Workshop on Digital Bioeconomy: Convergence towards a bio-based society



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## **Open Source Tools and FAIR Data Formats for Mass Spectrometry Lipidomics**

Tuesday 20 February 2024 10:45 (1 hour)

The Lipidomics Informatics for Life Science (LIFS) consortium, part of the German Network for Bioinformatics Infrastructure (de.NBI), pioneers advancements in lipidomics workflows through the development of a comprehensive suite of tools.

LipidCreator facilitates targeted LC-MS/MS assay generation and seamlessly integrates with Skyline for method file generation and data processing on state-of-the-art mass spectrometers from major vendors. LipidXplorer enables vendor-agnostic processing of untargeted, shotgun lipidomics data, allowing users to define custom lipid fragment patterns and rules using the mass spectrometry fragment query language (MFQL). Goslin is a polyglot grammar-based parsing and conversion library, harmonizing and mapping different lipid nomenclatures to the latest endorsed by LIPID MAPS and the lipidomics standards initiative (LSI). Finally, LUX Score, extended by LIFS, and its successor, LipidSpace, offer qualitative lipidome comparisons and similarity calculations. LipidSpace further facilitates interactive quantitative comparison of lipidomes on matching structural hierarchy levels, serving as an effective tool for post-hoc analysis, comparison, and visualization of published lipidomics data.

Collaborating with HUPO-PSI MS, we introduced mzTab-M, a tabular reporting format now widely supported by metabolomics and lipidomics tools and repositories. Simultaneously, we are standardizing the mzQC data format to capture typical and user-defined QC metrics for mass spectrometry experiments in proteomics, metabolomics, and lipidomics.

In summary, the LIFS consortium's comprehensive suite of tools, including LipidCreator, LipidXplorer, Goslin, LUX Score, and LipidSpace, empowers high-throughput, quantitative lipidomics. Our commitment to FAIR data principles ensures seamless data handling, submission, and integration, furthering the accessibility and interoperability of lipidomics research.

## Consent

Yes

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