Bioinformatic Services for Proteomics

BioInfra.Prot Bochum

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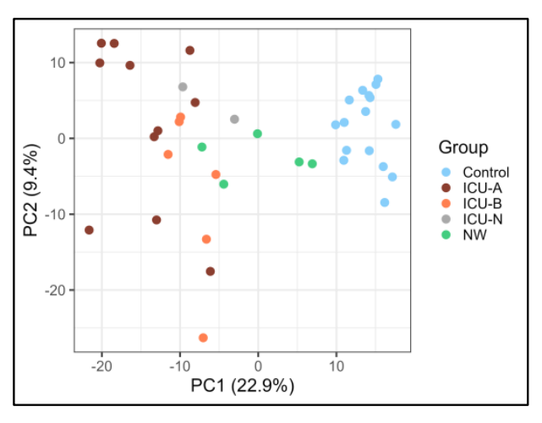
Contract Nr. W-de.NBI-005

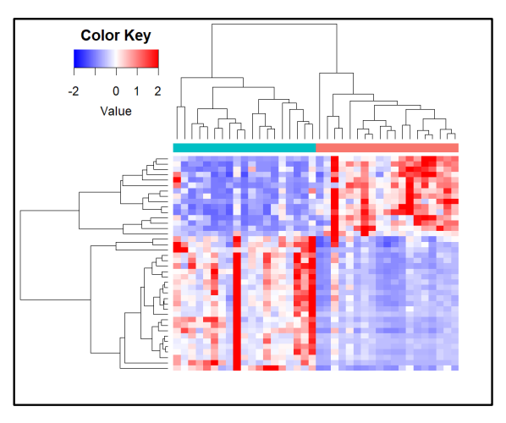
Short description of the project

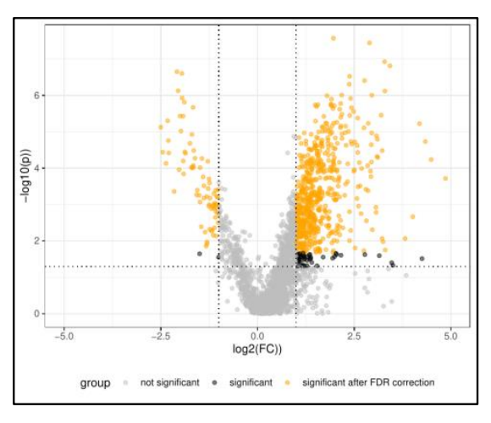
As a recently established core unit within the Medical Faculty of the Ruhr University Bochum we are complementing the BioInfra.Prot service center of the German Network for Bioinformatics Infrastructure - de.NBI 2.0, which realizes the German node ELIXIR-DE of the European ELIXIR infrastructure. We provide a comprehensive portfolio of Bioinformatics cooperation and infrastructure possibilities to clinical, biological, and mass spectrometry users.

de.NBI services

Computational & Statistical Analysis and Consulting for proteomics and corresponding clinical data





