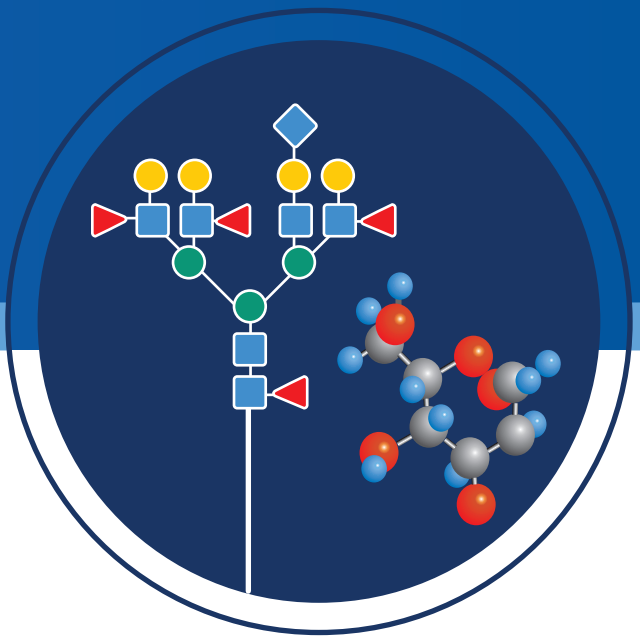
PREMIER Biosoft

SimGlycan®

A high-throughput glycan and glycopeptide data analysis tool for LC-, MALDI-, ESI- Mass Spectrometry workflows



SimGlycan software processes and interprets the MS/MS and higher multi-stage/sequential (MS^n) data generated by LC-, MALDI-, ESI- Mass Spectrometry based glycomics and glycopeptide workflows. The software automatically matches experimental mass spectra against a comprehensive database and generates a scored list of candidate structures.

In addition to the built-in master database of over 9000 unique glycan structures, you can also create custom databases storing curated glycans from different biological sources. The glycan structures can be stored along with retention times and other chromatographic details. The retention times, biological source, fragment information etc. can later be used as search predicates for glycan identification.**

The program accepts raw data in:

