



LIFS2 Systematic Lipidome Comparisons

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Short description of the project

LIFS2 implements algorithms for systematic lipidome comparison, scoring of lipid identifications and supports the integration of database services for lipidometers.

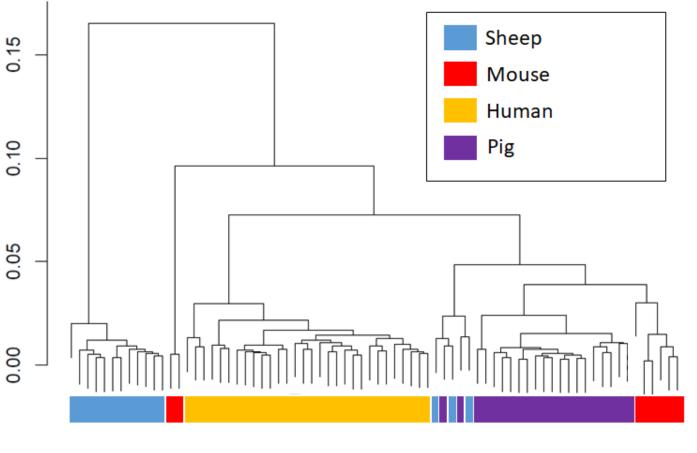
Progress report

		ID Validation	Data Interpretation
Shotgun	Import Speed	Quantitation	Lipidome
Lipidomics	Noise Reduction	Output Formats	Homology



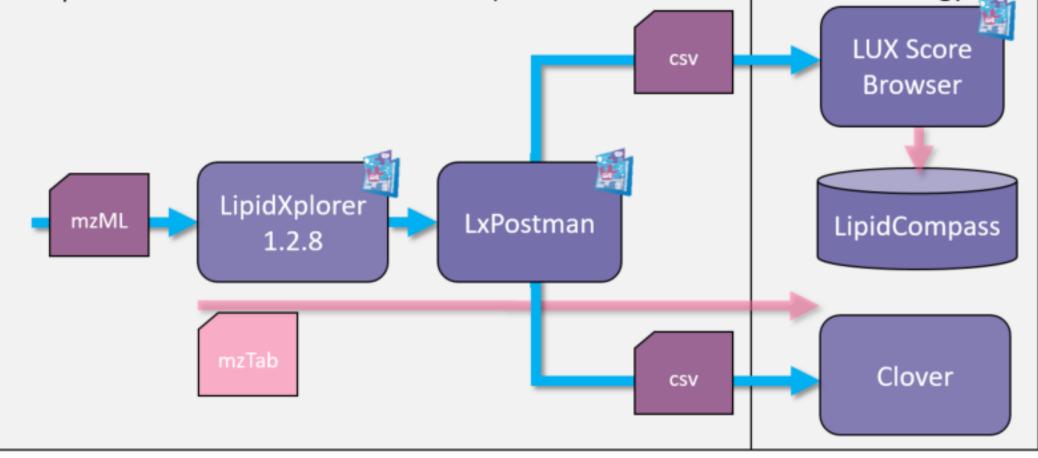
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Work Packages	6	12	18	24	30	36	42	48	54	60
WP 1 Lipidomics Software			•				•			
Implementation of data filters and converters										
Services for raw data conversion to LIFS format										
Optimization of data conversion algorithms										
Implementation of LUX score pipeline as web application										
WP 2 LIFS Web Portal										
Integration of LUX score browser										
Implementation of Scorelip on the LIFS portal										
WP 3 LIFS Reference DB										
Integration of Scorelip and LUX score into LIFS DB										
WP 4 LIFS Training and Education										
Workshops DGMS, Lipidomics Forum, Summer Schools										
Development of tutorials for LUX score and Scorelip										
WP 5 LIFS after extension										
Backend integration of LUX Score in LIPIDCOMPASS										
Reference lung lipidomes published										
Integration of data validation processes IxPostman										
Implementation of mzTab format										

LUX Score based homology analysis between lung lipidomes of different and long lipidomes and human.