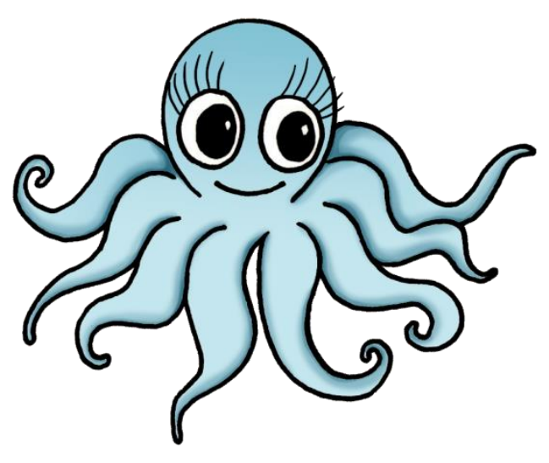


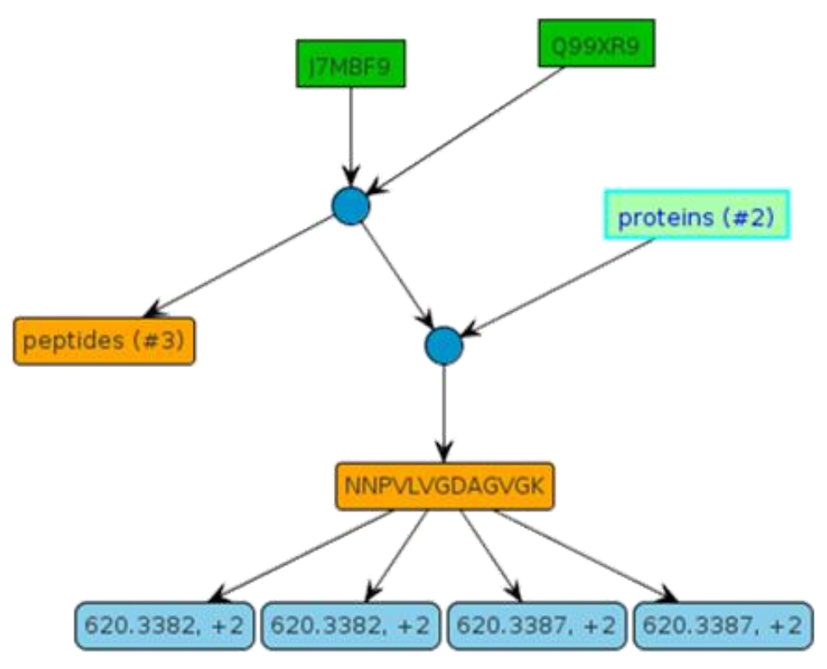
- *Study planning*
- *Normalization and quality control*
- *Statistic analysis*
- *Survival analysis*
- *Classification and Clustering*
- *Mashing Learning*

Tools:

Protein Inference Algorithms (PIA)[1]:

A toolbox for MS based protein inference and identification analysis.

