Metadata Management in Scientific Research: an overview

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iEntrance Advanced School, 22.02.2024

Outline

1.
Introduction

Motivation and recap of the FAIR principles

2.
Effective Metadata Management

Best practices and tools to implement them

3.
Metadata Management in practice

Top 10 management steps in real projects

4.
Conclusions

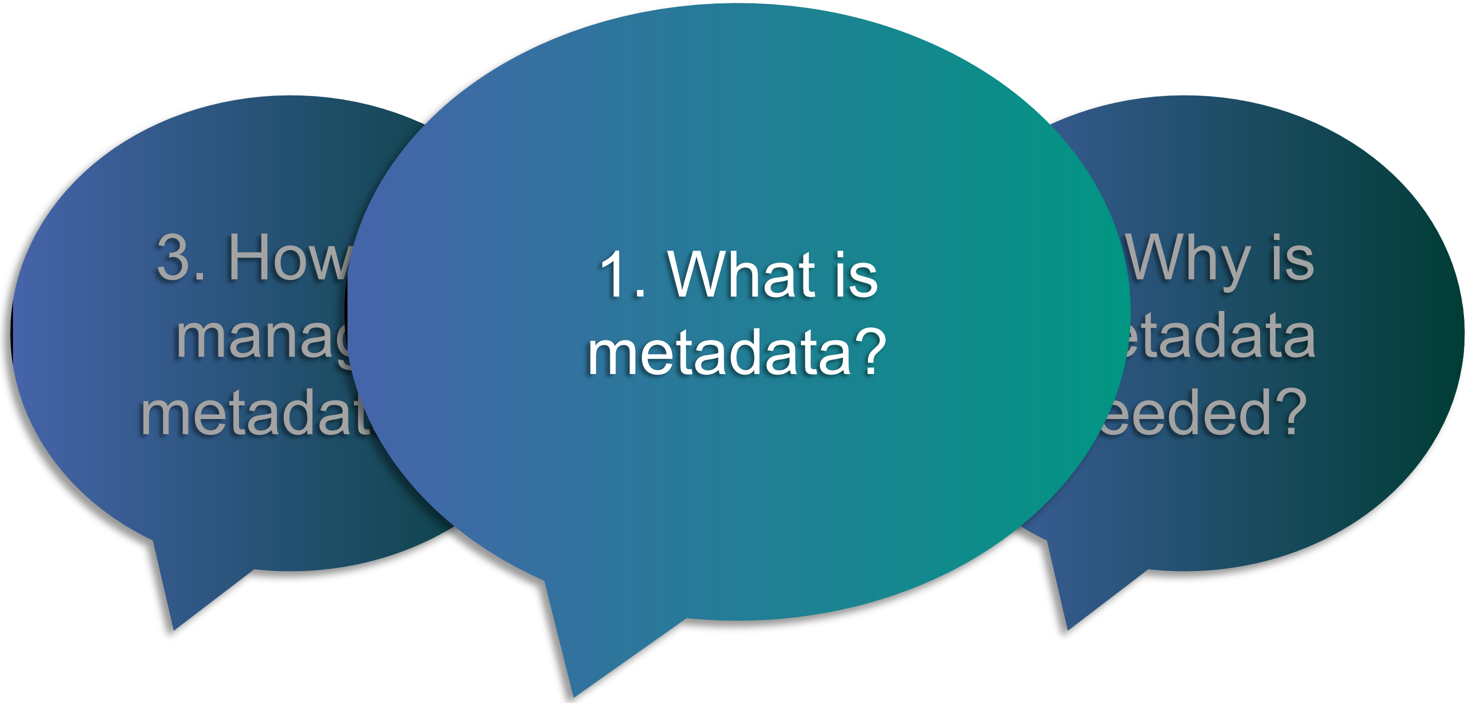
Summary and main takeaways

1. Introduction

Motivation

Powered by Bing Image Creator

Metadata



Data describing other data

Metadata

1. Wha metada

2. Why is metadata needed?

How to anage etadata?

To add context and meaning to data

Metadata

2. Why metada needed

3. How to manage metadata?

What is tadata?

We will see it throughout the next slides…

The FAIR Guiding Principles

Findable

Accessible

Interoperable

Reusable

https://www.go-fair.org/fair-principles/

The FAIR Guiding Principles

Findable	Accessible	Interoperable	Reusable

(Meta)data should be easy to find for both humans and computers

Globally unique persistent identifiers (PID)

https://www.go-fair.org/fair-principles/

The FAIR Guiding Principles

Findable | **Accessible** | Interoperable | Reusable

It should be known how (meta)data can be accessed

(Meta)data repositories, authorization & authentication

https://www.go-fair.org/fair-principles/

The FAIR Guiding Principles

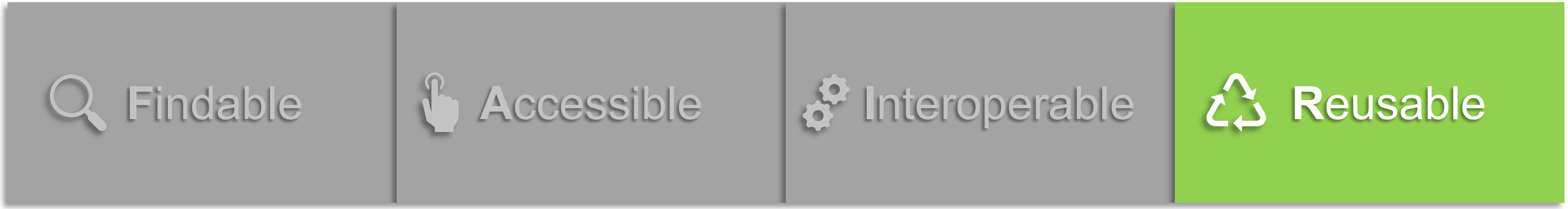
Findable | Accessible | **Interoperable** | Reusable

Data should be exchanged and interpreted by humans and computers

Structured metadata (schemas, vocabularies)

https://www.go-fair.org/fair-principles/

The FAIR Guiding Principles



Findable

Accessible

Interoperable

Reusable

It should be clear how data can be reused and/or replicated

Licences, rich (provenance) metadata

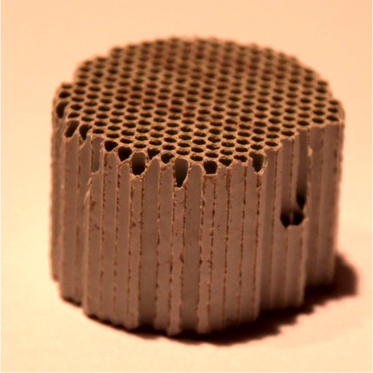
https://www.go-fair.org/fair-principles/

2. Effective Metadata Management

What to describe?

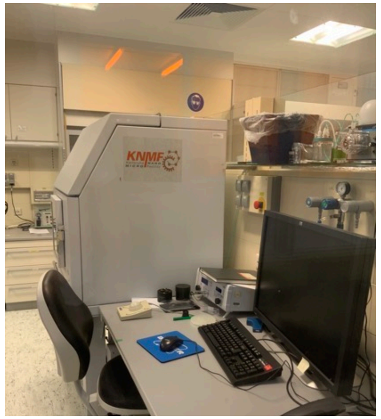
R1: Metadata should richly describe the data with a plurality of accurate and relevant attributes.

Sample



Sample Holder

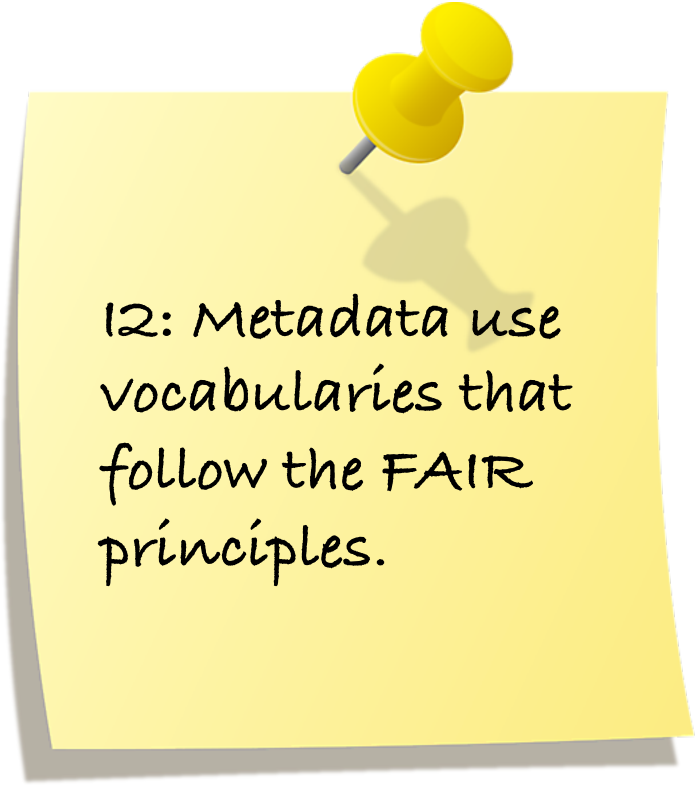
Instrument



Research data

Images: courtesy of R. Thelen and M. Mail. Powered by Bing Image Creator

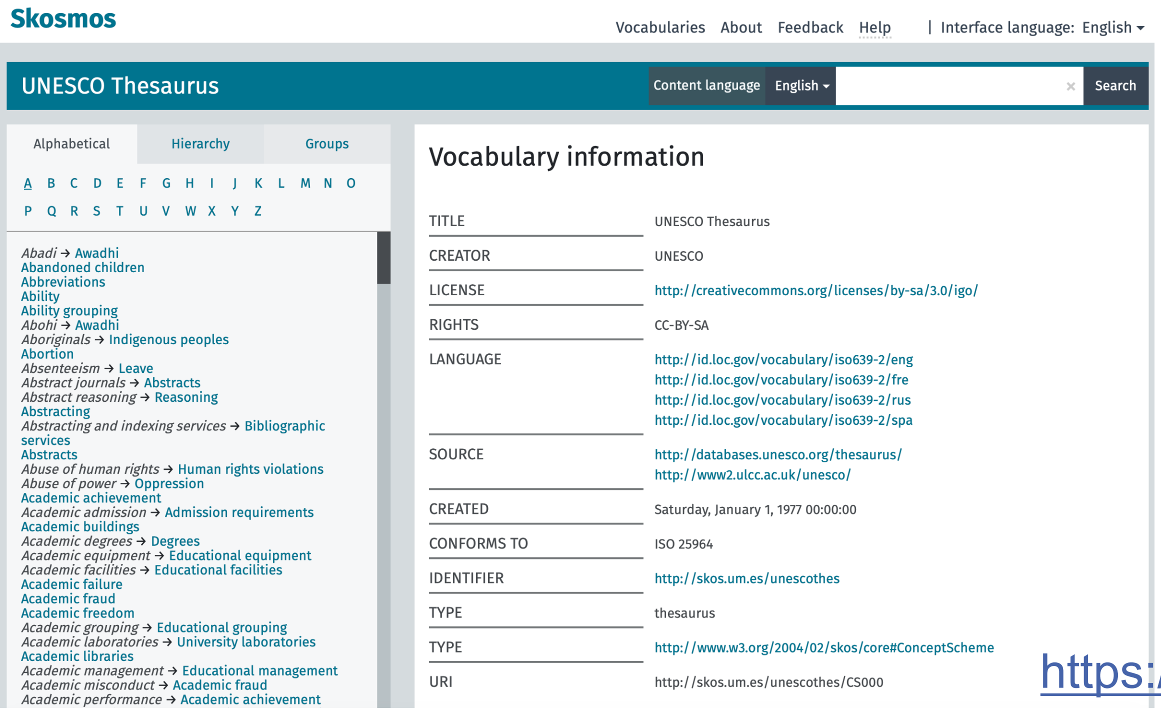
How to describe data?



I2: Metadata use vocabularies that follow the FAIR principles.

Minimal requirements:

- The vocabulary and its terms have globally unique PIDs
- The vocabulary and its terms are documented
- The documentation is findable and accessible by users



Skosmos
Vocabularies About Feedback Help | Interface language: English
UNESCO Thesaurus
Content language English
Search
Alphabetical Hierarchy Groups
A B C D E F G H I J K L M N O
P Q R S T U V W X Y Z

Abadi → Awadhi
Abandoned children
Abbreviations
Ability
Ability grouping
Abohi → Awadhi
Aboriginals → Indigenous peoples
Abortion
Absenteeism → Leave
Abstract journals → Abstracts
Abstract reasoning → Reasoning
Abstracting
Abstracting and indexing services → Bibliographic services
Abstracts
Abuse of human rights → Human rights violations
Abuse of power → Oppression
Academic achievement
Academic admission → Admission requirements
Academic buildings
Academic degrees → Degrees
Academic equipment → Educational equipment
Academic facilities → Educational facilities
Academic failure
Academic fraud
Academic freedom
Academic grouping → Educational grouping
Academic laboratories → University laboratories
Academic libraries
Academic management → Educational management
Academic misconduct → Academic fraud
Academic performance → Academic achievement

Vocabulary information

TITLE	UNESCO Thesaurus
CREATOR	UNESCO
LICENSE	http://creativecommons.org/licenses/by-sa/3.0/igo/
RIGHTS	CC-BY-SA
LANGUAGE	http://id.loc.gov/vocabulary/iso639-2/eng http://id.loc.gov/vocabulary/iso639-2/fre http://id.loc.gov/vocabulary/iso639-2/rus http://id.loc.gov/vocabulary/iso639-2/spa
SOURCE	http://databases.unesco.org/thesaurus/ http://www2.ulcc.ac.uk/unesco/
CREATED	Saturday, January 1, 1977 00:00:00
CONFORMS TO	ISO 25964
IDENTIFIER	http://skos.um.es/unescothes
TYPE	thesaurus
TYPE	http://www.w3.org/2004/02/skos/core#ConceptScheme
URI	http://skos.um.es/unescothes/CS000

https://skosmos.org

How to represent metadata?

