Center for Integrative Bioinformatics (CIBI Halle)
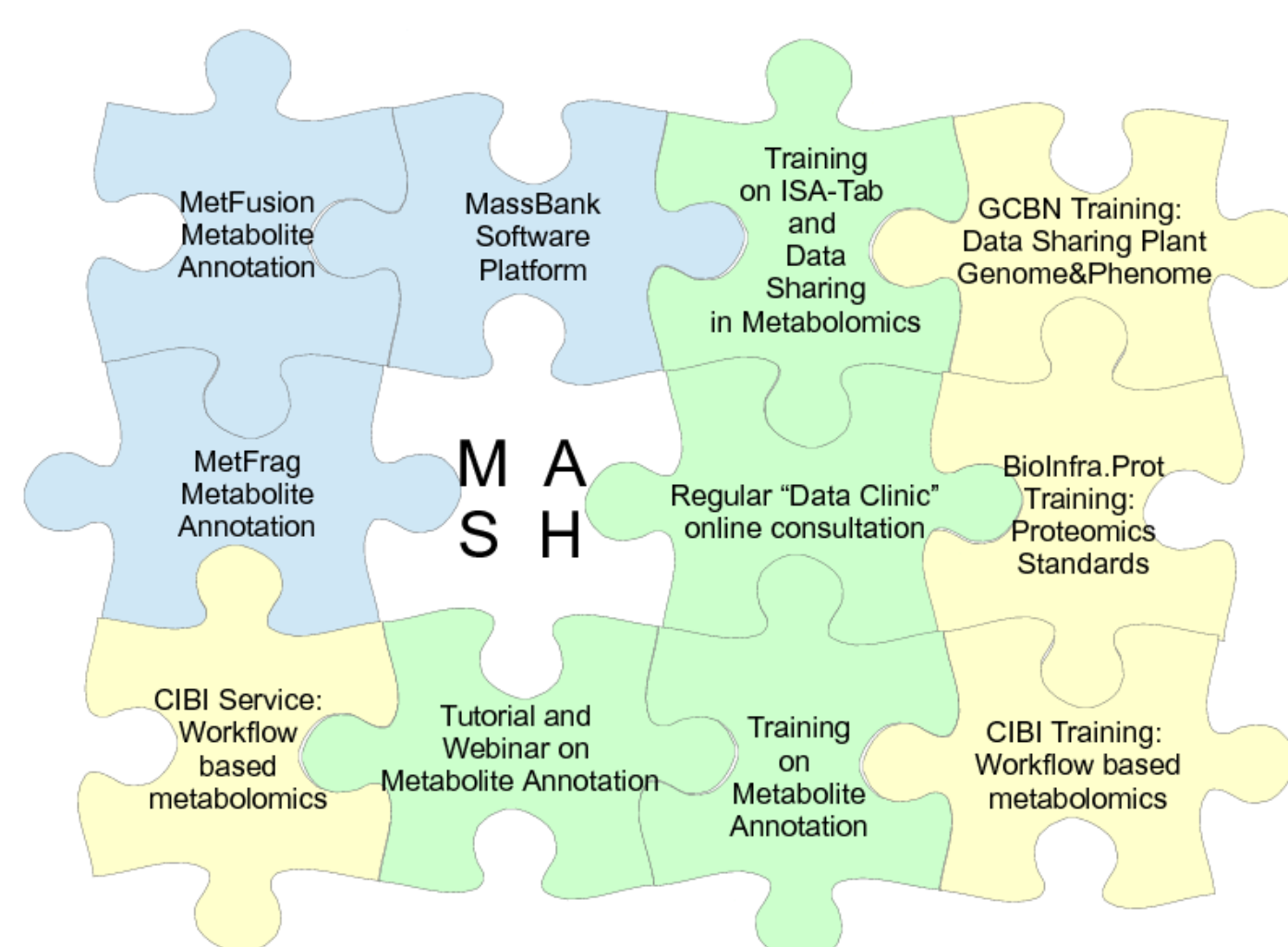# MASH: Metabolite Annotation and Sharing – Halle
FKZ 031L0107