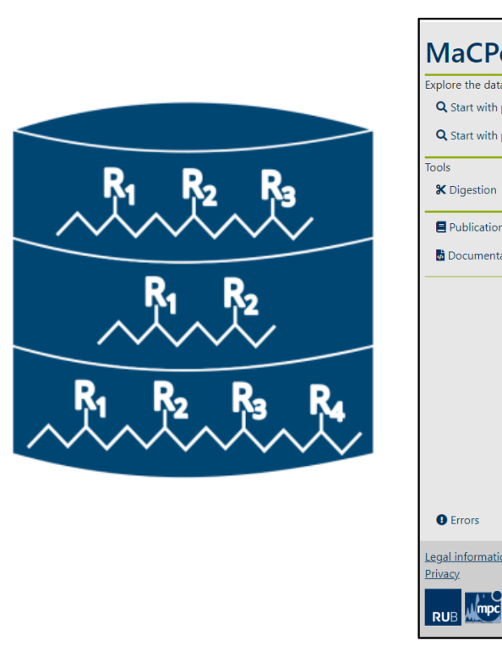


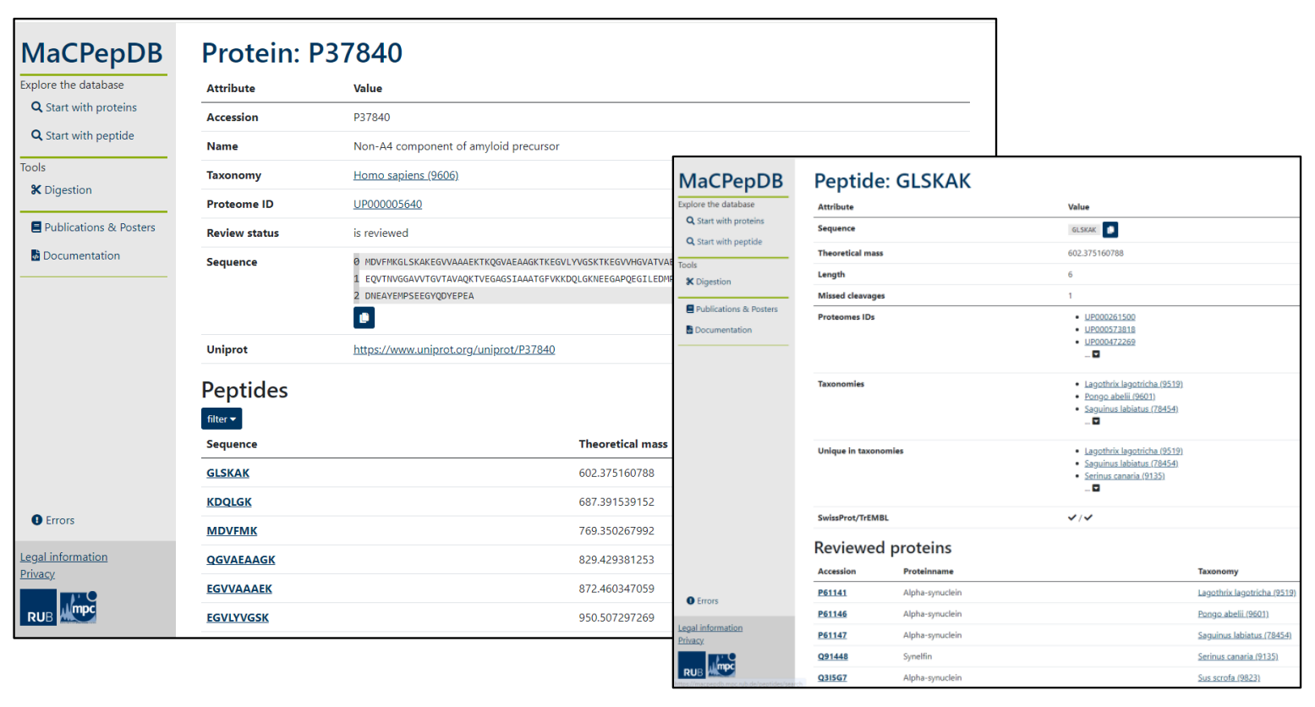


- *Inspect search results*
- *Combine and conduct statistical analysis*
- *Visualize the correspondence between PSMs, peptides and proteins*

Mass Centric Peptide Database (MaCPepDB)[2]:

Peptide database, that consists of the complete tryptic digest of the Swiss-Prot and TrEMBL parts of UniProtKB.

