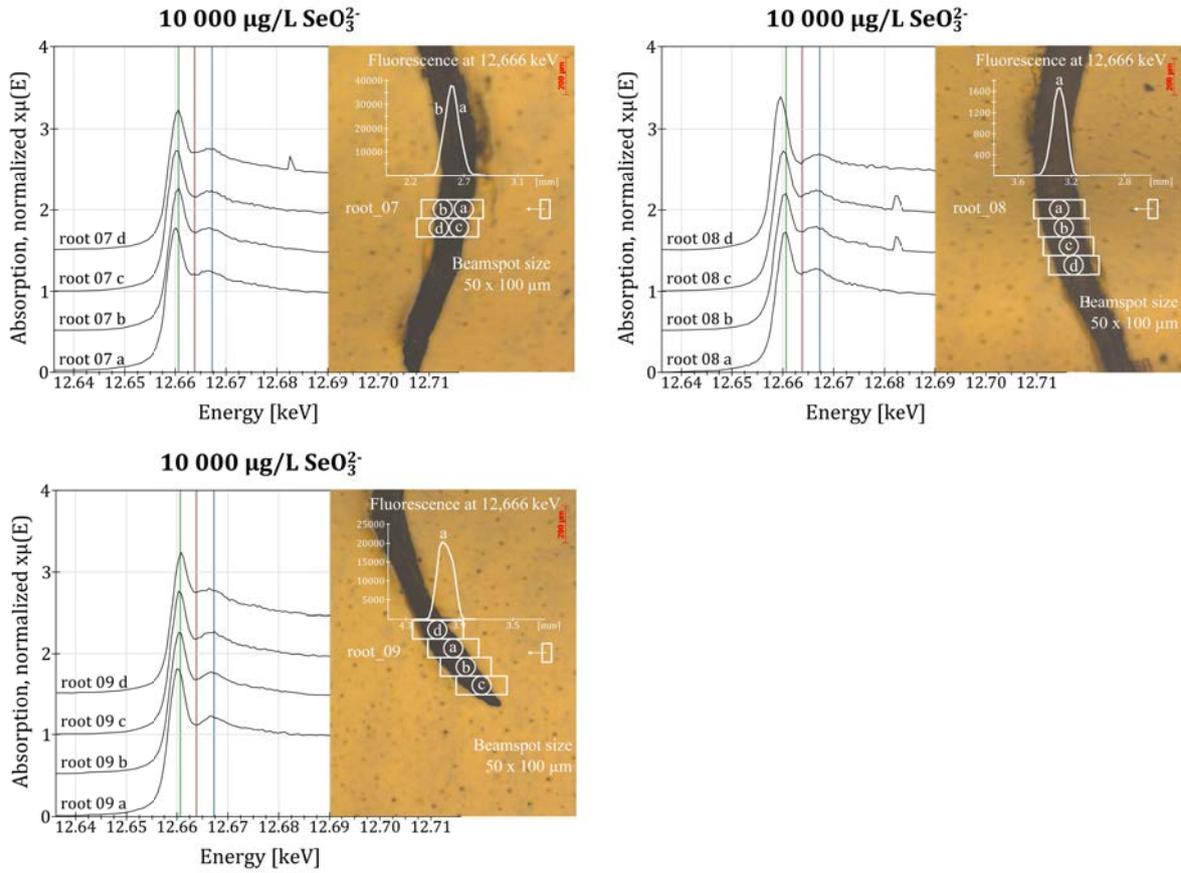


Figure C.24.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 10000 µg/L Se as Na₂SeO₃; right: microscope image (200 µm length indicated in red) of the ROI; super-imposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

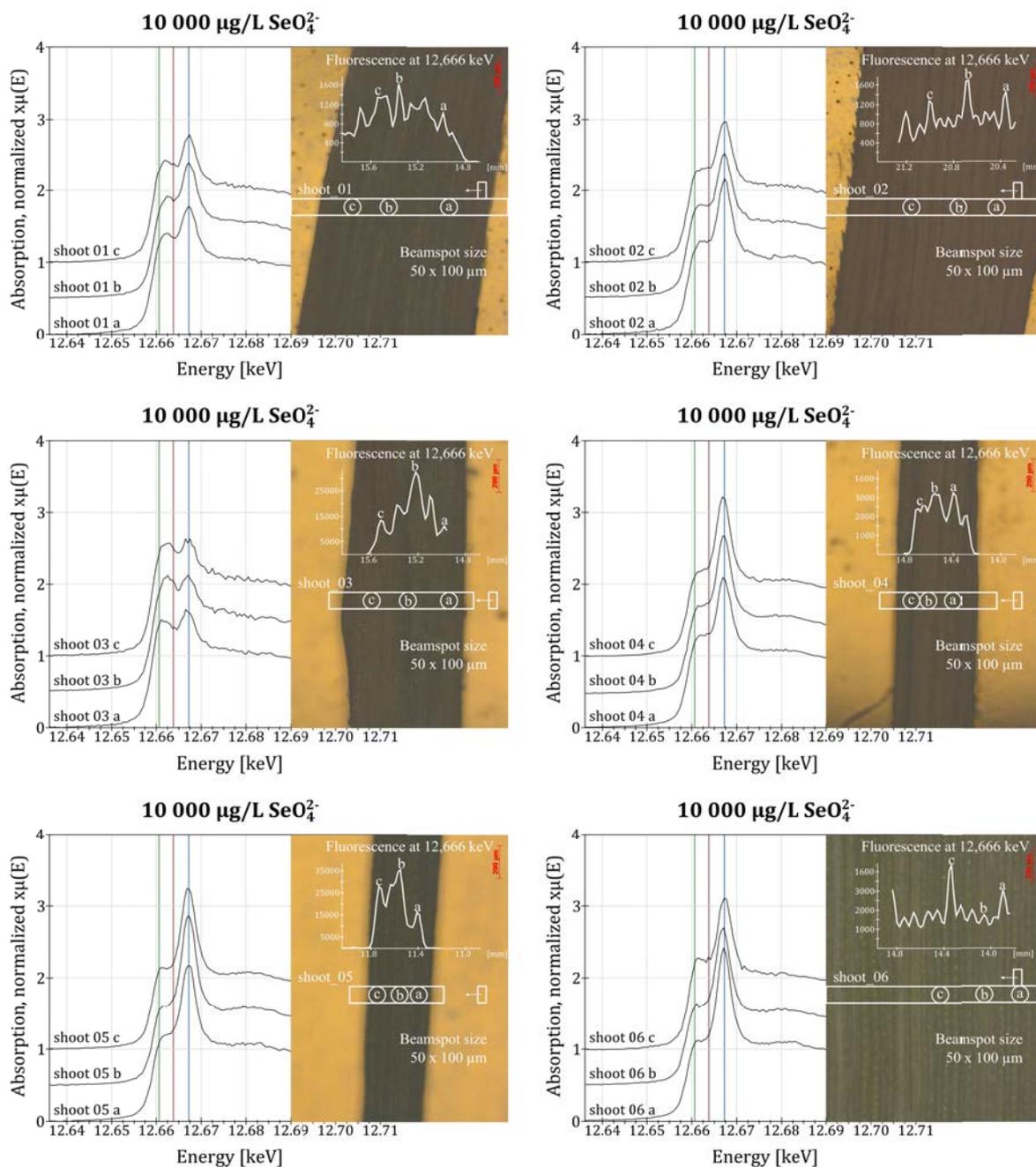


Figure C.25.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with $10000 \mu\text{g/L Se as Na}_2\text{SeO}_4$; right: microscope image ($200 \mu\text{m}$ length indicated in red) of the ROI; superimposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

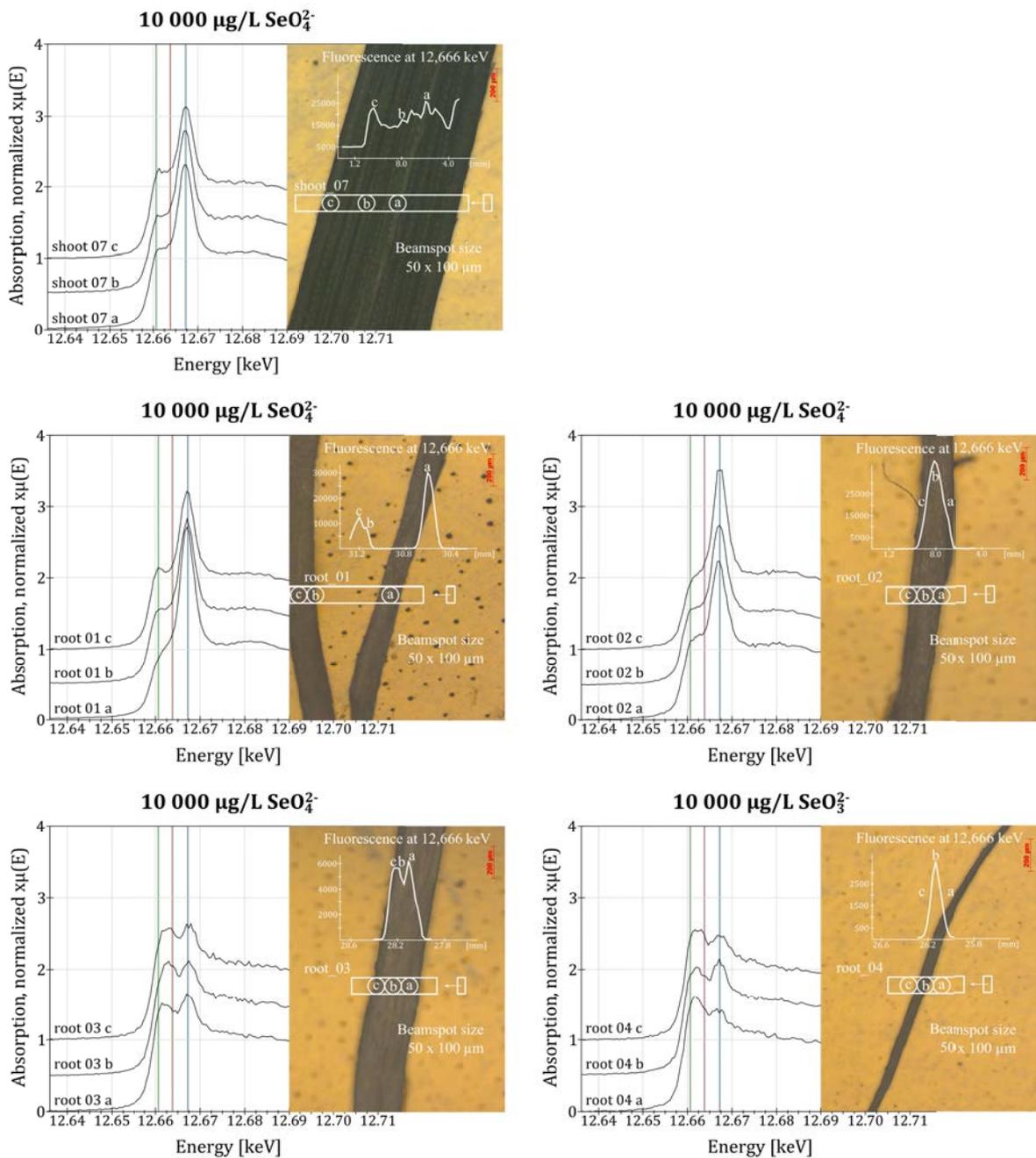


Figure C.26.: *all XANES spectra of each region of interest (ROI) on a rice plant treated with 10000 µg/L Se as Na₂SeO₄; right: microscope image (200 µm length indicated in red) of the ROI; superimposed: result of a fluorescence scan at 12.66 keV across the ROI; letters of the alphabet show where XANES spectra were measured; below each graph: area of XANES spectra on the microscopic image; left: XANES spectra of ROI (each a merge of 2 spectra taken at the exact same spot); green, red & blue indicating peak lines for selenomethionine (12.661 keV), selenite (12.664 keV) and selenate (12.667 keV), respectively)*

Table C.19.: C results for linear combination fitting of merged XANES spectra between 12628 and 12688 eV, fitting all combinations

