

MCP MOLECULAR & CELLULAR PROTEOMICS

Checklist for Publication of Mass Spectrometry-based Glycomic Identification Data

The identification of free or released glycans, glycopeptides or glycolipids is commonly accomplished by a combination of approaches. Many studies depend on acquiring mass spectra and the conversion of this data into a format suitable for analysis and interpretation. The following information is required by the journal for articles reporting mass spectrometric glycoconjugate analyses.

To aid authors in preparing their manuscripts, the check list of the items that must be included is given below. Authors are encouraged to print out this document and use it to ascertain that the complete set of required information has been included. [Click here to open a set of guidelines](#) that explains each point on the list, and why it has been included. Authors submitting this type of data for the first time are particularly encouraged to use both the checklist and guidelines.

The following information must be included in the *Experimental Procedures* section:

Section I

Clearly defined degree of analysis in support of reported structures is provided (assumptions regarding linkage, monosaccharide identity, etc. are provided)

Y

N/A

Page

Section II

Name of peaklist-generating software and release version (number or date) is given

Y

N/A

Page

Parameters and thresholds used are provided including the exclusion of contaminant peaks and/or consideration of degradation products

Y

N/A

Name of search engine and release version (number or date) is given

Y

N/A

Database/spectral library version (number or date) including number of entries searched is given

Y

N/A

Search Parameters including:

Fixed/variable modifications considered are given

Y

N/A

Enzyme/chemical release specificity and efficiency, if measured, are given

Y

N/A

Justification of the threshold employed for assignment provided including that for isobaric/isomeric species is described

Y

N/A

For quantitative data (same as peptide, proteins, and PTM checklist except for glycans/glycoconjugates) including:

Rationale for quantification of isobaric/isomeric structures is provided

Y

N/A

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The following information must be included in the *Results* or *Supplemental* sections:

Section III

For each glycan identified the following should be reported in a table:

			Page
Glycan assignment (suggest using the symbol methodology Outlined in Essentials of Glycobiology)	Y	N/A	
Precursor Mass/Charge and charge observed	Y	N/A	
Deviation between experimental and theoretical mass	Y	N/A	
Any modifications observed (reducing end, adducts, etc.)	Y	N/A	
Number of matched fragments above threshold for MS data	Y	N/A	
Number of assigned and unassigned mass values above threshold for MS-only data	Y	N/A	
Relevant scores, if software used for assignment	Y	N/A	
MS/MS (and full MS) annotated spectra should be included for all assignments	Y	N/A	
For quantitative studies, measurement and accuracy (e.g. mean and error) provided	Y	N/A	