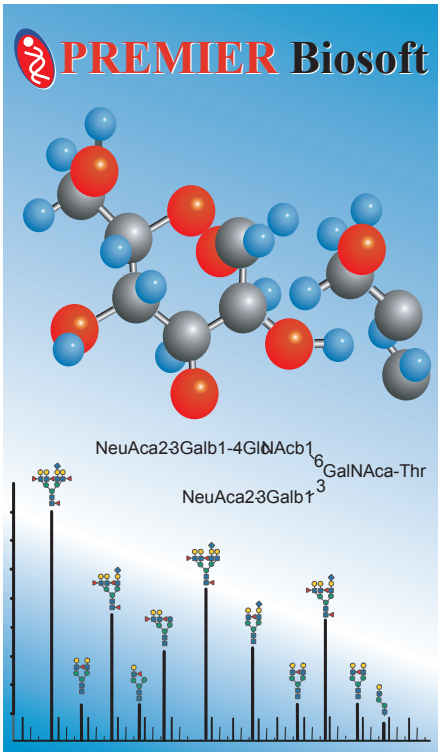
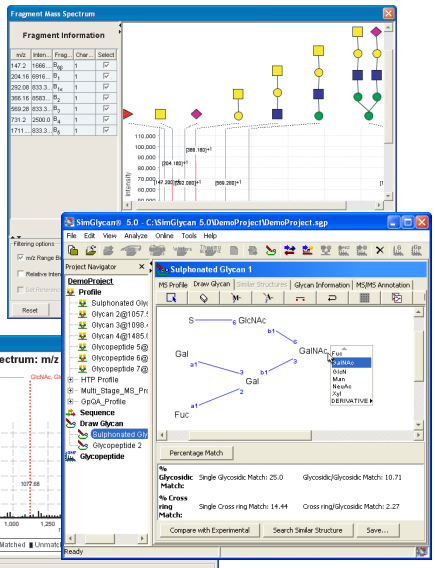


SimGlycan®

High throughput glycan & glycopeptide identification tool using mass spectrometry data

Enterprise Edition Available



SimGlycan® predicts structure of glycans from the MS/MS and multi-stage mass spectrometry (MS^n) data. Furthermore, comprehensive support for resolving glycopeptides using LC-MS/MS glycopeptide data facilitates glycosylation studies. SimGlycan® accepts experimental MS/MS data, matches them with its own database and finally generate a list of ranked candidate structures. Rank of each candidate indicates the proximity between the candidate structure and the experimental glycan. The rank is calculated based on a robust scoring mechanism that considers structure specific diagnostic ions observed in the experimental MS/MS spectra as well as the intensity of those observed peaks. SimGlycan® also supports multistage mass spectrometry (MS^n) data analysis for isomers differentiation.

LC-MS and LC-MS/MS Data Processing

SimGlycan® can read LC-MS data from .raw (Thermo ScientificTM), .baf, .yep, .fid (Bruker Corporation), .mzData and .mzXML files to generate LC-MS compound list for 100 raw data files in a single run. Users can import peaklists from Agilent's compound exchange files (CEF).The program automatically deconvolutes isomeric compounds that coelute. It identifies isotope clusters that enable accurate selection of precursor m/z values for MS/MS scans that were acquired for non-monoisotopic peaks. The peaks detected are aligned based on the agreement of retention time, m/z value, observed intensity and charge state. Glycan and glycopeptide identification results can be exported to HTML, CSV, MS Excel and CEF formats.

Glycan Quantitation

SimGlycan® now supports mass spectrometry-based quantitative glycomics workflow using aminoxyTMT™ reagents. Glycans are quantified by measuring reporter ion peak intensities from the corresponding MS/MS spectra. The oxyTMT reporter ion signals are adjusted to account for isotopic impurities in each TMT variant. Users can select the sum/average/median reporter ion intensities across all glycan-spectral matches as the quantity of a glycan. Various charts such as bar chart, cluster dot-plot etc. are plotted to facilitate visualization of glycan quantities in different TMT channels.

Robust Database

SimGlycan® database is a large relational database containing 9,165 glycans, 22,814 glycoproteins*, 6,027 glycans with known biological sources and 5,874 glycans with known classes. The database is continuously updated as information on additional glycans is published.