c(Se) 500 µg/L	Na ₂ SeO ₃						R-factor [-]	Na ₂ SeO ₄								
	org. Se [%]	SD	SeO ₃ ²⁻ [%]	SD	SeO ₄ ²⁻ [%]	SD		c(Se) 500 µg/L	org. Se [%]	SD	SeO ₃ ²⁻ [%]	SD	SeO ₄ ²⁻ [%]	SD	[-]	
root 01	73.32	10.11	26.68	2.50	0.00	0.00	1.57	root 01	31.01	1.94	5.72	2.26	63.27	3.13	0.75	
root 02	76.02	11.10	23.98	2.05	0.00	0.00	1.07	root 02	32.12	2.05	6.11	2.38	61.77	3.14	0.89	
root 03	78.59	7.44	21.41	13.91	0.00	0.00	0.96									
root 04	83.97	9.96	16.03	1.65	0.00	0.00	0.78	root 04	52.71	2.12	17.27	2.46	30.01	3.48	1.08	
root 05	85.21	12.69	14.79	1.52	0.00	0.00	0.67									
root 06	90.75	25.02	9.25	1.38	0.00	0.00	0.56	root 06	50.03	2.17	18.43	2.52	31.55	4.60	1.23	
root 07	100.00	10.59	0.00	0.00	0.00	0.00	0.51	root 07	42.67	19.42	16.01	1.57	41.32	0.76	0.47	
root 08	91.76	1.52	8.24	0.14	0.00	0.00	0.71									
mean	84.95	11.05	15.05	2.89	0.00	0.00	0.85	mean	41.71	5.54	12.71	2.24	45.58	3.02	0.88	
SD	8.97	6.59	8.97	4.54	0.00	0.00	0.35	SD	9.97	7.76	6.26	0.39	16.07	1.40	0.29	
shoot 01	63.98	2.65	36.02	2.65	0.00	0.00	1.97	shoot 01	44.92	2.69	22.78	4.33	32.30	1.51	2.02	
shoot 02	63.31	3.75	36.69	3.75	0.00	0.00	3.59	shoot 02	32.87	2.37	9.47	2.76	57.65	3.64	1.25	
shoot 03	66.58	2.39	33.42	2.39	0.00	0.00	1.63	shoot 03	41.39	2.24	27.74	3.76	30.87	1.26	1.39	
shoot 04	73.90	2.08	26.10	2.08	0.00	0.00	1.22	shoot 04	29.68	1.36	5.59	1.56	64.72	0.77	0.38	
shoot 05	71.45	3.49	28.55	3.49	0.00	0.00	2.94	shoot 05	56.49	1.25	11.04	3.68	32.47	0.71	0.46	
shoot 06	49.72	2.90	50.28	2.90	0.00	0.00	2.20	shoot 06	26.65	1.85	5.91	2.15	67.44	3.40	0.65	
shoot 07	65.40	2.93	34.60	2.93	0.00	0.00	2.25	shoot 07	33.27	2.80	15.57	2.29	51.16	1.11	0.88	
mean	64.90	2.88	35.10	2.88	0.00	0.00	2.26	mean	37.90	2.08	14.02	2.93	48.09	1.77	1.00	
SD	7.75	0.59	7.75	0.59	0.00	0.00	0.80	SD	10.39	0.61	8.50	1.01	16.03	1.23	0.59	
2000 µg/L								2000 µg/L								
root 01	89.13	13.20	10.87	1.61	0.00	0.70	0.43	root 01	13.79	24.36	15.07	2.65	71.14	1.28	0.92	
root 02	97.01	145.02	1.01	1.51	1.98	0.72	0.48	root 02	32.47	1.59	10.39	1.85	57.14	14.30	0.55	
root 03	100.00	1.00	0.00	0.00	0.00	0.00	0.62	root 03	63.97	3.04	26.78	1.82	9.25	0.88	0.71	
root 04	97.08	17.34	0.00	0.00	2.92	0.52	0.34									
root 05	94.09	35.21	4.02	1.51	1.89	0.71	0.48	root 05	80.12	2.37	14.86	1.56	5.02	0.76	0.55	
mean	95.46	42.35	3.18	0.92	1.36	0.53	0.47	mean	47.59	7.84	16.77	1.97	35.64	4.31	0.68	
SD	4.11	58.69	4.60	0.85	1.30	0.31	0.10	SD	29.99	11.03	7.01	0.47	33.45	6.67	0.17	
shoot 01	68.76	2.94	31.24	2.94	0.00	0.00	2.31	shoot 01	55.90	1.37	22.32	3.73	21.78	0.77	0.54	
shoot 02	63.31	3.75	36.69	3.75	0.00	0.00	3.59									
shoot 03	72.93	2.00	27.07	4.13	0.00	0.00	1.11	shoot 03	55.90	1.37	22.32	1.59	21.78	2.10	0.5433	
shoot 04	67.75	3.16	32.25	2.41	0.00	0.00	1.54	shoot 04	38.20	1.50	17.77	1.75	44.03	2.54	0.5436	
shoot 05	69.12	2.58	30.88	2.58	0.00	0.00	1.76	shoot 05	50.25	1.19	19.78	1.36	29.97	0.67	0.3636	
shoot 06	75.89	1.89	24.11	3.74	0.00	0.00	1.01	shoot 06	25.31	2.86	10.03	3.29	64.66	1.61	1.4508	
shoot 07	68.84	3.21	31.16	3.21	0.00	0.00	2.57	shoot 07	33.31	1.71	17.18	1.99	49.51	2.85	0.6466	
shoot 08	74.78	1.82	25.22	4.31	0.00	0.00	0.92	shoot 08	51.95	6.07	17.57	1.59	30.49	0.77	0.5189	
shoot 09	100.00	2.73	0.00	2.41	0.00	0.00	1.78	shoot 09	47.62	1.29	13.18	7.51	39.20	0.73	0.4220	
mean	73.49	2.68	26.51	3.28	0.00	0.00	1.84	mean	44.80	2.17	17.52	2.85	37.68	1.50	0.63	
SD	10.67	0.67	10.67	0.74	0.00	0.00	0.86	SD	11.28	1.66	4.25	2.07	14.77	0.90	0.34	
10000 µg/L								10000 µg/L								
root 01	100.00	1.78	0.00	0.00	0.00	0.00	1.38	root 01	42.53	21.03	6.11	1.52	51.36	0.74	0.39	
root 02	94.64	1.68	2.54	1.95	2.83	2.58	0.84	root 02	47.50	1.15	8.41	1.33	44.09	1.76	0.32	
root 03	100.00	1.13	0.00	0.00	0.00	0.00	0.74	root 03	56.60	17.46	31.33	2.09	12.07	1.01	0.89	
root 04	100.00	1.22	0.00	0.00	0.00	0.00	0.89	root 04	68.20	2.35	23.31	1.79	8.49	0.87	0.66	
root 05	99.40	1.80	0.60	1.80	0.00	0.00	0.97									
root 06	100.00	2.91	0.00	0.00	0.00	0.00	1.87									
root 07	100.00	2.05	0.00	2.05	0.00	0.00	1.26									
root 08	100.00	1.78	0.00	0.00	0.00	0.00	1.98									
root 09	100.00	1.50	0.00	0.00	0.00	0.00	1.35									
mean	99.34	1.76	0.35	0.64	0.31	0.29	1.25	mean	53.71	10.49	17.29	1.69	29.00	1.09	0.56	
SD	1.77	0.52	0.84	0.97	0.94	0.86	0.44	SD	11.28	10.22	12.07	0.33	21.87	0.46	0.26	
shoot 01	75.49	2.53	24.51	1.99	0.00	0.00	1.12	shoot 01	58.43	17.5	19.88	1.65	21.69	0.80	0.52	
shoot 02	74.26	138.12	25.74	1.87	0.00	0.00	0.97	shoot 02	55.80	16.68	12.70	1.59	31.50	0.77	0.52	
shoot 03	80.66	1.45	19.34	1.45	0.00	0.00	0.62	shoot 03	66.46	1.36	22.27	4.18	11.27	0.77	0.51	
shoot 04	81.12	1.41	18.88	1.41	0.00	0.00	0.57	shoot 04	51.80	19.02	12.24	1.51	35.96	0.73	0.45	
shoot 05	75.75	1.75	24.25	1.75	0.00	0.00	0.87	shoot 05	47.58	8.24	9.52	1.48	42.90	0.72	0.41	
shoot 06	80.61	1.54	19.39	1.54	0.00	0.00	0.70	shoot 06	50.05	1.62	6.79	1.46	43.16	0.71	0.40	
								shoot 07	49.91	7.81	9.13	1.24	40.97	0.60	0.29	
mean	77.98	24.47	22.02	1.67	0.00	0.00	0.81	mean	54.29	10.32	13.22	1.87	32.49	0.73	0.44	
SD	3.13	55.68	3.13	0.24	0.00	0.00	0.21	SD	6.53	7.46	5.76	1.03	12.07	0.07	0.09	

C.5.3. C analytical data

Table C.20.: C analytical data - HG-FIAS measurement I

Technique	AA FIAS-MHS							
Spectrometer Model	Aanalyst 200 S/N 200S6110908							
Autosampler Model	AS-90plus							
Batch ID	Plant Digestions							
Results Data Set	Nothstein_2014_07_01							
Date Measured	01.07.2014							
Method Name	Se Nothstein calib 6c							
correl. coeff.	PQL (= lowest calib-10 %)	0.450						
0.999458	LOQ (= 7-wash)	-0.252						
calib. slope	LOD (= 3-wash)	-0.108						
0.01021	analytical quality [%]	117.935						
Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]		
1	Blank	0.0000	0.0018	0.0	0.00	0.00		
2	0.5 ppb	0.0044	0.0008	0.5	0.43	0.08		
3	0.75 ppb	0.0069	0.0008	0.75	0.68	0.08		
4	1.0 ppb	0.0100	0.0014	1.0	0.98	0.14		
5	2.0 ppb	0.0212	0.0018	2.0	2.07	0.18		
6	4.0 ppb	0.0397	0.0007	4.0	3.89	0.07		
7	5.0 ppb	0.0517	0.0017	5.0	5.06	0.17		
8	6.0 ppb	0.0614	0.0008	6.0	6.01	0.08		
Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.116	0.192	0.116	0.192	1	0.12	0.19
2	wash	-0.086	0.105	-0.086	0.105	1	-0.09	0.11
3	6M HCl Blank	-0.123	0.103	-0.141	0.117	4	-0.56	0.47
4	Trace Metal 252 µg/L	2.605	0.157	2.519	0.151	120	302.26	18.18
5	wash	0.072	0.100	0.072	0.100	1	0.07	0.10
6	Se_Std_0	0.002	0.202	0.002	0.202	1	0.00	0.20
7	Se_Std_0.5	0.374	0.084	0.374	0.084	1	0.37	0.08
8	Se_Std_0.75	0.688	0.140	0.688	0.140	1	0.69	0.14
9	Se_Std_1	0.824	0.171	0.824	0.171	1	0.82	0.17
10	Se_Std_2	2.140	0.046	2.140	0.046	1	2.14	0.05
11	Se_Std_4	4.499	0.205	4.499	0.205	1	4.50	0.21
12	Se_Std_5	5.400	0.118	5.400	0.118	1	5.40	0.12
13	Se_Std_6	6.620	0.181	6.620	0.181	1	6.62	0.18
14	wash	-0.137	0.178	-0.137	0.178	1	-0.14	0.18
15	wash	-0.067	0.076	-0.067	0.076	1	-0.07	0.08
16	2014-06-16 digestion blank	0.117	0.271	0.129	0.299	8	< PQL	< PQL
17	2014-06-16 digestion Std Wheat 1567a	1.450	0.159	1.550	0.170	8	12.40	1.36
18	2014-06-16 0 µg/L Shoot	-0.029	0.080	-0.032	0.088	8	< PQL	< PQL
19	2014-06-16 0 µg/L Root	0.005	0.074	0.005	0.082	8	< PQL	< PQL
20	2014-06-16 20 µg/L Shoot	2.108	0.126	1.925	0.115	4	7.70	0.46
21	2014-06-16 20 µg/L Root	0.260	0.109	0.286	0.120	4	1.14	0.48
22	2014-06-16 50 µg/L Shoot	5.757	0.213	5.220	0.193	8	41.76	1.54
23	2014-06-16 50 µg/L Root	1.018	0.163	0.930	0.149	8	7.44	1.19
24	2014-06-16 100 µg/L Shoot	3.720	0.143	3.085	0.119	40	123.40	4.75
25	2014-06-16 100 µg/L Root	0.439	0.089	0.400	0.081	40	16.02	3.25
26	wash	-0.083	0.106	-0.083	0.106	1	-0.08	0.11
27	Se_Std_0	-0.098	0.058	-0.098	0.058	1	-0.10	0.06
28	Se_Std_0.5	0.407	0.140	0.407	0.140	1	0.41	0.14
29	Se_Std_0.75	0.812	0.143	0.812	0.143	1	0.81	0.14
30	Se_Std_1	0.999	0.127	0.999	0.127	1	1.00	0.13
31	Se_Std_2	2.362	0.072	2.362	0.072	1	2.36	0.07
32	Se_Std_4	4.599	0.193	4.599	0.193	1	4.60	0.19
33	Se_Std_5	5.671	0.143	5.671	0.143	1	5.67	0.14
34	Se_Std_6	6.845	0.192	6.845	0.192	1	6.84	0.19
35	wash	-0.032	0.133	-0.032	0.133	1	-0.03	0.13
36	wash	-0.053	0.071	-0.053	0.071	1	-0.05	0.07
37	2014-06-17 digestion blank	-0.101	0.077	-0.107	0.082	8	< PQL	< PQL
38	2014-06-17 digestion Std Wheat 1567a	1.447	0.104	1.372	0.098	8	10.98	0.79
39	2014-06-17 200 µg/L Shoot	4.851	0.212	3.931	0.172	40	157.23	6.88
40	2014-06-17 200 µg/L Root	0.693	0.129	0.578	0.108	40	23.12	4.32
41	2014-06-17 500 µg/L Shoot	8.031	0.171	7.082	0.151	80	> calib	> calib
42	2014-06-17 500 µg/L Root	1.562	0.050	1.378	0.044	80	110.23	3.54
43	2014-06-17 1000 µg/L Shoot	13.127	0.517	11.576	0.456	80	> calib	> calib
44	2014-06-17 1000 µg/L Root	2.438	0.118	2.151	0.104	80	172.04	8.33
45	2014-06-17 2000 µg/L Shoot	7.425	0.198	6.548	0.174	400	> calib	> calib
46	2014-06-17 2000 µg/L Root	2.154	0.136	1.900	0.120	200	379.99	23.92
47	wash	-0.019	0.104	-0.019	0.104	1	-0.02	0.10
48	Se_Std_0	-0.020	0.130	-0.020	0.130	1	-0.02	0.13
49	Se_Std_0.5	0.405	0.144	0.405	0.144	1	0.41	0.14
50	Se_Std_0.75	0.767	0.096	0.767	0.096	1	0.77	0.10
51	Se_Std_1	1.060	0.126	1.060	0.126	1	1.06	0.13
52	Se_Std_2	2.268	0.129	2.268	0.129	1	2.27	0.13
53	Se_Std_4	4.647	0.222	4.647	0.222	1	4.65	0.22
54	Se_Std_5	5.554	0.025	5.554	0.025	1	5.55	0.02
55	Se_Std_6	6.600	0.172	6.600	0.172	1	6.60	0.17
56	wash	-0.171	0.121	-0.171	0.121	1	-0.17	0.12
57	wash	-0.001	0.098	-0.001	0.098	1	0.00	0.10
58	2014-06-20 digestion blank	-0.080	0.066	-0.082	0.067	8	< PQL	< PQL
59	2014-06-20 digestion Std Wheat 1567a	1.470	0.201	1.421	0.195	8	11.37	1.56
60	2014-06-20 5000 µg/L Shoot	13.901	0.384	12.218	0.337	400	> calib	> calib
61	2014-06-20 5000 µg/L Root	5.147	0.237	4.672	0.215	200	934.41	43.07
62	2014-06-20 10 000 µg/L Shoot	17.572	0.117	15.445	0.103	400	> calib	> calib
63	2014-06-20 10 000 µg/L Root	8.103	0.077	7.122	0.068	200	> calib	> calib
64	2014-06-20 0 µg/L Shoot	0.011	0.117	0.011	0.119	8	< PQL	< PQL
65	2014-06-20 0 µg/L Root	-0.105	0.061	-0.106	0.062	8	< PQL	< PQL
66	2014-06-20 20 µg/L Shoot	1.214	0.082	1.174	0.080	8	9.39	0.64
67	2014-06-20 20 µg/L Root	1.293	0.180	1.250	0.174	8	10.00	1.39