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

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

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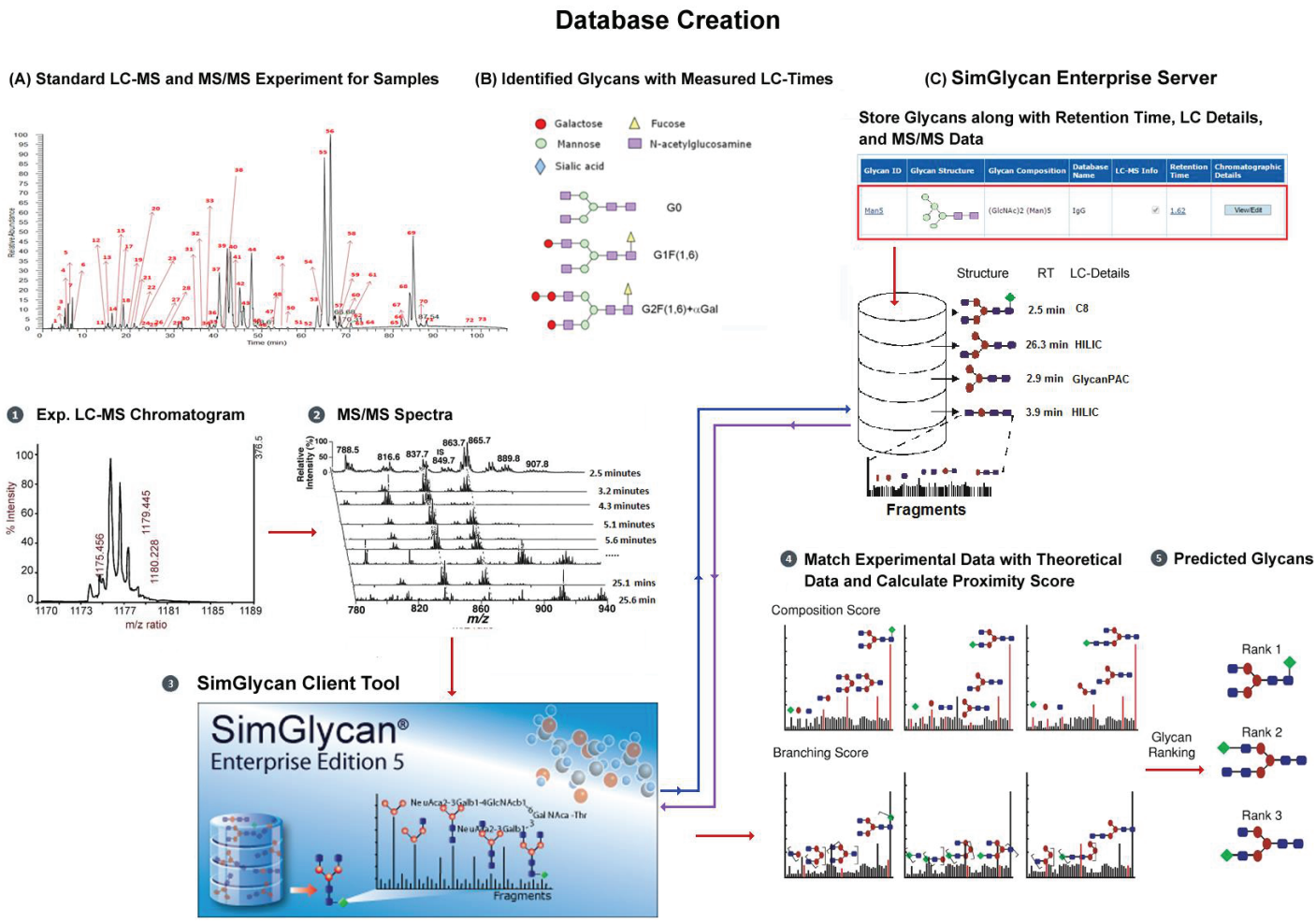

Figure 1: Schematic representation of glycan and glycopeptide data analysis workflow using SimGlycan

SALIENT FEATURES

1. LC-MS Data Processing: A fast and efficient algorithm performs peak detection, feature finding, and accurate precursor m/z selection for MS/MS data, making LC-MS glycomic data analysis – from structural identification to relative quantitation - simple, quick, and efficient.

