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mzIdentML: exchange format for peptides and proteins identified from mass spectra

Status of This Document

This document presents a final specification for the mzIdentML data format developed by the HUPO Proteomics Standards Initiative. Distribution is unlimited.

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Abstract

The Human Proteome Organisation (HUPO) Proteomics Standards Initiative (PSI) defines community standards for data representation in proteomics to facilitate data comparison, exchange and verification. The Proteomics Informatics Working Group is developing standards for describing the results of identification and quantitation processes for proteins, peptides and protein modifications from mass spectrometry. This document defines an XML schema that can be used to describe the outputs of proteomics search engines or similar software for peptide/protein identification from mass spectrometry (MS) data.

Contents

1. Introduction

1.1 Background

This document addresses the systematic description of (poly)peptide identification and characterisation based upon mass spectrometry (MS). A large number of different proteomics search engines are available that produce output in a variety of different formats. It is intended that mzIdentML will provide a common standard format for identification results to support a range of scenarios encountered in proteome informatics. mzIdentML has been developed with a view to supporting the following general tasks (more specific use cases are provided in Section 2):

T1. *The discovery of relevant results,* so that, for example, data sets in a database that use a particular technique or combination of techniques can be identified and studied by experimentalists during experiment design or data analysis.
T2. *The sharing of best practice*, so that, for example, analyses that have been particularly successful at identifying a certain group of peptides/proteins can be interpreted by consumers of the data.
T3. *The evaluation of results*, so that, for example, sufficient information is provided about how a particular analysis was performed to allow the results to be critically evaluated.
T4. *The sharing of data sets,* so that, for example, public repositories can import or export data, or multi-site projects can share results to support integrated analysis.
T5. *The creation of a format for input to analysis software*, for example, allowing software to be designed that provides a meta-score over the output from several search engines.
T6. *An internal format for pipeline analysis software*, for example, allowing analysis software to store intermediate results from different stages of an identification pipeline, prior to the final results being assembled in a single mzIdentML file.

This document presents a specification, not a tutorial. As such, the presentation of technical details is deliberately direct. The role of the text is to describe the model and justify design decisions made. The document does not discuss how the models should be used in practice, consider tool support for data capture or storage, or provide comprehensive examples of the models in use. Tutorial material can be located on the PSI website (see http://www.psidev.info/mzidentml).

1.2 Document Structure

The remainder of this document is structured as follows. Section 2 lists use cases mzIdentML is designed to support. Section 3 describes the terminology used. Section 4 describes how the specification presented in Section 4 relates to other specifications, both those that it extends and those that it is intended to complement. Section 6 contains the documentation for the XML schema which is generated automatically and several parts of the schema are documented in more detail in Section 7. Conclusions are presented in Section 8.

2. Use Cases for mzIdentML

The following use cases have driven the development of the mzIdentML data model and XML schema, and are used to define the scope of the format in the current version.

1. It should be possible to create a tool that loads an mzIdentML document and enables users to examine results from an MS or MSn analysis. However, there is no support for aggregating evidence from multiple MS levels. There should be sufficient information for the tool to generate output reports that conform to the requirements made by journals for publication and that conform to the relevant MIAPE guidelines. For example:
   · For a Peptide Mass Fingerprint (PMF) search, it should be possible to display the spectrum and show the matches of the peaks to the relevant peptides.
   · For an MS/MS search, it should be possible to locate which spectrum matched to which peptide in the original file.
2. There should be sufficient information stored in the instance document to enable a user to run the same or a similar search on the same or another search engine. This means that all search parameters should be described in sufficient detail and that sufficient information is available to determine which database (if any) the data were searched against. The peak lists data do not need to be included in the instance document, but do need to be suitably referenced.
3. It should be possible to save the results of searching a decoy database in the same instance document as the results from the target database. It should then be possible to write a viewer application that enables a user to investigate the effect of changing, for example, a threshold value on the false discovery rate. This would only be possible if results that are generally considered lower quality from the search are also saved in the mzIdentML document (rather than just top matches) and if the results from the decoy search are also saved. It would only be possible to do this at the peptide level for an MS/MS search, because changing thresholds would normally have some effect on the protein grouping algorithm.
4. It should be possible to save manual or automated annotation of proteins/peptides in an instance document. A third party tool could be used to save annotations and validations of identified proteins/peptides to an existing instance document.

5. It should be possible to save the results from a search of a metabolically labelled sample. For example, with a 14N/15N experiment, two separate sets of amino acid masses are used, and it must be possible to tell which masses were used for each peptide result.
6. For a search of multiple peak lists, it should be possible to identify the spectrum that matched a particular peptide or protein reported by the search engine. For example, in an LC-MS/MS run, it should be possible to refer back to the spectrum in the peak list file that was searched and from there, if the information is available, to be able to determine the retention time of the spectrum.
7. It should be possible to search a file to retrieve all molecules that have a specified modification.
8. It should be possible to store the results of a search of spectra against other spectra - i.e. a spectral library search.
9. It should be possible to store the results of a top down search i.e. analysis of complete proteins.
10. Support should be provided for storing fragmentation data so that for example viewers could display which ions in the input data match predicted ion fragment masses.
11. There should be support for storing the results of searches of peptides against nucleic acid databases, including the information about which translation frame the matches were found in.
12. It should be possible to combine the results from multiple search engines into one mzIdentML document. For example, the peptide spectrum matches (PSMs) from two or more different search engines could be combined using a third tool to give one set of protein results.
13. It should be possible to store *de novo* peptide sequencing results, to the extent that it will be possible to enumerate and record all possible matches found by a *de novo* technique. However, we anticipate that this can produce large files.
14. It should be possible to store the results of MS/MS cross-linking approaches, whereby two peptides cross-linked using chemical reagents or biologically occurring modifications have been identified (newly added in mzIdentML 1.2).
15. It should be possible to store at a basic level of detail the molecular interaction data that can be inferred from cross-linking approaches (newly added in mzIdentML 1.2).
16. It should be possible to represent statistical values or scores associated with the positions of modifications on a peptide chain (newly added in mzIdentML 1.2).
17. It should be possible to represent statistical values or scores associated with peptide identifications, formed from groups of redundant peptide-spectrum matches (PSMs) reporting on the same peptide (newly added in mzIdentML 1.2).
18. It should be possible to capture the output of proteogenomics analyses such as the mapping of peptides to gene models and chromosomes (newly added in mzIdentML 1.2).

There should be limited support for:
1. Sequence tagging, in which short sequences defined by a *de novo* process are used to characterize spectra. The final results from a sequence-tag-filtered search can be stored in mzIdentML, but the details of tag generation and filtering cannot.

The following use cases will not be supported in version 1.2 of mzIdentML:
1. It should be possible to store relative and absolute quantitation information at the peptide and protein level using all the popular techniques – this is captured in mzQuantML and also in mzTab.
2. Support for complex workflows where multiple data processing algorithms are combined in a pipeline; i.e. only “final” results are represented in mzIdentML v1.2 in one protein list.

3. Concepts and Terminology

This document assumes familiarity with XML Schema notation (www.w3.org/XML/Schema). The key words “MUST,” “MUST NOT,” “REQUIRED,” “SHALL,” “SHALL NOT,” “SHOULD,” “SHOULD NOT,” “RECOMMENDED,” “MAY,” and “OPTIONAL” are to be interpreted as described in RFC-2119 (http://www.ietf.org/rfc/rfc2119.txt).

4. Relationship to Other Specifications

The specification described in this document is not being developed in isolation; indeed, it is designed to be complementary to, and thus used in conjunction with, several existing and emerging models. Related specifications include the following:

1. *MIAPE MSI* (http://www.psidev.info/groups/miape) The Minimum Information About a Proteomics Experiment: Mass spectrometry Informatics document defines a checklist of information that should be reported about such a study.
2. *mzML* (http://www.psidev.info/mzml). mzML is the PSI standard for capturing mass spectra / peak lists resulting from MS in proteomics. It is RECOMMENDED that mzIdentML should be used in conjunction with mzML, although it is possible to use mzIdentML with other formats of mass spectra. This document does not assume familiarity with mzML (1).
3. *mzQuantML* (http://www.psidev.info/mzquantml). mzQuantML is the PSI standard for capturing quantitative proteomics data from MS (2) mzQuantML files that report quantitative data MAY reference mzIdentML files containing the detailed identification data.
4. *mzTab* (http://www.psidev.info/mztab). mzTab is the PSI standard that can represent identification and quantification results at different levels of detail, in a tab-delimited format (3). mzTab results can represent a subset of all the information included in a mzidentML file. However, in mzTab 1.0 while there is support for some of the new features represented in mzidentML 1.2 (e.g. ambiguity in the modification position), other features are not explicitly supported (e.g. cross-linking). mzTab files MAY reference mzIdentML files.
5. *PSI-MI XML / MITAB* (http://www.psidev.info/groups/molecular-interactions). The PSI has developed specifications for molecular interaction evidence in XML format (PSI-MI) and tab-separated (MITAB). When MS cross-linking data is stored in mzIdentML, including evidence for protein interactions, the file can act in a complementary manner (e.g. providing source data) to a PSI-MI (4) or MITAB file.

4.1 The PSI Mass Spectrometry Controlled Vocabulary (CV)

The PSI-MS controlled vocabulary (CV) (5) is intended to provide terms for annotation of mzML, mzIdentML, mzQuantML and other PSI standard file formats. The CV has been generated by collection of terms from software vendors and academic groups working in the area of MS and proteome informatics. Some terms describe attributes that must be coupled with a numerical value attribute in the <cvParam> element (e.g. MS:1001191 “p-value”) and optionally a unit for that value (e.g. MS:1001117, “theoretical mass”, units = dalton). The terms that require a value are denoted by having a “datatype” key-value pair in the CV itself: MS:1001172 "mascot:expectation value" value-type:xsd:double. Terms that need to be qualified with units are denoted by having a “has_units” key in the CV itself (relationship: has_units: UO:0000221 ! dalton). The details of which terms are allowed or required in a given schema section is reported in the mapping file (Section 4.2).

As recommended by the PSI CV guidelines, psi-ms.obo should be dynamically maintained *via* the psidev-ms-vocab@lists.sourceforge.net mailing list that allows any user to request new terms, in agreement with the community involved. Once a consensus is reached among the community the new terms are added within a few business days.

In general, modifications SHOULD be sourced from Unimod (http://www.unimod.org/obo/unimod.obo) where possible. For encoding cross-linking results, the XLMOD-CV SHOULD be used (https://raw.githubusercontent.com/HUPO-PSI/mzIdentML/master/cv/XLMOD.obo), unless suitable terms can be obtained from Unimod at a later date.

The following ontologies or controlled vocabularies specified below may also be suitable or required in certain instances:

- Unit Ontology (http://bioportal.bioontology.org/ontologies/UO?p=classes&conceptid=root).
- ChEBI (http://www.ebi.ac.uk/chebi/).
- For describing sample types, any suitable and stable ontologies MAY be used.

The PSI Protein modifications CV (http://psidev.cvs.sourceforge.net/viewvc/psidev/psi/mod/data/PSI-MOD.obo) is now DEPRECATED for use in mzIdentML. It is RECOMMENDED to use Unimod wherever possible.

4.2 Validation of controlled vocabulary terms

The correct usage of controlled vocabulary terms within mzIdentML is governed by the use of a mapping file that defines each XML location (XPath) where a <cvParam> instance can be used, and the allowed terms from the PSI-MS, or other CVs. The mapping file is read and interpreted by validation software, checking that the data annotation is consistent. The mapping file needs to be checked and updated when the structure of the CV is

changed, and in some instances when new terms are added to the CV. XML paths are associated with CV terms along with a requirement level (MAY, SHOULD or MUST) defining what should be reported by validation software if one of the mapped terms is not provided in an instance document. Syntactic and semantic validation SHOULD be checked using the official Java-based validator available from http://www.psidev.info/mzidentml.

4.3 Changes from version 1.1.0 to version 1.2.0

The primary update requiring the change from version 1.1.0 to version 1.2.0 is in the inclusion of guidelines for encoding protein group results (Section 5.2.1). Several examples referenced throughout the document are annotated with version 1.1.0. In these cases, it can be assumed that these files are also valid 1.2.0 files, since they do not include protein inference results. Other minor changes have been made to the specification since version 1.1.0, with regards to the encoding of specific workflows – notably searches where pre-fractionation has been performed (Section 5.2.5), searches employing multiple search engines (Section 5.2.4), *de novo* sequencing (Section 5.2.2) and spectral library searches (5.2.3).

Several new CV terms are now mandatory within the <SpectrumIdentificationProtocol> element - enabling the new features to be differentiated and recognised automatically by processing software, as follows. **1…*n* of the following terms MUST be present:**

CV term name	Accession	Reference to section within this document
peptide-level scoring	MS:1002490	5.2.7
modification localization scoring	MS:1002491	5.2.8
consensus scoring	MS:1002492	5.2.4
sample pre-fractionation	MS:1002493	5.2.5
cross-linking search	MS:1002494	5.2.9
de novo search	MS:1001010	5.2.2
spectral library search	MS:1001031	5.2.3
proteogenomics search	MS:1002635	5.2.10
no special processing	MS:1002495	Used to indicate that none of the above (new) features have been included in the file.

Table 1 New CV terms now mandatory (1...*n* terms MUST be present) within the <SpectrumIdentificationProtocol> element in mzIdentML 1.2. Terms “de novo search” and “spectral library search” MUST appear under the <SearchType> element. All other terms MUST appear under the <AdditionalSearchParams> element.

5. Format scope and specific use cases

5.1.1 Handling updates to the controlled vocabulary

In brief, when a new term is required, the file producers must contact the CV working group *via* e-mail (psidev-ms-vocab@lists.sourceforge.net) and request the new term. It is anticipated that problems may arise if a consumer of the file encounters a new CV term and they are not working from the latest version of the CV file. It has been decided that rather than aim for a workaround to this issue, it can be expected that data file consumers must ensure that the OBO file is up-to-date.

5.1.2 Identifying the input spectrum for each result

A <SpectrumIdentificationResult> is linked to the source spectrum (in an external file) from which the identifications are made by way of a reference in the spectrumID attribute and *via* the <SpectraData> element which stores the URL of the file in the location attribute. It is advantageous if there is a consistent system for identifying spectra in different file formats. The following table is implemented in the PSI-MS CV for providing consistent identifiers for different spectrum file formats. A CV term MUST be imported into the <SpectraData> element to demonstrate which system for identifying input spectra is being used in the spectrumID attribute of <SpectrumIdentificationResult>.

It is encouraged but not mandatory that a valid mzIdentML file is accompanied by the set of spectra that were searched. It is acknowledged that in many cases it will be useful to have an mzIdentML file and the input spectra together, there are practical problems processing such data depending on the spectrum file format (e.g. in case of proprietary formats), and cases where an mzIdentML is useful even if the spectra data is not available.

Update in version 1.2:
Version 1.1.0 of the specification document states "the CV holds the definite specification for legal encodings of spectrumID values". In version 1.2, the only legal ways of referencing a spectrum identification format are provided below in Table 1. Any new spectral formats that cannot fit into this schema require an update to this document.

ID	Term	Data type	Comment
MS:1000768	Thermo nativeID format	controllerType=xsd:nonNegativeInteger controllerNumber=xsd:positiveInteger scan=xsd:positiveInteger	controller=0 is usually the mass spectrometer. Space-separated values.
MS:1000769	Waters nativeID format	function=xsd:positiveInteger process=xsd:nonNegativeInteger scan=xsd:nonNegativeInteger	Space-separated values.
MS:1000770	WIFF nativeID format	sample=xsd:nonNegativeInteger period=xsd:nonNegativeInteger cycle=xsd:nonNegativeInteger experiment=xsd:nonNegativeInteger	Space-separated values.
MS:1000771	Bruker/Agilent YEP nativeID format	scan=xsd:nonNegativeInteger	
MS:1000772	Bruker BAF nativeID format	scan=xsd:nonNegativeInteger	
MS:1000773	Bruker FID nativeID format	file=xsd:IDREF	The nativeID must be the same as the source file ID.
MS:1000774	multiple peak list nativeID format	index=xsd:nonNegativeInteger	Used for referencing peak list files with multiple spectra, i.e. MGF, PKL, merged DTA files. Index is the spectrum number in the file, starting from 0.
MS:1000775	single peak list nativeID format	file=xsd:IDREF	The nativeID must be the same as the source file ID. Used for referencing peak list files with one spectrum per file, typically in a folder of PKL or DTAs, where each sourceFileRef is different.
MS:1000776	scan number only nativeID format	scan=xsd:nonNegativeInteger	Used for referencing mzXML, or a DTA folder where native scan numbers can be derived.
MS:1000777	spectrum identifier nativeID format	spectrum=xsd:nonNegativeInteger	Used for referencing mzData. The spectrum ID attribute is referenced.
MS:1001530	mzML unique identifier	xsd:string	Used for referencing mzML. The value of the spectrum ID attribute is referenced directly.
MS:1002647	Thermo nativeID format, combined spectra	controllerType=xsd:nonNegativeInteger controllerNumber=xsd:positiveInteger scan=xsd:positiveInteger,	Thermo nativeID comma separated list of spectra that have been combined prior to searching or interpretation.

		controllerType=xsd:nonNegativeInteger controllerNumber=xsd:positiveInteger scan=xsd:positiveInteger…	
MS:1002648	Waters nativeID format, combined spectra	function=xsd:positiveInteger process=xsd:nonNegativeInteger scan=xsd:nonNegativeInteger, function=xsd:positiveInteger process=xsd:nonNegativeInteger scan=xsd:nonNegativeInteger…	Waters nativeID comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002649	WIFF nativeID format, combined spectra	sample=xsd:nonNegativeInteger period=xsd:nonNegativeInteger cycle=xsd:nonNegativeInteger experiment=xsd:nonNegativeInteger, sample=xsd:nonNegativeInteger period=xsd:nonNegativeInteger cycle=xsd:nonNegativeInteger experiment=xsd:nonNegativeInteger	WIFF nativeID comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002650	Bruker/Agilent YEP nativeID format, combined spectra	scan=xsd:nonNegativeInteger, scan=xsd:nonNegativeInteger, scan=xsd:nonNegativeInteger…	Bruker/Agilent YEP comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002651	Bruker BAF nativeID format, combined spectra	scan=xsd:nonNegativeInteger, scan=xsd:nonNegativeInteger, scan=xsd:nonNegativeInteger…	Bruker BAF comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002652	Bruker FID nativeID format, combined spectra	file=xsd:IDREF, file=xsd:IDREF, file=xsd:IDREF…	Bruker FID comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002653	multiple peak list nativeID format, combined spectra	index=xsd:nonNegativeInteger, index=xsd:nonNegativeInteger, index=xsd:nonNegativeInteger…	Multiple peak list nativeID comma separated list of spectra that have been merged prior to searching or used together in some other manner intrinsic to the search.
MS:1002654	single peak list nativeID format, combined spectra	file=xsd:IDREF, file=xsd:IDREF, file=xsd:IDREF…	Single peak list nativeID comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002655	scan number only nativeID format, combined spectra	scan=xsd:nonNegativeInteger, scan=xsd:nonNegativeInteger, scan=xsd:nonNegativeInteger…	Scan number only nativeID comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002656	spectrum identifier nativeID format, combined spectra	spectrum=xsd:nonNegativeInteger, spectrum=xsd:nonNegativeInteger, spectrum=xsd:nonNegativeInteger…	Spectrum identifier nativeID comma separated list of spectra that have been combined prior to searching or interpretation.
MS:1002657	mzML unique identifier, combined spectra	xsd:string, xsd:string, xsd:string…	Comma separated list of spectra that have been combined prior to searching or interpretation.

Table 2. CV terms and rules implemented in the PSI-MS CV for formulating the “nativeID” to identify spectra in different file formats.

In mzIdentML, the spectrum ID attribute should be constructed following the data type specification in Table 2. As an example, to reference the third spectrum (index=2) in an MGF (Mascot Generic Format) file:

```
<SpectrumIdentificationResult id="Res1" spectrumID="index=2" SpectraData_ref="InputSpectra1">

...

<SpectraData location="local/mgf/merge.mgf" id="SD_1" >
  <FileFormat>
    <cvParam accession="MS:1001062" name="Mascot MGF file" cvRef="PSI-MS" />
  </FileFormat>
  <SpectrumIDFormat>
    <cvParam accession="MS:1000774" name="multiple peak list nativeID format" cvRef="PSI-MS" />
  </SpectrumIDFormat>
</SpectraData>
```

5.2 Comments on Specific use cases

Many special use cases for mzIdentML were considered during its development. Each of these use cases has a corresponding example file that exercises the relevant part of the schema and provides a reference implementation example (see supporting documentation). Authors of software that create mzIdentML are encouraged to examine the examples that accompany this format release before implementing the writer. Further, such authors are encouraged to use the validator before releasing any new writer code and working with the PSI PI Working Group to resolve any issues. In the subsections below, we comment on a few of the notable use cases that were considered – in particular those newly added in mzIdentML 1.2.

5.2.1 Protein grouping encoding

This section is newly inserted in the mzIdentML version 1.2.0 specifications. In version 1.1.0, CV terms had been proposed for representing set relationships between different proteins within groups, but there was not a requirement that particular terms were used. A given data structure from software could be mapped onto the hierarchy <ProteinAmbiguityGroup> and <ProteinDetectionHypothesis> in mzIdentML in different ways, leading to difficulties for data consumers. As such, a working group has now agreed a more rigid encoding detailed as follows and in (6).

1. As in mzIdentML version 1.1, a single protein accession that has been cited by software is captured in mzIdentML in <ProteinDetectionHypothesis> (PDH).
    a. A PDH MAY contain scores or statistical values produced by the export software, encoded as CV terms.
2. A “protein group”, representing a “biological entity” for which the software claims independent evidence is present, MUST be mapped onto <ProteinAmbiguityGroup> (PAG).
    a. A PAG MAY have additional scores produced by the export software, encoded as CV terms.
3. The reporting of protein identification thresholds is now mapped onto PAGs. There is no desire to change the core XML Schema Document (XSD) for mzIdentML and as such, a new CV term “protein group passes threshold” value= “xsd:boolean” MUST be present on every PAG (MS:1002415). If no thresholding has been done by the software, all protein groups MUST be annotated as “protein group passes threshold” value= “true”.
    a. The attribute *passThreshold* = “true|false” remains present on PDH and MAY be used if software packages wish to report a two-level hierarchy of thresholds applied. However, it is not expected that consuming software will use this attribute to determine which proteins have been reported as identified.
4. The <ProteinDetectionList> MUST contain the CV term “count of identified proteins” value= “xsd:integer” (MS:1002404). The value MUST be derived from the count of PAGs passing the threshold reported in the file and will be checked by validation software.
5. Few software packages report “protein clusters” at present, but for those packages that wish to report clusters, a CV term “cluster identifier” value = “xsd:integer” SHOULD be used (MS:1002407). The integer identifier MUST be shared by all PAGs belonging to the same cluster. An optional term “count of identified clusters” value = “xsd:integer” (MS:1002406) MAY be annotated on the <ProteinDetectionList>.

6. Every PDH MUST be annotated as either a “leading protein” (MS:1002401) or a “non-leading protein” (MS:1002402), as defined in Table 2, within a PAG. This recommendation thus makes it explicit for consuming software whether one or more proteins have stronger evidence than others in the group (see Table 2 for examples).
    a. An additional term, “group representative” (MS:1002403) MAY be used to annotate one PDH, which is also flagged as a “leading protein”, if the export software wishes to enforce that only one of potential several “leading proteins” will be interpreted by the consuming software as the representative of the group, for example acting as a tiebreaker.
    b. If the export software does not explicitly flag one protein as the “group representative”, it is assumed that if consuming software requires a single accession to represent the group, an arbitrary choice will be made (among “leading proteins” only if these exist).
7. Any PDHs MAY be annotated with terms present in the CV for spectrum/sequence same-set, spectrum/sequence subset, spectrum/sequence subsumable, marginally distinguished and so on (Table 2).
    a. A PDH MAY be annotated with more than one of these terms if appropriate to describe the complex set relationships that exist within a group.
    b. Developers of software packages MAY propose additional terms for describing group membership of PDHs, which will be incorporated into the CV.
    c. The associated value for these CV terms MAY be used to annotate which PDH(s) are the super/same-set of the annotated PDH.
    d. There is no expectation that consuming software should be aware of these terms, but they may be useful in internal pipeline or visualization software packages that are specifically designed to work with this terminology set.
8. Some PDHs could be mapped to more than one PAG, for example where proteins are multiply subsumed. To capture these cases, multiple PDHs in different PAGs MAY reference the same <DBSequence>.

The semantic validation software has been updated to encode these rules and report errors (“MUST” rule), warnings (“SHOULD” rule) or informational messages (“MAY” rule).

mzIdentML context	CV term	Values	Require-ment level	Description
ProteinDetection-List	count of identified proteins	xsd:integer	MUST	The value reported MUST equal the number of PAGs with “protein group passes threshold” value = “true”
ProteinDetection-List	count of identified clusters	xsd:integer	MAY	If protein clusters have been reported in the file, the exporter may choose to annotate the ProteinDetectionList with the number identified above threshold.
ProteinAmbiguity-Group	number of distinct protein sequences	xsd:integer	MAY	The number of distinct protein sequences among the PDHs in the group. For example, if there are two PDHs with different identifiers that have identical full length sequences, the value would be 1.
ProteinAmbiguity-Group	cluster identifier	xsd:integer	MAY	An identifier applied to protein groups to indicate that they are linked by shared peptides.
ProteinDetection-Hypothesis	leading protein OR non-leading protein	-	MUST OR MUST	Every PDH in each PAG MUST be flagged as a leading protein or a non-leading protein and each PAG MUST contain at least one leading protein, but MAY contain more than one. A “leading protein” is defined as a protein that has the strongest or near strongest (further explained in Table 3) set of evidence for being present in the sample studied, amongst the grouped protein accessions. A “non-leading protein” is defined as a protein that has (substantially) less evidence than other proteins within the same group, and is thus less likely to have been present in the sample studied.
ProteinDetection-Hypothesis	group representative	-	MAY	Each PAG MAY contain zero or one PDH flagged as the group representative, if the software wishes to flag a preference (often arbitrary or for example based on alphabetical ordering) amongst the leading proteins. The group representative term can thus be viewed a “tiebreaker” if the export software wishes to make this distinction.
ProteinAmbiguity-Group	protein group passes threshold	xsd:Boolean	MUST	Each PAG MUST be annotated with a Boolean CV term indicating whether the PAG has passed the threshold reported in the ProteinDetectionProtocol.

ProteinDetection-Hypothesis	sequence same-set protein	xsd: "list_of_ strings" space separated list of PDH IDs that are same-set.	MAY	A protein that is indistinguishable or equivalent to another protein in the group, having matches to an identical set of peptide sequences.
ProteinDetection-Hypothesis	spectrum same-set protein	xsd: "list_of_ strings" space separated list of PDH IDs that are same-set.	MAY	A protein that is indistinguishable or equivalent to another protein in the group, having PSMs derived from the same set of spectra.
ProteinDetection-Hypothesis	sequence sub-set protein	xsd: "list_of_ strings" space separated list of PDH IDs that are super-set.	MAY	A protein for which the matched peptide sequences are a subset of the matched peptide sequences for another protein in the group.
ProteinDetection-Hypothesis	spectrum sub-set protein	xsd: "list_of_ strings" space separated list of PDH IDs that are super-set.	MAY	A protein for which the matched spectra are a subset of the matched spectra for another protein in the group.
ProteinDetection-Hypothesis	sequence multiply subsumable protein	xsd: "list_of_ strings" space separated list of PDH IDs that subsume this PDH.	MAY	A protein for which the matched peptide sequences are the same, or a subset of, the matched peptide sequences for two or more other proteins combined. These other proteins need not all be in the same group.
ProteinDetection-Hypothesis	spectrum multiply subsumable protein	xsd: "list_of_ strings" space separated list of PDH IDs that subsume this PDH.	MAY	A protein for which the matched spectra are the same, or a subset of, the matched spectra for two or more other proteins combined. These other proteins need not all be in the same group.
ProteinDetection-Hypothesis	marginally distinguished protein	-	MAY	Assigned to a non-leading PDH that has some independent evidence to support its presence relative to the leading protein(s) e.g. the PDH may have a unique peptide but not sufficient to be promoted as, for example, a leading protein of another a PAG.

Table 3. New CV terms for reporting protein set (group) relationships and global statistics about the protein identification results. The semantic validation software for mzIdentML version 1.2.0 reports an error (MUST), a warning (SHOULD) or an informational message (MAY) if these terms are not reported within the file.

Scenario	Software preference	Encoding
Software scores A and B as same-set, C and D as subset.	Software wishes to make A the group representative (arbitrary)	A = leading protein & group representative B = leading protein C = non-leading protein D = non-leading protein (Use of formal same-set and subset notation is also allowed but optional)
As above	Software does not wish to choose which is the group representative	A = leading protein B = leading protein C = non-leading protein D = non-leading protein
Software scores A as best protein, B, C and D are all subset or subsumed	N/A	A = leading protein B = non-leading protein C = non-leading protein D = non-leading protein
Software scores all four proteins as same-set or more generally as having equal evidence	Software wishes to make A the group representative (arbitrary)	A = leading protein & group representative B = leading protein C = leading protein D = leading protein

As above	Software does not wish to choose which is the group representative	A = leading protein B = leading protein C = leading protein D = leading protein
Software scores A as having slightly more evidence than B. B has additional weak independent evidence relative to A. C and D have less evidence than either A or B.	Software wishes to assign A as the leading protein and the independent evidence for B is not sufficient for it to form a new PAG.	A = leading protein B = non-leading protein & marginally distinguished (optional) C = non-leading protein D = non-leading protein
As above	Software does not wish to choose which is the leading protein out of A and B or group representative	A = leading protein B = leading protein C = non-leading protein D = non-leading protein
As above	Software does not wish to choose which is the leading protein but does select a group representative	A = leading protein & group representative B = leading protein C = non-leading protein D = non-leading protein

Table 4. A summary of grouping options and recommendation for CV term annotations, assuming a group of four related proteins A-D.

5.2.2 Support for *de novo* sequencing approaches

In mzIdentML version 1.1, <SpectrumIdentificationItem> had a mandatory sub-element <PeptideEvidenceRef> to link each PSM to all the proteins from which it could have originated. The inclusion of these mandatory requriements makes it difficult to represent results from *de novo* sequencing and spectral library search approaches where PSMs may not necessarily have originated from a protein database search. As such, in mzIdentML 1.2.0 <PeptideEvidenceRef> has a cardinality of 0...many. In all cases of sequence database search, export software MUST include all <PeptideEvidenceRef> elements for every PSM. *De novo* sequencing approaches are therefore supported, but only in a relatively straightforward manner, where complete peptide sequences are identified. Proposals for representing partial peptide sequences or sequence tags are encouraged for future iterations of the standard.

5.2.3 Spectral library searches

An alternative to sequence database searches for identifying peptides from MS data is to search a pre-compiled library (spectral library) of PSMs. These spectral library searches are supported in mzIdentML. The recommended encoding is similar to sequence database search results. The main difference is that a <Peptide> entity SHOULD record each library entry that has been matched against. Additional scores or metadata about the library entity SHOULD be included as <cvParam> elements on <Peptide>. For searches against spectral archives i.e. where the identity of the library entry is unknown (there is no a peptide sequence assignment to the spectrum in the library), the encoding SHOULD include an empty string in <PeptideSequence>.

Note – there has been no formal change to the schema or CV requirements from mzIdentML 1.1 to 1.2.0 around spectral library encoding, but the intended encoding has changed. The mzIdentML 1.1. specifications stated that spectral library entries should be encoded within <DBSequence>, which does not well model the data produced.

5.2.4 Multiple database search engines

Proteomics research groups now commonly analyze MS data using multiple search engines and combine results to improve the number of peptide and protein identifications that can be made. The output of such approaches can be represented in mzIdentML as follows (see Section 6 for documentation of the model elements). Note that the RECOMMENDED encoding has changed since the version 1.1.0 specification as a result of community feedback. It has been decided that throughout mzIdentML, the spectrum referenced from a <SpectrumIdentificationResult> MUST be unique within a file i.e. only one set of ranked results can be provided per spectrum. This has implications for encoding the results of multiple search engines, as only consensus results (after they have been combined) can be represented in a valid mzIdentML 1.2.0 file. If exporters wish to maintain the original search engine results, these MAY be encoded using <cvParam> elements within

<SpectrumIdentificationItem> containing additional scores, statistics and indicating the original rankings from the source search engine.

The <SpectrumIdentification> element MUST reference a <SpectrumIdentificationProtocol> holding representative parameters used across all search engines (i.e. search tolerances, enzyme and modifications), since these are MANDATORY elements. If the same search parameters were not employed in all source searches, the parameters should be set with superset or widest values i.e. all modifications that have been searched, widest tolerances and so on. All search engines that have been employed SHOULD be represented within the <AnalysisSoftwareList>. The <AnalysisSoftwareList> SHOULD also record the software used to combine results. It must also be highlighted that mzIdentML cannot be used to model the order in which the software was used (it does not support workflows).

