PSI Recommendation
PSI Mass Spectrometry Working Group

Eric W. Deutsch, Institute for Systems Biology
Matthew Chambers, Vanderbilt University
Steffen Neumann, IPB Halle
Fredrik Levander, Lund University
et al.

December 2011

TraML: Transitions Markup Language

Status of This Document

This document presents the draft specification for the TraML (Transitions Markup Language) data format developed by the Institute for Systems Biology and the HUPO Proteomics Standards Initiative. Distribution is unlimited.

Version of This Document

The current version of this document is: Version 1.0.0.0; December 12, 2011.

The version of this document matches the schema version with one trailing decimal point and integer to denote specification documentation updates that do not correspond to a schema update. Thus the version numbers correspond to:
majorVersion.minorVersion.maintenanceVersion.documentationOnlyUpdateVersion.
Every new release of the specification document will be available in the PSI code repository.

Change Log since 0.0.0.0

- 2009-01-29: Very early draft version 0.1.1 still under development
- 2009-08-10: Draft version 0.9.0 released for comment
- 2009-10-27: Draft version 0.9.1 released for comment
- 2009-11-19: Draft version 0.9.2 released for comment
- 2010-01-05: Draft version 0.9.3 released for comment
- 2010-03-31: Draft version 0.9.4 released for comment
- 2010-04-05: Minor edits to spec doc. No format change.
- 2011-08-23: Draft version 0.9.5 released for comment
- 2011-12-12: Official version 1.0.0 released after addressing journal article reviewer comments and adding userParam element to conform with other PSI formats

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 Mass Spectrometry Working Group (PSI-MS WG) develops standards for use in mass spectrometry analysis. This document presents information to the mass spectrometry community about the modelling in XML of transitions used by mass spectrometric analysis of biomolecular compounds. These transitions are designed to be optimal signatures that allow mass spectrometers to monitor for the presence of these compounds. This XML format is designed to replace the common use of over a half dozen different tab-separated-value formats by different applications. This document should be read in conjunction with a kit of auxiliary files, including the example instance documents, the controlled vocabulary file, and the xsd file. All files related to this proposal are available for download at http://psidev.info/traml.

Contents

1. Introduction

1.1 Background

Mass spectrometry (MS) is a popular method to analyse bio-molecules by measuring the intact mass-to-charge ratios of their in-situ generated ionised forms or the mass-to-charge ratios of in situ-generated fragments of these ions. MS enables proteomics experiments in which thousands of proteins can be identified and quantified in complex samples.

Targeted proteomics via selected reaction monitoring (SRM) is a powerful technique affording better specificity and sensitivity than other methods. However, it does require more preparation in the form of selecting appropriate signatures, called transitions, for the proteins and peptides that are to be targeted. There are a growing number of software programs and resources for selecting optimal transitions, but the exchange of such transitions is hindered by a lack of a standard format.

We have developed a new format, called TraML (Transitions Markup Language), for encoding transition lists and the metadata associated with these lists. The format is encoded using Extensible Markup Language (XML) and this document provides a detailed specification of the format.

1.2 Previous formats

The formats currently used for storage and exchange of transitions are a variety of non-standardized tab-delimited or Excel-based files. The columns vary from lab to lab or project to project, and change over time. Instrument vendors accept a variety of different formats, but none are standard or necessarily applicable to other instruments. This is the situation that TraML aims to remedy.

1.3 Use cases

TraML is designed as a format to encode information needed to configure and perform targeted MS experiments. This includes SRM/MRM (selected/multiple reaction monitoring) experiments, especially for quantitation, and inclusion-list-based MS/MS (tandem mass spectrometry) experiments, e.g. for identification. The following subsections describe a variety of intended uses of the TraML format.

1.3.1 SRM experiments

A quantification experiment is typically performed on a set of known proteins or compounds, and for each, the instrument measures one or more transitions (defined as precursor m/z and product m/z pairs).

The selection of transitions can be accomplished in a variety of ways, including retrieval from spectral libraries or prediction from sequences, using desktop software applications or web-based resources. Detailed metadata describing how the transitions were selected should be stored. Those transitions MAY be validated (measured) on one or more instruments, and the analytical configuration(s) are stored with the transition. Scheduled SRM is commonly used to refer to the addition of a retention time component to each transition so that the transition is not monitored over an entire run, but rather just the time window within a run within which the peptide or compound is known to elute.

The TraML documents can be translated into vendor-dependent files suitable to create/configure an SRM/MRM experiment on a Triple-Quad, Ion Trap or other suitable mass spectrometer using external software. Ideally, the machine configuration can be obtained or derived from the set of validated transitions.

1.3.2 Targeted Inclusion-list MS/MS experiments

A TraML file can describe a targeted MS/MS (or MS^n) experiment via the specification of targets as retention time windows and precursor mass, both through inclusion and exclusion lists.

