LIFS2 Systematic Lipidome Comparisons

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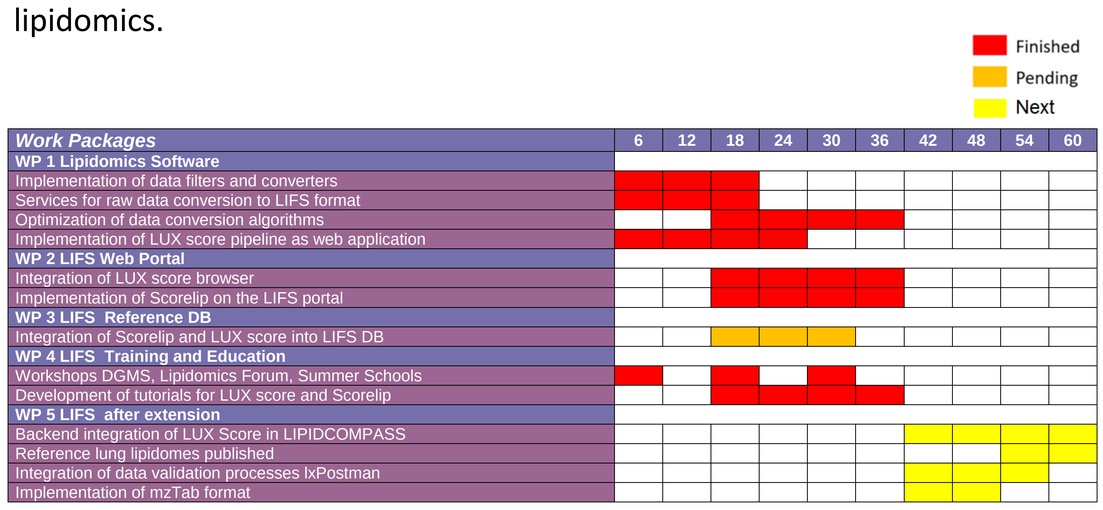
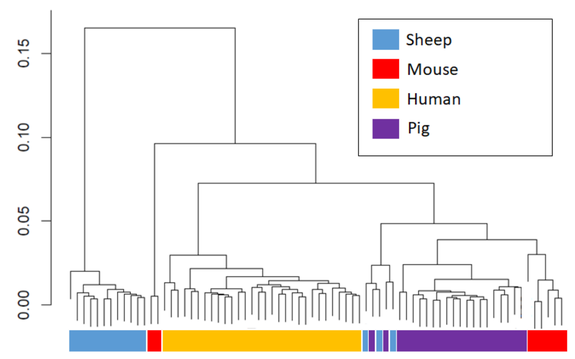
Short description of the project

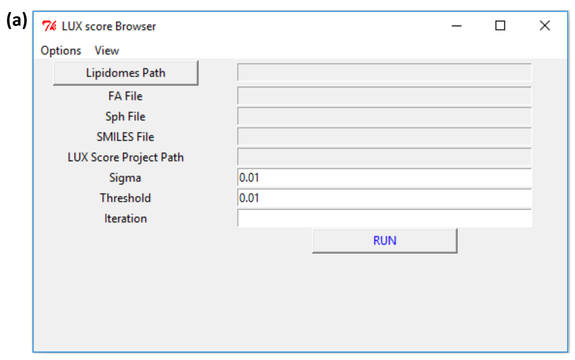
LIFS2 implements algorithms for systematic lipidome comparison, scoring of lipid identifications and supports the integration of database services for lipidomics.

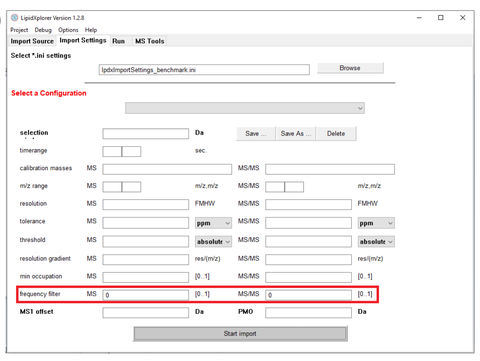


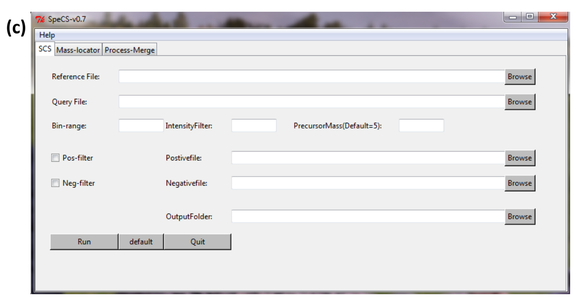
LUX Score based homology analysis between lung lipidomes of different model organisms and human.

