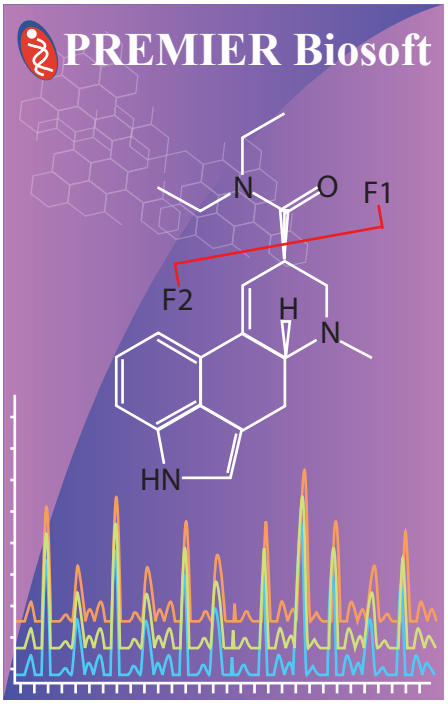
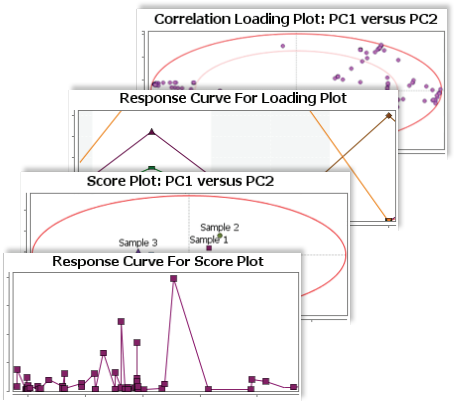


SimMet®

A comprehensive software suite for mass spectrometry metabolite data analysis that facilitates LC-MS data processing, metabolite identification, quantification and statistical analysis

SimMet® processes LC-MS data for peak detection, peak picking and retention time alignment. It enables users to identify metabolites using MS and MS/MS data in batch mode. Besides quantitative data analysis of identified metabolites, it facilitates differential analysis of metabolites across biological samples.



Single Platform for All Your Analysis

SimMet's comprehensive platform eliminates the need of managing and using multiple tools for metabolite research. All the metabolite data analysis, right from LC-MS data processing and subsequent peak identification to statistical analyses such as Principal Component Analysis is available in a single workspace. Loading Plots and Score Plots coupled with Confidence Ellipses (Correlation Loadings and Hotelling's T^2 ellipses) are supported to help researchers in understanding the relationship between metabolites and samples. Metabolite response curves are also provided to display the change in abundance of metabolites in different samples.

Manage Large Data Easily

SimMet® is engineered to handle massive volumes of data effectively which are typical of mass spectrometry based metabolomics workflows. Users can load two million scans in a single project as well as export analysis results of 50,000 scans at a time. All standard vendor formats are supported to seamlessly integrate qualitative and quantitative workflow solutions.

SimMet supports 2,34,284 MS/MS spectra for 9,345 metabolites and 354 adducts from NIST MS/MS database.

Accurate identification of metabolites by matching observed MS/MS spectra against standard MS/MS spectra of metabolites.

Annotated mass spectra with the identified metabolites and their fragment ions.

Sorting of the peak lists on the basis of Precursor Ion m/z, Charge State, Retention Time, Intensity, Drift Time, Probability Score & Pattern Score facilitates convenient investigation of data scattered across different scans or profiles.

Enables high throughput metabolite identification for 10,000 MS & MS/MS spectra in a single run.

Supports LC-MS & LC-MS/MS high throughput data processing methods such as peak detection, smoothing, chromatogram deconvolution, peak alignment, peak deisotoping & adduct identification.

Enables differential metabolomics via Principal Component Analysis (PCA) with 2D plots viz. Scores plot & Loadings plot supported along with Confidence Ellipses to pinpoint probable biomarkers.

Intuitive graphical interpretation of metabolite profiles using pie & bar charts.

Comparative analysis of metabolite profiles across samples using frequency tables.

Predicts amount of analyte for the samples using regression line fitted for the plots.

Mirror plot showing Observed Vs Standard spectra of the identified metabolites.

Comprehensive report by combining MS metabolite profile & its complementary MS/MS metabolite profiles in HTML/ CSV/ XLS formats for sharing information with colleagues.

To activate & evaluate, follow these steps
- Install SimMet® 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

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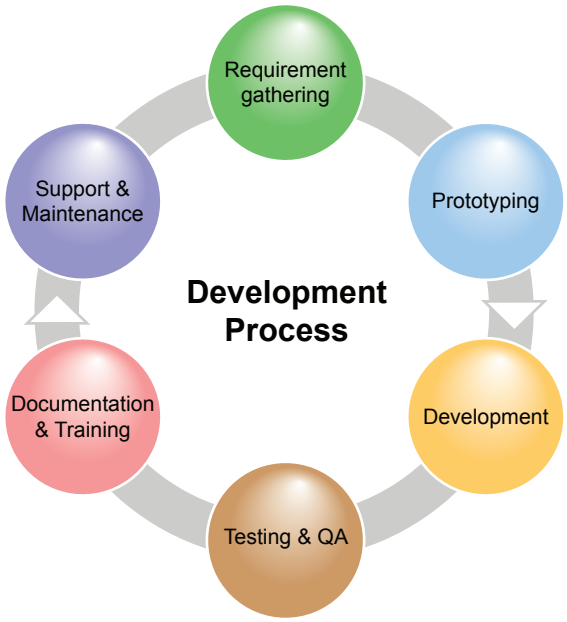

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Array Designer	For fast and efficient design of specific oligos for whole genome arrays, tiling arrays and resequencing arrays. (for Win & Linux)
Beacon Designer™	Design specific and efficient oligos for all major qPCR assays. (for Win & Mac)
LAMP 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)
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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)
SimVector	A tool for drawing publication, vector catalog quality maps & designing cloning experiments. (for Win & Mac)
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