Table C.21.: C analytical data - HG-FIAS measurement I (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
68	wash	-0.098	0.086	-0.098	0.086	1	-0.10	0.09
69	Se_Std_0	-0.045	0.047	-0.045	0.047	1	-0.05	0.05
70	Se_Std_0.5	0.449	0.142	0.449	0.142	1	0.45	0.14
71	Se_Std_0.75	0.739	0.053	0.739	0.053	1	0.74	0.05
72	Se_Std_1	0.963	0.034	0.963	0.034	1	0.96	0.03
73	Se_Std_2	2.300	0.296	2.300	0.296	1	2.30	0.30
74	Se_Std_4	4.464	0.170	4.464	0.170	1	4.46	0.17
75	Se_Std_5	5.506	0.092	5.506	0.092	1	5.51	0.09
76	Se_Std_6	6.879	0.133	6.879	0.133	1	6.88	0.13
77	wash	0.002	0.075	0.002	0.075	1	0.00	0.07
78	wash	-0.077	0.106	-0.077	0.106	1	-0.08	0.11
79	2014-06-23 digestion blank	-0.053	0.156	-0.058	0.171	8	< PQL	< PQL
80	2014-06-23 digestion Std Wheat 1567a	1.535	0.084	1.433	0.078	8	11.47	0.63
81	2014-06-23 50 µg/L Shoot	3.917	0.176	3.219	0.145	8	25.75	1.16
82	2014-06-23 50 µg/L Root	4.072	0.129	3.346	0.106	8	26.77	0.85
83	2014-06-23 100 µg/L Shoot	0.828	0.062	0.787	0.059	40	31.48	2.36
84	2014-06-23 100 µg/L Root	0.418	0.108	0.458	0.118	40	18.33	4.74
85	2014-06-23 200 µg/L Shoot	3.863	0.146	3.175	0.120	40	126.98	4.81
86	2014-06-23 200 µg/L Root	4.150	0.122	3.410	0.101	40	136.42	4.02
87	2014-06-23 500 µg/L Shoot	3.335	0.080	2.741	0.066	80	219.24	5.27
88	2014-06-23 500 µg/L Root	4.402	0.227	3.617	0.187	80	289.40	14.95
89	wash	-0.061	0.136	-0.061	0.136	1	-0.06	0.14
90	Se_Std_0	-0.018	0.189	-0.018	0.189	1	-0.02	0.19
91	Se_Std_0.5	0.336	0.129	0.336	0.129	1	0.34	0.13
92	Se_Std_0.75	0.682	0.112	0.682	0.112	1	0.68	0.11
93	Se_Std_1	1.125	0.186	1.125	0.186	1	1.13	0.19
94	Se_Std_2	2.275	0.103	2.275	0.103	1	2.27	0.10
95	Se_Std_4	4.693	0.049	4.693	0.049	1	4.69	0.05
96	Se_Std_5	5.827	0.164	5.827	0.164	1	5.83	0.16
97	Se_Std_6	6.777	0.229	6.777	0.229	1	6.78	0.23
98	wash	0.058	0.144	0.058	0.144	1	0.06	0.14
99	wash	-0.033	0.070	-0.033	0.070	1	-0.03	0.07
100	2014-06-24 digestion blank	-0.067	0.114	-0.073	0.125	8	< PQL	< PQL
101	2014-06-24 digestion Std Wheat 1567a	1.495	0.175	1.290	0.151	8	10.32	1.21
102	2014-06-24 1000 µg/L Shoot	7.286	0.136	6.132	0.115	80	> calib	> calib
103	2014-06-24 1000 µg/L Root	9.085	0.204	7.646	0.171	80	> calib	> calib
104	2014-06-24 2000 µg/L Shoot	2.127	0.106	1.814	0.091	400	725.40	36.24
105	2014-06-24 2000 µg/L Root	6.997	0.243	5.889	0.204	200	> calib	> calib
106	2014-06-24 5000 µg/L Shoot	2.674	0.108	2.280	0.092	400	911.87	36.90
107	2014-06-24 5000 µg/L Root	11.693	0.371	9.842	0.312	200	> calib	> calib
108	2014-06-24 10 000 µg/L Shoot	1.326	0.092	1.144	0.080	400	457.57	31.82
109	2014-06-24 10 000 µg/L Root	10.627	0.282	8.944	0.237	200	> calib	> calib
110	wash	0.022	0.113	0.022	0.113	1	0.02	0.11
111	Se_Std_0	-0.032	0.120	-0.032	0.120	1	-0.03	0.12
112	Se_Std_0.5	0.449	0.121	0.449	0.121	1	0.45	0.12
113	Se_Std_0.75	0.871	0.165	0.871	0.165	1	0.87	0.16
114	Se_Std_1	1.101	0.163	1.101	0.163	1	1.10	0.16
115	Se_Std_2	2.478	0.073	2.478	0.073	1	2.48	0.07
116	Se_Std_4	4.747	0.065	4.747	0.065	1	4.75	0.06
117	Se_Std_5	5.892	0.154	5.892	0.154	1	5.89	0.15
118	Se_Std_6	7.151	0.162	7.151	0.162	1	7.15	0.16
119	wash	-0.014	0.127	-0.014	0.127	1	-0.01	0.13
120	wash	-0.045	0.120	-0.045	0.120	1	-0.05	0.12
121	2014-06-17 500 µg/L Shoot	4.324	0.180	3.293	0.137	160	526.93	21.98
122	2014-06-17 1000 µg/L Shoot	3.192	0.127	2.431	0.096	400	972.45	38.55
123	2014-06-17 2000 µg/L Shoot	4.071	0.277	3.101	0.211	800	2480.51	168.82
124	2014-06-20 5000 µg/L Shoot	3.484	0.110	2.654	0.083	2000	5307.36	166.85
125	2014-06-20 10 000 µg/L Shoot	2.487	0.054	2.091	0.046	4000	8362.85	182.62
126	2014-06-20 10 000 µg/L Root	2.715	0.291	2.282	0.244	600	1369.43	146.65
127	2014-06-24 1000 µg/L Shoot	3.708	0.210	2.824	0.160	160	451.86	25.65
128	2014-06-24 1000 µg/L Root	4.966	0.158	4.045	0.129	160	647.14	20.63
129	2014-06-24 2000 µg/L Root	3.584	0.341	2.730	0.260	400	1091.88	103.97
130	2014-06-24 5000 µg/L Root	6.510	0.197	5.323	0.161	400	2129.21	64.33
131	2014-06-24 10 000 µg/L Root	5.860	0.217	4.792	0.177	400	1916.89	70.92
132	wash	-0.118	0.178	-0.118	0.178	1	-0.12	0.18
133	6M HCl Blank	-0.064	0.081	-0.072	0.092	4	-0.29	0.37
134	Trace Metal 252 µg/L	2.773	0.124	2.434	0.109	120	292.13	13.07
135	wash	-0.105	0.117	-0.105	0.117	1	-0.10	0.12
136	Se_Std_0	-0.096	0.060	-0.096	0.060	1	-0.10	0.06
137	Se_Std_0.5	0.378	0.090	0.378	0.090	1	0.38	0.09
138	Se_Std_0.75	0.695	0.074	0.695	0.074	1	0.70	0.07
139	Se_Std_1	0.945	0.103	0.945	0.103	1	0.95	0.10
140	Se_Std_2	2.324	0.138	2.324	0.138	1	2.32	0.14
141	Se_Std_4	4.877	0.085	4.877	0.085	1	4.88	0.09
142	Se_Std_5	6.113	0.049	6.113	0.049	1	6.11	0.05
143	Se_Std_6	7.064	0.105	7.064	0.105	1	7.06	0.10
144	wash	-0.031	0.160	-0.031	0.160	1	-0.03	0.16
145	wash	0.097	0.129	0.097	0.129	1	0.10	0.13

Table C.22.: C analytical data - HG-FIAS measurement II

Technique	AA FIAS-MHS							
Spectrometer Model	Aanalyst 200 S/N 200S6110908							
Autosampler Model	AS-90plus							
Batch ID	Plant Digestions							
Results Data Set	Nothstein_2014_07_11							
Date Measured	11.07.2014							
Method Name	Se Nothstein calib 6c							
correl. coeff.	PQL (= lowest calib-10 %)	0.450						
0.995864	LOQ (= 7-wash)	0.237						
calib. slope	LOD (= 3-wash)	-0.102						
0.00912	analytical quality [%]	132.162						
Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]		
1	Blank	0.0000	0.0003	0.0	0.00	0.00		
2	0.5 ppb	0.0026	0.0010	0.5	0.29	0.11		
3	0.75 ppb	0.0045	0.0010	0.75	0.49	0.11		
4	1.0 ppb	0.0065	0.0008	1.0	0.71	0.09		
5	2.0 ppb	0.0166	0.0010	2.0	1.82	0.11		
6	4.0 ppb	0.0363	0.0021	4.0	3.98	0.23		
7	5.0 ppb	0.0455	0.0011	5.0	4.99	0.12		
8	6.0 ppb	0.0560	0.0008	6.0	6.14	0.09		
Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	-0.071	0.055	-0.093	0.072	1	-0.09	0.07
2	wash	0.003	0.001	0.004	0.001	1	0.00	0.00
3	6M HCl Blank	0.004	0.001	0.004	0.001	4	0.01	0.00
4	Trace Metal 252 µg/L	2.051	0.175	2.100	0.180	120	252.00	21.54
5	wash	0.155	0.066	0.203	0.086	1	0.20	0.09
6	Se_Std_0	0.025	0.038	0.033	0.050	1	0.03	0.05
7	Se_Std_0.5	0.384	0.119	0.501	0.155	1	0.50	0.16
8	Se_Std_0.75	0.619	0.232	0.808	0.303	1	0.81	0.30
9	Se_Std_1	0.958	0.147	1.250	0.192	1	1.25	0.19
10	Se_Std_2	2.212	0.117	2.887	0.153	1	2.89	0.15
11	Se_Std_4	4.597	0.159	5.999	0.208	1	6.00	0.21
12	Se_Std_5	5.567	0.188	7.265	0.245	1	7.26	0.25
13	Se_Std_6	6.743	0.134	8.800	0.175	1	8.80	0.18
14	wash	0.093	0.167	0.121	0.218	1	0.12	0.22
15	wash	0.083	0.124	0.108	0.162	1	0.11	0.16
16	2014-06-25 digestion blank	0.018	0.072	0.011	0.046	8	< PQL	< PQL
17	2014-06-25 digestion Std Wheat 1567a	1.331	0.136	0.962	0.098	8	7.70	0.79
18	2014-06-25 0 µg/L Shoot	0.040	0.079	0.025	0.050	8	< PQL	< PQL
19	2014-06-25 0 µg/L Root	-0.013	0.077	-0.008	0.048	8	< PQL	< PQL
20	2014-06-25 20 µg/L Shoot	1.300	0.113	1.248	0.109	5	6.24	0.54
21	2014-06-25 20 µg/L Root	0.329	0.190	0.207	0.119	4	0.83	0.48
22	2014-06-25 50 µg/L Shoot	0.988	0.419	1.111	0.471	8	8.89	3.76
23	2014-06-25 50 µg/L Root	0.465	0.161	0.446	0.154	8	3.57	1.24
24	2014-06-25 100 µg/L Shoot	0.803	0.173	0.864	0.186	40	34.56	7.44
25	2014-06-25 100 µg/L Root	0.127	0.071	0.122	0.068	40	4.87	2.72
26	wash	0.049	0.207	0.064	0.270	1	0.06	0.27
27	Se_Std_0	0.010	0.099	0.013	0.129	1	0.01	0.13
28	Se_Std_0.5	0.497	0.110	0.648	0.144	1	0.65	0.14
29	Se_Std_0.75	0.822	0.085	1.073	0.111	1	1.07	0.11
30	Se_Std_1	1.099	0.077	1.434	0.100	1	1.43	0.10
31	Se_Std_2	2.391	0.183	3.121	0.239	1	3.12	0.24
32	Se_Std_4	4.756	0.126	6.206	0.165	1	6.21	0.16
33	Se_Std_5	5.795	0.304	7.562	0.397	1	7.56	0.40
34	Se_Std_6	7.079	0.312	9.238	0.407	1	9.24	0.41
35	wash	0.059	0.110	0.077	0.143	1	0.08	0.14
36	wash	0.076	0.059	0.099	0.078	1	0.10	0.08
37	2014-06-26 digestion blank	0.068	0.114	0.031	0.052	8	< PQL	< PQL
38	2014-06-26 digestion Std Wheat 1567a	1.338	0.036	0.848	0.023	8	6.79	0.18
39	2014-06-26 200 µg/L Shoot	2.828	0.144	3.144	0.160	40	125.76	6.39
40	2014-06-26 200 µg/L Root	0.324	0.155	0.232	0.111	40	9.27	4.44
41	2014-06-26 500 µg/L Shoot	2.888	0.156	3.233	0.174	80	258.68	13.94
42	2014-06-26 500 µg/L Root	0.539	0.051	0.515	0.048	80	41.23	3.88
43	2014-06-26 1000 µg/L Shoot	4.526	0.278	5.067	0.311	80	405.39	24.86
44	2014-06-26 1000 µg/L Root	0.815	0.153	0.779	0.146	80	62.32	11.67
45	2014-06-26 2000 µg/L Shoot	2.013	0.126	2.254	0.141	480	1082.03	67.59
46	2014-06-17 2000 µg/L Root	0.662	0.189	0.632	0.181	240	151.77	43.41
47	wash	-0.044	0.121	-0.057	0.158	1	-0.06	0.16
48	Se_Std_0	0.001	0.095	0.002	0.124	1	0.00	0.12
49	Se_Std_0.5	0.461	0.126	0.602	0.164	1	0.60	0.16
50	Se_Std_0.75	0.610	0.090	0.796	0.117	1	0.80	0.12
51	Se_Std_1	1.055	0.062	1.377	0.080	1	1.38	0.08
52	Se_Std_2	2.223	0.163	2.901	0.213	1	2.90	0.21
53	Se_Std_4	4.381	0.427	5.718	0.558	1	5.72	0.56
54	Se_Std_5	5.503	0.229	7.182	0.299	1	7.18	0.30
55	Se_Std_6	6.946	0.163	9.066	0.213	1	9.07	0.21
56	wash	0.049	0.177	0.064	0.231	1	0.06	0.23
57	wash	-0.022	0.109	-0.028	0.142	1	-0.03	0.14
58	2014-06-27 digestion blank	0.015	0.177	0.006	0.077	8	< PQL	< PQL
59	2014-06-27 digestion Std Wheat 1567a	1.365	0.096	0.876	0.061	8	7.01	0.49
60	2014-06-27 5000 µg/L Shoot	2.636	0.166	2.790	0.175	480	1339.03	84.20
61	2014-06-27 5000 µg/L Root	0.882	0.086	0.930	0.091	240	223.25	21.84
62	2014-06-27 10 000 µg/L Shoot	4.507	0.126	4.771	0.133	480	2289.99	63.98
63	2014-06-27 10 000 µg/L Root	1.429	0.048	1.512	0.051	240	362.92	12.15
64	2014-06-27 0 µg/L Shoot	0.132	0.134	0.057	0.058	8	< PQL	< PQL
65	2014-06-27 0 µg/L Root	0.035	0.096	0.015	0.042	8	< PQL	< PQL
66	2014-06-27 20 µg/L Shoot	0.422	0.055	0.271	0.035	4	1.08	0.14
67	2014-06-27 20 µg/L Root	0.052	0.065	0.033	0.042	4	< PQL	< PQL

Table C.23.: C analytical data - HG-FIAS measurement II (continued from previous page)