The definition for targets for the inclusion/exclusion lists has to be created based on a preselection of known (un-)desired compounds or proteins retrieved from databases, or (potentially unidentified) precursor mass and retention time windows measured during preceding profiling experiments. Known proteins and compounds are annotated as well.

The TraML documents can then be translated into vendor-dependent files suitable to create/configure an MS/MS experiment on a Triple-Quad, QqTOF, Ion Trap or other suitable mass spectrometer. Ideally, the machine configuration can be obtained or derived from the set of validated transitions.

The list of inclusion/exclusion list targets is unrelated to the list of transitions, and in most cases, a single TraML document will only contain either a transition list or a inclusion/exclusion list. Although the format is primarily intended for transition lists, the ability to encode inclusion/exclusion targets was added because of the similarity of datatype and since there is no alternative format for such data.

1.3.3 Support for all current TSV formats

It is intended as a use case that all current tab-delimited transition formats, no matter how simple, can be converted to a valid TraML document. TraML is able to encode very rich annotation of transitions, but due to mostly optional elements, can also encode very simple ones.

1.3.4 Retention time optimization

There may be stored with the compounds one or more instances of measured or predicted retention times. They can be interpreted as input-, archived- or generic retention times. One step in the processing of a TraML file is the selection/merging (and optionally calibrating) of these retention times into the "local" retention time under the target- and transition lists.

This local retention time SHOULD be used for the export to the instrument method in an export / conversion into e.g. a TSV file that the instrument can import.

1.3.5 Neutral loss scans not supported

A TraML file cannot describe neutral loss scans. There is no <neutralLoss> as an alternative to the <precursor><product> pair. This may be desirable in the future and will be considered for future releases if there is a demonstrated need. Note that transitions that monitor a product ion with a neutral loss are certainly supported.

1.4 Design Philosophy

The design of TraML uses many of the design concepts and constructs of mzML and mzIdentML. This reuse will simplify and accelerate the implementation of tools that support TraML as there was already existing code for several components first developed for mzML.

Following the design of mzML and mzIdentML, the format is defined by three components: 1) the XML schema (xsd file); 2) the controlled vocabulary file, which provides terms and definitions that are useful to describe information; and 3) a mapping file that allows semantic validation of the use of controlled vocabulary terms in TraML.

We use the standard PSI semantic validator (used by several of the other PSI formats), which enforces many rules as to how controlled vocabulary terms are used, not only making sure that the terms are in the CV, but also that the correct terms are used in the correct location in the document and the required terms are present the correct number of times. This allows greater flexibility in the schema, but enforces order in how the CV terms are used. This will require the discipline of using the semantic validator, not just an XML validator. The result is that new technologies or information can be accommodated with adjustments to the controlled vocabulary and validator, not to the schema.

The remainder of this document is structured as follows. Section 2.1 describes a number of concepts and information about the implementation of mzML, including aspects of terminology, design issues, the controlled vocabulary, etc. The schema model itself is presented in XML schema (XSD) notation in Section 3; some conclusions are presented in Section 4.

2. Implementation of the Format

2.1 Concepts and Terminology

This document assumes familiarity with one data modelling notation, namely XML Schema (www.w3.org/XML/Schema). Models are described using XML schema.

The keywords “MUST,” “MUST NOT,” “REQUIRED,” “SHALL,” “SHALL NOT,” “SHOULD,” “SHOULD NOT,” “RECOMMENDED,” “MAY,” and “OPTIONAL” are to be interpreted as described in RFC-2119 (Bradner 1997).

2.2 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 MS* (http://www.psidev.info/index.php?q=node/91) The “Minimum Information About a Proteomics Experiment: Mass Spectrometry” module document identifies the minimum information required to report the use of a mass spectrometer in a proteomics experiment. The mzML format has been designed to encode the requirements specified in MIAPE MS. At present, there is no module for MIAPE that corresponds to the information encoded in TraML. This shortcoming may be addressed later if there is support for it.
2. *mzML* (http://www.psidev.info/index.php?q=node/257). The mzML format is designed to encode all relevant information from the output of a run on a mass spectrometer. TraML, however, is solely designed as the input for a targeted mass spectrometry run. Some future version of mzML may allow a TraML document to be embedded in it, but for now TraML and mzML documents can be used complementarily.
3. *mzIdentML* (http://www.psidev.info/index.php?q=node/319). The mzIdentML specification has been developed by the PSI as a standard to capture the output of search engines that assign mass spectra to protein or peptide sequences. It is FuGE-based and will provide a UML model as well as an XML schema. This document does not assume familiarity with mzIdentML or FuGE.

