



SimLipid 4.20

Opis produktu

SimLipid?

A comprehensive high throughput informatics tool for characterizing lipids using precursors and product ions data from MS and MS/MS data

Lipidomics is an emerging field of systems biology being applied to disease research, drug discovery and biomarker identification. Mass spectrometry is one of the most sophisticated technologies for identification and quantification of lipids from biological mixtures. However, the major challenge in mass spectrometric data analysis is the huge amount of data generated in the process. Some of the most important aspects of mass spectrometric lipidome data analysis are the high throughput quantitative analysis of crude lipid extracts and structural identification of lipids using precursor and product ion data.

The structural analysis of lipid molecular species has been challenging owing to their diversity and quantity, complicating lipid identification. Analyzing complex lipid extracts from biological sources and obtaining a lipid profile provides information on the changes in lipid species composition as a result of a change in biological condition such as stimulation by receptor activator, progress of a disease or comparison between normal and transformed cell. Due to the technical limitations in characterizing lipids, the characterization of the complete lipidome of a cell or tissue is very challenging.

SimLipid? is a high throughput lipid identification and quantification

software. It analyzes hundreds of lipid MS, MS/MS and MS^E scans for structural elucidation, correction of experimental peak intensities (for their isotopic overlaps) and quantification of profiled lipids by specifying internal standards. The program facilitates specification of endogenous/exogenous lipids as internal standards. The program accepts experimental MS and MS/MS (m/z and intensity values) obtained by mass spectrometry in text, MS Excel, mzData, mzXML, Waters Corporation MS^E, DDA and direct infusion data, Bruker Corporation native files (*.fid, *.baf and *.yep), AB SCIEX binary files (*.t2d and *.wiff), Thermo Scientific? native file format (*.raw) and Agilent's Compound Exchange File (*.cef). The software enables lipid identification and profiling by searching precursors against the known lipid structures available in SimLipid? database. Additional information such as lipid ID, lipid abbreviation, systematic name, composition and other database links are also made available for easy reference.

