BioInfra.Prot - Dortmund

Bioinformatics for MS-based Proteomics Services

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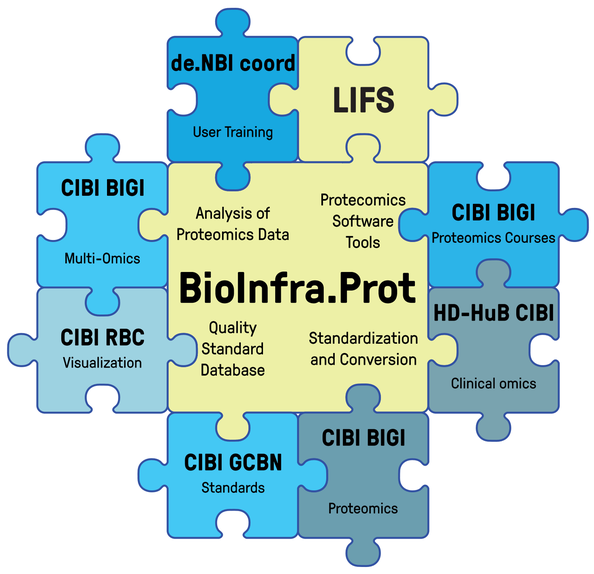
Fkz 031A534B

Short description of the project



BioInfra.Prot - Dortmund implements and provides bioinformatics for MS-based proteomics services like tools and databases. We put high importance on easy and intuitive usability to bridge the gap between pure informatics tools and end users. Additionally, we organize workshops and trainings as a de.NBI service unit.

de.NBI services

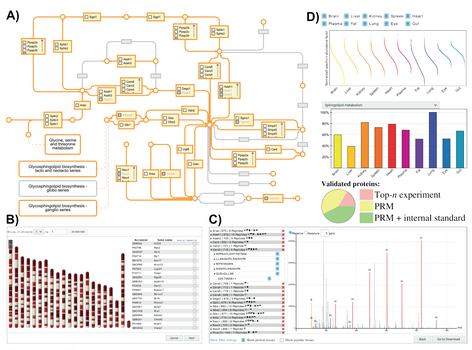


Figure 1: STAMPS in a nutshell. (A) Interactive graph-based pathway interface. (B) Different protein selection methods are available, for instance a chromosome browser. (C) Reviewing protein selection; all spectra / peptides / proteins can be examined on the fly. (D) External quality control.

STAMPS

- **S**imple **T**argeted **A**ssays for **M**etabolic **P**athways and **S**ignaling
- Spectral library containing ~160,000 high-quality, high-resolution peptide MS-spectra (manually curated)
- About 12,000 proteins and 130,000 peptides stored
- Pathway-based graph view for easy protein selection

SearchGUI

- Management tool for launching up to eight peptide search engines and two *de novo* tools at once
- Contains extensive command line interface for high-throughput batches
- High user acceptance, analyses launched over 67,000 times in 2019

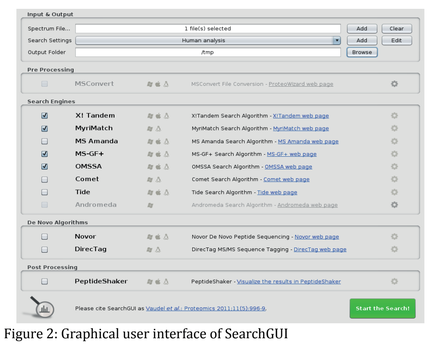


Figure 2: Graphical user interface of SearchGUI

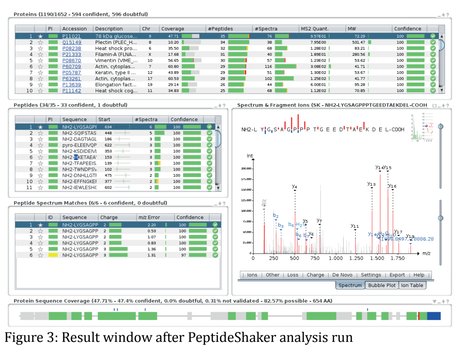


Figure 3: Result window after PeptideShaker analysis run

PeptideShaker

- Builds consensus protein identification lists from several runs
- Contains extensive command line interface for high-throughput batches
- Connected with proteomics data repository Pride
- High user acceptance, launched over 77,000 times in 2019

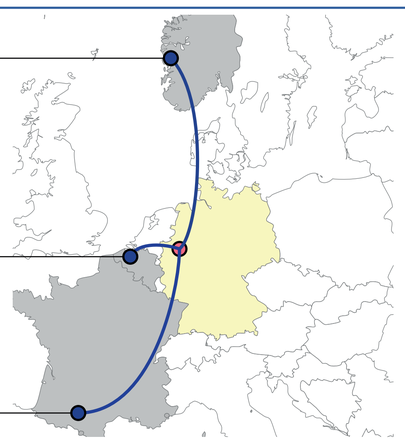
General information on the project

Cooperation partners

Bergen, Norway
Marc Vaudel
Harald Barsnes

Ghent, Belgium
Lennart Martens

Toulouse, France
David Bouyssié



BioInfra.Prot - Dortmund, ISAS (2019):

