

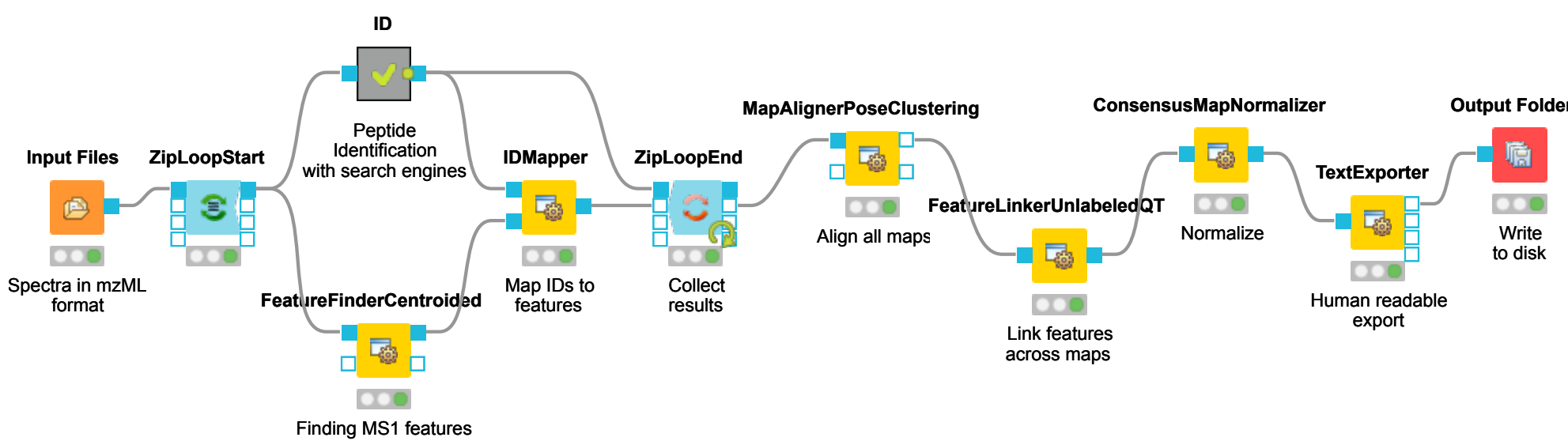
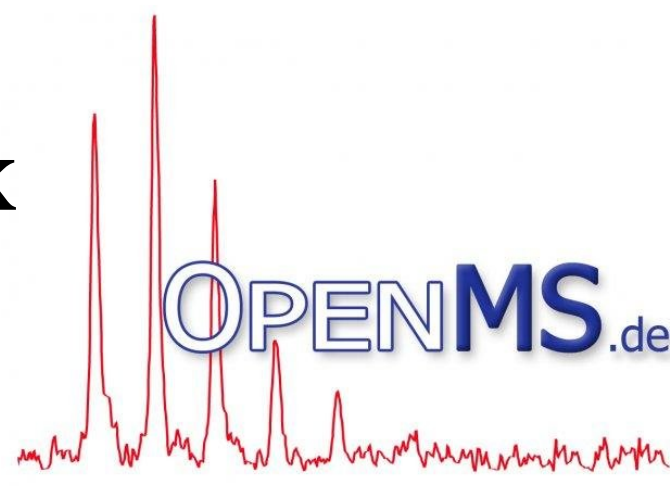
OpenMS – software framework and tools for computational mass spectrometry