I1: (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.

W3C Semantic Web

Resource Description Framework: metadata model to represent interconnected data.
https://www.w3.org/RDF/

Simple Knowledge Organization System: standard to represent knowledge organization systems using RDF
https://www.w3.org/2004/02/skos/

Web Ontology Language: computational logic-based language to represent complex knowledge.
https://www.w3.org/OWL/

How to structure metadata?

Karlsruhe Institute of Technology

R1.3: Metadata meet domain-relevant community standards or best practices.

General purpose

DublinCore http://dublincore.org/schemas/

DataCite http://schema.datacite.org

Schema.org https://schema.org

Neutron, x-ray, muon

NeXus http://www.nexusformat.org

Crystallography

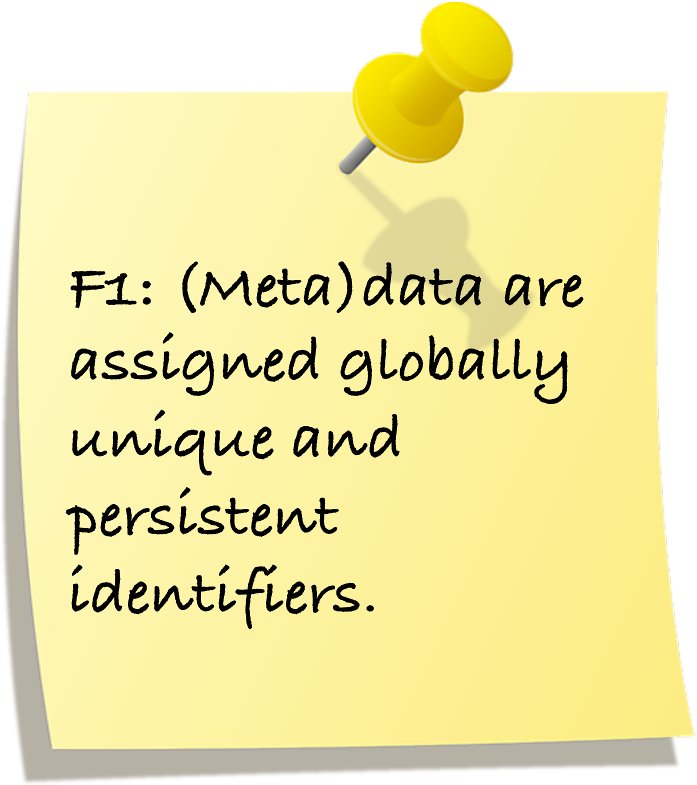
CIF https://www.iucr.org/resources/cif

How to represent structured metadata?

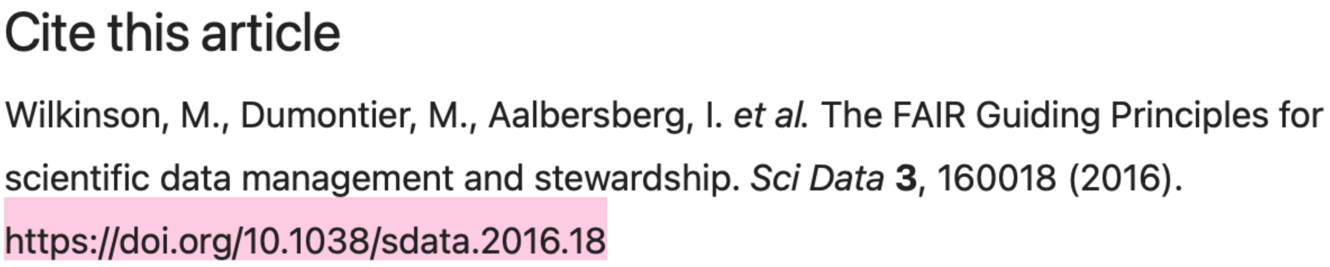
I1: Metadata use a formal, accessible, shared and broadly applicable language for knowledge representation.

- XML (eXtensible Markup Language)
- JSON (JavaScript Object Notation)
- JSON Schema https://json-schema.org
- JSON-LD (JSON for Linked Data)

How to publish (meta)data?

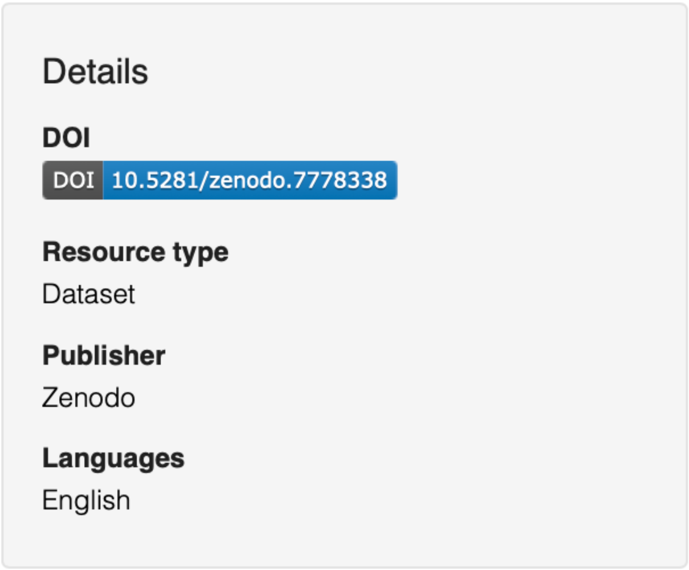


F1: (Meta)data are assigned globally unique and persistent identifiers.



Cite this article

Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* **3**, 160018 (2016). https://doi.org/10.1038/sdata.2016.18



Details

DOI

DOI 10.5281/zenodo.7778338

Resource type

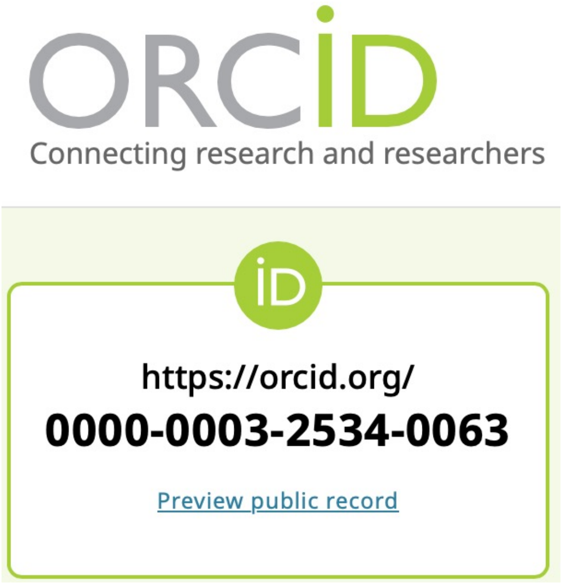
Dataset

Publisher

Zenodo

Languages

English



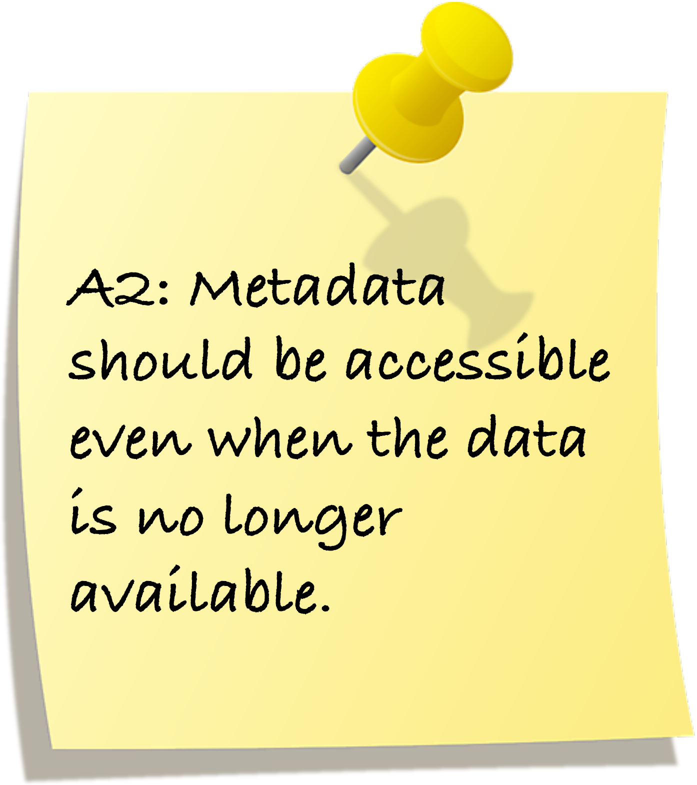
ORCID

Connecting research and researchers

https://orcid.org/
0000-0003-2534-0063

Preview public record

How to publish metadata?



A2: Metadata should be accessible even when the data is no longer available.

Not Found

The requested

Apache Serve

found on this ser

Something Went Wrong

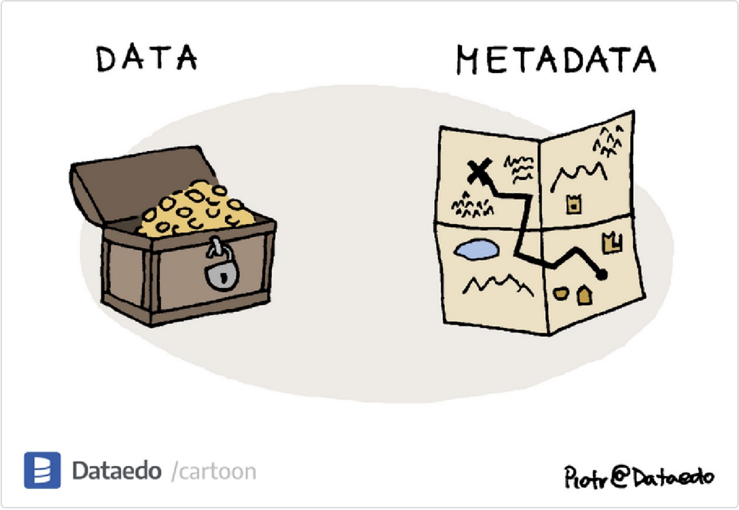
:/

Oops, this URL is invalid...

Error 404 - the requested U

Bad Request - Invalid URL

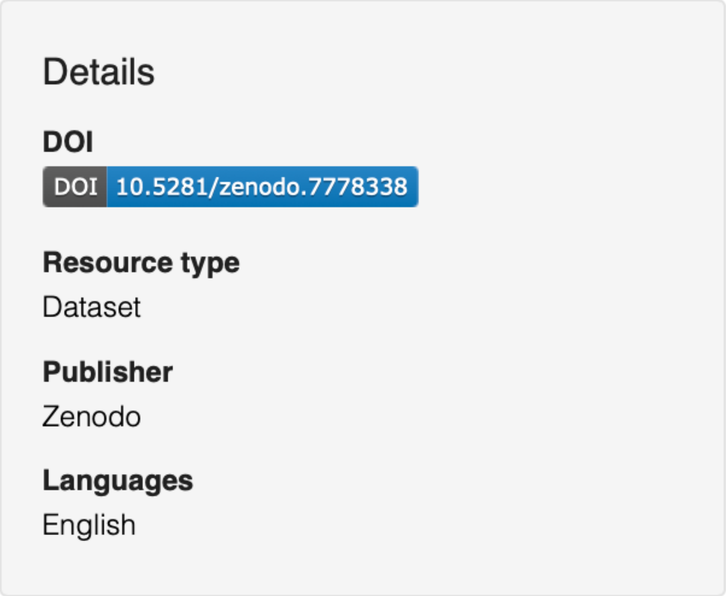
HTTP Error 400. The request URL is invalid.



Metadata Repositories!

How to find data from metadata?

F3: Metadata clearly and explicitly include the identifier of the data they describe.



