MIAPE: Mass Spectrometry

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This module identifies the minimum information required to report the use of a mass spectrometer in a proteomics experiment, sufficient to support both the effective interpretation and assessment of the data and the potential recreation of the work that generated it.

Introduction

The modern mass spectrometer is a rather complex instrument with many operational parameters; the data sets generated are similarly complex, and often rather voluminous. These guidelines for the reporting of mass spectrometry do not prescribe that all of that information be captured; and given the diversity of instruments currently available, the utility of such detail is clearly open to question.

However, it is possible to specify parameters that are representative of the way in which the mass spectrometer was used, to contextualise the data generated and thereby enable a better-informed process of assessment and interpretation.

These guidelines cover both the operation of a mass spectrometer and the generation of mass spectra from the 'raw' data. They do not cover the delivery of sample to the mass spectrometer, or the interpretation of spectra by search engines; these details are captured in separate MIAPE modules, the latest versions of which can be obtained from the HUPO Proteomics Standards Initiative website (http://psidev.sf.net/gps/miape/). Note also that these guidelines do not cover all the available components of a mass spectrometer (for example, some of the less frequently used ion sources); subsequent versions of this document will have expanded coverage, as will almost certainly be the case for all the MIAPE modules.

The following section, detailing the reporting requirements for the use of a mass spectrometer, is subdivided as follows:

1. General features; summary statistics such as mass accuracy; the software used to run the machine and the parameters supplied to it.
2. Ion sources; for example, matrix-assisted laser desorption ionisation (MALDI), electrospray ionisation, surface-enhanced laser desorption ionisation (SELDI).
3. All major components after the ion source; for example, ion traps, collision cells, time-of-flight tubes, detectors (including Fourier Transform Ion Cyclotron Resonance detection). Note that where a collision cell is an ion trap (including FT-ICR cells), the requirements for the relevant components should be combined.
4. The data resulting from the procedure; the method of generation of peak lists and the location of the raw data from which they were generated; the method by which quantitation was performed (where appropriate) and the resultant quantitative data set.

Reporting requirement for mass spectrometry

1. General features

a) Global descriptors
- Date stamp (as YYYY-MM-DD)
- Responsible person (or institutional role if more appropriate); provide name, affiliation and stable contact information.
- Machine manufacturer and model
- Significant customisations (summary)
- Resolution (*m*/*z*); state 'Baseline' or 'FWHM'
- Mass accuracy (Daltons); give estimates for each MS mode where appropriate.
- Ion mode

b) Control and analysis software
- Software description and version
- Switching criteria (tandem only); parent ion mass lists, neutral loss criteria *etc.*
- Location of 'parameters' file, as a file name and Uniform Resource Indicator (URI)

2. Ion sources

a) Electrospray Ionisation (ESI)
- Supply type (static, or LC-fed)

- Interface manufacturer, model and catalog number (where available)
- Sprayer type, coating, manufacturer, model and catalog number (where available)
- Tip voltage and temperature (Celsius)
- Tip-to-cone angle and distance (millimetres)
- Nebulising gas, and pressure (bar)
- Cone voltage (V)

b) MALDI
- Plate composition
- Matrix composition
- Spot deposition technique; where layers are applied, describe in order of application
- Grid voltage (V)
- Acceleration voltage (V)
- Whether extraction was delayed
- Laser type (*e.g.* nitrogen), wavelength (nm), pulse energy (μJ), pulse duration (ns at FWHM) and frequency (Hz)

c) SELDI
- *As for 'MALDI' (2b), plus the following*
- Chip manufacturer, model and catalog number (where available)
- Surface chemistry
- Incubation conditions
- Wash conditions

3. Post-source componentry

a) Ion optics, 'simple' quadrupoles, hexapoles
- *No parameters to be captured*

b) Time-of-flight drift tube (TOF)
- Total path length (millimetres)
- Reflectron status (on, off, none)

c) Ion trap
- Final MS exponent
- Isolation width (global, or by MS level)

d) Collision cell
- Gas type and pressure (bar)
- Collision energy; the gradient of energies used should be described (list *m*/*z* windows, and associated collision energies in eV); state also whether the gradient is stepped or continuous.

e) FT-ICR
- *As for 'Ion trap' (3c) and 'Collision cell' (3d) combined, plus the following*
- Magnetic field strength (T)

f) Detectors (not cyclotron resonance)
- Detector type

4. 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.

