

# LIFS3 Dresden

# Bioinformatics Services for Shotgun Lipidomics


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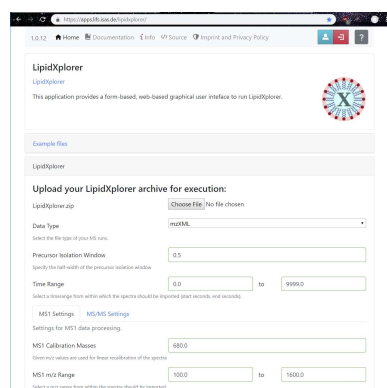
## Short description of the project

- We made the download and installation of LipidXplorer and Peakstrainer, simpler and easier by creating a single file installer.
- We also made LipidXplorer web accessible and reduce upload times by using PeakStrainer.
- Supplementary modules for calculating resolution curves, processing proprietary spectra and quantification based on lipid standards have been developed.
- Currently updates to the codebase show a substantial time performance improvement and facilitate streamlining the core functionality;
- lowering the barrier-to-entry of use of the software and making additional and modified functionality possible.
- LipidXplorer has been integrated into consortium software to calculate LUX score, and in lab tools for PUFA lipid quantification.
- A curated set of MFQL resources is being collected to provide users with a catalog of options for lipid identification.
- Python 3.X, linux and Dockers are available

## de.NBI services

 **LipidXplorer** is a tool for lipid identification by shotgun mass spectrometry, using the MFQL query language to specify the structural composition of the intact molecule as well as the fragments generated by MS/MS. This means that there is no database required for lipid identification (DOI 10.17617/1.47)  
Downloaded over 500 times, ca 200 in the last year, with multiple feature requests and bug fixes

 **PeakStrainer** is a tool to remove noise data from shotgun mass spectra, it is based on detecting the repetition of signals across multiple scans. In contrast to other approaches this maintains low intensity signals and only signals that are reproducible. Downloaded approximately 150 times, with some bugfixes and feature requests.



## Web service

- identifies *lipids of any class*
- works with *any mass spectrometer*
- supports *any shotgun experiment*
- identifies *unknown lipids*
- supports *high-throughput screens*

## General information on the project

One Post-doc position is paid from de.NBI grant  
Other staff involved: Kai Schuhmann, Henrik Thomas, Oskar Knittelfelder, Olga Vvedenskaya

## Progress report

Project runtime: November 2016 - October 2019

### Completed:

- Completion of Web version of LipidXplorer on LIFS servers
  - Release of LipidXplorer and PeakStrainer as single file installer, for easy installation.
- Source base is free and open source online.  
Example files and instructions available online.
- Integration of additional software and development of support applications, as well as Analysis and development of best practices for Lipidomics analysis of plasma
- Next Steps:** Testing and release of LipidXplorer 2.0 that performs faster and more transparent, configuration is automatically generated and results are visually verifiable. Where identification rules and warning can be encoded and molar quantification is supported.

## de.NBI Training and education

- SLAS 2018 Poster, San Diego, California, USA
- ASMS 2018 Poster, San Diego, California, USA
- 7th European Lipidomics Meeting 2018, Leipzig, Poster and Workshop
- Lipidomics Forum 2018 Dortmund Germany, Workshop
- Lipidomics workshop at DGMS, March 2019, Rostock, Germany
- e:Med summer school LipoSysMed, March 2019, Leipzig, Germany
- Lipidomics Forum 2019 LIFS workshop at, Borstel, Germany
- NASH Summit 2019 workshop at London UK

## Publications

- Intensity-Independent Noise Filtering in FT MS and FT MS/MS Spectra for Shotgun Lipidomics (DOI: 10.1021/acs.analchem.7b00794)
- Analytical challenges in human plasma lipidomics: A winding path towards the truth (DOI: 10.1021/acs.analchem.7b00794)
- Schuhmann, Kai, et al. "Quantitative Fragmentation Model for Bottom-Up Shotgun Lipidomics." *Analytical chemistry* 91.18 (2019): 12085-12093.
- Analytical challenges in human plasma lipidomics: A winding path towards the truth (DOI: 10.1016/j.trac.2018.10.013)
- Shotgun lipidomics-based characterization of the landscape of lipid metabolism in colorectal cancer (DOI: 10.1016/j.bbali.2019.158579)