

LIFS1 Lipidomics Informatics for Life Science

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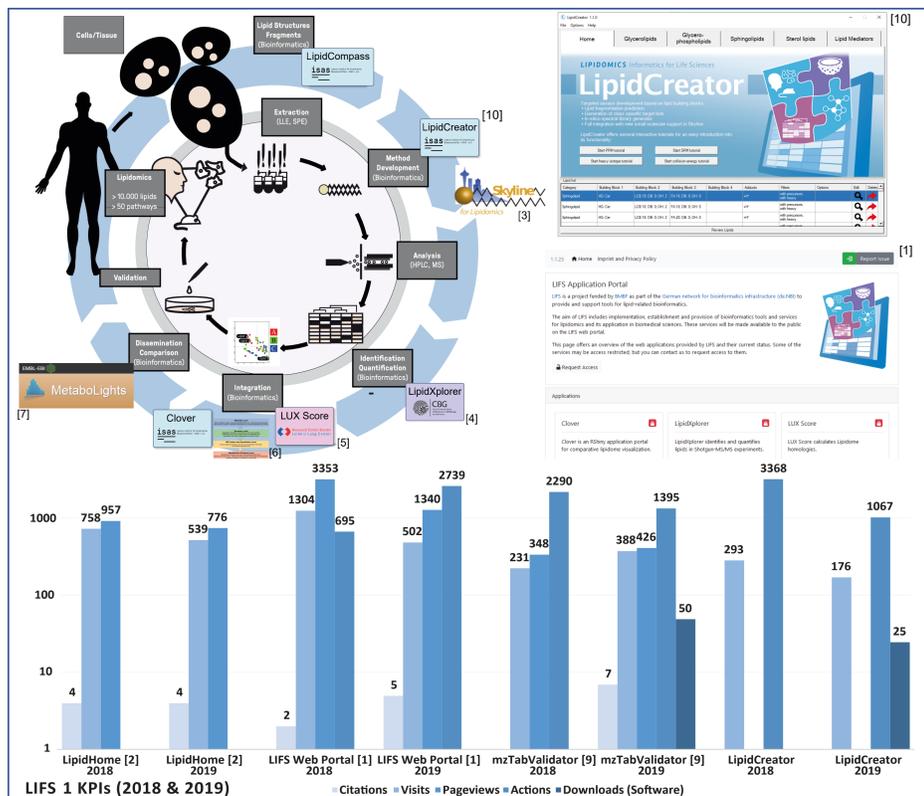
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Short description of the project

LIFS implements and provides bioinformatics for lipidomics services within one web portal, offers bioinformatics consulting services and organizes workshops and informatics courses as part of the de.NBI education activities [1,12].

LIFS1 provides integration with the tools *LipidXplorer*, *LipidCreator*, and *LUX Score* via the web portal and the exchange format *mzTab-M* and develops a new and redesigned database of theoretical lipids based on *Lipid-Home*. It further provides computational resources for the web-based services of the LIFS partners, as well as technical systems for support and collaboration, building, testing, and deployment of these services.

de.NBI services



General information on the project

LIFS 1, ISAS Dortmund:
PostDoc Position (1FTE)
funded by de.NBI
Other staff:
2x PostDoc (0.25 FTE each)
2x PhD Student (0.25 FTE each)

Seattle, USA:
Brian Pratt (Developer)
Brendan MacLean (Coordinator)

Hinxton, UK:
Kenneth Haug
Claire O'Donovan (PI)

ISAS Dortmund: LIFS 1
Nils Hoffmann (PostDoc)
Robert Ahrends (PI) (Vienna)
Albert Sickmann

RU Bochum: BioInfra.Prot
Martin Eisenacher (PI)

FZ Borstel: LIFS 2
Fadi Al Machot (PostDoc)
Dominik Schwudke (PI)

MPI-CBG Dresden: LIFS 3
Jacobina Miranda Ackerman (PostDoc)
Andrej Shevchenko (PI)

Progress report

Completed:

- LIFS web application portal with LUX Score, LipidXplorer, Clover, Ix Postman, PaLiNom and mzTab Validator web application [9] available since September 2018, continued updates, ~50 registered users.
- Platelet Lipidome publication [8] (data comparison and visualization)
- Reference implementations of mzTab-M [6, 9, 11].
- LipidCreator & Skyline, LipidCreator available as plugin from Skyline Tool Store [10].
- Backend of LipidCompass running internally, first data imports.
- Support of mzTab-M in LDA2, GNPS, MS-DIAL (external of LIFS).