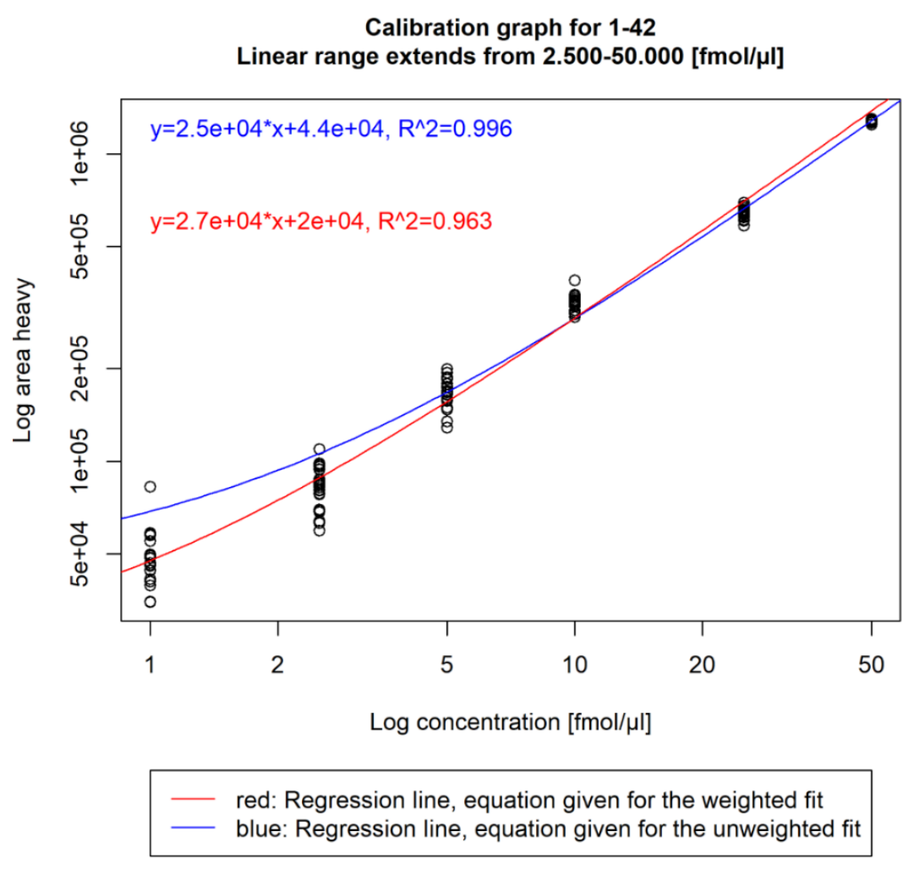




- *Web interface*
- *REST API available*
- *Peptide selection for targeted proteomics*
- *Proteins or peptide search*
- *PTMs support*

CalibraCurve[3]:

A tool for generating and visualizing calibration curves for targeted proteomics data