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
68	wash	0.074	0.072	0.096	0.094	1	0.10	0.09
69	Se_Std_0	-0.021	0.110	-0.028	0.144	1	-0.03	0.14
70	Se_Std_0.5	0.506	0.195	0.661	0.254	1	0.66	0.25
71	Se_Std_0.75	0.780	0.149	1.017	0.195	1	1.02	0.19
72	Se_Std_1	1.090	0.087	1.423	0.113	1	1.42	0.11
73	Se_Std_2	2.612	0.077	3.408	0.100	1	3.41	0.10
74	Se_Std_4	5.245	0.133	6.845	0.173	1	6.84	0.17
75	Se_Std_5	6.386	0.375	8.334	0.489	1	8.33	0.49
76	Se_Std_6	7.654	0.215	9.989	0.281	1	9.99	0.28
77	wash	-0.043	0.075	-0.056	0.098	1	-0.06	0.10
78	wash	0.007	0.096	0.009	0.125	1	0.01	0.12
79	2014-06-30 digestion blank	-0.031	0.065	-0.008	0.016	8	< PQL	< PQL
80	2014-06-30 digestion Std Wheat 1567a	1.430	0.217	0.682	0.103	8	5.46	0.83
81	2014-06-30 50 µg/L Shoot	0.063	0.147	0.054	0.128	8	< PQL	< PQL
82	2014-06-30 50 µg/L Root	0.059	0.130	0.051	0.113	8	< PQL	< PQL
83	2014-06-30 100 µg/L Shoot	-0.037	0.080	-0.013	0.028	40	< PQL	< PQL
84	2014-06-30 100 µg/L Root	0.069	0.101	0.017	0.025	40	< PQL	< PQL
85	2014-06-30 200 µg/L Shoot	0.032	0.095	0.028	0.082	40	< PQL	< PQL
86	2014-06-30 200 µg/L Root	0.131	0.106	0.113	0.092	40	< PQL	< PQL
87	2014-06-30 500 µg/L Shoot	0.045	0.133	0.039	0.115	80	< PQL	< PQL
88	2014-06-30 500 µg/L Root	0.009	0.122	0.007	0.106	80	< PQL	< PQL
89	wash	-0.046	0.111	-0.060	0.145	1	-0.06	0.14
90	Se_Std_0	-0.013	0.114	-0.017	0.149	1	-0.02	0.15
91	Se_Std_0.5	0.545	0.170	0.711	0.222	1	0.71	0.22
92	Se_Std_0.75	0.931	0.095	1.214	0.124	1	1.21	0.12
93	Se_Std_1	1.234	0.077	1.610	0.100	1	1.61	0.10
94	Se_Std_2	2.632	0.128	3.435	0.166	1	3.44	0.17
95	Se_Std_4	5.381	0.127	7.022	0.165	1	7.02	0.17
96	Se_Std_5	6.695	0.192	8.737	0.250	1	8.74	0.25
97	Se_Std_6	7.709	0.163	10.061	0.213	1	10.06	0.21
98	wash	0.060	0.119	0.078	0.156	1	0.08	0.16
99	wash	0.138	0.117	0.180	0.153	1	0.18	0.15
100	2014-07-01 digestion blank	0.026	0.059	0.036	0.081	8	< PQL	< PQL
101	2014-07-01 digestion Std Wheat 1567a	1.173	0.152	1.690	0.220	8	13.52	1.76
102	2014-07-01 1000 µg/L Shoot	-0.037	0.145	-0.049	0.192	80	< PQL	< PQL
103	2014-07-01 1000 µg/L Root	0.116	0.096	0.154	0.127	80	< PQL	< PQL
104	2014-07-01 2000 µg/L Shoot	0.018	0.033	0.016	0.029	480	< PQL	< PQL
105	2014-07-01 2000 µg/L Root	0.064	0.076	0.085	0.101	248	< PQL	< PQL
106	2014-07-01 5000 µg/L Shoot	0.042	0.133	0.037	0.118	480	< PQL	< PQL
107	2014-07-01 5000 µg/L Root	0.225	0.086	0.298	0.115	240	< PQL	< PQL
108	2014-07-01 10 000 µg/L Shoot	0.059	0.089	0.085	0.128	480	< PQL	< PQL
109	2014-07-01 10 000 µg/L Root	0.241	0.098	0.320	0.130	240	< PQL	< PQL
110	wash	0.061	0.087	0.080	0.114	1	0.08	0.11
111	6M HCl Blank	-0.051	0.109	-0.054	0.116	4	-0.22	0.46
112	Trace Metal 252 µg/L	2.839	0.124	3.451	0.151	120	414.10	18.09
113	wash	-0.030	0.090	-0.040	0.117	1	-0.04	0.12
114	Se_Std_0	0.016	0.072	0.021	0.094	1	0.02	0.09
115	Se_Std_0.5	0.586	0.080	0.765	0.104	1	0.77	0.10
116	Se_Std_0.75	0.760	0.200	0.992	0.262	1	0.99	0.26
117	Se_Std_1	1.227	0.149	1.601	0.194	1	1.60	0.19
118	Se_Std_2	2.825	0.140	3.687	0.182	1	3.69	0.18
119	Se_Std_4	5.648	0.127	7.371	0.165	1	7.37	0.17
120	Se_Std_5	6.595	0.132	8.606	0.172	1	8.61	0.17
121	Se_Std_6	8.309	0.203	10.844	0.265	1	10.84	0.26
122	wash	0.034	0.117	0.045	0.153	1	0.04	0.15
123	wash	0.026	0.096	0.034	0.125	1	0.03	0.13

Table C.24.: C analytical data - HG-FIAS measurement III

Technique	AA FIAS-MHS		
Spectrometer Model	Analyst 200 S/N 200S6110908		
Autosampler Model	AS-90plus		
Batch ID	Plant Digestions		
Results Data Set	Nothstein_2014_09_29		
Date Measured	29.09.2014		
Method Name	Se Nothstein calib 6c		
correl. coeff.	PQL (= lowest calib-10 %)	0.450	
0.996469	LOQ (= 7-wash)	-0.214	
calib. slope	LOD (= 3-wash)	-0.092	
0.01055	analytical quality [%]	115.433	

Calibration	Sample ID	Mean signal [-]	SD [-]	entered c(Se) [µg/L]	calc. c(Se) [µg/L]	SD [µg/L]
1	Blank	0.0000	0.0012	0.0	0.00	0.00
2	0.5 ppb	0.0017	0.0024	0.5	0.16	0.23
3	0.75 ppb	0.0056	0.0024	0.75	0.53	0.23
4	1.0 ppb	0.0083	0.0018	1.0	0.79	0.17
5	2.0 ppb	0.0208	0.0015	2.0	1.97	0.14
6	4.0 ppb	0.0425	0.0017	4.0	4.03	0.16
7	5.0 ppb	0.0527	0.0017	5.0	4.99	0.16
8	6.0 ppb	0.0639	0.0014	6.0	6.05	0.13

Sequence No.	Sample ID	c(Se) diluted [µg/L]	SD [µg/L]	c(Se) driftcorr. [µg/L]	SD driftcorr. [µg/L]	dilution factor [-]	c(Se) conc. [µg/L]	SD [µg/L]
1	Wash Milli-Q	0.011	0.155	0.011	0.155	1	0.01	0.16
2	wash	-0.092	0.136	-0.092	0.136	1	-0.09	0.14
3	6M HCl Blank	-0.089	0.095	-0.001	0.001	4	0.00	0.00
4	Trace Metal 252 µg/L	2.918	0.117	2.554	0.103	100	255.45	10.29
5	wash	-0.032	0.109	-0.032	0.109	1	-0.03	0.11
6	Se_Std_0	-0.089	0.066	-0.089	0.066	1	-0.09	0.07
7	Se_Std_0.5	0.320	0.148	0.320	0.148	1	0.32	0.15
8	Se_Std_0.75	0.644	0.241	0.644	0.241	1	0.64	0.24
9	Se_Std_1	0.947	0.074	0.947	0.074	1	0.95	0.07
10	Se_Std_2	2.219	0.072	2.219	0.072	1	2.22	0.07
11	Se_Std_4	4.589	0.137	4.589	0.137	1	4.59	0.14
12	Se_Std_5	5.561	0.213	5.561	0.213	1	5.56	0.21
13	Se_Std_6	6.637	0.189	6.637	0.189	1	6.64	0.19
14	wash	-0.021	0.097	-0.021	0.097	1	-0.02	0.10
15	wash	-0.061	0.121	-0.061	0.121	1	-0.06	0.12
16	2014-06-27 digestion blank	0.012	0.067	0.000	0.002	8	< PQL	< PQL
17	2014-06-27 digestion Std Wheat 1567a	1.367	0.101	0.911	0.068	8	7.29	0.54
18	2014-06-27 0 µg/L SeO3 Shoot	0.031	0.158	0.001	0.005	8	< PQL	< PQL
19	2014-06-27 0 µg/L SeO3 Root	0.022	0.124	0.001	0.004	8	< PQL	< PQL
20	2014-06-27 20 µg/L SeO3 Shoot	0.043	0.030	0.001	0.001	8	< PQL	< PQL
21	2014-06-27 20 µg/L SeO3 Root	0.056	0.220	0.002	0.007	8	< PQL	< PQL
22	2014-06-30 digestion blank	-0.104	0.089	-0.003	0.003	8	< PQL	< PQL
23	2014-06-30 digestion Std Wheat 1567a	1.486	0.113	0.990	0.075	8	7.92	0.60
24	2014-06-30 50 µg/L SeO3 Shoot	0.028	0.066	0.001	0.002	8	< PQL	< PQL
25	2014-06-30 50 µg/L SeO3 Root	0.016	0.175	0.001	0.006	8	< PQL	< PQL
26	2014-06-30 100 µg/L SeO3 Shoot	0.197	0.207	0.110	0.116	8	< PQL	< PQL
27	2014-06-30 100 µg/L SeO3 Root	0.207	0.089	0.116	0.050	8	< PQL	< PQL
28	wash	-0.135	0.100	-0.135	0.100	1	-0.14	0.10
29	Se_Std_0	-0.068	0.052	-0.068	0.052	1	-0.07	0.05
30	Se_Std_0.5	0.313	0.127	0.313	0.127	1	0.31	0.13
31	Se_Std_0.75	0.887	0.060	0.887	0.060	1	0.89	0.06
32	Se_Std_1	1.158	0.140	1.158	0.140	1	1.16	0.14
33	Se_Std_2	2.608	0.179	2.608	0.179	1	2.61	0.18
34	Se_Std_4	5.045	0.226	5.045	0.226	1	5.05	0.23
35	Se_Std_5	6.257	0.282	6.257	0.282	1	6.26	0.28
36	Se_Std_6	7.424	0.115	7.424	0.115	1	7.42	0.12
37	wash	-0.076	0.111	-0.076	0.111	1	-0.08	0.11
38	wash	0.063	0.517	0.063	0.517	1	0.06	0.52
39	2014-06-30 200 µg/L SeO3 Shoot	0.109	0.217	0.081	0.162	8	< PQL	< PQL
40	2014-06-30 200 µg/L SeO3 Root	0.018	0.136	0.001	0.005	8	< PQL	< PQL
41	2014-06-30 500 µg/L SeO3 Shoot	0.017	0.095	0.001	0.003	8	< PQL	< PQL
42	2014-06-30 500 µg/L SeO3 Root	0.155	0.081	0.005	0.003	8	< PQL	< PQL
43	2014-07-01 digestion blank	0.022	0.075	0.001	0.003	8	< PQL	< PQL
44	2014-07-01 digestion Std Wheat 1567a	1.622	0.097	1.397	0.083	8	11.17	0.67
45	2014-07-01 1000 µg/L SeO3 Shoot	0.110	0.146	0.004	0.005	8	< PQL	< PQL
46	2014-07-01 1000 µg/L SeO3 Root	1.186	0.162	1.022	0.139	8	8.17	1.11
47	2014-07-01 2000 µg/L SeO3 Shoot	0.294	0.081	0.010	0.003	8	< PQL	< PQL
48	2014-07-01 2000 µg/L SeO3 Root	2.360	0.089	2.125	0.080	8	17.00	0.64
49	2014-07-01 5000 µg/L SeO3 Shoot	1.180	0.127	1.016	0.109	8	8.13	0.87
50	2014-07-01 5000 µg/L SeO3 Root	4.992	0.101	4.783	0.096	8	38.26	0.77
51	2014-07-01 10000 µg/L SeO3 Shoot	2.702	0.175	2.432	0.157	8	19.46	1.26
52	2014-07-01 10000 µg/L SeO3 Root	6.525	0.063	6.647	0.064	8	53.17	0.52
53	wash	0.254	0.190	0.254	0.190	1	0.25	0.19
54	6M HCl Blank	-0.089	0.095	-0.001	0.001	4	0.00	0.00
55	Trace Metal 252 µg/L	2.908	0.119	3.263	0.133	100	326.33	13.32
56	wash	-0.007	0.358	-0.007	0.358	1	-0.01	0.36
57	Se_Std_0	-0.089	0.066	-0.089	0.066	1	-0.09	0.07
58	Se_Std_0.5	0.320	0.148	0.320	0.148	1	0.32	0.15
59	Se_Std_0.75	0.449	0.097	0.449	0.097	1	0.45	0.10
60	Se_Std_1	0.639	0.101	0.639	0.101	1	0.64	0.10
61	Se_Std_2	1.732	0.183	1.732	0.183	1	1.73	0.18
62	Se_Std_4	3.818	0.068	3.818	0.068	1	3.82	0.07
63	Se_Std_5	4.149	0.916	4.149	0.916	1	4.15	0.92
64	Se_Std_6	4.457	0.177	4.457	0.177	1	4.46	0.18
65	wash	-0.175	0.068	-0.175	0.068	1	-0.18	0.07
66	wash	-0.097	0.032	-0.097	0.032	1	-0.10	0.03

Table C.25.: *C* analytical data - IC measurement I

Technique	Ion Chromatography									
System	ICS-1000									
Quantification:	AnionenAS14									
Injection volume	25 µL									
Run time [min]	14									
Date Measured	24.04.2014									
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]		
Calib_1	4.14	Cl ⁻	XQOff	5	-0.004	0.153	0.001	99.9973		
Calib_2	6.70	NO ₃ ⁻	XQOff	5	-0.013	0.080	0.000	99.9992		
Calib_3	8.34	PO ₄ ³⁻	XQOff	5	-0.001	0.042	0.000	99.9999		
Calib_4	9.86	SO ₄ ²⁻	XQOff	5	-0.020	0.107	0.000	99.9997		
mean:					-0.0094	0.0954	0.0004	99.9990		
		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻					
standard repetition mean [mg/L]		10.40	21.01	31.76	21.14					
standard repetition SD [mg/L]		0.13	0.23	0.34	0.26					
standard repetition RSD [%]		1.20	1.01	1.06	1.25					
analytical quality [%]		105.44								
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	Retention time PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	Ion concentration NO ₃ ⁻ [mg/L]		PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.09	6.70	8.10	9.46	2.02	3.99	6.00	4.00	
2	Standard_2	4.09	6.68	8.09	9.46	4.92	9.99	15.00	9.98	
3	Standard_3	4.09	6.66	8.07	9.44	10.01	20.10	30.05	20.07	
4	Standard_4	4.10	6.62	8.06	9.43	20.06	39.89	59.95	39.94	
5	Standard_5	4.11	6.57	8.03	9.40	39.98	80.03	120.01	80.01	
6	wash-1	4.11	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
7	Standard_3-1	4.14	6.76	8.33	9.87	10.29	20.77	31.30	20.84	
8	wash-2	4.10	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
9	autoclave_blind_2014_03_25	4.14	6.70	8.34	9.86	3.28	264.59	31.73	67.36	
10	initisol_Na2SeO4_0000ppbSe_2014_03_25	4.14	6.70	8.34	9.86	4.48	301.75	33.44	67.83	
11	initisol_Na2SeO4_0020ppbSe_2014_03_25	4.14	6.69	8.34	9.86	6.71	309.98	34.61	70.07	
12	initisol_Na2SeO4_0050ppbSe_2014_03_25	4.14	6.70	8.34	9.86	4.77	309.44	34.22	71.13	
13	initisol_Na2SeO4_0100ppbSe_2014_03_25	4.14	6.74	8.35	9.86	3.09	170.59	20.59	52.63	
14	initisol_Na2SeO4_0200ppbSe_2014_03_25	4.14	6.70	8.34	9.86	4.61	313.56	33.90	70.71	
15	initisol_Na2SeO4_0500ppbSe_2014_03_25	4.14	6.70	8.34	9.86	5.17	324.67	36.75	70.75	
16	initisol_Na2SeO4_1000ppbSe_2014_03_25	4.14	6.73	8.35	9.87	4.73	214.76	26.87	62.38	
17	initisol_Na2SeO4_2000ppbSe_2014_03_25	4.14	6.75	8.34	9.87	2.78	143.01	17.77	43.65	
18	initisol_Na2SeO4_5000ppbSe_2014_03_25	4.14	6.72	8.34	9.86	3.40	206.48	24.12	57.74	
19	initisol_Na2SeO4_10000ppbSe_2014_03_25	4.14	6.72	8.35	9.87	6.00	252.07	29.97	63.58	
20	wash-3	4.17	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
21	Standard_3-2	4.15	6.78	8.33	9.86	10.31	20.90	31.71	21.07	
22	wash-4	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
23	K-sorp_Na2SeO4_0000ppbSe_2014_04_13	4.14	6.70	8.36	9.86	4.53	290.90	8.37	66.20	
24	K-sorp_Na2SeO4_0020ppbSe_2014_04_13	4.14	6.70	8.35	9.86	4.19	298.95	7.81	69.84	
25	K-sorp_Na2SeO4_0050ppbSe_2014_04_13	4.13	6.69	8.34	9.86	4.55	320.66	12.00	70.38	
26	K-sorp_Na2SeO4_0100ppbSe_2014_04_13	4.14	6.71	8.36	9.87	4.25	282.69	7.41	67.69	
27	K-sorp_Na2SeO4_0200ppbSe_2014_04_13	4.14	6.69	8.35	9.87	5.62	322.04	11.58	69.48	
28	K-sorp_Na2SeO4_0500ppbSe_2014_04_13	4.14	6.70	8.35	9.87	0.09	0.64	0.11	0.75	
29	K-sorp_Na2SeO4_1000ppbSe_2014_04_13	4.14	6.70	8.36	9.87	4.51	275.87	8.60	69.19	
30	K-sorp_Na2SeO4_2000ppbSe_2014_04_13	4.14	6.71	8.35	9.87	4.72	263.37	8.65	67.05	
31	K-sorp_Na2SeO4_5000ppbSe_2014_04_13	4.13	6.69	8.36	9.86	4.60	313.80	8.38	70.98	
32	K-sorp_Na2SeO4_10000ppbSe_2014_04_13	4.14	6.70	8.36	9.87	4.22	304.69	10.24	68.83	
33	wash-5	4.11	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
34	Standard_3-3	4.15	6.78	8.32	9.86	10.47	21.08	32.03	21.20	
35	wash-6	4.17	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
36	K-sorp+plant_Na2SeO4_0000ppbSe_2014_04_13	4.13	6.73	8.35	9.86	3.11	197.45	2.38	59.77	
37	K-sorp+plant_Na2SeO4_0020ppbSe_2014_04_13	4.14	6.73	8.37	9.86	4.01	194.86	1.34	63.14	
38	K-sorp+plant_Na2SeO4_0050ppbSe_2014_04_13	4.13	6.72	8.34	9.86	4.07	236.28	4.97	65.43	
39	K-sorp+plant_Na2SeO4_0100ppbSe_2014_04_13	4.14	6.73	8.34	9.86	4.16	217.83	4.41	64.48	
40	K-sorp+plant_Na2SeO4_0200ppbSe_2014_04_13	4.13	6.71	8.35	9.86	4.95	257.97	6.84	67.17	
41	K-sorp+plant_Na2SeO4_0500ppbSe_2014_04_13	4.14	6.72	8.38	9.86	4.34	222.12	3.48	64.30	
42	K-sorp+plant_Na2SeO4_1000ppbSe_2014_04_13	4.14	6.72	8.33	9.86	3.36	232.07	4.93	63.56	
43	K-sorp+plant_Na2SeO4_2000ppbSe_2014_04_13	4.14	6.73	8.34	9.86	3.68	211.02	3.55	59.76	
44	K-sorp+plant_Na2SeO4_5000ppbSe_2014_04_13	4.14	6.72	8.35	9.86	3.43	241.42	4.68	63.05	
45	K-sorp+plant_Na2SeO4_10000ppbSe_2014_04_13	4.14	6.72	8.34	9.87	3.13	232.85	5.60	62.17	
46	wash-7	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
47	Standard_3-4	4.14	6.77	8.32	9.86	10.54	21.29	31.99	21.47	
48	wash-8	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
49	Std_Riverwater	4.16	6.86	n.a.	9.82	45.23	0.64	n.a.	155.27	
50	wash-9	4.13	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
51	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	

