# Center for Integrative Bioinformatics (CIBI Tübingen)

## Tools for the Reproducible Analysis of Mass Spectrometric Data

**FKZ: 31A535A**

Oliver Alka, Felix Bartusch, Leon Bichmann, Benjamin Gläßle, Maximilian Hanussek, Julianus Pfeuffer, Oliver Kohlbacher, Jens Krüger, Timo Sachsenberg

---

### Short description of the project

**OpenMS:**
- Cross-platform mass spectrometry data analysis framework and programming library
- More than 180 tools for proteomics and metabolomics analysis tasks
- Tools can be chained into complex analysis workflows
- Workflows for high-throughput data analysis on HPC and cloud resources
- Consulting, training, and support for users and developers

**de.NBI cloud site Tübingen:**
- State-of-the-art technologies
- Access to more than 1,650 compute cores, 15 TB RAM, 13 PB storage
- Easy application and fast setup of own projects

**de.NBI services**

- Consulting and software support for both users and developers
- Integration of external code, data repositories, or software contributions into OpenMS
- Train users and external developers
- Improvements to software documentation and teaching material
- Two software releases per year, including: binary installer, container, KNIME plugins, python packages, bioconda packages, and integration into commercial platforms
- Maintenance of build and test infrastructure

### Progress report

**OpenMS:**
- Infrastructure development with focus on cloud
  - Automatic container builds for cloud computing
  - KNIME and Nextflow cloud workflows (nf-core)
  - Increased interoperability with public repositories (PRIDE)
  - Consulting and software support

**Elixir activities**
- Involved in four implementation studies
- Training coordination (O. Kohlbacher ELIXIR-DE TC)
- Involvement in EXCELERATE WP (Proteomics Beacon)
- Communities: proteomics (coord.), metabolomics

**Training and education**
- Revised training material
- Developer, user meetings, and conferences
- Online lectures and tutorials
- Training coordination (O. Kohlbacher de.NBI TC)

**Translation to industry**
- STORM Therapeutics, detection of modified RNAs
- Workflow integration in *Thermo Fisher ProteomeDiscoverer*

**Interaction w/ other activities**
- Close interaction with Medical Informatics Initiative (DIFUTURE consortium) on omics data analysis
- Interaction with GO-FAIR initiative and Personal Health Train implementation network

**de.NBI Cloud services**
- Support of bioinformatics tool integration and service
- Specific data mirroring for proteomics and proteogenomics (CPTAC, TCGA, ICGC)

### de.NBI cloud activities

- Established de.NBI cloud site in Tübingen
- Upcoming extension with 30 high-memory nodes
- Network infrastructure upgrade (Infiniband, 40GE)
- Currently more than 20 active projects with more than 60 individual users
- Two computationally intensive mass spectrometry projects started
  - KNIME in the cloud
  - *de novo* Metabolite identification

**Staff**

- 3 FTE for CIBI-1 and de.NBI Cloud paid through de.NBI and an additional 3 FTE own contribution
- All positions are currently filled

### Selected Publications

OpenMS: a flexible open-source software platform for mass spectrometry data analysis

OpenMS: applications for reproducible analysis of mass spectrometry data

OpenMS: applications for reproducible analysis of mass spectrometry data

OpenMS: applications for reproducible analysis of mass spectrometry data

---

www.denbi.de