MIAPE: Mass spectrometry

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Abstract
"MIAPE - Mass spectrometry" (MIAPE-MS) is one module of the Minimal Information About a Proteomics Experiment (MIAPE) documentation system. MIAPE is developed by the Proteomics Standards Initiative of the Human Proteome Organisation (HUPO-PSI). It aims at delivering a set of technical guidelines representing the minimal information required to report and sufficiently support assessment and interpretation of a proteomics experiment. This MIAPE-MS module is the result of a joint effort between the Mass Spectrometry group of HUPO-PSI and the proteomics community. It has been designed to specify a minimal set of information to document a mass spectrometry experiment. As for all MIAPE documents, these guidelines evolve and are made available on the PSI website at the url http://psidev.info.

MIAPE: Mass Spectrometry

Version 2.98, 13th August, 2012.

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 (re-)interpretation and (re-) assessment of the data and the potential reproduction of the work that generated it.

Introduction

This document is one of a collection of technology-specific modules that together constitute the Minimum Information about a Proteomics Experiment (MIAPE) reporting guidelines produced by the Proteomics Standards Initiative. MIAPE is structured around a parent document that lays out the principles to which the individual reporting guidelines adhere. In brief, a MIAPE module represents the minimum information that should be reported about a data set or an experimental process, to allow a reader to interpret and critically evaluate the conclusions reached, and to support their experimental corroboration. In practice a MIAPE module comprises a checklist of information that should be provided (for example about the protocols employed) when a data set is submitted to a public repository or when an experimental step is reported in a scientific publication (for instance in the materials and methods section). The MIAPE modules specify neither the format that information should be transferred in, nor the structure of the repository/text. However, PSI is not developing the MIAPE modules in isolation; several compatible data exchange standards are now well established and supported by public databases and data processing software in proteomics (for details see the PSI website www.psidev.info). For instance, the PSI Mass Spectrometry Standards Working Group has developed mzML, a data exchange standards in xml format that can store data and meta-data from a mass spectrometry experiment.

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. For a full discussion of the principles underlying this specification, please refer to the MIAPE parent document, which can be found on the MIAPE website http://psidev.info/miape.

These guidelines cover both the operation of a mass spectrometer and the generation of mass spectra from the 'raw' data. They do neither cover the delivery of sample to the mass spectrometer, nor 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.info/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 it will almost certainly be the case for all the MIAPE modules.

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

1. General features; summary information such as instrument manufacturer and model.
2. Ion sources; for example, matrix-assisted laser desorption ionisation (MALDI), electrospray ionisation.
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) or if the instrument has a hybrid

architecture, the requirements for the relevant components must be combined.

4. The data resulting from the procedure; the acquisition procedure, the method of generation of peak lists and the location of the raw data from which they were generated..

Changes relative to the previous release of MIAPE-MS (v.2.24): The elements related to quantitation have been deleted and are moved to a separate MIAPE module dedicated to quantitation aspects; a number of explicit terms have been removed to avoid overspecification; some elements have been restructured to improve clarity; other minor changes including improved definitions in the appendix.

Reporting guidelines for mass spectrometry

1. General features

1.1 Global descriptors
- Responsible person (or institutional role if more appropriate); provide name, affiliation and stable contact information
- Instrument manufacturer and model
- Customisations (summary)

2. Ion sources

As each spectrum is acquired using only one ionisation source, select the one that applies

2.1 Electrospray Ionisation (ESI)
- Supply type (static, or fed)
- Interface manufacturer, model
- Sprayer type, manufacturer, model
- Other parameters if discriminant for the experiment

2.2 MALDI
- Plate composition (or type)
- Matrix composition
- PSD (or LID/ISD) summary, if performed
- Laser type and wavelength,
- Other laser and source related parameters, if discriminating for the experiment

2.3 Other ionisation source
- Description of the ion source and relevant parameters

3. Post-source component

As an MS spectrum or chromatogram performed on one instrument cannot be acquired using all existing analysers and detectors, select the elements that apply

3.1 Analyser
- Ion optics, 'simple' quadrupole, hexapole, Paul trap, linear trap, magnetic sector, FT-ICR, Orbitrap: name of the analyser(s)
- Time-of-flight drift tube (TOF): Reflectron status

3.2 Activation / dissociation

The associated acquisition parameters are covered in 4.1
- Instrument component where the activation / dissociation occurs
- Gas type (when used)
- Activation / dissociation type

4. Spectrum and peak list generation and annotation

4.1 Data acquisition
- Software name and version
- Acquisition parameters

4.2 Data analysis
- Software name and version
- Parameters used in the generation of peak lists or processed spectra

4.3 Resulting data

The following information should be provided for each dataset
- Location of source ("raw") and processed files
- The chromatogram(s) for SRM data and other relevant cases

The following information should be provided for each spectrum or peaklist
- *m/z* and intensity values
- MS level
- Ion mode
- For MS level 2 and higher, precursor *m/z* and charge if known, with the full mass spectrum / peaklist containing that precursor peak, where available.

Summary

The MIAPE: MS minimum reporting guidelines 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. Providing the information required by this document will enable both the effective interpretation and assessment of mass spectral data and potentially, the reproduction of the work that generated it. Much of the required information should be reusable from existing files, or exportable from the instrument; we expect 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.info.