Rene Meier, Kristian Peters, Steffen Neumann, Leibniz Institute of Plant Biochemistry, Halle, Germany
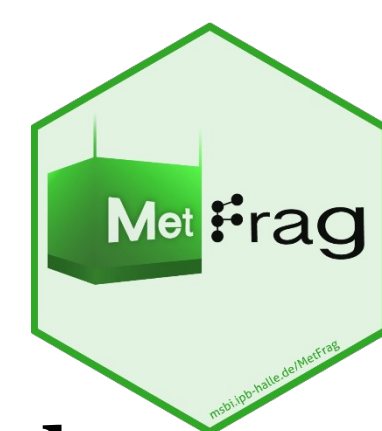
MASH provides …

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

MetFrag software maintenance & integration

de.NBI service: Metabolite annotation tools
- running MetFrag infrastructure on local site and on the de.NBI cloud
- deployment on de.NBI K8S cloud
- online and offline trainig materials
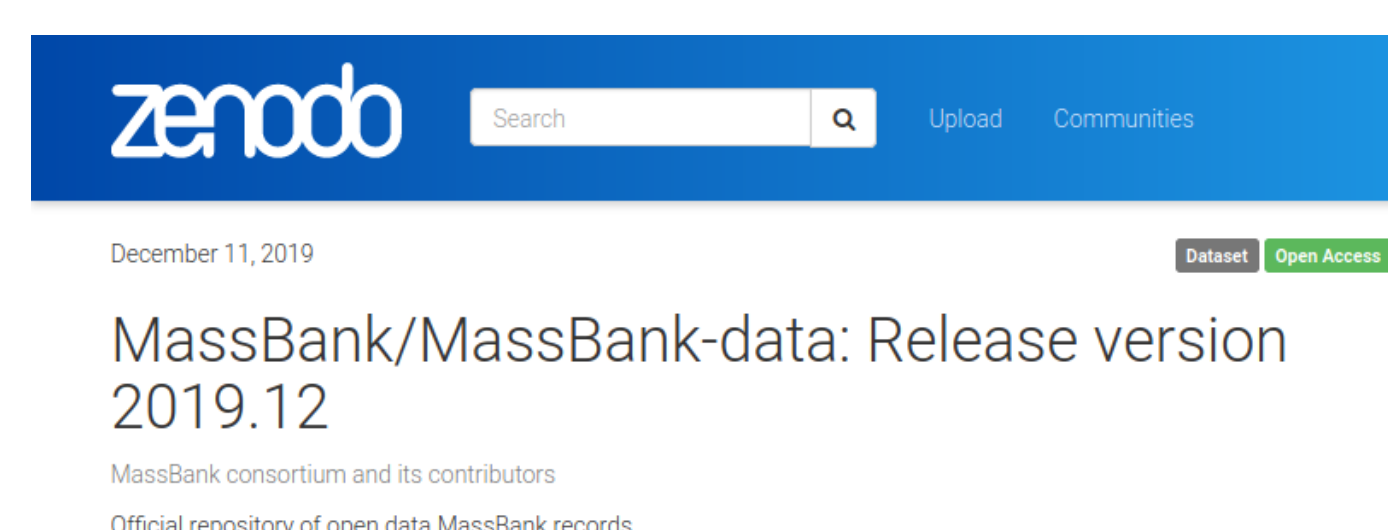- infrastructure deployments for workshops

MassBank software maintenance

de.NBI service: MassBank
- continous support for user and maintainance of data repository
- continous development of documentation for developer and contributors of MassBank
- support for 11 new contributors

FAIR MassBank
- automatic generation of sitemap on MassBank servers to increase findability of data
- Semantic annotation with *schema.org* and *Bioschemas* in the web application
- regular releases for web service and data repository with stable identifier *DOI*
- Implemented advanced search capabilities for via spectral identifier *SPLASH* and compound identifier *InChi-Key*

