MIRAGE MS guidelines

Guidelines for reporting mass spectrometric analysis data of glycans

Based on the MIAPE guidelines template, MIAPE-MS version 2.24

Version 1.0, April 24, 2013

Classification	Definition	Mandatory
1. General features — (a) Global descriptors		
Date stamp	The date on which the work described was completed; given in the standard 'YYYY-MM-DD' format (with hyphens).	?
Responsible person or role (or institutional role if more appropriate); provide name, affiliation and stable contact information	The (stable) primary contact person for this data set; this could be the experimenter, lab head, line manager etc. Where responsibility rests with an institutional role (e.g., one of a number of duty officers) rather than a person, give the official name of the role rather than any one person. In all cases give affiliation and stable contact information. This information can be made available as part of an authors' list or in an acknowledgment section	yes in supp. info.
Instrument manufacturer, model	The manufacturing company and model name for the mass spectrometer.	yes
Customizations	Any significant (i.e., affecting behaviour) deviations from the manufacturer's specification for the mass spectrometer.	yes
1. General features — (b) Control and analysis software		
Software name and version	The instrument management and data analysis package name, and version; where there are several pieces of software involved, give name, version and role for each one. Also mention upgrades not reflected in the version number.	yes
Switching criteria (tandem only)	The list of conditions that cause the switch from survey or zoom mode (MS^1) to or tandem mode (MS^n where n > 1); e.g., 'parent ion' mass lists, neutral loss criteria and so on.	yes
Isolation width (global, or by MS level)	For tandem instruments (i.e., multi-stage instruments such as triple quads and TOF-TOFs, plus ion traps and equivalents) the total width (i.e., not half for plus-or-minus) of the gate applied around a selected precursor ion m/z, provided for all levels or by MS level.	yes
Location of 'parameters' file	The location and name under which the mass spectrometer's parameter settings file for the run is stored, if available. Ideally this should be a URI including filename, or most preferably an LSID, where feasible. Location of file should be mentioned.	yes

2. Ion sources — (a) Electrospray Ionisation (ESI)		
Supply type (static, or fed)	Whether the sprayer is fed (by, for example, chromatography or CE) or is loaded with sample once (before spraying).	yes
Interface manufacturer, model and catalog number (where available)	Where the interface was bought from, plus its name and catalog number; list any modifications made to the standard specification. If the interface is entirely custom-built, describe it or provide a reference if available.	yes
Sprayer type, coating, manufacturer, model and catalog number (where available)	Where the sprayer was bought from, plus its name and catalog number; list any modifications made to the standard specification. If the sprayer is entirely custom-built, describe it briefly or provide a reference if available.	yes
Relevant voltages where appropriate (tip, cone, acceleration)	Voltages that are considered as discriminating from an understood standard measurement mode, or important for the interpretation of the data. These might include the voltage applied to the sprayer tip, the voltage applied to the sampling cone, the voltage used to accelerate the ions into the rest of the mass spectrometer (mass analysis + detection) by MS level.	yes
Degree of prompt fragmentation evaluated	Yes/No. If yes, provide data showing results.	yes
Whether in-source dissociation performed	State whether in-source dissociation was performed (increased voltage between sample orifice and first skimmer).	yes
Other parameters if discriminant for the experiment (such as nebulizing gas and pressure)	Where appropriate, and if considered as discriminating elements of the source parameters, describe these values.	yes
2. Ion sources — (b) MALDI		
Plate composition (or type)	The material of which the target plate is made (usually stainless steel, or coated glass); if the plate has a special construction then that should be briefly described and catalogue and lot numbers given where available.	yes
Matrix composition (if applicable)	The material in which the sample is embedded on the target (e.g., 2,5-dihydroxybenzoic acid (DHB)).	yes
Deposition technique	The method of laying down (matrix and) sample on the target plate (including matrix concentration and solvents applied); for example, matrix+sample in single deposition; or matrix, then matrix+sample (if several matrix substances are used, name each), Recrystallization using volatile solvent; where chromatographic eluent is directly applied to the plate by apparatus, or for other approaches, describe the process and instrumentation involved very briefly and cross-reference.	yes
Relevant voltages where appropriate	Voltages considered as relevant for the interpretation of the data. This might include the grid voltage (applied to the grid that sits just in front of the target), the acceleration voltage (used to accelerate the ions into the analyzer part of the mass spectrometer (mass analysis + detection), etc.	yes
Degree of prompt fragmentation evaluated	Yes/No. If yes, provide data showing results.	yes

