mzTab 1.1 Proteomics specific parts

There are no immediate plans to begin work on a proteomics version 1.1, but this document serves as a placeholder for notes and sections removed from the 1.1-M draft.

## Proteomics Metadata

The metadata fields in this section MAY be reported in a proteomics type file, but MUST NOT be reported in a metabolomics file.

### protein\_search\_engine\_score[1-n]

|  |  |
| --- | --- |
| **Description:** | The type of protein search engine score MUST be reported as a CV parameter [1-n].  The order of the search engine scores SHOULD reflect their importance for the identification and be used to determine the identification’s rank. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | ✓ | ✓ | | Identification | ✓ | ✓ | |
| **Example:** | MTD protein\_search\_engine\_score[1] [MS, MS:1001171, Mascot:score,] |

### peptide\_search\_engine\_score[1-n]

|  |  |
| --- | --- |
| **Description:** | The type of peptide search engine score MUST be reported as a CV parameter [1-n].  The order of the search engine scores SHOULD reflect their importance for the identification and be used to determine the identification’s rank. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | ✓ | ✓ | | Identification | ✓ | ✓ | |
| **Example:** | MTD peptide\_search\_engine\_score[1] [MS, MS:1001171, Mascot:score,] |

### psm\_search\_engine\_score[1-n]

|  |  |
| --- | --- |
| **Description:** | The type of psm search engine score MUST be reported as a CV parameter [1-n].  The order of the search engine scores SHOULD reflect their importance for the identification and be used to determine the identification’s rank. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | ✓ | ✓ | | Identification | ✓ | ✓ | |
| **Example:** | MTD psm\_search\_engine\_score[2] [MS, MS:1001330, X!Tandem:expect,] |

### fixed\_mod[1-n]

|  |  |
| --- | --- |
| **Description:** | A parameter describing a fixed modifications searched for. Multiple fixed modifications are numbered 1..n. If no fixed modifications are searched, include the CV param MS:1002453: No fixed modifications searched. |
| **Type:** | Param |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | ✓ | ✓ | | Identification | ✓ | ✓ | |
| **Example:** | MTD fixed\_mod[1] [UNIMOD, UNIMOD:4, Carbamidomethyl, ]  MTD fixed\_mod[2] [UNIMOD, UNIMOD:35, Oxidation, ]  MTD fixed\_mod[3] [CHEMMOD, CHEMMOD:-18.0913, , ] |

### fixed\_mod[1-n]-site

|  |  |
| --- | --- |
| **Description:** | A string describing a fixed modifications site. Following the unimod convention, modification site is a residue (e.g. “M”), terminus (“N-term” or “C-term”) or both (e.g. “N-term Q” or “C-term K”). |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD fixed\_mod[1] [UNIMOD, UNIMOD:35, Oxidation, ]  MTD fixed\_mod[1]-site M  …  MTD fixed\_mod[2] [UNIMOD, UNIMOD:1, Acetyl, ]  MTD fixed\_mod[2]-site N-term  …  MTD fixed\_mod[3] [UNIMOD, UNIMOD:2, Amidated, ]  MTD fixed\_mod[3]-site C-term |

### fixed\_mod[1-n]-position

|  |  |
| --- | --- |
| **Description:** | A string describing the term specifity of a fixed modification. Following the unimod convention, term specifity is denoted by the strings “Anywhere”, “Any N-term”, “Any C-term”, “Protein N-term”, “Protein C-term”. |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD fixed\_mod[1] [UNIMOD, UNIMOD:35, Oxidation, ]  MTD fixed\_mod[1]-site M  …  MTD fixed\_mod[2] [UNIMOD, UNIMOD:1, Acetyl, ]  MTD fixed\_mod[2]-site N-term  MTD fixed\_mod[2]-position Protein N-term  …  MTD fixed\_mod[3] [UNIMOD, UNIMOD:2, Amidated, ]  MTD fixed\_mod[3]-site C-term  MTD fixed\_mod[3]-position Protein C-term |