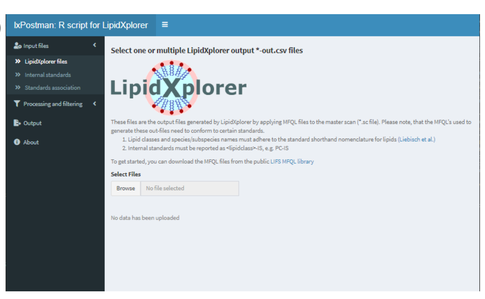


de.NBI Services









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 well-defined quality control approach for PRM based quantitation of lipid mediators
d) lxPostman: a post-processing tool for LipidXplorer that enables quality control of lipid identification, automated quantification and formatting of results

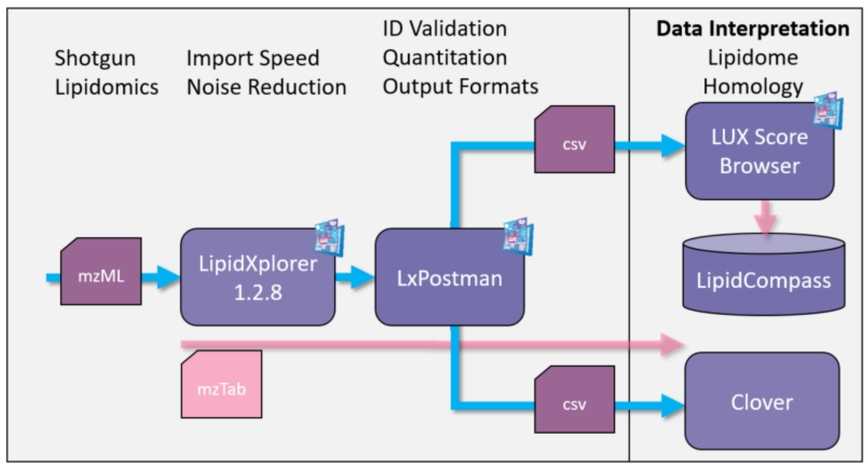
General information on the project

- 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)

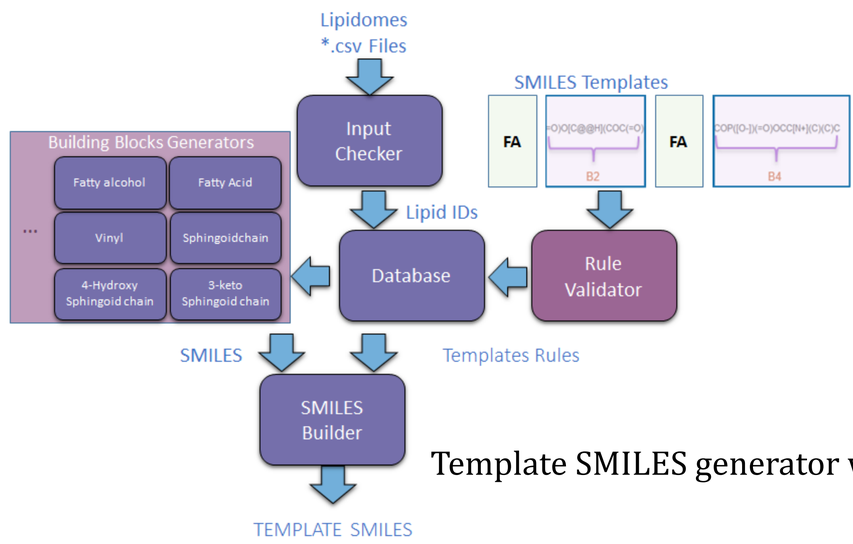
Progress report



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>

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



Template SMILES generator workflow

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

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)
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)

Publications

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)