



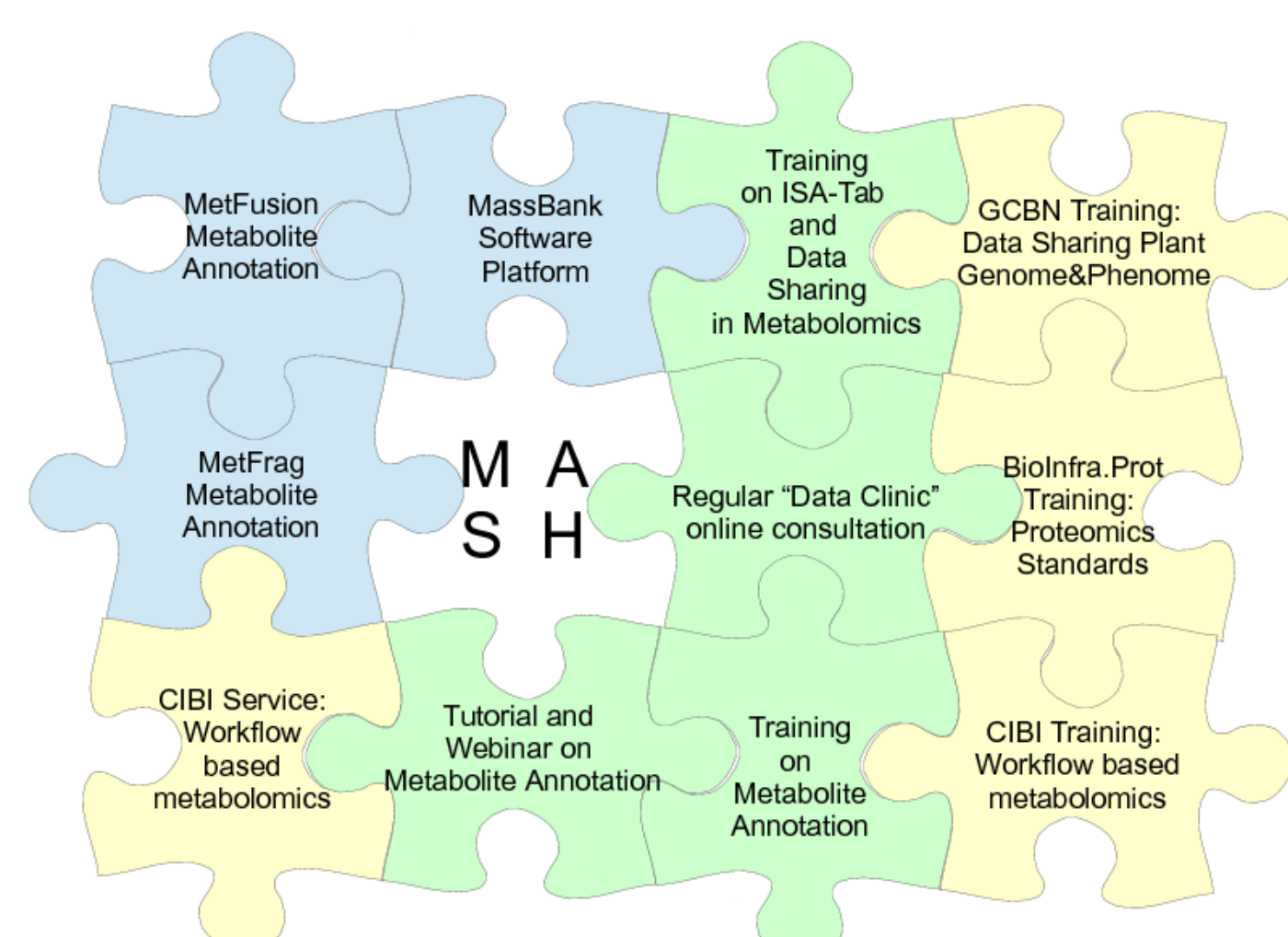
Center for Integrative Bioinformatics Metabolite Annotation & Sharing Halle (MASH)

Steffen Neumann, Guillaume Patoine
Leibniz Institute of Plant Biochemistry, Halle, Germany

Contract Nr. W-de.NBI-011

MASH provides ...

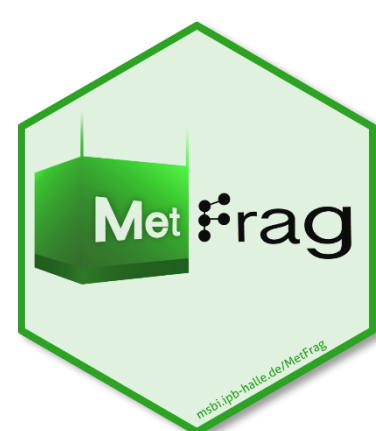
... training, maintenance and workflow integration of metabolite annotation software, and support for standards-compliant metabolomics and data sharing.



MASH services ...