2.2.1 The PSI Mass Spectrometry Controlled Vocabulary (CV)

A comprehensive collection of terms has been defined (mostly extracted from vocabulary and definitions in chapter 12 of the IUPAC nomenclature book) and structured in an mzML- and TraML-friendly way, hopefully facilitating the browsing of the terms. Almost all first-level branch terms (the direct children of the root term) have a homonymous XML element in mzML or TraML. Their children, the second-level terms, are relevant topics or categories that need CV support for their description. The leaf nodes under their respective parent categories should be used in a cvParam under the appropriate XML element in the TraML schema.

Some terms describe attributes that must be coupled with a numerical value attribute in the CvParam element (e.g. dwell time MS:1000039) and optionally a unit for that value (e.g. second MS:1000502). The terms that require a value are denoted by having a “datatype” key-value pair in the CV itself. Similarly, terms that need to be qualified with units are denoted by a “needs_units” key in the CV itself.

Although the structures of the CV and the TraML schema are related, the details of which terms are allowed/recommended in a given schema section are reported in the mapping file. The mapping file is a list of associations between a cvParam element in a specific schema location (described with an Xpath) and the branches of the CV terms expected in that location. This file is read and interpreted by the validator, checking that the data annotation is consistent. The mapping file needs to be checked and eventually updated when the CV terms or structure are changed.

As recommended by the PSI CV guidelines, psi-ms.obo should be dynamically maintained via the psidev-ms-vocab mailing lists, which allow 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 days. If there is no obvious consensus, the CV coordinators committee should vote and make a decision. A new psi-ms.obo should then be released by updating the file on the CVS server without changing the name of the file (this would alter the propagation of the file to the OBO website and to other ontology services that rely on file stable URI). For this reason, an internal version number with two decimals (x.y.z) should be increased:

- x should be increased when a first level term is renamed, added, deleted or rearranged in the structure. Such rearrangement is supposed to be rare and is very likely to have repercussions on the mapping.
- y should be increased when any other term, except the first level one, is altered.
- z should be increased when there is no term addition or deletion, but just editing on the definitions or other minor changes.

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

- Unit Ontology (http://www.obofoundry.org/cgi-bin/detail.cgi?id=unit)
- ChEBI (http://www.ebi.ac.uk/chebi/)
- OBI (Ontology of Biological Investigations - http://obi.sourceforge.net/) (formerly called FuGO)

2.3 Resolved Design Issues

There were several issues regarding the design of the format that were not clear, and a design choice was made that was not completely agreeable to everyone. So that these issues do not keep coming up, we document here the issues and the basis for the implemented design choice.

2.3.1 Merging <Transition> and <Target> elements

It was suggested during development that <Transition>s and <Target>s are inherently quite similar, whereby <Transition>s contain both a precursor and product element, and <Target>s contain only a precursor. The idea of merging these into the same structure (e.g. everything would be a <Target> and transitions would just have more information) was discussed extensively. In the end, we concluded that attempting to merge these elements would make validation of transitions much more difficult (e.g. disallowing transitions with no product ion information). Since our primary use case (and probably 90+% of instances of TraML) is for transitions, it seemed unwise to complicate the format and validation to satisfy some perception of unified elegance with a minor add-on (inclusion list targets). For this reason, <Transition>s and <Target>s, although similar in several ways, are completely separate entities.

2.3.2 Local retention times in <Transition>

Although retention time is generally an attribute of a peptide or a compound, and one may specify one or more retention times (predicted, calibrated, etc.) with peptides or compounds, we have also added the functionality to allow a single local retention time with transitions and targets. There are two reasons for this. First, with the very simplest of lists, there may only be Q1, Q3, and retention time values, and it seemed undesirable for the TraML file to require the creation of peptide or compound elements just to hold a single retention time value. In the worst-case scenario, the information may not be known, and the TraML writer would need to create fake entries to hold retention time. Second, in most instrumental setups, the retention time window can be specified for each transition. One can imagine some slightly contrived examples where one may want to specify one transition with a wide retention time window to guard against “out-of-window” problems, but then include more transitions per peptide with a smaller window to enable more transitions to be packed into the run. Further, the emergence of optimal scheduling algorithms may provide slightly different windows for some sibling transitions to optimize the density of transitions in a run. For this reason, it seems appropriate to allow one retention time for each transition.

2.3.3 Specifying groups of peptide ions

Often multiple highly-related peptide ions are monitored together and need to be processed together. The classic example is the case of a natural (light) peptide and its heavy-labeled reference peptides. Such related peptide ions may be labelled with a group label like this in the <Peptide> element:
<cvParam cvRef="MS" accession="MS:1000893" name="peptide group label" value="G1"/>

where the values are arbitrary. This mechanism will allow downstream processing software to group peptide ions with the same group label.

