

NIST Human Plasma Glycopeptide Libraries (June 2025)

This document describes the three varieties of NIST human plasma glycopeptide libraries.

1. A tryptic glycopeptide MSMS library (nist-plasma-proteins-msms). This is in the format of earlier NIST peptide libraries long available on the NIST library website. The highest scoring and highest purity spectra for each glycopeptide ion is selected and peaks are fully annotated.
2. A GADS (Glycopeptide Abundance Distribution Spectrum) library (nist-plasma-proteins-gads) is provided in the format of previous GADS libraries. These libraries are available along with this library in the same section of the NIST downloadable libraries site. Methods for validating GADS are described in these earlier GADS publications.
3. A glycan fragmentation library (nist-plasma-proteins-glycan), derived from selected spectra in MSMS library above. It contains a novel variety of “spectra” that represent glycan containing fragments according to the glycan contained in the precursor ion. This includes oxonium and glycopeptide fragment ions only. This can be searched by Glycan, using x as the first letter in the Name search window. For example, all G4H5FS containing glycopeptides can be found by entering xG4H5FS in the Name search tab in the NISTMS program (note G=GlcNac or GalNac, H=Hexose, F=Fucose, S=Sialyl). It can also be searched by peptide sequence

Libraries 1 and 2 are described in the document “nist-gads-glycopeptide-user-guide.pdf” in the same folder as this file in the downloaded file. Also, each of these libraries is available in NIST “.msp” format – a simple text (ASCII) format for special processing.

Library 3 is created from high resolution ion trap and stepped energy spectra in the MSMS Library 1. The x-axis corresponds to the glycan mass of the oxonium fragment ion or the mass of the LOSS of glycan from the precursor glycopeptide (i.e., the difference in mass of the precursor glycopeptide ion and product glycopeptide ion). The charge(s) of the latter are given in the annotation of each peak are these two varieties of fragment ions are aligned.

To access this library, run the accompanying “nistms-glyco.exe” program and selecte the default folder (it contains the 3 libraries above). Documentation concerning other features of the library are available in other PDF files. Library contents are more directly observed in the ‘Names’ tab after selecting one of the 3 libraries.