Table C.26.: C analytical data - IC measurement II

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	25.04.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.16	Cl ⁻	XQOff	5	-0.004	0.153	0.001	99.9973	
Calib_2	6.76	NO ₃ ⁻	XQOff	5	-0.013	0.080	0.000	99.9992	
Calib_3	8.48	PO ₄ ³⁻	XQOff	5	-0.001	0.042	0.000	99.9999	
Calib_4	10.02	SO ₄ ²⁻	XQOff	5	-0.020	0.107	0.000	99.9997	
mean:					-0.0094	0.0954	0.0004	99.9990	
		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
standard repetition mean [mg/L]		10.32	20.97	31.89	20.95				
standard repetition SD [mg/L]		0.08	0.14	0.30	0.19				
standard repetition RSD [%]		0.75	0.66	0.94	0.89				
analytical quality [%]		106.63							
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	Retention time PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	Ion concentration		
							NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	3.09	5.84	6.70	8.10	2.02	3.99	6.00	4.00
2	Standard_2	3.09	5.83	6.68	8.09	4.92	9.99	15.00	9.98
3	Standard_3	3.09	5.82	6.66	8.07	10.01	20.10	30.05	20.07
4	Standard_4	3.10	5.81	6.62	8.06	20.06	39.89	59.95	39.94
5	Standard_5	3.10	5.79	6.57	8.03	39.98	80.03	120.01	80.01
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	3.13	5.95	6.83	8.47	5.12	10.41	15.76	10.34
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	initsol_blind_2014_03_27	n.a.	n.a.	6.74	8.47	4.08	298.14	34.11	66.34
10	initsol_Na2SeO3_0000ppbSe_2014_03_27	n.a.	n.a.	6.76	8.48	2.96	224.19	26.63	62.00
11	initsol_Na2SeO3_0020ppbSe_2014_03_27	n.a.	n.a.	6.75	8.47	5.40	270.07	31.57	66.56
12	initsol_Na2SeO3_0050ppbSe_2014_03_27	n.a.	n.a.	6.76	8.47	2.86	217.83	26.71	57.29
13	initsol_Na2SeO3_0100ppbSe_2014_03_27	n.a.	n.a.	6.77	8.47	3.30	191.94	23.13	52.69
14	initsol_Na2SeO3_0200ppbSe_2014_03_27	n.a.	n.a.	6.76	8.46	3.99	236.96	28.22	61.07
15	initsol_Na2SeO3_0500ppbSe_2014_03_27	n.a.	n.a.	6.75	8.47	3.70	267.77	31.73	66.99
16	initsol_Na2SeO3_1000ppbSe_2014_03_27	n.a.	n.a.	6.74	8.46	3.96	297.71	35.86	68.43
17	initsol_Na2SeO3_2000ppbSe_2014_03_27	n.a.	n.a.	6.75	8.46	3.40	282.94	35.66	68.26
18	initsol_Na2SeO3_5000ppbSe_2014_03_27	n.a.	n.a.	6.76	8.45	3.23	229.34	31.80	60.16
19	initsol_Na2SeO3_10000ppbSe_2014_03_27	n.a.	n.a.	6.75	8.44	4.56	276.59	44.69	69.34
20	wash-3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Standard_2-2	3.13	5.96	6.84	8.46	5.14	10.45	15.90	10.49
22	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	K-sorp_Na2SeO3_0000ppbSe_2014_04_15	3.13	n.a.	6.73	8.47	5.32	314.98	14.02	70.55
24	K-sorp_Na2SeO3_0020ppbSe_2014_04_15	3.13	n.a.	6.74	8.48	4.37	305.60	11.85	68.22
25	K-sorp_Na2SeO3_0050ppbSe_2014_04_15	3.13	n.a.	6.74	8.46	4.49	310.42	13.10	69.25
26	K-sorp_Na2SeO3_0100ppbSe_2014_04_15	3.13	n.a.	6.74	8.48	4.35	312.90	12.34	69.48
27	K-sorp_Na2SeO3_0200ppbSe_2014_04_15	3.13	n.a.	6.74	8.47	4.49	309.41	12.85	69.17
28	K-sorp_Na2SeO3_0500ppbSe_2014_04_15	3.13	n.a.	6.75	8.47	3.51	247.89	8.66	52.78
29	K-sorp_Na2SeO3_1000ppbSe_2014_04_15	3.13	n.a.	6.73	8.46	4.58	315.48	14.58	69.73
30	K-sorp_Na2SeO3_2000ppbSe_2014_04_15	3.13	n.a.	6.74	8.46	4.46	308.41	12.38	68.23
31	K-sorp_Na2SeO3_5000ppbSe_2014_04_15	3.13	n.a.	6.73	8.44	4.48	322.72	19.06	71.77
32	K-sorp_Na2SeO3_10000ppbSe_2014_04_15	3.13	n.a.	6.73	8.42	4.56	312.94	24.78	69.07
33	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Standard_2-3	3.13	5.95	6.83	8.46	5.19	10.53	16.02	10.51
35	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
36	K-sorp+plant_Na2SeO3_0000ppbSe_2014_04_15	3.13	n.a.	6.75	8.47	3.95	242.62	4.16	63.16
37	K-sorp+plant_Na2SeO3_0020ppbSe_2014_04_15	3.13	n.a.	6.76	8.48	3.40	220.96	4.15	60.64
38	K-sorp+plant_Na2SeO3_0050ppbSe_2014_04_15	3.13	n.a.	6.77	8.47	2.52	195.65	5.18	61.59
39	K-sorp+plant_Na2SeO3_0100ppbSe_2014_04_15	3.13	n.a.	6.76	8.46	4.37	238.48	5.19	64.05
40	K-sorp+plant_Na2SeO3_0200ppbSe_2014_04_15	3.13	n.a.	6.75	8.47	3.33	240.57	4.22	62.26
41	K-sorp+plant_Na2SeO3_0500ppbSe_2014_04_15	3.13	n.a.	6.76	8.46	2.47	207.10	4.72	60.63
42	K-sorp+plant_Na2SeO3_1000ppbSe_2014_04_15	3.13	n.a.	6.75	8.47	3.38	246.93	7.64	63.07
43	K-sorp+plant_Na2SeO3_2000ppbSe_2014_04_15	n.a.	n.a.	6.75	8.43	3.68	257.06	5.48	61.81
44	K-sorp+plant_Na2SeO3_5000ppbSe_2014_04_15	3.13	n.a.	6.76	8.44	4.49	238.25	14.35	60.34
45	K-sorp+plant_Na2SeO3_10000ppbSe_2014_04_15	3.13	n.a.	6.81	8.42	5.91	95.08	23.51	67.80
46	wash-7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
47	Standard_2-4	3.13	5.96	6.84	8.46	5.20	10.56	16.09	10.56
48	wash-8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
49	Std_Riverwater	3.13	n.a.	n.a.	n.a.	45.66	n.a.	n.a.	157.30
50	wash-9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
51	StopMeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table C.27.: *C* analytical data - IC measurement III

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	15.07.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.07	Cl ⁻	XQOff	5	-0.004	0.153	0.001	99.9973	
Calib_2	6.60	NO ₃ ⁻	XQOff	5	-0.013	0.080	0.000	99.9992	
Calib_3	8.48	PO ₄ ³⁻	XQOff	5	-0.001	0.042	0.000	99.9999	
Calib_4	9.58	SO ₄ ²⁻	XQOff	5	-0.020	0.107	0.000	99.9997	
mean:					-0.0094	0.0954	0.0004	99.9990	
		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
standard repetition mean [mg/L]		9.99	20.21	30.22	20.24				
standard repetition SD [mg/L]		0.15	0.56	0.63	0.25				
standard repetition RSD [%]		1.52	2.79	2.00	1.24				
analytical quality [%]		102.14							
Seq. No.	Sample ID	Cl ⁻ [min]	Retention time NO ₃ ⁻ [min]	Retention time PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	Ion concentration NO ₃ ⁻ [mg/L]		SO ₄ ²⁻ [mg/L]
1	Standard_1	4.09	6.70	8.10	9.46	2.02	3.99	6.00	4.00
2	Standard_2	4.09	6.68	8.09	9.46	4.92	9.99	15.00	9.98
3	Standard_3	4.09	6.66	8.07	9.44	10.01	20.10	30.05	20.07
4	Standard_4	4.10	6.62	8.06	9.43	20.06	39.89	59.95	39.94
5	Standard_5	4.11	6.57	8.03	9.40	39.98	80.03	120.01	80.01
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.07	6.60	8.12	9.58	9.95	20.30	29.42	19.88
8	wash-2	4.15	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	initsol_blind_2014_05_08	4.07	6.65	n.a.	n.a.	25.48	6.24	n.a.	n.a.
10	initsol_Na2SeO4_0000ppbSe_2014_05_08	4.07	6.55	8.14	9.59	3.79	295.49	23.71	61.05
11	initsol_Na2SeO4_0020ppbSe_2014_05_08	4.07	6.55	8.13	9.58	4.48	297.19	23.51	62.27
12	initsol_Na2SeO4_0050ppbSe_2014_05_08	4.07	6.55	8.13	9.59	3.84	291.69	24.73	62.05
13	initsol_Na2SeO4_0100ppbSe_2014_05_08	4.07	6.55	8.13	9.59	4.16	290.40	23.04	60.69
14	initsol_Na2SeO4_0200ppbSe_2014_05_08	4.07	6.56	8.13	9.59	8.33	275.55	22.47	59.95
15	initsol_Na2SeO4_0500ppbSe_2014_05_08	4.07	6.55	8.13	9.59	4.22	295.29	22.38	62.41
16	initsol_Na2SeO4_1000ppbSe_2014_05_08	4.06	6.55	8.13	9.58	4.29	307.54	25.23	63.29
17	initsol_Na2SeO4_2000ppbSe_2014_05_08	4.07	6.56	8.13	9.59	3.76	274.22	22.01	58.39
18	initsol_Na2SeO4_5000ppbSe_2014_05_08	4.06	6.56	8.13	9.58	3.37	253.66	23.84	61.63
19	initsol_Na2SeO4_10000ppbSe_2014_05_08	4.07	6.56	8.14	9.59	3.45	265.19	26.44	58.83
20	wash-3	4.09	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Standard_3-2	4.07	6.61	8.12	9.58	9.95	19.57	30.17	20.28
22	wash-4	4.07	6.62	8.12	9.57	n.a.	n.a.	n.a.	n.a.
23	G-sorp_Na2SeO4_0000ppbSe_2014_05_27	4.06	6.55	n.a.	9.58	4.94	292.64	n.a.	54.74
24	G-sorp_Na2SeO4_0020ppbSe_2014_05_27	4.07	6.55	n.a.	9.59	5.29	294.36	n.a.	56.72
25	G-sorp_Na2SeO4_0050ppbSe_2014_05_27	4.06	6.54	n.a.	9.58	5.95	289.65	n.a.	55.85
26	G-sorp_Na2SeO4_0100ppbSe_2014_05_27	4.07	6.55	n.a.	9.58	3.70	287.99	n.a.	60.31
27	G-sorp_Na2SeO4_0200ppbSe_2014_05_27	4.07	6.56	n.a.	9.58	3.71	241.99	n.a.	55.82
28	G-sorp_Na2SeO4_0500ppbSe_2014_05_27	4.06	6.55	n.a.	9.59	3.34	291.73	n.a.	54.06
29	G-sorp_Na2SeO4_1000ppbSe_2014_05_27	4.07	6.55	n.a.	9.59	3.82	286.65	n.a.	60.39
30	G-sorp_Na2SeO4_2000ppbSe_2014_05_27	4.06	6.55	n.a.	9.58	3.50	292.04	n.a.	57.49
31	G-sorp_Na2SeO4_5000ppbSe_2014_05_27	4.07	6.57	n.a.	9.59	3.09	226.98	n.a.	57.60
32	G-sorp_Na2SeO4_10000ppbSe_2014_05_27	4.06	6.55	n.a.	9.58	4.05	286.23	n.a.	54.07
33	wash-5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Standard_3-3	4.07	6.61	8.11	9.58	9.88	20.93	30.45	20.46
35	wash-6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
36	G-sorp+plant_Na2SeO4_0000ppbSe_2014_05_27	4.07	6.58	n.a.	9.58	4.74	196.44	n.a.	65.45
37	G-sorp+plant_Na2SeO4_0020ppbSe_2014_05_27	4.07	6.60	n.a.	9.58	2.93	134.62	n.a.	66.37
38	G-sorp+plant_Na2SeO4_0050ppbSe_2014_05_27	4.07	6.60	n.a.	9.58	3.45	151.78	n.a.	74.12
39	G-sorp+plant_Na2SeO4_0100ppbSe_2014_05_27	4.07	6.58	n.a.	9.58	4.64	212.79	n.a.	65.20
40	G-sorp+plant_Na2SeO4_0200ppbSe_2014_05_27	4.07	6.58	n.a.	9.58	3.96	197.81	n.a.	64.96
41	G-sorp+plant_Na2SeO4_0500ppbSe_2014_05_27	4.06	6.59	n.a.	9.58	3.52	158.48	n.a.	65.65
42	G-sorp+plant_Na2SeO4_1000ppbSe_2014_05_27	4.07	6.57	n.a.	9.58	5.04	226.89	n.a.	66.63
43	G-sorp+plant_Na2SeO4_2000ppbSe_2014_05_27	4.07	6.58	n.a.	9.58	4.32	188.81	n.a.	71.58
44	G-sorp+plant_Na2SeO4_5000ppbSe_2014_05_27	4.07	6.59	n.a.	9.58	3.85	176.88	n.a.	54.47
45	G-sorp+plant_Na2SeO4_10000ppbSe_2014_05_27	4.07	6.58	n.a.	9.58	4.84	205.44	n.a.	65.52
46	wash-7	4.07	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
47	Standard_3-4	4.07	6.62	8.11	9.58	10.22	20.04	30.85	20.33
48	wash-8	4.06	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
49	Std_Riverwater	4.09	n.a.	n.a.	9.54	43.29	n.a.	n.a.	152.23
50	wash-9	4.09	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
51	Stopmeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table C.28.: C analytical data - IC measurement IV

