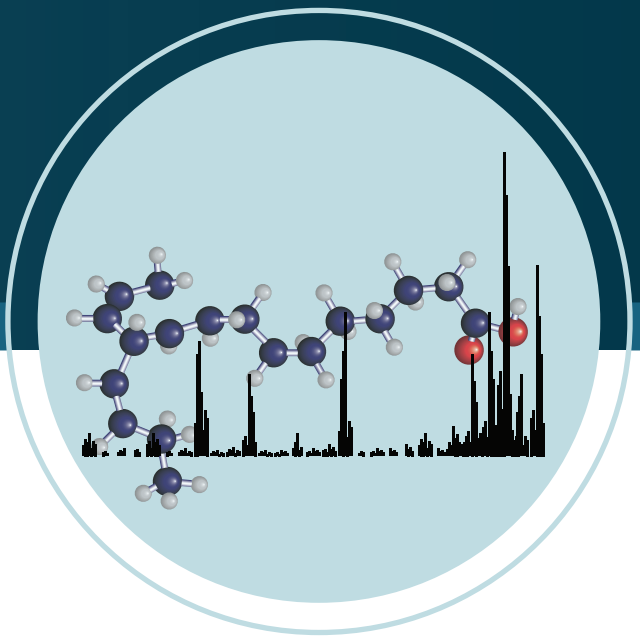
PREMIER Biosoft

# SimLipid®

## High throughput lipid identification and quantitation tool using data from LC-, MALDI-, and Shotgun-Mass Spectrometry workflows



SimLipid® Software is a high throughput mass spectrometric lipid data analysis software which identifies and quantifies lipid species from LC-, MALDI-, ESI-, Precursor Ion scan, and Neutral Loss Scan- MS data. It supports all data types from Triple Quad, qTOF, TOF, QqTOF, Ion Mobility, ITMS systems from all the major mass spectrometry manufacturing vendors and aims to provide a full solution for discovery and target lipidomics research.

The program accepts raw data in:

- **Vendor-specific native data file formats –** *.raw (Waters Corporation), *.lcd (Shimadzu Corporation), *.fid, *.baf and *.yep (Bruker Daltonics), *.wiff, and *.t2d (SCIEX), *.raw (Thermo Scientific™), and *.cef (Agilent Technologies)

- **Standard data file formats namely –** text, MS Excel, mzData, and mzXML

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The software enables identification of lipid species through searching of a proprietary and carefully curated database of precursor and fragment ion masses, retention times (optional), and drift times (optional). SimLipid® Software implements three separate workflows namely,

**1. MS and MS/MS Data Analysis:** You can perform direct database search for lipid identification using ESI-, MALDI- MS, and MS/MS data. The complete raw data from an experimental MS run- total ion chromatogram, Mass spectrum -, identified lipids, and their corresponding database information are displayed in a single workbench.