2.4 Other supporting materials

This document cannot be fully judged on its own. It is important to study the accompanying sample instance documents, controlled vocabulary, schema files, and the software that implements this pre-release version of TraML. In fact, the content of section 3 in this document (as well as the on-line HTML documentation) is completely autogenerated from these files and not maintained by hand.

All these files and programs are available at:
http://psidev.info/index.php?q=node/405

They are:

Filename	Description
TraML0.9.5.xsd	Main mzML XML schema definition file
TraML0.9.5.html	HTML documentation of the model
psi-ms.obo	PSI-MS controlled vocabulary in OBO format
specialNotes.txt	A set of special notes associated with individual elements (these are incorporated into the autogenerated documentation)
TraML-mapping.txt	XML-encoded rules for where certain CvParams MAY/MUST appear in the document.
ToyExample1.TraML	Tiny hand-crafted document including most available elements and attributes for demonstration purposes
Yeast_ATAQS_gen.TraML	A set of yeast transitions generated by the ATAQS software suite
Yeast_InclusionList.TraML	A set of inclusion list targets for yeast generated by Proteios

Additional material is referenced with hyperlinks at the same URL.

2.5 Open Issues

All open issues were resolved by the end of the TraML 1.0.0.0 design phase. This may be an appropriate section to describe issues that arise after the 1.0 release and are considered sufficiently disruptive that they require a new major or minor release number. Such disruptive changes to the schema are expected to be rare. It is hoped that it will be several years before the next major revision.

2.6 Implementations

There are a number of implementations already for TraML, most notably in the ProteoWizard toolkit, in ATAQS, and in Computils. The ProteoWizard implementation is the reference implementation as members of the ProteoWizard team are actively participating in the TraML design and implemenatation.

3. Model in XML Schema

The TraML model is described in the XML schema below.