m/z,m/z

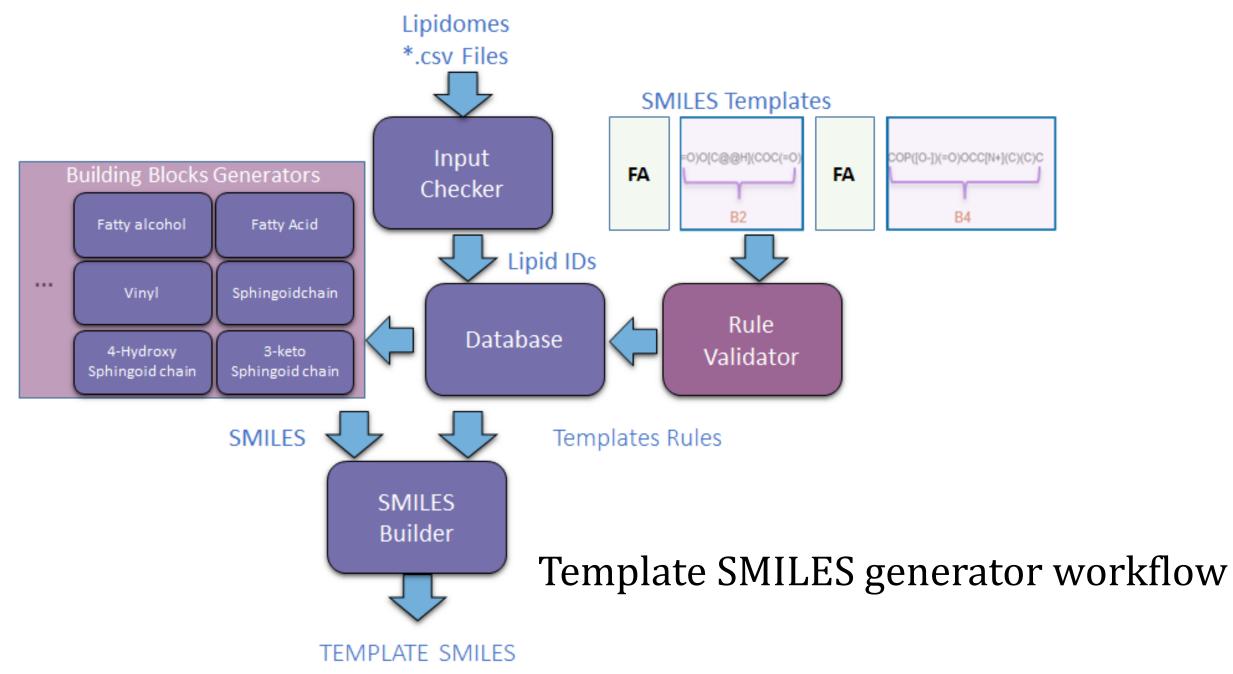


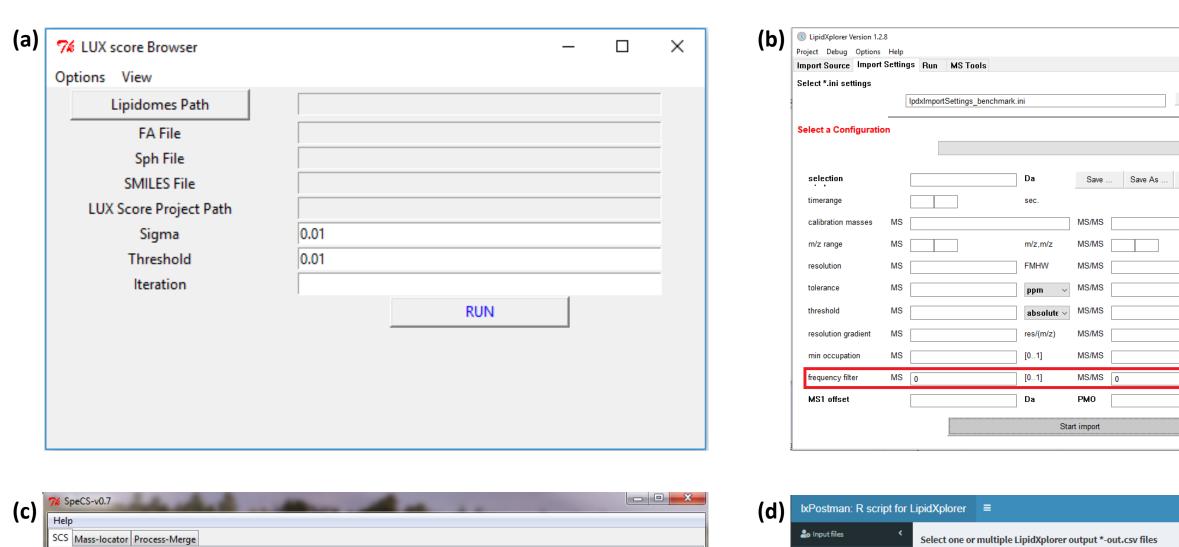


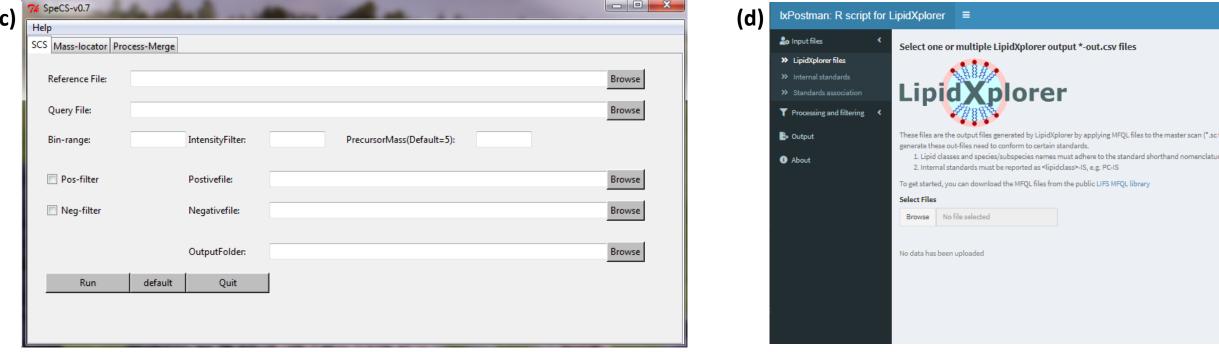
Shotgun Lipidomics workflow from start to finish of the LIFS consortia. Implementation of mzTab as unified reporting standard is on the way. LIFS2 () contribution.

<u>Performance indicators for LUX score web application</u>

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	<u>Period</u>	<u>Visits</u>	Visit Duration (s)	<u>Views</u>	<u>Actions</u>	<u>Actions per Visit</u>	<u>Tickets</u>	Reg. Users	<u>Downloads</u>
	2018	208	504	484	6938	33,36	1	23	2
	2019	284	598	553	20575	72.2	2	53	3







- a) LUX Score Browser: Fully implemented Template SMILES generator
- b) LipidXplorer 1.2.8: Improved import module and implemented frequency filters for MS and MS/MS.
- c) SpeCS: The spectral comparison score (SCS) algorithm provides a welldefined quality control approach for PRM based quantitation of lipid mediators

Next Steps:

- Integration of chemical space model and Template-SMILES in LIPIDCOMPASS for generalized lipidome homology
- Integration of automated data validators to improve user interaction
- Publication of in-depth homology analyses for lung lipidomes of mouse, pig, sheep and human with association to physiology
- Implementation of mzTab format as general exchange format of LIFS

de.NBI Training and education



Deutsche Gesellschaft für Massenspektrometrie



Publications

