

Lipidomics Data Pipeline (LDP)

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Contract Nr. W-de.NBI-006

Short description of the project

The LDP project focuses on further development and maintenance of software and resources that were created in the Lipidomics for Life Sciences (LIFS) network with our cooperation partners Robert Ahrends (University Vienna) and Andrej Shevchenko (MPI-CBG Dresden). Our focal points are:

a) streamlining and improvements of user experience of the established lipid identification and quantitation software pipeline for shotgun lipidomics consisting of **LipidXplorer** and **lxPostman**

b) contribute high quality datasets for the curation of **LipidCompass** and expand resource on verified **MFQL** libraires for shotgun lipidomics.

Vision:

Consolidate services that are supporting the community in LC - MSⁿ and shotgun based lipidomics approaches with the LIFS webportal as central entrie point to verified and user-friendly software.

Our service shall become a central hub for lipid related research and set standards in sustainable and user-friendly scientific software.

de.NBI services

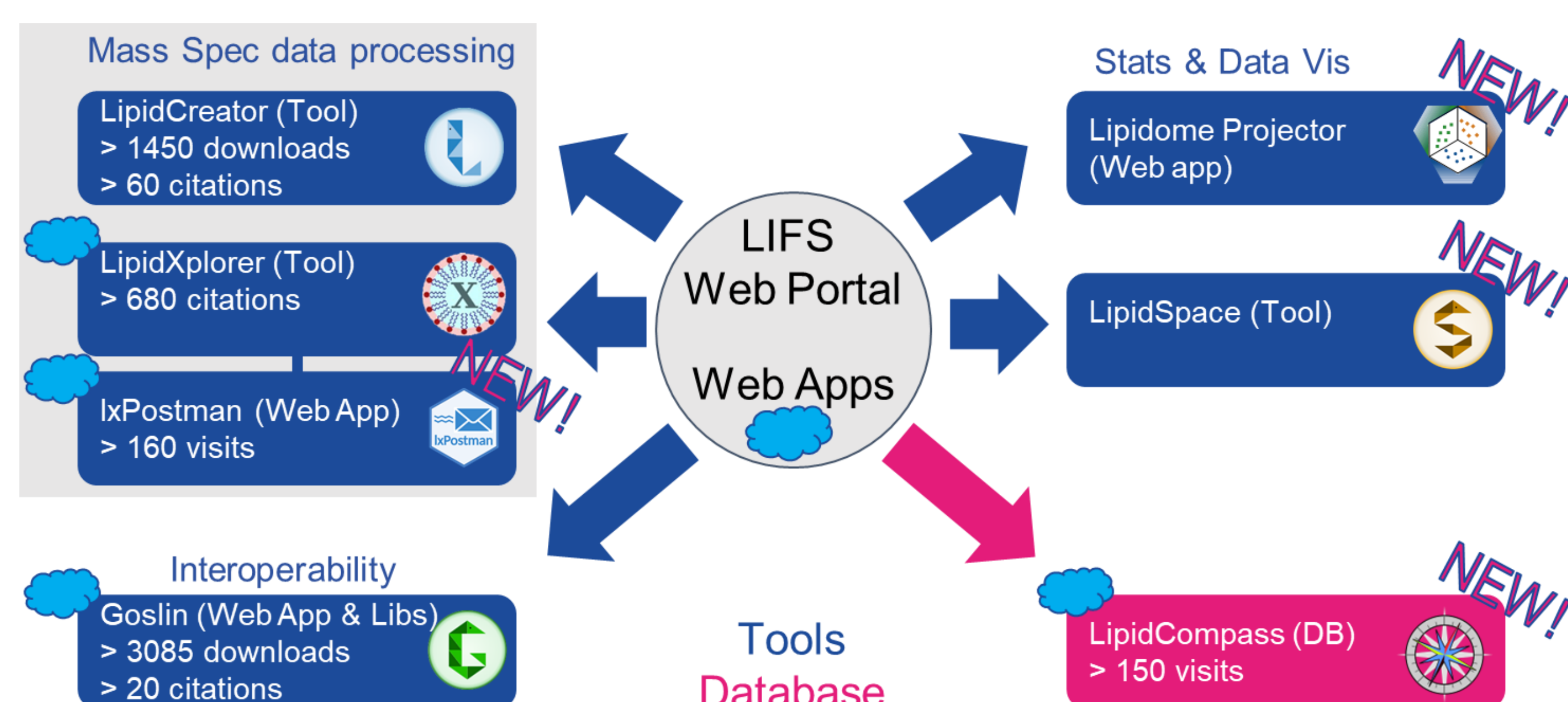


Table 1) Usage statistics of LDP services (Matomo).