### variable\_mod[1-n]

|  |  |
| --- | --- |
| **Description:** | A parameter describing a variable modification searched for. Multiple variable modifications are numbered 1.. n. If no variable modifications were searched, include the CV param MS:1002454: No variable modifications searched. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | ✓ | ✓ | | Identification | ✓ | ✓ | |
| **Example:** | MTD variable\_mod[1] [UNIMOD, UNIMOD:21, Phospho, ]  MTD variable\_mod[2] [UNIMOD, UNIMOD:35, Oxidation, ]  MTD variable\_mod[3] [CHEMMOD, CHEMMOD:-18.0913, , ] |

### variable\_mod[1-n]-site

|  |  |
| --- | --- |
| **Description:** | A string describing a variable modifications site. Following the unimod convention, modification site is a residue (e.g. “M”), terminus (“N-term” or “C-term”) or both (e.g. “N-term Q” or “C-term K”). |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD variable\_mod[1] [UNIMOD, UNIMOD:35, Oxidation, ]  MTD variable\_mod[1]-site M  …  MTD variable\_mod[2] [UNIMOD, UNIMOD:1, Acetyl, ]  MTD variable\_mod[2]-site N-term  …  MTD variable\_mod[3] [UNIMOD, UNIMOD:2, Amidated, ]  MTD variable\_mod[3]-site C-term |

### variable\_mod[1-n]-position

|  |  |
| --- | --- |
| **Description:** | A string describing the term specifity of a variable modification. Following the unimod convention, term specifity is denoted by the strings “Anywhere”, “Any N-term”, “Any C-term”, “Protein N-term”, “Protein C-term”. |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD variable\_mod[1] [UNIMOD, UNIMOD:35, Oxidation, ]  MTD variable\_mod[1]-site M  …  MTD variable\_mod[2] [UNIMOD, UNIMOD:1, Acetyl, ]  MTD variable\_mod[2]-site N-term  MTD variable\_mod[2]-position Protein N-term  …  MTD variable\_mod[3] [UNIMOD, UNIMOD:2, Amidated, ]  MTD variable\_mod[3]-site C-term  MTD variable\_mod[3]-position Protein C-term |

### protein-quantification\_unit

|  |  |
| --- | --- |
| **Description:** | Defines what type of units is reported in the protein quantification fields. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | (✓)1 | (✓)1 | | Identification |  |  |   1mandatory if protein section is present |
| **Example:** | MTD protein-quantification\_unit [PRIDE, PRIDE:0000395, Ratio, ] |

### peptide-quantification\_unit

|  |  |
| --- | --- |
| **Description:** | Defines what type of units is reported in the peptide quantification fields. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | (✓)1 | (✓)1 | | Identification |  |  |   1mandatory if peptide section is present |
| **Example:** | MTD peptide-quantification\_unit [PRIDE, PRIDE:0000395, Ratio, ] |

### colunit-protein

|  |  |
| --- | --- |
| **Description:** | Defines the unit for the data reported in a column of the protein section. The format of the value has to be {column name}={Parameter defining the unit}  This field MUST NOT be used to define a unit for quantification columns. The unit used for protein quantification values MUST be set in *protein-quantification\_unit*. |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD colunit-protein molecular\_mass=[UO, UO:0000222, kilodalton,] |

### colunit-peptide

|  |  |
| --- | --- |
| **Description:** | Defines the used unit for a column in the peptide section. The format of the value has to be {column name}={Parameter defining the unit}  This field MUST NOT be used to define a unit for quantification columns. The unit used for peptide quantification values MUST be set in peptide-quantification\_unit. |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD colunit-peptide retention\_time=[UO,UO:0000031, minute,] |

### colunit-psm

|  |  |
| --- | --- |
| **Description:** | Defines the used unit for a column in the PSM section. The format of the value has to be {column name}={Parameter defining the unit}  This field MUST NOT be used to define a unit for quantification columns. The unit used for peptide quantification values MUST be set in peptide-quantification\_unit. |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | |
| **Example:** | MTD colunit-psm retention\_time=[UO,UO:0000031, minute,] |