FKZ: 31A535A

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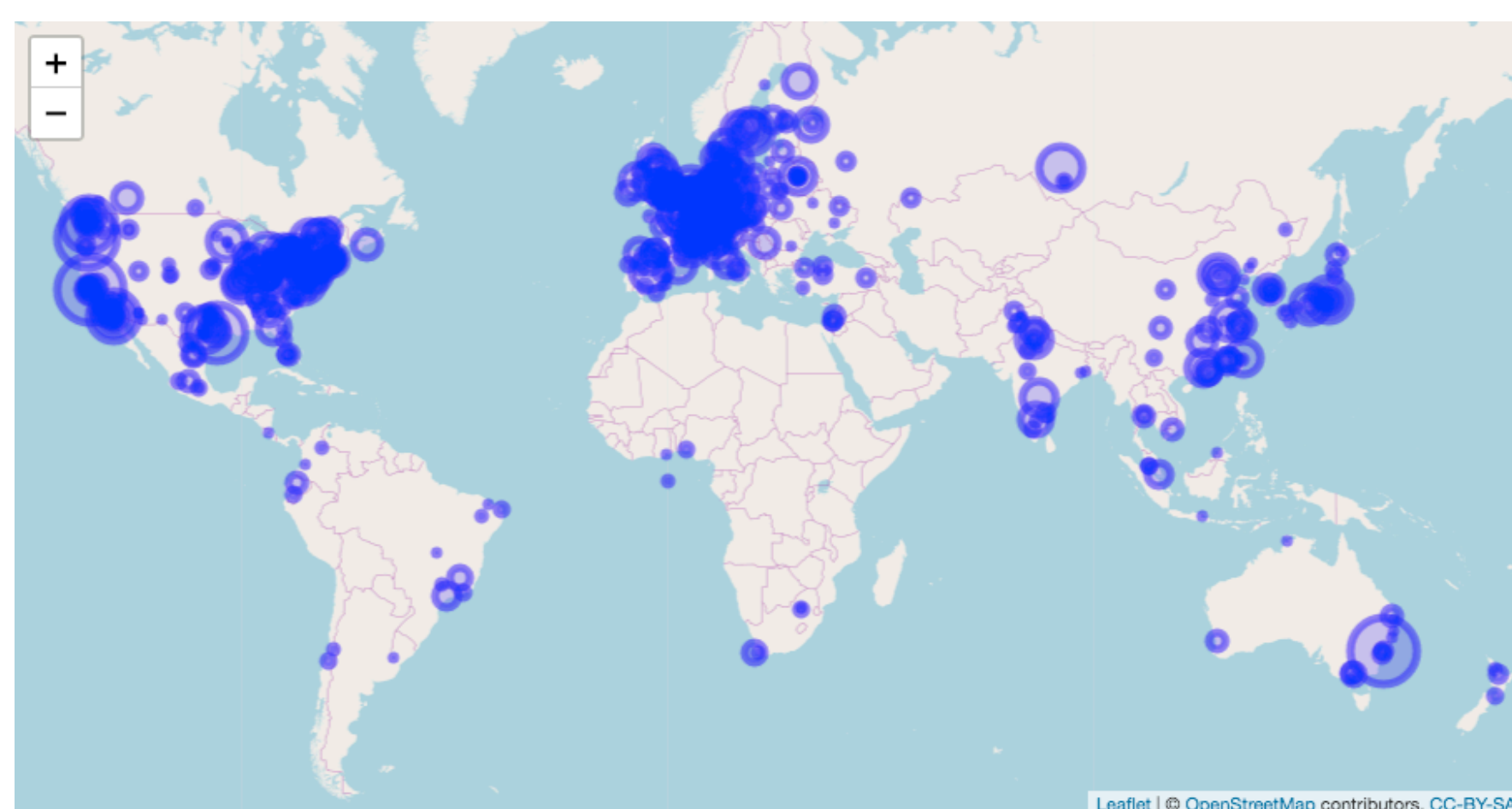
Short description of the project

- Mass spectrometry data analysis framework
- Cross-platform open-source software with active community
- More than 10 years of continuous development
- Builds on open, standardized data formats
- High-throughput data processing and analysis
- More than **180 cloud-ready tools for proteomics and metabolomics analysis tasks**
- Integrated into several workflow systems and portals