The same encoding MAY also be used to describe other approaches where different search protocols are applied to the same spectra (for example using different parameter sets with the same search engine), and subsequently combined. In this case, it is RECOMMENDED that only a single (assumed best) score of any given type is represented once per <SpectrumIdentificationItem>.

5.2.5 Pre-fractionation of samples prior to MS and splitting of searches

It is common in many workflows for pre-fractionation of a sample to be performed prior to MS, for example *via* 1D or 2D gel electrophoresis or 2D LC. In some scenarios results of database searches are combined prior to protein inference and in other instances there is no combination of results prior to protein inference. We have identified the following scenarios and describe the RECOMMENDED encoding in each case in Table 5 below.

Scenario	Encoding
Scenario 1. i) A sample is fractionated into *n* sub-samples, prior to *n* runs on the MS; ii) the search engine performs *n* searches, producing *n* protein-lists.	*n* mzIdentML files SHOULD be produced, each containing 1 <SpectrumIdentificationList>, 1 <SpectrumIdentificationProtocol>, 1<SpectrumIdentification>, 1 <ProteinDetection>, 1 <ProteinDetectionList>.
Scenario 2. i) A sample is fractionated into *n* sub-samples, prior to *n* runs on the MS; ii) the search engine imports *n* peak lists and performs *n* searches but internally integrates results to produce one protein list.	One single mzIdentML file SHOULD contain *n* <SpectrumIdentificationList>s, *n* <SpectrumIdentificationProtocol>s, *n* <SpectrumIdentification>s, 1 <ProteinDetection>, 1 <ProteinDetectionList>. The <SpectrumIdentificationProtocol>s MUST indicate that pre-fractionation has taken place, using the CV term indicated in Table 1.
Scenario 3. i) A sample is fractionated into *n* sub-samples, prior to *n* runs on the MS; ii) the search engine performs *n* searches, producing *n* lists of spectrum identifications; iii) post-processing software integrates results to produce one protein list.	As Scenario 2.
Scenario 4. i) There is no sample pre-fractionation and one run on the MS. ii) The spectra are split into *n* peak list files for searching (for example for parallelisation on a cluster), producing *n* lists of PSMs iii) post-processing software re-combines results into one mzIdentML file producing 1 protein list.	One single mzIdentML file SHOULD contain 1 <SpectrumIdentificationList>, 1 <SpectrumIdentificationProtocol>, 1 <SpectrumIdentification> referencing *n* <InputSpectra> sub-elements, 1 <ProteinDetection>, 1 <ProteinDetectionList>.

Table 5. A description of RECOMMENDED encodings in mzIdentML, where sample pre-fractionation has taken place.

5.2.6 Encoding replicate samples

One mzIdentML file is intended to capture the analysis of one sample, including rules for pre-fractionation as discussed in Section 5.2.5. For encoding replicate samples (biological or technical), separate mzIdentML files SHOULD be used. A naming convention using suffixes MAY be adopted but the specifications of such are beyond the scope of this document.

5.2.7 Peptide-level scores and statistical measures

The format was designed with explicit support for encoding scores or statistical measures for PSMs, for individual proteins and for protein groups. However, the original design contained no explicit (schema level) support for peptide-level scores i.e. after redundant PSMs reporting on the same peptide have been removed. One of the challenges in this space is defining the mechanism of grouping multiple PSMs for the same *distinct peptide* – since in different contexts a distinct peptide could encompass one of the following concepts:

- A peptide sequence with a given set of modifications – located in specified positions, identified from a single charge state.
- A peptide sequence with a given set of modifications – located in specified positions, identified from different charge state ions.
- A peptide sequence with a given set of modifications – regardless of the positions of modifications.
- A peptide sequence regardless of the presence/absence of different modifications.

A mechanism for encoding these different types of distinct peptide grouping in the mzIdentML 1.2.0 specifications has been defined, using CV terms as described in Figure 1. Three CV terms have currently been added to the PSI-MS CV: “group PSMs by sequence” (MS:1002496), “group PSMs by sequence with modifications” (MS:1002497) and “group PSMs by sequence with modifications and charge” (MS:1002498).

The following additional features have also been added to mzIdentML 1.2.0 to support peptide-level scores (Figure 1). First, an additional CV term “peptide-level scoring” (MS:1002490) MUST be included (when this process is being reported) in <SpectrumIdentificationProtocol>, as shown in Figure 1A and Table 1. In addition, the <SpectrumIdentificationProtocol> contains a <Threshold> element, used in previous versions, for representing the threshold applied at the PSM level. In mzIdentML 1.2, the element can now be used to demonstrate the threshold applied at the PSM and/or peptide-level, through the use of appropriate CV terms.

Additionally, a mechanism is needed for capturing how different PSMs are grouped into a single entity. This is achieved by adding a CV term to every PSM in the file “peptide group ID” (MS:1002520), whereby the associated value is a unique identifier shared between all PSMs in the same peptide group. In the example in Figure 1D, the unique identifier used is the peptide sequence itself (since when grouping by sequence irrespective of modification status this value must be unique), although this could be an arbitrary value such as an integer code.

The mzIdentML file must be able to record scores or statistical values at the peptide level. This is achieved *via* adding CV terms with identical values to all PSMs within the same peptide-group, with an indication that it is a peptide-level value, *via* the convention of the prefix “peptide:” in the CV term name (Figure 1E). Finally, a mechanism has been added for recording peptides both above and below the threshold, to allow complete statistical re-evaluation by downstream software. PSM-level threshold is covered *via* the *passThreshold* attribute on the <SpectrumIdentificationItem> element. To enable additional thresholding at the peptide-level, a new CV term is required for all PSMs (“peptide passes threshold”, MS:1002500) as shown in Figure 1F.

Guidelines for Peptide-level scoring

```
<SpectrumIdentificationProtocol analysisSoftware_ref="ID_software" id="SearchProtocol_1">
    <SearchType>
      <cvParam accession="MS:1001083" cvRef="PSI-MS" name="ms-ms search"/>
    </SearchType>
    <AdditionalSearchParams>
      <cvParam accession="MS:1001211" cvRef="PSI-MS" name="parent mass type mono"/>
      <cvParam accession="MS:1001256" cvRef="PSI-MS" name="fragment mass type mono"/>
      <cvParam accession="MS:1002490" cvRef="PSI-MS" name="peptide-level scoring"/>
      <cvParam accession = " MS:1002496" cvRef="PSI-MS" name="group PSMs by sequence"/>
    </AdditionalSearchParams>
    <ModificationParams>
      <SearchModification residues="C" massDelta="57.021465" fixedMod="true">
        <cvParam accession="UNIMOD:4" cvRef="UNIMOD" name="Carbamidomethyl"/>
      </SearchModification>
      <SearchModification residues="M" massDelta="15.994915" fixedMod="false">
        <cvParam accession="UNIMOD:35" cvRef="UNIMOD" name="Oxidation"/>
      </SearchModification>
    </ModificationParams>
    <Enzymes independent="false">
      <Enzyme missedCleavages="1" semiSpecific="false" cTermGain="OH" nTermGain="H" id="Enz1">
        <EnzymeName>
          <cvParam accession="MS:1001251" cvRef="PSI-MS" name="Trypsin"/>
        </EnzymeName>
      </Enzyme>
    </Enzymes>
    <FragmentTolerance>
      <cvParam accession="MS:1001412" cvRef="PSI-MS" unitCvRef="UO" unitName="dalton" unitAccession="UO:0000221" value="0.8" name="search tolerance plus value"/>
      <cvParam accession="MS:1001413" cvRef="PSI-MS" unitCvRef="UO" unitName="dalton" unitAccession="UO:0000221" value="0.8" name="search tolerance minus value"/>
    </FragmentTolerance>
    <ParentTolerance>
      <cvParam accession="MS:1001412" cvRef="PSI-MS" unitCvRef="UO" unitName="dalton" unitAccession="UO:0000221" value="1.5" name="search tolerance plus value"/>
      <cvParam accession="MS:1001413" cvRef="PSI-MS" unitCvRef="UO" unitName="dalton" unitAccession="UO:0000221" value="1.5" name="search tolerance minus value"/>
    </ParentTolerance>
    <Threshold>
      <cvParam accession="MS:1001868" cvRef="PSI-MS" name="distinct peptide-level q-value" value="0.01"/>
      <cvParam accession="MS:1002354" cvRef="PSI-MS" name="PSM-level q-value" value="0.01"/>
    </Threshold>
  </SpectrumIdentificationProtocol>
```

A B C

```
<SpectrumIdentificationResult spectraData_ref="SID_1" spectrumID="index=145" id="SIR_5">
  <SpectrumIdentificationItem passThreshold="false" rank="1" peptide_ref="SSHAPVPHGVRLWK" calculatedMassToCharge="523.284" experimentalMassToCharge="523.194" chargeState="3" id="SII_5_1">
    <PeptideEvidenceRef peptideEvidence_ref="PE5_2_9"/>
    <cvParam accession="MS:1001328" cvRef="PSI-MS" value="3.05370337630321" name="OMSSA:evalue"/>
    <cvParam accession="MS:1001329" cvRef="PSI-MS" value="6.82544339808495E-4" name="OMSSA:pvalue"/>
    <cvParam accession="MS:1002520" cvRef="PSI-MS" value="SSHAPVPHGVRLWK" name="peptide group ID"/>
    <cvParam accession="MS:1001868" cvRef="PSI-MS" value="distinct peptide-level q-value" name="6.82544339808495E-4"/>
    <cvParam accession="MS:1002500" cvRef="PSI-MS" value="peptide passes threshold" name="true"/>
  </SpectrumIdentificationItem>
  <cvParam accession="MS:1000796" cvRef="PSI-MS" value="55.6021.6024.3.dta" name="spectrum title"/>
</SpectrumIdentificationResult>
<SpectrumIdentificationResult spectraData_ref="SID_1" spectrumID="index=121" id="SIR_6">
  <SpectrumIdentificationItem passThreshold="false" rank="1" peptide_ref="SSHAPVPHGVRLWK" calculatedMassToCharge="523.284" experimentalMassToCharge="523.194" chargeState="3" id="SII_6_1">
    <PeptideEvidenceRef peptideEvidence_ref="PE5_2_9"/>
    <cvParam accession="MS:1001328" cvRef="PSI-MS" value="4.05370337630321" name="OMSSA:evalue"/>
    <cvParam accession="MS:1001329" cvRef="PSI-MS" value="7.82544339808495E-4" name="OMSSA:pvalue"/>
    <cvParam accession="MS:1002520" cvRef="PSI-MS" value="SSHAPVPHGVRLWK" name="peptide group ID"/>
    <cvParam accession="MS:1001868" cvRef="PSI-MS" value="distinct peptide-level q-value" name="6.82544339808495E-4"/>
    <cvParam accession="MS:1002500" cvRef="PSI-MS" value="peptide passes threshold" name="true"/>
  </SpectrumIdentificationItem>
  <cvParam accession="MS:1000796" cvRef="PSI-MS" value="55.6021.6025.3.dta" name="spectrum title"/>
</SpectrumIdentificationResult>
```

D E F

D E F

Feature	Explanation
A	cvParam indicating that peptide-level scoring has been done and that feature B MAY be present and features D, E and F MUST be present. A cvParam MUST also be present indicating the type of grouping of PSMs to peptides done.
B	The threshold used to determine whether each distinct peptides group has been confidently identified – used to set the value of feature F
C	As for regular mzIdentML files, a threshold can be applied at the level of PSMs – which is used to set the passThreshold attribute on <SpectrumIdentificationItem>
D	If feature A is present , exactly one cvParam “peptide group ID” MUST be present in which the value slot contains a unique identifier (string) that MUST be given to all <SpectrumIdentificationItem> elements within the same distinct peptide group. There is no expectation that meaningful information SHOULD be conveyed by the value slot, but implementers MAY choose to use the peptide sequence or peptide sequence and a modification string (depending on the grouping mechanism) as the value.
E	A cvParam containing the peptide-level score used for ordering *distinct peptide* entities, which MUST be given to all <SpectrumIdentificationItem> elements within the same distinct peptide group with the same value.
F	If feature A is present , every <SpectrumIdentificationItem> element MUST contain the “peptide passes threshold” cvParam with a Boolean value. All <SpectrumIdentificationItem> elements within the same distinct peptide group MUST have the same value.

Figure 1. The mechanism for encoding peptide-level statistics in mzIdentML 1.2.0.

5.2.8 Encoding modification localisation scores

A new addition to mzIdentML 1.2.0 is the ability to attach scores or statistical values to the position of a modification, with regards to the peptide sequence. A variety of software packages now export such values, since it is common for there to be more than one possible site of modification. Evidence from the presence or absence of fragment ions can enable a calculation of the likelihood of different possibilities. Such evidence trail is particularly important for some downstream uses of the data, such as profiling motifs for positions of modifications or populating databases with “experimentally observed” modification sites.

The encoding of such scores is achieved in mzIdentML 1.2.0 by making use of a regular expression attached within a <cvParam> at the level of <SpectrumIdentificationItem>. The following additional features to be present in mzIdentML 1.2.0 (Figure 2).

To ensure that downstream software is aware that a file contains modification scores, a CV term is added to the <SpectrumIdenticationProtocol> - “Modification localization scoring” (MS:1002491), as shown in Figure 2A and Table 1. Some approaches apply a statistical threshold for accepting or rejecting that a modification position has been confidently identified. The (re-usable) <Peptide> element has an attribute *via* which the residue and location of a modification can be recorded. To remain backwards compatible, we recommend that the software implementing mod scoring (and export) in mzIdentML should continue to use these attributes, populating with the most likely modification position (Figure 2C). A new CV term (REQUIRED when MS:1002491 is present in the protocol) must be added to every <Modification> element – called “modification index” (MS:1002504), where the value serves as a unique identifier (local only to the containing <Peptide>) to be referenced from the PSM (Figure 2D).

The modification scores themselves are added as CV terms to the <SpectrumIdentificationItem> element referencing the peptide (e.g. “phosphoRS score”, Figure 2E), with a value provided as a regular expression of four values in a defined order - MOD_INDEX, SCORE, POSITION, PASS_THRESHOLD. MOD_INDEX is a reference to the “modification index” identifier provided in the referenced <Peptide> - <Modification> element. SCORE represents the score or statistical value (double data type) for the given position. POSITION is the scored modification position with respect to the peptide sequence (where position = 0 is the N-terminus, and the peptide length + 1 is used to indicate the C-terminus). The POSITION can include the bar symbol ‘|’, as a logical OR, if the score relates to multiple positions that can be distinguished. PASS_THRESHOLD holds a Boolean (true, false) value to indicate whether the modification position passes the threshold described above.

```
<cvParam accession="MS:1002380" cvRef="PSI-MS" value="1:0.03:2|3:true" name="modification rescored by
false localization rate"/>
<cvParam accession="MS:1002380" cvRef="PSI-MS" value="1:0.97:8|9:false" name="modification rescored by
false localization rate"/>
```

The mechanism described MAY be used in conjunction with peptide-level scoring, using specific CV terms for peptide-level modification re-scoring.

Guidelines for Mod position scoring

```
<SpectrumIdentificationProtocol analysisSoftware_ref="ID_software" id="SearchProtocol_1">
  <SearchType>
   <cvParam accession="MS:1001083" cvRef="PSI-MS" name="ms-ms search"/>
  </SearchType>
  <AdditionalSearchParams>
   <cvParam accession="MS:1001211" cvRef="PSI-MS" name="parent mass type mono"/>
   <cvParam accession="MS:1001256" cvRef="PSI-MS" name="fragment mass type mono"/>
   <cvParam accession="MS:1002491" cvRef="PSI-MS" name="Modification localization scoring"/>
  </AdditionalSearchParams>
  ....
  <Threshold>
   <cvParam accession="MS:1002354" cvRef="PSI-MS" name="PSM-level q-value" value="0.01"/>
   <cvParam accession="MS:1002380" cvRef="PSI-MS" name="false localization rate" value="0.05"/>
  </Threshold>
```

A

B

```
<Peptide id="KYYGNVVYYIGER_p@2|3">
  <PeptideSequence>KYYGNVVYYIGER</PeptideSequence>
  <Modification monoisotopicMassDelta="79.966331" location="2" residues="Y">
   <cvParam accession="UNIMOD:21" cvRef="UNIMOD" name="Phospho"/>
   <cvParam accession="MS:1002504" cvRef="PSI-MS" name="modification index" value="1"/>  </Modification>
 </Peptide>
 <Peptide id="KYYGNVVYYIGER_p@2|3_p@8|9">
  <PeptideSequence>KYYGNVVYYIGER</PeptideSequence>
  <Modification monoisotopicMassDelta="79.966331" location="2" residues="Y">
   <cvParam accession="UNIMOD:21" cvRef="UNIMOD" name="Phospho"/>
   <cvParam accession="MS:1002504" cvRef="PSI-MS" name="modification index" value="1"/>
  </Modification>
  <Modification monoisotopicMassDelta="79.966331" location="8" residues="Y">
   <cvParam accession="UNIMOD:21" cvRef="UNIMOD" name="Phospho"/>
   <cvParam accession="MS:1002504" cvRef="PSI-MS" name="modification index" value="2"/>
  </Modification>
 </Peptide>
```

C

D

```
<SpectrumIdentificationResult spectraData_ref="qExactive01819.mgf" spectrumID="index=2727" id="SIR_4207">
  <SpectrumIdentificationItem passThreshold="true" rank="1"  peptide_ref="DNSTMGYMMAK_15.99491461956_15.99491461956"
    calculatedMassToCharge="640.751423992447"  experimentalMassToCharge="640.751992494115"
    chargeState="2" id="SII_4207_1">
  <PeptideEvidenceRef peptideEvidence_ref="PepEv_9145"/>
  <cvParam cvRef="PSI-MS" accession="MS:1001969" name="phosphoRS score" value="1:66.66666666:5:false"/>
  <cvParam cvRef="PSI-MS" accession="MS:1001969" name="phosphoRS score" value="1:66.66666666:8:false"/>
  <cvParam cvRef="PSI-MS" accession="MS:1001969" name="phosphoRS score" value="1:66.66666666:9:false"/>

  <cvParam cvRef="PSI-MS" accession="MS:1002539" name="D-score" value="1:62.37587272987858:5:false"/>
  <cvParam cvRef="PSI-MS" accession="MS:1002539" name="D-score" value="1:14.141586139372523:8:false"/>
  <cvParam cvRef="PSI-MS" accession="MS:1002539" name="D-score" value="1:36.626793239964236:9:false"/>
  <!--  Other PSM-level scores not shown...  -->
 </SpectrumIdentificationItem>
 <!--  Other ranked identifications not shown...  -->
</SpectrumIdentificationResult>
```

E

F

Feature	Explanation
A	If modification rescoring has been performed, this cvParam MUST be present.
B	A Threshold for modification localizations MAY be inserted into the <SpectrumIdentificationProtocol>
C	The ambiguity with respect to modification location is present at the level of <SpectrumIdentificationItem> but rescored software SHOULD use the residues and location attribute to insert the most likely location for the modification
D	If Feature A is present, every <Modification> element MUST have the cvParam used as a unique identifier to be referenced by Feature F.
E	If Feature A is present, every <SpectrumIdentificationItem> referencing a peptide with a variable modification MUST have a cvParam for the location score. The value slot takes the following format MOD_INDEX:SCORE:POSITION:PASS_THRESHOLD **MOD_INDEX** = <Modification> index attribute in the referenced <Peptide> object **SCORE** = Score or statistical measure associated with the modification position **POSITION** = Position of the modification on the peptide (N-terminus = 0, C-terminus = peptide length + 1). If the score pertains to grouped positions, different positions MUST be separated by "|" **PASS_THRESHOLD** = true | false with regards to the threshold specified in Feature A. If no Threshold has been specified, this MUST always be true.
F	The modification position rescoring software SHOULD NOT include additional equal or lower ranked <SpectrumIdentificationItem> elements referencing a different <Peptide> element with the same peptide sequence and the same set of modifications (but with different modification positions) i.e. the only expected mechanism for specifying modification position is the cvParam specified in Feature D.

Figure 2. The specification in mzIdentML 1.2.0 for encoding modification localization scores, using CV terms.

5.2.9 Encoding results of cross-linking searches

A new mechanism has been added in mzIdentML 1.2.0 to encode results from search engines that support identification of cross-linked peptides. This presents a new challenge for mzIdentML, since more than one peptide can be identified from the same spectrum – here termed the alpha and beta peptides, along with cross-linker modifications, linked across the two chains ("donor" and "acceptor" cross-link sites). The encoding, as exemplified in Figure 3, enables scores or statistical measures to be assigned jointly to identification of the alpha-beta pair, or independently to the alpha and beta peptide chain. To fulfil these requirements in mzIdentML 1.2, the following adaptations were made.

Encoding a cross-linked peptide pair identification

First of all, the <SpectrumIdentificationProtocol> must contain the CV term "cross-linking search" (MS:1002494) as shown in Figure 3A and Table 1. To represent the cross-linkers, we have added a mechanism for relating two different <Peptide> elements together, using the CV terms "cross-link donor" (MS:1002509) and "cross-link acceptor" (MS:1002510), where an identical value indicates that they are grouped together (Figure 3B). The <Modification> element has an attribute *monoisotopicMassDelta*, and the cross-link donor SHOULD contain the complete mass delta introduced by the cross-linking reagent, and that the cross-link acceptor reports a mass shift delta of zero. It is RECOMMENDED that the "donor" peptide SHOULD be the longer peptide, followed by alphabetical order for equal length peptides.

For reporting the evidence associated with the identification, within a given <SpectrumIdentificationResult>, a pair of cross-linked peptides MUST be reported as two instances of <SpectrumIdentificationItem> through having a shared local unique identifier as the value for the CV term "cross-link spectrum identification item" (MS:1002511), as shown in Figure 3D. The two instances of <SpectrumIdentificationItem> MUST also share the same value for the rank attribute.

If the search engine has produced a single score for the cross-linked pair, both <SpectrumIdentificationItem> elements must carry the identical score (CV term and value, as in Figure 3E), but the two chains may also have additional, independent scores if needed (not shown).

Both <*SpectrumIdentificationItem*> elements MUST have the same value for experimentalMassToCharge (i.e. the measured precursor mass value) and for *calculatedMassToCharge* representing the theoretical mass of the pair of peptides plus the cross-link.

Encoding information from stable isotope labelling or multiple fragmentation approaches

In some workflows, a consensus spectrum or collection of spectra is interpreted together to arrive at an identification of the cross-linked pair. For cases where data are *post-processed* to arrive at a confident identification, the mechanism for peptide-level scoring SHOULD be used. However, there are some search approaches that intrinsically take into account multiple spectra to arrive at the identification: i) where "light" and "heavy" isotopes of the cross-linker are used as a pair, combined together and searched once; ii) different fragmentation modes applied to the same precursor e.g. ETD and HCD; iii) MS^3 fragmentation of particular MS^2 products. In these cases, the <SpectraData> element SHOULD specify that it is using a "combined spectra" type of input file format (Table 2). The referenced spectrum (*via* the *spectrumID* attribute) SHOULD contain a comma-separated list of identifiers e.g. *spectrumID= "index=1001, index=1007"*. For each peptide chain identified from the combined set of spectra (as a grouped identification of one cross-linked pair), there SHOULD be exactly one <SpectrumIdentificationItem> - all sharing the same identifier under "cross-link spectrum identification item".

In the case of different fragmentation approaches (e.g. MS^2 and MS^3) applied to a single pair of cross-linked peptides, there SHOULD be exactly two <SpectrumIdentificationItem> elements sharing the same identifier under "cross-link spectrum identification item". In the case, of "light" and "heavy" cross-linked peptides, there SHOULD be exactly four <SpectrumIdentificationItem> elements, all sharing the same identifier under "cross-link spectrum identification item" (light alpha chain, light beta chain, heavy alpha chain, heavy beta chain).

Guidelines for cross-linking results encoding

```
<AnalysisProtocolCollection>
  <SpectrumIdentificationProtocol analysisSoftware_ref="ID_software" id="SearchProtocol_1">
    <SearchType>
      <cvParam accession="MS:1001083" cvRef="PSI-MS" name="ms-ms search"/>
    </SearchType>
    <AdditionalSearchParams>
      <cvParam accession="MS:1001211" cvRef="PSI-MS" name="parent mass type mono"/>
      <cvParam accession="MS:1001256" cvRef="PSI-MS" name="fragment mass type mono"/>
      <cvParam accession="MS:1002494" cvRef="PSI-MS" name="cross-linking search"/>
    </AdditionalSearchParams>
```

A

AAFTKQAADK
▮
AMYPPKEDR

```
  <Peptide id="30491856_30492180_2_4_p1">
    <PeptideSequence>AAFTKQAADK</PeptideSequence>
    <Modification monoisotopicMassDelta="138.0680796"  location="5">
      <cvParam accession="XL:00002" cvRef=" PSI-MS " name="Xlink:DSS"/>
      <cvParam accession="MS:1002509" cvRef="PSI-MS" name="cross-link donor" value="5448"/>
    </Modification>
  </Peptide>
  <Peptide id="30491856_30492180_2_4_p2">
    <PeptideSequence>AMYPPKEDR</PeptideSequence>
    <Modification monoisotopicMassDelta="0.0" location="6">
      <cvParam accession="MS:1002510" cvRef="PSI-MS" name="cross-link receiver" value="5448"/>
    </Modification>
  </Peptide>
```

B

C

B

```
<SpectrumIdentificationResult spectraData_ref="SID_1" spectrumID="index=2776" id="SIR_1">
    <SpectrumIdentificationItem passThreshold="true" rank="1" peptide_ref="30491856_30492180_2_4_p1"
experimentalMassToCharge= "569.7912" calculatedMassToCharge= "569.79054" chargeState="4" id="SII_1_1">
      <PeptideEvidenceRef peptideEvidence_ref="pepevid_psm121558473_pep30491845_protP02768-A_target_535"/>
      <cvParam accession="MS:1002511" cvRef="PSI-MS" value="1" name="cross-link spectrum identification item"/>
     <cvParam accession="MS:1002545" cvRef="PSI-MS" value="1.3111826921077734" name="xi:score"/>
   </SpectrumIdentificationItem>
    <SpectrumIdentificationItem passThreshold="true" rank="1" peptide_ref="30491715_30491845_3_7_p0"
experimentalMassToCharge= "569.7912" calculatedMassToCharge= "569.79054" chargeState="4" id="SII_1_2">
      <PeptideEvidenceRef peptideEvidence_ref="pepevid_psm121558473_pep30491715_protP02768-A_target_411"/>
      <cvParam accession="MS:1002511" cvRef="PSI-MS" value="1" name="cross-link spectrum identification item"/>
      <cvParam accession="MS:1002545" cvRef="PSI-MS" value="1.3111826921077734" name="xi:score"/>
    </SpectrumIdentificationItem>
  </SpectrumIdentificationResult>
```

D

E

Feature	Explanation
A	If a cross-linking search has been performed, this cvParam MUST be present.
B	If a pair of cross-linked peptides has been identified, one peptide's Modification element MUST be flagged as "cross-link donor" and one MUST be flagged as "cross-link receiver". The export software SHOULD use the following rules to choose the crosslink donor as the: longer peptide, then higher peptide neutral mass, then alphabetical order. The cross-link donor Modification element MUST have the attribute monoisotopicMassDelta = the mass gain from the crosslink reagent. The cross-link receiver peptide's Modification element MUST have monoisotopicMassDelta = 0. A unique identifier linking these two Modification elements together MUST be in the value slot.
C	The cross-link donor peptide's Modification element MUST have a suitably sourced cvParam for the crosslink. The cross-link acceptor peptide's Modification element MUST not have a cvParam for the reagent.
D	If a cross-linked pair of peptides has been identified, there MUST be two <SpectrumIdentificationItem> elements with the same rank value. Both MUST have the "cross-link spectrum identification item" cvParam, and the value acts as a local identifier within the <SpectrumIdentificationResult> to group these two elements together. The experimentalMassToCharge, calculateMassToCharge and chargeState MUST be identical over both SII elements, indicating the overall values for the pair.
E	If the search engine applies a score to the paired identification, both <SpectrumIdentificationItem> elements MUST have the same cvParam capturing the value. The two <SpectrumIdentificationItem> elements MAY also have independent scores for the two chains.

Figure 3. The encoding in mzIdentML 1.2.0 for annotating results of searches including cross-linked peptides.

Encoding evidence associated with cross-linked position
The encoding for cross-linked peptides MAY be combined with the encoding for modification localisation scoring, using the same mechanism (Section 5.2.8).

Encoding peptide-level rescoring of cross-linking data
The cross-linking approach MAY also be combined with peptide-level re-scoring (Section 5.2.7, with specific CV terms for scores associated with cross-linked peptides rather than PSM-level terms), for approaches that do not follow the consensus spectrum approach outlined above.

Encoding protein-level interaction evidence
In cross-linking, protein identification, grouping or inference SHOULD follow the general encoding as decribed in Section 5.2.1. Where software has evidence that a pair of proteins is interacting due to the presence of cross-linked peptides, such evidence can be encoded through adding CV terms to the <ProteinDetectionHypothesis> elements elements representing the two interacting proteins (Figure 4). The value slot of the CV term MUST have the exact structure as shown in Figure 4.

If evidence exists that the same protein forms a homo-dimer, then the same protein accession can be used (*via* two <ProteinDetectionHypothesis> elements) in two different <ProteinAmbiguityGroup> elements, and using the same interaction score mechanism as above.

This way to encode molecular interaction data does not intend to capture all the details related to the interaction. There are other formats developed by the PSI-MI (Molecular Interactions) working group (e.g. PXI-MI XML and MITAB) that can be used to achieve this (see Section 4).

Encoding modifications searched
The <SpectrumIdentificationProtocol> element encodes, amongst other items, the modifications that were searched for. When encoding cross-linking modifications, it is expected that at least two <SearchModification> elements SHOULD be used to encode each cross-link reagent used, to encode the site specificity of both the donor and acceptor termini of the reagent, as shown below. The value slot of the cross-link donor and acceptor pair CV terms, is interpreted as a local unique identifier for the pair.

```
<SearchModification fixedMod="false" massDelta="138.06808" residues="S T Y K">
  <cvParam cvRef="XLMOD" accession="XLMOD:02000" name="BS3"/>
  <cvParam cvRef="PSI-MS" accession="MS:1002509" name="cross-link donor" value="0"/>
</SearchModification>
<SearchModification fixedMod="false" massDelta="0.0" residues="S T Y K">
  <cvParam cvRef="XLMOD" accession="XLMOD:02000" name="BS3"/>
  <cvParam cvRef="PSI-MS" accession="MS:1002510" name="cross-link acceptor" value="0"/>
</SearchModification>
```

Hypothetical/stylized example of encoding evidence for protein interactions

PAG 1

PDH 1.1
accession = Prot A.1
name="protein-pair-level global FDR" value="1001.a:256:0.001:TRUE"
name="protein-pair-level global FDR" value="1002.a:478:0.07:FALSE"

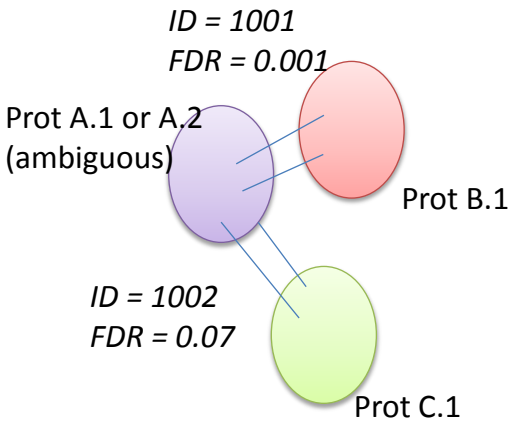
PDH 1.2
accession = Prot A.2
name="protein-pair-level global FDR" value="1001.a:258:0.001:TRUE"
name="protein-pair-level global FDR" value="1002.a:480:0.07:TRUE

PAG 2

PDH 2.1
accession = Prot B.1
name="protein-pair-level global FDR" value="1001.b:135:0.001:TRUE"

PAG 3

PDH 1.1
accession = Prot A.1
name="protein-pair-level global FDR" value="1002.b:135:0.07:FALSE"



Explanation

IDs on Proteins are to name and describe the overall interaction evidence (potentially based off multiple peptides) for the pairwise interaction.

In mzIdentML, they will be represented by different ProteinDetectionHypothesis (PDH) elements within different ProteinAmbiguityGroup (PAG) elements, sharing the same ID and score.

These CV terms must have a paired structure of int_ID.a|b:POS|null:SCORE_OR_VALUE:PASS_THRESHOLD

1) The two partners in the interaction share the same *integer* value for ID followed by *a* or *b*. If there is ambiguity in protein identification, two different ProteinDetectionHypothesis (PDH) elements, within the same ProteinAmbiguityGroup (PAG), MAY share the same ID and suffix (a or b). A given identifier (integer and suffix) value MUST NOT be used in more than PAG.
2) The export software MAY indicate the general position of the interaction (potentially taking on board multiple pairs of cross-linked peptides), with respect to the protein sequence – using a 1-based counting system. A "null" MAY be used if the export software does not wish to include a value.
3) The score or statistical value for the interaction.
4) "true" or "false" to indicate whether the score or value has passed a reported threshold in the file. If no threshold is defined, then PASS_THRESHOLD is always true.