Tool	2023		2024 (November, 15)		Citations (Web of Science)
	Visits	Pageviews	Visits	Pageviews	
Clover	6	10	1	1	NA
LIFS APPS	74	133	76	158	NA
LIFS Goslin Webapp	21.463	22.582	1.159	2.017	23
Goslin Sparql	0	0	1	2	NA
LIFS Webportal	662	1.857	753	2.172	NA
LipidCompass	205	1.711	160	1.477	NA
LipidCreator	1.343	2	1.449	0	63
Lipidomics Checklist	280	4	312	0	51
LipidSpace	105	0	3	0	2
LipidXplorer	78	2	67	1.719	681
LipidXplorer Wiki	366	1.02	268	731	NA
Lux Score	18	73	0	0	17
lxPostman	57	184	160	476	NA
MzTabValidator	292	706	277	1.103	50

General information on the project

- de.NBI staff:
 - Lukas Müller (2023 - 24, 0.5 FTE)
 - Timur Olzhabaev (2023 - 24, 0.5 FTE)
 - Wiebke Gauda (2024, RCB, 0.65 FTE)
- other staff:
 - Daniel Krause (alumni, RCB)
 - Nils Hoffmann (FZ-Jülich)
- from Feb. 2025: doctoral student identified (0.65 FTE)

Progress report

- Postprocessing software **lxPostman** was further developed and tested with complex data sets, made available for registered users on the LIFS webportal
- Contributed to implementation of **lipidomics minimal reporting** (3) checklist to standardize documentation of experimental studies and utilized software
- Prepared well described and published datasets for the **LipidCompass** database (1, 4)
- Contributed to novel approach for systematic comparison of lipidomes provided within the software **LipidSpace** (2)
- Performed maintenance and bug fixes on **LipidXplorer** with planned new release of version 1.2.9. in December 2024
- Expanded libraries of MFQL scripts for **LipidXplorer** for the lipidome of *M. tuberculosis* (doctoral project of Wiebke Gauda, inhouse financed doctoral student, – reference lipidome) and *S. pneumoniae* (Dissertation of Belal Alshaar – reference lipidome to be published)
- Designed novel approach and software package **Lipidome Projector** for visualization and basic comparison of lipidomes (5)
- Took part in the ILS - CLIG ring trial on plasma lipidomics to further evaluate our software pipeline in context of regulated analyses – data evaluation ongoing
- We had a long and intensive search in three rounds for doctoral student in the team. One promising candidate was interviewed on November 14, 2024. Planned start employment February 2025.

de.NBI Training and education



Organization of LIFS Hands On Course and Lipidomics Forum 2025 in Vienna

September 14th - 17th, 2025

- LIFS Workshops: 2023 - Vienna; 2024 - Borstel – Hands on training on software tools for lipidomics data analysis.
- Lipidomics Forum 2023 / 2024 member of organization team for conference series on lipidomics and related topics

Table 2) Details on LIFS Hands On Courses

Year	Participants	PI, PostDoc, Grad, Undergrad, non acad.	from Germany	International
2023	26	2, 9, 13, 0, 2	9	17
2024	18	2, 5, 7, 0, 4	13	5

Detailed feedback forms were collected with an overall positive response.

Publications

- Global analysis of putative phospholipases in *Plasmodium falciparum* reveals an essential role of the phosphoinositide-specific phospholipase C in parasite maturation.
Burda PC, Ramaprasad A, Bielfeld S, Pietsch E, Woitalla A, Söhnchen C, Singh MN, Strauss J, Sait A, Collinson LM, [Schwudke D](#), Blackman MJ, Gilberger TW.
mBio. 2023. doi: 10.1128/mbio.01413-23. PMID: 37489900 - **Dataset for LipidCompass**
- LipidSpace: Simple Exploration, Reanalysis, and Quality Control of Large-Scale Lipidomics Studies.
Kopczynski D, Ejlsing CS, McDonald JG, Bamba T, Baker ES, Bertrand-Michel J, Brügger B, Coman C, Ellis SR, Garrett TJ, Griffiths WJ, Guan XL, Han X, Höring M, Holčapek M, Hoffmann N, Huynh K, Lehmann R, Jones JW, Kaddurah-Daouk R, Köfeler HC, Meikle PJ, Metz TO, O'Donnell VB, Saigusa D, [Schwudke D](#), Shevchenko A, Torta F, Vizcaino JA, Welti R, Wenk MR, Wolrab D, Xia Y, Ekroos K, Ahrends R, Liebisch G.
J Lipid Res. 2024. doi: 10.1016/j.jlir.2024.100621. PMID: 39151590
- Glycerophospholipid remodeling is critical for orthoflavivirus infection.
Hehner J, Schneider L, Woitalla A, Ott B, Vu KCT, Schöbel A, Hain T, [Schwudke D](#), Herker E.*
Nat Commun. 2024. doi: 10.1038/s41467-024-52979-y. PMID: 39375358 - **Dataset for LipidCompass**
- Lipidome visualisation, comparison, and analysis in a vector space.
[Olzhabaev T](#), [Müller L](#), [Krause D](#), [Schwudke D](#),* Torda AE.* **preprint bioRxiv** 2024. doi: 10.1101/2024.08.02.606134
in review PLOS Computational Biology

underlined - LDP personal; * shared last authorships