Resource Summary Report

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GlycoPeptideSearch

RRID:SCR_005767
Type: Tool

Proper Citation

GlycoPeptideSearch (RRID:SCR_005767)

Resource Information

URL:
https://edwardslab.bmcb.georgetown.edu/trac/GlycoPeptideSearch/#WelcometoGlycoPeptideSearch

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Description: GlycoPeptideSearch (GPS) simplifies data interpretation of N-glycopeptide CID MS/MS datasets by searching for glycopeptide results consistent with MS/MS spectra. Results are tabulated in Excel format. Accelerate and simplify interpretation of N-glycopeptide CID MS/MS spectra using GlycoPeptideSearch (GPS). This tool is designed for tandem mass-spectra acquired from proteolytic digests of purified glycoproteins modified with N-glycans and analyzed by LC-MS/MS and CID. The search yields an Excel spreadsheet of N-glycopeptide matches consistent with the spectra. GPS requires two files as input - an mzXML (or other open spectral format) file of glycopeptide CID tandem mass-spectra and a text file (.txt) of peptide sequences containing the N-linked glycosylation motif NXS/T. Spectral datafiles must be converted from raw vendor formats, such as .RAW or .wiff, to an open peak list format (mzXML preferred). In addition to these two input files, the user must specify one or more glycan databases (provided in the software package). The database(s) selected by the user will be used to match glycan structures in the glycopeptide spectra. The output is an Excel spreadsheet with one or more rows for spectra within the dataset that contain evidence of glycoprotein fragmentation, paired with one or more proposed glycopeptide matches for each spectrum. Glycopeptide matches consist of a peptide-glycan pair, with the peptide drawn from the user-supplied peptide file, and the glycan selected from a glycan database(s). The human subset of the GlycomeDB glycan database is provided, and N-linked glycans are automatically selected from it. GPS interprets glycopeptide CID MS/MS spectra by first requiring MS/MS spectra contain evidence of glycopeptide fragmentation - the oxonium ion peaks (m/z 204 - Hex, m/z 366 - HexNAc), and N-glycopeptide core specific peaks (peptide, peptide + HexNAc, peptide + HexNAc-HexNAc, peptide + HexNAc-HexNAc-Hex). For spectra that meet these initial criteria, for a particular peptide, a mass-based search of one or more glycan databases looks for glycans which capture the remaining mass of the spectral precursor. Additional spectral information may be used to narrow the number of matches, and equivalent glycan topologies may be collapsed to a single

peptide-glycan pair. GPS also provides N-glycan compositions with the necessary additional mass, even if no glycan with the composition is present in the glycan database(s). GPS can either be run from the command-line or by using its graphical user interface. We recommend the msconvert (or MSConvertGUI) software from the ProteoWizard project to convert spectral datafiles from vendor formats such as .wiff and .RAW into mzXML.

Abbreviations: GPS

Resource Type: software resource

Defining Citation: PMID:22239659

Keywords: peptide, glyopeptide, glycoprotein, mass-spectra, ms/ms spectra

Resource Name: GlycoPeptideSearch

Resource ID: SCR_005767

Alternate IDs: nlx_149231

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Record Last Update: 20260725T190609+0000

Ratings and Alerts

No rating or validation information has been found for GlycoPeptideSearch.

No alerts have been found for GlycoPeptideSearch.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We have not found any literature mentions for this resource.