Summer school (LipoSysMed): Integration of Large Scale Lipidomics Data in Systems Medicine Research 22 March 2019, Center of Biotechnology and Biomedicine (BBZ), Leipzig, Germany

Workshop: Bioinformatics for Lipidomics

50th Annual meeting of the German Society for Mass Spectrometry (DGMS)

 d) IxPostman: a post-processing tool for LipidXplorer that enables quality control of lipid identification, automated quantification and formatting of results

General information on the project

- de.NBI funded postdoctoral researcher (1 FTE) <u>Staff paid from additional resources:</u>
- postdoctoral researcher (0.25 FTE)
- PhD student (0.25 FTE)
- Technician (0.25 FTE)

5. March 2017, Kiel (25 participants)

Workshop: Lipidomics Forum

12 November 2017, Borstel (20 participants)11 November 2018, Dortmund (19 participants)10 November 2019, Borstel (18 participants)

- 1) Eggers et al. Lipidomes of lung cancer and tumour-free lung tissues reveal distinct molecular signatures for cancer differentiation, age, inflammation, and pulmonary emphysema. Scientific Reports (2017)
- 2) Schwudke et al. *Lipidomics informatics for life-science*. J Biotechnol. (2017)
- 3) Wutkowski et al. Software-aided quality control of parallel reaction monitoring based quantitation of lipid mediators. Analytica Chimica Acta (2018)
- 4) Eggers et al. *Shotgun Lipidomics Approach for Clinical Samples.* Clinical Metabolomics. Methods in Molecular Biology (2018)