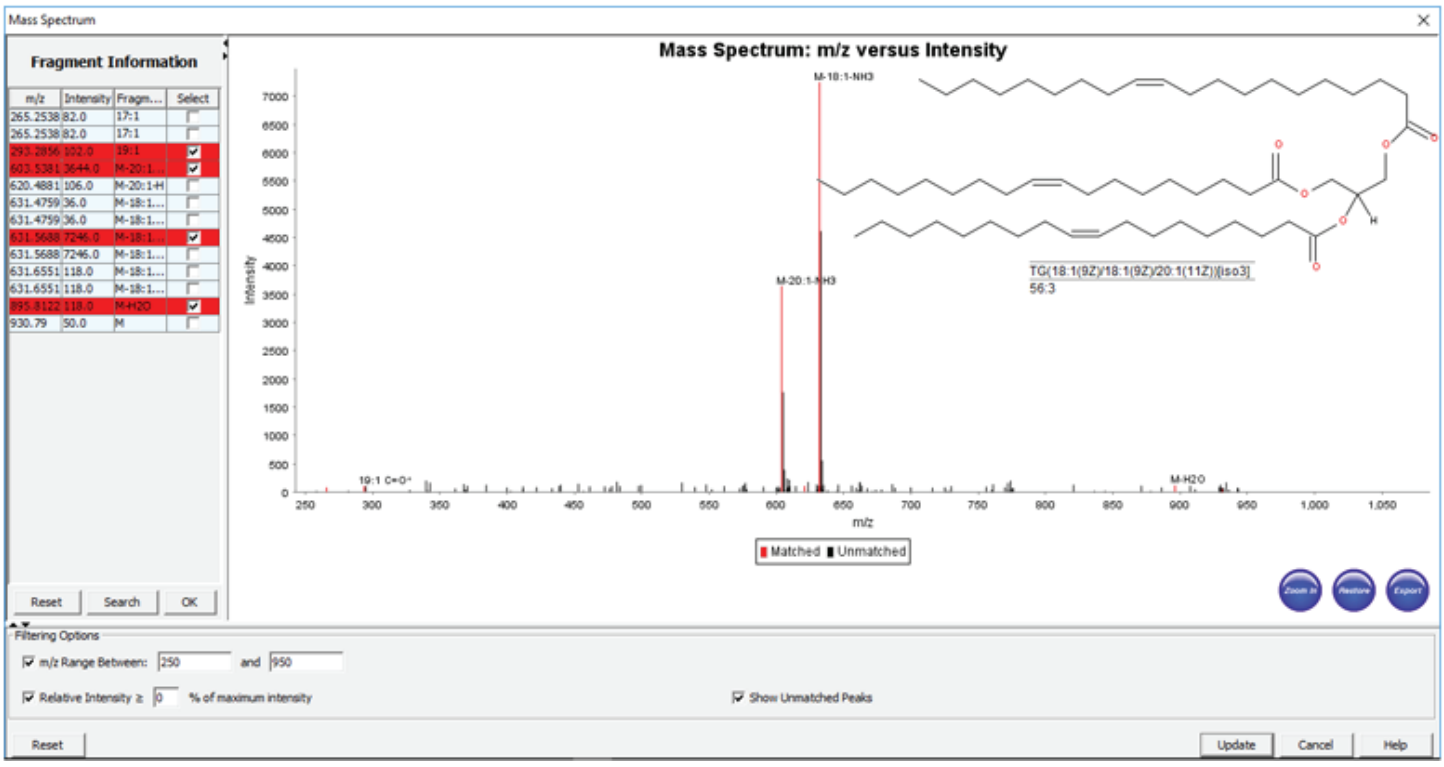


*Figure 1: Typical graphical user interface of SimLipid software: Annotated MS/MS spectrum of the identified lipid TG(56:3). The two most intense observed peaks in the spectrum correspond to the characteristic ions of the unique fatty acid chains 18:1, and 20:1 respectively of the structure*

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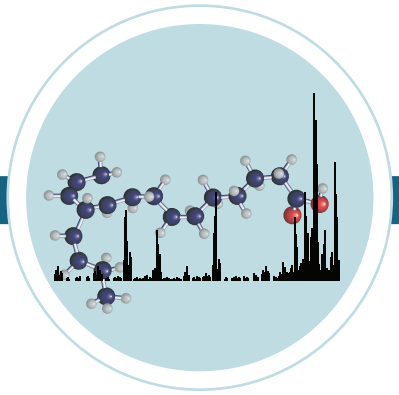

**2. Differential Analysis:** Automated LC-MS data processing for peak detection, peak picking, molecular feature finding, lipid species identification, retention time alignment across experimental LC-MS runs. Differential lipids across biological samples are identified using statistics such as fold change and p-value from ANOVA, and t-test.