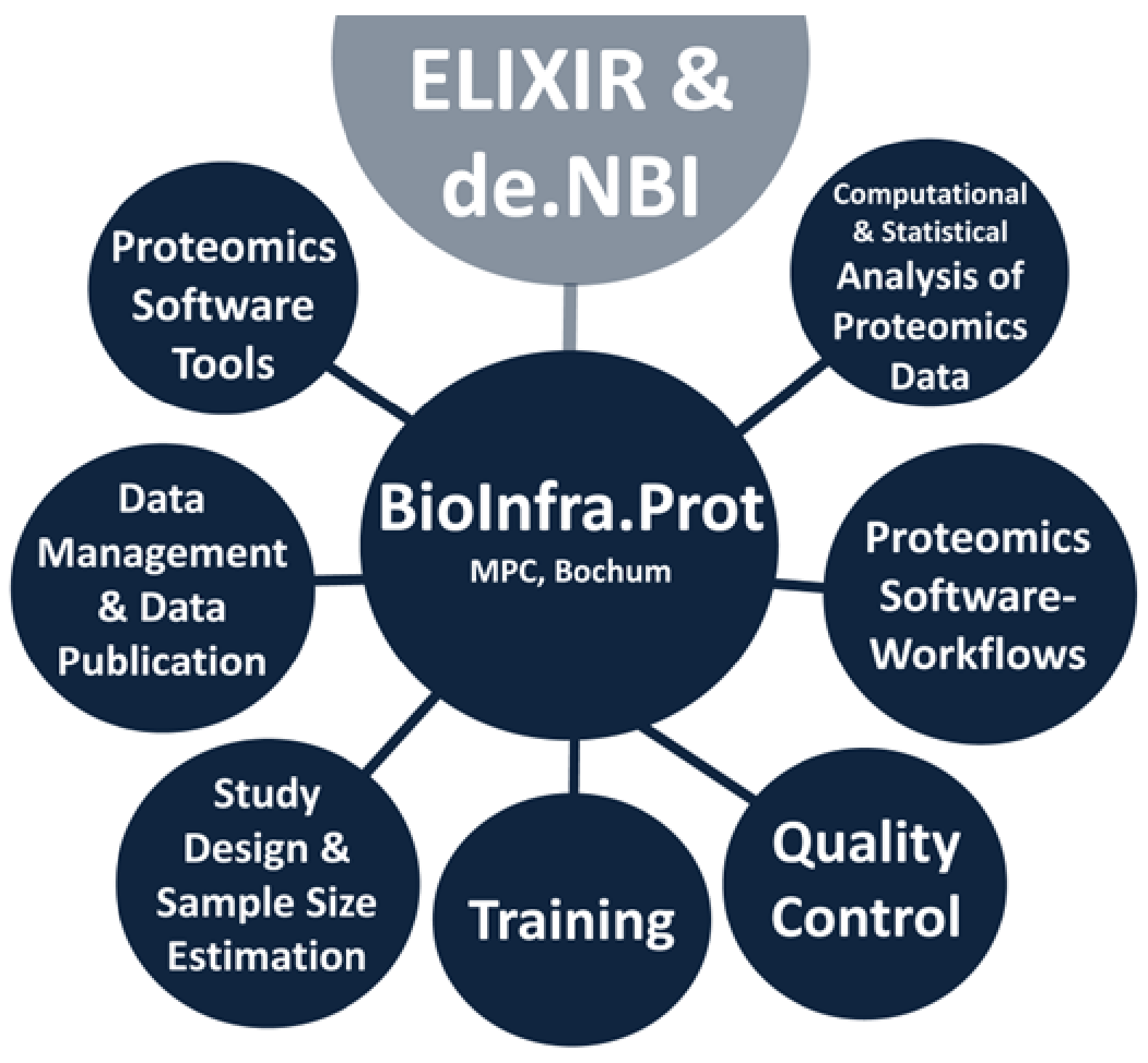


- *Dynamic linear range*
- *LOQ, ULQ*
- *Pre-filtering steps*
- *Intuitive visualization*