Technique	Ion Chromatography								
System	ICS-1000								
Quantification:	AnionenAS14								
Injection volume	25 µL								
Run time [min]	14								
Date Measured	16.07.2014								
Calibration ID	Ret. Time [min]	Peak Name	Cal. Type	Points	Offset (C0)	Slope (C1)	Curve (C2)	Coeff. Det. [%]	
Calib_1	4.07	Cl ⁻	XQOff	5	-0.004	0.153	0.001	99.9973	
Calib_2	6.60	NO ₃ ⁻	XQOff	5	-0.013	0.080	0.000	99.9992	
Calib_3	8.48	PO ₄ ³⁻	XQOff	5	-0.001	0.042	0.000	99.9999	
Calib_4	9.58	SO ₄ ²⁻	XQOff	5	-0.020	0.107	0.000	99.9997	
mean:					-0.0094	0.0954	0.0004	99.9990	
		Cl ⁻	NO ₃ ⁻	PO ₄ ³⁻	SO ₄ ²⁻				
standard repetition mean [mg/L]		10.35	21.23	30.74	20.59				
standard repetition SD [mg/L]		0.07	0.17	0.16	0.11				
standard repetition RSD [%]		0.67	0.81	0.51	0.52				
analytical quality [%]		103.67							
Seq. No.	Sample ID	Cl ⁻ [min]	NO ₃ ⁻ [min]	PO ₄ ³⁻ [min]	SO ₄ ²⁻ [min]	Cl ⁻ [mg/L]	NO ₃ ⁻ [mg/L]	PO ₄ ³⁻ [mg/L]	SO ₄ ²⁻ [mg/L]
1	Standard_1	4.09	6.70	8.10	9.46	2.02	3.99	6.00	4.00
2	Standard_2	4.09	6.68	8.09	9.46	4.92	9.99	15.00	9.98
3	Standard_3	4.09	6.66	8.07	9.44	10.01	20.10	30.05	20.07
4	Standard_4	4.10	6.62	8.06	9.43	20.06	39.89	59.95	39.94
5	Standard_5	4.11	6.57	8.03	9.40	39.98	80.03	120.01	80.01
6	wash-1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
7	Standard_3-1	4.09	6.63	8.15	9.65	10.27	20.99	30.66	20.44
8	wash-2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
9	nut_sol_blind_2014_05_15	4.09	n.a.	n.a.	n.a.	0.24	n.a.	n.a.	n.a.
10	nut_sol_0000ppbSe_2014_05_15	4.08	6.57	8.16	9.66	4.25	277.18	23.57	59.80
11	nut_sol_0020ppbSe_2014_05_15	4.08	6.60	8.17	9.66	2.39	153.46	15.97	36.53
12	nut_sol_0050ppbSe_2014_05_15	4.08	6.57	8.16	9.65	5.26	273.97	22.79	56.56
13	nut_sol_0100ppbSe_2014_05_15	4.08	6.58	8.17	9.66	3.26	244.44	25.09	58.14
14	nut_sol_0200ppbSe_2014_05_15	4.08	6.58	8.16	9.65	3.32	247.17	22.96	53.96
15	nut_sol_0500ppbSe_2014_05_15	4.08	6.56	8.16	9.65	4.58	294.59	26.30	62.03
16	nut_sol_1000ppbSe_2014_05_15	4.08	6.56	8.16	9.65	4.10	289.28	26.41	60.09
17	nut_sol_2000ppbSe_2014_05_15	4.08	6.57	8.16	9.66	3.90	291.39	26.76	62.71
18	nut_sol_5000ppbSe_2014_05_15	4.08	6.57	8.14	9.65	3.95	298.03	31.05	61.85
19	nut_sol_10000ppbSe_2014_05_15	4.08	6.58	8.14	9.65	3.63	269.62	38.64	60.24
20	wash-3	4.11	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
21	Standard_3-2	4.09	6.64	8.15	9.65	10.30	21.23	30.59	20.62
22	wash-4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
23	nut_sol_0000ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.65	3.60	280.26	n.a.	58.80
24	nut_sol_0020ppbSe_GB_2014_06_03	4.08	6.59	n.a.	9.65	3.42	232.54	n.a.	50.52
25	nut_sol_0050ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.64	3.73	289.92	n.a.	57.00
26	nut_sol_0100ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.64	3.87	275.68	n.a.	54.81
27	nut_sol_0200ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.64	3.91	283.05	n.a.	57.15
28	nut_sol_0500ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.64	3.82	285.01	n.a.	57.82
29	nut_sol_1000ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.65	3.62	284.65	n.a.	58.09
30	nut_sol_2000ppbSe_GB_2014_06_03	4.08	6.58	n.a.	9.64	3.73	288.76	n.a.	57.61
31	nut_sol_5000ppbSe_GB_2014_06_03	4.08	6.59	n.a.	9.65	3.43	279.05	n.a.	60.28
32	nut_sol_10000ppbSe_GB_2014_06_03	4.08	6.59	n.a.	9.65	3.59	277.43	n.a.	59.49
33	wash-5	4.18	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
34	Standard_3-3	4.09	6.65	8.14	9.65	10.40	21.33	30.75	20.69
35	wash-6	4.12	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
36	nut_sol_0000ppbSe_MB_2014_06_03	4.08	6.61	n.a.	9.65	3.98	208.21	n.a.	63.20
37	nut_sol_0020ppbSe_MB_2014_06_03	4.08	6.61	n.a.	9.64	3.82	182.02	n.a.	69.65
38	nut_sol_0050ppbSe_MB_2014_06_03	4.08	6.60	n.a.	9.65	3.63	220.01	n.a.	62.37
39	nut_sol_0100ppbSe_MB_2014_06_03	4.08	6.61	n.a.	9.65	3.20	197.35	n.a.	63.79
40	nut_sol_0200ppbSe_MB_2014_06_03	4.08	6.60	n.a.	9.65	3.27	206.42	n.a.	65.07
41	nut_sol_0500ppbSe_MB_2014_06_03	4.08	6.60	n.a.	9.64	4.05	215.97	n.a.	66.91
42	nut_sol_1000ppbSe_MB_2014_06_03	4.08	6.60	n.a.	9.64	3.39	212.00	n.a.	64.51
43	nut_sol_2000ppbSe_MB_2014_06_03	4.08	6.60	n.a.	9.65	5.78	210.51	n.a.	63.58
44	nut_sol_5000ppbSe_MB_2014_06_03	4.08	6.60	n.a.	9.65	3.42	219.96	n.a.	67.96
45	nut_sol_10000ppbSe_MB_2014_06_03	4.08	6.61	n.a.	9.65	3.84	179.76	n.a.	71.52
46	wash-7	4.11	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
47	Standard_3-4	4.09	6.64	8.15	9.65	10.41	21.38	30.96	20.62
48	wash-8	4.18	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
49	Std_Riverwater	4.11	n.a.	n.a.	9.61	43.82	n.a.	n.a.	154.94
50	wash-9	4.07	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
51	Stopmeth	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

Table C.29.: *C analytical data - ICP-MS measurement I; Na₂SeO₄ uptake into plants in the presence of kaolinite sorption*

Technique	ICP-MS Quadrupole						
System	X-Series Thermo Fischer						
Date measured	21.07.2014						
Isotope	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	dil. factor	Se mean ⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se	SD
	[µg/L]	[µg/L]	[µg/L]	[µg/L]	[-]	[µg/L]	[µg/L]
Analytical Quality							
wash-mean	0.05	0.04	0.07	0.08	1		
wash-SD	0.04	0.02	0.01	0.04	1		
LOD (= 3·wash)	0.12	0.05	0.04	0.12			
HighPurityStd ref. value	2.20	2.20	2.20	2.20	(5)		
Quality [%]	126.16	119.27	114.82	114.20			
Calibration							
Std 0ppb	0.15	0.01	0.07	0.06	1	0.08	0.07
Std 0.5ppb	4.93	4.88	5.05	4.99	1	4.96	0.09
Std 1ppb	10.09	10.23	10.25	10.14	1	10.19	0.09
Std 2.5ppb	25.07	25.56	25.24	25.16	1	25.29	0.25
Std 5ppb	50.30	50.24	50.35	50.75	1	50.30	0.06
Std 10ppb	99.71	100.70	100.40	99.94	1	100.27	0.51
Std 25ppb	248.40	251.30	251.00	249.40	1	250.23	1.59
Std 50ppb	494.80	497.90	498.60	499.20	1	497.10	2.02
Std 100ppb	1000.00	1001.00	1000.00	1001.00	1	1000.33	0.58
Samples							
wash 2	0.12	0.04	0.07	0.10	1		
HPS	2.66	2.62	2.61	2.61	(5)		
wash 3	0.15	0.05	0.08	0.14	1		
initsol_Na2SeO4_10000ppb	2401.00	2532.00	2525.00	2511.00	5	12430.00	368.48
initsol_Na2SeO4_05000ppb	1211.00	1278.00	1282.00	1278.00	5	6285.00	199.44
initsol_Na2SeO4_02000ppb	1182.00	1254.00	1251.00	1252.00	2	2458.00	81.46
initsol_Na2SeO4_01000ppb	603.00	638.60	640.30	641.90	2	1254.60	42.12
initsol_Na2SeO4_00500ppb	299.20	315.70	318.00	314.50	2	621.93	20.51
initsol_Na2SeO4_00200ppb	128.40	135.50	134.30	134.70	2	265.47	7.60
initsol_Na2SeO4_00100ppb	59.86	63.09	62.40	62.48	2	123.57	3.40
initsol_Na2SeO4_00050ppb	31.91	33.49	34.17	34.40	2	66.38	2.32
initsol_Na2SeO4_00020ppb	13.27	13.79	14.14	13.91	2	27.47	0.88
initsol_Na2SeO4_00000ppb	0.15	0.07	0.13	0.05	2	0.23	0.08
autoclave_blnd	0.16	0.10	0.11	0.10	2	0.25	0.07
wash 4	0.09	0.04	0.06	0.12	1		
test 5ppb	49.65	51.10	50.77	51.00	1		
HPS	2.85	2.48	2.39	2.47	5		
wash 5	0.16	0.03	0.09	0.05	1		
K-sorp+plant_Na2SeO4_10000ppb	1998.00	2106.00	2109.00	2105.00	5	10355.00	316.19
K-sorp+plant_Na2SeO4_05000ppb	1015.00	1073.00	1075.00	1073.00	5	5271.67	170.39
K-sorp+plant_Na2SeO4_02000ppb	964.70	1020.00	1022.00	1018.00	2	2004.47	65.04
K-sorp+plant_Na2SeO4_01000ppb	502.80	528.60	531.60	531.50	2	1042.00	31.67
K-sorp+plant_Na2SeO4_00500ppb	247.50	263.50	263.90	261.10	2	516.60	18.71
K-sorp+plant_Na2SeO4_00200ppb	106.30	113.20	112.80	112.60	2	221.53	7.75
K-sorp+plant_Na2SeO4_00100ppb	49.16	52.26	52.53	52.26	2	102.63	3.75
K-sorp+plant_Na2SeO4_00050ppb	27.35	29.06	29.06	29.24	2	56.98	1.97
K-sorp+plant_Na2SeO4_00020ppb	11.34	11.72	11.43	11.66	2	22.99	0.40
K-sorp+plant_Na2SeO4_00000ppb	0.78	0.61	0.76	0.85	2	1.44	0.18
wash 6	0.08	0.04	0.07	0.06	1		
test 5ppb	50.63	52.22	52.34	52.24	1		
wash 7	0.19	0.07	0.08	0.05	1		
wash 8	0.07	0.05	0.06	0.06	1		
K-sorp_Na2SeO4_10000ppb	2181.00	2302.00	2316.00	2322.00	5	11331.67	371.16
K-sorp_Na2SeO4_05000ppb	1114.00	1184.00	1176.00	1183.00	5	5790.00	191.57
K-sorp_Na2SeO4_02000ppb	1112.00	1171.00	1172.00	1172.00	2	2303.33	68.71
K-sorp_Na2SeO4_01000ppb	529.60	558.00	566.80	569.80	2	1102.93	38.88
K-sorp_Na2SeO4_00500ppb	258.10	275.20	274.40	278.50	2	538.47	19.30
K-sorp_Na2SeO4_00200ppb	116.00	122.80	123.30	123.30	2	241.40	8.16
K-sorp_Na2SeO4_00100ppb	50.10	52.85	53.43	54.09	2	104.25	3.56
K-sorp_Na2SeO4_00050ppb	29.60	30.99	31.53	31.65	2	61.41	1.99
K-sorp_Na2SeO4_00020ppb	11.51	12.44	12.24	12.35	2	24.13	0.98
K-sorp_Na2SeO4_00000ppb	0.66	0.35	0.54	0.54	2	1.03	0.31
wash 9	0.07	0.01	0.06	0.12	1		
test 5ppb	51.03	51.26	51.55	50.72	1		
wash 9 wdh	0.14	0.06	0.09	0.02	1		
HPS wdh	2.90	2.63	2.44	2.41	5		
wash 10	0.07	0.02	0.07	0.02	1		

Table C.30.: C analytical data - ICP-MS measurement II; Na₂SeO₃ uptake into plants in the presence of kaolinite sorption

