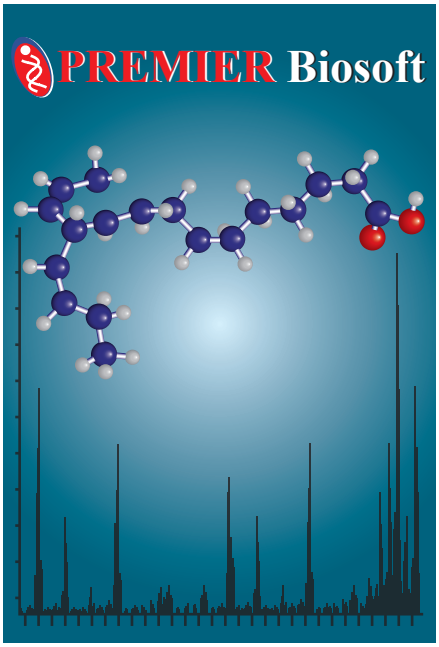
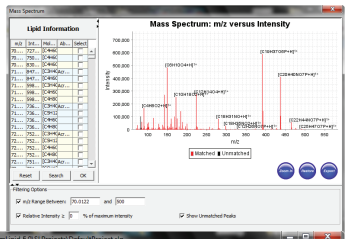


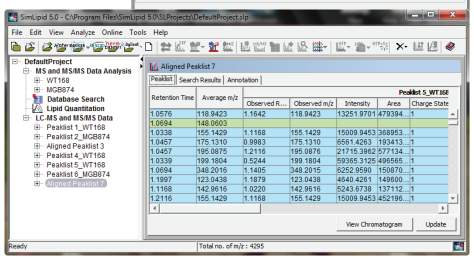
SimLipid®

High throughput lipid characterization tool for data from MS^E, TripleTOF, MALDI TOF/TOF, LC-MS, LC-MS/MS systems

Enterprise Edition Available

SimLipid is a comprehensive lipidome data analysis software, enabling users to identify lipids using LC and MALDI- MS, MS/MS & MS^E data, remove isotopic overlapping of peaks from multiple spectra in batch mode. SimLipid accepts experimental MS data (m/z and intensity values) in text, MS Excel, mzData, mzXML, Waters Corporation MS^E, DDA and direct infusion data, Bruker Corporation (.fid, .baf and .yep), SCIEX (*.t2d and *.wiff) and Thermo Scientific™ (.raw) and Agilent's Compound Exchange File (.cef).





High Throughput MS and MS/MS Data Analysis

SimLipid supports high throughput MS data (precursor m/z) search for Carnitines, Fatty acyls, Glycerolipids, Glycerophospholipids, Polyketides, Prenols, Saccharolipids, Sphingolipids and Sterols. The profiled lipids can further be verified using MS/MS product ions. SimLipid supports comprehensive structure specific characteristic ions from Carnitines, Fatty acyls, Glycerolipids, Glycerophospholipids, Prenols, Saccharolipids, Sphingolipids and Sterols.

Users can load data from 500,000 MS, MS/MS and MS^E scans in a single project and analyze up to 10000 spectra in batch mode. High Resolution Accurate Mass (HRAM) data with error tolerance between 0.1- 50 ppm can be analyzed, improving the accuracy of prediction. The results are sorted based on an innovating ranking algorithm that maps the degree of proximity of theoretical lipids with experimental data.

High Throughput Lipid Profiling and Quantitation

SimLipid enables quantification of analyte lipids present in biological samples based on internal standards. To enable data analysis from low resolution spectra, SimLipid corrects the intensities for isotopic overlaps for different lipid species. This facilitates accurate quantification of lipids from biological mixtures.

LC-MS and LC-MS/ MS High Throughput Data Processing

SimLipid can process up to 200 LC-MS and MS/MS raw data files to generate peaklists in a single run. It performs:

- Peak detection and peak picking.
- Separation of isomeric compounds that are eluted under single peaks.
- Identification of isotope clusters and ion species, selection correct precursor m/z for MS/MS scans.
- Align the peaks detected from different LC-MS runs using the RANSAC and Gale-Shapely (SMP) techniques.
- Overlay of extracted ion chromatograms from different samples facilitates comparative and quantitative analysis.
- Export results to HTML, CSV and MS Excel formats.

Note: Users do not need to perform LC-MS and MS/MS data processing for Agilent's Compound Exchange Files (.cef) as these already contains peaklist generated by Mass Hunter Qualitative Analysis Software.