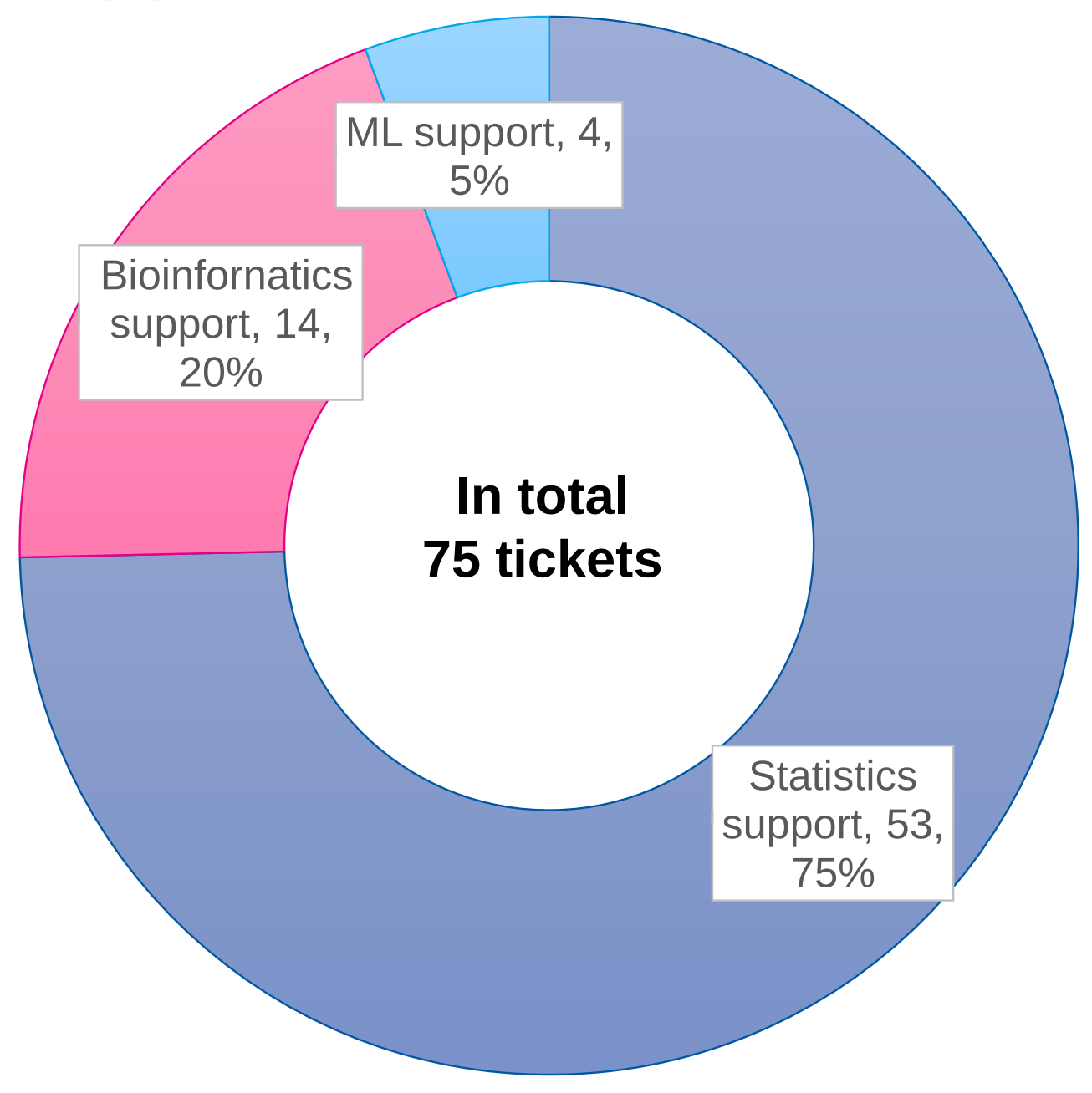
General information on the project

- No. of staff paid from de.NBI grant (FTE): 1.2
- Other staff involved (FTE): 5

Progress report



Supported tickets since 2023



- **CalibraCurve:** 181 downloads
- **PIA:** 3,941 downloads
- **MaCPepDB:** 5,179 visits

ELIXIR engagement

We continued the lead of the community led implementation study 2021 for proteomics and successfully finished the study. The active funding of the study ended in October 2023 (after an extension), but together with some partners we plan to further take advantage of the SDRF for proteomics file format for sample annotations and create tools and workflows for the automated (re-)analysis of proteomics datasets. Dirk Winkelhardt is active as the ELIXIR officer for proteomics.

Cloud activities

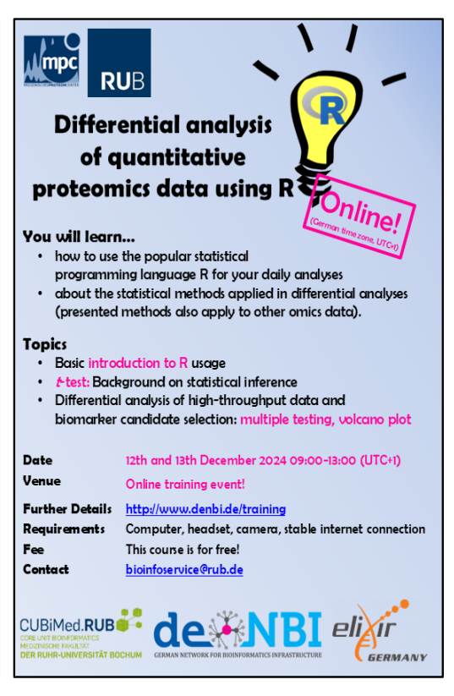
We calculated several own analysis projects in the de.NBI cloud. We advertise the cloud as free to use for German academic scientists.

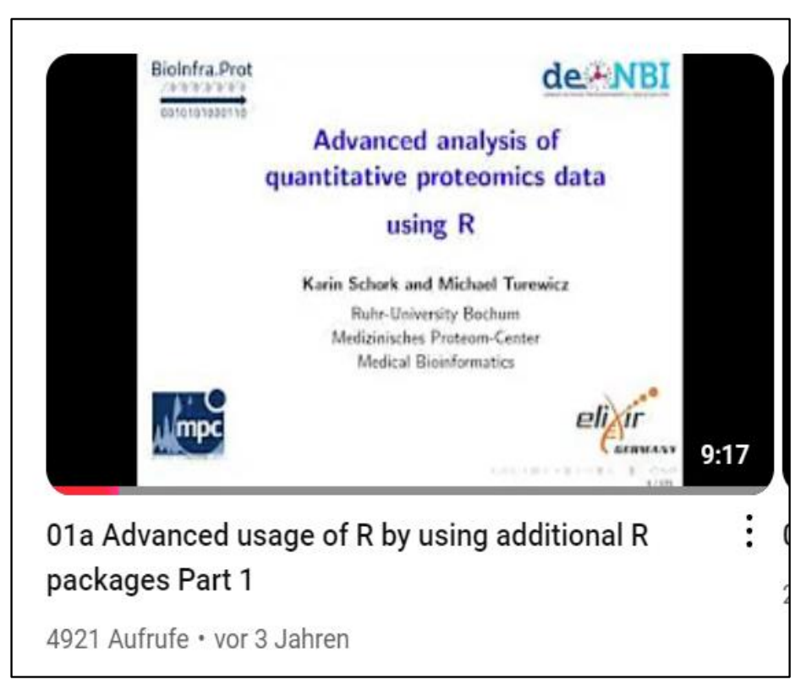
de.NBI **Training** and education

We proceeded with some trainings that were already established during the de.NBI-project and developed novel training concepts.