de.NBI services

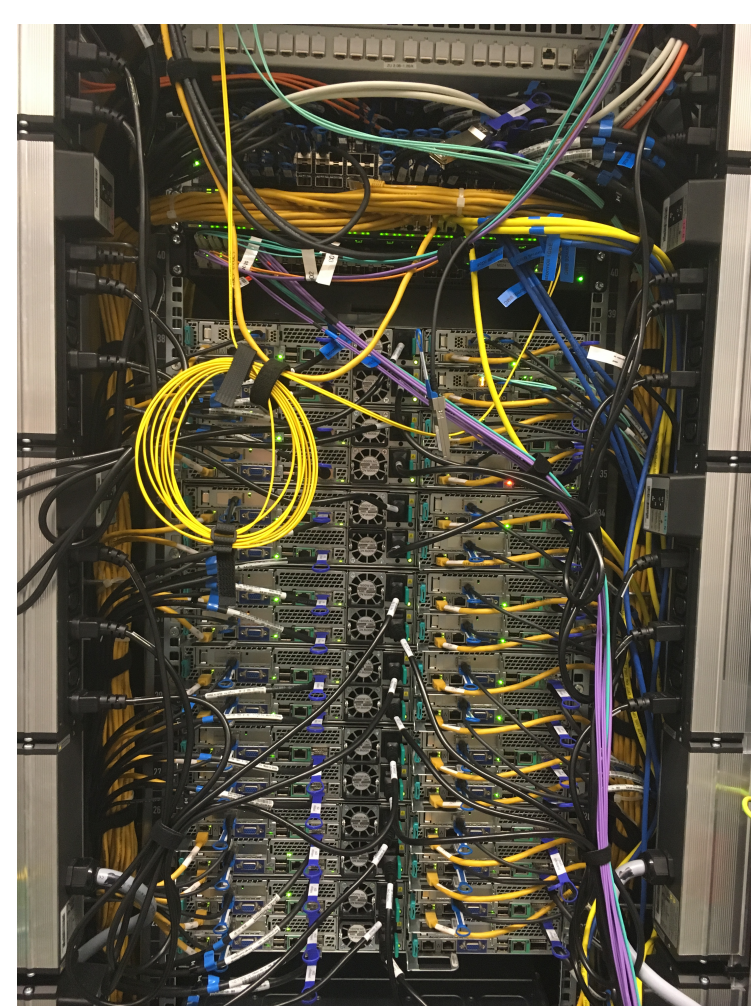
- **Maintenance** of build and test infrastructure
- Integration of **external contributions**
364 issues solved, 298 new contributions (PRs)
- New tools and algorithms
- **9.4k+ users**



- **3.2k downloads of OpenMS 2.4 installers**
- Consulting, training and software **support**
- **KNIME plugins** to visually construct workflows
- Integration into **commercial platforms**
- Available on **Bioconda** (8.4k downloads) and Biocontainer
- Workflows in nf-core

de.NBI Cloud activities

- Extension with **high-memory** nodes (1.5TB RAM)
- Virtual clusters
- Concepts for handling sensitive patient data
- Continuation of the BSI C5 Certification process
- Tender process published, extending the cloud site with GPUs