Technique	ICP-MS Quadrupole							
System	X-Series Thermo Fischer							
Date measured	22.07.2014							
Isotope	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	dil. factor	Se mean ⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se	SD	
	[µg/L]	[µg/L]	[µg/L]	[µg/L]	[-]	[µg/L]	[µg/L]	
Analytical Quality								
wash-mean	0.16	0.14	0.16	0.17				
wash-SD	0.09	0.09	0.08	0.07				
LOD (= 3·wash)	0.27	0.26	0.23	0.22				
HighPurityStd ref. value	2.20	2.20	2.20	2.20	(5)			
Quality [%]	129.82	109.68	114.45	114.11				
Calibration								
Std 0ppb	0.07	0.07	0.06	0.08	1	0.07	0.00	
Std 0.5ppb	5.26	5.09	4.81	5.17	1	5.05	0.22	
Std 1ppb	9.95	10.34	10.28	10.09	1	10.19	0.21	
Std 2.5ppb	25.16	25.30	25.41	24.79	1	25.29	0.13	
Std 5ppb	50.12	49.09	50.41	49.77	1	49.87	0.69	
Std 10ppb	100.30	100.00	99.39	100.40	1	99.90	0.46	
Std 25ppb	248.00	251.50	249.10	249.10	1	249.53	1.79	
Std 50ppb	496.40	498.80	500.60	498.00	1	498.60	2.11	
Std 100ppb	1002.00	1000.00	1000.00	1001.00	1	1000.67	1.15	
Samples								
wash 2	0.12	0.04	0.07	0.08	1			
HPS	2.71	2.32	2.41	2.36	5			
wash 3	0.08	0.04	0.07	0.05	1			
initsol_Na2SeO3_10000ppb	2199.00	2319.00	2309.00	2323.00	5	11378.33	332.92	
initsol_Na2SeO3_05000ppb	1102.00	1160.00	1162.00	1155.00	5	5706.67	170.39	
initsol_Na2SeO3_02000ppb	1146.00	1213.00	1206.00	1203.00	2	2376.67	73.66	
initsol_Na2SeO3_01000ppb	570.60	601.10	602.40	600.00	2	1182.73	35.99	
initsol_Na2SeO3_00500ppb	269.00	284.50	279.80	280.50	2	555.53	15.90	
initsol_Na2SeO3_00200ppb	112.60	118.30	118.60	117.60	2	233.00	6.76	
initsol_Na2SeO3_00100ppb	57.78	61.05	61.39	61.66	2	120.15	3.99	
initsol_Na2SeO3_00050ppb	28.53	30.85	30.07	30.06	2	59.63	2.36	
initsol_Na2SeO3_00020ppb	11.24	12.03	11.52	11.66	2	23.19	0.80	
initsol_Na2SeO3_00000ppb	0.53	0.45	0.43	0.46	2	0.94	0.10	
autoclave_blnd	0.51	0.61	0.59	0.61	2	1.14	0.11	
wash 4	0.17	0.12	0.18	0.20	1			
test 5ppb	49.27	51.19	50.03	49.19	1			
wash 5	0.11	0.13	0.16	0.13	1			
K-sorp+plant_Na2SeO3_10000ppb	1886.00	1981.00	1976.00	1976.00	5	9738.33	267.32	
K-sorp+plant_Na2SeO3_05000ppb	865.80	916.20	906.10	912.60	5	4480.17	133.33	
K-sorp+plant_Na2SeO3_02000ppb	783.60	824.30	824.60	829.90	2	1621.67	47.17	
K-sorp+plant_Na2SeO3_01000ppb	440.00	461.60	460.60	464.40	2	908.13	24.38	
K-sorp+plant_Na2SeO3_00500ppb	174.60	185.40	182.80	185.40	2	361.87	11.27	
K-sorp+plant_Na2SeO3_00200ppb	80.14	84.02	84.76	85.91	2	165.95	4.96	
K-sorp+plant_Na2SeO3_00100ppb	39.72	41.26	41.51	42.25	2	81.66	1.94	
K-sorp+plant_Na2SeO3_00050ppb	19.42	20.84	20.67	20.95	2	40.62	1.55	
K-sorp+plant_Na2SeO3_00020ppb	7.55	8.10	8.00	8.22	2	15.77	0.59	
K-sorp+plant_Na2SeO3_00000ppb	1.23	1.14	1.17	1.45	2	2.36	0.09	
wash 6	0.19	0.26	0.26	0.22	1			
test 5ppb	50.12	50.51	50.43	50.54	1			
wash 7	0.20	0.14	0.20	0.11	1			
K-sorp_Na2SeO3_10000ppb	2020.00	2137.00	2123.00	2127.00	5	10466.67	319.47	
K-sorp_Na2SeO3_05000ppb	1005.00	1055.00	1047.00	1053.00	5	5178.33	134.29	
K-sorp_Na2SeO3_02000ppb	938.00	989.80	988.50	997.10	2	1944.20	59.08	
K-sorp_Na2SeO3_01000ppb	492.90	518.50	517.50	520.50	2	1019.27	29.00	
K-sorp_Na2SeO3_00500ppb	229.60	244.60	240.90	242.70	2	476.73	15.63	
K-sorp_Na2SeO3_00200ppb	93.98	99.01	97.63	98.40	2	193.75	5.20	
K-sorp_Na2SeO3_00100ppb	46.53	48.76	49.06	49.36	2	96.23	2.76	
K-sorp_Na2SeO3_00050ppb	22.67	23.62	23.27	23.58	2	46.37	0.96	
K-sorp_Na2SeO3_00020ppb	8.99	9.13	9.25	9.28	2	18.24	0.26	
K-sorp_Na2SeO3_00000ppb	1.12	1.05	1.06	1.19	2	2.15	0.07	
wash 8	0.33	0.26	0.24	0.23	1			
HPS	3.01	2.51	2.63	2.67	(5)			
test 5ppb	50.62	49.88	50.43	51.01	1			
wash 9	0.20	0.21	0.24	0.23	1			

Table C.31.: C analytical data - ICP-MS measurement III; Na₂SeO₄ uptake into plants in the presence of goethite sorption

Technique	ICP-MS Quadrupole							
System	X-Series Thermo Fischer							
Date measured	23.07.2014							
Isotope	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	dil. factor	Se mean ⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se	SD	
	[µg/L]	[µg/L]	[µg/L]	[µg/L]	[-]	[µg/L]	[µg/L]	
Analytical Quality								
wash-mean	0.17	0.08	0.11	0.13				
wash-SD	0.06	0.04	0.04	0.03				
LOD (= 3·wash)	0.18	0.13	0.13	0.09				
HighPurityStd ref. value	2.20	2.20	2.20	2.20	(5)			
Quality [%]	130.86	103.43	108.64	111.34				
Calibration								
Std 0ppb	0.12	0.07	0.08	0.12	1	0.09	0.03	
Std 0.5ppb	5.44	5.03	4.95	5.01	1	5.14	0.26	
Std 1ppb	9.91	10.17	10.13	10.04	1	10.07	0.14	
Std 2.5ppb	24.90	24.49	24.99	25.41	1	24.79	0.27	
Std 5ppb	50.24	49.22	50.21	50.09	1	49.89	0.58	
Std 10ppb	100.30	98.40	100.10	98.78	1	99.60	1.04	
Std 25ppb	249.40	248.10	249.00	250.50	1	248.83	0.67	
Std 50ppb	496.90	495.60	500.50	498.80	1	497.67	2.54	
Std 100ppb	1002.00	1003.00	999.90	1001.00	1	1001.63	1.58	
Samples								
wash 2	0.07	0.06	0.09	0.10	1			
HPS	2.99	2.34	2.44	2.42	(5)			
wash 3	0.14	0.06	0.10	0.11	1			
initsol_Na2SeO4_10000ppb	888.30	932.40	930.50	922.90	5	4585.33	124.65	
initsol_Na2SeO4_05000ppb	431.90	452.50	451.90	451.20	5	2227.17	58.62	
initsol_Na2SeO4_02000ppb	1104.00	1164.00	1159.00	1155.00	2	2284.67	66.58	
initsol_Na2SeO4_01000ppb	553.00	585.70	584.70	582.70	2	1148.93	37.19	
initsol_Na2SeO4_00500ppb	272.80	287.00	290.00	285.80	2	566.53	18.38	
initsol_Na2SeO4_00200ppb	112.20	119.70	118.80	117.60	2	233.80	8.19	
initsol_Na2SeO4_00100ppb	55.09	57.67	58.62	58.56	2	114.25	3.65	
initsol_Na2SeO4_00050ppb	28.77	30.01	30.72	30.97	2	59.67	1.97	
initsol_Na2SeO4_00020ppb	12.56	12.79	13.09	12.90	2	25.63	0.53	
initsol_Na2SeO4_00000ppb	0.50	0.26	0.45	0.45	2	0.81	0.25	
autoclave_blnd	0.50	0.43	0.43	0.47	2	0.91	0.08	
wash 4	0.15	0.04	0.09	0.15	1			
test 5ppb	50.63	50.62	49.91	50.00	1			
wash 5	0.14	0.07	0.11	0.13	1			
G-sorp+plant_Na2SeO4_10000ppb	352.70	369.60	373.40	375.90	5	1826.17	55.10	
G-sorp+plant_Na2SeO4_05000ppb	135.90	144.20	145.10	144.20	5	708.67	25.36	
G-sorp+plant_Na2SeO4_02000ppb	477.70	499.20	502.30	501.80	2	986.13	26.80	
G-sorp+plant_Na2SeO4_01000ppb	236.10	248.70	247.40	245.00	2	488.13	13.86	
G-sorp+plant_Na2SeO4_00500ppb	129.00	134.50	136.10	135.40	2	266.40	7.45	
G-sorp+plant_Na2SeO4_00200ppb	48.25	49.64	49.14	49.46	2	98.02	1.41	
G-sorp+plant_Na2SeO4_00100ppb	23.84	24.94	25.17	25.69	2	49.30	1.42	
G-sorp+plant_Na2SeO4_00050ppb	14.47	14.99	15.47	15.63	2	29.95	1.00	
G-sorp+plant_Na2SeO4_00020ppb	5.75	6.06	5.99	6.35	2	11.86	0.32	
G-sorp+plant_Na2SeO4_00000ppb	0.43	0.34	0.31	0.72	2	0.72	0.13	
wash 6	0.19	0.08	0.10	0.13	1			
test 5ppb	51.02	50.95	51.42	50.65	1			
wash 7	0.24	0.09	0.10	0.08	1			
G-sorp_Na2SeO4_10000ppb	327.90	342.40	344.90	342.90	5	1692.00	45.89	
G-sorp_Na2SeO4_05000ppb	157.20	165.70	166.80	166.60	5	816.17	26.27	
G-sorp_Na2SeO4_02000ppb	402.00	417.30	419.30	416.80	2	825.73	18.93	
G-sorp_Na2SeO4_01000ppb	204.70	214.40	214.30	213.00	2	422.27	11.14	
G-sorp_Na2SeO4_00500ppb	94.60	98.42	100.50	98.07	2	195.68	5.98	
G-sorp_Na2SeO4_00200ppb	39.67	41.66	42.09	42.06	2	82.28	2.58	
G-sorp_Na2SeO4_00100ppb	21.51	22.98	22.44	22.46	2	44.62	1.49	
G-sorp_Na2SeO4_00050ppb	10.44	11.15	10.84	11.15	2	21.62	0.71	
G-sorp_Na2SeO4_00020ppb	5.01	5.15	5.22	5.32	2	10.25	0.21	
G-sorp_Na2SeO4_00000ppb	0.69	0.63	0.65	0.81	2	1.32	0.06	
wash 8	0.19	0.07	0.08	0.10	1			
HPS	2.77	2.22	2.34	2.48	(5)			
test 5ppb	50.43	51.01	50.98	50.60	1			
wash 9	0.27	0.19	0.22	0.17	1			

Table C.32.: C analytical data - ICP-MS measurement IV; Na₂SeO₃ uptake into plants in the presence of goethite sorption

Technique	ICP-MS Quadrupole							
System	X-Series Thermo Fischer							
Date measured	24.07.2014							
Isotope	⁷⁶ Se	⁷⁷ Se	⁷⁸ Se	⁸² Se	dil. factor	Se mean ⁷⁶ Se, ⁷⁷ Se, ⁷⁸ Se		SD
	[µg/L]	[µg/L]	[µg/L]	[µg/L]	[-]	[µg/L]		[µg/L]
Analytical Quality								
wash-mean	0.17	0.11	0.15	0.18				
wash-SD	0.07	0.08	0.06	0.04				
LOD (= 3·wash)	0.20	0.24	0.18	0.12				
HighPurityStd ref. value	2.20	2.20	2.20	2.20	(5)			
Quality [%]	135.05	111.55	110.75	110.52				
Calibration								
Std 0ppb	0.04	0.06	0.09	0.17	1	0.06	0.02	
Std 0.5ppb	5.02	4.95	5.11	5.12	1	5.03	0.08	
Std 1ppb	10.05	9.77	9.93	10.10	1	9.92	0.14	
Std 2.5ppb	25.12	25.20	25.07	24.95	1	25.13	0.07	
Std 5ppb	49.90	48.44	48.92	49.45	1	49.09	0.74	
Std 10ppb	99.74	100.40	99.26	99.33	1	99.80	0.57	
Std 25ppb	249.20	250.50	248.40	248.30	1	249.37	1.06	
Std 50ppb	498.10	502.30	500.70	501.00	1	500.37	2.12	
Std 100ppb	1001.00	998.70	1000.00	1000.00	1	999.90	1.15	
Samples								
wash 2	0.22	0.07	0.12	0.16	1			
HPS	3.06	2.46	2.43	2.52	(5)			
wash 3	0.15	0.06	0.10	0.16	1			
initsol_Na2SeO3_10000ppb	1942.00	2069.00	2070.00	2043.00	5	10135.00	368.07	
initsol_Na2SeO3_05000ppb	1036.00	1099.00	1087.00	1086.00	5	5370.00	167.26	
initsol_Na2SeO3_02000ppb	1015.00	1078.00	1073.00	1066.00	2	2110.67	70.04	
initsol_Na2SeO3_01000ppb	517.30	543.50	542.00	539.30	2	1068.53	29.43	
initsol_Na2SeO3_00500ppb	251.50	266.00	264.60	263.80	2	521.40	16.00	
initsol_Na2SeO3_00200ppb	102.50	107.80	107.40	107.80	2	211.80	5.90	
initsol_Na2SeO3_00100ppb	51.42	53.56	53.77	53.67	2	105.83	2.60	
initsol_Na2SeO3_00050ppb	26.72	27.93	28.21	28.13	2	55.24	1.58	
initsol_Na2SeO3_00020ppb	11.19	11.72	11.60	11.47	2	23.01	0.56	
initsol_Na2SeO3_00000ppb	0.95	0.84	0.91	0.99	2	1.80	0.11	
autoclave_blnd	0.85	0.91	0.90	0.94	2	1.78	0.06	
wash 4	0.21	0.13	0.21	0.21	1			
test 5ppb	49.86	48.14	49.35	48.87	1			
wash 5	0.17	0.24	0.23	0.22	1			
G-sorp_Na2SeO3_10000ppb	6.26	6.43	6.45	6.49	5	31.90	0.53	
G-sorp_Na2SeO3_05000ppb	3.07	3.09	3.05	3.13	5	15.35	0.11	
G-sorp_Na2SeO3_02000ppb	3.03	3.41	3.41	3.50	2	6.56	0.44	
G-sorp_Na2SeO3_01000ppb	1.52	1.68	1.74	2.07	2	3.29	0.23	
G-sorp_Na2SeO3_00500ppb	1.31	1.16	1.18	1.50	2	2.43	0.15	
G-sorp_Na2SeO3_00200ppb	1.18	1.01	0.98	1.31	2	2.11	0.21	
G-sorp_Na2SeO3_00100ppb	1.26	1.16	1.09	1.42	2	2.34	0.17	
G-sorp_Na2SeO3_00050ppb	1.47	1.40	1.41	1.74	2	2.85	0.08	
G-sorp_Na2SeO3_00020ppb	0.70	0.73	0.60	1.07	2	1.34	0.13	
G-sorp_Na2SeO3_00000ppb	0.61	0.47	0.52	0.81	2	1.06	0.14	
wash 6	0.20	0.08	0.14	0.15	1			
test 5ppb	50.22	49.32	49.60	49.32	1			
wash 7	0.11	0.07	0.12	0.14	1			
G-sorp+plant_Na2SeO3_10000ppb	4.29	4.19	4.23	4.18	5	21.19	0.25	
G-sorp+plant_Na2SeO3_05000ppb	2.28	2.54	2.46	2.53	5	12.13	0.67	
G-sorp+plant_Na2SeO3_02000ppb	2.51	2.66	2.63	2.65	2	5.20	0.15	
G-sorp+plant_Na2SeO3_01000ppb	1.70	1.60	1.62	1.73	2	3.28	0.11	
G-sorp+plant_Na2SeO3_00500ppb	1.11	0.96	0.95	1.22	2	2.01	0.18	
G-sorp+plant_Na2SeO3_00200ppb	0.81	0.80	0.81	0.92	2	1.61	0.02	
G-sorp+plant_Na2SeO3_00100ppb	0.62	0.56	0.57	0.69	2	1.17	0.06	
G-sorp+plant_Na2SeO3_00050ppb	0.63	0.59	0.59	0.58	2	1.20	0.05	
G-sorp+plant_Na2SeO3_00020ppb	0.77	0.61	0.68	0.78	2	1.37	0.15	
G-sorp+plant_Na2SeO3_00000ppb	1.78	1.83	1.86	1.90	2	3.64	0.08	
wash 8	0.18	0.05	0.10	0.13	1			
HPS wdh	2.88	2.45	2.44	2.35	(5)			
test 5ppb	50.21	49.75	50.40	50.20	1			
wash 9	0.30	0.27	0.25	0.17	1			