**The glycoproteins have been curated from The UniProt Consortium.*

UniProt: a hub for protein information; Nucleic Acids Res. 43: D204-D212 (2015)

Annotated Spectra

SimGlycan® facilitates automated interpretation of MS/MS and MS^n spectra. The program highlights the experimental peaks that match those of theoretical fragments and annotate the peaks using symbols or Domon-Costello fragment nomenclature. Successive loss of either carbohydrate residues or antennae of a glycan can be annotated between peaks in the spectra. The annotated spectra can be exported as image files for sharing the findings with your colleagues.

Supports MS/MS and MS^n dglycopeptide and released glycan data analysis.

Supports LC-MS and MS/MS data processing methods such as Peak detection, chromatogram deconvolution, precursor m/z selection and peak alignment.

Support for High Resolution Accurate (HRAM) data with an error tolerance of up to 0.1 ppm.

Support of H, Li, Na, Mg^{2+}, K, $HCOO^-$ and NH_4^+ adducts and their combinations.

Compatible with mass spectrometers from

- *AB SCIEX (TripleTOF™ 5600 System,TOF/TOF 5800, 4800 Plus MALDI TOF/TOF™ Analyzer, 4000 QTRAP® and QSTAR® Elite Systems).*
- *Bruker Corporation (ultrafleXtreme™ MALDI TOF/TOF, ultraflex™ MALDI TOF/TOF, autoflex™ TOF & TOF/TOF, maXis™ UHR-TOF, micrOTOF™, micrOTOF-Q™, solariX™ q-FTMS & amaZon™ ion trap series).*
- *Thermo ScientificTM (LTQ FT Ultra, LTQb Velos Dual-Pressure Ion Trap, LTQ XL Linear Ion Trap, LTQ Orbitrap Discovery, LTQ Orbitrap Velos, LTQ Orbitrap XL, LTQ Orbitrap XL ETD, MALDI LTQ Orbitrap).*
- *Waters Corporation (SYNAPT G2 HDMS, SYNAPT G2 MS, Xevo G2 QTof, Xevo QTof MS, Xevo TQ MS and Xevo TQ-S platforms).*
- *Agilent Technologies(6200 Series LC/TOF and the 6500 Series LC/Q-TOF).*

Supports .txt, .xls and mzXML & mzData files.

Fully annotated 2D glycan structure view along with their glycosidic and cross ring fragments.

Exports results in an html, spreadsheet or as a tab delimited file and generates a formatted report.

Generates comprehensive report that can include search results from 20,000 MS/MS spectra.

To activate & evaluate, follow these steps

- Install SimGlycan® 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

- E-mail: sales@premierbiosoft.com
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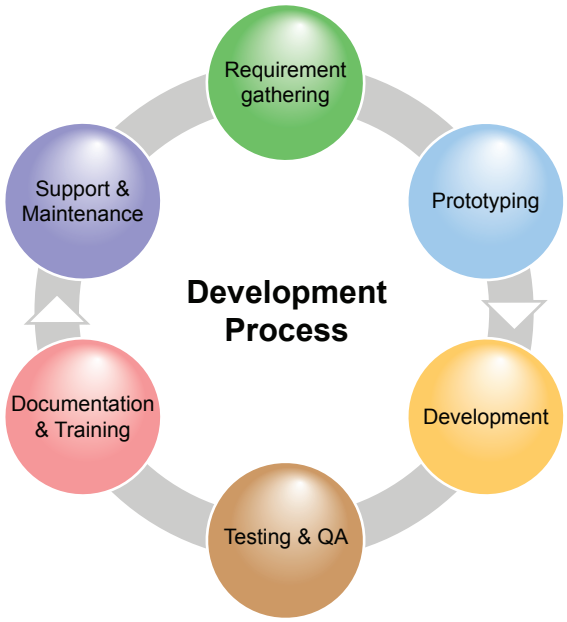

AlleleID®	A comprehensive tool designed to address the challenges of species identification & taxa discrimination using qPCR, xMAP® and microarrays. (for Win & Mac)
Array Designer	For fast and efficient design of specific oligos for whole genome arrays, tiling arrays and resequencing arrays. (for Win & 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)
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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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