XML Snippet

```
<ProteinAmbiguityGroup id="PAG_0">
    <ProteinDetectionHypothesis dBSequence_ref="dbseq_P02771" passThreshold="true" id="PAG_0_PDH_0">
      <PeptideHypothesis peptideEvidence_ref="pepevid_psm252637369_pep54601081">
        <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_1_1"/>
      </PeptideHypothesis>
    ...

      <cvParam cvRef="PSI-MS" accession="MS:1002676" name="protein-pair-level global FDR" value="100.b:null:0.001:true"/>
      <cvParam cvRef="PSI-MS" accession="MS:1002677" name="residue-pair-level global FDR" value="106.b:146:0.0294:true"/>
    </ProteinDetectionHypothesis>
    <cvParam cvRef="PSI-MS" accession="MS:1002415" name="protein group passes threshold" value="true"/>
</ProteinAmbiguityGroup>


<ProteinAmbiguityGroup id="PAG_1">
    <ProteinDetectionHypothesis dBSequence_ref="dbseq_P02768" passThreshold="true" id="PAG_1_PDH_0">
      <PeptideHypothesis peptideEvidence_ref="pepevid_psm252637369_pep54600650">
        <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_1_2"/>
      </PeptideHypothesis>
      <PeptideHypothesis peptideEvidence_ref="pepevid_psm252633422_pep54604445_protP02768-A_target_52">
        <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_2_1"/>
      </PeptideHypothesis>
    ....
    <cvParam cvRef="PSI-MS" accession="MS:1002676" name="protein-pair-level global FDR" value="100.a:null:0.001:true"/>
    <cvParam cvRef="PSI-MS" accession="MS:1002677" name="residue-pair-level global FDR" value="106.a:436:0.0294:true"/>
  </ProteinDetectionHypothesis>
  <cvParam cvRef="PSI-MS" accession="MS:1002415" name="protein group passes threshold" value="true"/>
</ProteinAmbiguityGroup>
```

Figure 4. Encoding of protein interaction scores or statistics from cross-linking in mzIdentML.

5.2.10 Encoding proteogenomics annotation data

It is now common to use tandem MS data to improve current gene model annotations, in so-called proteogenomics approaches, for example based on making peptide identifications against the official gene models or against alternative databases generated by gene finders, mapping mRNA transcripts or six frame genome translations. Where identifications do not match the official genes, they give evidence in support of updates to the gene models. One of the key concepts required is the mapping of peptides back to chromosomes, including, for example, where they map across splice junctions. File format specifications are under development that can be used directly for genome visualisation, such as adaptations of the BED and BAM (7) formats commonly used in genomics. To ensure a consistent export is possible from mzIdentML to formats designed for genome visualisation or annotation, in mzIdentML 1.2, a consistent encoding of the chromosomal mappings has been developed, as exemplified in Figure 5.

Guidelines for encoding proteogenomics results

```
<SpectrumIdentificationProtocol analysisSoftware_ref="ID_software" id="SearchProtocol_1">
    <SearchType>
      <cvParam cvRef="PSI-MS" accession="MS:1001083" name="ms-ms search"/>
    </SearchType>
    <AdditionalSearchParams>
      <cvParam cvRef="PSI-MS" accession="MS:1001211" name="parent mass type mono"/>
      <cvParam cvRef="PSI-MS" accession="MS:1001256" name="fragment mass type mono"/>
      <cvParam cvRef="PSI-MS" accession="MS:1002490" name="peptide-level scoring"/>
      <cvParam cvRef="PSI-MS" accession="MS:1002496" name="group PSMs by sequence"/>
      <cvParam cvRef="PSI-MS" accession="MS:1002635" name="proteogenomics search"/>
    </AdditionalSearchParams>
```

A

```
 <PeptideEvidence dBSequence_ref="dbseq_generic|A_ENSP00000354925|" peptide_ref="DVLEGDSSEDR_" start="23"
end="33" pre="A" post="A" isDecoy="false" id="DVLEGDSSEDR_generic|A_ENSP00000354925|_23_33">
    <cvParam cvRef="PSI-MS" accession="MS:1002640" name="peptide end on chromosome" value="156646808"/>
    <cvParam cvRef="PSI-MS" accession="MS:1002641" name="peptide exon count" value="2"/>
    <cvParam cvRef="PSI-MS" accession="MS:1002642" name="peptide exon nucleotide sizes" value="25,8"/>
    <cvParam cvRef="PSI-MS" accession="MS:1002643" name="peptide start positions on chromosome"
value="156646122,156646800"/>
  </PeptideEvidence>
```

B

C

```
<DBSequence searchDatabase_ref="SearchDB_1" accession="generic|A_ENSP00000389898|"
id="dbseq_generic|A_ENSP00000389898|">
   <cvParam cvRef="PSI-MS" accession="MS:1002637" name="chromosome name" value="1"/>
   <cvParam cvRef="PSI-MS" accession="MS:1002638" name="chromosome strand" value="+"/>
   <cvParam cvRef="PSI-MS" accession="MS:1002644" name="genome reference version" value="Ensembl release
84"/>
</DBSequence>
```

D

Feature	Explanation
A	If a proteogenomics search has been performed, this cvParam MUST be present.
B	Every PeptideEvidence that has isDecoy="false", MUST have either MS:1002740 "unmapped peptide" (for cases where a peptide could not be mapped) or the cv terms in bold MUST be present. For PeptideEvidence elements with isDecoy="true", all terms are OPTIONAL. In this example, peptide DVLEGDSSEDR crosses an exon boundary. The N-terminal region of the peptide is mapped to positions 156646123 – 156646148 (start + 25 from peptide exon nucleotide sizes). The C-terminal region of the peptide is mapped from 156646800 to 156646808 (second value of "peptide start positions on chromosome" + 8). Definitions of terms are provided below
C	Additional CV terms MAY be added at a later date to encode classifications of peptide types, such as "novel junction", "novel N-terminus" and so on. Such information MAY be encoded on SpectrumIdentificationItem, using the peptide-level scores type of encoding.
D	Each DBSequence value MUST store either: 1) the genome reference version, chromosome name and strand or 2) be annotated with the term MS:1002741 "unmapped protein".

Figure 5. The encoding for chromosomal coordinates in mzIdentML in support of proteogenomics approaches.

5.3 Other supporting materials

Example files demonstrating the different uses cases have been developed and are available from the following location: https://github.com/HUPO-PSI/mzIdentML/tree/master/examples/1_2examples. The sub-folder names indicate the features of the format being used in each example.

6. Model in XML Schema

An overview of the schema is presented in Figure 6. The following documentation is automatically generated from the XML Schema.

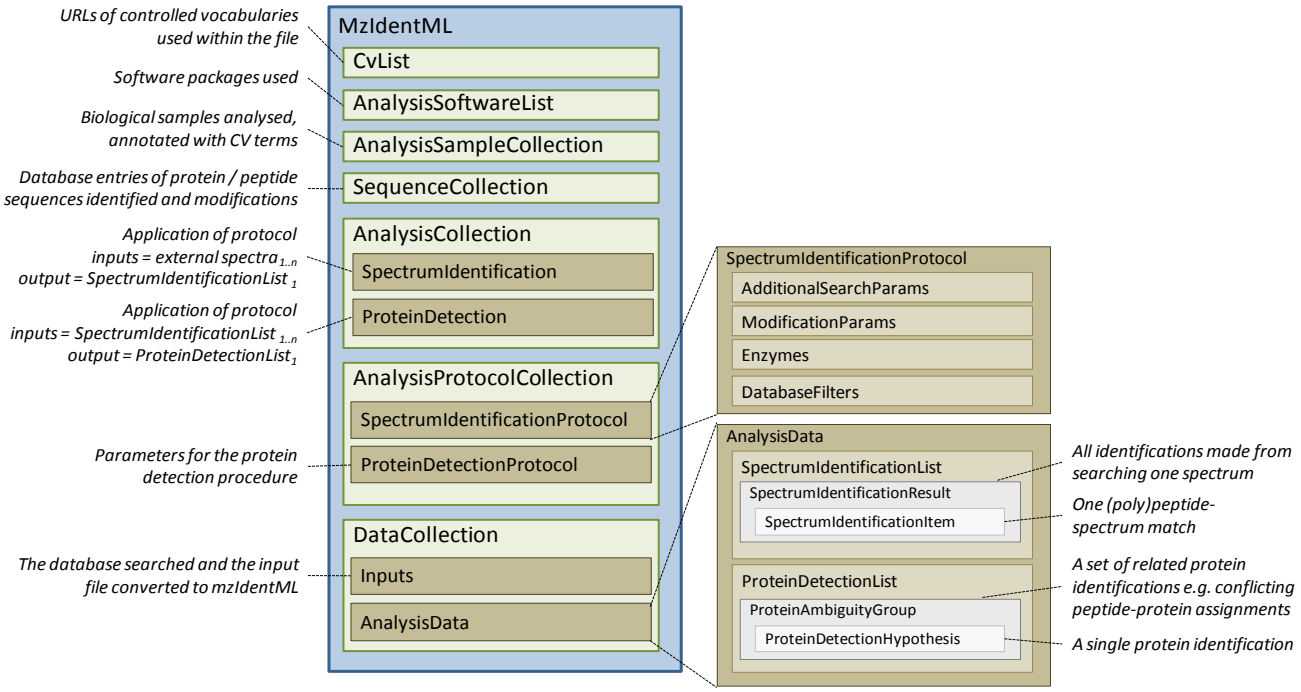


Figure 6. A diagrammatic overview of the mzIdentML schema.

6.1 Element <MzIdentML>

Definition: The upper-most hierarchy level of mzIdentML with sub-containers for example describing software, protocols and search results (spectrum identifications or protein detection results).

Type: MzIdentMLType

Attributes:

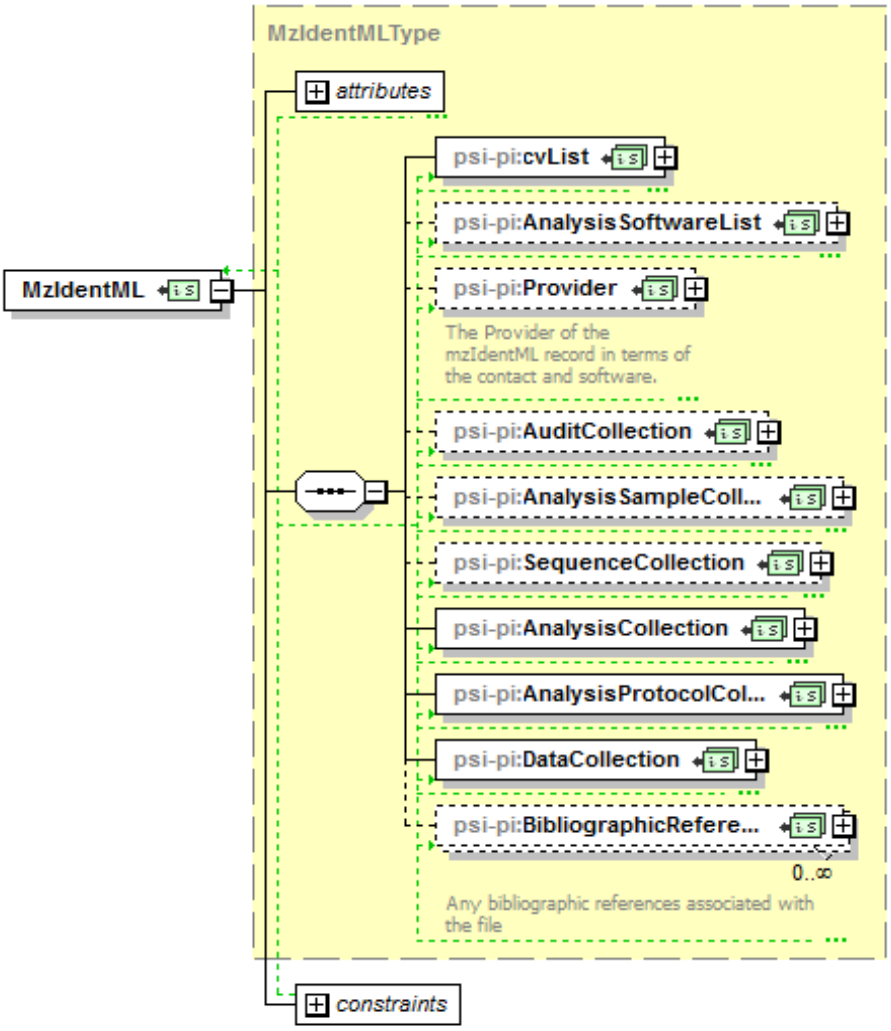
Attribute Name	Data Type	Use	Definition
creationDate	xsd:dateTime	optional	The date on which the file was produced.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
version	versionRegex	required	The version of the schema this instance document refers to, in the format x.y.z. Changes to z should not affect prevent instance documents from validating.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition

cvList	1	1	The list of controlled vocabularies used in the file.
AnalysisSoftwareList	0	1	The software packages used to perform the analyses.
Provider	0	1	The Provider of the mzIdentML record in terms of the contact and software.
AuditCollection	0	1	The complete set of Contacts (people and organisations) for this file.
AnalysisSampleCollection	0	1	The samples analysed can optionally be recorded using CV terms for descriptions. If a composite sample has been analysed, the subsample association can be used to build a hierarchical description.
SequenceCollection	0	1	The collection of sequences (DBSequence or Peptide) identified and their relationship between each other (PeptideEvidence) to be referenced elsewhere in the results.
AnalysisCollection	1	1	The analyses performed to get the results, which map the input and output data sets. Analyses are for example: SpectrumIdentification (resulting in peptides) or ProteinDetection (assemble proteins from peptides).
AnalysisProtocolCollection	1	1	The collection of protocols which include the parameters and settings of the performed analyses.
DataCollection	1	1	The collection of input and output data sets of the analyses.
BibliographicReference	0	unbounded	Any bibliographic references associated with the file

Graphical Context:



Example Context:

```
<MzIdentML xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xmlns:xsd="http://www.w3.org/2001/XMLSchema" id=""
xsi:schemaLocation="http://psidev.info/psi/pi/mzIdentML/1.2 mzIdentML1.2.0.xsd" creationDate="2014-
06-03T14:52:58.665376Z" version="1.2.0" xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
  <cvList>
    <cv fullName="Proteomics Standards Initiative Mass Spectrometry Vocabularies" version="2.32.0"
uri="https://raw.githubusercontent.com/HUPO-PSI/psi-ms-CV/master/psi-ms.obo" id="PSI-MS" />
    <cv fullName="UNIMOD" uri="http://www.unimod.org/obo/unimod.obo" id="UNIMOD" />
    <cv fullName="UNIT-ONTOLOGY"
uri="http://obo.cvs.sourceforge.net/*checkout*/obo/obo/ontology/phenotype/unit.obo" id="UO" />
  </cvList>
  <AnalysisSoftwareList>
  ...
</MzIdentML>
```

6.2 Element <AdditionalSearchParams>

Definition: The search parameters other than the modifications searched.

Type: ParamListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

userParam	1	unbounded	A single user-defined parameter.

Example Context:

```
      <AdditionalSearchParams>
        <cvParam cvRef="PSI-MS" accession="MS:1001211" name="parent mass type mono"/>
        <cvParam cvRef="PSI-MS" accession="MS:1001256" name="fragment mass type mono"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002492" name="consensus scoring"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002490" name="peptide-level scoring"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002497" name="group PSMs by sequence with
modifications"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002491" name="modification localization scoring"/>
  ...
</AdditionalSearchParams>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/AdditionalSearchParams
MAY supply a *child* term of MS:1001302 (search engine specific input parameter) one or more
times
  e.g.: MS:1001005 (SEQUEST:CleavesAt)
  e.g.: MS:1001007 (SEQUEST:OutputLines)
  e.g.: MS:1001009 (SEQUEST:DescriptionLines)
  e.g.: MS:1001026 (SEQUEST:NormalizeXCorrValues)
  e.g.: MS:1001028 (SEQUEST:SequenceHeaderFilter)
  e.g.: MS:1001032 (SEQUEST:SequencePartialFilter)
  e.g.: MS:1001037 (SEQUEST:ShowFragmentIons)
  e.g.: MS:1001038 (SEQUEST:Consensus)
  e.g.: MS:1001042 (SEQUEST:LimitTo)
  e.g.: MS:1001046 (SEQUEST:sort by dCn)
  et al.
MAY supply a *child* term of MS:1001066 (ions series considered in search) one or more times
MAY supply a *child* term of MS:1001210 (mass type settings) one or more times
  e.g.: MS:1001211 (parent mass type mono)
  e.g.: MS:1001212 (parent mass type average)
  e.g.: MS:1001255 (fragment mass type average)
  e.g.: MS:1001256 (fragment mass type mono)
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001211" name="parent mass type mono"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001256" name="fragment mass type mono"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002490" name="peptide-level scoring"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002496" name="group PSMs by sequence"></cvParam>
<cvParam accession="MS:1001118" cvRef="PSI-MS" name="param: b ion"/>
<cvParam accession="MS:1001149" cvRef="PSI-MS" name="param: b ion-NH3 DEPRECATED"/>
<cvParam accession="MS:1001150" cvRef="PSI-MS" name="param: b ion-H2O DEPRECATED"/>
<cvParam accession="MS:1001262" cvRef="PSI-MS" name="param: y ion"/>
<cvParam accession="MS:1001151" cvRef="PSI-MS" name="param: y ion-NH3 DEPRECATED"/>
<cvParam accession="MS:1001152" cvRef="PSI-MS" name="param: y ion-H2O DEPRECATED"/>
<cvParam accession="MS:1002494" cvRef="PSI-MS" name="cross-linking search"/>
<cvParam name="no special processing" cvRef="PSI-MS" accession="MS:1002495" />
<cvParam cvRef="PSI-MS" accession="MS:1002492" name="consensus scoring"/>
<cvParam cvRef="PSI-MS" accession="MS:1002497" name="group PSMs by sequence with modifications"/>
<cvParam cvRef="PSI-MS" accession="MS:1002491" name="modification localization scoring"/>
```

Example userParams:

```
<userParam value="true" name="TargetDecoyApproach"/>
<userParam value="-1" name="MinIsotopeError"/>
<userParam value="2" name="MaxIsotopeError"/>
<userParam value="HCD" name="FragmentMethod"/>
<userParam value="QExactive" name="Instrument"/>
<userParam value="iTRAQ" name="Protocol"/>
<userParam value="2" name="NumTolerableTermini"/>
<userParam value="1" name="NumMatchesPerSpec"/>
<userParam value="2" name="MaxNumModifications"/>
<userParam value="6" name="MinPepLength"/>
<userParam value="40" name="MaxPepLength"/>
<userParam value="2" name="MinCharge"/>
<userParam value="3" name="MaxCharge"/>
<userParam value="2a_uniprot" name="Mascot User Comment"/>
<userParam value="ESI-QUAD" name="Mascot Instrument Name"/>
<userParam name="input_consensusXML" unitName="xsd:string" value="leitner004.consensusXML"/>
<userParam name="input_decoys" unitName="xsd:string" value=""/>
<userParam name="decoy_prefix" unitName="xsd:integer" value="1"/>
<userParam name="decoy_string" unitName="xsd:string" value="decoy"/>
<userParam name="precursor:min_charge" unitName="xsd:integer" value="3"/>
<userParam name="precursor:max_charge" unitName="xsd:integer" value="7"/>
<userParam name="fragment:mass_tolerance_xlinks" unitName="xsd:double" value="0.3"/>
<userParam name="peptide:min_size" unitName="xsd:integer" value="5"/>
<userParam name="cross_link:residue1" unitName="xsd:string" value="[K]"/>
<userParam name="cross_link:residue2" unitName="xsd:string" value="[K]"/>
<userParam name="cross_link:mass" unitName="xsd:double" value="138.0680796"/>
<userParam name="cross_link:mass_isoshift" unitName="xsd:double" value="12.075321"/>
<userParam name="cross_link:mass_monolink" unitName="xsd:string" value="[156.07864431,
155.094628715]"/>
<userParam name="modifications:variable_max_per_peptide" unitName="xsd:integer" value="2"/>
<userParam name="algorithm:candidate_search" unitName="xsd:string" value="enumeration"/>
<userParam name="charges" unitName="xsd:string" value="2,3,4,5,6"/>
```

Example for peptide-level statistics:

```
<cvParam cvRef="PSI-MS" accession="MS:1001211" name="parent mass type mono"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001256" name="fragment mass type mono"></cvParam>
```

```
                <cvParam cvRef="PSI-MS" accession="MS:1002490" name="peptide-level scoring"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002496" name="group PSMs by sequence"></cvParam>
```

Example for sample pre-fractionation:

```
                <cvParam cvRef="PSI-MS" accession="MS:1001256" name="fragment mass type mono"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1001211" name="parent mass type mono"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002493" name="sample pre-fractionation"
        value="MudPIT"></cvParam>
```

Example for proteogenomics:

```
                <cvParam cvRef="PSI-MS" accession="MS:1002635" name="proteogenomics search" value=""></cvParam>
```

Example for cross-linking:

```
                <cvParam cvRef="PSI-MS" accession="MS:1001211" name="parent mass type mono"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002494" name="cross-linking search"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1001256" name="fragment mass type mono"></cvParam>
```

Example for modification position scoring:

```
                <cvParam cvRef="PSI-MS" accession="MS:1002491" name="modification localization scoring"></cvParam>
```

Example for de novo sequencing:

```
                <cvParam cvRef="PSI-MS" accession="MS:1001010" name=" de novo search "></cvParam>
```

Example for consensus scoring:

```
                <cvParam cvRef="PSI-MS" accession="MS:1002492" name="consensus scoring"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002392" name="PIA:PSM sets created" value="true"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002391" name="PIA:Combined FDRScore calculated"
        value="true"></cvParam>
```

6.3 Element <Affiliation>

Definition: The organization a person belongs to.

Type: AffiliationType

Attributes:

Attribute Name	Data Type	Use	Definition
organization_ref	xsd:string	required	A reference to the organization this contact belongs to.

Subelements: none

Example Context:

```
<Affiliation organization_ref="ORG_DOC_OWNER"></Affiliation>
```

6.4 Element <AmbiguousResidue>

Definition: Ambiguous residues e.g. X can be specified by the Code attribute and a set of parameters for example giving the different masses that will be used in the search.

Type: AmbiguousResidueType

Attributes:

Attribute Name	Data Type	Use	Definition
code	chars	required	The single letter code of the ambiguous residue e.g. X.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	1	unbounded	A single user-defined parameter.

Example Context:

```
<AmbiguousResidue code="X">
    <cvParam accession="MS:1001360" cvRef="PSI-MS" value="A C D E F G H I K L M N O P Q R S T U V W
Y" name="alternate single letter codes"/>
</AmbiguousResidue>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/MassTable/AmbiguousResidue
MAY supply a *child* term of MS:1001359 (ambiguous residues) one or more times
  e.g.: MS:1001360 (alternate single letter codes)
  e.g.: MS:1001361 (alternate mass)
```

Example cvParams:

```
<cvParam accession="MS:1001360" cvRef="PSI-MS" value="D N" name="alternate single letter codes"/>
```

6.5 Element <AnalysisCollection>

Definition: The analyses performed to get the results, which map the input and output data sets. Analyses are for example: SpectrumIdentification (resulting in peptides) or ProteinDetection (assemble proteins from peptides).

Type: AnalysisCollectionType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SpectrumIdentification	1	unbounded	An Analysis which tries to identify peptides in input spectra, referencing the database searched, the input spectra, the output results and the protocol that is run.
ProteinDetection	0	1	An Analysis which assembles a set of peptides (e.g. from a spectra search analysis) to proteins.

Example Context:

```
<AnalysisCollection >
  <SpectrumIdentification spectrumIdentificationProtocol_ref="SearchProtocol_1_4299"
spectrumIdentificationList_ref="SII_LIST_1_1_4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-3_Din.raw"
id="SpecIdent__4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-3_Din.raw">
    <InputSpectra spectraData_ref="SD_4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-
3_Din.raw"></InputSpectra>
    <SearchDatabaseRef searchDatabase_ref="SDB_4299_203"></SearchDatabaseRef>
  </SpectrumIdentification>
  <SpectrumIdentification spectrumIdentificationProtocol_ref="SearchProtocol_1_4299"
spectrumIdentificationList_ref="SII_LIST_1_1_4299_120114_09_Orbi2_ZC_QC_220_HSAd0-d4-1to4-2_Din.raw"
id="SpecIdent__4299_120114_09_Orbi2_ZC_QC_220_HSAd0-d4-1to4-2_Din.raw">
    <InputSpectra spectraData_ref="SD_4299_120114_09_Orbi2_ZC_QC_220_HSAd0-d4-1to4-
2_Din.raw"></InputSpectra>
  ...
</AnalysisCollection>
```

6.6 Element <AnalysisData>

Definition: Data sets generated by the analyses, including peptide and protein lists.

Type: AnalysisDataType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SpectrumIdentificationList	1	unbounded	Represents the set of all search results from SpectrumIdentification.
ProteinDetectionList	0	1	The protein list resulting from a protein detection process.

Example Context:

```
<AnalysisData>
<SpectrumIdentificationList xmlns="http://psidev.info/psi/pi/mzIdentML/1.2" id="SII_LIST_1">
  <SpectrumIdentificationResult spectrumID="index=6451" spectraData_ref="SD_COMBINED_SE_0"
id="SIR_8947">
    <SpectrumIdentificationItem chargeState="2" experimentalMassToCharge="679.817322"
calculatedMassToCharge="679.818488" peptide_ref="AVMDDFAAFVEK_##Oxidation(M):3" rank="1"
passThreshold="false" id="SIR_8947_SII_1">
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000401820|p:known_378_389"></PeptideEvidenceRef>
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000421027|p:putative_420_431"></PeptideEvidenceRef>
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000483421|p:known_357_368"></PeptideEvidenceRef>
  ...
</AnalysisData>
```

6.7 Element <AnalysisParams>

Definition: The parameters and settings for the protein detection given as CV terms.

Type: ParamListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	1	unbounded	A single user-defined parameter.

Example Context:

```
<AnalysisParams>
  <cvParam name="mascot:SigThreshold" value="0.05" cvRef="PSI-MS" accession="MS:1001316" />
  <cvParam name="mascot:MaxProteinHits" value="Auto" cvRef="PSI-MS" accession="MS:1001317" />
  <cvParam name="mascot:ProteinScoringMethod" value="MudPIT" cvRef="PSI-MS"
accession="MS:1001318" />
  <cvParam name="mascot:MinMSMSThreshold" value="0" cvRef="PSI-MS" accession="MS:1001319" />
  <cvParam name="mascot:ShowHomologousProteinsWithSamePeptides" value="1" cvRef="PSI-MS"
accession="MS:1001320" />
  <cvParam name="mascot:ShowHomologousProteinsWithSubsetOfPeptides" value="10" cvRef="PSI-MS"
accession="MS:1001321" />
  ...
</AnalysisParams>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/ProteinDetectionProtocol/AnalysisParams
MAY supply a *child* term of MS:1001302 (search engine specific input parameter) one or more
times
  e.g.: MS:1001005 (SEQUEST:CleavesAt
  e.g.: MS:1001007 (SEQUEST:OutputLines)
  e.g.: MS:1001009 (SEQUEST:DescriptionLines)
  e.g.: MS:1001026 (SEQUEST:NormalizeXCorrValues)
  e.g.: MS:1001028 (SEQUEST:SequenceHeaderFilter)
  e.g.: MS:1001032 (SEQUEST:SequencePartialFilter)
  e.g.: MS:1001037 (SEQUEST:ShowFragmentIons)
  e.g.: MS:1001038 (SEQUEST:Consensus)
  e.g.: MS:1001042 (SEQUEST:LimitTo)
  e.g.: MS:1001046 (SEQUEST:sort by dCn)
  et al.
MAY supply a *child* term of MS:1001194 (quality estimation with decoy database) one or more
times
```

Example cvParams:

```
<cvParam name="mascot:SigThreshold" value="0.05" cvRef="PSI-MS" accession="MS:1001316" />
<cvParam name="mascot:MaxProteinHits" value="Auto" cvRef="PSI-MS" accession="MS:1001317" />
<cvParam name="mascot:ProteinScoringMethod" value="MudPIT" cvRef="PSI-MS"
accession="MS:1001318" />
<cvParam name="mascot:MinMSMSThreshold" value="0" cvRef="PSI-MS" accession="MS:1001319" />
<cvParam name="mascot:ShowHomologousProteinsWithSamePeptides" value="1" cvRef="PSI-MS"
accession="MS:1001320" />
<cvParam name="mascot:ShowHomologousProteinsWithSubsetOfPeptides" value="10" cvRef="PSI-MS"
accession="MS:1001321" />
<cvParam name="mascot:RequireBoldRed" value="0" cvRef="PSI-MS" accession="MS:1001322" />
<cvParam name="mascot:UseUnigeneClustering" value="false" cvRef="PSI-MS" accession="MS:1001323"
/>
<cvParam name="mascot:IncludeErrorTolerantMatches" value="1" cvRef="PSI-MS"
accession="MS:1001324" />
<cvParam name="mascot:ShowDecoyMatches" value="0" cvRef="PSI-MS" accession="MS:1001325" />
```

6.8 Element <AnalysisProtocolCollection>

Definition: The collection of protocols which include the parameters and settings of the performed analyses.

Type: AnalysisProtocolCollectionType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SpectrumIdentificationProtocol	1	unbounded	The parameters and settings of a SpectrumIdentification analysis.
ProteinDetectionProtocol	0	1	The parameters and settings of a ProteinDetection process.

Example Context:

```
<AnalysisProtocolCollection xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <SpectrumIdentificationProtocol analysisSoftware_ref="AS_mascot_server" id="SIP">
        <SearchType>
            <cvParam accession="MS:1001083" cvRef="PSI-MS" value="" name="ms-ms search"/>
        </SearchType>
        <AdditionalSearchParams>
            <cvParam accession="MS:1001211" cvRef="PSI-MS" name="parent mass type mono"/>
  ...
</AnalysisProtocolCollection>
```

6.9 Element <AnalysisSampleCollection>

Definition: The samples analysed can optionally be recorded using CV terms for descriptions. If a composite sample has been analysed, the subsample association can be used to build a hierarchical description.

Type: AnalysisSampleCollectionType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Sample	1	unbounded	A description of the sample analysed by mass spectrometry using CVParams or UserParams. If a composite sample has been analysed, a parent sample should be defined, which references subsamples. This represents any kind of substance used in an experimental workflow, such as whole organisms, cells, DNA, solutions, compounds and experimental substances (gels, arrays etc.).

Example Context:

6.10 Element <AnalysisSoftware>

Definition: The software used for performing the analyses.

Type: AnalysisSoftwareType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
uri	xsd:anyURI	optional	URI of the analysis software e.g. manufacturer's website
version	xsd:string	optional	The version of Software used.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ContactRole	0	1	The Contact that provided the document instance.
SoftwareName	1	1	The name of the analysis software package, sourced from a CV if available.
Customizations	0	1	Any customizations to the software, such as alternative scoring mechanisms implemented, should be documented here as free text.

Example Context:

```
<AnalysisSoftware uri="http://code.google.com/p/ehu-bio/downloads/list" version="1.1-beta4"
name="PAnalyzer (v1.1-beta4)" id="PAnalyzer">
    <ContactRole contact_ref="PAnalyzer_Author">
        <Role>
            <cvParam accession="MS:1001271" cvRef="PSI-MS" name="researcher"/>
        </Role>
    </ContactRole>
    <SoftwareName>
  ...
</AnalysisSoftware>
```

6.11 Element <AnalysisSoftwareList>

Definition: The software packages used to perform the analyses.

Type: AnalysisSoftwareListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
AnalysisSoftware	1	unbounded	The software used for performing the analyses.

Example Context:

```
<AnalysisSoftwareList xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <AnalysisSoftware version="Beta (v9979)" name="MS-GF+" id="ID_software">
        <SoftwareName>
            <cvParam accession="MS:1002048" cvRef="PSI-MS" name="MS-GF+"/>
        </SoftwareName>
    </AnalysisSoftware>
    <AnalysisSoftware name="FalseDiscoveryRate_2014-07-02 12-04-18" id="FalseDiscoveryRate_2014-
07-02 12-04-18">
  ...
</AnalysisSoftwareList>
```

6.12 Element <AuditCollection>

Definition: The complete set of Contacts (people and organisations) for this file.

Type: AuditCollectionType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Person	1	1	A person's name and contact details. Any additional information such as the address, contact email etc. should be supplied using CV parameters or user parameters.
Organization	1	1	Organizations are entities like companies, universities, government agencies. Any additional information such as the address, email etc. should be supplied either as CV parameters or as user parameters.