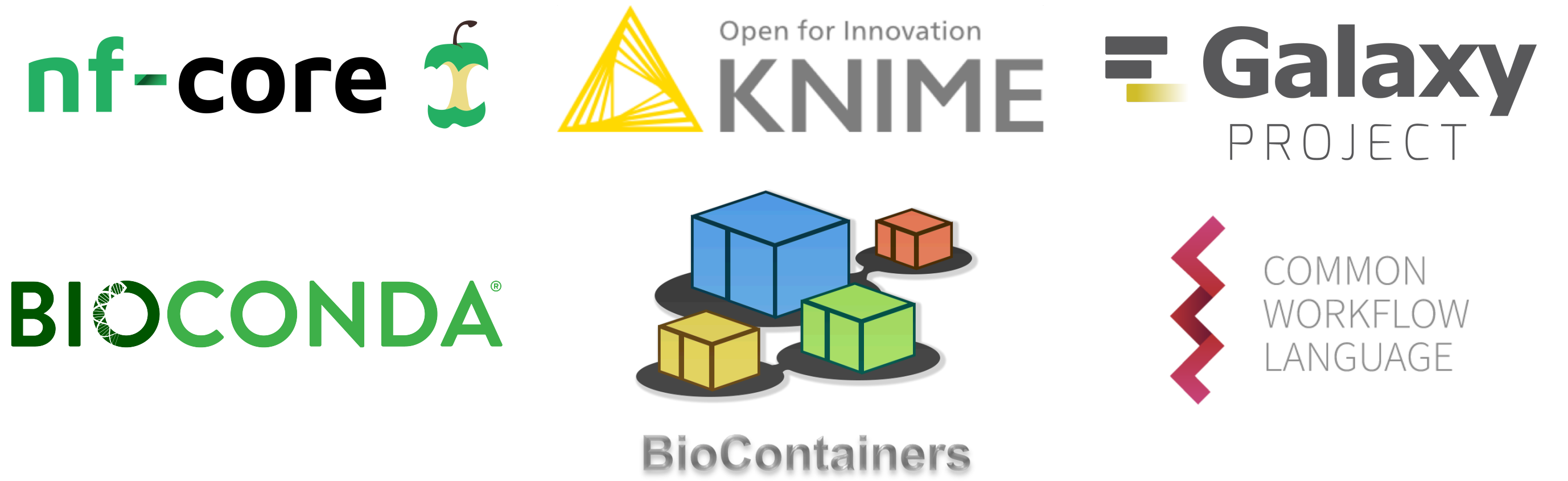
Staff

- 5.0 FTE for CIBI-1 (2), Elixir (1) and de.NBI Cloud (2) projects

Progress report

Infrastructure development

- Extended continuous integration matrices and services
- Compiler and dependency updates
- New and updated Bioconda recipes and (Bio-)containers
- Consolidation of various tools into mini-workflows for increased performance and userfriendliness
- pyOpenMS for rapid prototyping of MS visualizations
- Workflows for cloud deployment
- Completion of the initial audit to achieve the BSI C5 security certificate