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

Classification	*Definition*
1. General features — 1.1 Global descriptors	
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.
Instrument manufacturer, model	The manufacturing company and model name for the mass spectrometer.
Customisations (summary)	Any significant (*i.e.* affecting behaviour) deviations from the manufacturer's specification for the mass spectrometer.
2. Ion sources — 2.1 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, such as in static infusion.
Interface manufacturer, model	The manufacturing company and model name for the interface; list any modifications made to the standard specification. If the interface is entirely custom-built, describe it or provide a reference if available.
Sprayer type, manufacturer, model	The manufacturing company and model name for the sprayer; list any modifications made to the standard specification. If the sprayer is entirely custom-built, describe it briefly or provide a reference if available.
Other parameters if discriminant for the experiment	Where appropriate, and if considered as discriminating elements of the source parameters, describe these values.
2. Ion sources — 2.2 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.
Matrix composition	The material in which the sample is embedded on the target (*e.g.* alpha-cyano-4-hydroxycinnamic acid).
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, summarise the stepwise reduction of reflector voltage).
Laser type and wavelength	The type of laser and the wavelength (nm) of the generated pulse. For instance nitrogen, 337 nm.
Other laser and source related parameters, if discriminating for the experiment	Other details of the laser used to shoot at the matrix-embedded sample if considered important for the interpretation of data; this might include the pulse energy, focus diameter, attenuation details, pulse duration at full-width half maximum, frequency of shots in Hertz and average number of shots fired to generate each combined mass spectrum.
2. Ion sources — 2.3 Other ion source	
Description of the ion source and relevant parameters	Describe the ion source and provide relevant and discriminating parameters for its use.

3. Post source component — 3.1 Analyser	
Ion optics, 'simple' quadrupole, hexapole, Paul trap, linear trap, magnetic sector, FT-ICR, Orbitrap: name of the analyser(s)	Describe the analyser(s) used in the MS experiment. Example might be MS1 survey scans in an Orbitrap and MSn analysed in a linear trap; No other parameters to be captured here.
Time-of-Flight drift tube: Reflectron status	Reflectron status (on, off, none) when status can be set.
3. Post-source component — 3.2 Activation / dissociation	
Instrument component where the activation / dissociation occurs	The hardware element where activation and/or dissociation occurs. For instance a quadrupole collision cell, a 3D ion trap, the ion source (for ISD, PSD, LID, isCID)
Gas type (when used)	The composition and pressure of the gas used to fragment ions, for instance in the collision cell.
Activation / dissociation type	The type of activation an/or dissociation used in the fragmentation process. Examples might include Collision Induced Dissociation (CID) with a static or spread collision energy, Electron Transfer Dissociaton (ETD) with provided activator molecules.
4. Spectrum and peak list generation and annotation — 4.1 Data acquisition	
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 of them. Mention also upgrades not reflected in the version number.
Acquisition parameters	The information on how the MS data have been generated. It describes the instrument's parameter settings / acquisition method file or information describing the acquisition conditions and settings of the MS run. Ideally this should be a URI+filename, for example an export of the acquisition method (and Tune page or other relevant information where appropriate). This includes for instance if the data are acquired and primarily stored in a profile or centroid mode. An explicit text description of the acquisition process is also desirable. This includes the acquisition sequence (for instance as simplified as top-five method with a cycle made of one full MS1 scan in the Orbitrap, followed by a precursor selection of 5 most intense ions applying an exclusion window of 30 seconds and followed by the acquisition of 5 product ion scans generated in the LTQ analyser, and detected in the LTQ). This allows to differentiate between the use of a selected precursor window vs unselected fragmentation (MS`E/bbCID/AIF). This also allows to explicitely describe pre-defined the acquisition method of a SRM experiment where all transitions and detection windows are specified.
4. Spectrum and peak list generation and annotation — 4.2 Data analysis	
Software name and version	The MS data analysis package name, and version; where there are several pieces of software involved, give name, version and role for each one. Mention also upgrades not reflected in the version number.
Parameters used in the generation of peak lists or processed spectra	The information on how the spectra have been processed. This include the list of parameters triggering the generation of peak lists, chromatograms, images from raw data or already processed data and the order in which they have been used. This can be a list or a parameters file.
4. Spectrum and peak list generation and annotation — 4.3 Resulting data	
Location of source ('raw') and processed files	The location and filename under which the original raw data file(s) from the mass spectrometer and the processed file(s) are stored. Also give the type of the file where appropriate. Ideally this should be a URI+filename.
The chromatogram(s) for SRM data and other	The chromatogram as array of time and intensity values. Provide the type and descriptors (for instance the explicit

relevant cases	transition for a SRM trace, TIC with selected mass range when available, XIC with selected m/z and tolerance, BPC with the m/z range considered).
m/*z* and intensity values	The actual data (m/z and intensity) for each spectrum. This is most often provided in the spectra and/or peaklist file.
MS level	The MS level (*e.g.* MS^2) at which each spectrum was acquired. This is most often provided in the spectra or peaklist file
Ion mode	The ion mode (positive or negative). This is most often provided in the spectra or peaklist file.
For MS level 2 and higher, precursor m/z and charge if known, with the full mass spectrum / peaklist containing that precursor peak, where available.	For tandem spectra; in addition to the preceeding information,the precursor m/z value and the charge state of the precursor ion should also be given; the mass spectrum used to deduce the precursor information should also be provided.