Example Context:

```
<AuditCollection xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
  <Person lastName="secondName" firstName="firstname" id="PERSON_DOC_OWNER">
    <cvParam cvRef="PSI-MS" accession="MS:1000587" name="contact address" value="address"></cvParam>
    <Affiliation organization_ref="ORG_DOC_OWNER"></Affiliation>
  </Person>
  <Organization id="ORG_DOC_OWNER" name="myworkplace">
    <cvParam cvRef="PSI-MS" accession="MS:1000586" name="contact name" value="address"></cvParam>
  ...
</AuditCollection>
```

6.13 Element <BibliographicReference>

Definition: Any bibliographic references associated with the file

Type: BibliographicReferenceType

Attributes:

Attribute Name	Data Type	Use	Definition
authors	xsd:string	optional	The names of the authors of the reference.
doi	xsd:string	optional	The DOI of the referenced publication.
editor	xsd:string	optional	The editor(s) of the reference.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
issue	xsd:string	optional	The issue name or number.

name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
pages	xsd:string	optional	The page numbers.
publication	xsd:string	optional	The name of the journal, book etc.
publisher	xsd:string	optional	The publisher of the publication.
title	xsd:string	optional	The title of the BibliographicReference.
volume	xsd:string	optional	The volume name or number.
year	xsd:int	optional	The year of publication.

Subelements: none

Example Context:

```
<BibliographicReference id="10.1002/(SICI)1522-2683(19991201)20:18<3551::AID-ELPS3551>3.0.CO;2-2"
name="Probability-based protein identification by searching sequence databases using mass
spectrometry data" authors="David N. Perkins, Darryl J. C. Pappin, David M. Creasy, John S.
Cottrell" publication="Electrophoresis" publisher="Wiley VCH" editor="" year="1999" volume="20"
issue="18" pages="3551-3567" title="Probability-based protein identification by searching sequence
databases using mass spectrometry data" />
```

6.14 Element <ContactRole>

Definition:

Depending on context:
1: The contact details of the organisation or person that produced the software
2: Contact details for the Material. The association to ContactRole could specify, for example, the creator or provider of the Material.
3: The Contact that provided the document instance.

Type: ContactRoleType

Attributes:

Attribute Name	Data Type	Use	Definition
contact_ref	xsd:string	required	When a ContactRole is used, it specifies which Contact the role is associated with.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Role	1	1	The roles (lab equipment sales, contractor, etc.) the Contact fills.

Example Context:

```
<ContactRole contact_ref="PERSON_DOC_OWNER">
  <Role>
    <cvParam cvRef="PSI-MS" accession="MS:1001271" name="researcher"></cvParam>
  </Role>
</ContactRole>
```

6.15 Element <Customizations>

Definition: Any customizations to the software, such as alternative scoring mechanisms implemented, should be documented here as free text.

Type: xsd:string

Attributes: none

Subelements: none

Example Context:

```
<Customizations>
  No customisations
</Customizations>
```

6.16 Element <cv>

Definition: A source controlled vocabulary from which cvParams will be obtained.

Type: cvType

Attributes:

Attribute Name	Data Type	Use	Definition

fullName	xsd:string	required	The full name of the CV.
id	xsd:string	required	The unique identifier of this cv within the document to be referenced by cvParam elements.
uri	xsd:anyURI	required	The URI of the source CV.
version	xsd:string	optional	The version of the CV.

Subelements: none

Example Context:

```
<cv fullName="Proteomics Standards Initiative Mass Spectrometry Vocabularies" version="2.32.0"
uri=" https://raw.githubusercontent.com/HUPO-PSI/psi-ms-CV/master/psi-ms.obo" id="PSI-MS" />
```

6.17 Element <cvList>

Definition: The list of controlled vocabularies used in the file.

Type: CVListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cv	1	unbounded	A source controlled vocabulary from which cvParams will be obtained.

Example Context:

```
<cvList>
   <cv id="PSI-MS" fullName="Proteomics Standards Initiative Mass Spectrometry Vocabularies"
uri="https://raw.githubusercontent.com/HUPO-PSI/psi-ms-CV/master/psi-ms.obo" version="3.15.0"></cv>
   <cv id="UNIMOD" fullName="UNIMOD" uri="http://www.unimod.org/obo/unimod.obo"></cv>
  <cv id="UO"     fullName="UNIT-ONTOLOGY" uri="https://raw.githubusercontent.com/bio-ontology-
research-group/unit-ontology/master/unit.obo"></cv>
  <cv id="XLMOD" fullName="PSI cross-link modifications"
uri="https://raw.githubusercontent.com/HUPO-PSI/mzIdentML/master/cv/XLMOD-1.0.0.obo"></cv>
</cvList>
```

6.18 Element <cvParam>

Definition: A single entry from an ontology or a controlled vocabulary.

Type: CVParamType

Attributes:

Attribute Name	Data Type	Use	Definition
accession	xsd:string	required	The accession or ID number of this CV term in the source CV.
cvRef	xsd:string	required	A reference to the cv element from which this term originates.
name	xsd:string	required	The name of the parameter.
unitAccession	xsd:string	optional	An accession number identifying the unit within the OBO foundry Unit CV.
unitCvRef	xsd:string	optional	If a unit term is referenced, this attribute MUST refer to the CV 'id' attribute defined in the cvList in this file.
unitName	xsd:string	optional	The name of the unit.
value	xsd:string	optional	The user-entered value of the parameter.

Subelements: none

Example Context:

```
<cvParam cvRef="PSI-MS" accession="MS:1002520" name="peptide group ID"
value="CCPQCCSSGCSQNLCGPLCVTTPYYCTR_##Carbamidomethyl(C):1##Carbamidomethyl(C):2##Carbamidomethyl(C
:5##Carbamidomethyl(C):6##Carbamidomethyl(C):10##Carbamidomethyl(C):15##Carbamidomethyl(C
:19##Carbamidomethyl(C):26"></cvParam>
```

6.19 Element <DatabaseFilters>

Definition: The specification of filters applied to the database searched.

Type: DatabaseFiltersType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Filter	1	unbounded	Filters applied to the search database. The filter MUST include at least one of Include and Exclude. If both are used, it is assumed that inclusion is performed first.

Example Context:

```
<DatabaseFilters>
    <Filter>
        <FilterType>
            <cvParam accession="MS:1001020" cvRef="PSI-MS" name="DB filter taxonomy"/>
        </FilterType>
    </Filter>
</DatabaseFilters>
```

6.20 Element <DatabaseName>

Definition: The database name may be given as a cvParam if it maps exactly to one of the release databases listed in the CV, otherwise a userParam should be used.

Type: ParamType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.
userParam	1	1	A single user-defined parameter.

Example Context:

```
        <DatabaseName>
          <userParam name="uniprot-human-reviewed-trypsin-april-
2016_concatenated_target_decoy.fasta"/>
        </DatabaseName>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/Inputs/SearchDatabase/DatabaseName
MAY supply a *child* term of MS:1001013 (database name) one or more times
  e.g.: MS:1001084 (database nr)
  e.g.: MS:1001104 (database UniProtKB/Swiss-Prot)
  e.g.: MS:1001142 (database IPI_human)
  e.g.: MS:1001285 (database IPI_mouse)
  e.g.: MS:1001286 (database IPI_rat)
  e.g.: MS:1001287 (database IPI_zebrafish)
  e.g.: MS:1001288 (database IPI_chicken)
  e.g.: MS:1001289 (database IPI_cow)
  e.g.: MS:1001290 (database IPI_arabidopsis)
  e.g.: MS:1002060 (database UniProtKB/TrEMBL)
```

Example cvParams:

```
<cvParam accession="MS:1001197" cvRef="PSI-MS" name="DB composition target+decoy"/>
<cvParam accession="MS:1001283" cvRef="PSI-MS" value="^XXX" name="decoy DB accession regexp"/>
<cvParam accession="MS:1001195" cvRef="PSI-MS" name="decoy DB type reverse"/>
<cvParam accession="MS:1001073" cvRef="PSI-MS" name="database type amino acid"/>
```

Example userParams:

```
<userParam name="fawaz_PXD000652_combined_concatenated_target_decoy.fasta"></userParam>
<userParam name="no description"/>
<userParam name="Rosetta_uniprot_20130402_mouse_SWISS_can_iso_ECOLI.fasta"/>
<userParam name="Ros_Uniprot_20130402.fasta"/>
<userParam name="26Syeast_test.fasta"/>
<userParam name="Ros_Uniprot_Ecoli_20130402.fasta" />
<userParam name="uniprot-human-reviewed-trypsin-april-2016_concatenated_target_decoy.fasta"/>
<userParam name="HSA-Active.FASTA"></userParam>
```

6.21 Element <DatabaseTranslation>

Definition: A specification of how a nucleic acid sequence database was translated for searching.

Type: DatabaseTranslationType

Attributes:

Attribute Name	Data Type	Use	Definition
frames	listOfAllowedFrames	optional	The frames in which the nucleic acid sequence has been translated as a space separated list

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
TranslationTable	1	unbounded	The table used to translate codons into nucleic acids e.g. by reference to the NCBI translation table.

Example Context:

6.22 Element <DataCollection>

Definition: The collection of input and output data sets of the analyses.

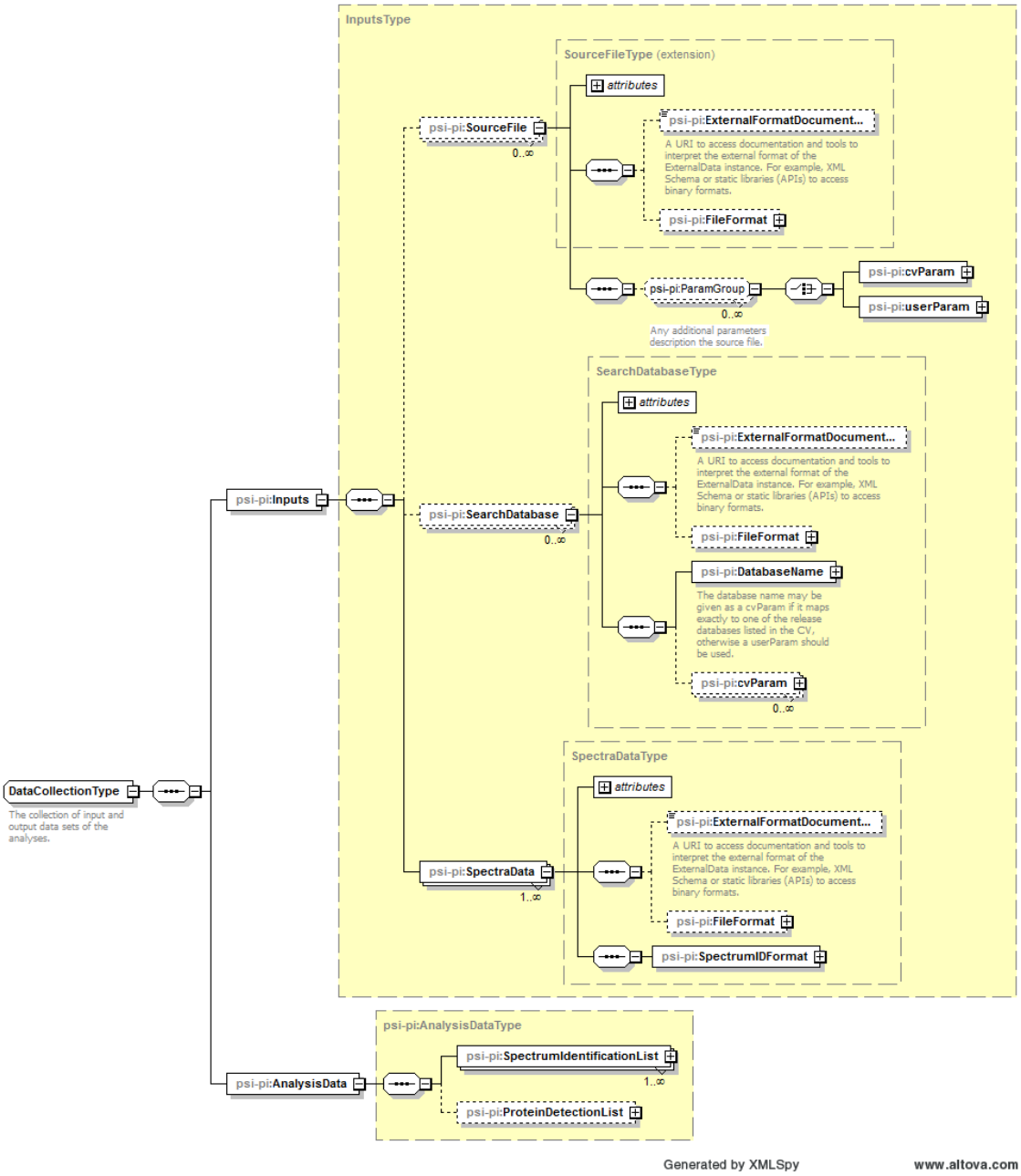
Type: DataCollectionType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Inputs	1	1	The inputs to the analyses including the databases searched, the spectral data and the source file converted to mzIdentML.
AnalysisData	1	1	Data sets generated by the analyses, including peptide and protein lists.

Graphical Context:



Example Context:

```
<DataCollection>
<Inputs xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <SearchDatabase numDatabaseSequences="57566"
location="E:\Work\PSI\mzIdentML\ProteinInference\Rosetta2\FASTAswithecoli\Rosetta_uniprot_20130402_
mouse_SWISS_can_iso_ECOLI.fasta" id="SearchDB_1">
        <FileFormat>
            <cvParam accession="MS:1001348" cvRef="PSI-MS" name="FASTA format"/>
        </FileFormat>
        <DatabaseName>
  ...
</DataCollection>
```

6.23 Element <DBSequence>

Definition: A database sequence from the specified SearchDatabase (nucleic acid or amino acid). If the sequence is nucleic acid, the source nucleic acid sequence should be given in the seq attribute rather than a translated sequence.

Type: DBSequenceType

Attributes:

Attribute Name	Data Type	Use	Definition
accession	xsd:string	required	The unique accession of this sequence.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
length	xsd:int	optional	The length of the sequence as a number of bases or residues.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
searchDatabase_ref	xsd:string	required	The source database of this sequence.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Seq	0	1	The actual sequence of amino acids or nucleic acid.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<DBSequence accession="sp|P20029|GRP78_MOUSE 78 kDa glucose-regulated protein OS=Mus musculus
GN=Hspa5
PE=1..." searchDatabase_ref="SearchDB_1" length="655" name="sp|P20029|GRP78_MOUSE 78 kDa glucose-
regula
ted protein OS=Mus musculus GN=Hspa5 PE=1 SV=3" id="dbseq_sp|P20029|GRP78_MOUSE 78 kDa glucose-
regulated
protein OS=Mus musculus GN=Hspa5 PE=1...">

<Seq>MMKFTVVAAALLLLGAVRAEEEDKKEDVGTVVGIDLGTTYSCVGVFKNGRVEIIANDQGNRITPSYVAFTPEGERLIGDAAKNQLTSNPENTVFDA
KRLIGRTWNDPSVQQDIKFLPFKVVEKKTKPYIQVDIGGGQTKTFAPEEISAMVLTKMKETAEAYLGKKVTHAVVTVPAYFNDAQRQATKDAGTIAGLNVM
RIINEPTAAAIAYGLDKREGEKNILVFDLGGGTFDVSLLTIDNGVFEVVATNGDTHLGGEDFDQRVMEHFIKLYKKKTGKDVRKDNRAVQKLRREVEKAKR
ALSSQHQARIEIESFFEGEDFSETLTRAKFEELNMDLFRSTMKPVQKVLEDSDLKKSDIDEIVLVGGSTRIPKIQQLVKEFFNGKEPSRGINPDEAVAYGA
AVQAGVLSGDQDTGDLVLLDVCPLTLGIETVGGVMTKLIPRNTVVPTKKSQIFSTASDNQPTVTIKVYEGERPLTKDNHLLGTFDLTGIPPAPRGVPQIEV
TFEIDVNGILRVTAEDKGTGNKNKITITNDQNRLTPEEIERMVNDAEKFAEEDKKLKERIDTRNELESYAYSLKNQIGDKEKLGGKLSSEDKETMEKAVEE
KIEWLESHQDADIEDFKAKKKELEEIVQPIISKLYGSGGPPPTGEEDTSEKDEL</Seq>
</DBSequence>
```

cvParam Mapping Rules:

```
Path /MzIdentML/SequenceCollection/DBSequence
MAY supply a *child* term of MS:1001342 (database sequence details) one or more times
  e.g.: MS:1001088 (protein description)
  e.g.: MS:1001090 (taxonomy nomenclature)
  e.g.: MS:1001343 (NA sequence)
  e.g.: MS:1001344 (AA sequence)
  e.g.: MS:1001467 (taxonomy: NCBI TaxID)
  e.g.: MS:1001468 (taxonomy: common name)
  e.g.: MS:1001469 (taxonomy: scientific name)
  e.g.: MS:1001470 (taxonomy: Swiss-Prot ID)
MAY supply a *child* term of MS:1001089 (molecule taxonomy) one or more times
  e.g.: MS:1001090 (taxonomy nomenclature)
  e.g.: MS:1001467 (taxonomy: NCBI TaxID)
  e.g.: MS:1001468 (taxonomy: common name)
  e.g.: MS:1001469 (taxonomy: scientific name)
  e.g.: MS:1001470 (taxonomy: Swiss-Prot ID)
```

Example cvParams:

```
<cvParam accession="MS:1001088" cvRef="PSI-MS" value="sp|P36938|PGM_ECOLI Phosphoglucomutase
OS=Escherichia coli (strain K12) GN=pgm PE=1 SV=1" name="protein description"/>
```

Example for proteogenomics search:

```
        <DBSequence searchDatabase_ref="SearchDB_1" accession="generic|A_ENSP00000284981|"
id="dbseq_generic|A_ENSP00000284981|">
                <cvParam cvRef="PSI-MS" accession="MS:1002637" name="chromosome name" value="21"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002638" name="chromosome strand" value="-"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002644" name="genome reference version"
        value="Homo_sapiens.GRCh38.77.gff3"></cvParam>
        </DBSequence>
```

6.24 Element <Enzyme>

Definition: The details of an individual cleavage enzyme should be provided by giving a regular expression or a CV term if a "standard" enzyme cleavage has been performed.

Type: EnzymeType

Attributes:

Attribute Name	Data Type	Use	Definition
cTermGain	xsd:string with restriction `[A-Za-z0-9 ]+`	optional	Element formula gained at CTerm.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
minDistance	xsd:int	optional	Minimal distance for another cleavage (minimum: 1).
missedCleavages	xsd:int	optional	The number of missed cleavage sites allowed by the search. The attribute MUST be provided if an enzyme has been used.
nTermGain	xsd:string with restriction `[A-Za-z0-9 ]+`	optional	Element formula gained at NTerm.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
semiSpecific	xsd:boolean	optional	Set to true if the enzyme cleaves semi-specifically (i.e. one terminus MUST cleave according to the rules, the other can cleave at any residue), false if the enzyme cleavage is assumed to be specific to both termini (accepting for any missed cleavages).

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SiteRegexp	0	1	Regular expression for specifying the enzyme cleavage site.
EnzymeName	0	1	The name of the enzyme from a CV.

Example Context:

```
<Enzyme missedCleavages="1" semiSpecific="false" cTermGain="OH" nTermGain="H" id="ENZ_0">
    <SiteRegexp>(?<=[KR])</SiteRegexp>
    <EnzymeName>
        <cvParam accession="MS:1001313" cvRef="PSI-MS" name="Trypsin/P"/>
    </EnzymeName>
</Enzyme>
```

6.25 Element <EnzymeName>

Definition: The name of the enzyme from a CV.

Type: ParamListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	1	unbounded	A single user-defined parameter.

Example Context:

```
<EnzymeName>
  <cvParam cvRef="PSI-MS" accession="MS:1001251" name="Trypsin"/>
</EnzymeName>
```

cvParam Mapping Rules:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/Enzymes/Enzyme/EnzymeName
MAY supply a *child* term of MS:1001045 (cleavage agent name) only once
  e.g.: MS:1001091 (NoEnzyme)
  e.g.: MS:1001251 (Trypsin)
  e.g.: MS:1001303 (Arg-C)
```

```
  e.g.: MS:1001304 (Asp-N)
  e.g.: MS:1001305 (Asp-N_ambic)
  e.g.: MS:1001306 (Chymotrypsin)
  e.g.: MS:1001307 (CNBr)
  e.g.: MS:1001308 (Formic_acid)
  e.g.: MS:1001309 (Lys-C)
  e.g.: MS:1001310 (Lys-C/P)
  et al.
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001251" name="Trypsin"></cvParam>
<cvParam accession="MS:1001313" cvRef="PSI-MS" name="Trypsin/P"/>
```

6.26 Element <Enzymes>

Definition: The list of enzymes used in experiment

Type: EnzymesType

Attributes:

Attribute Name	Data Type	Use	Definition
independent	xsd:boolean	optional	If there are multiple enzymes specified, this attribute is set to true if cleavage with different enzymes is performed independently.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Enzyme	1	unbounded	The details of an individual cleavage enzyme should be provided by giving a regular expression or a CV term if a "standard" enzyme cleavage has been performed.

Example Context:

```
<Enzymes>
    <Enzyme missedCleavages="1" semiSpecific="false" cTermGain="OH" nTermGain="H" id="ENZ_0">
        <SiteRegexp>(?<=[KR])</SiteRegexp>
        <EnzymeName>
            <cvParam accession="MS:1001313" cvRef="PSI-MS" name="Trypsin/P"/>
        </EnzymeName>
    </Enzyme>
  ...
</Enzymes>
```

6.27 Element <Exclude>

Definition: All sequences fulfilling the specifed criteria are excluded.

Type: ParamListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	1	unbounded	A single user-defined parameter.

Example Context:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/DatabaseFilters/Filter/Exclude
```

cvParam Mapping Rules:

```
MAY supply a *child* term of MS:1001512 (Sequence database filters) one or more times
  e.g.: MS:1001090 (taxonomy nomenclature)
  e.g.: MS:1001201 (DB MW filter maximum)
  e.g.: MS:1001202 (DB MW filter minimum)
  e.g.: MS:1001203 (DB PI filter maximum)
  e.g.: MS:1001204 (DB PI filter minimum)
  e.g.: MS:1001467 (taxonomy: NCBI TaxID)
  e.g.: MS:1001468 (taxonomy: common name)
  e.g.: MS:1001469 (taxonomy: scientific name)
  e.g.: MS:1001470 (taxonomy: Swiss-Prot ID)
  e.g.: MS:1001513 (DB sequence filter pattern)
  et al.
```

6.28 Element <ExternalFormatDocumentation>

Definition: A URI to access documentation and tools to interpret the external format of the ExternalData instance. For example, XML Schema or static libraries (APIs) to access binary formats.

Type: xsd:anyURI

Attributes: none

Subelements: none

Example Context:

6.29 Element <FileFormat>

Definition: The format of the ExternalData file, for example "tiff" for image files.

Type: FileFormatType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
<FileFormat>
  <cvParam cvRef="PSI-MS" accession="MS:1001401" name="X!Tandem xml format"/>
</FileFormat>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/Inputs/SearchDatabase/FileFormat
MUST supply a *child* term of MS:1001347 (database file formats) one or more times
  e.g.: MS:1001348 (FASTA format)
  e.g.: MS:1001349 (ASN.1)
  e.g.: MS:1001350 (NCBI *.p*)
  e.g.: MS:1001351 (clustal aln)
  e.g.: MS:1001352 (embl em)
  e.g.: MS:1001353 (NBRF PIR)
  e.g.: MS:1001462 (PEFF format)
  e.g.: MS:1002659 (UniProtKB text sequence format)
  e.g.: MS:1002660 (UniProtKB XML sequence format)
Path /MzIdentML/DataCollection/Inputs/SourceFile/FileFormat
MUST supply a *child* term of MS:1001040 (intermediate analysis format) only once
  e.g.: MS:1000742 (Bioworks SRF format)
  e.g.: MS:1001107 (data stored in database)
  e.g.: MS:1001199 (Mascot DAT format)
  e.g.: MS:1001200 (SEQUEST out file format)
  e.g.: MS:1001242 (SEQUEST out folder)
  e.g.: MS:1001243 (SEQUEST summary)
  e.g.: MS:1001275 (ProteinScape SearchEvent)
  e.g.: MS:1001276 (ProteinScape Gel)
  e.g.: MS:1001399 (OMSSA csv format)
  e.g.: MS:1001400 (OMSSA xml format)
  et al.
Path /MzIdentML/DataCollection/Inputs/SpectraData/FileFormat
MUST supply a *child* term of MS:1000560 (mass spectrometer file format) one or more times
  e.g.: MS:1000526 (Waters raw format)
  e.g.: MS:1000562 (ABI WIFF format)
  e.g.: MS:1000563 (Thermo RAW format)
  e.g.: MS:1000564 (PSI mzData format)
  e.g.: MS:1000565 (Micromass PKL format)
  e.g.: MS:1000566 (ISB mzXML format)
  e.g.: MS:1000567 (Bruker/Agilent YEP format)
  e.g.: MS:1000584 (mzML format)
  e.g.: MS:1000613 (DTA format)
  e.g.: MS:1000614 (ProteinLynx Global Server mass spectrum XML format)
  et al.
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001400" name="OMSSA xml file"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001348" name="FASTA format"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001062" name="Mascot MGF file"></cvParam>
<cvParam accession="MS:1001401" cvRef="PSI-MS" name="X\!Tandem xml file"/>
<cvParam accession="MS:1001199" cvRef="PSI-MS" name="Mascot DAT format"/>
<cvParam accession="MS:1000584" cvRef="PSI-MS" name="mzML format"/>
<cvParam cvRef="PSI-MS" accession="MS:1000563" name="Thermo Raw file"></cvParam>
```

6.30 Element <Filter>

Definition: Filters applied to the search database. The filter MUST include at least one of Include and Exclude. If both are used, it is assumed that inclusion is performed first.

Type: FilterType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
FilterType	1	1	The type of filter e.g. database taxonomy filter, pi filter, mw filter
Include	0	1	All sequences fulfilling the specifed criteria are included.
Exclude	0	1	All sequences fulfilling the specifed criteria are excluded.

Example Context:

```
<Filter>
    <FilterType>
        <cvParam accession="MS:1001020" cvRef="PSI-MS" name="DB filter taxonomy"/>
    </FilterType>
</Filter>
```

6.31 Element <FilterType>

Definition: The type of filter e.g. database taxonomy filter, pi filter, mw filter

Type: ParamType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.
userParam	1	1	A single user-defined parameter.

Example Context:

```
<FilterType>
    <cvParam accession="MS:1001020" cvRef="PSI-MS" name="DB filter taxonomy"/>
</FilterType>
```

cvParam Mapping Rules:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/DatabaseFilters/Filter/FilterTyp
e
MUST supply a *child* term of MS:1001511 (Sequence database filter types) one or more times
  e.g.: MS:1001020 (DB filter taxonomy)
  e.g.: MS:1001021 (DB filter on accession numbers)
  e.g.: MS:1001022 (DB MW filter)
  e.g.: MS:1001023 (DB PI filter)
  e.g.: MS:1001027 (DB filter on sequence pattern)
```

Example cvParams:

```
<cvParam accession="MS:1001020" cvRef="PSI-MS" name="DB filter taxonomy"/>
```

6.32 Element <FragmentArray>

Definition: An array of values for a given type of measure and for a particular ion type, in parallel to the index of ions identified.

Type: FragmentArrayType

Attributes:

Attribute Name	Data Type	Use	Definition
measure_ref	xsd:string	required	A reference to the Measure defined in the FragmentationTable
values	listOfFloats	required	The values of this particular measure, corresponding to the index defined in ion type

Subelements: none

Example Context:

```
                <FragmentArray measure_ref="Measure_Error" values="4.173258879802688E-4 -
1.9794682032170385E-5 1.618474794895519E-5 0.001690052197886871 -0.0037214683721344954
0.0020060110579152024 -2.3719321211501665E-4 2.7168621795681247E-4 -0.0019049343519554895
0.0019553613780090018 2.6704080801209784E-4 0.007734020238103767 0.0013568713879976713
1.571508180404635E-4 -0.0017703817320580129 0.013774177127970688 0.0056154565579618065
0.004415735988004599 0.006145015418042021 -0.005059517131940083 0.01419863401793009
0.007626913448120831 0.007892192877989146"/>
```

6.33 Element <Fragmentation>

Definition: The product ions identified in this result.

Type: FragmentationType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
IonType	1	unbounded	IonType defines the index of fragmentation ions being reported, importing a CV term for the type of ion e.g. b ion. Example: if b3 b7 b8 and b10 have been identified, the index attribute will contain 3 7 8 10, and the corresponding values will be reported in parallel arrays below

Example Context:

```
          <Fragmentation>
            <IonType charge="1" index="1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
23">
              <FragmentArray measure_ref="Measure_MZ" values="175.1193695 232.1403961 289.1618958
452.2268982 509.2429504 566.2701416 653.2999268 710.3218994 767.3411865 854.3770752 911.3968506
968.4257813 1065.472168 1122.492432 1285.553833 1399.612305 1456.62561 1513.645874 1570.669067
1733.721191 1830.793213 1887.808105 1944.829834"/>
              <FragmentArray measure_ref="Measure_Int" values="5939.5844726563 4933.5014648438
13310.7265625 5077.6694335938 5685.9287109375 13253.552734375 7620.0947265625 7724.3696289063
16868.541015625 10552.126953125 11589.0576171875 7839.9741210938 47821.64453125 60335.71484375
21759.3984375 8742.5595703125 11512.0908203125 18130.890625 30577.375 3801.3923339844 8051.07421875
1954.5501708984 4844.9125976563"/>
              <FragmentArray measure_ref="Measure_Error" values="4.173258879802688E-4 -
1.9794682032170385E-5 1.618474794895519E-5 0.001690052197886871 -0.0037214683721344954
0.0020060110579152024 -2.3719321211501665E-4 2.7168621795681247E-4 -0.0019049343519554895
0.0019553613780090018 2.6704080801209784E-4 0.007734020238103767 0.0013568713879976713
1.571508180404635E-4 -0.0017703817320580129 0.013774177127970688 0.0056154565579618065
0.004415735988004599 0.006145015418042021 -0.005059517131940083 0.01419863401793009
0.007626913448120831 0.007892192877989146"/>
              <cvParam cvRef="PSI-MS" accession="MS:1001220" name="frag: y ion"/>
            </IonType>
  ...
</Fragmentation>
```

6.34 Element <FragmentationTable>

Definition: Contains the types of measures that will be reported in generic arrays for each SpectrumIdentificationItem e.g. product ion m/z, product ion intensity, product ion m/z error

Type: FragmentationTableType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Measure	1	unbounded	References to CV terms defining the measures about product ions to be reported in SpectrumIdentificationItem

Example Context:

```
        <FragmentationTable>
          <Measure id="Measure_MZ">
            <cvParam cvRef="PSI-MS" accession="MS:1001225" name="product ion m/z" unitCvRef="PSI-MS"
unitAccession="MS:1000040" unitName="m/z" />
          </Measure>
          <Measure id="Measure_Int">
            <cvParam cvRef="PSI-MS" accession="MS:1001226" name="product ion intensity"
unitCvRef="PSI-MS" unitAccession="MS:1000131" unitName="number of detector counts"/>
          </Measure>
  ...
</FragmentationTable>
```

6.35 Element <FragmentTolerance>

Definition: The tolerance of the search given as a plus and minus value with units.

Type: ToleranceType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
<FragmentTolerance>
  <cvParam cvRef="PSI-MS" accession="MS:1001412" name="search tolerance plus value" value="20.0
ppm" unitAccession="UO:0000169" unitName="parts per million" unitCvRef="UO"></cvParam>
  <cvParam cvRef="PSI-MS" accession="MS:1001413" name="search tolerance minus value" value="20.0
ppm" unitAccession="UO:0000169" unitName="parts per million" unitCvRef="UO"></cvParam>
</FragmentTolerance>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/FragmentTolerance
MUST supply term MS:1001412 (search tolerance plus value) only once
MUST supply term MS:1001413 (search tolerance minus value) only once
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001412" name="search tolerance plus value" value="0.7"
unitAccession="UO:0000221" unitName="dalton" unitCvRef="UO"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001413" name="search tolerance minus value" value="0.7"
unitAccession="UO:0000221" unitName="dalton" unitCvRef="UO"></cvParam>
```

6.36 Element <Include>

Definition: All sequences fulfilling the specifed criteria are included.

Type: ParamListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	1	unbounded	A single user-defined parameter.