Details

DOI

DOI 10.5281/zenodo.7778338

Resource type

Dataset

Publisher

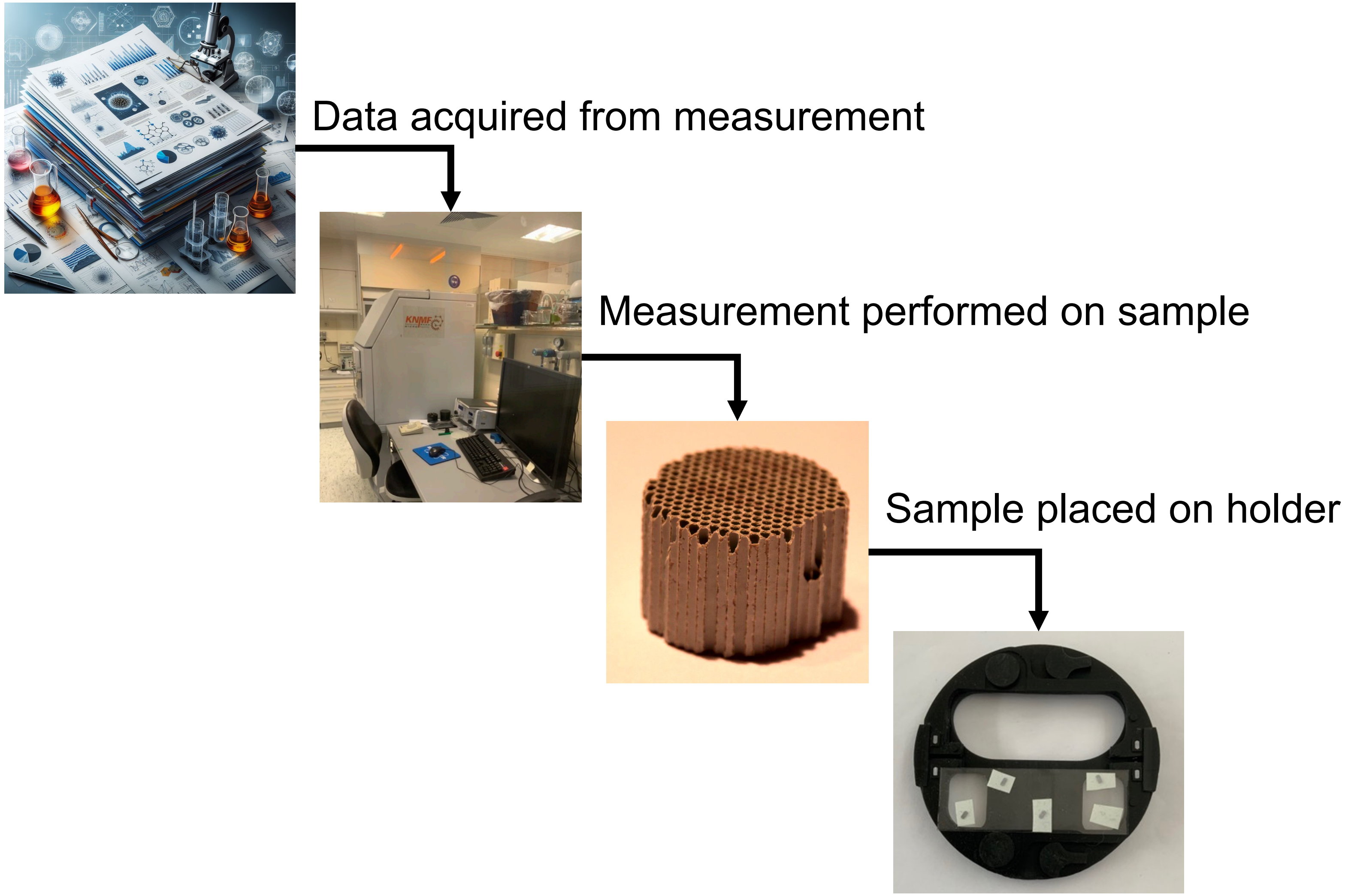
Zenodo

Languages

English

How to find data from metadata?

R1.2: Metadata are associated with detailed provenance.



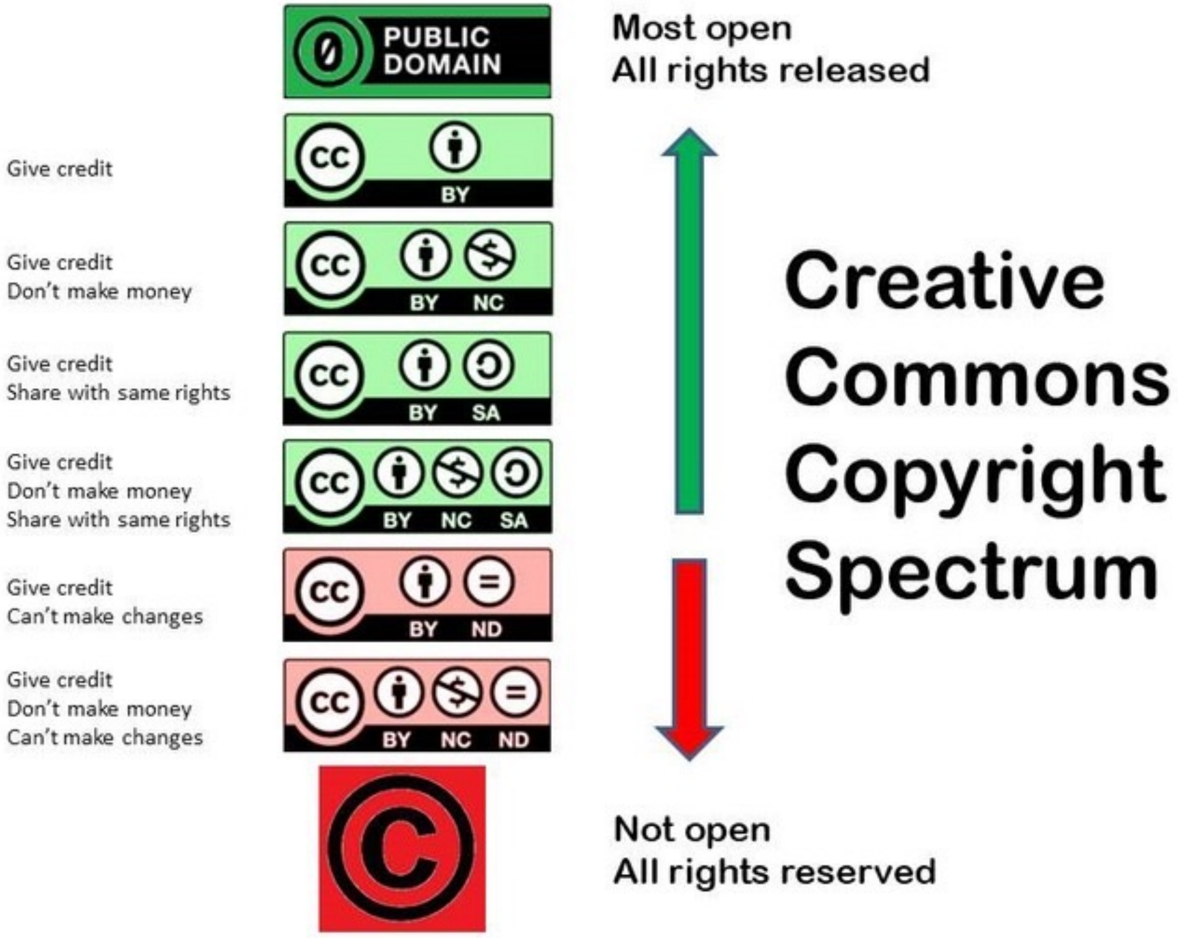
Data acquired from measurement

Measurement performed on sample

Sample placed on holder

How to reuse the data?

R1.1: (Meta)data are released with a clear and accessible data usage licence.



Most open
All rights released

Give credit

Give credit
Don't make money

Give credit
Share with same rights

Give credit
Don't make money
Share with same rights

Give credit
Can't make changes

Give credit
Don't make money
Can't make changes

Creative Commons Copyright Spectrum

Not open
All rights reserved

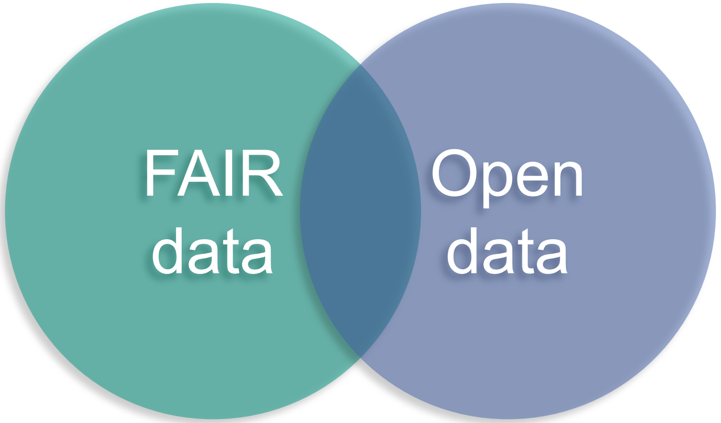
https://creativecommons.org/share-your-work/cclicenses/

Should FAIR data be open?

A1.2: The protocol allows for an authentication and authorization procedure where necessary.

Open data: “can be freely used, modified, and shared by anyone for any purpose” https://opendefinition.org

FAIR data: “as open as possible, as closed as necessary”



FAIR or open?

My data is copyright protected	FAIR	
My dataset can be used only by a specific group of scientists	FAIR	
An image is shared on a public website	Open	
A dataset is published on Zenodo with an open licence	FAIR	Open
A data file is on my Dropbox	None	

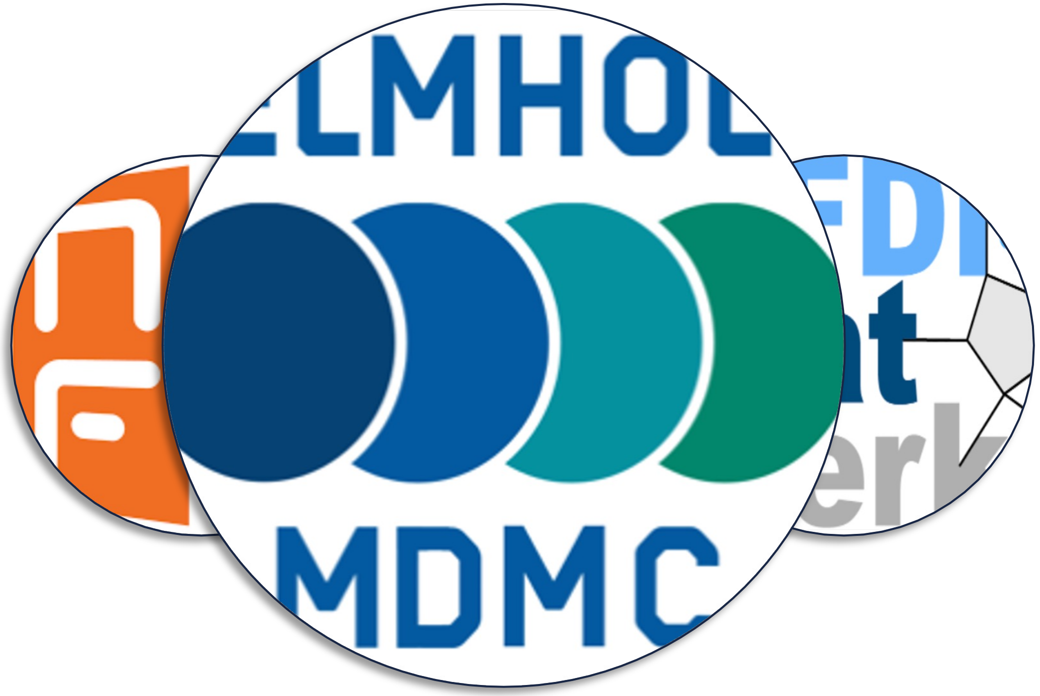
3. Metadata Management in practice

The projects

Nanoscience Foundries and Fine Analysis – Europe Pilot (NEP)
https://nffa.eu

Access to nanoscience research infrastructure
Synthesis, growth of nanostructures, fine analysis, theory and simulation

The projects



Joint-Lab Model and Data driven Materials Characterization (MDMC) of the Helmholtz Association
https://jl-mdmc-helmholtz.de

Platform for multiscale and multidimensional characterization, analytics and simulation methods

The projects

National Research Data Infrastructure for Materials Science and Engineering (NFDI-MatWerk)
https://nfdi-matwerk.de

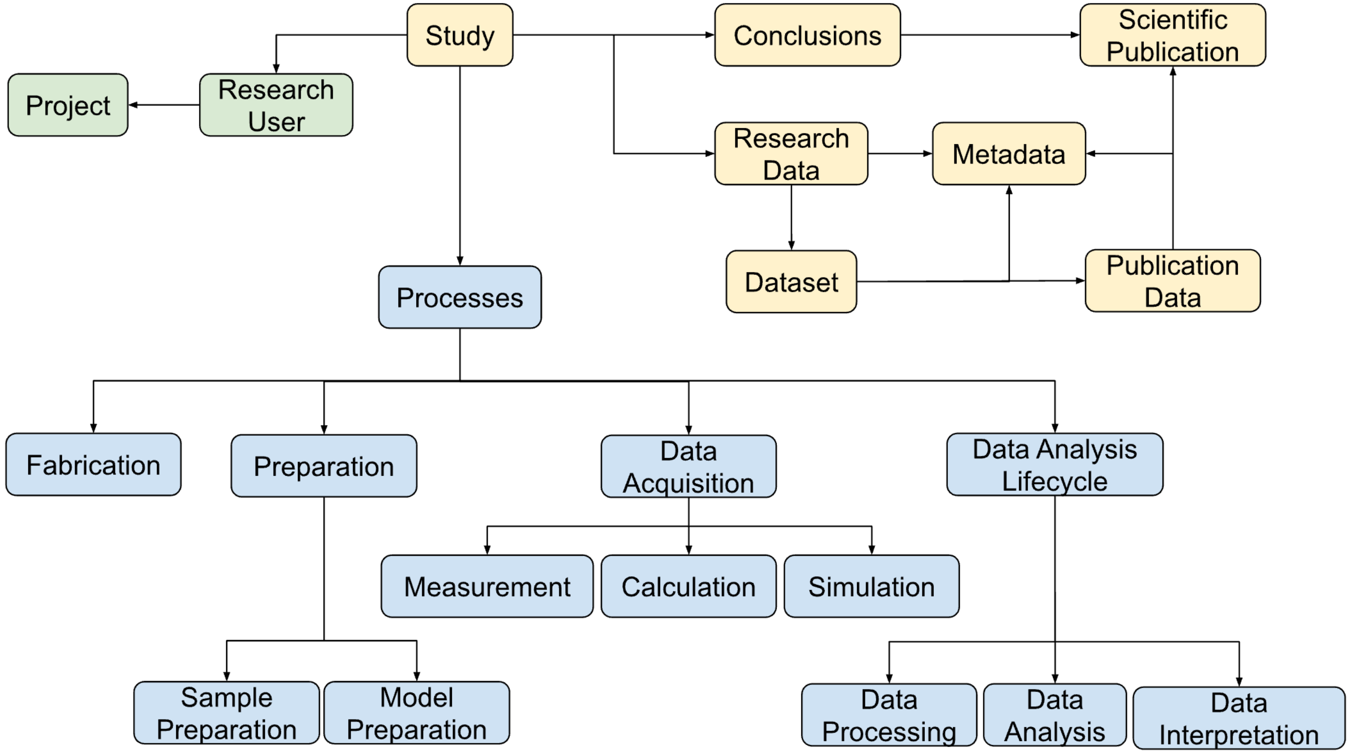
Infrastructure for the digital representation of materials and their relevant process