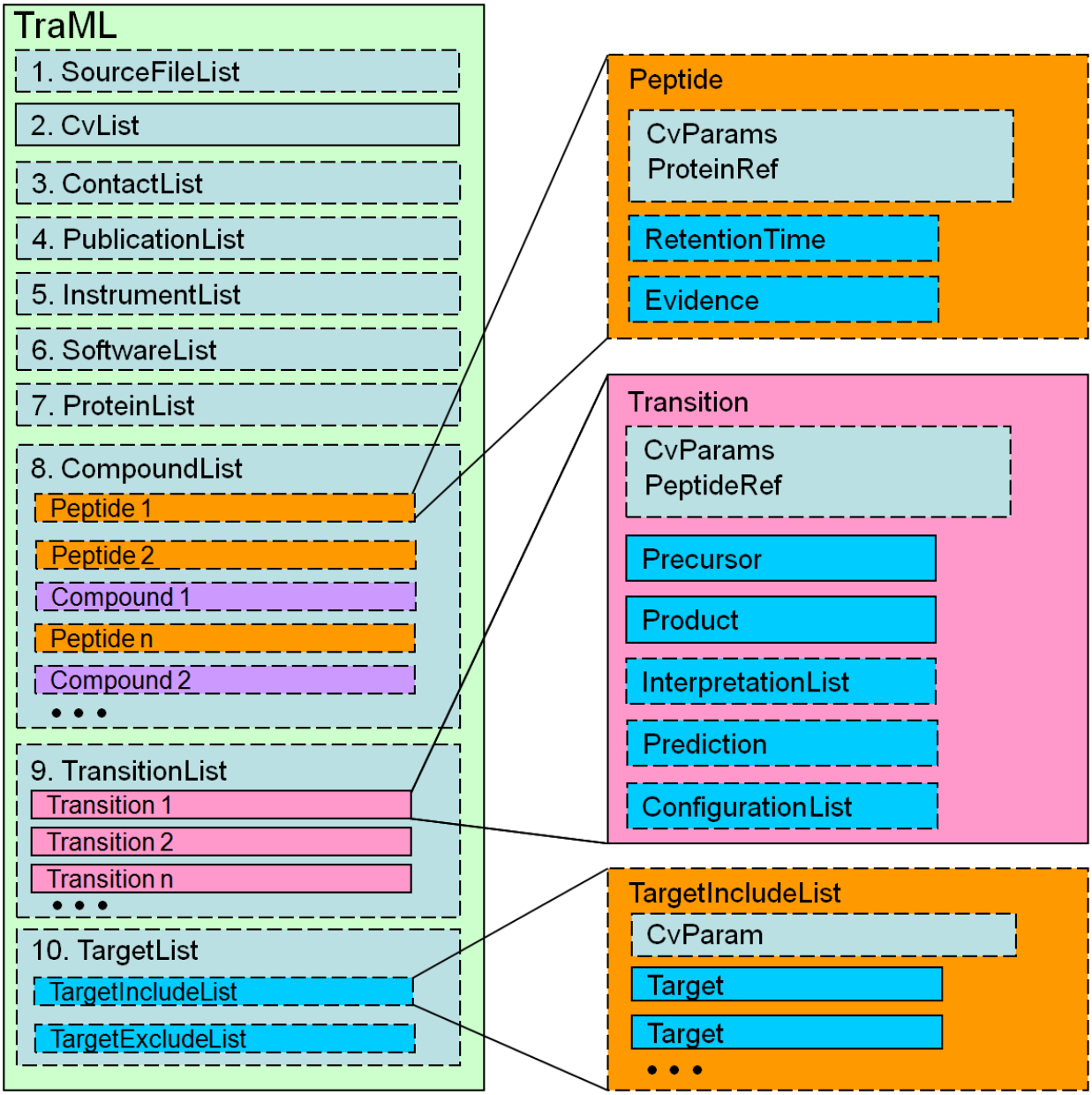

Figure 1: High-level overview of the XML elements for TraML. Each box represents an XML element, nested within other elements as shown. Boxes with dash outlines denote optional elements.

3.1 Element <TraML>

Definition: Container for the HUPO PSI TraML format for encoding selected reaction monitoring transitions and other target lists

Type: TraMLType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:string	optional	An optional id for the TraML document used for referencing from external files. It is recommended to use LSIDs when possible.
version	xs:string	required	Version of the TraML format used by this document

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvList	1	1	List of controlled vocabularies used in a TraML document
SourceFileList	0	1	List and descriptions of the source files this TraML document was generated or derived from
ContactList	0	1	List of contacts referenced in the generation or validation of transitions
PublicationList	0	1	List of publications from which the transitions were collected or wherein they are published
InstrumentList	0	1	List of instruments on which transitions are validated
SoftwareList	0	1	List of software packages used in the generation of one of more transitions described in the document
ProteinList	0	1	List of proteins for which one or more transitions are intended to identify
CompoundList	0	1	List of compounds (including peptides) for which one or more transitions are intended to identify
TransitionList	0	1	List of transitions
TargetList	0	1	List of precursor m/z targets to include or exclude

Example Context:

```
<TraML version="1.0.0" xmlns="http://psi.hupo.org/ms/traml"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xsi:schemaLocation="http://psi.hupo.org/ms/traml TraML1.0.0.xsd">
  <cvList>
    <cv id="MS" fullName="Proteomics Standards Initiative Mass Spectrometry Ontology"
version="2.31.0" URI="http://psidev.cvs.sourceforge.net/*checkout*/psidev/psi/psi-
ms/mzML/controlledVocabulary/psi-ms.obo"/>
    <cv id="UO" fullName="Unit Ontology" version="unknown"
URI="http://obo.cvs.sourceforge.net/obo/obo/ontology/phenotype/unit.obo"/>
    <cv id="UNIMOD" fullName="UNIMOD CV for modifications" version="unknown"
URI="http://www.unimod.org/obo/unimod.obo"/>
  </cvList>
  <SourceFileList>
  ...
</TraML>
```

3.2 Element <cvList>

Definition: List of controlled vocabularies used in a TraML document

Type: cvListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cv	1	unbounded	Controlled vocabulary used in a TraML document

Example Context:

```
<cvList>
  <cv id="MS" fullName="Proteomics Standards Initiative Mass Spectrometry Ontology"
version="2.31.0" URI="http://psidev.cvs.sourceforge.net/*checkout*/psidev/psi/psi-
ms/mzML/controlledVocabulary/psi-ms.obo"/>
  <cv id="UO" fullName="Unit Ontology" version="unknown"
URI="http://obo.cvs.sourceforge.net/obo/obo/ontology/phenotype/unit.obo"/>
```

```
  <cv id="UNIMOD" fullName="UNIMOD CV for modifications" version="unknown"
URI="http://www.unimod.org/obo/unimod.obo"/>
</cvList>
```

3.3 Element <SourceFileList>

Definition: List and descriptions of the source files this TraML document was generated or derived from

Type: SourceFileListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
SourceFile	1	unbounded	Description of the source file, including location and type.