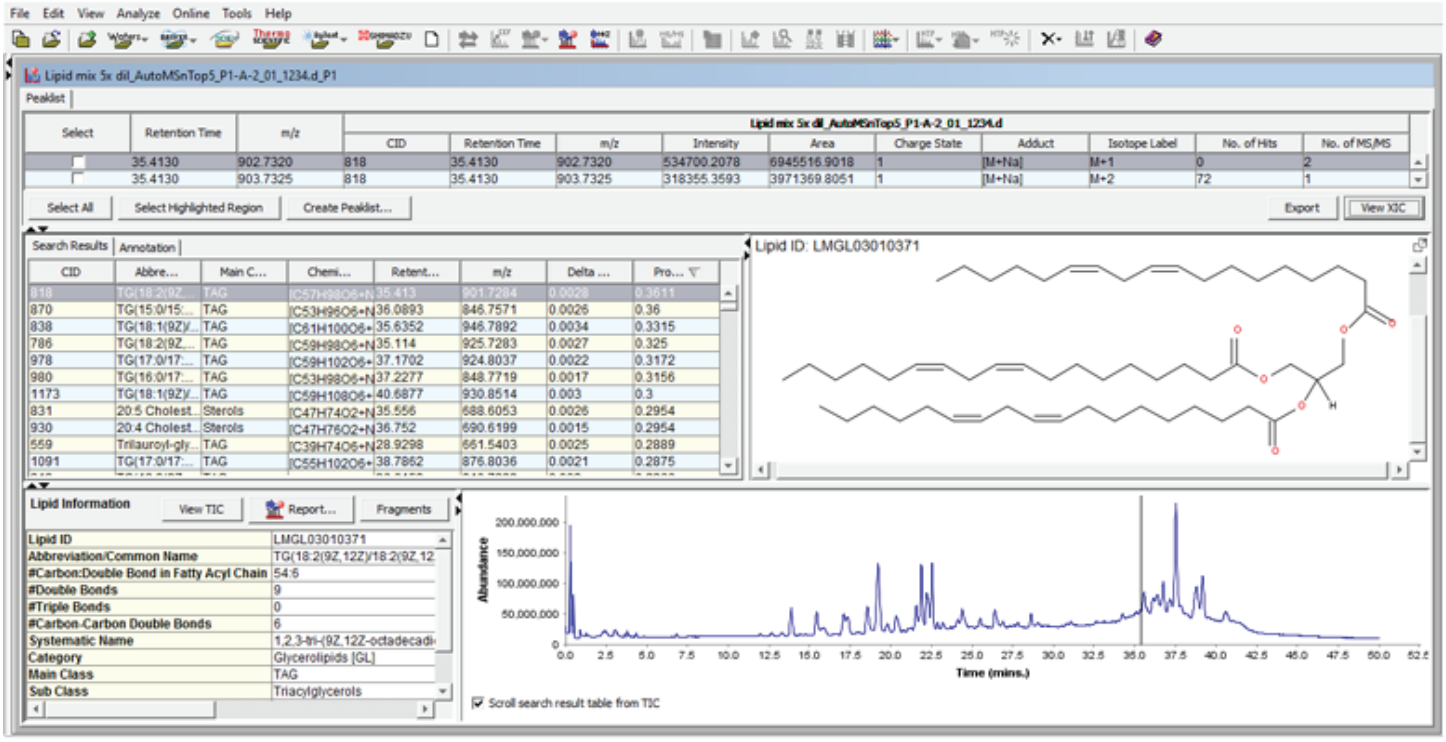


*Figure 2: Typical graphical user interface of SimLipid software: A single workbench view of LC-MS peaklist, list of identified lipids at retention time points, structure of a lipid at a selected retention time point, and chromatogram of the sample with a vertical line indicating the retention time point of the displayed lipid structure*

**3. Lipid Quantitation:** An automated data processing workflow to model experimental design, obtain lipid species identification using precursor ion/neutral loss target masses, correct isotope overlapping of species (with m/z values within error tolerance of peaks in their isotopic clusters), perform multiple internal standards-based quantification and align identified lipids across biological samples.