### assay[1-n]-quantification\_reagent

|  |  |
| --- | --- |
| **Description:** | The reagent used to label the sample in the assay. For label-free analyses the “unlabeled sample” CV term SHOULD be used for proteomics cases, optional for metabolomics. For the “light” channel in label-based experiments the appropriate CV term specifying the labelling channel should be used. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification | (✓)1 | ✓ | | Identification | 2 | 2 | | Metabolomics |  |  |   1mandatory if quantification is reported on assays  2not recommended for identification only files |
| **Example:** | MTD assay[1]-quantification\_reagent [PRIDE,PRIDE:0000114,iTRAQ reagent,114] MTD assay[2]-quantification\_reagent [PRIDE,PRIDE:0000115,iTRAQ reagent,115]  OR  MTD assay[1]-quantification\_reagent [MS,MS:1002038,unlabeled sample,]  OR  MTD assay[1]-quantification\_reagent [PRIDE, PRIDE:0000326, SILAC light]  MTD assay[2]-quantification\_reagent [PRIDE, PRIDE:0000325, SILAC heavy] |

### assay[1-n]-quantification\_mod[1-n]

|  |  |
| --- | --- |
| **Description:** | A parameter describing a modification associated with a quantification\_reagent. Multiple modifications are numbered 1..n. |
| **Type:** | Parameter |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification | 1 | 1 |   1 not recommended for identification only files |
| **Example:** | MTD assay[2]-quantification\_mod[1] [UNIMOD, UNIMOD:188, Label:13C(6), ] |

### assay[1-n]-quantification\_mod[1-n]-site

|  |  |
| --- | --- |
| **Description:** | A string describing the modifications site. Following the unimod convention, modification site is a residue (e.g. “M”), terminus (“N-term” or “C-term”) or both (e.g. “N-term Q” or “C-term K”). |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification | 1 | 1 |   1 not recommended for identification only files |
| **Example:** | MTD assay[2]-quantification\_mod[1] [UNIMOD, UNIMOD:188, Label:13C(6), ]  MTD assay[2]-quantification\_mod[2] [UNIMOD, UNIMOD:188, Label:13C(6), ]  MTD assay[2]-quantification\_mod[1]-site R  MTD assay[2]-quantification\_mod[2]-site K |

### assay[1-n]-quantification\_mod[1-n]-position

|  |  |
| --- | --- |
| **Description:** | A string describing the term specifity of the modification. Following the unimod convention, term specifity is denoted by the strings “Anywhere”, “Any N-term”, “Any C-term”, “Protein N-term”, “Protein C-term”. |
| **Type:** | String |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification | 1 | 1 |   1 not recommended for identification only files |
| **Example:** | MTD assay[2]-quantification\_mod[1] [UNIMOD, UNIMOD:188, Label:13C(6), ]  MTD assay[2]-quantification\_mod[2] [UNIMOD, UNIMOD:188, Label:13C(6), ]  MTD assay[2]-quantification\_mod[1]-site R  MTD assay[2]-quantification\_mod[2]-site K  MTD assay[2]-quantification\_mod[1]-position Anywhere  MTD assay[2]-quantification\_mod[2]-position Anywhere |

### false\_discovery\_rate

|  |  |
| --- | --- |
| **Description:** | The file’s false discovery rate(s) reported at the PSM, peptide, and/or protein level for proteomics, or for small molecules in Metabolomics. False Localization Rate (FLD) for the reporting of modifications can also be reported here. Multiple parameters MUST be separated by “|”. |
| **Type:** | Parameter List |
| **Mandatory** | |  |  |  | | --- | --- | --- | |  | Summary | Complete | | Quantification |  |  | | Identification |  |  | | Metabolomics |  |  | |
| **Example:** | MTD false\_discovery\_rate [MS, MS:1001364, pep:global FDR, 0.01]|…  [MS, MS:1001214, prot:global FDR, 0.08] |