**Appendix One .** The MIAPE-QC glossary of items

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| **Classification** | **References** | **Definition** | **Details** |
| 1. General features - 1.1 Global descriptors | | | |
| Contact attribute | PSI-MS: contact attribute/MS\_1000585  MIAPE-MS: responsible person or role  MIAPE-MSI: responsible person or role  MIAPE-Quant: responsible person or role  MIAPE-CC: responsible person or role | Details about a person or organization to contact in case of concern or discussion about the file. | 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. |
| Instrument model | PSI-MS: instrument model/MS\_1000031  MIAPE-MS: Instrument model | Instrument model name not including the vendor’s name. | The manufacturing company and model name for mass spectrometer. |
| Customization | PSI-MS: customization/MS\_1000032  MIAPE-MS: Instrument customisations | Free text description of a single customization made to the instrument; for several modifications, use several entries. | Any significant deviations from the manufacturer’s specification for the mass spectrometer. |
| Sample | PSI-MS: Sample/MS:1000457  MIAPE-CC: Brief description of sample | Terms to describe the sample. | A description of the source, such as means of collection, volume, concentration or previous step of processing. Include information about tags, molecular mass, pH and anything else relevant to experiment. In a multi-dimensional separation, this should contain the name of the fraction from the previous dimension. |
| Mass spectrometer file format | PSI-MS: mass spectrometer file format/MS\_1000560  MIAPE-MS: location of source and processed files | The format of the file being used. This could be a instrument or vendor specific proprietary file format or a converted open file format. | The location of the data generated. Ideally this should be an URI + filename. |
| 2. MS acquisition parameters - 2.1 Chromatography | | | |
| Chromatogram count | QCML: Chromatogram count/QC:0000008 | Contains the number of chromatograms recorded. | Contains the number of chromatograms recorded. |
| Fraction of repeat peptide identifications with divergent RT |  | Fraction of all peptides identified at least 4 min earlier/latter than max full MS scan. | Fraction of all peptides identified at least 4 min earlier/latter than max full MS scan. |
| Retention time (retention time ranges, max/min retention time and interquartile retention time period) | PSI-MS: retention time/MS\_1000894  QCML: MS RT acquisition ranges/QC:0000012 | A time interval from the start of chromatography when an analyte exits a chromatographic column. /  Contains the min/max RT range boundaries observed during MS acquisition. | Provide min/max retention time range observed, time period over which 50% of peptides were identified and rate of peptide identification during time period over which 50% of peptides were identified. |
| Peak widths at half-height for identifications |  |  | Provide median peak widths for all identified unique peptides and measure of the distribution of the peak widths. |
| Peak widths at half-max over RT deciles for identifications |  |  | Median peak width for identified peptides in last/first/median RT decile. |
| Average elution order difference |  |  | Provide average elution rank order difference for identified peptides between series and provide radio of average rank order difference between series to average rank order difference within a series(low values indicate similarity between series). |
| Fraction of early eluting peptides in row series |  |  | Estimates relative frequency of early/late eluting peptides. |
| 2. MS acquisition parameters - 2.2 Ion source | | | |
| MZ | QCML: MS MZ acquisition ranges/QC:0000009 |  | Provide median MZ for all identified peptides, min/max MZ range boundaries observed, minimum MZ detected and maximum MZ detected. |
| MS1 during middle(and early)peptide retention |  |  | Number of times where full MS scan signal greatly decreased between adjacent scans more/less than 10-fold. |
| Identifications by charge state |  |  | Number of 1+/3+/4+ peptides over 2+ peptides. |
| 2. MS acquisition parameters - 2.3 Full MS scan signal | | | |
| Ion injection time | QCML: MS1 injection time/QC:0000017 | Contains the accumulation time in the ion trap device used in machine settings during MS acquisition. | Full MS scan ion injection time. |
| Full MS scan time | QCML: MS1 scan time/QC:0000019 |  | Average scan time for Full MS scan used in machine settings. |
| Median signal-to-noise value |  |  | Median signal-to-noise value for full MS spectra up to and including time period over which 50% of peptides were identified. |
| XIC value | PSI-MS: Total XIC area/MS:1002412 | Summed area of all the extracted ion chromatogram for the peptide (e.g. of all the transitions in SRM). | Provide the median XIC value for identified peptides over same time period as used for median signal-to-noise value. |
| MS1 ID max |  |  | Ratio of 95th over 5th percentile full MS scan maximum intensity values for identified peptides and median maximum full MS scan value for identified peptides |
| MS1 intensity variation for peptides |  |  | Average of between series intensity variations for identified peptides and the ratio of average intensity variation between series to average intensity variation within a series. |
| Precursors |  |  | Provide table of measured precursor ions over retention time/mz. |
| Precursor m/z - Peptide ion m/z |  |  | Provide the median real value of precursor errors, the mean of the absolute precursor errors, the median real value of precursor errors in ppm, the Interquartile distance in ppm of the precursor errors. |