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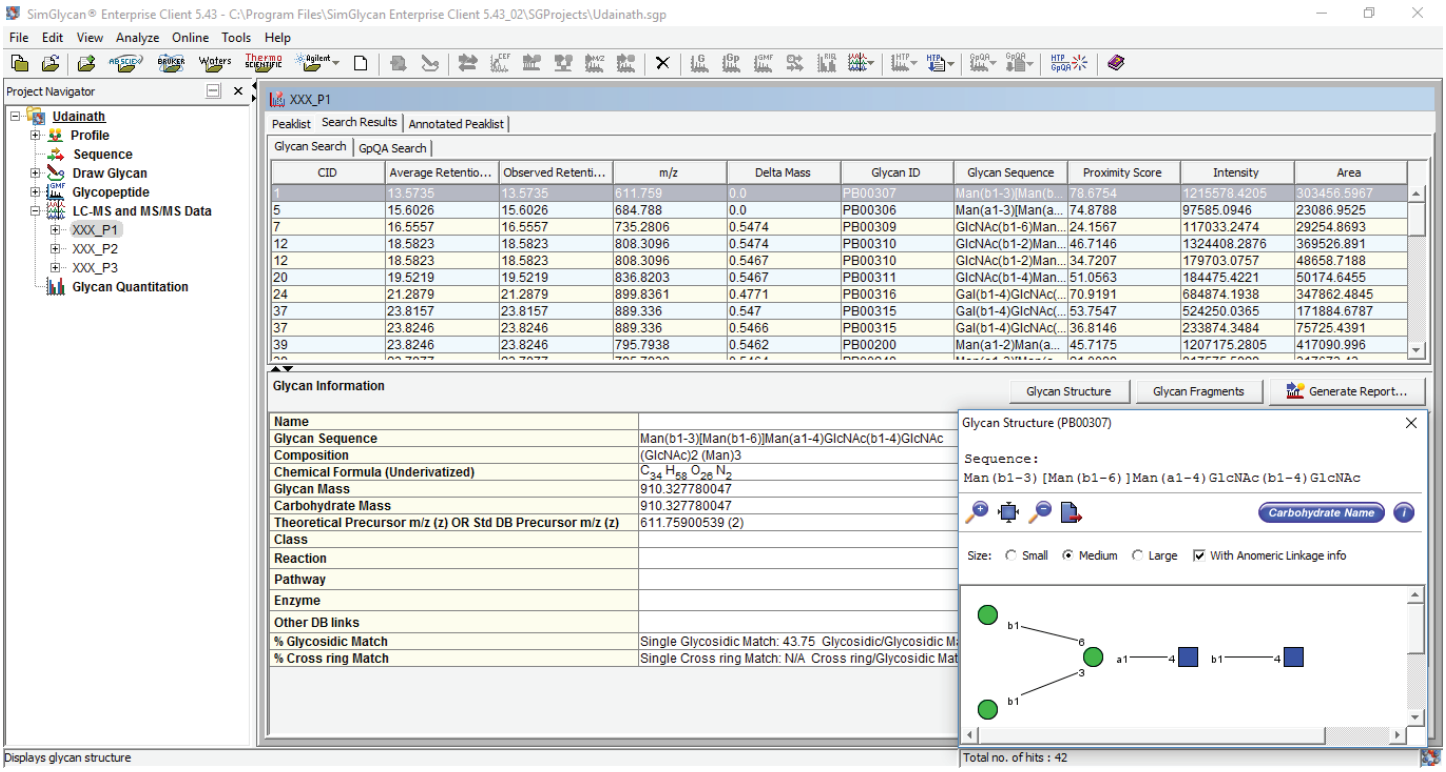

Figure 2: Typical SimGlycan interface showing the identified glycan structure of an LC detected compound

2. Glycan & Glycopeptide MS/MS Data Analysis: The program is capable of determining glycan, and glycopeptide heterogeneity and their isomeric forms. Additional key features are:

i. Processes MSn data to resolve glycan heterogeneity, branching patterns, & isobaric structures.
ii. Searches for glycans with various chemical derivatives used for reducing end modifications e.g., 2-AB, 2-AA, RapiFlour, etc., even if the derivative is not available in the database.
iii. Characterizes Na, Li, Mg, K, and formate adducts, & adduct combinations such as Na + H, etc.
iv. Identifies complex glycosaminoglycan structures, even when modified with substituents such as sulfate, phosphate, and ethanolamine.
v. Determines cross-ring and double glycosidic cleavages, through a combination of permethyl derivatization and MSn data.