Example Context:

cvParam Mapping Rules:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/DatabaseFilters/Filter/Include
MAY supply a *child* term of MS:1001512 (Sequence database filters) one or more times
  e.g.: MS:1001090 (taxonomy nomenclature)
  e.g.: MS:1001201 (DB MW filter maximum)
  e.g.: MS:1001202 (DB MW filter minimum)
  e.g.: MS:1001203 (DB PI filter maximum)
  e.g.: MS:1001204 (DB PI filter minimum)
  e.g.: MS:1001467 (taxonomy: NCBI TaxID)
  e.g.: MS:1001468 (taxonomy: common name)
  e.g.: MS:1001469 (taxonomy: scientific name)
  e.g.: MS:1001470 (taxonomy: Swiss-Prot ID)
  e.g.: MS:1001513 (DB sequence filter pattern)
  et al.
```

6.37 Element <Inputs>

Definition: The inputs to the analyses including the databases searched, the spectral data and the source file converted to mzIdentML.

Type: InputsType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SourceFile	0	unbounded	A file from which this mzIdentML instance was created.

SearchDatabase	0	unbounded	A database for searching mass spectra. Examples include a set of amino acid sequence entries, nucleotide databases (e.g. 6 frame translated) or annotated spectra libraries.
SpectraData	1	unbounded	A data set containing spectra data (consisting of one or more spectra).

Example Context:

```
<Inputs xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <SourceFile
location="C:\Work\PSI\mzIdentML\ProteinInference\Rosetta2\tandem\peaklist2a_plus_ecoli_versus_unimod_
full.xml" id="SourceFile_1">
        <FileFormat>
            <cvParam accession="MS:1001401" cvRef="PSI-MS" name="X\!Tandem xml file"/>
        </FileFormat>
    </SourceFile>
    <SearchDatabase numDatabaseSequences="163648"
location="C:/Work/PSI/mzIdentML/ProteinInference/Rosetta2/FASTAs,
neat/Rosetta_uniprot_20130402_mouse_FULL_UNIPROT_can+iso.fasta" id="SearchDB_1">
  ...
</Inputs>
```

6.38 Element <InputSpectra>

Definition: One of the spectra data sets used.

Type: InputSpectraType

Attributes:

Attribute Name	Data Type	Use	Definition
spectraData_ref	xsd:string	optional	A reference to the SpectraData element which locates the input spectra to an external file.

Subelements: none

Example Context:

```
<InputSpectra spectraData_ref="SD_4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-
3_Din.raw"></InputSpectra>
```

6.39 Element <InputSpectrumIdentifications>

Definition: The lists of spectrum identifications that are input to the protein detection process.

Type: InputSpectrumIdentificationsType

Attributes:

Attribute Name	Data Type	Use	Definition
spectrumIdentificationList_ref	xsd:string	required	A reference to the list of spectrum identifications that were input to the process.

Subelements: none

Example Context:

```
<InputSpectrumIdentifications spectrumIdentificationList_ref="SII_LIST_1"/>
```

6.40 Element <IonType>

Definition: IonType defines the index of fragmentation ions being reported, importing a CV term for the
Type of ion e.g. b ion. Example: if b3 b7 b8 and b10 have been identified, the index attribute
will contain 3 7 8 10, and the corresponding values will be reported in parallel arrays below

Type: IonTypeType

Attributes:

Attribute Name	Data Type	Use	Definition

charge	xsd:int	required	The charge of the identified fragmentation ions.
index	listOfIntegers	optional	The index of ions identified as integers, following standard notation for a-c, x-z e.g. if b3 b5 and b6 have been identified, the index would store "3 5 6". For internal ions, the index contains pairs defining the start and end point - see specification document for examples. For immonium ions, the index is the position of the identified ion within the peptide sequence - if the peptide contains the same amino acid in multiple positions that cannot be distinguished, all positions should be given. For precursor ions, including neutral losses, the index value MUST be 0. For any other ions not related to the position within the peptide sequence e.g. quantification reporter ions, the index value MUST be 0.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
FragmentArray	0	unbounded	An array of values for a given type of measure and for a particular ion type, in parallel to the index of ions identified.
userParam	0	unbounded	A single user-defined parameter.
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
            <IonType charge="1" index="1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
22 23">
              <FragmentArray measure_ref="Measure_MZ" values="175.1193695 232.1403961
289.1618958
452.2268982 509.2429504 566.2701416 653.2999268 710.3218994 767.3411865 854.3770752 911.3968506
968
4257813 1065.472168 1122.492432 1285.553833 1399.612305 1456.62561 1513.645874 1570.669067
1733.721191
1830.793213 1887.808105 1944.829834"/>
              <FragmentArray measure_ref="Measure_Int" values="5939.5844726563
4933.5014648438
13310.7265625 5077.6694335938 5685.9287109375 13253.552734375 7620.0947265625 7724.3696289063
16868.541015625 10552.126953125 11589.0576171875 7839.9741210938 47821.64453125 60335.71484375
21759.3984375 8742.5595703125 11512.0908203125 18130.890625 30577.375 3801.3923339844
8051.07421875
1954.5501708984 4844.9125976563"/>
              <FragmentArray measure_ref="Measure_Error" values="4.173258879802688E-4
-1.9794682032170385E-5 1.618474794895519E-5 0.001690052197886871 -0.0037214683721344954
0.0020060110579152024 -2.3719321211501665E-4 2.7168621795681247E-4 -0.0019049343519554895
0.0019553613780090018 2.6704080801209784E-4 0.007734020238103767 0.0013568713879976713
1.571508180404635E-4 -0.0017703817320580129 0.013774177127970688 0.0056154565579618065
0.004415735988004599 0.006145015418042021 -0.005059517131940083 0.01419863401793009
0.007626913448120831 0.007892192877989146"/>
              <cvParam cvRef="PSI-MS" accession="MS:1001220" name="frag: y ion"/>
            </IonType>
```

cvParam Mapping Rules:

```
Path
/MzIdentML/DataCollection/AnalysisData/SpectrumIdentificationList/SpectrumIdentificationResult/
SpectrumIdentificationItem/Fragmentation/IonType
MAY supply a *child* term of MS:1001221 (fragmentation information) one or more times
  e.g.: MS:1000903 (product ion series ordinal)
  e.g.: MS:1000904 (product ion m/z delta)
  e.g.: MS:1000926 (product interpretation rank)
  e.g.: MS:1001220 (frag: y ion)
  e.g.: MS:1001222 (frag: b ion - H2O)
  e.g.: MS:1001223 (frag: y ion - H2O)
  e.g.: MS:1001224 (frag: b ion)
  e.g.: MS:1001225 (product ion m/z)
  e.g.: MS:1001227 (product ion m/z error)
  e.g.: MS:1001228 (frag: x ion)
  et al.
```

Example cvParams:

```
<cvParam accession="MS:1001224" cvRef="PSI-MS" name="frag: b ion"/>
<cvParam accession="MS:1001220" cvRef="PSI-MS" name="frag: y ion"/>
<cvParam accession="MS:1002681" cvRef="PSI-MS" name="OpenXQuest:combined score"
value="21.9678562261903"/>
```

```
<cvParam accession="MS:1002511" cvRef="PSI-MS" name="cross-link spectrum identification item"
value="3050674907789158263"/>
<cvParam accession="MS:1000894" cvRef="PSI-MS" name="retention time" value="5468.0193"
unitAccession="second" unitName="" unitCvRef="se"/>
<cvParam cvRef="PSI-MS" accession="MS:1001523" name="frag: precursor ion"/>
<cvParam cvRef="PSI-MS" accession="MS:1002466" name="PeptideShaker PSM score" value="0.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002467" name="PeptideShaker PSM confidence"
value="0.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002469" name="PeptideShaker peptide confidence"
value="4.0000000000000036"/>
<cvParam cvRef="PSI-MS" accession="MS:1002468" name="PeptideShaker peptide score" value="-
0.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002500" name="peptide passes threshold" value="false"/>
<cvParam cvRef="PSI-MS" accession="MS:1002520" name="peptide group ID" value="QKAQAAATVVK"/>
<cvParam cvRef="PSI-MS" accession="MS:1001328" name="OMSSA:evalue" value="68.145917448381"/>
<cvParam cvRef="PSI-MS" accession="MS:1001117" name="theoretical mass"
value="1113.6506071554904" unitCvRef="UO" unitAccession="UO:0000221" unitName="dalton"/>
<cvParam cvRef="PSI-MS" accession="MS:1002540" name="PeptideShaker PSM confidence type"
value="Not Validated"/>
<cvParam cvRef="PSI-MS" accession="MS:1000796" name="spectrum title"
value="qExactive01819.13825.13825. File:"qExactive01819.raw", NativeID:"controllerType=0
controllerNumber=1 scan=13825""/>
<cvParam cvRef="PSI-MS" accession="MS:1001222" name="frag: b ion - H2O"/>
<cvParam cvRef="PSI-MS" accession="MS:1001239" name="frag: immonium ion"/>
<cvParam cvRef="PSI-MS" accession="MS:1001223" name="frag: y ion - H2O"/>
<cvParam cvRef="PSI-MS" accession="MS:1001233" name="frag: y ion - NH3"/>
<cvParam cvRef="PSI-MS" accession="MS:1001521" name="frag: precursor ion - H2O"/>
<cvParam cvRef="PSI-MS" accession="MS:1002536" name="D-Score"
value="2:99.6124031007752:1:true"/>
<cvParam cvRef="PSI-MS" accession="MS:1001330" name="X!Tandem:expect" value="0.0067"/>
<cvParam cvRef="PSI-MS" accession="MS:1001232" name="frag: b ion - NH3"/>
<cvParam cvRef="PSI-MS" accession="MS:1001522" name="frag: precursor ion - NH3"/>
<cvParam cvRef="PSI-MS" accession="MS:1002674" name="frag: b ion - CH4OS"/>
<cvParam cvRef="PSI-MS" accession="MS:1001969" name="phosphoRS score" value="1:50.0:4:false"/>
<cvParam cvRef="PSI-MS" accession="MS:1002550" name="peptide:phosphoRS score"
value="1:50.0:4:false"/>
<cvParam cvRef="PSI-MS" accession="MS:1002553" name="peptide:D-Score"
value="1:1.4263074484944571:4:false"/>
<cvParam cvRef="PSI-MS" accession="MS:1002694" name="frag: precursor ion - CH4OS"/>
<cvParam cvRef="PSI-MS" accession="MS:1002686" name="frag: y ion - CH4OS"/>
```

Example userParams:

```
<userParam name="cross-link_chain" unitName="xsd:string" values="alpha"/>
<userParam name="cross-link_ioncategory" unitName="xsd:string" values="ci"/>
```

6.41 Element <MassTable>

Definition: The masses of residues used in the search.

Type: MassTableType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
msLevel	listOfIntegers	required	The MS spectrum that the MassTable refers to e.g. "1" for MS1 "2" for MS2 or "1 2" for MS1 or MS2.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Residue	0	unbounded	The specification of a single residue within the mass table.
AmbiguousResidue	0	unbounded	Ambiguous residues e.g. X can be specified by the Code attribute and a set of parameters for example giving the different masses that will be used in the search.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<MassTable msLevel="1 2" id="MT">
    <Residue mass="71.03712" code="A"/>
    <Residue mass="103.009186" code="C"/>
    <Residue mass="115.02694" code="D"/>
    <Residue mass="129.04259" code="E"/>
    <Residue mass="147.06842" code="F"/>
    <Residue mass="57.021465" code="G"/>
  ...
</MassTable>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/MassTable
MAY supply a *child* term of MS:1001354 (mass table options) one or more times
  e.g.: MS:1001346 (AAIndex mass table)
```

6.42 Element <Measure>

Definition: References to CV terms defining the measures about product ions to be reported in SpectrumIdentificationItem

Type: MeasureType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
          <Measure id="Measure_Int">
            <cvParam cvRef="PSI-MS" accession="MS:1001226" name="product ion intensity"
unitCvRef="PSI-MS" unitAccession="MS:1000131" unitName="number of detector counts"/>
          </Measure>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/AnalysisData/SpectrumIdentificationList/FragmentationTable/Measure
MUST supply term MS:1001226 (product ion intensity) only once
MUST supply term MS:1001225 (product ion m/z) only once
MUST supply term MS:1001227 (product ion m/z error) only once
```

Example cvParams:

```
<cvParam accession="MS:1001225" cvRef="PSI-MS" unitCvRef="PSI-MS" unitName="m/z"
unitAccession="MS:1000040" name="product ion m/z"/>
<cvParam accession="MS:1001226" cvRef="PSI-MS" unitCvRef="PSI-MS" unitName="number of detector
counts" unitAccession="MS:1000131"  name="product ion intensity"/>
<cvParam accession="MS:1001227" cvRef="PSI-MS" unitCvRef="PSI-MS" unitName="m/z"
unitAccession="MS:1000040" name="product ion m/z error"/>
```

6.43 Element <Modification>

Definition: A molecule modification specification. If n modifications have been found on a peptide, there should be n instances of Modification. If multiple modifications are provided as cvParams, it is assumed that the modification is ambiguous i.e. one modification or another. A cvParam MUST be provided with the identification of the modification sourced from a suitable CV e.g. UNIMOD. If the modification is not present in the CV (and this will be checked by the semantic validator within a given tolerance window), there is a â€œunknown modificationâ€• CV term that MUST be used instead. A neutral loss should be defined as an additional CVParam within Modification. If more complex information should be given about neutral losses (such as presence/absence on particular product ions), this can additionally be encoded within the FragmentationArray.

Type: ModificationType

Attributes:

Attribute Name	Data Type	Use	Definition
avgMassDelta	xsd:double	optional	Atomic mass delta considering the natural distribution of isotopes in Daltons.

location	xsd:int	optional	Location of the modification within the peptide - position in peptide sequence, counted from the N-terminus residue, starting at position 1. Specific modifications to the N-terminus should be given the location 0. Modification to the C-terminus should be given as peptide length + 1. If the modification location is unknown e.g. for PMF data, this attribute should be omitted.
monoisotopicMassDelta	xsd:double	optional	Atomic mass delta when assuming only the most common isotope of elements in Daltons.
residues	listOfChars	optional	Specification of the residue (amino acid) on which the modification occurs. If multiple values are given, it is assumed that the exact residue modified is unknown i.e. the modification is to ONE of the residues listed. Multiple residues would usually only be specified for PMF data.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
    <Modification location="10" residues="K" monoisotopicMassDelta="138.0680796">
      <cvParam accession="XLMOD:02001" cvRef="XLMOD" name="DSS"/>
      <cvParam accession="MS:1002509" cvRef="PSI-MS" name="cross-link donor"
value="11309529182388590588"/>
    </Modification>
```

Example cvParams:

```
<cvParam cvRef="UNIMOD" accession="UNIMOD:35" name="Oxidation"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:37" name="Trimethyl"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:4" name="Carbamidomethyl"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:27" name="Glu->pyro-Glu"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:1" name="Acetyl"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:385" name="Ammonia-loss"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:28" name="Gln->pyro-Glu"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:575" name="Gly->Val"></cvParam>
<cvParam accession="UNIMOD:214" cvRef="UNIMOD" name="iTRAQ4plex"/>
<cvParam accession="UNIMOD:7" cvRef="UNIMOD" name="Deamidated"/>
<cvParam accession="UNIMOD:39" cvRef="UNIMOD" name="Methylthio"/>
<cvParam accession="XLMOD:02001" cvRef="XLMOD" name="DSS"/>
<cvParam accession="MS:1002509" cvRef="PSI-MS" name="cross-link donor"
value="11309529182388590588"/>
<cvParam accession="MS:1002510" cvRef="PSI-MS" name="cross-link acceptor"
value="23992940650693606606"/>
<cvParam accession="UNIMOD:1020" name="xlink:DSS" cvRef="UNIMOD"/>
<cvParam cvRef="XLMOD" accession="XLMOD:01000" name="hydrolyzed BS3"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01001" name="amidated BS3"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:02000" name="BS3"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01008" name="hydrolyzed BS3-d4"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01009" name="amidated BS3-d4"></cvParam>
```

Example for cross-linking:

```
<Modification location="2" residues="Y" monoisotopicMassDelta="156.07864430999996">
        <cvParam cvRef="XLMOD" accession="XLMOD:01000" name="hydrolysed BS3"></cvParam>
</Modification>
```

6.44 Element <ModificationParams>

Definition: The specification of static/variable modifications (e.g. Oxidation of Methionine) that are to be considered in the spectra search.

Type: ModificationParamsType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition

SearchModification	1	unbounded	Specification of a search modification as parameter for a spectra search. Contains the name of the modification, the mass, the specificity and whether it is a static modification.

Example Context:

```
<ModificationParams>
    <SearchModification residues="M" massDelta="15.9949" fixedMod="false">
        <cvParam accession="UNIMOD:35" cvRef="UNIMOD" name="Oxidation"/>
    </SearchModification>
    <SearchModification residues="." massDelta="144.102" fixedMod="false">
        <cvParam accession="UNIMOD:214" cvRef="UNIMOD" name="iTRAQ4plex"/>
        <cvParam accession="MS:1001189" cvRef="PSI-MS" name="modification specificity peptide N-
term"/>
  ...
</ModificationParams>
```

6.45 Element <Organization>

Definition: Organizations are entities like companies, universities, government agencies. Any additional information such as the address, email etc. should be supplied either as CV parameters or as user parameters.

Type: OrganizationType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.
Parent	0	1	The containing organization (the university or business which a lab belongs to, etc.)

Example Context:

```
    <Organization name="PeptideShaker developers" id="PS_DEV">
      <cvParam cvRef="PSI-MS" accession="MS:1000586" name="contact name" value="PeptideShaker
developers"/>
      <cvParam cvRef="PSI-MS" accession="MS:1000587" name="contact address" value="Proteomics
Unit, Building for Basic Biology, University of Bergen, Jonas Liesvei 91, N-5009 Bergen,
Norway"/>
      <cvParam cvRef="PSI-MS" accession="MS:1000588" name="contact URL"
value="http://compomics.github.io/projects/peptide-shaker.html"/>
      <cvParam cvRef="PSI-MS" accession="MS:1000589" name="contact email" value="peptide-
shaker@googlegroups.com"/>
    </Organization>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AuditCollection/Organization
SHOULD supply term MS:1000588 (contact URL) one or more times
SHOULD supply term MS:1000587 (contact address) one or more times
SHOULD supply term MS:1000589 (contact email) one or more times
SHOULD supply term MS:1000586 (contact name) one or more times
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1000586" name="contact name" value="address"></cvParam>
<cvParam accession="MS:1000588" cvRef="PSI-MS" value="http://www.matrixscience.com" name="contact
URL"/>
<cvParam cvRef="PSI-MS" accession="MS:1000587" name="contact address" value="test"/>
<cvParam cvRef="PSI-MS" accession="MS:1000589" name="contact email" value="test"/>
```

6.46 Element <Parent>

Definition: The containing organization (the university or business which a lab belongs to, etc.)

Type: ParentOrganizationType

Attributes:

Attribute Name	Data Type	Use	Definition
organization_ref	xsd:string	required	A reference to the organization this contact belongs to.

Subelements: none

Example Context:

6.47 Element <ParentTolerance>

Definition: The tolerance of the search given as a plus and minus value with units.

Type: ToleranceType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
<ParentTolerance>
  <cvParam cvRef="PSI-MS" accession="MS:1001412" name="search tolerance plus value" value="6.0 ppm"
unitAccession="UO:0000169" unitName="parts per million" unitCvRef="UO"></cvParam>
  <cvParam cvRef="PSI-MS" accession="MS:1001413" name="search tolerance minus value" value="6.0
ppm" unitAccession="UO:0000169" unitName="parts per million" unitCvRef="UO"></cvParam>
</ParentTolerance>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/ParentTolerance
MUST supply term MS:1001412 (search tolerance plus value) only once
MUST supply term MS:1001413 (search tolerance minus value) only once
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001412" name="search tolerance plus value" value="10.0"
unitAccession="UO:0000221" unitName="dalton" unitCvRef="UO"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001413" name="search tolerance minus value" value="10.0"
unitAccession="UO:0000221" unitName="dalton" unitCvRef="UO"></cvParam>
```

6.48 Element <Peptide>

Definition: One (poly)peptide (a sequence with modifications). The combination of Peptide sequence and modifications MUST be unique in the file.

Type: PeptideType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
PeptideSequence	1	1	The amino acid sequence of the (poly)peptide. If a substitution modification has been found, the original sequence should be reported.
Modification	0	unbounded	A molecule modification specification. If n modifications have been found on a peptide, there should be n instances of Modification. If multiple modifications are provided as cvParams, it is assumed that the modification is ambiguous i.e. one

			modification or another. A cvParam MUST be provided with the identification of the modification sourced from a suitable CV e.g. UNIMOD. If the modification is not present in the CV (and this will be checked by the semantic validator within a given tolerance window), there is a â€œunknown modificationâ€• CV term that MUST be used instead. A neutral loss should be defined as an additional CVParam within Modification. If more complex information should be given about neutral losses (such as presence/absence on particular product ions), this can additionally be encoded within the FragmentationArray.
SubstitutionModification	0	unbounded	A modification where one residue is substituted by another (amino acid change).
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<Peptide
id="CCPQCCSSGCSQNLCGPLCVTTPYYCTR_##Carbamidomethyl(C):1##Carbamidomethyl(C):2##Carbamidomethyl(C):
5##Carbamidomethyl(C):6##Carbamidomethyl(C):10##Carbamidomethyl(C):15##Carbamidomethyl(C):
19##Carbamidomethyl(C):26">
  <PeptideSequence>CCPQCCSSGCSQNLCGPLCVTTPYYCTR</PeptideSequence>
  <Modification location="1" residues="C" monoisotopicMassDelta="57.02147">
    <cvParam cvRef="UNIMOD" accession="UNIMOD:4" name="Carbamidomethyl"></cvParam>
  </Modification>
  <Modification location="2" residues="C" monoisotopicMassDelta="57.02147">
    <cvParam cvRef="UNIMOD" accession="UNIMOD:4" name="Carbamidomethyl"></cvParam>
  ...
</Peptide>
```

cvParam Mapping Rules:

```
Path /MzIdentML/SequenceCollection/Peptide
MAY supply a *child* term of MS:1001355 (peptide descriptions) one or more times
```

Example for cross-linking:

```
<Peptide id="54603257_54604608_2_1_p1">
  <PeptideSequence>KYLYEIAR</PeptideSequence>
  <Modification location="2" residues="Y" monoisotopicMassDelta="156.07864430999996">
    <cvParam cvRef="XLMOD" accession="XLMOD:01000" name="hydrolysed BS3"></cvParam>
  </Modification>
  <Modification location="4" residues="Y" monoisotopicMassDelta="155.094628715">
    <cvParam cvRef="XLMOD" accession="XLMOD:01001" name="amidated BS3"></cvParam>
  </Modification>
  <Modification location="2" monoisotopicMassDelta="0.0">
    <cvParam cvRef="PSI-MS" accession="MS:1002510" name="cross-link acceptor" value="1"></cvParam>
  </Modification>
</Peptide>
<Peptide id="54603257_54604608_2_1_p0">
  <PeptideSequence>LSVEAFEK</PeptideSequence>
  <Modification location="3" monoisotopicMassDelta="138.06807961">
    <cvParam cvRef="XLMOD" accession="XLMOD:02000" name="BS3"></cvParam>
    <cvParam cvRef="PSI-MS" accession="MS:1002509" name="cross-link donor" value="1"></cvParam>
  </Modification>
</Peptide>
```

6.49 Element <PeptideEvidence>

Definition: PeptideEvidence links a specific Peptide element to a specific position in a DBSequence. There MUST only be one PeptideEvidence item per Peptide-to-DBSequence-position.

Type: PeptideEvidenceType

Attributes:

Attribute Name	Data Type	Use	Definition

dBSequence_ref	xsd:string	required	A reference to the protein sequence in which the specified peptide has been linked.
end	xsd:int	optional	The index position of the last amino acid of the peptide inside the protein sequence, where the first amino acid of the protein sequence is position 1. Must be provided unless this is a de novo search.
frame	allowed_frames	optional	The translation frame of this sequence if this is PeptideEvidence derived from nucleic acid sequence
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
isDecoy	xsd:boolean	optional	Set to true if the peptide is matched to a decoy sequence.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
peptide_ref	xsd:string	required	A reference to the identified (poly)peptide sequence in the Peptide element.
post	xsd:string with restriction `[ABCDEFGHIJKLMNOPQRSTUVWXYZ?\-]{1}`	optional	Post flanking residue. If the peptide is C-terminal, post="-" and not post="". If for any reason it is unknown (e.g. denovo), post="?" should be used.
pre	xsd:string with restriction `[ABCDEFGHIJKLMNOPQRSTUVWXYZ?\-]{1}`	optional	Previous flanking residue. If the peptide is N-terminal, pre="-" and not pre="". If for any reason it is unknown (e.g. denovo), pre="?" should be used.
start	xsd:int	optional	Start position of the peptide inside the protein sequence, where the first amino acid of the protein sequence is position 1. Must be provided unless this is a de novo search.
translationTable_ref	xsd:string	optional	A reference to the translation table used if this is PeptideEvidence derived from nucleic acid sequence

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.

userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<PeptideEvidence dBSequence_ref="dbseq_generic|B_GENSCAN00000036974_REVERSED|p:genscan"
peptide_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_##Carbamidomethyl(C):1##Carbamidomethyl(C):
3##Carbamidomethyl(C):12##Carbamidomethyl(C):18##Carbamidomethyl(C):25##Carbamidomethyl(C):
31##Ammonia-loss(C):1" start="494" end="531" pre="R" post="L" isDecoy="true"
id="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_generic|B_GENSCAN00000036974_REVERSED|p:genscan_494_531">
</PeptideEvidence>
```

Example for proteogenomics search:

```
        <PeptideEvidence dBSequence_ref="dbseq_generic|A_ENSP00000287611|" peptide_ref="YNSQNQSNNQFVLYR_" start="44"
end="58" pre="K" post="I" isDecoy="false" id="YNSQNQSNNQFVLYR_generic|A_ENSP00000287611|_44_58">
                <cvParam cvRef="PSI-MS" accession="MS:1002640" name="peptide end on chromosome"
        value="186717716"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002641" name="peptide exon count" value="1"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002642" name="peptide exon nucleotide sizes"
        value="45"></cvParam>
                <cvParam cvRef="PSI-MS" accession="MS:1002643" name="peptide start positions on chromosome"
        value="186717673"></cvParam>
        </PeptideEvidence>
```

6.50 Element <PeptideEvidenceRef>

Definition: Reference to the PeptideEvidence element identified. If a specific sequence can be assigned to multiple proteins and or positions in a protein all possible PeptideEvidence elements should be referenced here.

Type: PeptideEvidenceRefType

Attributes:

Attribute Name	Data Type	Use	Definition
peptideEvidence_ref	xsd:string	required	A reference to the PeptideEvidenceItem element(s).

Subelements: none

Example Context:

```
<PeptideEvidenceRef
peptideEvidence_ref="GEGGAQDGSGTEGVGATGAAGGRGAQGAPGGTGGAGSGSGLHHQQDSGYQGASGSGGAQSGGR_generic|A_ENSP
00000352272_REVERSED|p:known_125_187"></PeptideEvidenceRef>
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1002356" name="PSM-level combined FDRScore"
value="3.9523759266648643E-7"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002359" name="distinct peptide-level local FDR"
value="0.0"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001868" name="distinct peptide-level q-value"
value="0.0"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002360" name="distinct peptide-level FDRScore"
value="3.0117913560694526E-7"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002500" name="peptide passes threshold"
value="true"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002520" name="peptide group ID"
value="AVMDDFAAFVEK_##Oxidation(M):3"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002439" name="final PSM list UNDER DISCUSSION"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002511" name="Cross-linked spectrum identification item."
value="21"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002545" name="The xi result 'Score'."
value="2.769918944845425"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1000797" name="peak list scans" value="6655"></cvParam>
```

Example userParams:

```
<userParam name="search engines identifying PSM" value="12"></userParam>
```

6.51 Element <PeptideHypothesis>

Definition: Peptide evidence on which this ProteinHypothesis is based by reference to a PeptideEvidence element.

Type: PeptideHypothesisType

Attributes:

Attribute Name	Data Type	Use	Definition
peptideEvidence_ref	xsd:string	required	A reference to the PeptideEvidence element on which this hypothesis is based.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SpectrumIdentificationItemRef	1	unbounded	Reference(s) to the SpectrumIdentificationItem element(s) that support the given PeptideEvidence element. Using these references it is possible to indicate which spectra were actually accepted as evidence for this peptide identification in the given protein.

Example Context:

```
            <PeptideHypothesis peptideEvidence_ref="PepEv_1864">
              <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_1780_1"/>
              <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_2217_1"/>
              <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_3245_1"/>
              <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_4362_1"/>
              <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_5349_1"/>
              <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_5621_1"/>
  ...
</PeptideHypothesis>
```

Example cvParams:

```
<cvParam accession="MS:1001097" cvRef="PSI-MS" value="1" name="distinct peptide sequences"/>
<cvParam accession="MS:1002235" cvRef="PSI-MS" value="81.01860914459425" name="ProteoGrouper:PDH
score"/>
<cvParam accession="MS:1002401" cvRef="PSI-MS" name="leading protein"/>
<cvParam accession="MS:1002403" cvRef="PSI-MS" name="group representative"/>
<cvParam accession="MS:1001594" cvRef="PSI-MS" value="PDH_15" name="sequence same-set protein"/>
<cvParam accession="MS:1002415" cvRef="PSI-MS" value="true" name="protein group passes threshold"/>
<cvParam accession="MS:1002236" cvRef="PSI-MS" value="43.73236628236426" name="ProteoGrouper:PAG
score"/>
<cvParam accession="MS:1002407" cvRef="PSI-MS" value="2" name="cluster identifier"/>
<cvParam accession="MS:1002404" cvRef="PSI-MS" value="4" name="count of identified proteins"/>
<cvParam accession="MS:1001596" cvRef="PSI-MS" value="PDH_239" name="sequence sub-set protein"/>
<cvParam accession="MS:1002402" cvRef="PSI-MS" name="non-leading protein"/>
<cvParam accession="MS:1001598" cvRef="PSI-MS" value="PDH_167" name="sequence subsumable protein"/>
<cvParam name="mascot:score" value="1416.6296969697" cvRef="PSI-MS" accession="MS:1001171" />
<cvParam name="PAnalyzer:conclusive protein" cvRef="PSI-MS" accession="MS:1002213" />
<cvParam name="PAnalyzer:non-conclusive protein" cvRef="PSI-MS" accession="MS:1002215" />
<cvParam name="PAnalyzer:indistinguishable protein" cvRef="PSI-MS" accession="MS:1002214" />
<cvParam cvRef="PSI-MS" accession="MS:1001093" name="sequence coverage" value="0.19"/>
<cvParam cvRef="PSI-MS" accession="MS:1002470" name="PeptideShaker protein group score"
value="100.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002471" name="PeptideShaker protein group confidence"
value="100.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002542" name="PeptideShaker protein confidence type"
value="Confident"/>
```

Example userParams:

```
<userParam value="IINEPTAAAIAYGLDK" name="razor peptides"/>
<userParam value="SLSDTLEEVLSSSGEK" name="unique peptides"/>
```

6.52 Element <PeptideSequence>

Definition: The amino acid sequence of the (poly)peptide. If a substitution modification has been found, the original sequence should be reported.

Type: sequence

Attributes: none

Subelements: none

Example Context:

```
<PeptideSequence>GEGGAQDGSGTEGVGATGAAGGRGAQGAPGGTGGAGSGSGLHHQQDSGYQGASGSGGAQSGGR</PeptideSequence>
```

6.53 Element <Person>

Definition: A person's name and contact details. Any additional information such as the address, contact email etc. should be supplied using CV parameters or user parameters.

Type: PersonType

Attributes:

Attribute Name	Data Type	Use	Definition
firstName	xsd:string	optional	The Person's first name.

id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
lastName	xsd:string	optional	The Person's last/family name.
midInitials	xsd:string	optional	The Person's middle initial.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.
Affiliation	0	unbounded	The organization a person belongs to.

Example Context:

```
<Person firstName="test" lastName="test" id="PROVIDER">
  <cvParam cvRef="PSI-MS" accession="MS:1000587" name="contact address" value="test"/>
  <cvParam cvRef="PSI-MS" accession="MS:1000588" name="contact URL" value="test"/>
  <cvParam cvRef="PSI-MS" accession="MS:1000589" name="contact email" value="testtest"/>
  <Affiliation organization_ref="ORG_DOC_OWNER"/>
</Person>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AuditCollection/Person
SHOULD supply term MS:1000588 (contact URL) one or more times
SHOULD supply term MS:1000587 (contact address) one or more times
SHOULD supply term MS:1000589 (contact email) one or more times
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1000587" name="contact address" value="address"></cvParam>
<cvParam accession="MS:1000589" cvRef="PSI-MS" value="smartinez@proteored.org" name="contact email"/>
<cvParam cvRef="PSI-MS" accession="MS:1000588" name="contact URL" value="test"/>
```

6.54 Element <ProteinAmbiguityGroup>

Definition: A set of logically related results from a protein detection, for example to represent conflicting assignments of peptides to proteins.