Table C.33.: C analytical data - ICP-MS measurement V; Exp. C desorption from kaolinite using K_2HPO_4

Technique	ICP-MS Quadrupole						
System	X-Series Thermo Fischer						
Date measured	17.07.2014						
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean (drift.-corr.) $^{77}\text{Se},^{78}\text{Se}$	SD
	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[-]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]
Analytical Quality							
wash-mean	0.37	0.05	0.08	0.25			
wash-SD	0.12	0.02	0.03	0.03			
LOD (= 3-wash)	0.37	0.06	0.09	0.09			
HighPurityStd ref. value	5.50	5.50	5.50	5.50			
Quality [%]	146.29	110.53	110.29	110.35			
Calibration							
Std 0ppb	0.04	0.02	0.08	0.21		0.05	0.04
Std 5ppb Se	4.87	5.00	5.12	5.31		5.06	0.08
Std 10ppb Se	10.33	10.06	10.15	10.06		10.11	0.06
Std 25ppb Se	25.80	24.88	25.17	25.30		25.03	0.21
Std 50ppb Se	49.72	50.93	50.82	50.04		50.88	0.08
Std 100ppb Se	97.88	100.60	99.56	100.30		100.08	0.74
Std 250ppb Se	249.60	250.30	248.00	247.70		249.15	1.63
Std 500ppb Se	503.00	502.90	501.50	501.00		502.20	0.99
Std 1000ppb Se	998.80	998.40	999.80	1000.00		999.10	0.99
Samples							
wash 2	0.27	0.10	0.15	0.21			
HPS	7.26	5.44	5.58	5.88	(2)		
wash 3	0.19	0.06	0.09	0.23			
K-desorp_sorp+plant_SeO4_10000ppb	61.30	58.21	57.42	57.70	10	572.34	0.48
K-desorp_sorp+plant_SeO4_05000ppb	29.91	28.88	28.23	28.91	10	281.24	0.40
K-desorp_sorp+plant_SeO4_02000ppb	13.93	13.02	12.84	12.82	10	126.70	0.09
K-desorp_sorp+plant_SeO4_01000ppb	6.87	6.27	6.28	6.52	10	61.19	0.03
K-desorp_sorp+plant_SeO4_00500ppb	4.09	3.33	3.16	3.50	10	31.47	0.10
K-desorp_sorp+plant_SeO4_00200ppb	1.67	0.99	1.00	1.33	10	9.57	0.01
K-desorp_sorp+plant_SeO4_00100ppb	1.48	0.71	0.78	1.10	10	7.15	0.05
K-desorp_sorp+plant_SeO4_00050ppb	0.87	0.34	0.39	0.75	10	3.47	0.03
K-desorp_sorp+plant_SeO4_00020ppb	0.88	0.23	0.34	0.63	10	2.74	0.08
K-desorp_sorp+plant_SeO4_00000ppb	0.77	0.14	0.23	0.65	10	1.75	0.06
wash 4	0.46	0.04	0.11	0.26	1		
Test 25ppb	27.39	26.62	26.64	26.57	1		
wash 5	0.37	0.05	0.07	0.26	1		
K-desorp_sorp_SeO4_10000ppb	67.73	63.59	63.02	61.50	10	594.95	0.21
K-desorp_sorp_SeO4_05000ppb	40.77	38.59	38.43	37.75	10	361.95	0.29
K-desorp_sorp_SeO4_02000ppb	14.72	13.29	13.27	13.64	10	124.82	0.14
K-desorp_sorp_SeO4_01000ppb	9.02	8.44	8.22	8.39	10	78.31	0.05
K-desorp_sorp_SeO4_00500ppb	4.35	3.78	3.77	3.80	10	35.49	0.04
K-desorp_sorp_SeO4_00200ppb	1.73	1.21	1.18	1.52	10	11.27	0.00
K-desorp_sorp_SeO4_00100ppb	1.94	0.83	1.02	1.40	10	8.74	0.14
K-desorp_sorp_SeO4_00050ppb	1.10	0.44	0.51	0.69	10	4.48	0.06
K-desorp_sorp_SeO4_00020ppb	0.88	0.21	0.28	0.74	10	2.30	0.05
K-desorp_sorp_SeO4_00000ppb	0.72	0.09	0.12	0.62	10	0.98	0.03
wash 6	0.50	0.04	0.07	0.30			
Test 25ppb	27.30	26.86	26.37	26.63			
wash 7	0.43	0.03	0.07	0.29			
K-desorp_sorp+plant_SeO3_10000ppb	42.00	38.85	38.72	38.57	10	364.88	0.67
K-desorp_sorp+plant_SeO3_05000ppb	28.09	26.13	26.05	25.76	10	245.50	0.45
K-desorp_sorp+plant_SeO3_02000ppb	12.82	12.50	11.70	11.58	10	113.83	0.30
K-desorp_sorp+plant_SeO3_01000ppb	6.73	6.19	5.85	6.01	10	56.66	0.11
K-desorp_sorp+plant_SeO3_00500ppb	4.93	4.15	4.17	4.29	10	39.17	0.10
K-desorp_sorp+plant_SeO3_00200ppb	2.64	1.87	1.95	2.32	10	17.97	0.09
K-desorp_sorp+plant_SeO3_00100ppb	2.18	1.49	1.49	1.78	10	14.04	0.02
K-desorp_sorp+plant_SeO3_00050ppb	1.34	0.73	0.87	1.28	10	7.53	0.11
K-desorp_sorp+plant_SeO3_00020ppb	1.10	0.35	0.49	0.86	10	3.96	0.10
K-desorp_sorp+plant_SeO3_00000ppb	0.85	0.12	0.25	0.84	10	1.72	0.09
wash 8	0.45	0.04	0.07	0.28			
Test 25ppb	27.41	26.75	26.34	26.31			
wash 9	0.44	0.04	0.08	0.22			
K-desorp_sorp_SeO3_10000ppb	52.90	50.87	49.38	49.14	10	470.42	0.14
K-desorp_sorp_SeO3_05000ppb	19.93	18.34	18.29	18.36	10	171.53	0.27
K-desorp_sorp_SeO3_02000ppb	16.18	14.51	14.64	14.65	10	136.21	0.31
K-desorp_sorp_SeO3_01000ppb	9.28	8.64	8.51	8.59	10	79.94	0.04
K-desorp_sorp_SeO3_00500ppb	5.29	4.95	4.82	5.15	10	45.46	0.01
K-desorp_sorp_SeO3_00200ppb	3.24	2.16	2.40	2.75	10	21.18	0.19
K-desorp_sorp_SeO3_00100ppb	2.04	1.33	1.36	1.90	10	12.43	0.04
K-desorp_sorp_SeO3_00050ppb	1.47	0.86	0.81	1.26	10	7.70	0.02
K-desorp_sorp_SeO3_00020ppb	0.93	0.36	0.43	0.75	10	3.64	0.05
K-desorp_sorp_SeO3_00000ppb	0.75	0.09	0.16	0.46	10	1.13	0.05
wash 10	0.44	0.03	0.07	0.24			
HPS wdh	8.05	6.08	6.07	6.07	(2)		
Test 25ppb	28.67	27.34	27.19	27.37			
wash 11	0.43	0.03	0.07	0.27			

Table C.34.: C analytical data - ICP-MS measurement VI; Exp. C desorption from goethite using K_2HPO_4

Technique	ICP-MS Quadrupole						
System	X-Series Thermo Fischer						
Date measured	28.07.2014						
Isotope	^{76}Se	^{77}Se	^{78}Se	^{82}Se	dil. factor	Se mean $^{77}\text{Se}, ^{78}\text{Se}$	SD
	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]	[-]	[$\mu\text{g/L}$]	[$\mu\text{g/L}$]
Analytical Quality							
wash-mean	0.11	0.08	0.11	0.10			
wash-SD	0.06	0.03	0.03	0.05			
LOD (= 3·wash)	0.17	0.09	0.09	0.16			
HighPurityStd ref. value	5.50	5.50	5.50	5.50	2		
Quality [%]	137.87	104.48	104.98	104.21			
Calibration							
Std 0ppb	0.06	0.07	0.08	0.06	1	0.77	0.00565685
Std 5ppb Se	4.81	4.95	4.89	5.07	1	49.20	0.03818377
Std 10ppb Se	9.75	10.17	9.89	10.24	1	100.32	0.19516147
Std 25ppb Se	24.42	24.93	25.16	24.27	1	250.45	0.16263456
Std 50ppb Se	50.67	49.96	50.00	50.35	1	499.80	0.02828427
Std 100ppb Se	101.00	99.29	100.00	99.98	1	996.45	0.50204581
Std 250ppb Se	249.90	250.20	251.10	249.20	1	2506.50	0.6363961
Std 500ppb Se	498.90	500.30	498.80	501.30	1	4995.50	1.06066017
Std 1000ppb Se	1000.00	999.90	1000.00	999.50	1	9999.50	0.07071068
Samples							
wash 2	0.39	0.40	0.40	0.48			
HPS	7.58	5.85	5.90	5.71	(2)		
wash 3	0.19	0.15	0.19	0.19			
G-desorp_sorp+plant_SeO4_10000ppb	141.60	138.30	139.20	137.10	10	1387.5	0.64
G-desorp_sorp+plant_SeO4_05000ppb	123.30	119.20	117.60	118.60	10	1184.0	1.13
G-desorp_sorp+plant_SeO4_02000ppb	67.11	64.83	65.10	64.53	10	649.7	0.19
G-desorp_sorp+plant_SeO4_01000ppb	38.69	36.11	36.92	36.94	10	365.2	0.57
G-desorp_sorp+plant_SeO4_00500ppb	18.98	18.69	18.59	18.76	10	186.4	0.07
G-desorp_sorp+plant_SeO4_00200ppb	7.99	7.05	7.13	7.26	10	70.9	0.06
G-desorp_sorp+plant_SeO4_00100ppb	4.28	3.79	3.72	4.04	10	37.6	0.05
G-desorp_sorp+plant_SeO4_00050ppb	2.18	1.93	1.91	2.20	10	19.2	0.01
G-desorp_sorp+plant_SeO4_00020ppb	1.31	1.10	1.08	1.19	10	10.9	0.01
G-desorp_sorp+plant_SeO4_00000ppb	0.48	0.31	0.23	0.41	10	2.69	0.06
wash 4	0.15	0.09	0.10	0.11			
Test 25ppb	26.20	25.79	25.78	25.38			
wash 5	0.14	0.09	0.12	0.11			
G-desorp_sorp_SeO4_10000ppb	267.50	262.60	262.10	260.10	10	2623.5	0.35
G-desorp_sorp_SeO4_05000ppb	128.30	124.00	123.70	121.80	10	1238.5	0.21
G-desorp_sorp_SeO4_02000ppb	129.20	126.70	126.10	124.00	10	1264.0	0.42
G-desorp_sorp_SeO4_01000ppb	63.16	62.85	61.31	60.52	10	620.8	1.09
G-desorp_sorp_SeO4_00500ppb	32.28	31.64	30.90	31.15	10	312.7	0.52
G-desorp_sorp_SeO4_00200ppb	13.01	12.01	12.43	12.23	10	122.2	0.30
G-desorp_sorp_SeO4_00100ppb	6.14	5.64	5.66	5.57	10	56.5	0.01
G-desorp_sorp_SeO4_00050ppb	3.66	3.51	3.40	3.48	10	34.6	0.08
G-desorp_sorp_SeO4_00020ppb	1.45	1.24	1.21	1.34	10	12.2	0.03
G-desorp_sorp_SeO4_00000ppb	1.46	0.88	1.14	1.33	10	10.07	0.19
wash 6	0.15	0.04	0.09	0.06			
Test 25ppb	25.93	25.86	25.71	25.62			
wash 7	0.16	0.06	0.10	0.12			
G-desorp_sorp+plant_SeO3_10000ppb	784.60	773.70	767.40	766.40	10	7705.5	4.45
G-desorp_sorp+plant_SeO3_05000ppb	444.30	437.20	432.50	432.50	10	4348.5	3.32
G-desorp_sorp+plant_SeO3_02000ppb	150.80	147.00	145.50	146.30	10	1462.5	1.06
G-desorp_sorp+plant_SeO3_01000ppb	74.50	73.62	74.10	72.16	10	738.6	0.34
G-desorp_sorp+plant_SeO3_00500ppb	40.18	38.94	38.26	38.39	10	386.0	0.48
G-desorp_sorp+plant_SeO3_00200ppb	15.93	15.39	15.42	15.02	10	154.1	0.02
G-desorp_sorp+plant_SeO3_00100ppb	8.63	7.72	7.77	7.90	10	77.5	0.04
G-desorp_sorp+plant_SeO3_00050ppb	4.06	3.82	3.87	4.20	10	38.5	0.04
G-desorp_sorp+plant_SeO3_00020ppb	2.11	1.73	1.62	1.78	10	16.8	0.08
G-desorp_sorp+plant_SeO3_00000ppb	0.97	0.72	0.70	0.89	10	7.11	0.01
wash 8	0.12	0.07	0.09	0.04			
Test 25ppb	25.78	25.10	25.68	25.44			
wash 9	0.07	0.08	0.14	0.06			
G-desorp_sorp_SeO3_10000ppb	767.70	752.60	752.80	751.30	10	7527.0	0.14
G-desorp_sorp_SeO3_05000ppb	381.50	374.20	374.70	370.50	10	3744.5	0.35
G-desorp_sorp_SeO3_02000ppb	155.20	151.30	151.90	152.00	10	1516.0	0.42
G-desorp_sorp_SeO3_01000ppb	71.78	71.31	70.58	71.92	10	709.5	0.52
G-desorp_sorp_SeO3_00500ppb	34.14	32.77	32.99	33.29	10	328.8	0.16
G-desorp_sorp_SeO3_00200ppb	13.41	14.05	13.52	13.54	10	137.9	0.37
G-desorp_sorp_SeO3_00100ppb	8.29	8.01	8.04	7.93	10	80.2	0.02
G-desorp_sorp_SeO3_00050ppb	3.66	3.32	3.42	3.34	10	33.7	0.07
G-desorp_sorp_SeO3_00020ppb	1.77	1.70	1.67	1.94	10	16.9	0.02
G-desorp_sorp_SeO3_00000ppb	3.03	2.64	2.67	2.83	10	26.5	0.02
wash 10	0.03	0.06	0.10	0.10			
Test 25ppb	25.37	25.19	25.28	24.98			
HPS	7.59	5.64	5.65	5.76	(2)		
wash 11	0.05	0.10	0.11	0.04			