Data Clinic to support data sharing

de.NBI service:
Regular videoconferences with online support
- User support to create and deposit studies following FAIR principles
- Data standards for metabolomics (e.g. mzTab-M)
- Coordination of software support to increase standards adoption (active in PSI-MS)
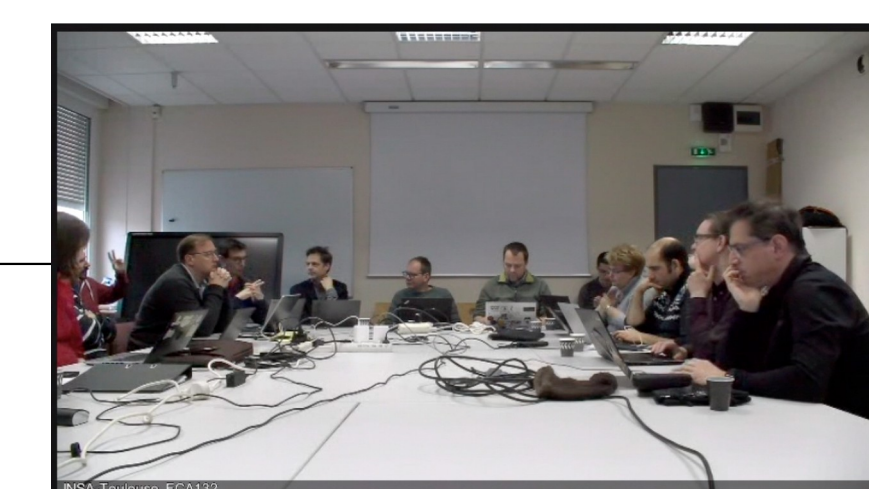
de.NBI cloud Activities
- Adaptation of software towards cloud-native architecture
- Deployment of software to de.NBI cloud
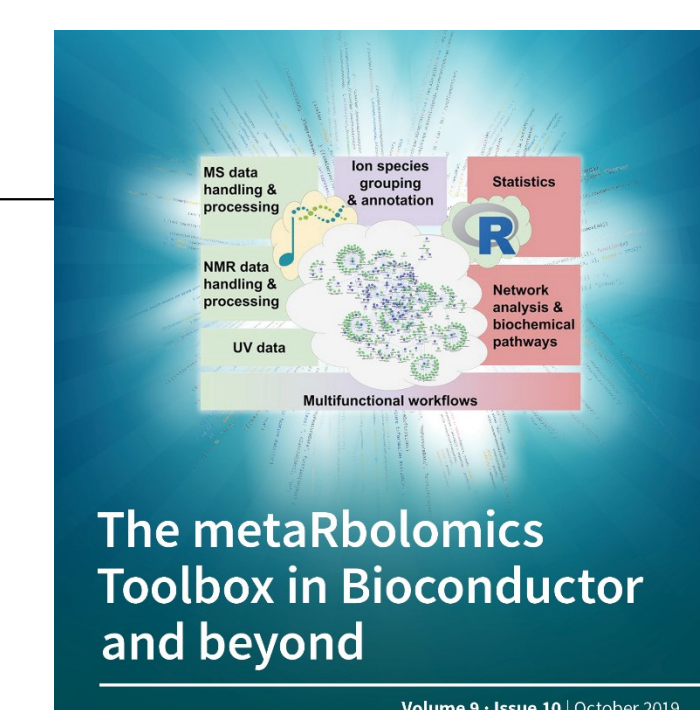- Supporting users to run our software on the de.NBI cloud

ELIXIR Activities
- 20. – 21.01.2020 **Toulouse** *„Strategies for standards compliant reporting and data sharing"* ELIXIR Metabolomics Community Meeting
- Part of ELIXIR Metabolomics community

de.NBI **Training** and education
- 01. – 03.04.2019 **Wittenberg** *„de.NBI CompMS metaRbolomics Hackathon"*
- 24.06.2019 **Den Haag** Workshop *„Towards FAIR Spectral Libraries: a workshop for Maintainers, Developers and Power Users"* at Metabolomics Conference 2019
- 15. – 19.07.2019 **Halle** BioBYTE Summer School 2019 for curious pupils
- 02. – 06.09. 2019 **Gatersleben** de.NBI Summer School 2019 *„(Bio)Data Science"*

General information on the project
- 2 FTE, all positions are currently filled
- Research group MSBI involved

Publications

- **The metaRbolomics Toolbox in Bioconductor and beyond.** Stanstrup, J. *et al.*; Metabolites 2019 9(10), 200. doi: 10.3390/metabo9100200
- **FAIR Computational Workflows.** Goble C *et al.*; Data Intelligence 2020 2:1-2, 108-121. doi: 10.1162/dint_a_00033
- **mzTab-M: a data standard for sharing quantitative results in mass spectrometry metabolomics.** Hoffmann N, *et al.*; Analytical chemistry 2019. doi:10.1021/acs.analchem.8b04310