PSD (or LID/ISD) summary, if performed	Confirm whether post-source decay, laser-induced decomposition, or in-source dissociation was performed; if so provide a brief description of the process (for example, summarize the stepwise reduction of reflector voltage).	yes
Operation with or without delayed extraction	State whether a delay between laser shot and ion acceleration is employed.	yes
Laser type (e.g., nitrogen) and wavelength (nm)	The type of laser and the wavelength of the generated pulse (in nanometers).	yes
Other laser related parameters, if discriminating for the experiment (such as pulse energy (J), attenuation, focus diameter (m), pulse duration (ns at FWHM), frequency (Hz) and average shots fired per spectrum	Other details of the laser used to irradiate the matrix-embedded sample if considered as important for the interpretation of data; this might include the pulse energy in microJoules, focus diameter in microns, attenuation details, pulse duration in nanoseconds at full-width half maximum, frequency of shots in Hertz and average number of shots fired to generate each combined mass spectrum.	yes
3. Ion transfer optics		
Hardware options	e.g. ‘simple’ quadrupoles, hexapoles, stacked ring electrodes, TOF, ...	yes
3. Post-source componentry — (a) Collision cell		
Gas type and pressure (bar) CID	The composition and pressure of the gas used to fragment ions in the collision cell (TOF-TOF, linear trap, Paul trap, or FT- ICR cell).	if applicable
Collision energy CID	The specifics for the process of imparting a particular impetus to ions with a given m/z value, as they travel into the collision cell for fragmentation. This could be a global figure (e.g., for tandem TOFs), or a complex function; for example a gradient (stepped or continuous) of m/z values (for quads) or activation frequencies (for traps) with associated collision energies (given in eV).	if applicable
Electron transfer dissociation ETD	Reagent gas, pressure, reaction time, number of reagent ions	if applicable
Electron capture dissociation ECD	Emitter type, Voltage, Current	if applicable
3. Post-source componentry — (b) TOF drift tube		
Reflectron status (on, off, none)	Whether a Reflectron is present, and if so, whether it is used. Depending on the type of instrument provide exact details on the reflectron mode (e.g. V or W mode).	yes
3. Post-source componentry — (c) Ion trap		
Final MS stage achieved	The final MS level achieved in generating this data set with an ion trap or equivalent (e.g., MS^10).	yes
3. Post-source componentry – (d) Ion mobility		
Specific Ion mobility parameters	gas, pressure, instrument-specific parameters e.g. wave velocity/height depending on the particular vendor's options for tuning this component	if applicable
3. Post-source componentry — (e) FT-ICR		
Excitation and detection parameters	Peak selection, pulse width, voltage, decay time, ... other important experiment parameters e.g. IR, ...	if applicable