Example Context:

```
<SourceFileList>
  <SourceFile id="sf1" name="OneTransition.tsv" location="file:///F:/data/Exp01">
    <cvParam cvRef="MS" accession="MS:1000914" name="tab delimited text file" value=""/>
    <cvParam cvRef="MS" accession="MS:1000569" name="SHA-1"
value="71be39fb2700ab2f3c8b2234b91274968b6899b1"/>
  </SourceFile>
</SourceFileList>
```

3.4 Element <ContactList>

Definition: List of contacts referenced in the generation or validation of transitions

Type: ContactListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Contact	1	unbounded	Contact person referenced in the generation or validation of transitions

Example Context:

```
<ContactList>
  <Contact id="CS">
    <cvParam cvRef="MS" accession="MS:1000586" name="contact name" value="Eric Deutsch"/>
    <cvParam cvRef="MS" accession="MS:1000590" name="contact organization" value="Institute
for Systems Biology"/>
    <cvParam cvRef="MS" accession="MS:1000587" name="contact address" value="1441 NE 34th
St, Seattle WA 98103, USA"/>
    <cvParam cvRef="MS" accession="MS:1000588" name="contact URL"
value="http://www.systemsbiology.org/"/>
    <cvParam cvRef="MS" accession="MS:1000589" name="contact email"
value="example@systemsbiology.org"/>
  ...
</ContactList>
```

3.5 Element <PublicationList>

Definition: List of publications from which the transitions were collected or wherein they are published

Type: PublicationListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Publication	1	unbounded	Reference to a publication in which one or more transitions were published

Example Context:

```
<PublicationList>
  <Publication id="PMID12748199">
    <cvParam cvRef="MS" accession="MS:1000879" name="PubMed identifier" value="12748199"/>
  </Publication>
</PublicationList>
```

3.6 Element <InstrumentList>

Definition: List of instruments on which transitions are validated

Type: InstrumentListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Instrument	1	unbounded	Instrument on which transitions are validated

Example Context:

```
<InstrumentList>
  <Instrument id="LCQ_Deca">
    <cvParam cvRef="MS" accession="MS:1000554" name="LCQ Deca"/>
  </Instrument>
  <Instrument id="QTRAP">
    <cvParam cvRef="MS" accession="MS:1000870" name="4000 QTRAP"/>
  </Instrument>
  ...
</InstrumentList>
```

3.7 Element <SoftwareList>

Definition: List of software packages used in the generation of one of more transitions described in the document

Type: SoftwareListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Software	1	unbounded	Description of a software package used in the generation of one or more transitions described in the document

Example Context:

```
<SoftwareList>
  <Software id="MaRiMba" version="1.0">
    <cvParam cvRef="MS" accession="MS:1000872" name="MaRiMba"/>
  </Software>
  <Software id="SSRCalc3.0" version="3.0">
    <cvParam cvRef="MS" accession="MS:1000874" name="SSRCalc"/>
  </Software>
  ...
</SoftwareList>
```

3.8 Element <ProteinList>

Definition: List of proteins for which one or more transitions are intended to identify

Type: ProteinListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Protein	1	unbounded	Protein for which one or more transitions are intended to identify

Example Context:

```
<ProteinList>
  <Protein id="Q12149">
    <cvParam cvRef="MS" accession="MS:1000885" name="protein accession" value="Q00613"/>
    <cvParam cvRef="MS" accession="MS:1000883" name="protein short name" value="HSF 1"/>
    <cvParam cvRef="MS" accession="MS:1000886" name="protein name" value="Heat shock factor
protein 1"/>

<Sequence>MSTEMETKAEDVETFAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLDNGKE</Sequence>
  </Protein>
  ...
```

```
</ProteinList>
```

3.9 Element <CompoundList>

Definition: List of compounds (including peptides) for which one or more transitions are intended to identify

Type: CompoundListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
Peptide	0	unbounded	Peptide for which one or more transitions are intended to identify
Compound	0	unbounded	Chemical compound other than a peptide for which one or more transitions

Example Context:

```
<CompoundList>
  <Peptide id="ADTHFLLNIYDQLR-M1" sequence="ADTHFLLNIYDQLR">
    <cvParam cvRef="MS" accession="MS:1000891" name="heavy labeled peptide"/>
    <cvParam cvRef="MS" accession="MS:1000893" name="peptide group label" value="G1"/>
    <cvParam cvRef="MS" accession="MS:1000863" name="predicted isoelectric point"
value="5.22"/>
    <cvParam cvRef="MS" accession="MS:1001117" name="theoretical mass" value="1189.22"
unitCvRef="UO" unitAccession="UO:0000221" unitName="dalton"/>
    <userParam name="isomerization potential" value="0.583" type="xsd:float"/> <!-- Additional
information may be added as a userParams if it is not possible and not appropriate to encode
the information as a cvParam -->
  ...
</CompoundList>
```

3.10 Element <TransitionList>

Definition: List of transitions

Type: TransitionListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Transition	1	unbounded	Information about a single transition for a peptide or other compound

Example Context:

```
<TransitionList>
  <Transition id="ADTHFLLNIYDQLR-M1-T1" peptideRef="ADTHFLLNIYDQLR-M1">
    <Precursor>
      <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
      <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
    </Precursor>
    <Product>
  ...
</TransitionList>
```