- Dominik Kopczynski - 1 FTE, de.NBI
- 1 PhD student (1/4 FTE)
- Albert Sickmann, PI
- Robert Ahrends, Coordinator

Progress report

Completed:

- BioInfra.Prot - Dortmund has provided tools for services and has started teaching and education activities
- Tools: SearchGUI, PeptideShaker, and STAMPS
- Usage numbers confirm the high acceptance of our tools within the community

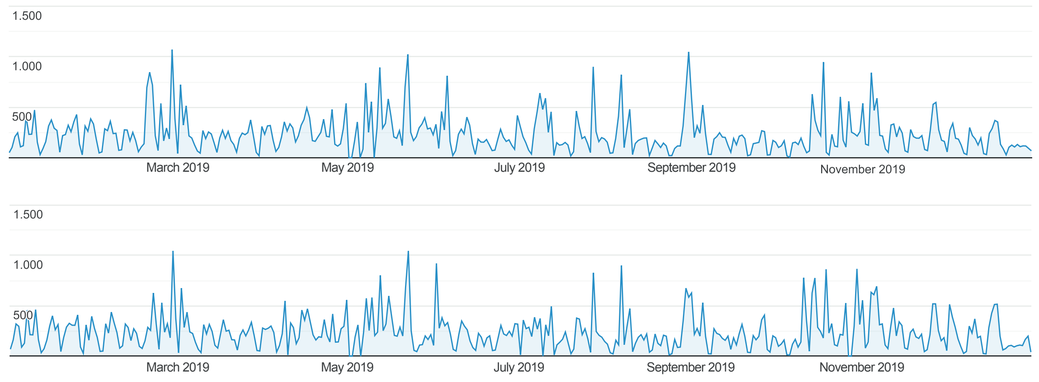


Figure 4: Diagram of SearchGUI (top) and PeptideShaker (bottom) analysis start events from January 2017 until December 2019 (included)

- All workshops, courses and summer schools were always fully booked and well rated by the participants
- Close collaboration with:
  - Compomics group in Ghent / Belgium headed by Lennart Martens
  - Bioinformatics group in Bergen / Norway headed by Harald Barsnes
  - Proteomics group in Toulouse / France in coop. with David Bouyssié

Further steps:

- Publishing STAMPS
- Finishing refactoring of new database system in PeptideShaker
- Extending STAMPS for new species and metabolic spectra

de.NBI Training and education

Past:

- Workshop: “Computational Protein Identification with SearchGUI & PeptideShaker”, Proteomics Forum 2019, Potsdam, Germany
- Workshop: “Lipid Pathways: the Proteomics Side of the coin - STAMPS”, LipoSysMed Summer School 2019, Leipzig, Germany
- Workshop: “Basics in Computational Protein Identification”, EuPA Congress 2018, Santiago de Compostela, Spain
- Workshop: “Computational and Bioinf. Tools for Proteomics“, European Mass Spectrometry Conference (EMSC) 2018, Saarbrücken, DE

User satisfaction of workshops during period of March 2015 until September 2019

General workshop satisfaction		*Teaching materials*		*Hands-on exercises*	
Poor	0%	Poor	0%	Poor	0%
Weak	8.45%	Weak	7.63%	Weak	7.27%
Good	22.07%	Good	24.43%	Good	27.88%
Excellent	69.48%	Excellent	67.94%	Excellent	64.85%

Upcoming:

- Workshop at Lipidomics Forum, Sep. 2020, Regensburg, Germany
- Proteomics Summer School, 2021

Publications

[1] Kopczynski, D., Barsnes, H., Njølstad, P. R., Sickmann, A., Vaudel, M., & Ahrends, R. (2017). PeptideMapper: efficient and versatile amino acid sequence and tag mapping. Bioinformatics, 33(11): 2042–2044.

[2] Kopczynski, D., Coman, C., Zahedi, R. P., Lorenz, K., Sickmann, A., & Ahrends, R. (2017). Multi-OMICS: a critical technical perspective on integrative lipidomics approaches. Biochimica et Biophysica Acta (BBA)-Molecular and Cell Biology of Lipids, 1862(8): 808–811.

[3] Kopczynski, D., Sickmann, A., & Ahrends, R. (2017). Computational proteomics tools for identification and quality control. Journal of Biotechnology.

[4] Vögtle, F. N., Burkhart, J. M., Gonczarowska-Jorge, H., Kücükköse, C., Taskin, A. A., Kopczynski, D., Ahrends, R., Mossmann, D., Sickmann, A., Zahedi, R.P., & Meisinger, C. (2017). Landscape of submitochondrial protein distribution. Nature Communications, 8(290).

[5] Kopczynski, D., *et al.* (2020). Simple targeted assays for metabolic pathways and signaling: a powerful tool for targeted proteomics. In submission.

[6] Peng, B., ..., Kopczynski, D., *et al.* (2018). Identification of key lipids critical for platelet activation by comprehensive analysis of the platelet lipidome. Blood, 132(5):e1-e12.

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