3. Post-source componentry — (f) Detectors		
Detector type	Needs defintion if non OEM detector were used (e.g. microchannel plate, channeltron etc.)	if applicable
4. Spectrum and peak list generation and annotation		
For this section, if software other than that listed in 1b (Control and analysis software) is used to perform a task, the producer, name and version of that software must be supplied in each case.		
4. Spectrum and peak list generation and annotation — (a) Spectrum description		
Location of source ('raw') file including file name and type	The location and filename under which the original raw data file from the mass spectrometer is stored, if available. Also give the type of the file where appropriate, or else a description of the software or reference resource used to generate it. Ideally this should be a URI or filename, or most preferably an LSID, where feasible. Due to the nature of the raw files (proprietary formats, no open source software, licensing, etc), the validation of raw data can only be possible if the information is provided in an open XML format (mzXML, mzData, mzML)	on request
Identifying information for the target area	Either a spot number, or some other form of coordinates if more appropriate, that link the spectrum to the analzsed area of the sample (2D imaging).	if applicable
4. Peak list generation and annotation — (b) Peak list generation		
Since several different applications may be used for the data acquisition, data post processing and spectrum annotation each software used should be recorded separately together with the information what modification has been done to the data.		
Software	This includes the name of the software, the manufacturers and the version number. It should also include the availability of the software (e.g. open source, commercial) and if applicable the URI for the software (e.g. project homepage).	yes
Software type	Type of data processing that was performed with the software (e.g. data acquisition, de-isotoping, charge deconvolution, peak picking, and annotation).	yes
Customizations made to the software	Any changes made to the original program code that may affect the results.	yes
Software settings	Any settings made in the software that may affect the results (e.g. thresholds). For the annotation software this parameters are recorded in the Annotation parameter section.	yes
Data file	Information about the produced data file. This includes the file format, the availability of the file and if applicable the URI to access the file.	On request
Acquisition number (from the 'raw' file) for all acquisitions combined in the peak list, total number and whether summed or averaged.	Where available, the reference numbers of all the scans (as numbered in the raw file) that were combined to produce a peak list, the total number of acquisitions combined to produce the peak list, and whether the peak list was produced by summing or averaging the scans that are listed.	yes

Parameters triggering the generation of peak lists from raw data, where appropriate	The total ion count or S/N threshold for a spectrum and the minimum number of ions detected in that scan, for it to be a candidate for grouping in a peak list; plus the mass tolerance (Da) on the precursor ion masses for MS/MS spectra.	yes
Raw data scoring	Describe methode and software for selection of peaks for inclusion in the peaklist	yes
Smoothing; whether applied, parameters	Any peak smoothing should be described, along with the parameters supplied to the algorithm.	yes
Background threshold, or algorithm used	The intensity or S/N cut-off used to filter background noise; or a description of the algorithm used to gate the noise, if complex.	yes
Signal-to-noise estimation and method	The ratio of signal to noise for each significant peak in a peak list; significance is defined as being above a given intensity (which should be supplied) or being otherwise of interest; the method of calculation should also be named (if available).	no
Percentage peak height for centroiding; or algorithm used, if appropriate	The percentage peak height at which centroids are calculated; if a more complex algorithm is used to perform the process, it should be named here.	yes
Retention times for all acquisitions combined in the peak list	The times relative to the start of the MS run for all acquisitions that were combined in the peak list so that those acquisitions may later be correlated to a chromatogram (continuously-fed electrospray sources only).	yes
m/z and intensity values	The actual data (m/z versus intensity); as described in the preceding sections.	yes
4. Peak list generation and annotation — (c) Annotation		
Since several different applications may be used for the data acquisition, data post processing and spectrum annotation each used software should be recorded separately together with the information what modification has been done to the data.		
Software	This includes the name of the software, the manufacturers and the version number. It should also include the availability of the software (e.g. open source, commercial) and if applicable the URI for the software (e.g. project homepage).	yes
Software type	Type of data processing that was performed with the software.	yes
Customizations made to the software	Any changes made to the original program code that may affect the results.	yes
Software settings	Any settings made in the software that may affect the results (e.g. thresholds). For the annotation software this parameters are recorded in the Annotation parameter section.	yes
Data file	Information about the annotation data file. This includes the file format, the availability of the file and if applicable the URI to access the file.	yes
Database queried	List of databases used for the annotation of the data. Also specify databases version, annotation date and number of entries.	yes