Next Steps:

- mzTab-M support in LipidXplorer, Skyline, LUX Score, Clover, IxPostman to simplify exchange of result data and import into LipidCompass.
- Testing phase and release of LipidCompass (LipidHome + LIPID-DB).
- Make web applications available via de.NBI Cloud.
- Integration of mzTab-M data import from MetaboLights.
- Extend international lipidomics standardization efforts [13].

de.NBI Training and education

- 2018:**
- LIFS software and pipelines workshop at Lipidomics Forum, Nov. 2018, Dortmund, Germany (20 applicants, 19 participants)
- 2019:**
- Lipidomics workshop at DGMS, March 2019, Rostock, Germany (6 applicants, 6 participants)
 - e:Med summer school LipoSysMed, March 2019, Leipzig, Germany (25 applicants, 19 participants)
 - LIFS MS Data Processing & LIFS Statistical Analysis workshops at Lipidomics Forum, Nov. 2019, Borstel, Germany (13 & 6 applicants, 13 & 6 participants)

Publications

- D. Schwudke *et al.*, "Lipidomics informatics for life-science", *Journal of Biotechnology*, Aug. 2017.
- J. M. Foster *et al.*, "LipidHome: A Database of Theoretical Lipids Optimized for High Throughput Mass Spectrometry Lipidomics", *PLOS ONE*, vol. 8, no. 5, p. e61951, May 2013.
- B. Peng *et al.*, "Adaptation of Skyline for Targeted Lipidomics", *Journal of Proteome Research*, vol. 15, no. 1, pp. 291-301, Jan. 2016.
- R. Herzog *et al.*, "LipidXplorer: A Software for Consensual Cross-Platform Lipidomics", *PLOS ONE*, vol. 7, no. 1, p. e29851, Jan. 2012.
- C. Marella, A. E. Torda, and D. Schwudke, "The LUX Score: A Metric for Lipidome Homology", *PLOS Computational Biology*, vol. 11, no. 9, p. e1004511, Sep. 2015.
- N. Hoffmann *et al.*, "mzTab-M: a data standard for sharing quantitative results in mass spectrometry metabolomics", *Analytical Chemistry*, vol. 91, no. 5, pp. 3302-3310, Jan. 2019.
- K. Haug *et al.*, "MetaboLights-an open-access general-purpose repository for metabolomics studies and associated metadata", *Nucleic Acids Research*, vol. 41, no. D1, pp. D781-D786, Jan. 2013.
- B. Peng *et al.*, "Identification of key lipids critical for platelet activation by comprehensive analysis of the platelet lipidome", *Blood*, vol. 132, no. 5, pp. e1-e12, Aug. 2018.
- N. Hoffmann *et al.*, "jmxTab-M: A Reference Parser, Writer, and Validator for the Proteomics Standards Initiative mzTab 2.0 Metabolomics Standard", *Analytical Chemistry*, vol. 91, no. 20, pp. 12615-12618, Sep. 2019.
- Peng *et al.*, "LipidCreator: A workbench to probe the lipidomic landscape", submitted, 2020.
- J. Stanstrup *et al.*, "The metaBonomics toolbox in Bioconductor and beyond", *Metabolites*, vol. 9, no. 200, Sep. 2019.
- D. Wibberg *et al.*, "The de.NBI / ELIXIR-DE training platform - Bioinformatics training in Germany and across Europe within ELIXIR", *F1000 Research*, vol. 8, p. 1877, Nov. 2019.
- LSI Consortium, "Lipidomics needs more standardization", *Nature Metabolism*, vol. 1, pp. 745-747, Jul. 2019.