Type: ProteinAmbiguityGroupType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ProteinDetectionHypothesis	1	unbounded	A single result of the ProteinDetection analysis (i.e. a protein).
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<ProteinAmbiguityGroup id="PAG_1">
    <ProteinDetectionHypothesis passThreshold="true" dBSequence_ref="dbseq_sp|Q64467|G3PT_MOUSE Glyceraldehyde-3-phosphate dehydrogenase, testis-specific OS=Mus..." id="PDH_11">
        <PeptideHypothesis peptideEvidence_ref="PE13_2_63">
            <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_13_1"/>
        </PeptideHypothesis>
        <cvParam accession="MS:1001097" cvRef="PSI-MS" value="1" name="distinct peptide sequences"/>
        <cvParam accession="MS:1002235" cvRef="PSI-MS" value="34.57557513936462" name="ProteoGrouper:PDH score"/>
```

cvParam Mapping Rules:

```
  ...
</ProteinAmbiguityGroup>
Path /MzIdentML/DataCollection/AnalysisData/ProteinDetectionList/ProteinAmbiguityGroup
MUST supply term MS:1002415 (protein group passes threshold) only once
MAY supply a *child* term of MS:1001147 (protein ambiguity group result details) one or more times
  e.g.: MS:1001164 (Paragon:unused protscore)
  e.g.: MS:1001165 (Paragon:total protscore)
  e.g.: MS:1001301 (protein rank)
  e.g.: MS:1002236 (ProteoGrouper:PAG score)
  e.g.: MS:1002407 (cluster identifier)
  e.g.: MS:1002415 (protein group passes threshold)
  e.g.: MS:1002474 (ProteoAnnotator:non-canonical gene model score)
  e.g.: MS:1002475 (ProteoAnnotator:count alternative peptides)
  e.g.: MS:1002663 (Morpheus:summed Morpheus score)
```

Example for protein grouping:

```
<ProteinAmbiguityGroup id="PAG_4266">
        <ProteinDetectionHypothesis dBSequence_ref="DBSeq_RRRRRQ7TMJ9|Q7TMJ9_MOUSE" passThreshold="true"
id="PDH_RRRRRQ7TMJ9|Q7TMJ9_MOUSE_PAG_4266">
                <PeptideHypothesis peptideEvidence_ref="PE_APVPPSQAR(0;144.1021)-332-340-
        RRRRRQ7TMJ9|Q7TMJ9_MOUSE">
                <SpectrumIdentificationItemRef
        spectrumIdentificationItem_ref="2:[0,144.1021]:APVPPSQAR:index=26699"></SpectrumIdentificationItemRef
        >
        </PeptideHypothesis>
        <cvParam cvRef="PSI-MS" accession="MS:1002394" name="PIA:protein score"
value="2.0881360887005513"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002401" name="leading protein"></cvParam>
</ProteinDetectionHypothesis>
        cvParam cvRef="PSI-MS" accession="MS:1002415" name="protein group passes threshold"
value="true"></cvParam>
        cvParam cvRef="PSI-MS" accession="MS:1002407" name="cluster identifier" value="2814"></cvParam>
</ProteinAmbiguityGroup>
```

6.55 Element <ProteinDetection>

Definition: An Analysis which assembles a set of peptides (e.g. from a spectra search analysis) to proteins.

Type: ProteinDetectionType

Attributes:

Attribute Name	Data Type	Use	Definition
activityDate	xsd:dateTime	optional	When the protocol was applied.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
proteinDetectionList_ref	xsd:string	required	A reference to the ProteinDetectionList in the DataCollection section.
proteinDetectionProtocol_ref	xsd:string	required	A reference to the detection protocol used for this ProteinDetection.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
InputSpectrumIdentifications	1	unbounded	The lists of spectrum identifications that are input to the protein detection process.

Example Context:

```
<ProteinDetection id="PD_1" activityDate="2014-01-11T19:42:49"
proteinDetectionList_ref="PDL_PAnalyzer" proteinDetectionProtocol_ref="PDP_PAnalyzer">
  <InputSpectrumIdentifications spectrumIdentificationList_ref="SIL_1" />
</ProteinDetection>
```

6.56 Element <ProteinDetectionHypothesis>

Definition: A single result of the ProteinDetection analysis (i.e. a protein).

Type: ProteinDetectionHypothesisType

Attributes:

Attribute Name	Data Type	Use	Definition
dBSequence_ref	xsd:string	required	A reference to the corresponding DBSequence entry. Note - this attribute was optional in mzIdentML 1.1 but is now mandatory in mzIdentML 1.2. Consuming software should assume that the DBSequence entry referenced here is the definitive identifier for the protein.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
passThreshold	xsd:boolean	required	Set to true if the producers of the file has deemed that the ProteinDetectionHypothesis has passed a given threshold or been validated as correct. If no such threshold has been set, value of true should be given for all results.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
PeptideHypothesis	1	unbounded	Peptide evidence on which this ProteinHypothesis is based by reference to a PeptideEvidence element.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<ProteinDetectionHypothesis passThreshold="true" dBSequence_ref="dbseq_tr|Q3V2I5|Q3V2I5_MOUSE
Glyceraldehyde-3-phosphate dehydrogenase (Fragment) OS=Mus..." id="PDH_10">
    <PeptideHypothesis peptideEvidence_ref="PE13_2_62">
        <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_13_1"/>
    </PeptideHypothesis>
    <cvParam accession="MS:1001097" cvRef="PSI-MS" value="1" name="distinct peptide sequences"/>
    <cvParam accession="MS:1002235" cvRef="PSI-MS" value="34.57557513936462" name="ProteoGrouper:PDH
score"/>
    <cvParam accession="MS:1001594" cvRef="PSI-MS" value="PDH_11" name="sequence same-set protein"/>
  ...
</ProteinDetectionHypothesis>
```

cvParam Mapping Rules:

```
Path
/MzIdentML/DataCollection/AnalysisData/ProteinDetectionList/ProteinAmbiguityGroup/ProteinDetection
Hypothesis
MAY supply term MS:1002403 (group representative) only once
MAY supply a *child* term of MS:1001116 (single protein result details) one or more times
  e.g.: MS:1001088 (protein description)
  e.g.: MS:1001093 (sequence coverage)
  e.g.: MS:1001097 (distinct peptide sequences)
  e.g.: MS:1001098 (confident distinct peptide sequences)
  e.g.: MS:1001099 (confident peptide qualification)
  e.g.: MS:1001100 (confident peptide sequence number)
  e.g.: MS:1001125 (manual validation)
  e.g.: MS:1001157 (SEQUEST:sp)
  e.g.: MS:1001158 (SEQUEST:Uniq) WARNING: Term has no definition!
  e.g.: MS:1001169 (Paragon:expression change p-value)
  et al.
MUST supply term MS:1002402 (non-leading protein) only once
MAY supply a *child* term of MS:1001153 (search engine specific score) one or more times
  e.g.: MS:1001154 (SEQUEST:probability)
  e.g.: MS:1001155 (SEQUEST:xcorr)
  e.g.: MS:1001156 (SEQUEST:deltacn)
  e.g.: MS:1001157 (SEQUEST:sp)
  e.g.: MS:1001158 (SEQUEST:Uniq) WARNING: Term has no definition!
  e.g.: MS:1001159 (SEQUEST:expectation value)
  e.g.: MS:1001160 (SEQUEST:sf)
  e.g.: MS:1001161 (SEQUEST:matched ions)
  e.g.: MS:1001162 (SEQUEST:total ions)
  e.g.: MS:1001163 (SEQUEST:consensus score)
  et al.
MAY supply a *child* term of MS:1001060 (quality estimation method details) one or more times
  e.g.: MS:1001058 (quality estimation by manual validation)
  e.g.: MS:1001194 (quality estimation with decoy database)
```

```
    e.g.: MS:1001364 (distinct peptide-level global FDR)
    e.g.: MS:1001447 (prot:FDR threshold)
    e.g.: MS:1001448 (pep:FDR threshold)
    e.g.: MS:1001454 (quality estimation with implicite decoy sequences)
    e.g.: MS:1001491 (percolator:Q value)
    e.g.: MS:1001494 (no threshold)
    e.g.: MS:1001574 (report only spectra assigned to identified proteins)
    e.g.: MS:1002055 (MS-GF:PepQValue)
    et al.
  MAY supply a *child* term of MS:1001101 (protein group or subset relationship) one or more times
    e.g.: MS:1001591 (anchor protein)
    e.g.: MS:1001592 (family member protein)
    e.g.: MS:1001593 (group member with undefined relationship OR ortholog protein)
    e.g.: MS:1001594 (sequence same-set protein)
    e.g.: MS:1001595 (spectrum same-set protein)
    e.g.: MS:1001596 (sequence sub-set protein)
    e.g.: MS:1001597 (spectrum sub-set protein)
    e.g.: MS:1001598 (sequence subsumable protein)
    e.g.: MS:1001599 (spectrum subsumable protein)
    e.g.: MS:1002213 (PAnalyzer:conclusive protein)
    et al.
  MUST supply term MS:1002401 (leading protein) only once
```

Example for protein grouping:

```
        <cvParam cvRef="PSI-MS" accession="MS:1002394" name="PIA:protein score"
value="107.73038501509386"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002401" name="leading protein"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1001594" name="sequence same-set protein"
value="PDH_Q3TWF2_PAG_2106 PDH_Q3U7T8_PAG_2106 PDH_Q3U9G2_PAG_2106"></cvParam>
</ProteinDetectionHypothesis>
```

6.57 Element <ProteinDetectionList>

Definition: The protein list resulting from a protein detection process.

Type: ProteinDetectionListType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ProteinAmbiguityGroup	0	unbounded	A set of logically related results from a protein detection, for example to represent conflicting assignments of peptides to proteins.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<ProteinDetectionList id="PDL_1" xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <ProteinAmbiguityGroup id="PAG_0">
        <ProteinDetectionHypothesis passThreshold="true"
dBSequence_ref="dbseq_sp|P16627|HS71L_MOUSE Heat shock 70 kDa protein 1-like OS=Mus musculus
GN=Hspa11..." id="PDH_15">
            <PeptideHypothesis peptideEvidence_ref="PE16_2_69">
                <SpectrumIdentificationItemRef spectrumIdentificationItem_ref="SII_16_1"/>
            </PeptideHypothesis>
            <PeptideHypothesis peptideEvidence_ref="PE17_2_107">
  ...
</ProteinDetectionList>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/AnalysisData/ProteinDetectionList
MAY supply a *child* term of MS:1001184 (search statistics) one or more times
  e.g.: MS:1001035 (date / time search performed)
  e.g.: MS:1001036 (search time taken)
  e.g.: MS:1001177 (number of molecular hypothesis considered)
  e.g.: MS:1002404 (count of identified proteins)
MUST supply term MS:1002404 (count of identified proteins) only once
```

6.58 Element <ProteinDetectionProtocol>

Definition: The parameters and settings of a ProteinDetection process.

Type: ProteinDetectionProtocolType

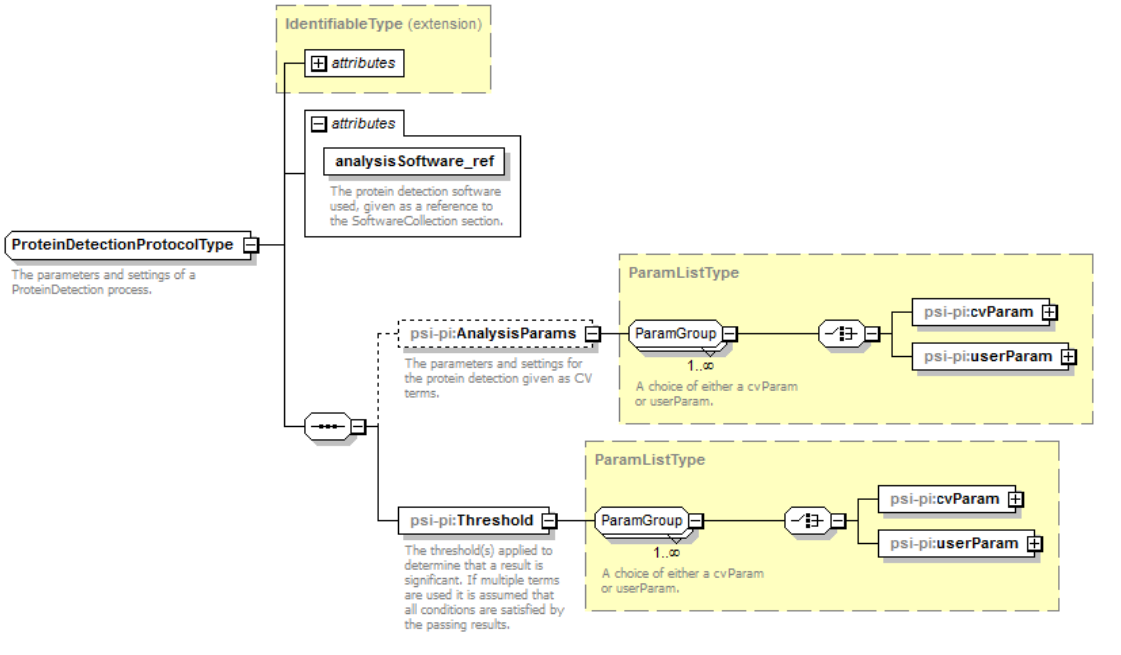
Attributes:

Attribute Name	Data Type	Use	Definition
analysisSoftware_ref	xsd:string	required	The protein detection software used, given as a reference to the SoftwareCollection section.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
AnalysisParams	0	1	The parameters and settings for the protein detection given as CV terms.
Threshold	1	1	The threshold(s) applied to determine that a result is significant. If multiple terms are used it is assumed that all conditions are satisfied by the passing results.

Graphical Context:



Example Context:

```
<ProteinDetectionProtocol id="PDP_PAnalyzer" analysisSoftware_ref="PAnalyzer">
  <AnalysisParams>
    <cvParam name="mascot:SigThreshold" value="0.05" cvRef="PSI-MS" accession="MS:1001316" />
    <cvParam name="mascot:MaxProteinHits" value="Auto" cvRef="PSI-MS" accession="MS:1001317" />
    <cvParam name="mascot:ProteinScoringMethod" value="MudPIT" cvRef="PSI-MS" accession="MS:1001318"
/>
    <cvParam name="mascot:MinMSMSThreshold" value="0" cvRef="PSI-MS" accession="MS:1001319" />
    <cvParam name="mascot:ShowHomologousProteinsWithSamePeptides" value="1" cvRef="PSI-MS"
accession="MS:1001320" />
  ...
</ProteinDetectionProtocol>
```

6.59 Element <Provider>

Definition: The Provider of the mzIdentML record in terms of the contact and software.

Type: ProviderType

Attributes:

Attribute Name	Data Type	Use	Definition
analysisSoftware_ref	xsd:string	optional	The Software that produced the document instance.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ContactRole	0	1	The Contact that provided the document instance.

Example Context:

```
<Provider id="PROVIDER" xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <ContactRole contact_ref="PERSON_DOC_OWNER">
        <Role>
            <cvParam accession="MS:1001271" cvRef="PSI-MS" name="researcher"/>
        </Role>
    </ContactRole>
</Provider>
```

6.60 Element <Residue>

Definition: The specification of a single residue within the mass table.

Type: ResidueType

Attributes:

Attribute Name	Data Type	Use	Definition
code	chars	required	The single letter code for the residue.
mass	xsd:float	required	The residue mass in Daltons (not including any fixed modifications).

Subelements: none

Example Context:

```
<Residue code="C" mass="103.009186" />
```

6.61 Element <Role>

Definition: The roles (lab equipment sales, contractor, etc.) the Contact fills.

Type: RoleType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
        <Role>
          <cvParam cvRef="PSI-MS" accession="MS:1001267" name="software vendor"/>
        </Role>
```

cvParam Mapping Rules:

```
Path /MzIdentML/Provider/ContactRole/Role
MUST supply a *child* term of MS:1001266 (role type) one or more times
  e.g.: MS:1001267 (software vendor)
  e.g.: MS:1001268 (programmer)
  e.g.: MS:1001269 (instrument vendor)
  e.g.: MS:1001270 (lab personnel)
  e.g.: MS:1001271 (researcher)
Path /MzIdentML/AnalysisSoftwareList/AnalysisSoftware/ContactRole/Role
MUST supply a *child* term of MS:1001266 (role type) one or more times
  e.g.: MS:1001267 (software vendor)
  e.g.: MS:1001268 (programmer)
  e.g.: MS:1001269 (instrument vendor)
```

```
    e.g.: MS:1001270 (lab personnel)
    e.g.: MS:1001271 (researcher)
  Path /MzIdentML/AnalysisSampleCollection/Sample/ContactRole/Role
  MUST supply a *child* term of MS:1001266 (role type) one or more times
    e.g.: MS:1001267 (software vendor)
    e.g.: MS:1001268 (programmer)
    e.g.: MS:1001269 (instrument vendor)
    e.g.: MS:1001270 (lab personnel)
    e.g.: MS:1001271 (researcher)
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001271" name="researcher"></cvParam>
<cvParam accession="MS:1001267" cvRef="PSI-MS" name="software vendor"/>
```

6.62 Element <Sample>

Definition: A description of the sample analysed by mass spectrometry using CVParams or UserParams. If a composite sample has been analysed, a parent sample should be defined, which references subsamples. This represents any kind of substance used in an experimental workflow, such as whole organisms, cells, DNA, solutions, compounds and experimental substances (gels, arrays etc.).

Type: SampleType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ContactRole	0	unbounded	The Contact that provided the document instance.
SubSample	0	unbounded	References to the individual component samples within a mixed parent sample.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

6.63 Element <SearchDatabase>

Definition: A database for searching mass spectra. Examples include a set of amino acid sequence entries, nucleotide databases (e.g. 6 frame translated) or annotated spectra libraries.

Type: SearchDatabaseType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
location	xsd:anyURI	required	The location of the data file.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

numDatabaseSequences	xsd:long	optional	The total number of sequences in the database.
numResidues	xsd:long	optional	The number of residues in the database.
releaseDate	xsd:dateTime	optional	The date and time the database was released to the public; omit this attribute when the date and time are unknown or not applicable (e.g. custom databases).
version	xsd:string	optional	The version of the database.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ExternalFormatDocumentation	0	1	A URI to access documentation and tools to interpret the external format of the ExternalData instance. For example, XML Schema or static libraries (APIs) to access binary formats.
FileFormat	1	1	The format of the ExternalData file, for example "tiff" for image files.
DatabaseName	1	1	The database name may be given as a cvParam if it maps exactly to one of the release databases listed in the CV, otherwise a userParam should be used.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
      <SearchDatabase numDatabaseSequences="40400"
location="C:\Users\hba041\My_Git_Applications\peptide-shaker.wiki\data\2016_04_05\uniprot-human-
reviewed-trypsin-april-2016_concatenated_target_decoy.fasta" id="SearchDB_1">
        <FileFormat>
          <cvParam cvRef="PSI-MS" accession="MS:1001348" name="FASTA format"/>
        </FileFormat>
        <DatabaseName>
          <userParam name="uniprot-human-reviewed-trypsin-april-
2016_concatenated_target_decoy.fasta"/>
        </DatabaseName>
  ...
</SearchDatabase>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/Inputs/SearchDatabase
MAY supply a *child* term of MS:1000561 (data file checksum type) one or more times
  e.g.: MS:1000568 (MD5)
  e.g.: MS:1000569 (SHA-1)
MAY supply a *child* term of MS:1001011 (search database details) one or more times
  e.g.: MS:1001014 (database local file path)
  e.g.: MS:1001015 (database original uri)
  e.g.: MS:1001016 (database version)
  e.g.: MS:1001017 (database release date)
  e.g.: MS:1001020 (DB filter taxonomy)
  e.g.: MS:1001021 (DB filter on accession numbers)
  e.g.: MS:1001022 (DB MW filter)
  e.g.: MS:1001023 (DB PI filter)
  e.g.: MS:1001024 (translation frame)
  e.g.: MS:1001025 (translation table)
  et al.
```

6.64 Element <SearchDatabaseRef>

Definition: One of the search databases used.

Type: SearchDatabaseRefType

Attributes:

Attribute Name	Data Type	Use	Definition
searchDatabase_ref	xsd:string	optional	A reference to the database searched.

Subelements: none

Example Context: `<SearchDatabaseRef searchDatabase_ref="SDB_4299_203"></SearchDatabaseRef>`

6.65 Element <SearchModification>

Definition: Specification of a search modification as parameter for a spectra search. Contains the name of the modification, the mass, the specificity and whether it is a static modification.

Type: SearchModificationType

Attributes:

Attribute Name	Data Type	Use	Definition
fixedMod	xsd:boolean	required	True, if the modification is static (i.e. occurs always).
massDelta	xsd:float	required	The mass delta of the searched modification in Daltons.
residues	listOfCharsOrAny	required	The residue(s) searched with the specified modification. For N or C terminal modifications that can occur on any residue, the . character should be used to specify any, otherwise the list of amino acids should be provided.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SpecificityRules	0	unbounded	The specificity rules of the searched modification including for example the probability of a modification's presence or peptide or protein termini. Standard fixed or variable status should be provided by the attribute fixedMod.
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
        <SearchModification residues="E" massDelta="-18.010565" fixedMod= "false" >
          <SpecificityRules>
            <cvParam cvRef="PSI-MS" accession="MS:1001189" name="modification specificity peptide N-
term"/>
          </SpecificityRules>
          <cvParam cvRef="UNIMOD" accession="UNIMOD:27" name="Glu->pyro-Glu"/>
          <cvParam cvRef="PSI-MS" accession="MS:1002504" name="modification index" value="3"/>
        </SearchModification>
```

cvParam Mapping Rules:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/ModificationParams/
SearchModification
MAY supply term MS:1002509 (cross-link donor) only once
MAY supply term MS:1002510 (cross-link acceptor) only once
MAY supply a *child* term of UNIMOD:0 (unimod root node) only once
MAY supply a *child* term of MS:1001471 (peptide modification details) only once
  e.g.: MS:1001460 (unknown modification)
  e.g.: MS:1001524 (fragment neutral loss)
  e.g.: MS:1001525 (precursor neutral loss)
  e.g.: MS:1001972 (PTM scoring algorithm version)
  e.g.: MS:1002028 (nucleic acid base modification)
  e.g.: MS:1002029 (original nucleic acid sequence)
  e.g.: MS:1002030 (modified nucleic acid sequence)
MUST supply term MS:1001460 (unknown modification) only once
MAY supply a *child* term of XLMOD:00002 (cross-linker related PTM) only once
MAY supply term MS:1002504 (modification index) only once
MAY supply a *child* term of XLMOD:00004 (cross-linker) only once
MAY supply a *child* term of MOD:00000 (protein modification) only once
```

Example cvParams:

```
<cvParam cvRef="UNIMOD" accession="UNIMOD:35" name="Oxidation"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:4" name="Carbamidomethyl"></cvParam>
<cvParam accession="UNIMOD:214" cvRef="UNIMOD" name="iTRAQ4plex"/>
<cvParam accession="MS:1001189" cvRef="PSI-MS" name="modification specificity peptide N-
term"/>
<cvParam accession="UNIMOD:39" cvRef="UNIMOD" name="Methylthio"/>
<cvParam accession="UNIMOD:7" cvRef="UNIMOD" name="Deamidated"/>
<cvParam cvRef="PSI-MS" accession="MS:1002504" name="modification index" value="0"/>
<cvParam cvRef="XLMOD" accession="XLMOD:02000" name="BS3"></cvParam>
```

```
<cvParam cvRef="PSI-MS" accession="MS:1002509" name="cross-link donor"
value="0"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002510" name="cross-link acceptor"
value="0"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:02004" name="BS3-d4"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01001" name="amidated BS3"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01000" name="hydrolyzed BS3"></cvParam>
<cvParam cvRef="UNIMOD" accession="UNIMOD:1020" name="Xlink:DSS"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01009" name="amidated BS3-d4"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:01008" name="hydrolyzed BS3-d4"></cvParam>
```

6.66 Element <SearchType>

Definition: The type of search performed e.g. PMF, Tag searches, MS-MS

Type: ParamType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.
userParam	1	1	A single user-defined parameter.

Example Context:

```
<SearchType>
    <cvParam accession="MS:1001083" cvRef="PSI-MS" value="" name="ms-ms search"/>
</SearchType>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/SearchType
MUST supply a *child* term of MS:1001080 (search type) one or more times
  e.g.: MS:1001010 (de novo search)
  e.g.: MS:1001031 (spectral library search)
  e.g.: MS:1001081 (pmf search)
  e.g.: MS:1001082 (tag search)
  e.g.: MS:1001083 (ms-ms search)
  e.g.: MS:1001584 (combined pmf + ms-ms search)
  e.g.: MS:1002490 (peptide-level scoring)
  e.g.: MS:1002491 (modification localization scoring)
  e.g.: MS:1002492 (consensus scoring)
  e.g.: MS:1002493 (sample pre-fractionation)
  et al.
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001083" name="ms-ms search"></cvParam>
```

6.67 Element <Seq>

Definition: The actual sequence of amino acids or nucleic acid.

Type: sequence

Attributes: none

Subelements: none

Example Context:

```
<Seq>MMKFTVVAAALLLLGAVRAEEEDKKEDVGTVVGIDLGTTYSCVGVFKNGRVEIIANDQGNRITPSYVAFTPEGERLIGDAAKNQLTSNPENTVFDA
KRLIGRTWNDPSVQQDIKFLPFKVVEKKTKPYIQVDIGGGQTKTFAPEEISAMVLTKMKETAEAYLGKKVTHAVVTVPAYFNDAQRQATKDAGTIAGLNVM
RIINEPTAAAIAYGLDKREGEKNILVFDLGGGTFDVSLLTIDNGVFEVVATNGDTHLGGEDFDQRVMEHFIKLYKKKTGKDVRKDNRAVQKLRREVEKAKR
ALSSQHQARIEIESFFEREDFSETLTRAKFEELNMDLFRSTMKPVQKVLEDSDLKKSDIDEIVLVGGSTRIPKIQQLVKEFFNGKEPSRGINPDEAVAYGA
AVQAGVLSGGQDTGDLVLLDVCPLTLGIETVGGVMTKLIPRNTVVPTKKSQIFSTASDNQPTVTIKVYEGERPLTKDNHLLGTFDLTGIPPAPRGVPQIEV
TFEIDVNGILRVTAEDKGTGNKNKITITNDQNRLTPEEIERMVNDAEKFAEEDKKLKERIDTRNELESYAYSLKNQIGDKEKLGGKLSSEDKETMEKAVEE
KIEWLESHQDADIEDFKAKKKELEEIVQPIISKLYGSGGPPPTGEEDTSEKDEL</Seq>
```

6.68 Element <SequenceCollection>

Definition: The collection of sequences (DBSequence or Peptide) identified and their relationship between each other (PeptideEvidence) to be referenced elsewhere in the results.

Type: SequenceCollectionType

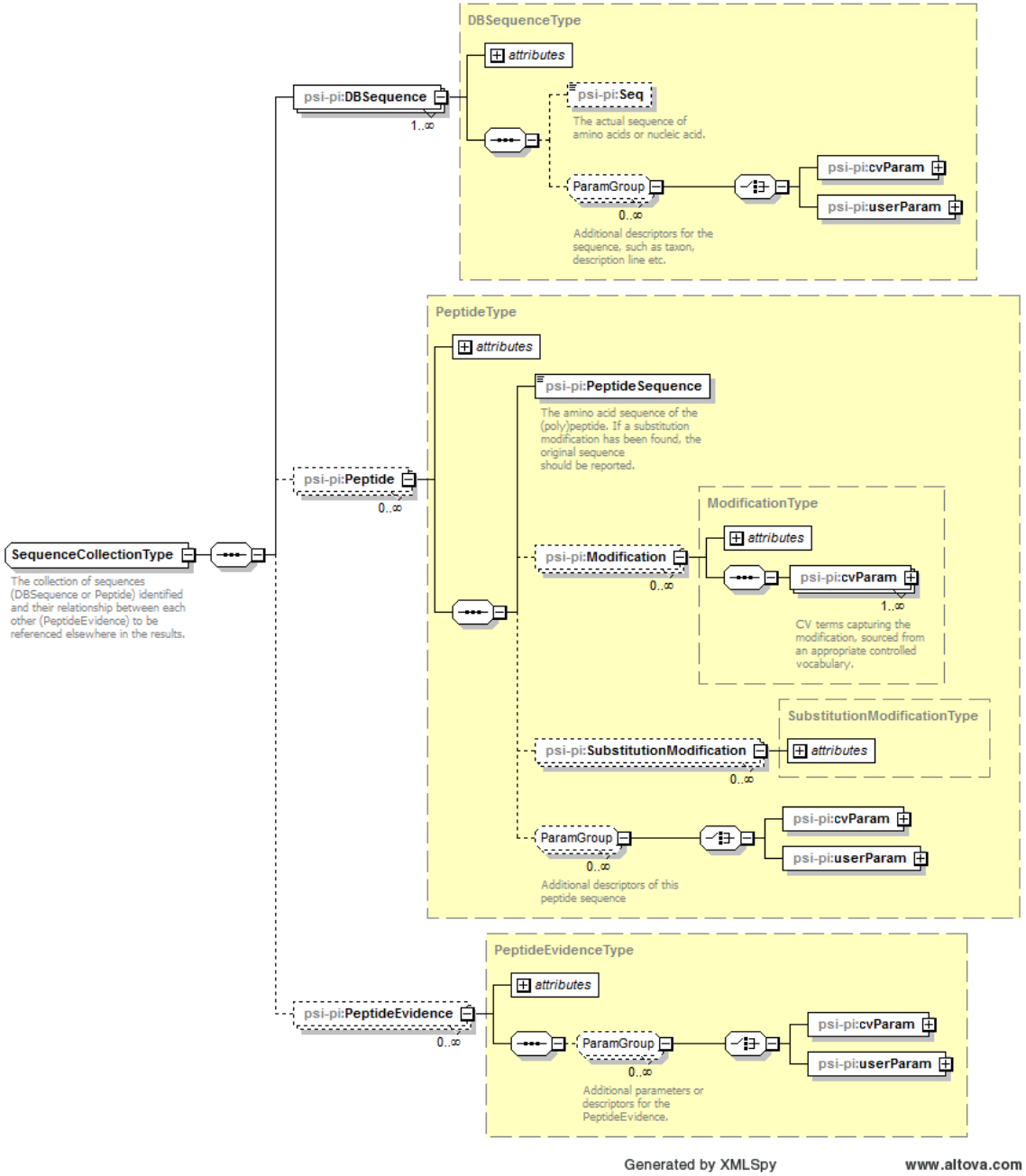
Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
DBSequence	0	unbounded	A database sequence from the specified SearchDatabase (nucleic acid or amino acid).

			If the sequence is nucleic acid, the source nucleic acid sequence should be given in the seq attribute rather than a translated sequence.
Peptide	0	unbounded	One (poly)peptide (a sequence with modifications). The combination of Peptide sequence and modifications MUST be unique in the file.
PeptideEvidence	0	unbounded	PeptideEvidence links a specific Peptide element to a specific position in a DBSequence. There MUST only be one PeptideEvidence item per Peptide-to-DBSequence-position.

Graphical Context:



Example Context:

```
<SequenceCollection xmlns="http://psidev.info/psi/pi/mzIdentML/1.2">
    <DBSequence accession="sp|Q64467|G3PT_MOUSE Glyceraldehyde-3-phosphate dehydrogenase, testis-
speci
fic OS=Mus..." searchDatabase_ref="SearchDB_1" length="440" name="sp|Q64467|G3PT_MOUSE
Glyceraldehyde-3
-phosphate dehydrogenase, testis-specific OS=Mus musculus GN=Gapdhs PE=1 SV=1"
id="dbseq_sp|Q64467|G3PT
_MOUSE Glyceraldehyde-3-phosphate dehydrogenase, testis-specific OS=Mus...">
        <Seq>MSRRDVVLTNVTVVQLRRDRCPCPCPCPCPCPCPVIRPPPPKLEDPPPTVEEQPPPPPPPPPPPPPPPPPPPPQIEPDKFEEAPPPPP
PPPPPPPPPP
PPLQKPARELTVGINGFGRIGRLVLRVCMEKGIRVVAVNDPFIDPEYMVYMFKYDSTHGRYKGNVEHKNGQLVVDNLEINTYQCKDPKEIPWSSIGNPYVV
EC
TGVYLSIEAASAHISSGARRVVVTAPSPDAPMFVMGVNEKDYNPGSMTIVSNASCTTNCLAPLAKVIHENFGIVEGLMTTVHSYTATQKTVDGPSKKDWRG
GR
GAHQNIIPSSTGAAKAVGKVIPELKGKLTGMAFRVPTPNVSVVDLTCRLAKPASYSAITEAVKAAAKGPLAGILAYTEDQVVSTDFNGNPHSSIFDAKAGI
AL
NDNFVKLVAWYDNEYGYSNRVVDLLRYMFSREK</Seq>
    </DBSequence>
    <DBSequence accession="tr|Q3UEM8|Q3UEM8_MOUSE Putative uncharacterized protein (Fragment) OS=Mus
musculus..." searchDatabase_ref="SearchDB_1" length="520" name="tr|Q3UEM8|Q3UEM8_MOUSE Putative
unchar
acterized protein (Fragment) OS=Mus musculus GN=Hspa5 PE=2 SV=1" id="dbseq_tr|Q3UEM8|Q3UEM8_MOUSE
Puta
tive uncharacterized protein (Fragment) OS=Mus musculus...">

<Seq>MMKFTVVAAALLLLGAVRAEEEDKKEDVGTVVGIDLGTTYSCVGVFKNGRVEIIANDQGNRITPSYVAFTPEGERLIGDAAKNQLTSNP
ENTVFDAK
RLIGRTWNDPSVQQDIKFLPFKVVEKKTKPYIQVDIGGGQTKTFAPEEISAMVLTKMKETAEAYLGKKVTHAVVTVPAYFNDAQRQATKDAGTIAGLNVMR
I
INEPTAAAIAYGLDKREGEKNILVFDLGGGTFDVSLLTIDNGVFEVVATNGDTHLGGEDFDQRVMEHFIKLYKKKTGKDVRKDNRAVQKLRREVEKAKRAL
S
SQHQARIEIESFFEGEDFSETLTRAKFEELNMDLFRSTIKPVQKVLEDSDLKKSDIDEIVLVGGSTRIPKIQQLVKEFFNGKEPSRGINPDEAVAYGAAVQ
A
GVLSGDQDTGDLVLLDVCPLTLGIETVGGVMTKLIPRNTVVPTKKSQIFSTASDNQPTVTIKVYEGERPLTKDNHLLGTFDLTGIPPAPRGVPQIEVTFEI
D
VNGILRVTAEDKGTG</Seq>
    </DBSequence>
  ...
</SequenceCollection>
```

6.69 Element <SiteRegexp>

Definition: Regular expression for specifying the enzyme cleavage site.

Type: xsd:string

Attributes: none

Subelements: none

Example Context:

```
<SiteRegexp>(?<=[KR])</SiteRegexp>
```

6.70 Element <SoftwareName>

Definition: The name of the analysis software package, sourced from a CV if available.

Type: ParamType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.
userParam	1	1	A single user-defined parameter.

Example Context:

```
<SoftwareName>
    <cvParam accession="MS:1002244" cvRef="PSI-MS" name="mzidLib:FalseDiscoveryRate"/>
</SoftwareName>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisSoftwareList/AnalysisSoftware/SoftwareName
MUST supply a *child* term of MS:1001456 (analysis software) one or more times
  e.g.: MS:1000532 (Xcalibur)
  e.g.: MS:1000533 (Bioworks)
  e.g.: MS:1000534 (MassLynx)
  e.g.: MS:1000535 (FlexAnalysis)
  e.g.: MS:1000536 (Data Explorer)
  e.g.: MS:1000537 (4700 Explorer)
  e.g.: MS:1000539 (Voyager Biospectrometry Workstation System)
  e.g.: MS:1000551 (Analyst)
  e.g.: MS:1000600 (Proteios)
```

Example cvParams:

```
  e.g.: MS:1000601 (ProteinLynx Global Server)
  et al.
<cvParam cvRef="PSI-MS" accession="MS:1001475" name="OMSSA"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002237" name="mzidLib"></cvParam>
<cvParam accession="MS:1001476" cvRef="PSI-MS" name="X\!Tandem"/>
<cvParam accession="MS:1002239" cvRef="PSI-MS" name="mzidLib:Tandem2Mzid"/>
<cvParam accession="MS:1002244" cvRef="PSI-MS" name="mzidLib:FalseDiscoveryRate"/>
<cvParam accession="MS:1002242" cvRef="PSI-MS" name="mzidLib:Thresholder"/>
<cvParam accession="MS:1002241" cvRef="PSI-MS" name="mzidLib:ProteoGrouper"/>
<cvParam accession="MS:1002048" cvRef="PSI-MS" name="MS-GF+"/>
<cvParam accession="MS:1001207" cvRef="PSI-MS" name="Mascot"/>
<cvParam accession="MS:1001478" cvRef="PSI-MS" name="Mascot Parser"/>
<cvParam accession="MS:1002076" cvRef="PSI-MS" name="PAnalyzer"/>
<cvParam accession="MS:1001456" cvRef="PSI-MS" name="analysis software"/>
<cvParam accession="MS:1000752" cvRef="PSI-MS" name="TOPP software"/>
<cvParam cvRef="PSI-MS" accession="MS:1002458" name="PeptideShaker"/>
<cvParam cvRef="PSI-MS" accession="MS:1002544" name="xiFDR"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002543" name="xiFDR"></cvParam>
```

6.71 Element <SourceFile>

Definition: A file from which this mzIdentML instance was created.

Type: SourceFileType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
location	xsd:anyURI	required	The location of the data file.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ExternalFormatDocumentation	0	1	A URI to access documentation and tools to interpret the external format of the ExternalData instance. For example, XML Schema or static libraries (APIs) to access binary formats.
FileFormat	1	1	The format of the ExternalData file, for example "tiff" for image files.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
      <SourceFile location="C:\Users\hba041\My_Git_Applications\peptide-
shaker.wiki\data\2016_04_05\.PeptideShaker_unzip_temp\searchgui_out_PeptideShaker_temp\qExactive01819
.t.xml" id="SourceFile_2">
        <FileFormat>
          <cvParam cvRef="PSI-MS" accession="MS:1001401" name="X!Tandem xml format"/>
        </FileFormat>
      </SourceFile>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/Inputs/SourceFile
MAY supply a *child* term of MS:1000561 (data file checksum type) one or more times
  e.g.: MS:1000568 (MD5)
  e.g.: MS:1000569 (SHA-1)
```

6.72 Element <SpecificityRules>

Definition: The specificity rules of the searched modification including for example the probability of a modification's presence or peptide or protein termini. Standard fixed or variable status should be provided by the attribute fixedMod.