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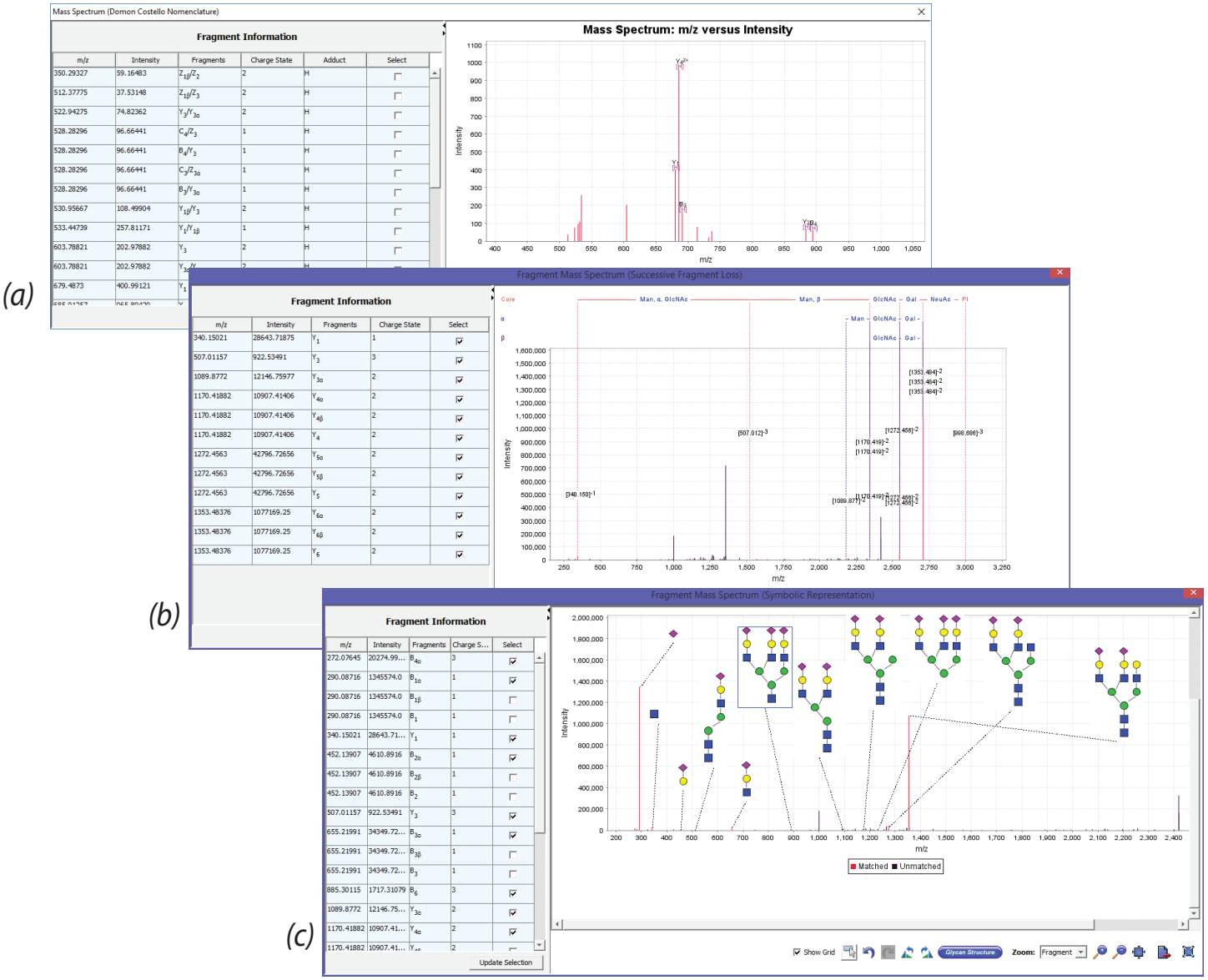

Figure 3: Typical SimGlycan software interface displaying mass spectrum annotated with (a) fragment names in Domon Costello Nomenclature, (b) successive fragment loss, and (c) symbolic representation of the fragments

3. Glycan Quantitation Using aminoxyTMT6 Reagent: Glycans labeled with aminoxyTandem Mass Tags (TMT) are quantified by measuring reporter ion peak intensities from MS/MS spectra. Various charts such as bar chart, dot-plot etc., enable visualization of the abundance of each glycan across biological samples.**

