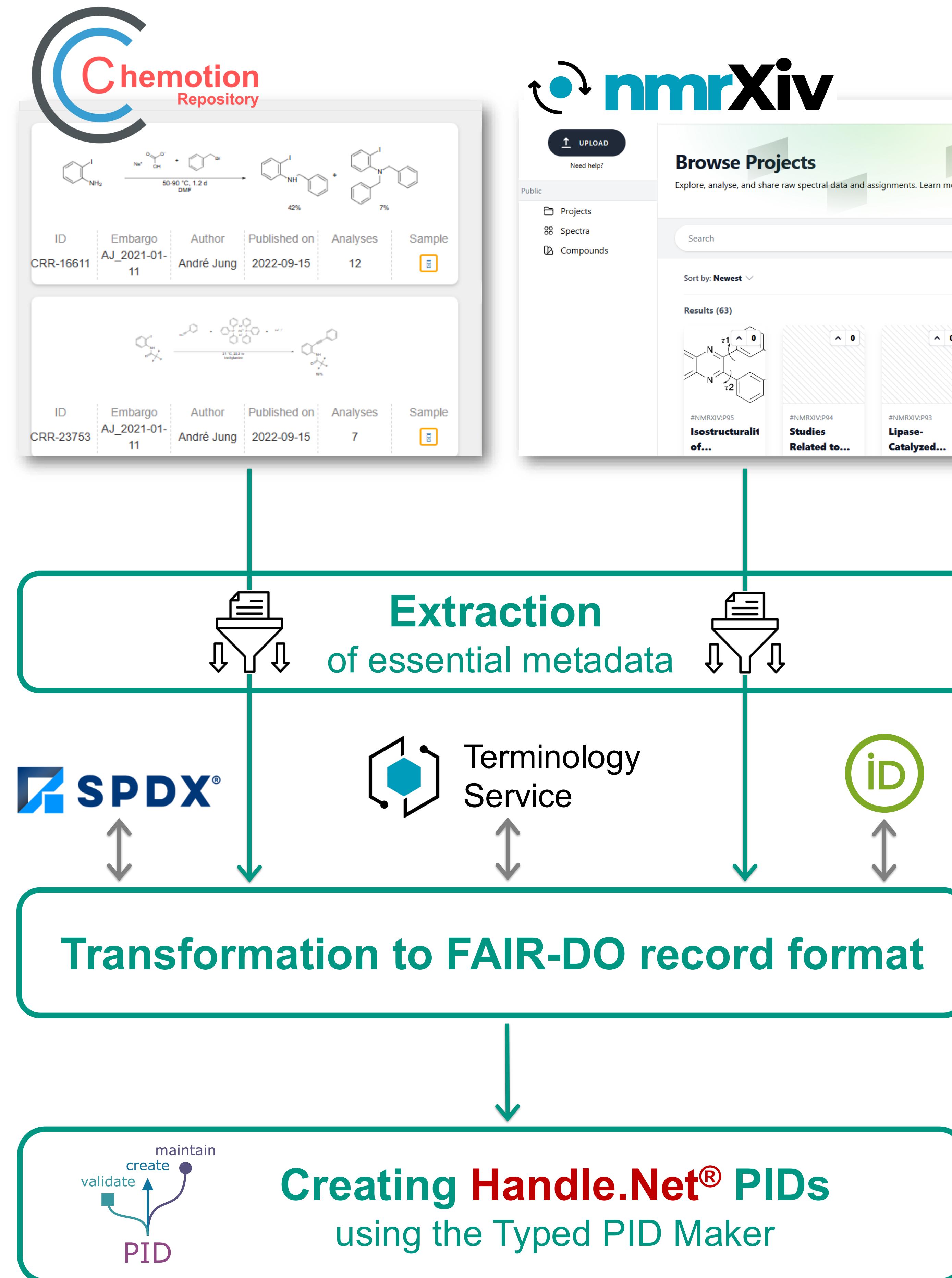


# Using FAIR Digital Objects for a Harmonized Representation of NMR Spectroscopy Data

Maximilian Inckmann, Christopher Raquet, Rossella Aversa



**Problem:** Researchers have to search through multiple non-interoperable databases to find artifacts

**Solution:** FAIR Digital Objects as a harmonization layer<sup>1</sup>

- Extract essential metadata out of existing systems without need for modification to support FAIR-DOs
- Heuristics ensure high-quality metadata by using existing vocabularies (SPDX), ontologies (NFDI4Chem Terminology Service), and identifier systems (ORCID)
- Harmonized selected domain-agnostic<sup>2,3</sup> and domain-specific metadata across systems based on MChl community standard<sup>4</sup>

**Benefits:** Uniform entry point to multiple systems

- See “FAIR Digital Objects” poster
- FAIR and AI-ready (meta)data
- Search using commodity search software
- User-friendly and highly customizable search with powerful filtering and graph-based inspection

[1] Blumenröhrl, Nicolas, Philipp-Joachim Ost, Felix Kraus, and Achim Streit. “FAIR Digital Objects for the Realization of Globally Aligned Data Spaces”. 2024 IEEE International Conference on Big Data, IEEE, 2024, <https://doi.org/10.1109/BigData62323.2024.10825796>

[2] Weigel, Tobias, Beth Plale, Mark Parsons, et al. “RDA Recommendation on PID Kernel Information”. Recommendation. Research Data Alliance, 2019. <https://doi.org/10.15497/rdarec00031>

[3] Curdt, Constanze, Gerrit Günther, Thomas Jeikal, et al. “Helmholtz Metadata Collaboration, Helmholtz Kernel Information Profile”. Report. HMC Office, GEOMAR Helmholtz Centre for Ocean Research, 2022. [https://doi.org/10.3289/HMC\\_publ\\_03](https://doi.org/10.3289/HMC_publ_03)

[4] Rayya, Noura, Philip Strömer, Stefan Kuhn, Stuart Chalk, Tillmann Fischer, Robert Hanson, Nicole Jung, et al. “MARGARITAS: MChl Standard for Reporting Liquid-State NMR Experiments of Small Molecules”. NFDI4Chem, 2024

<https://nfdi4chem.github.io/workshops/docs/category/version-1>

Icons: chemotion.net, nmrxiv.org, flaticon.com, spdx.org, terminology.nfdi4chem.de, ericid.org, elastic.co, fairdo.org, nfa.eu, helmholtz-metadaten.de, nfdi.de