The projects

Common aims:

- Implement (meta)data management practices following the FAIR principles
- Develop tools and infrastructure solutions guided by community requirements
- Agree on common descriptions
- Collaborate on interoperable results

1. Definition of terms

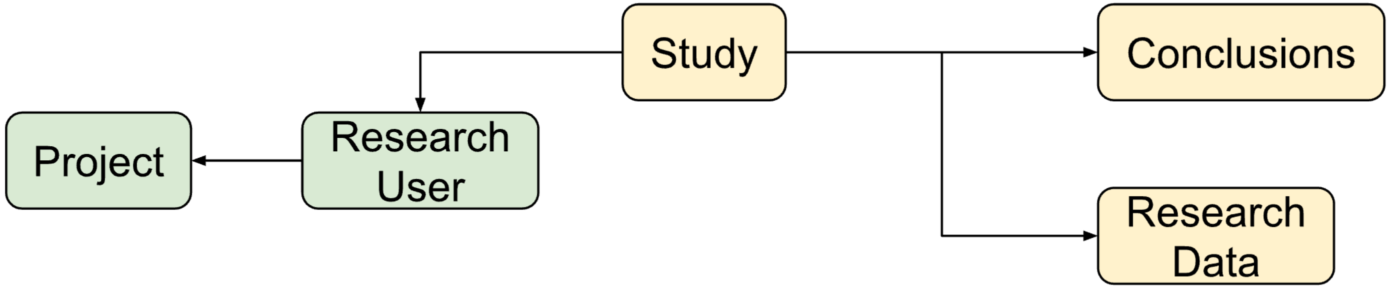


Glossary of Terms

- High-level description of experimental and computational workflows
- Framed in the management infrastructure of the projects
- Allows to track the provenance information
- Adopts existing terms

MDMC-NEP Glossary of Terms. DOI: [10.5281/zenodo.10663833](https://doi.org/10.5281/zenodo.10663833)

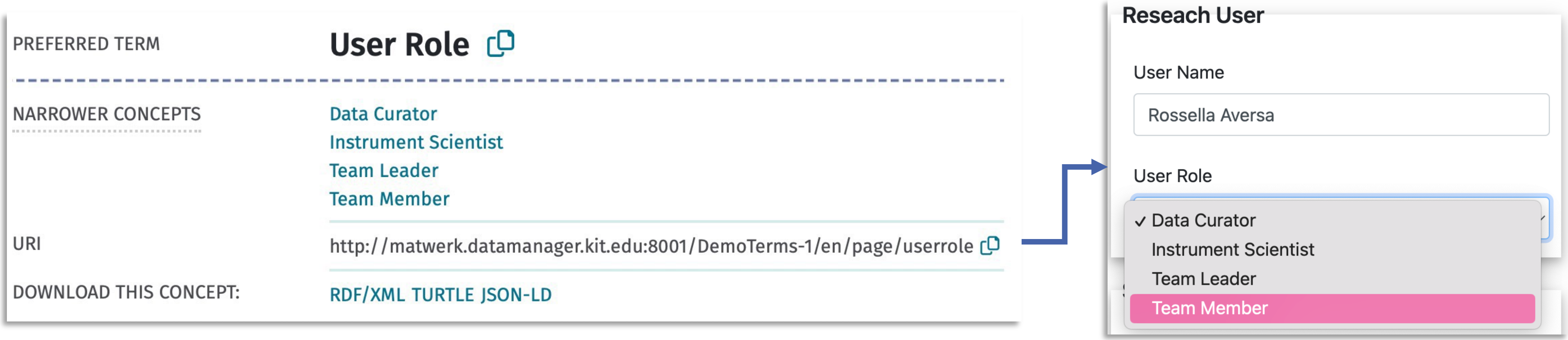
1. Definition of terms



Research User
Person, usually member of a **Project**, who conducts any part of the **Study**, in order to collect and/or analyse **Research Data** or is interested in reusing **Research Data** by a third party (e.g., **Reference Data**) with the final aim to extract insights that support the answer to some specific research question (i.e., **Conclusions**). **Research Users** may be assigned with a role (data curator, instrument scientist, team leader, team member).

MDMC-NEP Glossary of Terms. DOI: [10.5281/zenodo.10663833](https://doi.org/10.5281/zenodo.10663833)

2. Terms in a Vocabulary Service



PREFERRED TERM: **User Role**

NARROWER CONCEPTS: Data Curator, Instrument Scientist, Team Leader, Team Member

URI: http://matwerk.datamanager.kit.edu:8001/DemoTerms-1/en/page/userrole

DOWNLOAD THIS CONCEPT: RDF/XML TURTLE JSON-LD

Reseach User

User Name: Rossella Aversa

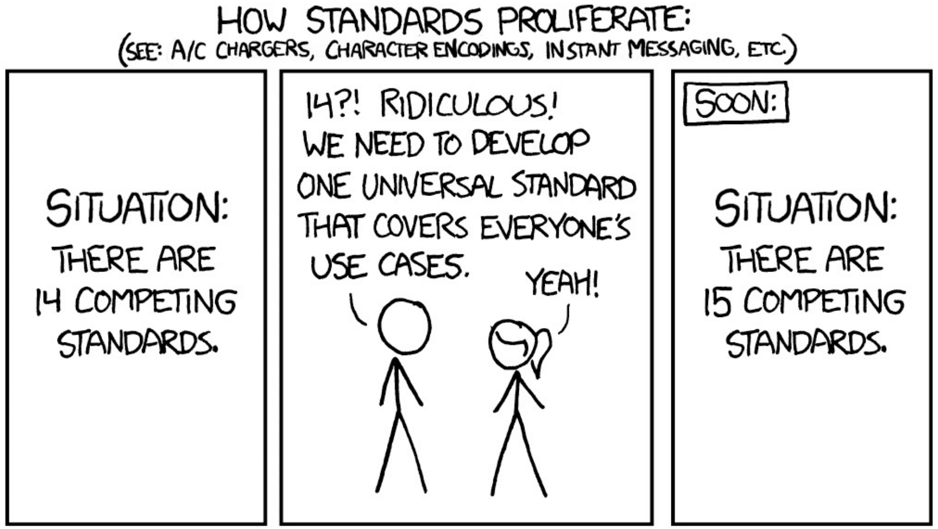
User Role:
- ✓ Data Curator
- Instrument Scientist
- Team Leader
- Team Member

EVOKS Vocabulary Service: Collaborative online vocabulary editor

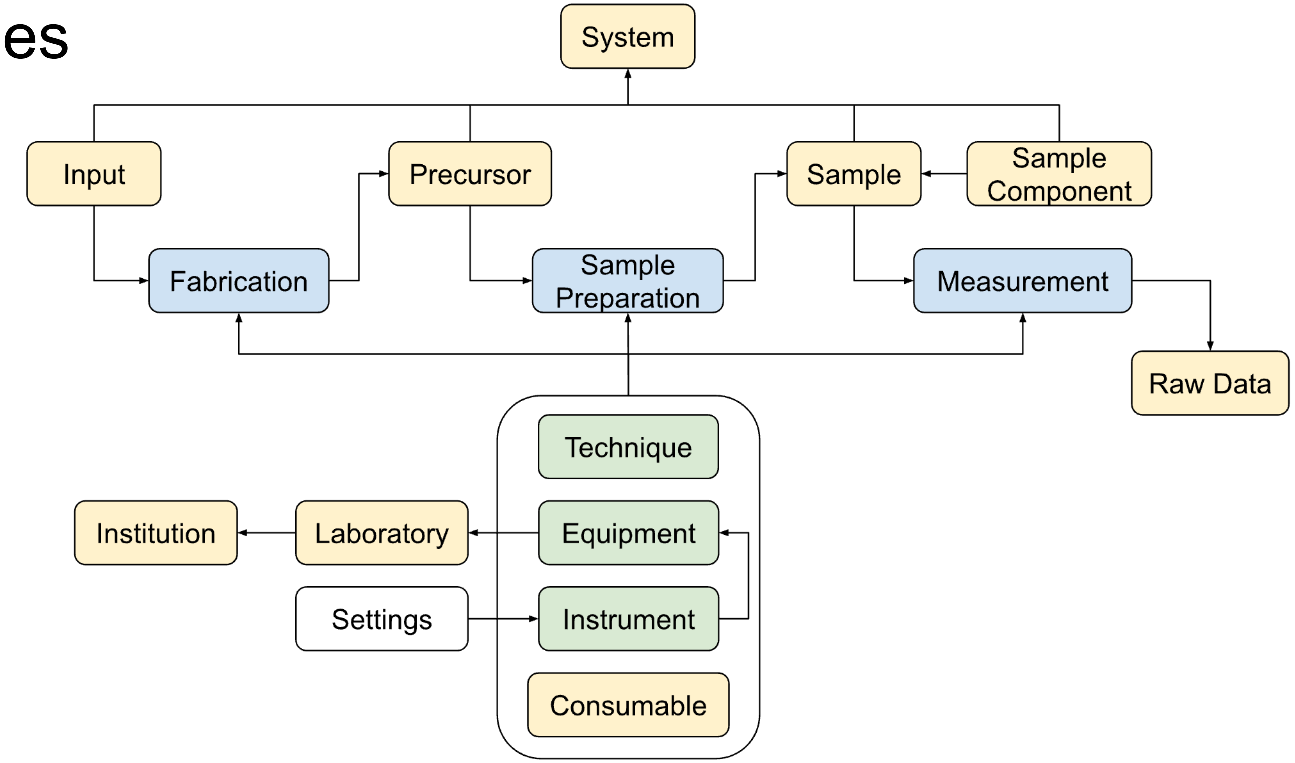
- RDF model + SKOS model
- Persistent identifier to each term
- Can be resolved in interfaces, websites, automatic processes…
- Centrally maintained
- Public read-only Skosmos instance

3. Metadata schemas

- Describe inputs/outputs of processes
- JSON schema
- Adopt existing solutions
- Avoid proliferation of schemas

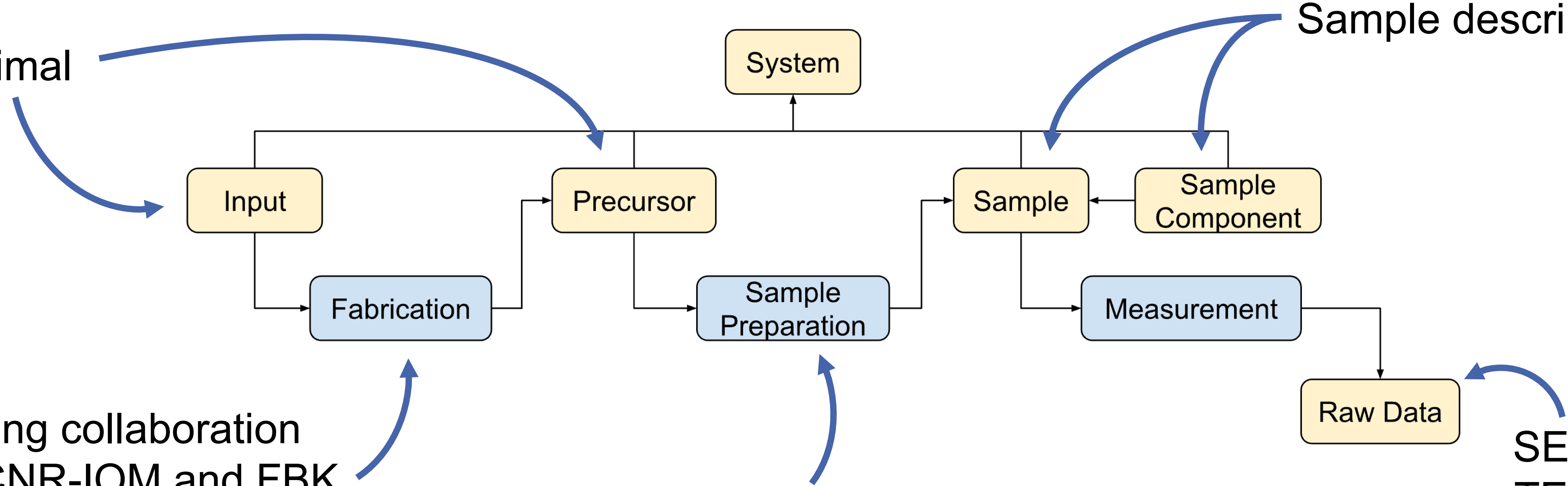

HOW STANDARDS PROLIFERATE:
(SEE: A/C CHARGERS, CHARACTER ENCODINGS, INSTANT MESSAGING, ETC.)
SITUATION: THERE ARE 14 COMPETING STANDARDS.
14?! RIDICULOUS! WE NEED TO DEVELOP ONE UNIVERSAL STANDARD THAT COVERS EVERYONE'S USE CASES.
YEAH!
SOON:
SITUATION: THERE ARE 15 COMPETING STANDARDS.