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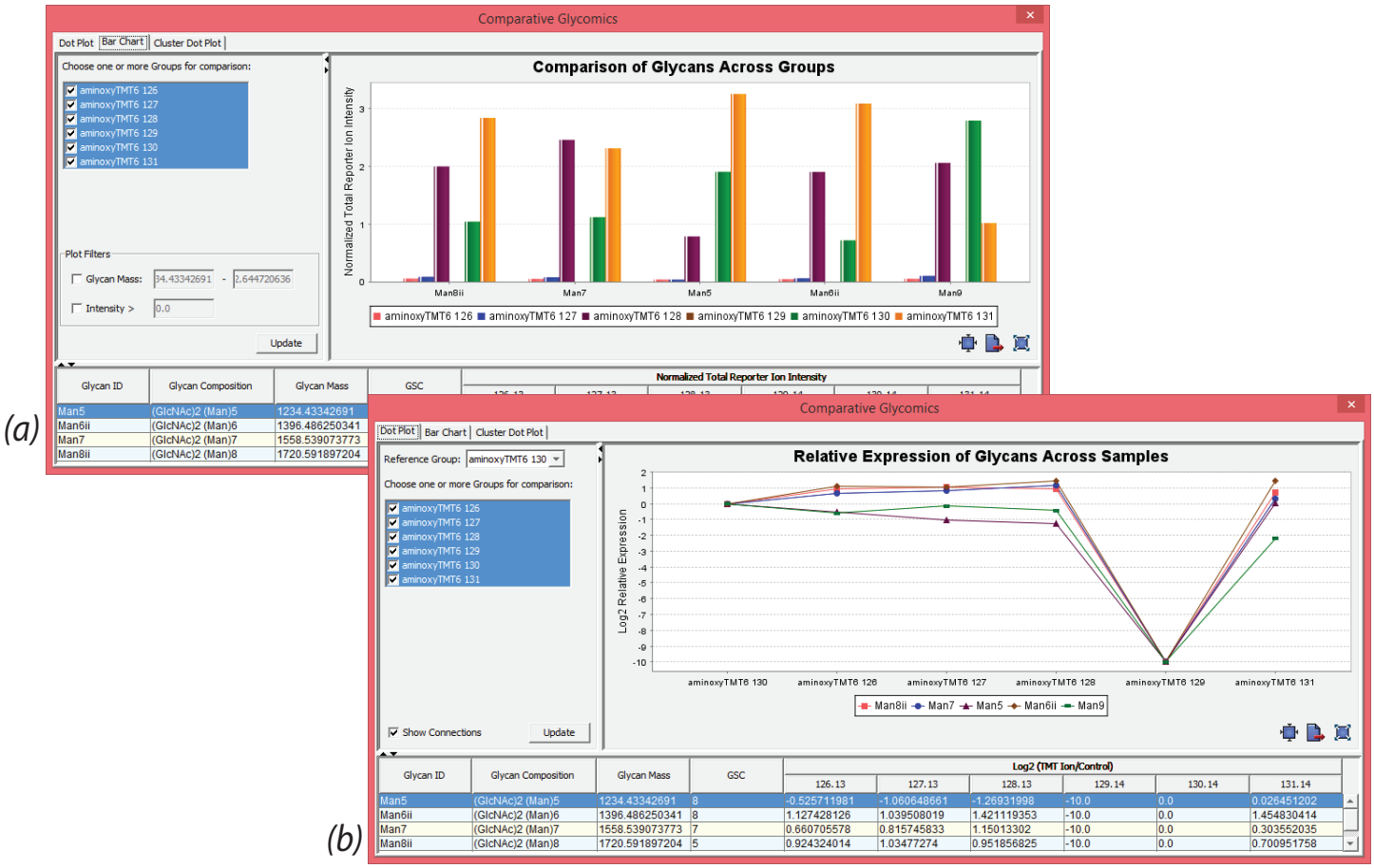

*Figure 4: Typical SimGlycan software charts: (a) Bar Chart displaying the abundance glycans in different samples; (b) Dot plot depicting relative expression of glycans across samples***

** Available in SimGlycan Enterprise Edition only

4. Powerful Reporting: Export your analysis results in HTML and Microsoft Excel format for easy sharing of findings and publishing data.

i. Creates reports that include glycan characteristics such as ID, name, composition, mass, precursor ion m/z, class, glycan image and theoretical fragments with corresponding mass and m/z values.

ii. Exports images of glycan structures, fragments, and spectra as JPEG or PNG files for use in publications.