a) Generation of 'stick' spectrum
- Location of source ('raw') file, as a file name, type and Uniform Resource Indicator (URI)
- Parameters triggering the generation of peak lists from raw data, where appropriate
- Acquisition number (from the 'raw' file) of all acquisitions combined in the peak list, and whether summed or averaged
- Signal-to-noise estimation for spectrum
- Smoothing; whether applied, plus algorithm
- Percentage peak height for centroiding
- Background threshold, or algorithm used
- Base peak *m*/*z*, where appropriate
- Whether charge states calculated, spectrum deconvoluted and peaks de-isotoped
- Precursor ion charge for tandem spectra
- Actual values of *m*/*z* and intensity

b) Quantitation for selected ions
- *As for 'Generation of stick spectrum' (4a), plus the following information*
- Experimental protocol (*e.g.* iTRAQ)
- Number of combined samples analysed
- Quantitation approach (*e.g.* integration)
- Normalisation technique
- Location of quantitation data, giving the file name, type (where appropriate) and URI

Summary

The MIAPE: MS minimum reporting requirements for the use of a mass spectrometer specify that a significant degree of detail be captured, for mass spectrometry, spectral data and its subsequent processing. It is clear however, that providing the information required by this document will enable both the effective interpretation and assessment of mass spectral data and potentially, the recreation of the work that generated it. Much of the required information should be reusable from existing files, or exportable from the instrument; we anticipate further automation of this process.

These guidelines will evolve. To contribute, or to track the process to remain 'MIAPE-compliant', browse to the website at http://psidev.sf.net/gps/

Appendix One. The MIAPE: MS glossary of required-parameter classifications

Classification	*Definition*
1. General features — (a) Global descriptors	
Date stamp	The date on which the work described was initiated; given in the standard 'YYYY-MM-DD' format (with hyphens).
Responsible person or role	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.
Machine manufacturer and model	The manufacturing company and model name for the mass spectrometer that generated this data set.
Significant customisations	Any significant (*i.e.* affecting behaviour) deviations from the manufacturer's specification for the mass spectrometer.
Resolution (*m*/*z*); state 'Baseline' or 'FWHM'	The *m*/*z* value above which peaks cannot be distinguished; specified either as baseline or full width at half maximum.
Mass accuracy (Daltons)	The margin of error in mass measurement by the mass spectrometer; specified as 'plus-or-minus *x* Da'.
Ion mode	Whether the mass spectrometer is operating in positive or negative ion mode.
1. General features — (b) Control and analysis software	
Software description 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.
Switching criteria (tandem only)	The list of conditions that cause the mass spectrometer to switch from survey or zoom mode (PMF) to 'tandem' or MS/MS mode; for ion traps, this should be specified either globally (if appropriate), or for each increment in MS level.
Location of 'parameters' file	The URI and filename under which the mass spectrometer's parameter settings file for the run is stored, if available.
2. Ion sources — (a) Electrospray Ionisation (ESI)	
Supply type (static, or LC-fed)	Whether the sprayer is fed by, for example, a chromatography column, or is loaded with sample once (before spraying).
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 briefly.
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.
Tip voltage and temperature (Celsius)	The voltage applied to the sprayer tip, and the temperature (°C) at which it is maintained during operation.
Tip-to-cone angle and distance (millimetres)	The angle subtended between the axis of the sprayer and the intake for the ion optics, plus the distance in millimetres.
Nebulising gas, and pressure (bar)	The elemental composition of the Nebulising gas, and the pressure of the supply (not the flow rate).
Cone voltage	The (fixed) voltage applied to the sampling cone.
2. Ion sources — (b) MALDI	
Plate composition	The material of which the target plate is made (usually stainless steel, or coated glass).