https://xkcd.com/927/



MDMC-NEP Glossary of Terms. DOI: 10.5281/zenodo.10663833

3. Metadata schemas



Minimal

Sample description

Ongoing collaboration with CNR-IOM and FBK (see talk by L. Ferrario)

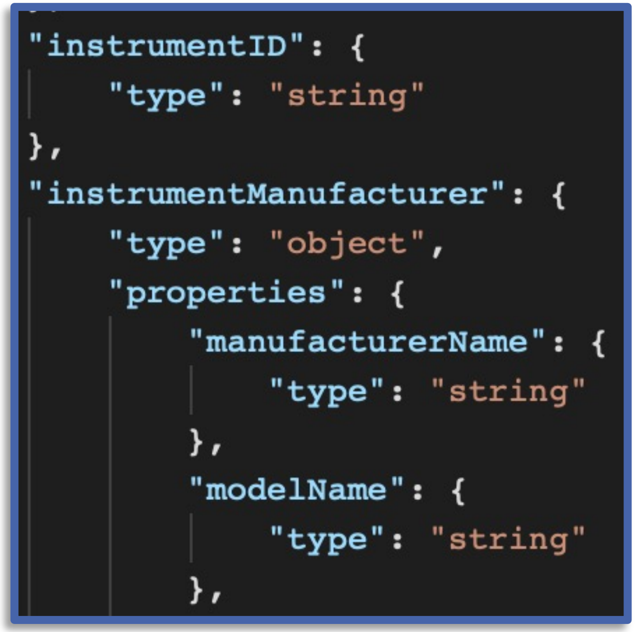
Adopted from the Materials Data Vocabulary
DOI: 10.5334/dsj-2021-018

SEM
TEM
MRI
STM
SEM/FIB Tomography
Nano CT/micro CT

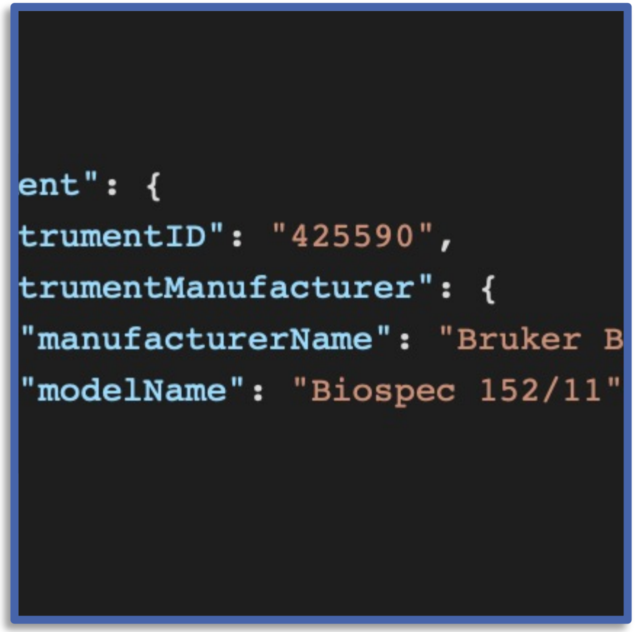
4. Metadata schemas and documents

Metadata Schema: outline of the overall structure of the metadata (elements, value types, rules, …)

Metadata Document: structured information about a data resource



```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```

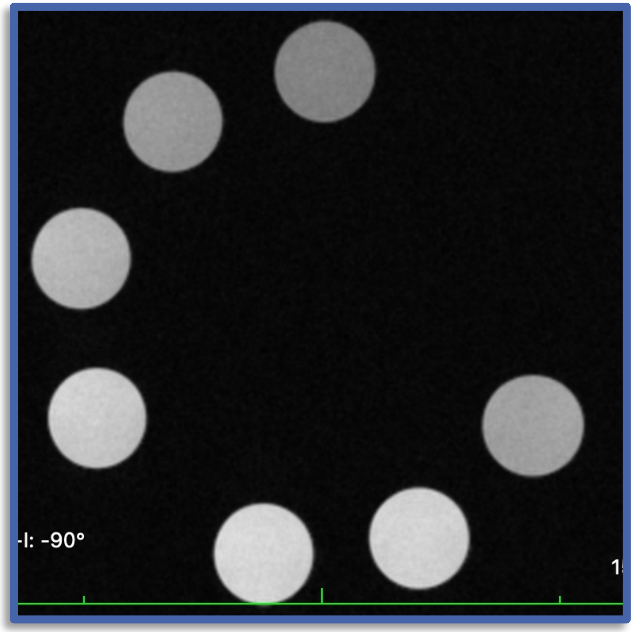


```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```

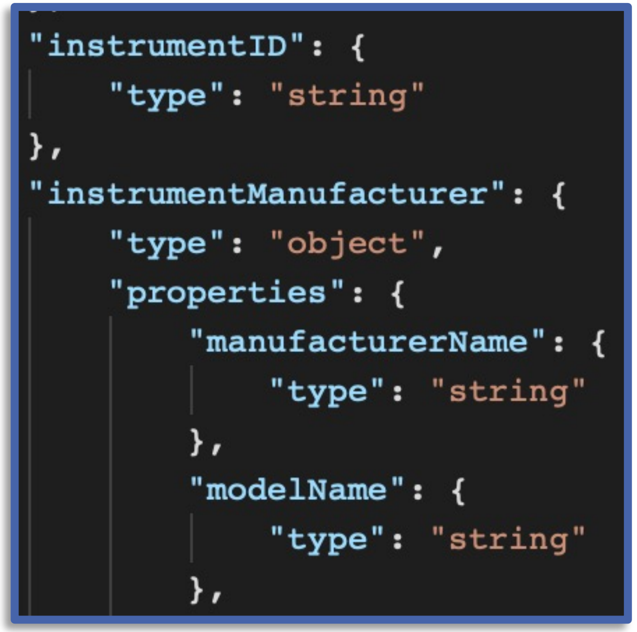
MRI schema, DOI: 10.5445/IR/1000159552

From data to metadata

Raw Data

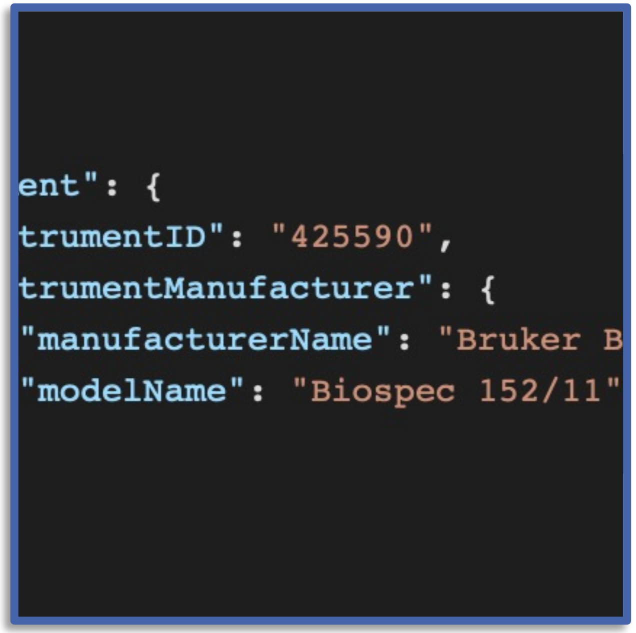


Metadata Schema



```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```

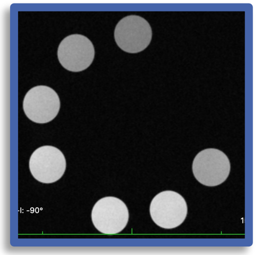
Metadata Document

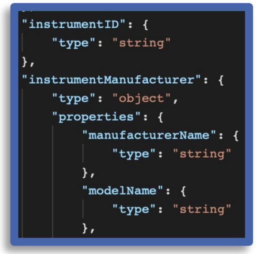


```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```

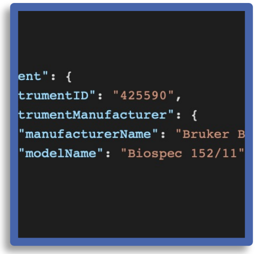
Image from Magnetic Resonance Imaging Copper Sulfate Dataset. DOI: 10.5281/zenodo.6107720

5. Mapping service



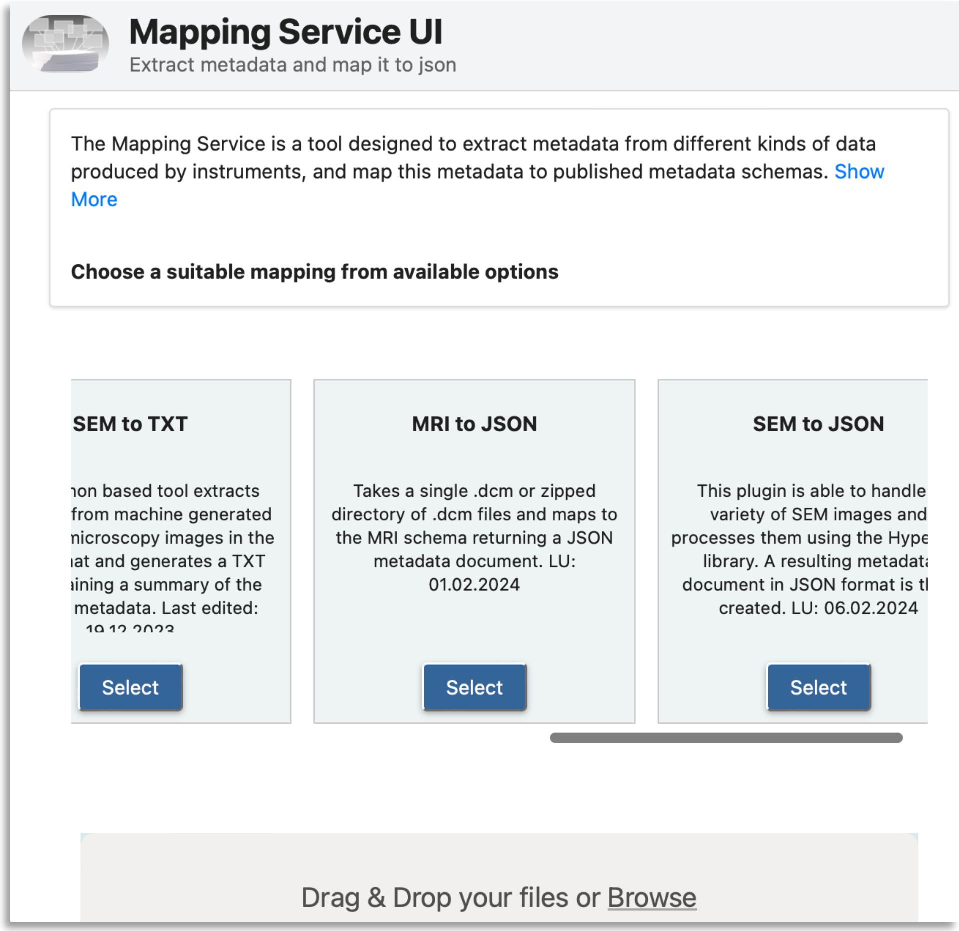


```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```



```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```

- Online service
- Input: data file(s)
- Extract unstructured metadata
- Map them to the metadata schema
- Output: structured metadata



Mapping Service UI

Extract metadata and map it to json

The Mapping Service is a tool designed to extract metadata from different kinds of data produced by instruments, and map this metadata to published metadata schemas. Show More

Choose a suitable mapping from available options

SEM to TXT

ion based tool extracts from machine generated nicroscopy images in the iat and generates a TXT iining a summary of the metadata. Last edited: 19.12.2023

MRI to JSON

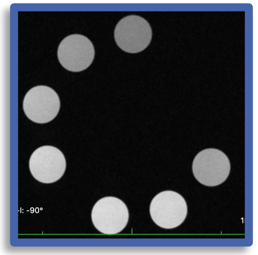
Takes a single .dcm or zipped directory of .dcm files and maps to the MRI schema returning a JSON metadata document. LU: 01.02.2024

