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

2 FTE paid from de.NBI grant, Research group MSBI involved

MetFrag software maintenance & integration
- MetFrag converted to Container technology deployment in Kubernetes cluster (IPB, de.NBI cloud)
- Integration into KNIME workflow engine

MassBank software maintenance
- Updated database schema, responsive design, software running MassBank.eu and mirror MassBank.jp
- schema.org for structured data markup in record pages
- MassBank-web running as containers (in classic VM) or on Kubernetes (de.NBI cloud-ready!)
- MassBank-data now also on github, data with continuous integration, issue tracking, pull requests

> software engineering approaches for data!
- Extensive debugging/curation of ~48,000 records
- Follow-up BMBF grant proposal Speculative between UFZ Leipzig (T. Schulze), BAM (J. Lisec) and IPB

Data Clinic to support data sharing
- Support users via online meetings and staff-exchange to deposit studies
- ISA-Tab metadata
- Collaboration with MetaboLights team @EMBL-EBI
- Sharing MS/MS spectra from 11 groups, common data extraction workflow

de.NBI cloud and PhenoMeNal/Elixir Cloud
- PhenoMeNal is H2020 project collaborating with EMBL-EBI TSI and Elixir cloud teams
- Advanced application stack deployment using the Infrastructure-as-Code on Bielefeld/Giessen/Tübingen cloud

de.NBI Training and education
- de.NBI CIBI Winter School on Computational Metabolomics from March 5-8, 2018 at Leucorea Wittenberg with 43 participants from seven European countries
- BioBYTE Summer School 2018 for 18 curious pupils from July 16 – 20, 2018 at MLU Halle and de.NBI partners IPK and Metabolomics@IPB
- de.NBI CIBI-MASH UM 19.09.-21.09.2018 in Berlin
- Educator in 1st de.NBI Cloud User Meeting
- Online training and documentation for MetFrag at github.com/c-ruttkies/MetFragTraining including video material of MetFrag usage
- de.NBI CompMS metaRbomolomics Hackathon Announced for 01.-03.04.2019 in Wittenberg covering RMassBank, metFrag, ...
- Application for workshop @ Metabolomics2019 (The Hague) in preparation