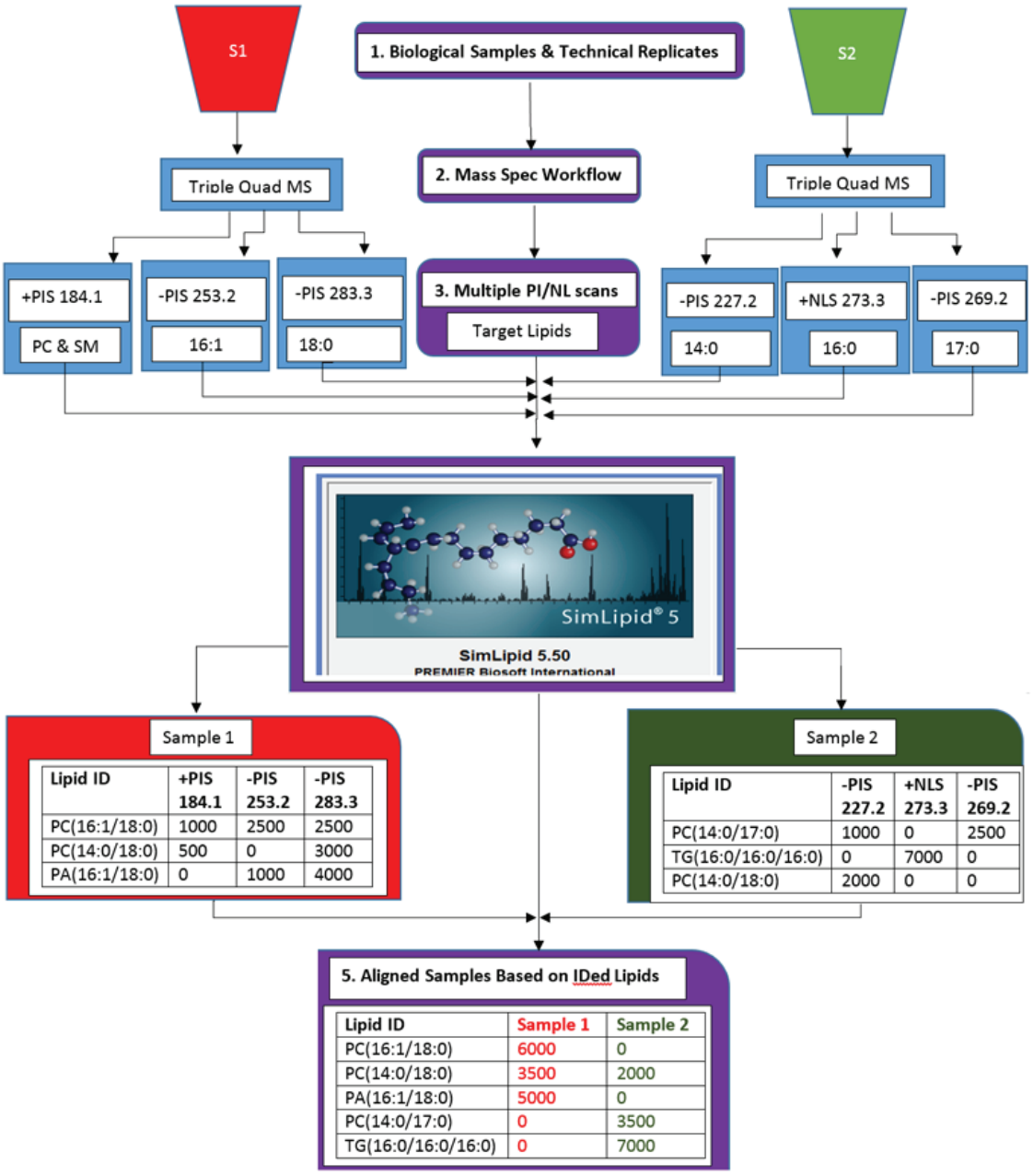


*Figure 3: Schematic representation of the lipid profiling and quantitation workflow of SimLipid software using data from MPIS/NLS QqQ MS method*

**Portable Reports:** Export data analysis results to customized reports in HTML/CSV/XLS formats for sharing information with colleagues or publishing data.