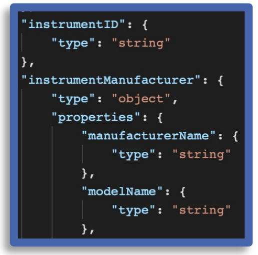
SEM to JSON

This plugin is able to handle variety of SEM images and processes them using the Hype library. A resulting metadat document in JSON format is tl created. LU: 06.02.2024

https://matwerk.datamanager.kit.edu/mapping-service-ui.html

6. Metadata Editor





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    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
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        "modelName": {
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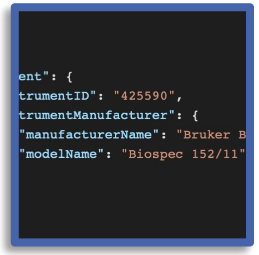
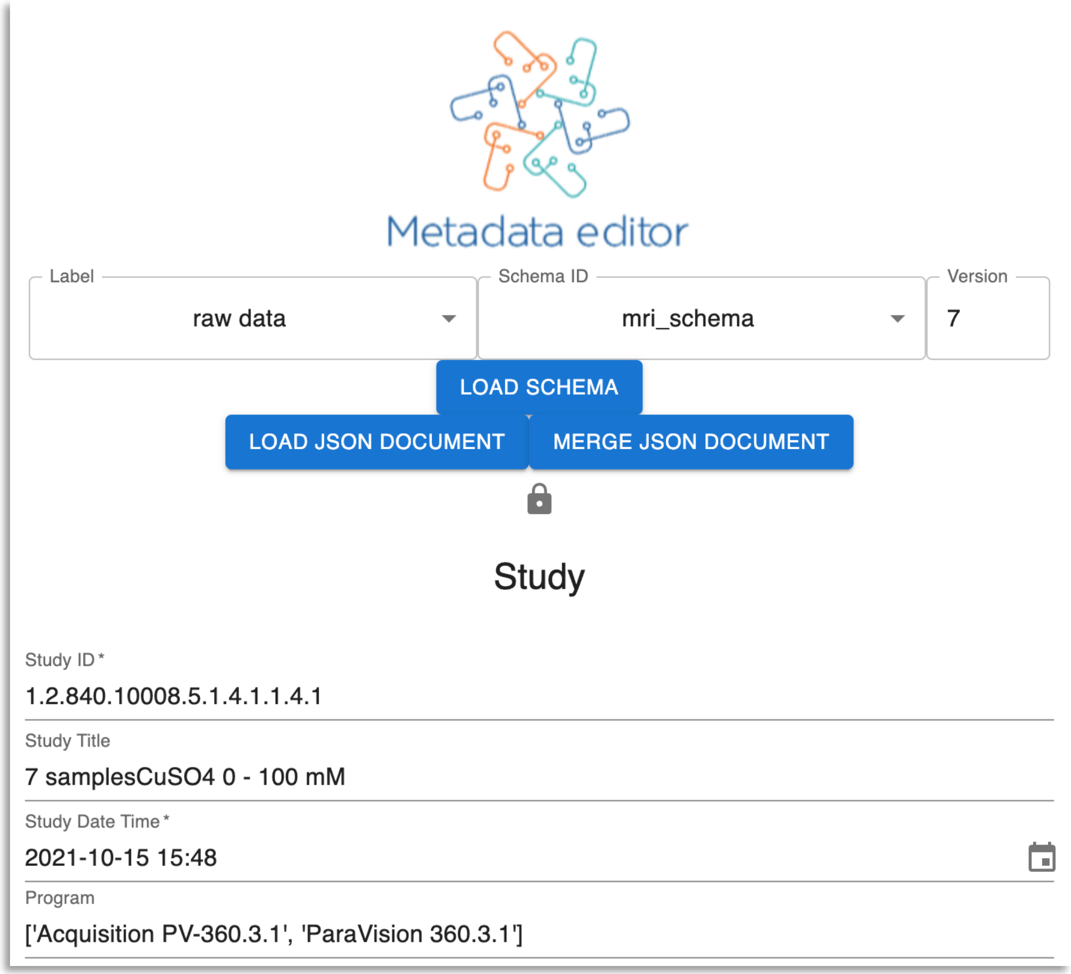
```



```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```

- Local service connected to the metadata repository
- Load schema from registered ones
- Load existing metadata documents
- Manually edit metadata documents
- Download metadata documents
- Register metadata documents
- Create the provenance file



Label: raw data

Schema ID: mri_schema

Version: 7

Study

Study ID *
1.2.840.10008.5.1.4.1.1.4.1

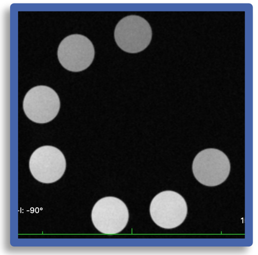
Study Title
7 samplesCuSO4 0 - 100 mM

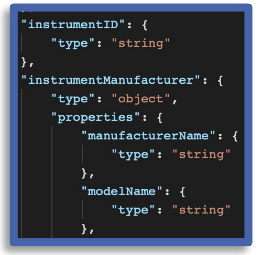
Study Date Time *
2021-10-15 15:48

Program
['Acquisition PV-360.3.1', 'ParaVision 360.3.1']

https://metadata-editor.gitlab.io/documentation/

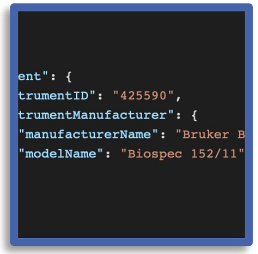
7. ELN and LIMS





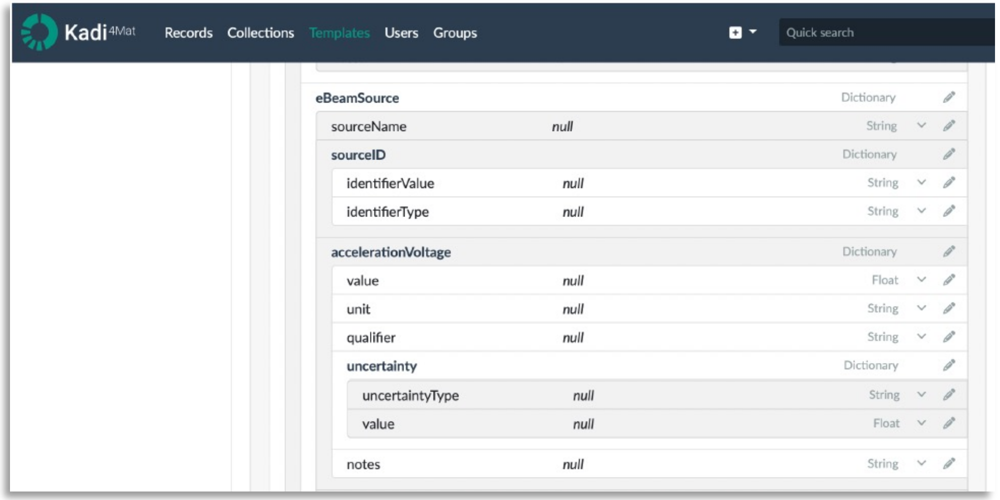
```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```

ELN
LIMS

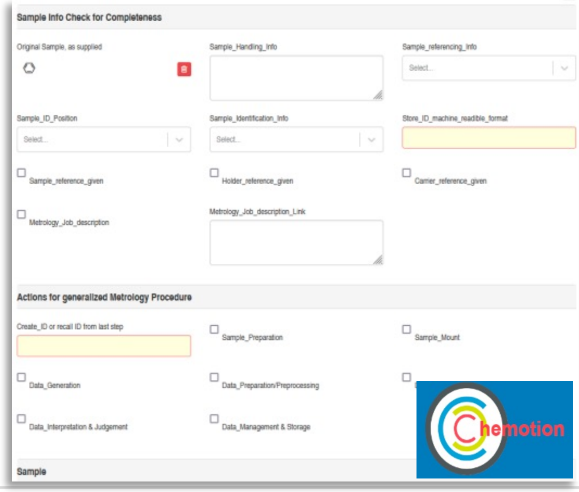


```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```

- Electronic Lab Notebooks
- Lab Information Management Systems
- Metadata schemas as templates
- Ongoing collaborations:
  - KIT
  - CNR-IOM
  - FBK (see talk L. Ferrario)



eBeamSource		Dictionary
sourceName	null	String
sourceID		Dictionary
identifierValue	null	String
identifierType	null	String
accelerationVoltage		Dictionary
value	null	Float
unit	null	String
qualifier	null	String
uncertainty		Dictionary
uncertaintyType	null	String
value	null	Float
notes	null	String



Sample Info Check for Completeness

Original Sample, as supplied

Sample_Handling_Info

Sample_referencing_Info: Select...

Sample_ID_Position: Select...

Sample_Identification_Info: Select...

Store_ID_machine_readible_format

□ Sample_reference_given

□ Holder_reference_given

□ Carrier_reference_given

□ Metrology_Job_description

Metrology_Job_description_Link

Actions for generalized Metrology Procedure

Create_ID or recall ID from last step

□ Sample_Preparation

□ Sample_Mount

□ Data_Generation

□ Data_Preparation/Preprocessing

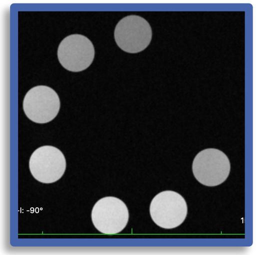
□

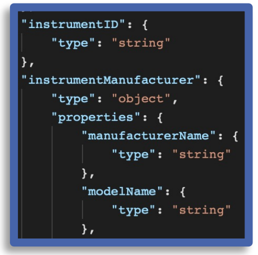
□ Data_Interpretation & Judgement

□ Data_Management & Storage

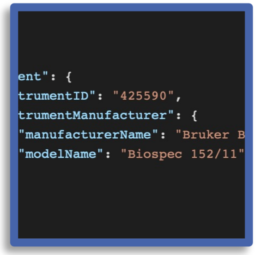
Sample

8. MetaStore

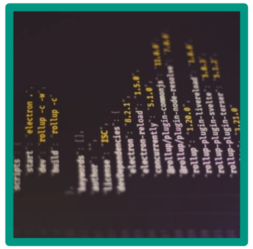




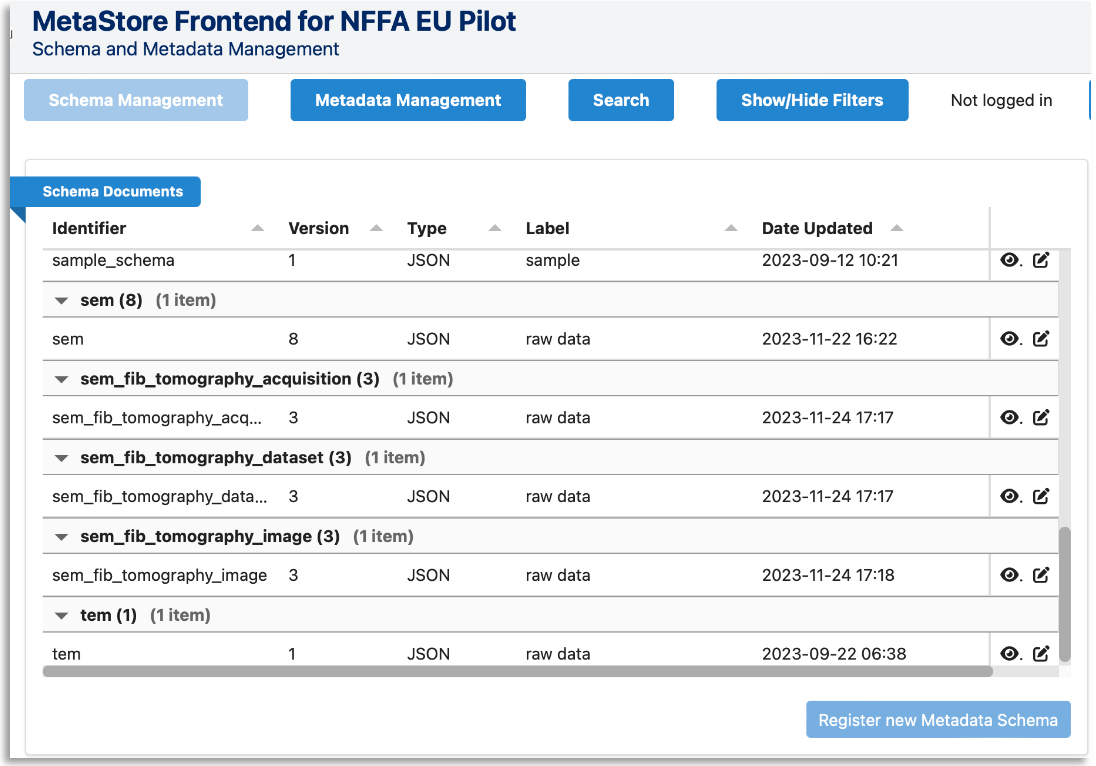
```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```



```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```



- Metadata repository
- Register/find metadata schemas
- Register/find metadata documents
- Validate metadata documents
- Versioning
- Access control management
- User authentication