Matrix composition	The material in which the sample is embedded on the target (*e.g.* alpha-cyano-4-hydroxycinnamic acid).
Spot deposition technique; where layers are applied, describe in order of application	The method of laying down matrix and sample on the target plate; for example, matrix+sample in single deposition; or matrix, then matrix+sample (if several matrix substances are used, name each).
Grid voltage	The voltage applied to the grid that sits just in front of the target.
Acceleration voltage	The voltage used to accelerate the ions into the rest of the mass spectrometer (mass analysis + detection).
Whether extraction was delayed	State whether a delay between laser shot and ion acceleration is employed.
Laser type (e.g. nitrogen), wavelength (nm), pulse energy (μJ), pulse duration (ns at FWHM) and frequency (Hz)	The full details of the laser used to shoot at the matrix-embedded sample; type of laser and wavelength of the generated pulse (in nanometres); energy in microJoules, duration in nanoseconds at full-width half maximum, and frequency of shots in Hertz.
2. Ion sources — (c) SELDI	
Chip manufacturer, model and catalog number (where available)	Where the SELDI chip was bought from, plus its name and catalog number; if the chip and/or surface are custom-made, describe them briefly; note that the application of sample to the chip is covered in the LC guidelines.
Surface chemistry	Nature of the reactive surface of the SELDI chip.
Incubation conditions	Time and temperature used when incubating sample on the chip surface.
Wash conditions	Solution and conditions used to remove unbound sample; note that matrix application is covered in 2(b).
3. Post-source componentry — (a) Ion optics, 'simple' quadrupoles, hexapoles	
No parameters to be captured	These components (focusing elements and ion guides) require no description at present.
3. Post-source componentry — (b) TOF drift tube	
Total path length (millimetres)	The average distance (both with and without reflection) travelled by ions (*i.e. not* the physical length of the drift tube).
Reflectron status (on, off, none)	Whether a Reflectron is present, and if so, whether it is used.
3. Post-source componentry — (c) Ion trap	
Final MS exponent	The final 'MS level' achieved when performing PFF with the ion trap (*e.g.* MS^10).
Isolation width (global, or by MS level)	The total width (*i.e.* not half for plus-or-minus) of the gate applied around a selected precursor ion.
3. Post-source componentry — (d) Collision cell	
Gas type and pressure (bar)	The composition and pressure of the gas used to fragment ions in the collision cell (linear trap, Paul trap, or FT-ICR cell).
Collision energy; the gradient of energies used should be described (list m/z windows, and associated collision energies in eV); state also whether the gradient is stepped or continuous	The specifics for the process of imparting a particular impetus to ions with an *m*/*z* value in a particular range, as they travel into the collision cell for fragmentation; this could be a global figure but is more commonly partitioned to impart more force to larger ions — in this case the cutoff values for each value of the collision energy should be provided, and the gradient described as stepped or continuous.
3. Post-source componentry — (e) FT-ICR	
Magnetic field strength (T)	The field strength in Tesla generated by the magnet surrounding an ICR cell.

3. Post-source componentry — (f) Detectors (not cyclotron resonance)	
Detector type	Short phrase describing the type of detector used in the machine (*e.g.* microchannel plate, channeltron *etc.*).
4. 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. Peak list generation and annotation — (a) Generation of 'stick' spectrum	
Location of source ('raw') file, giving file name, type and Uniform Resource Indicator	The URI 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.
Parameters triggering the generation of peak lists from raw data, where appropriate	For 'tandem' experiments only: The total ion count threshold for a product ion scan 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 those separate scans.
Acquisition number (from the 'raw' file) of all acquisitions combined in the peak list, and whether summed or averaged.	The reference numbers of all the scans (as numbered in the raw file) that were combined to produce a peak list, and whether the peak list was produced by summing or averaging those scans that are listed.
Signal-to-noise estimation for spectrum	The ratio of signal to noise in a peak list for use as a quality control measure for spectra.
Smoothing; whether applied, plus algorithm	Any peak smoothing should be described, and the algorithm outlined.
Percentage peak height for centroiding	The percentage peak height at which centroids are calculated.
Background threshold, or algorithm used	The intensity cutoff used to filter background noise; or a description of the algorithm used to gate the noise, if complex.
Base peak m/z, where appropriate	If the intensities are scaled to that of a 'base peak' then the *m/z* of that base peak should be given.
Whether charge states calculated, spectrum deconvoluted and peaks de-isotoped	Firstly, the use of any of these three techniques should be made explicit; secondly, wherever a piece of software other than that named in *1(b)* has been used, the software's manufacturer, and its version, should be provided.
Precursor ion charge for tandem spectra	For PFF spectra, the charge of the precursor ion should be given.
Actual values of m/z and intensity	Of course, the actual data should be provided also…
4. Peak list generation and annotation — (b) Quantitation for selected ions	
Experimental protocol (e.g. iTRAQ)	Which mass tag technology is being used (*e.g.* stable isotope labelling).
Number of combined samples analysed	The number of experimental classes that are represented, each with its own different tag.
Quantitation approach (e.g. integration)	Whether the measured value is the area under SIC curve, max peak height or something else.
Normalisation technique	Describe briefly the normalisation strategy employed; *e.g.* take ratios, then normalise to a global average.
Location of quantitation data, giving the file name, type and Uniform Resource Indicator	The URI and filename under which the quantitation data file from the statistical analysis is stored, if available. Also give the type of the file where appropriate, or else a description of the software used to generate it.