| Delta ppm | QCML: Delta ppm/QC:0000039 |  | Provide the deviation/mean deviation/median deviation of the precursor ion mass(es) from the theoretical mass(es) of the matched identification(s). |
| Full MS scan spectra count | QCML: MS1 spectra count/QC:0000006 | Contains the number of MS1 spectra recorded. | Number of full MS scan spectra. |
| 2. MS acquisition parameters - 2.4 Dynamic sampling | | | |
| Ratios of peptide ions IDed by different numbers of spectra |  |  | Ratio of peptides identified by 1 spectrum divided by number identified by 2 spectra. And Ratio of peptides identified by 2 spectrum divided by number identified by 3 spectra. |
| Spectrum counts |  |  | Number of full MS scans taken over time period over which 50% of peptides were identified and number of tandem MS scans taken over time period over which 50% of peptides were identified. |
| Full MS scan max/full MS scan sampled abundance ratio |  |  | Ratio of full MS scan maximum to full MS scan value at sampling for median decile of peptides by full MS scan maximum intensity. |
| 2. MS acquisition parameters - 2.5 Tandem MS scan signal | | | |
| Tandem MS spectra count | QCML: MS2 spectra count/QC:0000007 | Contains the number of MS2 spectra recorded. | Number of tandem MS scan spectra. |
| Tandem MS scan time | QCML: MS2 scan time/QC:0000012 | Contains the average scan time for a MS2 event used in machine settings during MS acquisition. | Average scan time for Tandem MS event used in machine settings. |
| Tandem MS injection time | QCML: MS2 injection time/QC: 0000018 | Contains the accumulation time in the ion trap device used in machine settings during MS acquisition. | Tandem MS ion injection time. |
| Tandem MS identification peaks |  |  | Provide the number and median number of peaks in an Tandem MS scan |
| Fracion of tandem MS at different full MS max quartiles |  |  | Fraction of total tandem MS scans identified in the first/second/third/last quartile of peptides sorted by full MS scans maximum intensity. |
| 3. MS identification parameters - 3.1 Spectrum identification | | | |
| Estimated spectra FDR |  |  | Provide the false discovery rate of the estimated spectra. |
| ID spectra ratio |  |  | The number of identified spectra vs. The number of total spectra. |
| Precursor error |  |  | Provide the maximum and median number of precursor error. |
| 3. MS identification parameters - 3.2 Peptide identification | | | |
| Estimated peptide FDR |  |  | Provide the false discovery rate of the estimated peptide. |
| ID peptide ratio |  |  | The number of identified peptides vs. The number of recorded Tandem MS spectrum. |
| Average spectra count per peptide |  |  | Average number of spectra matched to one peptide. |
| Average peptide ion count per peptide |  |  | Average peptide ion count per peptide. |
| Cleavages | QCML: total number of missed cleavages/QC:0000037 | This number indicates the number missed cleavages that were identified. | Total number of missed cleavages. |
| Peptide counts | QCML: total number of identified peptides | This number indicates the number peptides that were identified. | Provide ratio of semi/fully tryptic peptide IDs, ratio of non-tryptic peptide IDs as well as ratio of missed-cleavage peptide IDs. |
| Ions |  |  | Provide the number of tryptic peptide identified. |
| TIC | QCML: TIC slump/QC:0000023 | The percentage of tic slumps below 10k. | Provide table of total ion currents detected in each of a series of mass spectrum and the number of tic slumps below 10K. |
| Total number of PSMs | QCML: Total number of PSMs/QC:0000029 | This number indicates the number of spectra that were given peptide annotations. | This number indicates the number of spectra that were given peptide annotations. |
| 3.MS identification parameters - 3.2 Protein identification | | | |
| Protein count | QCML: total number of identified proteins/QC:0000032 | This number indicates the number proteins that were identified. | Total number of identified proteins. |
| Uniquely protein count | QCML: total number of uniquely identified proteins/QC: 0000033 | This number indicates the number proteins that were uniquely identified. | Total number of uniquely identified proteins. |
| Modified peptides count | QCML: total number of modified peptides/QC:0000034 | This number indicates the number modified peptide sequences that were identified (after FDR). | The number of spectra that were given peptide annotations. |
| Protein coverage |  |  | Provide median and average protein coverage. Meanwhile, provide protein coverage for each protein. |
| One peptide protein ratio |  |  | Provide the ratio of one peptide protein. |
| Estimated protein FDR |  |  | Provide the false discovery rate of the estimated protein. |
| Average spectra count per protein |  |  | Provide average spectra count per protein. |
| Average peptide count per protein |  |  | Provide average peptide count per protein. |
| 3.MS identification parameters - 3.3 Protein group and inference | | | |
| Protein count for parsimony protein group |  |  | Provide the average and median protein count for parsimony protein group. |
| Missed protein group |  |  | Missed protein group in the parsimony protein list. |
| Protein group ratio |  |  | Provide ratio of unique protein group to parsimony protein group |
| 4.MS quantification parameters - 4.1 Quantification parameters | | | |
| Features | QCML: Features/QC:0000047 | The tables of features over RT/mz. | Table of features over retention time/mz. |
| Number of features | QCML: Number of features/QC:0000046 | The number of features reported | The number of features reported. |
| Median quantification deviation |  |  | The median quantification deviation for each protein ions. |
| Median peptide quantification deviation |  |  | Provide the median peptide quantification deviation for same protein. |