MetaStore Frontend for NFFA EU Pilot

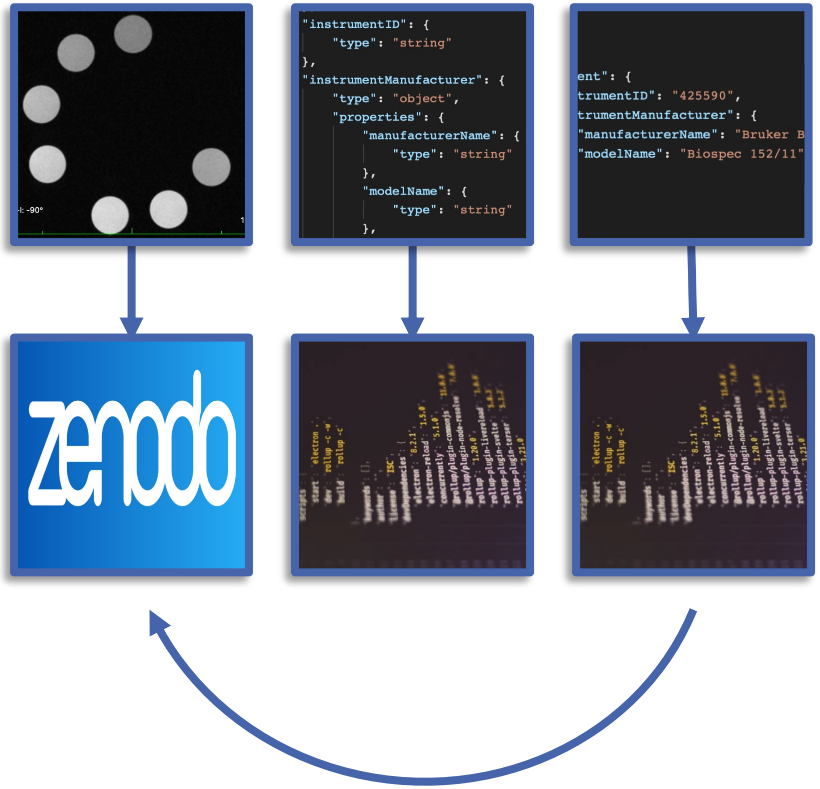
Schema and Metadata Management

Identifier	Version	Type	Label	Date Updated
sample_schema	1	JSON	sample	2023-09-12 10:21
▾ **sem (8)** (1 item)				
sem	8	JSON	raw data	2023-11-22 16:22
▾ **sem_fib_tomography_acquisition (3)** (1 item)				
sem_fib_tomography_acq...	3	JSON	raw data	2023-11-24 17:17
▾ **sem_fib_tomography_dataset (3)** (1 item)				
sem_fib_tomography_data...	3	JSON	raw data	2023-11-24 17:17
▾ **sem_fib_tomography_image (3)** (1 item)				
sem_fib_tomography_image	3	JSON	raw data	2023-11-24 17:18
▾ **tem (1)** (1 item)				
tem	1	JSON	raw data	2023-09-22 06:38

https://metarepo.nffa.eu/

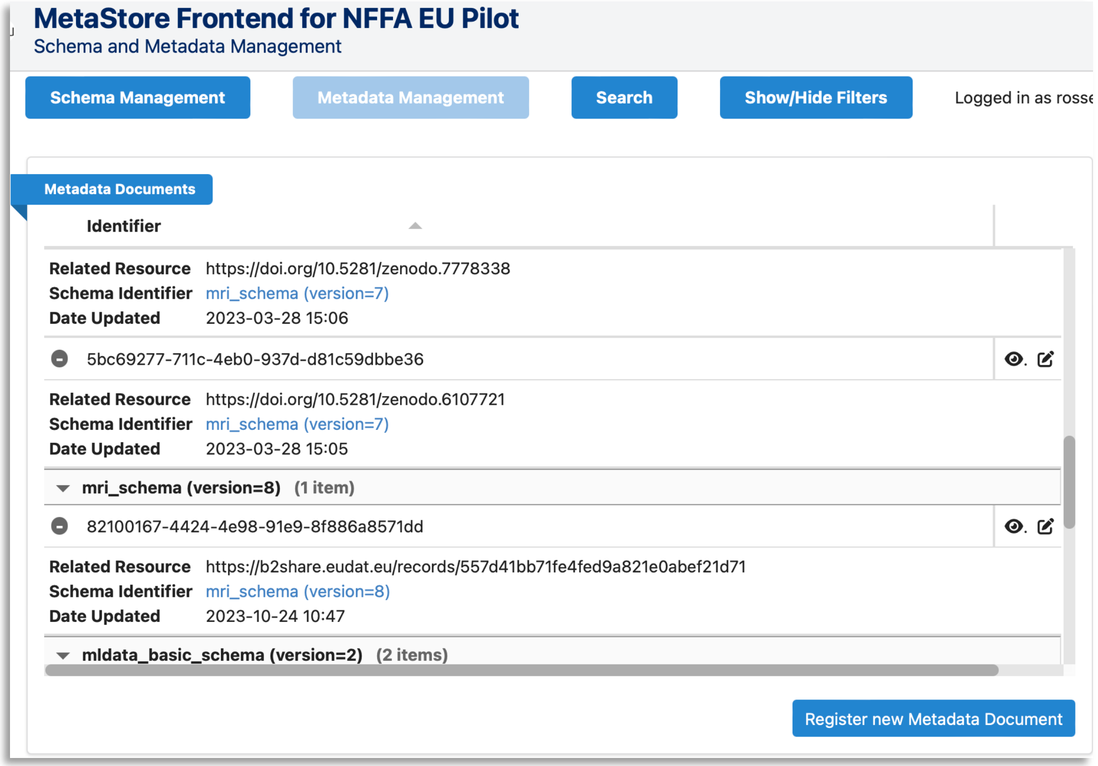
https://github.com/kit-data-manager/metastore2

9. Link metadata to data



```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```

```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```



MetaStore Frontend for NFFA EU Pilot

Schema and Metadata Management

Related Resource https://doi.org/10.5281/zenodo.7778338
Schema Identifier mri_schema (version=7)
Date Updated 2023-03-28 15:06

5bc69277-711c-4eb0-937d-d81c59dbbe36

Related Resource https://doi.org/10.5281/zenodo.6107721
Schema Identifier mri_schema (version=7)
Date Updated 2023-03-28 15:05

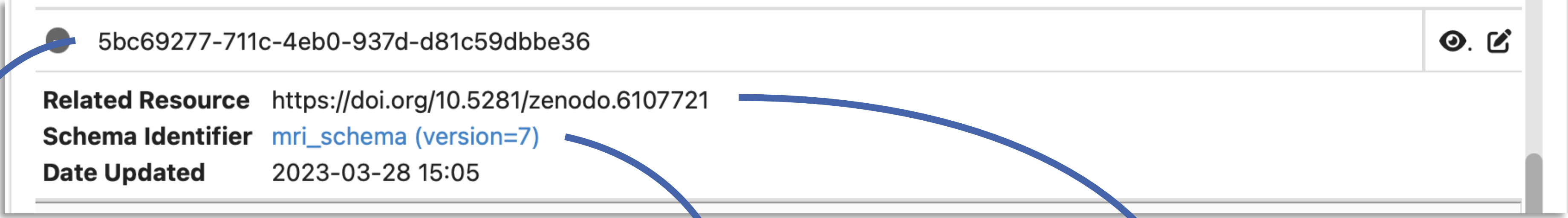
mri_schema (version=8) (1 item)

82100167-4424-4e98-91e9-8f886a8571dd

Related Resource https://b2share.eudat.eu/records/557d41bb71fe4fed9a821e0abef21d71
Schema Identifier mri_schema (version=8)
Date Updated 2023-10-24 10:47

mldata_basic_schema (version=2) (2 items)

9. Link metadata to data

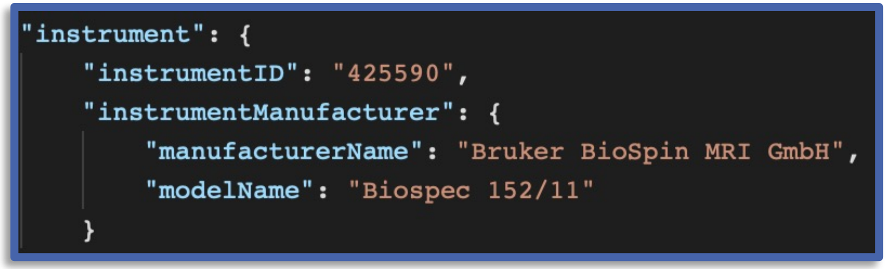


5bc69277-711c-4eb0-937d-d81c59dbbe36

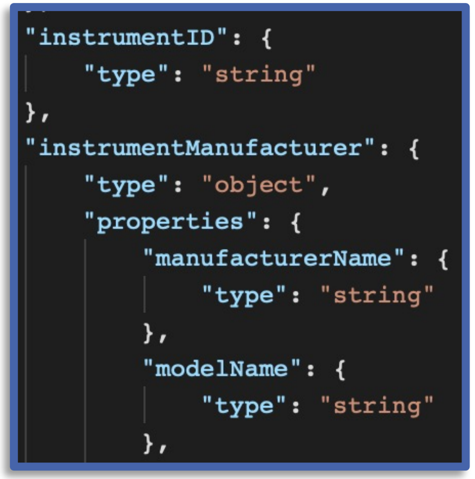
Related Resource https://doi.org/10.5281/zenodo.6107721

Schema Identifier mri_schema (version=7)

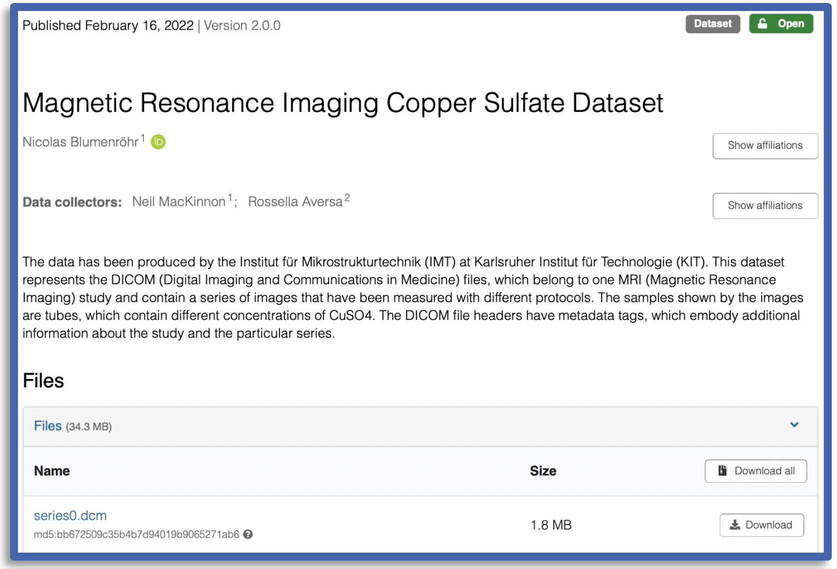
Date Updated 2023-03-28 15:05



```
"instrument": {
    "instrumentID": "425590",
    "instrumentManufacturer": {
        "manufacturerName": "Bruker BioSpin MRI GmbH",
        "modelName": "Biospec 152/11"
    }
```



```
"instrumentID": {
    "type": "string"
},
"instrumentManufacturer": {
    "type": "object",
    "properties": {
        "manufacturerName": {
            "type": "string"
        },
        "modelName": {
            "type": "string"
        },
```



Published February 16, 2022 | Version 2.0.0

Magnetic Resonance Imaging Copper Sulfate Dataset

Nicolas Blumenröhr[1]

Data collectors: Neil MacKinnon[1]; Rossella Aversa[2]

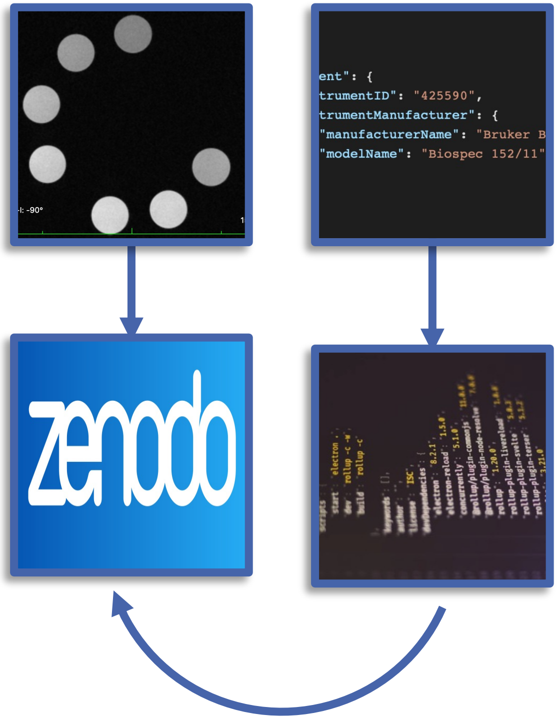
The data has been produced by the Institut für Mikrostrukturtechnik (IMT) at Karlsruher Institut für Technologie (KIT). This dataset represents the DICOM (Digital Imaging and Communications in Medicine) files, which belong to one MRI (Magnetic Resonance Imaging) study and contain a series of images that have been measured with different protocols. The samples shown by the images are tubes, which contain different concentrations of CuSO4. The DICOM file headers have metadata tags, which embody additional information about the study and the particular series.