Type: SpecificityRulesType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
          <SpecificityRules>
            <cvParam cvRef="PSI-MS" accession="MS:1002057" name="modification specificity protein N-
term"/>
          </SpecificityRules>
```

cvParam Mapping Rules:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/ModificationParams/SearchModifi
cation/SpecificityRules
MUST supply a *child* term of MS:1001056 (modification specificity rule) only once
  e.g.: MS:1001189 (modification specificity peptide N-term)
  e.g.: MS:1001190 (modification specificity peptide C-term)
  e.g.: MS:1001875 (modification motif)
  e.g.: MS:1001876 (modification probability)
  e.g.: MS:1002057 (modification specificity protein N-term)
  e.g.: MS:1002058 (modification specificity protein C-term)
```

Example cvParams:

```
<cvParam accession="MS:1001189" cvRef="PSI-MS" name="modification specificity peptide N-term"/>
<cvParam accession="UNIMOD:214" cvRef="UNIMOD" name="iTRAQ4plex"/>
<cvParam accession="MS:1002057" cvRef="PSI-MS" name="modification specificity protein N-term"/>
<cvParam accession="UNIMOD:1" cvRef="UNIMOD" name="Acetyl"/>
<cvParam cvRef="PSI-MS" accession="MS:1002504" name="modification index" value="2"/>
<cvParam cvRef="UNIMOD" accession="UNIMOD:27" name="Glu->pyro-Glu"/>
<cvParam cvRef="UNIMOD" accession="UNIMOD:28" name="Gln->pyro-Glu"/>
<cvParam cvRef="UNIMOD" accession="UNIMOD:385" name="Ammonia-loss"/>
<cvParam cvRef="XLMOD" accession="XLMOD:02000" name="BS3"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002509" name="cross-link donor" value="0"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002510" name="cross-link acceptor" value="0"></cvParam>
<cvParam cvRef="XLMOD" accession="XLMOD:02004" name="BS3-d4"></cvParam>
```

6.73 Element <SpectraData>

Definition: A data set containing spectra data (consisting of one or more spectra).

Type: SpectraDataType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
location	xsd:anyURI	required	The location of the data file.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
ExternalFormatDocumentation	0	1	A URI to access documentation and tools to interpret the external format of the ExternalData instance. For example, XML Schema or static libraries (APIs) to access binary formats.
FileFormat	1	1	The format of the ExternalData file, for example "tiff" for image files.
SpectrumIDFormat	1	1	The format of the spectrum identifier within the source file

Example Context:

```
<SpectraData
location="E:\Work\PSI\mzIdentML\ProteinInference\Rosetta2\Peaklistswithecoli\Rosetta2a_Ecoli_spectra
.mgf" name="Rosetta2a_Ecoli_spectra.mgf" id="SID_1">
    <FileFormat>
        <cvParam accession="MS:1001062" cvRef="PSI-MS" name="Mascot MGF format"/>
    </FileFormat>
    <SpectrumIDFormat>
        <cvParam accession="MS:1000774" cvRef="PSI-MS" name="multiple peak list nativeID format"/>
    </SpectrumIDFormat>
```

```
  ...
</SpectraData>
```

6.74 Element <SpectrumIdentification>

Definition: An Analysis which tries to identify peptides in input spectra, referencing the database searched, the input spectra, the output results and the protocol that is run.

Type: SpectrumIdentificationType

Attributes:

Attribute Name	Data Type	Use	Definition
activityDate	xsd:dateTime	optional	When the protocol was applied.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
spectrumIdentificationList_ref	xsd:string	required	A reference to the SpectrumIdentificationList produced by this analysis in the DataCollection section.
spectrumIdentificationProtocol_ref	xsd:string	required	A reference to the search protocol used for this SpectrumIdentification.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
InputSpectra	1	unbounded	One of the spectra data sets used.
SearchDatabaseRef	1	unbounded	One of the search databases used.

Example Context:

```
<SpectrumIdentification spectrumIdentificationProtocol_ref="SearchProtocol_1_4299"
spectrumIdentificationList_ref="SII_LIST_1_1_4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-3_Din.raw"
id="SpecIdent__4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-3_Din.raw">
  <InputSpectra spectraData_ref="SD_4299_120114_20_Orbi2_ZC_QC_220_HSAd0-d4-1to1-
3_Din.raw"></InputSpectra>
 <SearchDatabaseRef searchDatabase_ref="SDB_4299_203"></SearchDatabaseRef>
</SpectrumIdentification>
```

6.75 Element <SpectrumIdentificationItem>

Definition: An identification of a single (poly)peptide, resulting from querying an input spectra, along with the set of confidence values for that identification. PeptideEvidence elements should be given for all mappings of the corresponding Peptide sequence within protein sequences.

Type: SpectrumIdentificationItemType

Attributes:

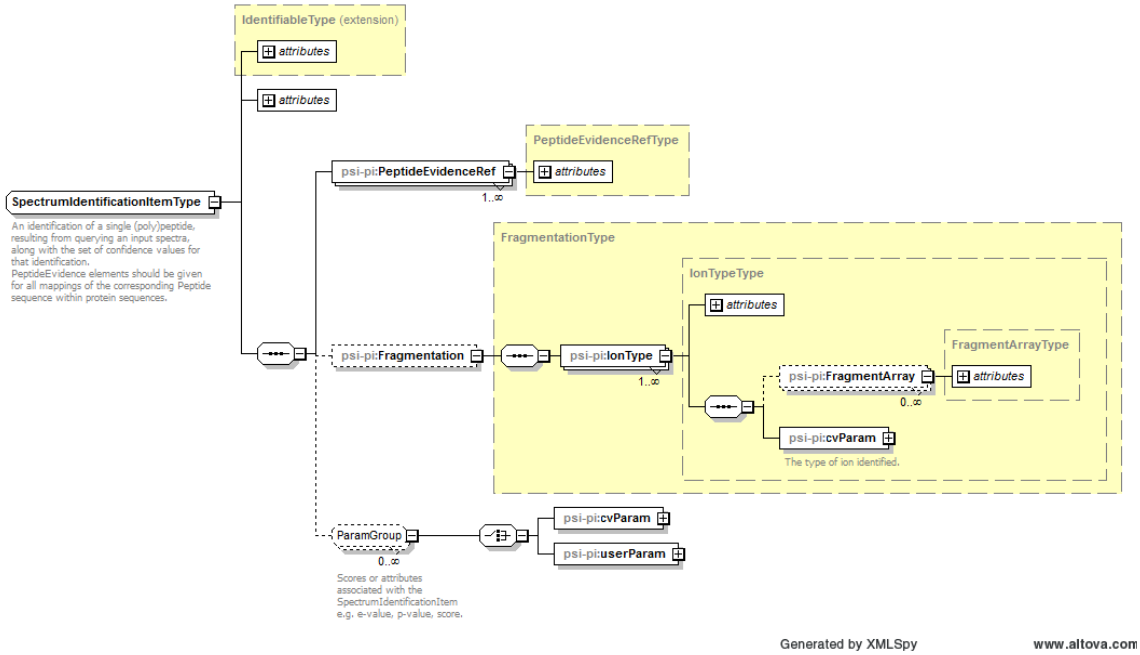
Attribute Name	Data Type	Use	Definition
calculatedMassToCharge	xsd:double	optional	The theoretical mass-to-charge value calculated for the peptide in Daltons / charge.
calculatedPI	xsd:float	optional	The calculated isoelectric point of the (poly)peptide, with relevant modifications included. Do not supply this value if the PI cannot be calcuated properly.
chargeState	xsd:int	required	The charge state of the identified peptide.
experimentalMassToCharge	xsd:double	required	The mass-to-charge value measured in the experiment in Daltons / charge.

id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
massTable_ref	xsd:string	optional	A reference should be given to the MassTable used to calculate the sequenceMass only if more than one MassTable has been given.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
passThreshold	xsd:boolean	required	Set to true if the producers of the file has deemed that the identification has passed a given threshold or been validated as correct. If no such threshold has been set, value of true should be given for all results.
peptide_ref	xsd:string	required	A reference to the identified (poly)peptide sequence in the Peptide element.
rank	xsd:int	required	For an MS/MS result set, this is the rank of the identification quality as scored by the search engine. 1 is the top rank. If multiple identifications have the same top score, they should all be assigned rank =1. For PMF data, the rank attribute may be meaningless and values of rank = 0 should be given.
sample_ref	xsd:string	optional	A reference should be provided to link the SpectrumIdentificationItem to a Sample if more than one sample has been described in the AnalysisSampleCollection.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
PeptideEvidenceRef	0	unbounded	Reference to the PeptideEvidence element identified. If a specific sequence can be assigned to multiple proteins and or positions in a protein all possible PeptideEvidence elements should be referenced here.
Fragmentation	0	1	The product ions identified in this result.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Graphical Context:



Example Context:

```
          <SpectrumIdentificationItem passThreshold="true" rank="1"
peptide_ref="NMGGPYGGGNYGPGGSGGSGGYGGR_15.99491461956-ATAA-2" calculatedMassToCharge="1103.45377262
38118" experimentalMassToCharge="1103.454029541017" chargeState="2" id="SII_1920_1">
            <PeptideEvidenceRef peptideEvidence_ref="PepEv_5164"/>
            <Fragmentation>
              <IonType charge="1" index="1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
23">
                <FragmentArray measure_ref="Measure_MZ" values="175.1193695 232.1403961 289.1618958
452.2268982 509.2429504 566.2701416 653.2999268 710.3218994 767.3411865 854.3770752 911.3968506
968.4257813 1065.472168 1122.492432 1285.553833 1399.612305 1456.62561 1513.645874 1570.669067
1733.721191 1830.793213 1887.808105 1944.829834"/>
                <FragmentArray measure_ref="Measure_Int" values="5939.5844726563 4933.5014648438
13310.7265625 5077.6694335938 5685.9287109375 13253.552734375 7620.0947265625 7724.3696289063
16868.541015625 10552.126953125 11589.0576171875 7839.9741210938 47821.64453125 60335.71484375
21759.3984375 8742.5595703125 11512.0908203125 18130.890625 30577.375 3801.3923339844 8051.07421875
1954.5501708984 4844.9125976563"/>
                <FragmentArray measure_ref="Measure_Error" values="4.173258879802688E-4
-1.9794682032170385E-5 1.618474794895519E-5 0.001690052197886871 -0.0037214683721344954
0.0020060110579152024 -2.3719321211501665E-4 2.7168621795681247E-4 -0.0019049343519554895
0.0019553613780090018 2.6704080801209784E-4 0.007734020238103767 0.0013568713879976713
1.571508180404635E-4 -0.0017703817320580129 0.013774177127970688 0.0056154565579618065
0.004415735988004599 0.006145015418042021 -0.005059517131940083 0.01419863401793009
0.007626913448120831 0.007892192877989146"/>
  ...
</SpectrumIdentificationItem>
```

cvParam Mapping Rules:

Path
/MzIdentML/DataCollection/AnalysisData/SpectrumIdentificationList/SpectrumIdentificationResult/Spect
rumIdentificationItem
MAY supply a *child* term of MS:1001405 (spectrum identification result details) one or more times
  e.g.: MS:1000016 (scan start time)
  e.g.: MS:1000796 (spectrum title)
  e.g.: MS:1000797 (peak list scans)
  e.g.: MS:1000798 (peak list raw scans)
  e.g.: MS:1000903 (product ion series ordinal)
  e.g.: MS:1000904 (product ion m/z delta)
  e.g.: MS:1000926 (product interpretation rank)
  e.g.: MS:1001030 (number of peptide seqs compared to each spectrum)
  e.g.: MS:1001035 (date / time search performed)
  e.g.: MS:1001036 (search time taken)
  et al.

Example cvParams:

```
<cvParam accession="MS:1001330" cvRef="PSI-MS" value="2.5E-6" name="X\!Tandem:expect"/>
<cvParam accession="MS:1001331" cvRef="PSI-MS" value="43.2" name="X\!Tandem:hyperscore"/>
<cvParam accession="MS:1001250" cvRef="PSI-MS" value="0.0" name="local FDR"/>
<cvParam accession="MS:1001868" cvRef="PSI-MS" value="0.0" name="distinct peptide-level q-value"/>
<cvParam accession="MS:1001874" cvRef="PSI-MS" value="3.1133250311332251E-4" name="FDRScore"/>
<cvParam accession="MS:1000796" cvRef="PSI-MS" value="Locus:11.1.1.4652.4 File:"R1 p450 iTRAQ QS
CEX11.wiff"" name="spectrum title"/>
<cvParam accession="MS:1002049" cvRef="PSI-MS" value="129" name="MS-GF:RawScore"/>
<cvParam accession="MS:1002050" cvRef="PSI-MS" value="143" name="MS-GF:DeNovoScore"/>
<cvParam accession="MS:1002052" cvRef="PSI-MS" value="6.3746987E-25" name="MS-GF:SpecEValue"/>
<cvParam accession="MS:1002053" cvRef="PSI-MS" value="1.3781529E-17" name="MS-GF:EValue"/>
<cvParam accession="MS:1002054" cvRef="PSI-MS" value="0.0" name="MS-GF:QValue"/>
<cvParam accession="MS:1002055" cvRef="PSI-MS" value="0.0" name="MS-GF:PepQValue"/>
```

```
<cvParam accession="MS:1002351" cvRef="PSI-MS" value="0.0" name="PSM-level local FDR"/>
<cvParam accession="MS:1002354" cvRef="PSI-MS" value="0.0" name="PSM-level q-value"/>
<cvParam accession="MS:1002355" cvRef="PSI-MS" value="1.5603866050496166E-18" name="PSM-level
FDRScore"/>
<cvParam accession="MS:1001171" cvRef="PSI-MS" value="25.37" name="Mascot:score"/>
<cvParam accession="MS:1001172" cvRef="PSI-MS" value="0.0813522191664226" name="Mascot:expectation
value"/>
<cvParam accession="MS:1001175" cvRef="PSI-MS" name="peptide shared in multiple proteins"/>
<cvParam accession="MS:1001363" cvRef="PSI-MS" name="peptide unique to one protein"/>
<cvParam accession="MS:1001371" cvRef="PSI-MS" value="40" name="Mascot:identity threshold"/>
<cvParam accession="MS:1001370" cvRef="PSI-MS" value="27" name="Mascot:homology threshold"/>
<cvParam accession="MS:1001030" cvRef="PSI-MS" value="10148" name="number of peptide seqs compared to
each spectrum"/>
<cvParam accession="MS:1001114" cvRef="PSI-MS" unitCvRef="UO" unitName="second"
unitAccession="UO:0000010" value="1741" name="retention time(s)"/>
<cvParam accession="MS:1002681" cvRef="PSI-MS" name="OpenXQuest:combined score"
value="0.552164719139592"/>
<cvParam accession="MS:1002511" cvRef="PSI-MS" name="cross-link spectrum identification item"
value="11309529182388590588"/>
<cvParam accession="MS:1000894" cvRef="PSI-MS" name="retention time" value="5468.0193"
unitAccession="second" unitName="" unitCvRef="se"/>
```

Example userParams:

```
<userParam value="0" name="IsotopeError"/>
<userParam value="HCD" name="AssumedDissociationMethod"/>
```

Example for peptide-level statistics:

```
<SpectrumIdentificationItem chargeState="3" experimentalMassToCharge="710.352539"
calculatedMassToCharge="710.352984" peptide_ref="KMDLSDEGGGGVRYPGLHPK_##Oxidation(M):2" rank="1"
passThreshold="false" id="SIR_3397_SII_1">
        <PeptideEvidenceRef
        peptideEvidence_ref="KMDLSDEGGGGVRYPGLHPK_generic|B_GENSCAN00000016205_REVERSED|p:genscan_42_61"></Pe
        ptideEvidenceRef>
        <cvParam cvRef="PSI-MS" accession="MS:1002356" name="PSM-level combined FDRScore"
        value="0.38641138028680944"></cvParam>
        <userParam name="search engines identifying PSM" value="2"></userParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002359" name="distinct peptide-level local FDR"
        value="0.419570671870644"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1001868" name="distinct peptide-level q-value"
        value="0.4192650334075724"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002360" name="distinct peptide-level FDRScore"
        value="0.41934590570107133"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002500" name="peptide passes threshold"
        value="true"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002520" name="peptide group ID"
        value="KMDLSDEGGGGVRYPGLHPK_##Oxidation(M):2"></cvParam>
</SpectrumIdentificationItem>
```

Example for cross-linking:

```
<SpectrumIdentificationItem chargeState="4" experimentalMassToCharge="0.0"
peptide_ref="54600873_54605193_9_1_p1" rank="1" passThreshold="false" id="SII_21_1">
        <PeptideEvidenceRef peptideEvidence_ref="pepevid_psm252621611_pep54605193_protP02768-
        A_target_137"></PeptideEvidenceRef>
        <cvParam cvRef="PSI-MS" accession="MS:1002511" name="Cross-linked spectrum identification item."
        value="21"></cvParam>
        <cvParam cvRef="PSI-MS" accession="MS:1002545" name="The xi result 'Score'."
        value="2.769918944845425"></cvParam>
</SpectrumIdentificationItem>
```

6.76 Element <SpectrumIdentificationItemRef>

Definition: Reference(s) to the SpectrumIdentificationItem element(s) that support the given PeptideEvidence element. Using these references it is possible to indicate which spectra were actually accepted as evidence for this peptide identification in the given protein.

Type: SpectrumIdentificationItemRefType

Attributes:

Attribute Name	Data Type	Use	Definition
spectrumIdentificationItem_ref	xsd:string	required	A reference to the SpectrumIdentificationItem element(s).

Subelements: none

Example Context:

```
<SpectrumIdentificationItemRef
spectrumIdentificationItem_ref="SII_1000_1"></SpectrumIdentificationItemRef>
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001591" name="anchor protein"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1001593" name="group member with undefined relationship OR
ortholog protein"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002676" name="protein-pair-level global FDR"
value="0.a:null:1.0:true"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002677" name="residue-pair-level global FDR"
value="0.a:58:0.04716981132075472:true"></cvParam>
```

```
<cvParam cvRef="PSI-MS" accession="MS:1002415" name="protein group passes threshold"
value="true"></cvParam>
<cvParam cvRef="PSI-MS" accession="MS:1002404" name="count of identified protein"
value="2"></cvParam>
```

6.77 Element <SpectrumIdentificationList>

Definition: Represents the set of all search results from SpectrumIdentification.

Type: SpectrumIdentificationListType

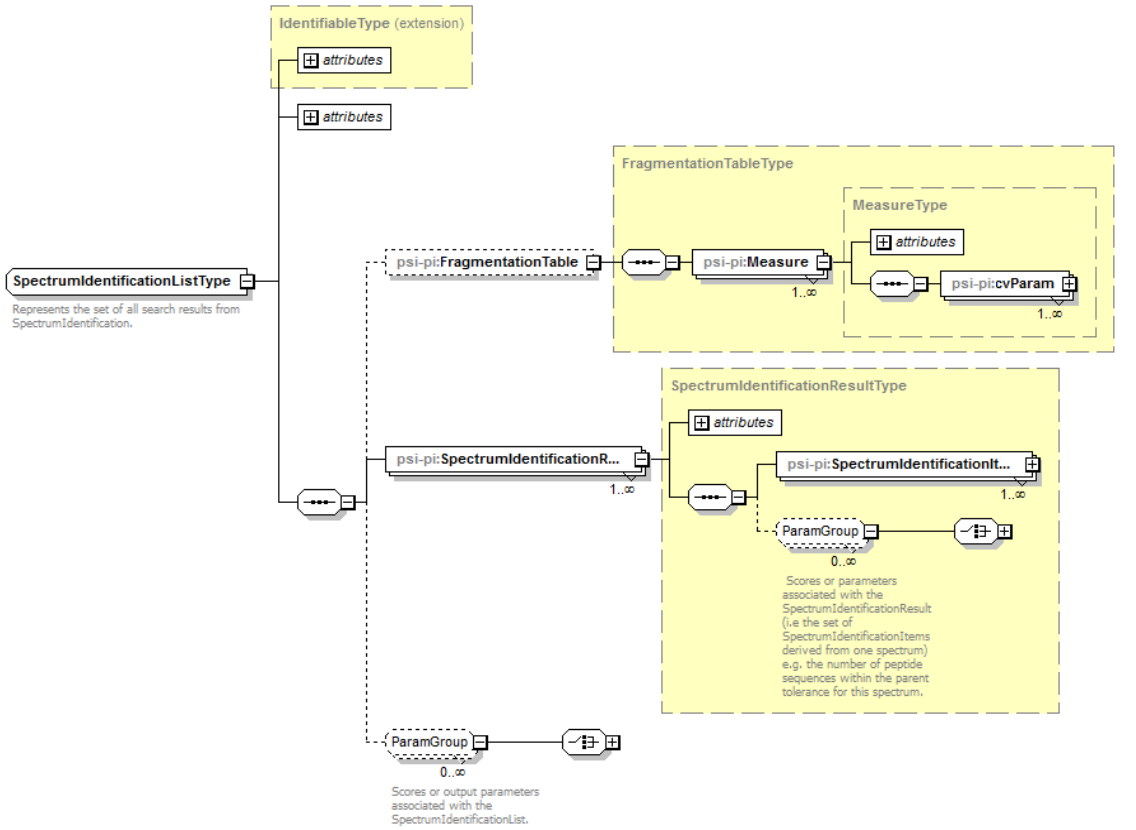
Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
numSequencesSearched	xsd:long	optional	The number of database sequences searched against. This value should be provided unless a de novo search has been performed.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
FragmentationTable	0	1	Contains the types of measures that will be reported in generic arrays for each SpectrumIdentificationItem e.g. product ion m/z, product ion intensity, product ion m/z error
SpectrumIdentificationResult	1	unbounded	All identifications made from searching one spectrum. For PMF data, all peptide identifications will be listed underneath as SpectrumIdentificationItems. For MS/MS data, there will be ranked SpectrumIdentificationItems corresponding to possible different peptide IDs.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Graphical Context:



Example Context:

```
<SpectrumIdentificationList xmlns="http://psidev.info/psi/pi/mzIdentML/1.2" id="SII_LIST_1">
  <SpectrumIdentificationResult spectrumID="index=6451" spectraData_ref="SD_COMBINED_SE_0"
id="SIR_8947">
    <SpectrumIdentificationItem chargeState="2" experimentalMassToCharge="679.817322"
calculatedMassToCharge="679.818488" peptide_ref="AVMDDFAAFVEK_##Oxidation(M):3" rank="1"
passThreshold="false" id="SIR_8947_SII_1">
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000401820|p:known_378_389"></PeptideEvidenceRef>
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000421027|p:putative_420_431"></PeptideEvidenceRef>
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000483421|p:known_357_368"></PeptideEvidenceRef>
      <PeptideEvidenceRef
peptideEvidence_ref="AVMDDFAAFVEK_generic|A_ENSP00000480485|p:known_357_368"></PeptideEvidenceRef>
  ...
</SpectrumIdentificationList>
```

6.78 Element <SpectrumIdentificationProtocol>

Definition: The parameters and settings of a SpectrumIdentification analysis.

Type: SpectrumIdentificationProtocolType

Attributes:

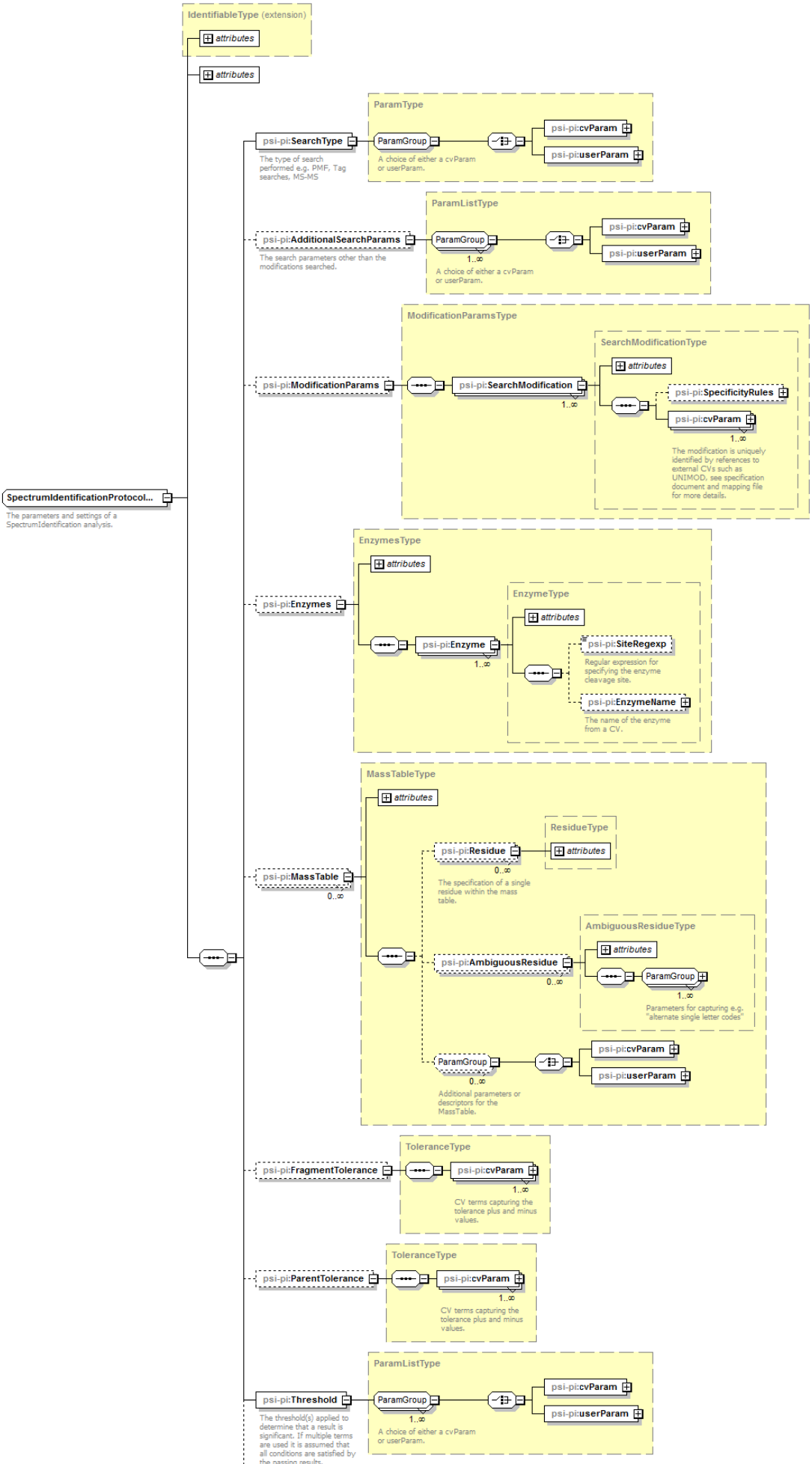
Attribute Name	Data Type	Use	Definition
analysisSoftware_ref	xsd:string	required	The search algorithm used, given as a reference to the SoftwareCollection section.
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition

SearchType	1	1	The type of search performed e.g. PMF, Tag searches, MS-MS
AdditionalSearchParams	0	1	The search parameters other than the modifications searched.
ModificationParams	0	1	The specification of static/variable modifications (e.g. Oxidation of Methionine) that are to be considered in the spectra search.
Enzymes	0	1	The list of enzymes used in experiment
MassTable	0	unbounded	The masses of residues used in the search.
FragmentTolerance	0	1	The tolerance of the search given as a plus and minus value with units.
ParentTolerance	0	1	The tolerance of the search given as a plus and minus value with units.
Threshold	1	1	The threshold(s) applied to determine that a result is significant. If multiple terms are used it is assumed that all conditions are satisfied by the passing results.
DatabaseFilters	0	1	The specification of filters applied to the database searched.
DatabaseTranslation	0	1	A specification of how a nucleic acid sequence database was translated for searching.

Graphical Context:



http://www.pside

Example Context:

```
  <SpectrumIdentificationProtocol id="SIP_10589554385233790425"
analysisSoftware_ref="SOF_10581839310406754333">
    <SearchType>
      <cvParam accession="MS:1001083" cvRef="PSI-MS" name="ms-ms search"/>
    </SearchType>
    <AdditionalSearchParams>
      <cvParam accession="MS:1002494" cvRef="PSI-MS" name="cross-linking search"/>
      <userParam name="input_consensusXML" unitName="xsd:string" value="leitner004.consensusXML"/>
  ...
</SpectrumIdentificationProtocol>
```

6.79 Element <SpectrumIdentificationResult>

Definition: All identifications made from searching one spectrum. For PMF data, all peptide identifications will be listed underneath as SpectrumIdentificationItems. For MS/MS data, there will be ranked SpectrumIdentificationItems corresponding to possible different peptide IDs.