Metabolite annotation tools

- running MetFrag infrastructure on local site and on the de.NBI cloud
- deployment on de.NBI K8S cloud
- online and offline training materials
- infrastructure deployments for workshops



MassBank spectral library

- continuous support for user and maintenance of data repository
- continuous development of documentation for developer and contributors of MassBank



FAIR MassBank

- Semantic annotation with schema.org and Bioschemas in web application & dumps
- regular releases for web service & data repository with stable DOI identifier



Data Clinic to support data sharing

- User support to create and deposit studies following FAIR principles
- Data standards for metabolomics (e.g. mzTab-M)
-  denbi-mash@ipb-halle.de

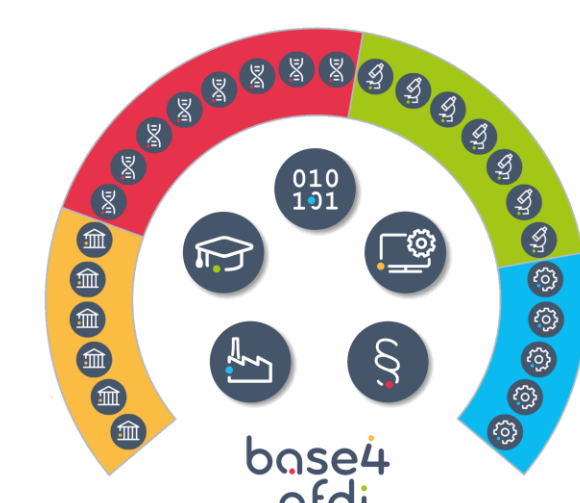
ELIXIR activities

- Steffen Neumann is Metabolomics community co-lead since 2022
- 2023 community meeting in Heidelberg
- Biohackathon activities
 - Bioschemas Resource Index for Chem & Plants
 - Ontologies & Terminology services ecosystem
 - Integrating BioC with bio.tools & EDAM
- ELIXIR AllHands 2023 *"The next Challenge: Data Management, Submission and FAIRness in Multi-Omics Experiments"*



German NFDI network

- IPB is Co-applicant  NFDI₄Chem
- NFDI Section Metadata
 - Bridge to ELIXIR w/ Bioschemas
 - Knowledge graphs & AI



de.NBI Training and education

- *"Introduction to Metabolite Identification in MS/MS Data"*, training workshop @DGMet 2023 in Halle



Team MASH

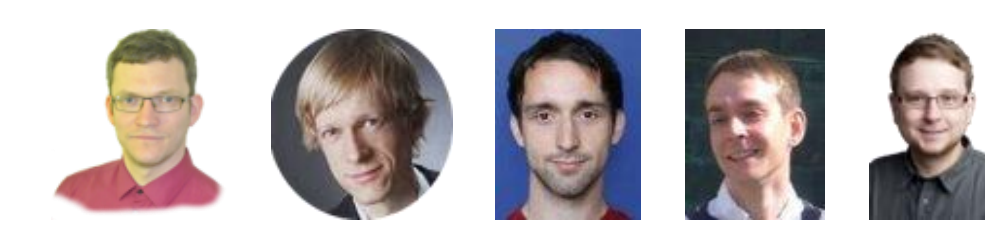


Guillaume Patoine



Steffen Neumann

Alumni: (left-to-right) Rene Meier, Kristian Peters, Christoph Ruttkies, Hendrik Treutler, Chris Ulpinnis



Publications

Arend, Daniel, Alessio Del Conte, Manuel Feser, Yojana Gadiya, Alban Gaignard, Leyla Jael Castro, Ivan Mičetić, et al. 2024. "Bioschemas Resource Index for Chem and Plants." <https://doi.org/10.37044/lof.io/xyxunp>.

Deutsch, Eric W., Juan Antonio Vizcaíno, Andrew R. Jones, Pierre-Alain Binz, Henry Lam, Joshua Klein, Wout Bittremieux, et al. 2023. "Proteomics Standards Initiative at Twenty Years: Current Activities and Future Work." *Journal of Proteome Research* 22 (2): 287–301. <https://doi.org/10.1021/acs.jproteome.2c00637>.

Giannattasio, Sergio, Katharina F. Heil, Henning Hermjakob, Rob W. W. Hooft, Maria I. Klapa, Fabrizio Mastroiocco, Steffen Neumann, et al. 2023. "The next Challenge: Data Management, Submission and FAIRness in Multi-Omics Experiments." *F1000 Research Limited*. <https://doi.org/10.7490/F1000RESEARCH.1119646.1>.

Klein, Joshua, Henry Lam, Tytus D. Mak, Wout Bittremieux, Yasset Perez-Riverol, Ralf Gabriels, Jim Shofstahl, et al. 2024. "The Proteomics Standards Initiative Standardized Formats for Spectral Libraries and Fragment Ion Peak Annotations: mzSpecLib and mzPAF." *Analytical Chemistry* 96 (46): 18491–501. <https://doi.org/10.1021/acs.analchem.4c04091>.

Peters, Kristian, Kaitlyn L. Blatt-Janmaat, Natalia Tkach, Nicole M. van Dam, and Steffen Neumann. 2023. "Untargeted Metabolomics for Integrative Taxonomy: Metabolomics, DNA Marker-Based Sequencing, and Phenotype Bioimaging." *Plants (Basel, Switzerland)* 12 (4). <https://doi.org/10.3390/plants12040881>.