Files

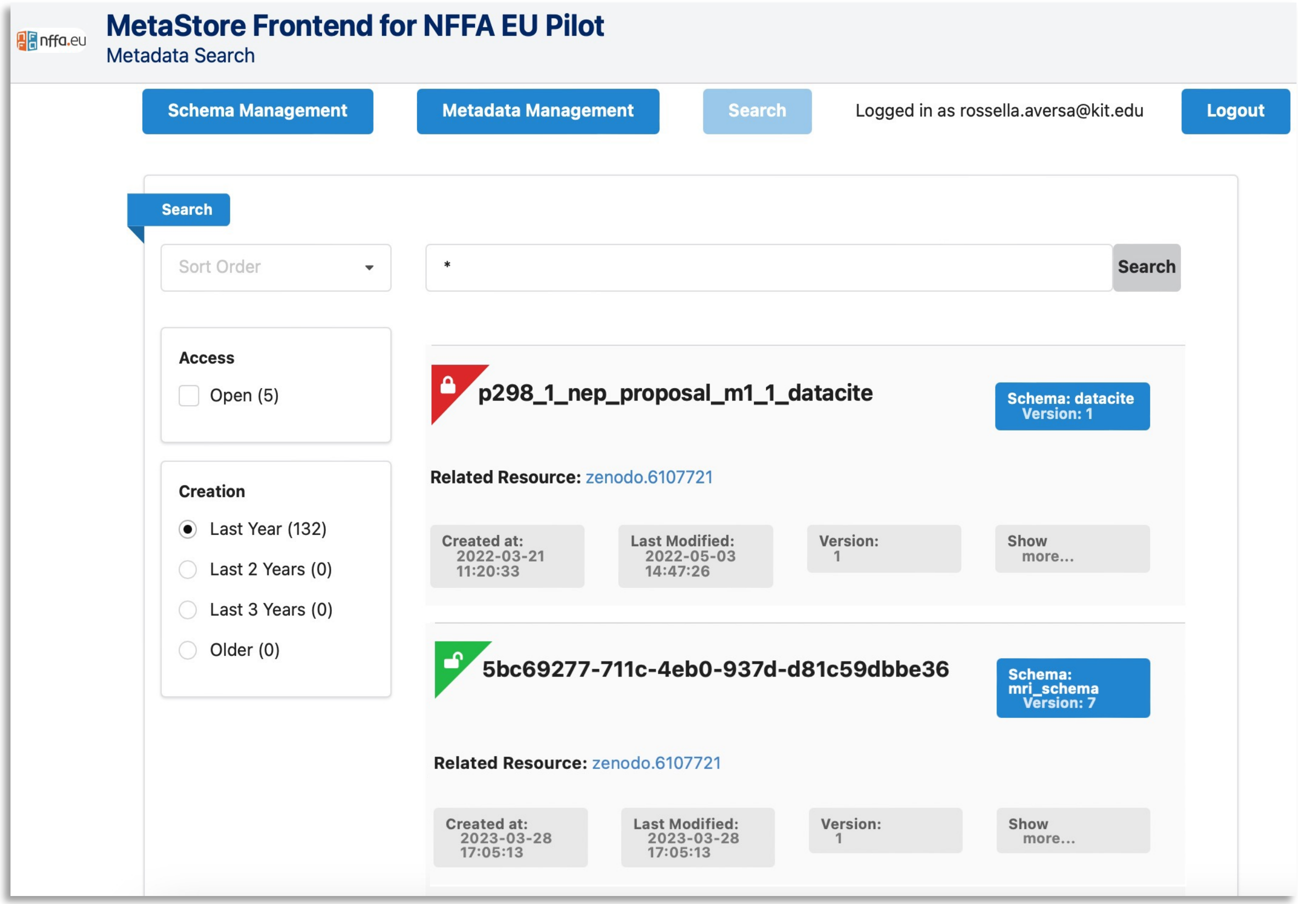
Files (34.3 MB)

Name	Size	Download all
series0.dcm md5:bb672509c35b4b7d94019b9065271ab6	1.8 MB	Download

10. Find data from metadata



```
ent": {
trumentID": "425590",
trumentManufacturer": {
"manufacturerName": "Bruker B
"modelName": "Biospec 152/11"
```



MetaStore Frontend for NFFA EU Pilot
Metadata Search

Logged in as rossella.aversa@kit.edu

Search: *

Access

□ Open (5)

Creation

● Last Year (132)
○ Last 2 Years (0)
○ Last 3 Years (0)
○ Older (0)

p298_1_nep_proposal_m1_1_datacite — Schema: datacite Version: 1

Related Resource: zenodo.6107721

Created at: 2022-03-21 11:20:33 | Last Modified: 2022-05-03 14:47:26 | Version: 1 | Show more...

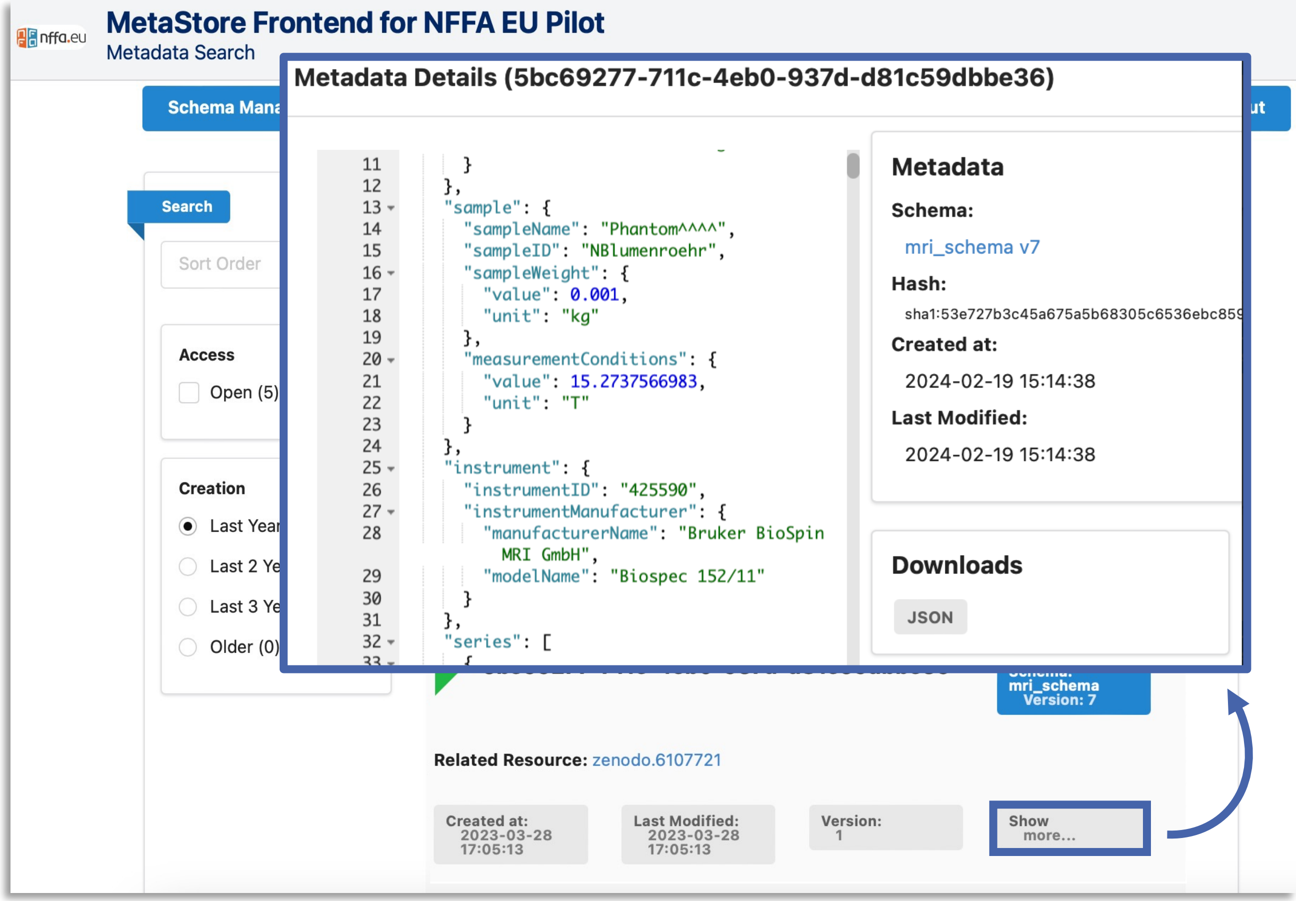
5bc69277-711c-4eb0-937d-d81c59dbbe36 — Schema: mri_schema Version: 7

Related Resource: zenodo.6107721

Created at: 2023-03-28 17:05:13 | Last Modified: 2023-03-28 17:05:13 | Version: 1 | Show more...

10. Find data from metadata

- Use the content of metadata documents to search for relevant data
- Private vs Public resources
- What is the data about? Is it useful for my needs?
- Full-text search
- (basic, customizable) faceted search



MetaStore Frontend for NFFA EU Pilot

Metadata Search

Metadata Details (5bc69277-711c-4eb0-937d-d81c59dbbe36)

```
    }
  },
  "sample": {
    "sampleName": "Phantom^^^^",
    "sampleID": "NBlumenroehr",
    "sampleWeight": {
      "value": 0.001,
      "unit": "kg"
    },
    "measurementConditions": {
      "value": 15.2737566983,
      "unit": "T"
    }
  },
  "instrument": {
    "instrumentID": "425590",
    "instrumentManufacturer": {
      "manufacturerName": "Bruker BioSpin
        MRI GmbH",
      "modelName": "Biospec 152/11"
    }
  },
  "series": [
```

Metadata

Schema:

mri_schema v7

Hash:

sha1:53e727b3c45a675a5b68305c6536ebc859

Created at:

2024-02-19 15:14:38

Last Modified:

2024-02-19 15:14:38

Downloads

JSON

Related Resource: zenodo.6107721

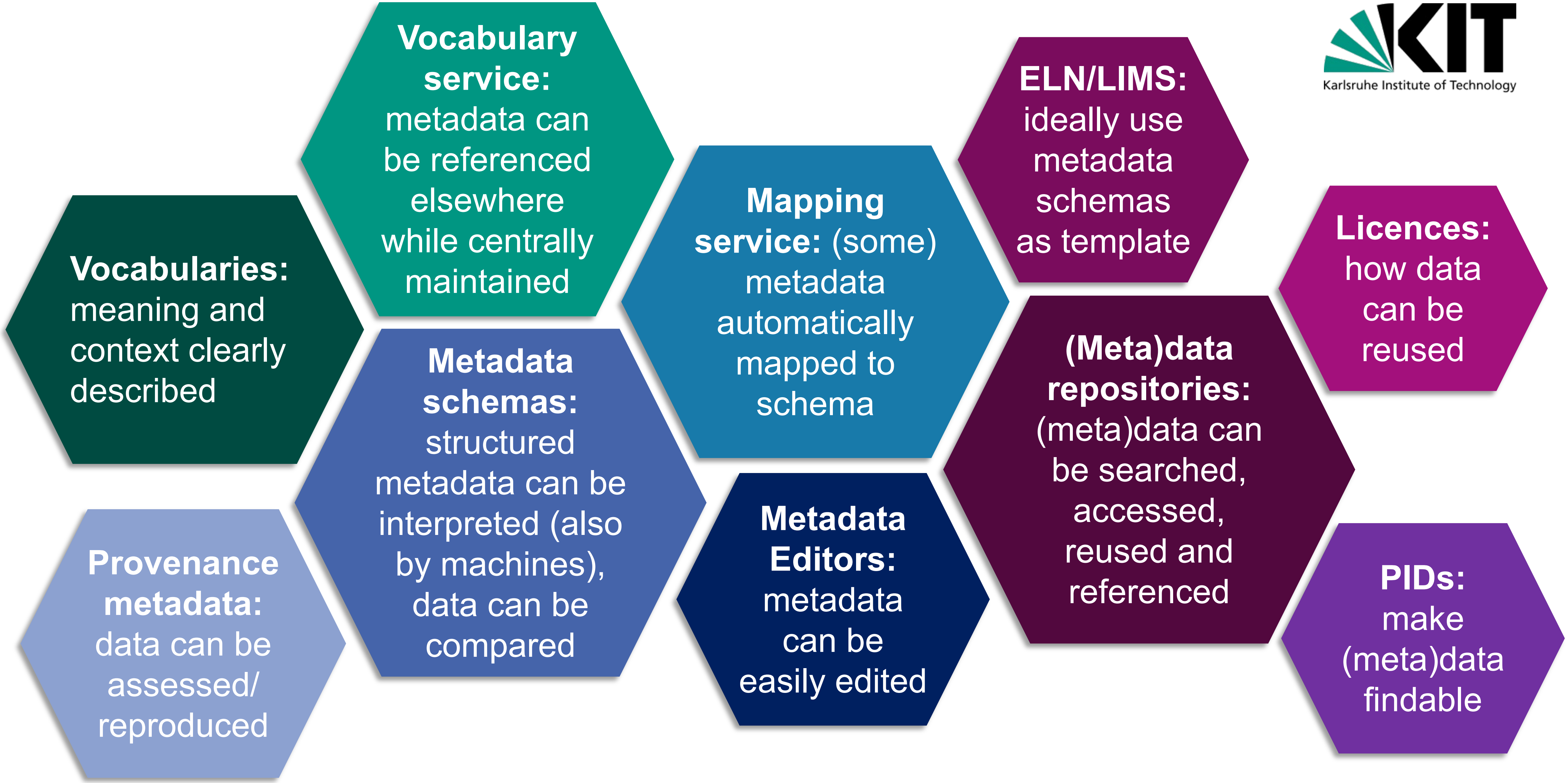
Created at: 2023-03-28 17:05:13

Last Modified: 2023-03-28 17:05:13

Version: 1

Show more...

4. Conclusions



Vocabularies: meaning and context clearly described

Provenance metadata: data can be assessed/ reproduced

Vocabulary service: metadata can be referenced elsewhere while centrally maintained

Metadata schemas: structured metadata can be interpreted (also by machines), data can be compared

Mapping service: (some) metadata automatically mapped to schema

Metadata Editors: metadata can be easily edited

ELN/LIMS: ideally use metadata schemas as template

(Meta)data repositories: (meta)data can be searched, accessed, reused and referenced

Licences: how data can be reused

PIDs: make (meta)data findable

Contacts: rossella.aversa@kit.edu

Acknowledgements to:
G. Abdildina, N. Blumenröhr, F. Ernst, V. Haltmann, M. Inkmann, T. Jejkal, A. Kirar, E. Vitali, NEP JA6, JL-MDMC Metadata WG.

Founded by:
The Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under the National Research Data Infrastructure – NFDI 38/1 – project number 460247524; the Joint Laboratory Model and Data driven Materials Characterization (JL MDMC), a cross-centre platform of the Helmholtz Association: NFFA-Europe-Pilot (EU H2020 – n. 101007417); the research program “Engineering Digital Futures” of the Helmholtz Association of German Research Centers; the Helmholtz Metadata Collaboration Platform.