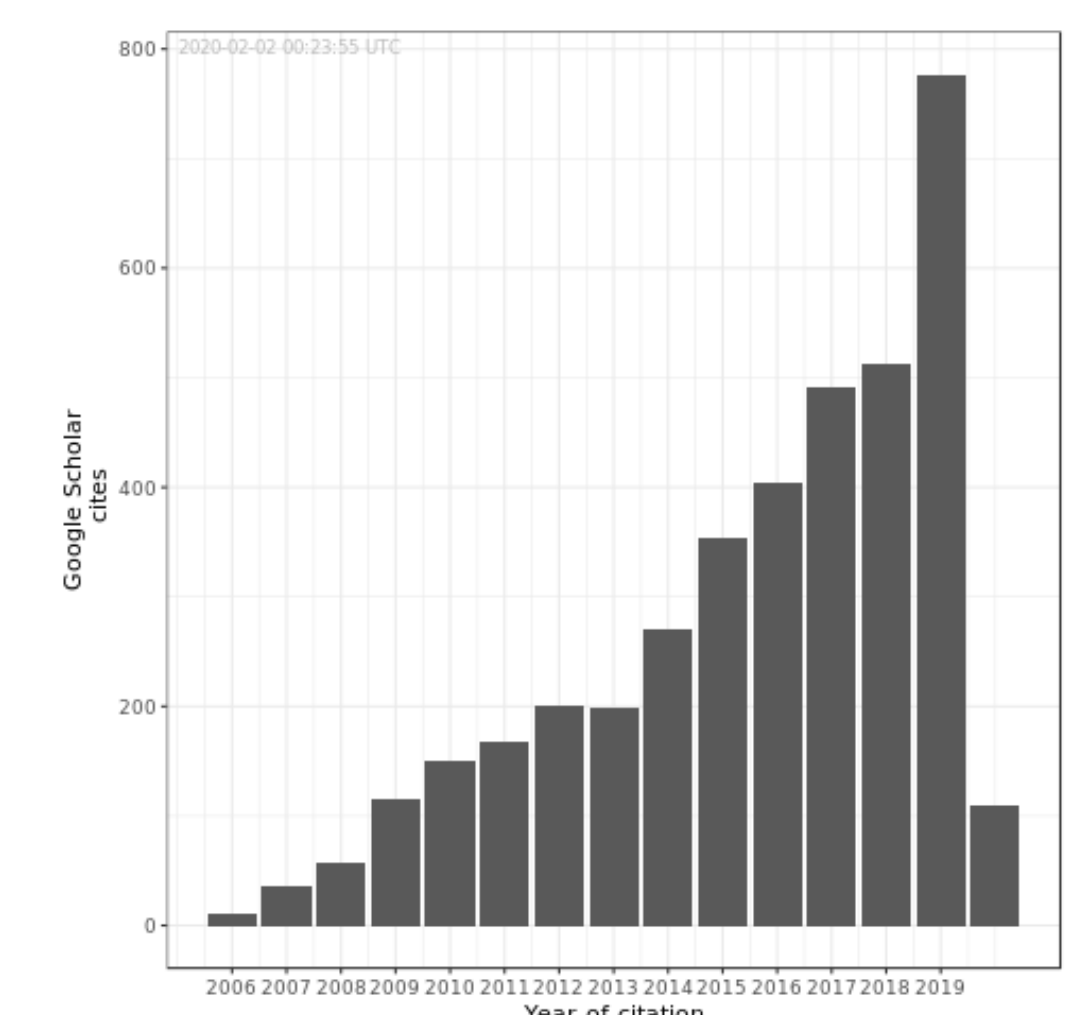
Training and education

- Revised training material (on- and offline)
- Trainings using cloud resources

de.NBI Training and education

5 national and 4 international training events in 2019

- 15 Jan 2019 (Zakopane, EUBIC WS): Label-free quantification with OpenMS/OpenSWATH
- 18 Mar 2019 (Berlin): SeqAn & OpenMS (CIBI) Integration Workshop at the KNIME Spring Summit
- 7 Apr 2019 (Belgrade): OpenMS Developer Meeting
- 29 Apr 2019 (Boston): 3 days workshop *MayInstitute* Proteomics and Metabolomics with OpenMS
- 03 Sep 2019 (Heidelberg): 3 days de.NBI cloud user meeting, Virtual Cluster deployment with Terraform
- 16 Sep 2019 (Heidelberg GCB): Proteomics and metabolomics with OpenMS and pyOpenMS
- 3 Nov 2019 (Göttingen SSP): Protein-RNA cross-linking with RNPxl/OpenMS
- 11 Nov 2019 (Salerno NETTAB): Label-free quantification with OpenMS
- 2 Dec 2019 (Tübingen): 2 days training course on de.NBI cloud resources: Analyzing epiGBS data



Selected Publications

OpenMS: a flexible open-source software platform for mass spectrometry data analysis
HL Röst, T Sachsenberg, S Aiche, C Bielow, H Weissner, et al. – *Nat. Methods*

OpenMS – A platform for reproducible analysis of mass spectrometry data
Pfeuffer, J, Sachsenberg, T, Alka, O, Walzer, M, Füllbrunn, A, Nilse, L., Schilling O, Reinert K, Kohlbacher, O. *Journal of Biotechnology*

LFQProfiler and RNPxl: Open-Source Tools for Label-Free Quantification and Protein-RNA Cross-Linking Integrated into Proteome Discoverer
J Veit, T Sachsenberg, et al. – *Journal of Proteome Research*

BioContainers: An open-source and community-driven framework for software standardization.
Leprevost FD, Grünig BA, Alves Afritas S, Röst HL, Uszkoreit J, Barsnes H, Vaudel M, Moreno P, Gatto L, Weber J, Bai M, Jimenez RC, Sachsenberg T, Pfeuffer J, Vera Alvarez R, Griss J, Nesvizhskii AI, Perez-Riverol Y, *Bioinformatics*

MHCquant: Automated and Reproducible Data Analysis for Immunopeptidomics.
Bichmann, A Nelde, M Ghosh, L Heumos, C Mohr, A Peltzer, L Kuchenbecker, T Sachsenberg, J Walz, S Stevanović, HG Rammensee, O Kohlbacher, *Journal of Proteome Research*

EPIFANY - A method for efficient high-confidence protein inference.
J Pfeuffer, T Sachsenberg, T M H Dijkstra, O Serang, K Reinert and Oliver Kohlbacher, *Journal of Proteome Research*

In-depth analysis of protein inference algorithms using multiple search engines and well-defined metrics
E Audain, J Uszkoreit, T Sachsenberg, J Pfeuffer, X Liang, et al. – *Journal of proteomics*

Recognizing millions of consistently unidentified spectra across hundreds of shotgun proteomics datasets
J Griss, Perez-Riverol, Y, Lewis, S, Tabb, DL, Dians, JA, del-Toro, N, Rurik, M, Walzer, MM, Kohlbacher, O, Hermjakob, H, Wang, R, and Vizcaino, JA – *Nat. Methods*