Type: SpectrumIdentificationResultType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.
spectraData_ref	xsd:string	required	A reference to a spectra data set (e.g. a spectra file).
spectrumID	xsd:string	required	The locally unique id for the spectrum in the spectra data set specified by SpectraData_ref. External guidelines are provided on the use of consistent identifiers for spectra in different external formats.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SpectrumIdentificationItem	1	unbounded	An identification of a single (poly)peptide, resulting from querying an input spectra, along with the set of confidence values for that identification. PeptideEvidence elements should be given for all mappings of the corresponding Peptide sequence within protein sequences.
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	0	unbounded	A single user-defined parameter.

Example Context:

```
<SpectrumIdentificationResult spectrumID="index=7665" spectraData_ref="SD_COMBINED_SE_0"
id="SIR_7191">
  <SpectrumIdentificationItem chargeState="4" experimentalMassToCharge="1123.974121"
calculatedMassTo
Charge="1123.968707"
peptide_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_##Carbamidomethyl(C):1##Carba
midomethyl(C):3##Carba
midomethyl(C):12##Carbamidomethyl(C):18##Carbamidomethyl(C):25##Carbamidomethyl(C):31##Ammonia-
loss(C):
1" rank="1" passThreshold="false" id="SIR_7191_SII_1">
    <PeptideEvidenceRef
peptideEvidence_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_generic|A_ENSP00000376692_REVERSED|p:
novel_575_612"></PeptideEvidenceRef>
    <PeptideEvidenceRef
peptideEvidence_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_generic|B_GENSCAN00000036974_REVERSED|p:
genscan_494_531"></PeptideEvidenceRef>
    <PeptideEvidenceRef
peptideEvidence_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_generic|A_ENSP00000471297_REVERSED|p:
putative_641_678"></PeptideEvidenceRef>
    <PeptideEvidenceRef
peptideEvidence_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_generic|A_ENSP00000319883_REVERSED|p:
known_633_670"></PeptideEvidenceRef>
```

```
    <PeptideEvidenceRef
peptideEvidence_ref="CRCQYSGVNNLCHTSSHCPNQGSTCENVDTCLKPDEPK_generic|A_ENSP00000472280_REVERSED|p:
putative_622_659"></PeptideEvidenceRef>
  ...
</SpectrumIdentificationResult>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/AnalysisData/SpectrumIdentificationList/SpectrumIdentificationResult
MAY supply a *child* term of MS:1001405 (spectrum identification result details) one or more times
  e.g.: MS:1000016 (scan start time)
  e.g.: MS:1000796 (spectrum title)
  e.g.: MS:1000797 (peak list scans)
  e.g.: MS:1000798 (peak list raw scans)
  e.g.: MS:1000903 (product ion series ordinal)
  e.g.: MS:1000904 (product ion m/z delta)
  e.g.: MS:1000926 (product interpretation rank)
  e.g.: MS:1001030 (number of peptide seqs compared to each spectrum)
  e.g.: MS:1001035 (date / time search performed)
  e.g.: MS:1001036 (search time taken)
  et al.
```

6.80 Element <SpectrumIDFormat>

Definition: The format of the spectrum identifier within the source file

Type: SpectrumIDFormatType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	A single entry from an ontology or a controlled vocabulary.

Example Context:

```
      <SpectrumIDFormat>
         <cvParam accession="MS:1000774" cvRef="PSI-MS" name="multiple peak list nativeID
format"/>
      </SpectrumIDFormat>
```

cvParam Mapping Rules:

```
Path /MzIdentML/DataCollection/Inputs/SpectraData/SpectrumIDFormat
MUST supply a *child* term of MS:1000767 (native spectrum identifier format) only once
  e.g.: MS:1000768 (Thermo nativeID format)
  e.g.: MS:1000769 (Waters nativeID format)
  e.g.: MS:1000770 (WIFF nativeID format)
  e.g.: MS:1000771 (Bruker/Agilent YEP nativeID format)
  e.g.: MS:1000772 (Bruker BAF nativeID format)
  e.g.: MS:1000773 (Bruker FID nativeID format)
  e.g.: MS:1000774 (multiple peak list nativeID format)
  e.g.: MS:1000775 (single peak list nativeID format)
  e.g.: MS:1000776 (scan number only nativeID format)
  e.g.: MS:1000777 (spectrum identifier nativeID format)
  et al.
MUST supply a *child* term of MS:1001529 (spectra data details) only once
  e.g.: MS:1001530 (mzML unique identifier)
  e.g.: MS:1001531 (spectrum from ProteinScape database nativeID format)
  e.g.: MS:1001532 (spectrum from database string nativeID format)
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1000774" name="multiple peak list nativeID
format"></cvParam>
```

6.81 Element <SubSample>

Definition: References to the individual component samples within a mixed parent sample.

Type: SubSampleType

Attributes:

Attribute Name	Data Type	Use	Definition
sample_ref	xsd:string	required	A reference to the child sample.

Subelements: none

Example Context:

6.82 Element <SubstitutionModification>

Definition: A modification where one residue is substituted by another (amino acid change).

Type: SubstitutionModificationType

Attributes:

Attribute Name	Data Type	Use	Definition

avgMassDelta	xsd:double	optional	Atomic mass delta considering the natural distribution of isotopes in Daltons. This should only be reported if the original amino acid is known i.e. it is not "X"
location	xsd:int	optional	Location of the modification within the peptide - position in peptide sequence, counted from the N-terminus residue, starting at position 1. Specific modifications to the N-terminus should be given the location 0. Modification to the C-terminus should be given as peptide length + 1.
monoisotopicMassDelta	xsd:double	optional	Atomic mass delta when assuming only the most common isotope of elements in Daltons. This should only be reported if the original amino acid is known i.e. it is not "X"
originalResidue	xsd:string with restriction `[ABCDEFGHIJKLMNOPQRSTUVWXYZ?\-]{1}`	required	The original residue before replacement.
replacementResidue	xsd:string with restriction `[ABCDEFGHIJKLMNOPQRSTUVWXYZ?\-]{1}`	required	The residue that replaced the originalResidue.

Subelements: none

Example Context:

```
<SubstitutionModification originalResidue="X" replacementResidue="I" location="10" />
```

6.83 Element <Threshold>

Definition:

Depending on context:
1: The threshold(s) applied to determine that a result is significant. If multiple terms are used it is assumed that all conditions are satisfied by the passing results.
2: The threshold(s) applied to determine that a result is significant. If multiple terms are used it is assumed that all conditions are satisfied by the passing results.

Type: ParamListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	A single entry from an ontology or a controlled vocabulary.
userParam	1	unbounded	A single user-defined parameter.

Example Context:

```
      <Threshold>
        <cvParam cvRef="PSI-MS" accession="MS:1001364" name="distinct peptide-level global FDR"
value="1.0"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002350" name="PSM-level global FDR" value="1.0"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002567" name="phosphoRS score threshold"
value="95.0"/>
        <cvParam cvRef="PSI-MS" accession="MS:1002557" name="D-Score threshold" value="95.0"/>
      </Threshold>
```

cvParam Mapping Rules:

```
Path /MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/Threshold
MUST supply a *child* term of MS:1001302 (search engine specific input parameter) one or more
times
```

```
  e.g.: MS:1001005 (SEQUEST:CleavesAt)
  e.g.: MS:1001007 (SEQUEST:OutputLines)
  e.g.: MS:1001009 (SEQUEST:DescriptionLines)
  e.g.: MS:1001026 (SEQUEST:NormalizeXCorrValues)
  e.g.: MS:1001028 (SEQUEST:SequenceHeaderFilter)
  e.g.: MS:1001032 (SEQUEST:SequencePartialFilter)
  e.g.: MS:1001037 (SEQUEST:ShowFragmentIons)
  e.g.: MS:1001038 (SEQUEST:Consensus)
  e.g.: MS:1001042 (SEQUEST:LimitTo)
  e.g.: MS:1001046 (SEQUEST:sort by dCn)
  et al.
MUST supply a *child* term of MS:1001153 (search engine specific score) one or more times
  e.g.: MS:1001154 (SEQUEST:probability)
  e.g.: MS:1001155 (SEQUEST:xcorr)
  e.g.: MS:1001156 (SEQUEST:deltacn)
  e.g.: MS:1001157 (SEQUEST:sp)
  e.g.: MS:1001158 (SEQUEST:Uniq)
  e.g.: MS:1001159 (SEQUEST:expectation value)
  e.g.: MS:1001160 (SEQUEST:sf)
  e.g.: MS:1001161 (SEQUEST:matched ions)
  e.g.: MS:1001162 (SEQUEST:total ions)
  e.g.: MS:1001163 (SEQUEST:consensus score)
  et al.
MUST supply term MS:1001494 (no threshold) only once
MUST supply term MS:1001448 (pep:FDR threshold) only once
Path /MzIdentML/AnalysisProtocolCollection/ProteinDetectionProtocol/Threshold
MUST supply a *child* term of MS:1001302 (search engine specific input parameter) one or more
times
  e.g.: MS:1001005 (SEQUEST:CleavesAt)
  e.g.: MS:1001007 (SEQUEST:OutputLines)
  e.g.: MS:1001009 (SEQUEST:DescriptionLines)
  e.g.: MS:1001026 (SEQUEST:NormalizeXCorrValues)
  e.g.: MS:1001028 (SEQUEST:SequenceHeaderFilter)
  e.g.: MS:1001032 (SEQUEST:SequencePartialFilter)
  e.g.: MS:1001037 (SEQUEST:ShowFragmentIons)
  e.g.: MS:1001038 (SEQUEST:Consensus)
  e.g.: MS:1001042 (SEQUEST:LimitTo)
  e.g.: MS:1001046 (SEQUEST:sort by dCn)
  et al.
MUST supply a *child* term of MS:1001153 (search engine specific score) one or more times
  e.g.: MS:1001154 (SEQUEST:probability)
  e.g.: MS:1001155 (SEQUEST:xcorr)
  e.g.: MS:1001156 (SEQUEST:deltacn)
  e.g.: MS:1001157 (SEQUEST:sp)
  e.g.: MS:1001158 (SEQUEST:Uniq)
  e.g.: MS:1001159 (SEQUEST:expectation value)
  e.g.: MS:1001160 (SEQUEST:sf)
  e.g.: MS:1001161 (SEQUEST:matched ions)
  e.g.: MS:1001162 (SEQUEST:total ions)
  e.g.: MS:1001163 (SEQUEST:consensus score)
  et al.
MUST supply term MS:1001447 (prot:FDR threshold) only once
MUST supply term MS:1001494 (no threshold) only once
```

Example cvParams:

```
<cvParam cvRef="PSI-MS" accession="MS:1001494" name="no threshold"></cvParam>
<cvParam accession="MS:1001874" cvRef="PSI-MS" value="0.01" name="FDRScore"/>
<cvParam accession="MS:1002351" cvRef="PSI-MS" value="0.01" name="PSM-level local FDR"/>
<cvParam accession="MS:1001316" cvRef="PSI-MS" value="0.05" name="Mascot:SigThreshold"/>
<cvParam cvRef="PSI-MS" accession="MS:1001364" name="distinct peptide-level global FDR"
value="1.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002350" name="PSM-level global FDR" value="1.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002567" name="phosphoRS score threshold" value="95.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002557" name="D-Score threshold" value="95.0"/>
<cvParam cvRef="PSI-MS" accession="MS:1002369" name="protein group-level global FDR"
value="0.01"/>
```

6.84 Element <TranslationTable>

Definition: The table used to translate codons into nucleic acids e.g. by reference to the NCBI translation table.

Type: TranslationTableType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xsd:string	required	An identifier is an unambiguous string that is unique within the scope (i.e. a document, a set of related documents, or a repository) of its use.
name	xsd:string	optional	The potentially ambiguous common identifier, such as a human-readable name for the instance.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	A single entry from an ontology or a controlled vocabulary.

Example Context:

cvParam Mapping Rules:

```
Path
/MzIdentML/AnalysisProtocolCollection/SpectrumIdentificationProtocol/DatabaseTranslation/Translation
Table
MUST supply term MS:1001410 (translation start codons) only once
MUST supply term MS:1001025 (translation table) only once
MUST supply term MS:1001423 (translation table description) only once
```

6.85 Element <userParam>

Definition: In case more information about the ions annotation has to be conveyed, that has no fit in FragmentArray. Note: It is suggested that the value attribute takes the form of a list of the same size as FragmentArray values. However, there is no formal encoding and it cannot be expeceted that other software will process or impart that information properly.

Type: UserParamType

Attributes:

Attribute Name	Data Type	Use	Definition
name	xsd:string	required	The name of the parameter.
type	xsd:string	optional	The datatype of the parameter, where appropriate (e.g.: xsd:float).
unitAccession	xsd:string	optional	An accession number identifying the unit within the OBO foundry Unit CV.
unitCvRef	xsd:string	optional	If a unit term is referenced, this attribute MUST refer to the CV 'id' attribute defined in the cvList in this file.
unitName	xsd:string	optional	The name of the unit.
value	xsd:string	optional	The user-entered value of the parameter.

Subelements: none

Example Context:

```
<userParam value="VLENAEGDR; ASSGLNEDEIQK; MQELAQVSQK; KTAEDYLGEPVTEAVITVPAYFNDAQR; SLGQFNLDGINPAPR;
MPMVQK; IIAADNGDAWVEVK; DVSIMPFK; KDVNPDEAVAIGAAVQGGVLTGDVK; KFEELVQTR; NDPLAMQR; VAEFFGK;
QVEEAGDKLPADDK; MAPPQISAEVLKK; KQVEEAGDKLPADDK; LINYLVEEFK; MAPPQISAEVLK; QAVTNPQNTLFAIK;
TFEVLATNGDTHLGGEDFDSR; VALQDAGLSVSDIDDVILVGGQTR; FQDEEVQR" name="unique peptides"/>
```

7. Specific Comments on schema

In this section, several points of documentation are elaborated beyond the core specification in Section 6.

7.1 File extension and compression

It is noted that standard file compression algorithms greatly reduce the mzIdentML file sizes, speeding up file transfers and uploads / downloads. It is also noted that software implementing mzIdentML import or export will be expected to benefit in performance from working with compressed mzIdentML, since the compression and decompression algorithms are expected to give significant performance gains over disk access times for non-compressed files. As such, it is RECOMMENDED that mzIdentML files are compressed using gzip from all software that exports mzIdentML and software that imports SHOULD be expected to read gzipped files, as well as native (non-compressed) mzIdentML files. The file extension for native mzIdentML files SHOULD be ".mzid" and for compressed files SHOULD be "mzid.gz".

7.2 Referencing elements within the document

A number of elements within the schema have an attribute which is used to reference an element elsewhere in the file using the unique identifier of the referenced element. These attributes are named following the convention: "[elementName]_ref". The uniqueness of the value in the "id" attribute of elements is validated using xsd:key, and the integrity of the reference is validated using xsd:keyref, defined within the schema.

7.3 Searches against nucleotide sequences

The “seq” attribute on <DBSequence> SHOULD contain the nucleic acid sequence if a nucleic acid database was searched (rather than up to six translated sequences). <Peptide> represents the identified amino acid sequence (including modifications) and, as such, the <peptideSequence> elements SHOULD store the translated amino acid sequences. <PeptideEvidence> contains the *DBSequence_Ref* together with the translation frame and a *TranslationTable_Ref* attribute (see below). The *Peptide_Ref* is done in <SpectrumIdentificationItem> as in the case for an amino acid database. If protein detection is performed, there are <PeptideHypothesis> elements referencing <PeptideEvidence> elements from <SpectrumIdentificationItem> sections. For clarification, see the example instance document for a nucleic acid search (Section 5.3).

In the <SpectrumIdentificationProtocol>, <TranslationTable> is used to specify how nucleic acid sequences are translated into amino acid sequences as follows:

```
<DatabaseTranslation frames="1 2 3 -1 -2 -3">
  <TranslationTable id="TT_1" name="Standard">
    <cvParam accession="MS:1001025" name="translation table" cvRef="PSI-MS"
value="FFLLSSSSYY**CC*WLLLLPPPPHHQQRRRRIIIMTTTTNNKKSSRRVVVVAAAADDEEGGGG" />
    <cvParam accession="MS:1001410" name="translation start codons" cvRef="PSI-MS" value="---M---------
------M---------------M----------------------------" />
    <cvParam accession="MS:1001423" name="translation table description" cvRef="PSI-MS"
value="http://www.ncbi.nlm.nih.gov/Taxonomy/taxonomyhome.html/index.cgi?chapter=cgencodes#SG1" />
  </TranslationTable>
  <TranslationTable id="TT_2" name="Vertebrate Mitochondrial">
    <cvParam accession="MS:1001025" name="translation table" cvRef="PSI-MS"
value="FFLLSSSSYY**CCWWLLLLPPPPHHQQRRRRIIMMTTTTNNKKSS**VVVVAAAADDEEGGGG" />
    <cvParam accession="MS:1001410" name="translation start codons" cvRef="PSI-MS" value="-------------
------------------MMMM---------------M------------" />
    <cvParam accession="MS:1001423" name="translation table description" cvRef="PSI-MS"
value="http://www.ncbi.nlm.nih.gov/Taxonomy/taxonomyhome.html/index.cgi?chapter=cgencodes#SG2" />
  </TranslationTable>
```

The attribute “frames” specifies which frames are considered and one or more translation tables can be specified using CV parameters. The translation table is defined here: http://www.ncbi.nlm.nih.gov/IEB/ToolBox/SDKDOCS/SEQFEAT.HTML#_Genetic_Codes:

"The genetic codes themselves are arrays of 64 amino acid codes. The index to the position in the array of the amino acid is derived from the codon by the following method:

index = (base1 16) + (base2 4) + (base3 1)
where T=0, C=1, A=2, G=3”

The same encoding technique is used to specify start codons. Alphabet names are prefixed with "s" (e.g. sncbieaa) to indicate start codon arrays. Each cell of a start codon array contains either the gap code ("-" for ncbieaa) or an amino acid code if it is valid to use the codon as a start codon. Currently all starts are set to code for methionine, since it has never been convincingly demonstrated that a protein can start with any other amino acid. However, if other amino acids are shown to be used as starts, this structure can easily accommodate that information.

For each peptide, the frame and translation table should be specified in the <PeptideEvidence> element:

```
<PeptideEvidence id=”1” TranslationTable_ref="TT_1" frame="1" />
```

7.4 Reporting peptide and protein identifications passing a significance threshold

The elements <SpectrumIdentificationItem> and <ProteinDetectionHypothesis> have a mandatory Boolean attribute *passThreshold* that allows a file producer to indicate that an identification has passed a given threshold or that it has been manually validated. Depending on the intended purpose of the file, the file producer MAY wish to report a number of identifications that fall below the given significance threshold, for example to allow global statistical analyses to be performed which are not possible if only identifications passing the threshold are reported. Thresholds for peptide-spectrum matches or for protein identification should be encoded as instances of <cvParam> within <SpectrumDetectionProtocol> or <ProteinDetectionProtocol> as follows. If the file producer does not want to indicate that a threshold has been set, all identifications MUST have passThreshold = “true” and the “no threshold” CV term should be given within the protocols.

```
<SpectrumIdentificationProtocol id="SIP" AnalysisSoftware_ref="AS_mascot_server">
        …
    <Threshold>
      <cvParam accession="MS:1001316" name="mascot:SigThreshold" cvRef="PSI-MS" value="0.05"/>
    </Threshold>


<ProteinDetectionProtocol id="PDP_MascotParser_1"  AnalysisSoftware_ref="AS_mascot_parser">
        …
  <Threshold>
    <cvParam accession="MS:1001316" name="mascot:SigThreshold" cvRef="PSI-MS" value="0.05"/>
  </Threshold>
```

The reporting of significance thresholds at the PSM and peptide level (mzIdentML 1.2) is explained in section 5.3.3. Reporting of threshold for modification position (also mzIdentML 1.2) is explained in section 5.3.4.

7.5 Using decoy databases to set different thresholds of false discovery rate

mzIdentML supports the reporting of searches against decoy databases, constructed and searched using many of the currently known methods. A <SpectrumIdentificationItem> can be marked as matching a decoy peptide using the *isDecoy* attribute of the referenced <PeptideEvidence> element, thus allowing the false discovery rate to be calculated across an entire file. The *DBSequence_Ref* references the decoy protein record.

Implementers of the format SHOULD report the peptide identifications that pass the threshold they wish to communicate to a consumer of the data. For example, a threshold could be set by p-value, false discovery rate, by a native search engine score (or a more complex system documented with CV terms in <Threshold>), and those peptides reported (passing the threshold) are used to determine which proteins have been detected. It is not guaranteed that a consumer of an mzIdentML file will be able to calculate other results, or global false discovery rates, using different thresholds from the reported information, although in some circumstances they may be able to, for example, if a user reports the complete output of a search against a target and decoy search.

```
<SearchDatabase location="/localdirectory/18.E_coli_K12_edit.fasta" id="K12_nosignal" name="K12"
numDatabaseSequences="9376" releaseDate="01-2008-08-2008" version="1.0" >
        <FileFormat>
                <cvParam accession="MS:1001348" name="FASTA format" cvRef="PSI-MS"/>
        </FileFormat>
        <DatabaseName>
                <userParam name="18.E_coli_K12_edit.fasta" />
        </DatabaseName>
        <cvParam accession="MS:1001197" name="DB composition target+decoy" cvRef="PSI-MS"/>
        <cvParam accession="MS:1001283" name="decoy DB accession regexp" value="Rnd" cvRef="PSI-MS"/>
        <cvParam accession="MS:1001195" name="decoy DB type reverse" cvRef="PSI-MS"/>
</SearchDatabase>

<SpectrumIdentificationItem passThreshold="false" rank="1"
                        peptide_ref="HAVGGRYSSLLCK__57.0215@C$403;_"
                        experimentalMassToCharge="1448.756" chargeState="2" id="SII_6_1">
                        <PeptideEvidenceRef peptideEvidence_ref="PE6_2_4"/>
            <PeptideEvidence isDecoy="true" post="D" pre="K" end="404"
                start="392" peptide_ref="HAVGGRYSSLLCK__57.0215@C$403;_"
                dBSequence_ref="dbseq_REV_psu|NC_LIV_113200" id="PE6_2_4"/>
               <cvParam accession="MS:1001329" name="OMSSA:pvalue" cvRef="PSI-MS"  value="0.00073351"
/>

…

</SpectrumIdentificationItem>
```

7.6 Database Filter

The format can specify that a sequence database has been filtered, for example based on pI, protein mass, taxonomy or even a set of accession numbers for a second pass search. For example, all animals except mice would be encoded as (NCBI:33208 is metazoa, NCBI:10090 is *Mus musculus*):

```
<DatabaseFilters>
  <Filter>
    <FilterType>
      <cvParam accession="MS:1001020" name="DB filter taxonomy" cvRef="PSI-MS" />
```

```
    </FilterType>
   <Include>
      <cvParam accession="MS:1001467" name="taxonomy: NCBI TaxID" cvRef="PSI-MS" value="33208"/>
   </Include>
   <Exclude>
     <cvParam accession="MS:1001467" name="taxonomy: NCBI TaxID" cvRef="PSI-MS" value="10090"/>
   </Exclude>
   </Filter>
</DatabaseFilters>
```

7.7 Types of parameters and values

There are several types for parameters that are used in the schema:

<ParamListType>: A list (i.e. unbounded number) of <ParamGroup> elements.
<ParamGroup>: A choice between <cvParam> or <userParam> elements.

<ParamType>: A single reference to <ParamGroup>, which allows a choice between either <cvParam> or <userParam> elements at the specified point in the schema.
<cvParamType>: A single entry from an ontology or a CV. Attributes: *accession*, *cvRef*, *name*, *value*, *unitAccession*, *unitName*, *unitCvRef*.
<userParamType>: A single user-defined parameter. Attributes: *name*, *value*, *unitAccession*, *unitName*, *unitCvRef*.

7.8 Reporting fragmentation ions

mzIdentML employs an array type structure to support the reporting of ion types identified in an MS/MS analysis, coupled with CV parameters to retain flexibility in the types of ions that can be reported.

A brief example is given here to explain how these structures should be used where *y11*, *y8* and *y7* have been identified with charge = 2+. First, the types of measures to be reported are given in the <FragmentationTable> using <cvParam> instances. Second, each <SpectrumIdentificationItem> contains an index of values (11, 8 and 7 for each y ion) and parallel arrays that reference back to each <Measure> defined in the <FragmentationTable>. In the example, the *y8* ion has a product ion *m/z* = 436.4, product ion intensity = 11 and product ion *m/z* error = 0.1284 (the second position in the index of each array).

```
<FragmentationTable>
  <Measure id="m_mz">
    <cvParam cvRef="PSI-MS" accession="MS:1001225" name="product ion m/z"/>
  </Measure>
  <Measure id="m_intensity">
    <cvParam cvRef="PSI-MS" accession="MS:1001226" name="product ion intensity"/>
  </Measure>
  <Measure id="m_error">
    <cvParam cvRef="PSI-MS" accession="MS:1001227" name="product ion m/z error"
unitAccession="MS:1000040" unitName="m/z" unitCvRef="PSI-MS"/>
  </Measure>
</FragmentationTable>
…

<IonType index="11 8 7" charge="2">
  <cvParam cvRef="PSI-MS" accession="MS:1001220" name="frag: y ion"/>
  <FragmentArray values="551.3 436.4 380.1 " measure_ref="m_mz"/>
  <FragmentArray values="800 11 46" measure_ref="m_intensity"/>
  <FragmentArray values="0.4752 0.1284 0.3704" measure_ref="m_error"/>
</IonType>
```

7.8.1 Internal fragments and immonium ions

mzIdentML supports the reporting of internal fragment ions, of which an immonium ion is a special case comprising a single side chain (http://www.matrixscience.com/help/fragmentation_help.html). For internal and immonium ions, the index is used in two different ways. Internal fragments are reported using the index structure to identify the start and end of the ion within the sequence. The example shows how the index performs this different role, as it identifies pairs of internal ions: *ya2-5*, *ya3-7*, *ya3-8*, *ya4-8*, *ya5-8*, *ya5-11*, *ya8-11*.

```
<IonType index="2 5 3 7 3 8 4 8 5 8 5 11 8 11" charge="1">
  <FragmentArray values="315.2 388.1 501.4 444.1 342.8 669.901495 412.4 " measure_ref="m_mz"/>
  <FragmentArray values="44 63 10430 75 48 6420 31" measure_ref="m_intensity"/>
```

```
  <FragmentArray values="-0.0027 -0.1191 0.0969 -0.1817 -0.4340 0.4721 0.1082" measure_ref="m_error"/>
  <cvParam cvRef="PSI-MS" accession="MS:1001366" name="frag: internal ya ion"/>
</IonType>
```

For immonium ions, the index is the position of the identified ion within the peptide sequence. If the peptide contains the same amino acid in multiple positions that cannot be distinguished, all positions should be given. Example, where immonium ions have been found matching T and G in the following peptide sequence FGGEENTY (positions 2 or 3, and position 7):

```
<IonType charge="1" index="2 3 7">
  <FragmentArray values="288.2 286.1 387.2 371.127841 " measure_ref="m_mz"/>
  <FragmentArray values="2137 83 656 1663" measure_ref="m_intensity"/>
  <FragmentArray values="0.0260 -0.1125 -0.0602 -0.1011" measure_ref="m_error"/>
  <cvParam cvRef="PSI-MS" accession="MS:1001239" name="frag: immonium ion"/>
</IonType>
```

7.8.2 Encoding Neutral loss fragment ions

The encoding of the identification of neutral loss fragment ions has changed from version 1.1 to version 1.2.0. The CV previously contained an attempt to enumerate all possible neutral losses from all types of fragment ions, leading to a long and incomplete list of possible terms. As such, pairs of CV terms are now allowed in version 1.2.0 to describe both the ion type and the type of neutral loss, as follows:

```
<IonType charge="2" index="3">
        <FragmentArray measure_ref="Measure_MZ" values="165.0899353"/>
        <FragmentArray measure_ref="Measure_Int" values="2058.2841796875"/>
        <FragmentArray measure_ref="Measure_Error" values="0.007899949187986977"/>
        <cvParam cvRef="PSI-MS" accession="MS:1001220" name="frag: y ion"/>
        <cvParam cvRef="PSI-MS" accession="MS:1000336" name="neutral loss" value="H3N"/>
</IonType>
```

7.9 Enzyme definition

The <SpectrumIdentificationProtocol> SHOULD contain a specification of which enzyme (if any) was applied in the search. The element <Enzyme> has optional sub-elements for specifying the <EnzymeName> using a CV term and the cleavage site, using a regular expression. Regular expressions should be encoded following the notation of Perl Compatible Regular Expressions (PCRE regex, http://www.pcre.org, matching the syntax and semantics of Perl version 5). The PSI-MS CV contains terms for the most common enzymes with pre-defined regular expressions (Table 6). If the enzyme used is present in the PSI-MS CV, the term MUST be encoded under <EnzymeName> unless the rule given in the CV does not match that used by the software or if the enzyme used is not present in the CV, in which case the regular expression used MUST be given in the element <SiteRegexp>. If the <EnzymeName> element is used, the regular expression MAY also be provided additionally. For a no enzyme search, (i.e. one where there may be a cleavage at any residue), the CV term MS:1001091 'NoEnzyme' MUST be specified, and the missedCleavages and semiSpecific attributes SHOULD NOT be specified. If two or more enzymes are used, multiple <Enzyme> elements SHOULD be provided rather than trying to build a regular expression covering all cleavage sites. If the software uses a name for an enzyme other than the one specified in the CV, a user param term MAY also be given.

The following guidelines SHOULD be followed when generating regular expressions in an instance document for enzymes not present in the CV: 1) use the PCRE supplied negation syntax for look-ahead and look-behind assertions and 2) use the most compact representation possible for a regex. The start of a match specifies the cleavage point. For example the enzyme trypsin, which cleaves following a K or R residue unless the next residue is P, has the regular expression:

```
(?<=[KR])(?!P)
```

The ?<= is a "zero-width positive look-behind assertion", and [] means one of this character set. So, this rule is to look behind for a K or R. ?! is a zero-width positive look-ahead assertion, and ?!P means any character that is not P. An example of an "N-term" enzyme is Asp-N which cleaves before D or B. This can be described using the PCRE:

```
  (?=[BD])
```

The ?= is a “zero-width positive look-ahead assertion.”

A simple 3 line perl program can be written to test a regular expression:

```
$protein = "ABCDKPEFGHIJKLMNOPQRSTUVWXYZ";
@peptides = split(/(?<=[KR])( ?!P)/, $protein);
print join "\n", @peptides;
```

The program returns:

```
ABCDKPEFGHIJK
LMNOPQR
STUVWXYZ
```

Enzyme Name	Regular expression
Trypsin	(?<=[KR])(?!P)
Arg-C	(?<=R)(?!P)
Asp-N	(?=[BD])
Asp-N_ambic	(?=[DE])
Chymotrypsin	(?<=[FYWL])(?!P)
CNBr	(?<=M)
Formic_acid	((?<=D))|((?=D))
Lys-C	(?<=K)(?!P)
Lys-C/P	(?<=K)
PepsinA	(?<=[FL])
TrypChymo	(?<=[FYWLKR])(?!P)
Trypsin/P	(?<=[KR])
V8-DE	(?<=[BDEZ])(?!P)
V8-E	(?<=[EZ])(?!P)
Leukocyte elastase	(?<=[ALIV])(?!P)
Proline endopeptidase	(?<=[HKR]P)(?!P)
Glutamyl endopeptidase	(?<=[^E]E)
2-iodobenzoate	(?<=W)

Table 6. Common enzymes and the cleavage site specified as regular expressions as represented in the PSI-MS CV.

7.10 Unknown modifications

In version 1.1.0 onwards of mzIdentML there has been a change with respect to how “unknown modifications” (i.e. those not present in an allowed CV) are reported on peptides. In version 1.0, <userParam> elements were allowed on <Peptide> to capture these modifications. In version 1.1.0 onwards, only <cvParam> elements can be given on <Peptide> and a term “unknown modification” has been added to the PSI-MS CV. This term MUST only be used if the identified modification is not present in Unimod (or other allowed CV such as PSI-MOD, although PSI-MOD is now deprecated), according to the identity of the residue modified and the delta mass, within the parent tolerance specified in the search. The semantic validator will check any uses of the “unknown modification” term (MS:1001460) and reject files if the modification is present in Unimod.

8. Conclusions

This document contains the specifications for using the mzIdentML format to represent results from peptide and protein identification pipelines, in the context of a proteomics investigation. This specification, in conjunction with the XML Schema, mapping file and CV constitute a proposal for a standard from the Proteomics Standards Initiative. These artefacts are currently undergoing the PSI document process standardization process, which will result in a standard officially sanctioned by PSI.

9. Authors and Contributors

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