3.11 Element <TargetList>

Definition: List of precursor m/z targets to include or exclude

Type: TargetListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
TargetIncludeList	0	1	List of precursor m/z targets to include
TargetExcludeList	0	1	List of precursor m/z targets to exclude

Example Context:

```
<TargetList>
  <cvParam cvRef="MS" accession="MS:1000920" name="includes supersede excludes"/>
  <TargetIncludeList>
    <Target id="PEPTIDEC2+" peptideRef="PEPTIDEC">
      <Precursor>
        <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
        <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
  ...
</TargetList>
```

cvParam Mapping Rules:

```
Path /TraML/TargetList
MUST supply a *child* term of MS:1000919 (target inclusion exclusion priority) only once
  e.g.: MS:1000920 (includes supersede excludes)
  e.g.: MS:1000921 (excludes supersede includes)
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000920" name="includes supersede excludes"/>
```

3.12 Element <cv>

Definition: Controlled vocabulary used in a TraML document

Type: cvType

Attributes:

Attribute Name	Data Type	Use	Definition
URI	xs:anyURI	required	Uniform Resource Identifier for the controlled vocabulary
fullName	xs:string	required	Full name of the controlled vocabulary
id	xs:ID	required	Identifier for the controlled vocabulary to be used for referencing within a document
version	xs:string	required	Version of controlled vocabulary in use when the document was created

Subelements: none

Example Context:

```
<cv id="MS" fullName="Proteomics Standards Initiative Mass Spectrometry Ontology"
version="2.31.0" URI="http://psidev.cvs.sourceforge.net/*checkout*/psidev/psi/psi-
ms/mzML/controlledVocabulary/psi-ms.obo"/>
```

3.13 Element <SourceFile>

Definition: Description of the source file, including location and type.

Type: SourceFileType

Attributes:

Attribute Name	Data Type	Use	Definition

id	xs:ID	required	Identifier for the sourceFile to be used for referencing within a document.
location	xs:anyURI	required	URI-formatted location where the file was retrieved.
name	xs:string	required	Name of the source file, without reference to location (either URI or local path).

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<SourceFile id="sf1" name="OneTransition.tsv" location="file:///F:/data/Exp01">
  <cvParam cvRef="MS" accession="MS:1000914" name="tab delimited text file" value=""/>
  <cvParam cvRef="MS" accession="MS:1000569" name="SHA-1"
value="71be39fb2700ab2f3c8b2234b91274968b6899b1"/>
</SourceFile>
```

cvParam Mapping Rules:

```
Path /TraML/SourceFileList/SourceFile
MAY supply a *child* term of MS:1000561 (data file checksum type) only once
  e.g.: MS:1000568 (MD5)
  e.g.: MS:1000569 (SHA-1)
MUST supply term MS:1001459 (file format) or any of its children only once
  e.g.: MS:1000526 (Waters raw file)
  e.g.: MS:1000562 (ABI WIFF file)
  e.g.: MS:1000563 (Thermo RAW file)
  e.g.: MS:1000564 (PSI mzData file)
  e.g.: MS:1000565 (Micromass PKL file)
  e.g.: MS:1000566 (ISB mzXML file)
  e.g.: MS:1000567 (Bruker/Agilent YEP file)
  e.g.: MS:1000584 (mzML file)
  e.g.: MS:1000613 (DTA file)
  e.g.: MS:1000614 (ProteinLynx Global Server mass spectrum XML file)
  et al.
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000914" name="tab delimited text file" value=""/>
<cvParam cvRef="MS" accession="MS:1000569" name="SHA-1"
value="71be39fb2700ab2f3c8b2234b91274968b6899b1"/>
```

3.14 Element <Contact>

Definition: Contact person referenced in the generation or validation of transitions

Type: ContactType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:ID	required	Identifier for the contact to be used for referencing within a document

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Contact id="CS">
  <cvParam cvRef="MS" accession="MS:1000586" name="contact name" value="Eric Deutsch"/>
  <cvParam cvRef="MS" accession="MS:1000590" name="contact organization" value="Institute
for Systems Biology"/>
  <cvParam cvRef="MS" accession="MS:1000587" name="contact address" value="1441 NE 34th St,
Seattle WA 98103, USA"/>
  <cvParam cvRef="MS" accession="MS:1000588" name="contact URL"
value="http://www.systemsbiology.org/"/>
  <cvParam cvRef="MS" accession="MS:1000589" name="contact email"
value="example@systemsbiology.org"/>
</Contact>
```

cvParam Mapping Rules:

```
Path /TraML/ContactList/Contact
MAY supply a *child* term of MS:1000585 (contact attribute) one or more times
  e.g.: MS:1000586 (contact name)
  e.g.: MS:1000587 (contact address)
  e.g.: MS:1000588 (contact URL)
  e.g.: MS:1000589 (contact email)
  e.g.: MS:1000590 (contact organization)
  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)
  et al.
MUST supply term MS:1000590 (contact organization) only once
MUST supply term MS:1000586 (contact name) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000586" name="contact name" value="Eric Deutsch"/>
<cvParam cvRef="MS" accession="MS:1000590" name="contact organization" value="Institute for
Systems Biology"/>
<cvParam cvRef="MS" accession="MS:1000587" name="contact address" value="1441 NE 34th St,
Seattle WA 98103, USA"/>
<cvParam cvRef="MS" accession="MS:1000588" name="contact URL"
value="http://www.systemsbiology.org/"/>
<cvParam cvRef="MS" accession="MS:1000589" name="contact email"
value="example@systemsbiology.org"/>
```

