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Link do produktu: http://www.novazym.sklep.pl/simglycan-500-p-878.html

SimGlycan 5.00

Opis produktu

SimGlycan?

An Innovative Glycan and Glycopeptide MS^n Data Analysis Tool

SimGlycan? predicts the structure of glycans and glycopeptides using mass spectrometry data. SimGlycan?accepts the experimental MS/MS and Multi Stage/Sequential mass spectrometry (MS^n, n>2) data, matches them with its own database of theoretical fragments and generates a list of probable candidate structures. Each structure is scored to reflect how closely it matches your experimental data. Apart from the structural information, other biological information for the probable molecular structures such as the glycan class (N-Linked, O-Linked heparin, lipopolysaccharide etc.), reaction, pathway and enzyme are also made available for easy reference in case of structural elucidation of glycans while in the case of glycopeptide qualitative analysis, information such as Protein ID, Protein Name, Source, Classification, Class, peptide sequence, peptide mass etc. are made available for identified glycopeptides.

These experimental mass spectrometry data can be uploaded in SimGlycan? using standard file formats or directly from mass spectrometer raw files from AB SCIEX (TripleTOF? 5600 System, TOF/TOF 5800, 4800 Plus MALDI TOF/TOF? Analyzer, QTRAP? 6500 System, 4000 QTRAP? and QSTAR? Elite Systems, 4000 QTRAP?and QSTAR? Elite Systems), Agilent Technologies (Agilent 6200 Series TOF LC/MS and Agilent 6500 Series Q-TOF LC/MS systems), Bruker Corporation (ultrafleXtreme? MALDI TOF/TOF, ultraflex? MALDI TOF/TOF, autoflex? TOF and TOF/TOF, maXis? UHR-TOF, micrOTOF?, micrOTOF-Q?, solariX? Qq-FTMS, and amaZon? ion trap series), Thermo Scientific? (LTQ FT Ultra, LTQ Velos, LTQ XL, LTQ Orbitrap Discovery, LTQ Orbitrap Velos, LTQ Orbitrap XL, MALDI LTQ Orbitrap, Orbitrap Elite, Q Exactive, Thermo Scientific? Orbitrap? Fusion? Tribrid mass spectrometer and Thermo Scientific? Q Exactive? hybrid quadrupole-Orbitrap mass spectrometer) and Waters Corporation (SYNAPT G2 HDMS, SYNAPT G2 MS, Xevo G2 QTof, Xevo QTof MS, Xevo TQ MS and Xevo TQ-S platforms).

For supporting automated data analysis of different instrument workflows, SimGlycan? includes comprehensive support for different adducts such as H, Li, Na, Mg^{2+}, K, $HCOO^-$ and $NH4^+$ and adduct combinations such as Na + H, Li + H etc. MS/MS fragmentation patterns of glycans and glycopeptides (based on different instrument settings) can be specified in order to enable the program to reduce false positives from the data analysis results.

SimGlycan® can analyze mass spectrometry data for released glycans that are underivatized, permethylated and reducing end modified. It also provides comprehensive support to perform MS^n data analysis, which assists in resolving heterogeneity, branching patterns and isobaric oligosaccharide structures. SimGlycan®can identify complex glycosaminoglycan structures even when some of the carbohydrate residues are modified with substituents such as sulfate, phosphate, ethanolamine etc.

SimGlycan® also includes comprehensive support for resolving glycopeptides obtained from a LC-MS/MS run of proteolytically digested purified glycoproteins. The Protein ID, Protein sequence or peptide sequences identified by a third party tool will be used as initial input in SimGlycan® in order to identify the glycopeptides from data dependent MS/MS data. SimGlycan® identifies probable glycan-peptide combinations and ranks them on the basis of observed peaks corresponding to diagnostic ions.

Glycan & Glycopeptide MS/MS Data Analysis for Studying Glycosylation

Protein Glycosylation, which is a key post-translational modification, is the result of addition of a glycan to a peptide sequence. Glycopeptides are known to exhibit multiple biological functions. In order to identify distinct functional properties for defined structural features, detailed information on the respective glycan moieties is essential. In order to understand all these phenomena, glycosylation analysis is an area of growing interest. Glycans have also been found to participate in many biological processes including embryonic development, inter and intracellular activities, coordination of immune functions, pathogens homing on their host tissues, cell division processes and protein regulations and interactions.

Glycoprotein glycosylation analysis has since long been a challenging task for biochemists. SimGlycan®assists in predicting the structure of a glycan from the released glycan MS/MS data or directly a glycopeptide (peptide chain modified with a single or two glycan structures) from glycopeptide MS/MS data acquired using various ionization techniques of mass spectrometry. Besides, it supports MS/MS data for released glycans with different chemical derivatives such as permethylation and various reducing terminal modifications. The facility to specify a user defined reducing end mass for permethylated glycans is also available. All these features facilitate accurate study of protein glycosylation providing a strong base for developing a sensitive analytic approach to achieve complete quality analysis of glycoprotein therapeutics.