Automatic Interpretation of MS and MS/MS Spectra

SimLipid annotates peaks observed in the MS and MS/MS spectra with the chemical composition of the identified lipids or fragments. The annotated mass spectra can be exported as image files in JPEG and PNG formats, facilitating information sharing amongst research groups.

Mass Spectrometry Workflows: *SimLipid supports analysis of MALDI, LC-MS and MS/MS besides product ions from UPLC-MS^E lipid data.*

Database Strength: *36,299 lipid species along with their additional information such as lipid structure, abbreviation, systematic name, mass, composition and links to the other databases.*

MS/MS Lipid Characteristic Ions: *Comprehensive structure specific diagnostic ions for Carnitines, Fatty acyls, Glycerophospholipids, Glycerolipids, Prenols, Sterols, Saccharolipids and Sphingolipids.*

LC-MS and LC-MS/MS *data processing methods.*

Intuitive GUI to Visualize and Review Data Analysis Results: *Sort MS & MS/MS spectra, compound list on the basis of precursor Ion m/z, charge, retention time, intensity and drift time besides naming a profile with the name of the identified lipid.*

Portable Reports: *Export data analysis results customized according to research needs into HTML/CSV/XLS formats.*

To activate & evaluate, follow these steps
- Install SimLipid from our website or the CD
- Launch the program and click 'Activate' on the first window
- Enter the 'Registration Number' requested from us and your e-mail address. Click 'Next'
- Update the registration information following the on-screen prompts and click 'Submit'

For a quick start
- Check the Multimedia Tutorial

Order on-line
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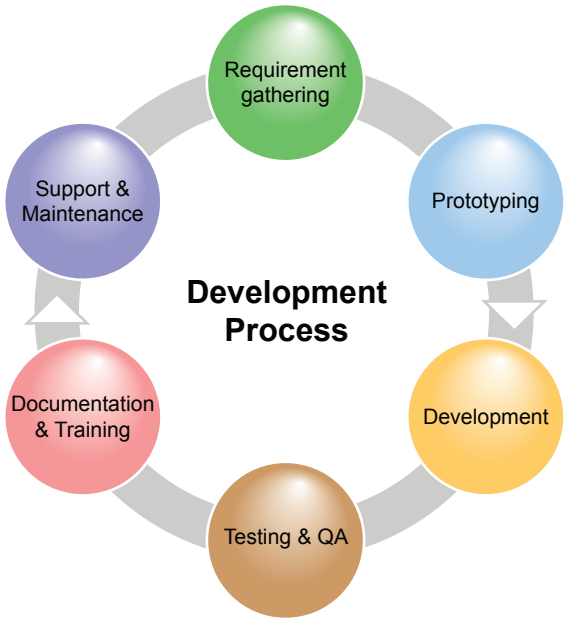

AlleleID®	A comprehensive tool designed to address the challenges of species identification & taxa discrimination using qPCR, xMAP® and microarrays. (for Win & Mac)
Array Designer	For fast and efficient design of specific oligos for whole genome arrays, tiling arrays and resequencing arrays. (for Win & Linux)
Beacon Designer™	Design specific and efficient oligos for all major qPCR assays. (for Win & Mac)
LAMP Designer	Design primers for Loop-mediated Isothermal Amplification. (for Win)
MALDIVision	A comprehensive data processing & visualization tool for MALDI IMS data. (for Win)
MLPA® Designer	A comprehensive tool co-developed with MRC-Holland to design highly specific oligos for MLPA assays. (for Win & Mac)
PrimerPleX	A multiplex PCR primer design tool. (for Win & Mac)
Primer Premier	A comprehensive primer design tool for standard PCR assays. (for Win and Mac)
PROTEOIQ	Right from validation to quantification, a powerful software that supports the entire proteomic data analysis pipeline. (for Win & Mac)
SimGlycan®	High throughput glycan & glycopeptide identification tool for data from TripleTOF, MALDI TOF/TOF, LC-MS/MS systems. (for Win)
SimLipid®	High throughput lipid characterization tool for data from Triple TOF, MALDI TOF/TOF, LC-MS, LC-MS/MS systems. (for Win)
SimMet®	A robust high throughput informatics software for qualitative and quantitative analysis of mass spectrometry metabolite data. (for Win)
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Xpression Primer	A novel tagged primer design tool for expression cloning and for designing sequencing primers to verify transcripts. (for Win & Mac)

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