Taxonomical restrictions	List of species the search was limited to.	yes
Other restrictions	Other settings to the software that filtered out certain sequences from the database (e.g. allow only certain glycan types (N-Glycan) or restriction by composition). This also includes the usage of threshold for scoring values.	yes
Allowed cleavages	List of allowed cleavages for the annotation run (A,B,C,X,Y,Z). This includes also the number of allowed cross-ring cleavages and glycosidic cleavages.	if applicable
Mass accuracy	Mass accuracy settings for the annotation run.	yes
Scoring algorithm	Used scoring function with a references to the algorithm and of software	yes
The following lines have to be repeated for each identified feature in the mass spectrum.		
Scan number	Scan number of the spectra	yes
Ion mode for this spectrum	The ion mode (positive or negative), which is assumed to be the same for all contributing acquisitions.	yes
MS level for this spectrum	The MS level (e.g., MS^2) at which this spectrum was acquired.	yes
Precursor m/z and charge	For tandem spectra only; the precursor m/z value and the charge state of the precursor ion should be given.	yes
Estimate of precursor ion stability, with the full mass spectrum containing that peak (for MS level 2 and higher)	The whole spectra generated before precursor isolation and that after precursor ion isolation prior to dissociation.	for appropriate reference glycan
Structure unique identifier (accession code)	Glycan identifier in the queried database(s).	if applicable
Deduced structure(s)	Description of the structural features supported by the data including provenance	if applicable
Validation status	Validation status for all glycan structures, specify if accepted without post-processing of database/de-novo interpretation or if manually accepted or rejected.	yes
Validation	Confirmation of preliminary assignment with tandem MS data. In the case of glycan tandem/multistage MS profiling (MSn) describe the number of fragmentation stages and m/z values associated to the identified glycan.	yes
In the case of MSn the number of matched/unmatched peaks	For MS level 2 and higher, the precursor m/z and charge, with full spectrum/peaklist comprising the select precursor ion, where available, should be accessible. The number of unmatched signals should be reported or alternatively the total number of m/z values can be extracted from the supporting datasets.	yes
Orthogonal approaches	Other additional information used for evaluation of confidence. This may include the use of retention time, exoglycosidase treatment, reference/internal database/standard etc (e.g. permethylation -> particular fragmentation pattern, PGC-specific retention time patterns,...).	yes

4. Peak list generation and annotation — (d) Quantification for selected ions (in addition to 4a and 4b))		
Experimental protocol, canonical reference where available with deviations	Which methodology is being used for quantification (e.g., duplex stable isotope labeling, multiplex isobaric tag labeling, label-free method based on spectral count, etc.); if a methods paper for the technique exists, a reference to it should be given and any significant deviations noted.	yes
Number of combined samples and MS runs analyzed	The number of experimental classes and MS runs (including number of replicates) that are represented, each with its own different tag.	yes
Quantitation approach (e.g., integration)	Whether the measured value is the area under the selected ion current, max peak height, or something else.	yes
Normalization technique	Briefly describe the normalization strategy employed; e.g., take ratios, then normalize to a global average.	yes
Location of quantification data, giving the file name, type and Uniform Resource Indicator	The location and filename under which the quantification data from the statistical analysis are stored, if available. Ideally this should be a URI or filename, or most preferably an LSID. Also give the type of the file where appropriate, or else a description of the software used to generate it.	on request
Quantity measurement	Absolute or relative quantification based on signal intensity or spectral counts. Were internal standards used.	yes
Data transformation technique	What are the input intensity values, how have they been filtered, transformed and processed?	yes
Acceptance criteria (including measure of errors).	Describe the evaluation method applied to the quantitation software (or manual calculation) result and the acceptance criteria and supply quantitative measures of variability (e.g. standard error)	yes
5. Interpretation and validation		
Confidence	Assessment and confidence given to the identification and quantitation (description of methods, thresholds, values, etc.) including the approach and software.	yes