Additionally, our YouTube tutorials on R courses have garnered significant attention, accumulating up to 4,700 views over the past three years.

Date	Course title	Location	Users
28.09.2023	“Data Exploration with Python - The Young Researcher’s Toolkit"	Bielefeld	19
17.11.2023	“Data Exploration with Python - The Young Researcher’s Toolkit"	Bochum	9
09.09.2024	“Data Exploration with Python - The Young Researcher’s Toolkit"	Bochum	4
06.12.2024	“Data Exploration with Python - The Young Researcher’s Toolkit"	Bochum	4 registered
12-13.12.2024	“Differential analysis of quantitative proteomics data using R”	Bochum	> 30 registered





Publications

1) **Uszkoreit J**, Perez-Riverol Y, Eggers B, Marcus K, **Eisenacher M**. Protein Inference Using PIA Workflows and PSI Standard File Formats. J Proteome Res. 2019 Feb 1;18(2):741-747. doi: 10.1021/acs.jproteome.8b00723. Epub 2018 Dec 5. PMID: 30474983.
2) **Uszkoreit J**, **Winkelhardt D**, Barkovits K, Wulf M, Roocke S, Marcus K, **Eisenacher M**. MaCPepDB: A Database to Quickly Access All Tryptic Peptides of the UniProtKB. J Proteome Res. 2021 Apr 2;20(4):2145-2150. doi: 10.1021/acs.jproteome.0c00967. Epub 2021 Mar 16. PMID: 33724838.
3) **Kohl M**, **Stepath M**, Bracht T, Megger DA, Sitek B, Marcus K, **Eisenacher M**. CalibraCurve: A Tool for Calibration of Targeted MS-Based Measurements. Proteomics. 2020 Jun;20(11):e1900143. doi: 10.1002/pmic.201900143. Epub 2020 Mar 6. PMID: 32086983
4) Hardt R, Dehghani A, Schoor C, Gödderz M, Cengiz Winter N, Ahmadi S, Sharma R, **Schork K**, **Eisenacher M**, Gieselmann V, Winter D. Proteomic investigation of neural stem cell to oligodendrocyte precursor cell differentiation reveals phosphorylation-dependent Dclk1 processing. Cell Mol Life Sci. 2023 Aug 18;80(9):260. doi: 10.1007/s00018-023-04892-8. PMID: 37594553; PMCID: PMC10439241.
5) **Rozanova S**, **Uszkoreit J**, **Schork K**, Serschnitzki B, **Eisenacher M**, Tönges L, Barkovits-Boeddinghaus K, Marcus K. Quality Control-A Stepchild in Quantitative Proteomics: A Case Study for the Human CSF Proteome. Biomolecules. 2023 Mar 7;13(3):491. doi: 10.3390/biom13030491. PMID: 36979426; PMCID: PMC10046854.
6) Guntermann A, Fatoba O, Kronenberg M, Reinehr S, Grotegut P, Schargus M, Tsai T, Ivanova S, Serschnitzki B, Kumowski N, Maier C, Marcus K, Dick HB, Joachim SC, May C. Investigation of Inter- and Intra-Day Variability of Tear Fluid Regarding Flow Rate, Protein Concentration as well as Protein Composition. Invest Ophthalmol Vis Sci. 2023 Oct 3;64(13):13. doi: 10.1167/iovs.64.13.13. PMID: 37815507; PMCID: PMC10573576. **(BioInfra.Prot acknowledged)**
7) Köhler CU, **Schork K**, **Turewicz M**, **Eisenacher M**, Roghmann F, Noldus J, Marcus K, Brüning T, Käfferlein HU. Use of Multiple Machine Learning Approaches for Selecting Urothelial Cancer-Specific DNA Methylation Biomarkers in Urine. Int J Mol Sci. 2024 Jan 6;25(2):738. doi: 10.3390/ijms25020738. PMID: 38255812; PMCID: PMC10815677.

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung