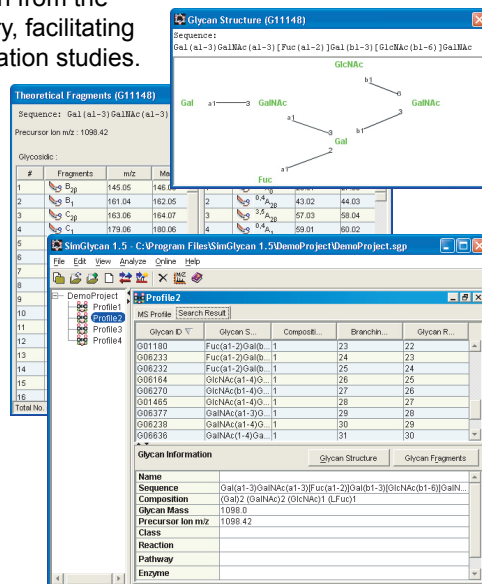


SimGlycan

An Innovative Tool for Glycan Mass Fingerprinting

SimGlycan predicts the structure of a glycan from the MS/MS data acquired by mass spectrometry, facilitating glycosylation and post translational modification studies.

SimGlycan accepts the experimental MS profiles generated by a mass spectrometer, matches them with its own database of over 7,000 glycans and generates a list of probable glycan structures. Each structure is scored to help you judge which results closely match your experimental data. Other biological information for the probable glycan structure such as the glycan class, reaction, pathway and enzyme are displayed. This helps you easily access all published information related to the glycan without referring to multiple sources.



Predict the glycan structure accurately using a comprehensive database of over 7000 glycans and 26 monosaccharides

Continuous updates to the database as additional glycan information is published.

Ranked list of probable glycans

Automatic retrieval of glycan information including biological source, class, enzyme, pathway and other database links

Fully annotated 2D glycan structure view

View glycosidic and cross ring fragments along with their mass and m/z values

Easily manage projects, associating results with input profile and search parameters

Theoretical fragments generated using standard Domon and Costello nomenclature

Terms and definitions specified in the Standard IUPAC guidelines are used

Export results in an html, spreadsheet or tab delimited file.

Generate an attractively formatted report for your lab notebook

Robust Glycan Database

The SimGlycan database is a large relational database populated with fragments of known glycan structures made up of 26 different monosaccharides. Every glycan in the database is fragmented for each of the possible thirty four reaction conditions using an intensive fragmentation algorithm. This ensures that the probable glycan fragments reported are comprehensive and accurate.

The SimGlycan database currently contains 8087 glycans, 7526 biological sources, 3418 glycan compositions, 5336 glycan classes, 196 biochemical reactions, 148 biochemical pathways, 177 glycan related enzymes and 7234 other database links. The database is continuously updated as information on additional glycans is published.

Comprehensive Analysis

SimGlycan accepts the experimental m/z and the intensity values of a glycan generated from a mass spectrometer and allows the user complete control to set experimental conditions that were used while generating the spectra. These conditions include precursor ion error, precursor ion m/z, spectrum peak m/z error, glycan derivatization, ion mode and the adduct.

Accurate Glycan Ranking

All possible glycan structures are ranked and scored based on our proprietary search and scoring mechanism. The ranking mechanism is based on calculating the glycan score which is a numerical representation of how closely the experimental mass of the glycan is to the mass of the glycans included in the database. The glycans that have the same mass are then ranked in decreasing order of their intensities.

Activate the program following these steps:

- Install and launch SimGlycan from the CD
- Click **Evaluate** on the first window that opens.
- Enter the evaluation key requested from us

Learn to use SimGlycan

- Multimedia tutorial is included on the CD

Order on-line

- E-mail: sales@PremierBiosoft.com
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