3.15 Element <Publication>

Definition: Reference to a publication in which one or more transitions were published

Type: PublicationType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:ID	required	Identifier for the publication to be used for referencing within a document

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Publication id="PMID12748199">
  <cvParam cvRef="MS" accession="MS:1000879" name="PubMed identifier" value="12748199"/>
</Publication>
```

cvParam Mapping Rules:

```
Path /TraML/PublicationList/Publication
MUST supply term MS:1000879 (PubMed identifier) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000879" name="PubMed identifier" value="12748199"/>
```

3.16 Element <Instrument>

Definition: Instrument on which transitions are validated

Type: InstrumentType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:ID	required	Identifier for the instrument to be used for referencing within a document

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Instrument id="LCQ_Deca">
  <cvParam cvRef="MS" accession="MS:1000554" name="LCQ Deca"/>
</Instrument>
```

cvParam Mapping Rules:

```
Path /TraML/InstrumentList/Instrument
MUST supply a *child* term of MS:1000031 (instrument model) only once
  e.g.: MS:1000139 (4000 QTRAP)
  e.g.: MS:1000140 (4700 Proteomics Analyzer)
  e.g.: MS:1000141 (apex IV)
  e.g.: MS:1000142 (apex Q)
  e.g.: MS:1000143 (API 150EX)
  e.g.: MS:1000144 (API 150EX Prep)
  e.g.: MS:1000145 (API 2000)
  e.g.: MS:1000146 (API 3000)
  e.g.: MS:1000147 (API 4000)
  e.g.: MS:1000148 (autoflex II)
  et al.
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000554" name="LCQ Deca"/>
<cvParam cvRef="MS" accession="MS:1000870" name="4000 QTRAP"/>
```

3.17 Element <Software>

Definition: Description of a software package used in the generation of one or more transitions described in the document

Type: SoftwareType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:ID	required	Identifier for the software to be used for referencing within a document
version	xs:string	required	Version of the software program described

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	1	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example

```
<Software id="SSRCalc3.0" version="3.0">
  <cvParam cvRef="MS" accession="MS:1000874" name="SSRCalc"/>
```

Context:

```
</Software>
```

cvParam Mapping Rules:

```
Path /TraML/SoftwareList/Software
MUST supply a *child* term of MS:1000531 (software) only once
  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:1000538 (massWolf)
  e.g.: MS:1000539 (Voyager Biospectrometry Workstation System)
  e.g.: MS:1000540 (FlexControl)
  e.g.: MS:1000541 (ReAdW)
  et al.
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000872" name="MaRiMba"/>
<cvParam cvRef="MS" accession="MS:1000874" name="SSRCalc"/>
<cvParam cvRef="MS" accession="MS:1000922" name="Skyline"/>
```

3.18 Element <Protein>

Definition: Protein for which one or more transitions are intended to identify

Type: ProteinType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:ID	required	Identifier for the protein to be used for referencing within a document

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
Sequence	0	1	Amino acid sequence of the protein

Example Context:

```
<Protein id="ENSP00000332698">
  <cvParam cvRef="MS" accession="MS:1000885" name="protein accession" value="ENSP00000332698"/>
  <cvParam cvRef="MS" accession="MS:1000883" name="protein short name" value="HSF 1"/>
  <cvParam cvRef="MS" accession="MS:1000886" name="protein name" value="Heat shock factor protein 1"/>

<Sequence>MSTEMETKAEDVETFAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLDNGKEELISNSSDALDKI</Sequence>
</Protein>
```

cvParam Mapping Rules:

```
Path /TraML/ProteinList/Protein
MAY supply a *child* term of MS:1000884 (protein attribute) one or more times
  e.g.: MS:1000883 (protein short name)
  e.g.: MS:1000885 (protein accession)
  e.g.: MS:1000886 (protein name)
  e.g.: MS:1000933 (protein modifications)
  e.g.: MS:1000934 (gene name)
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000885" name="protein accession" value="Q00613"/>
<cvParam cvRef="MS" accession="MS:1000883" name="protein short name" value="HSF 1"/>
<cvParam cvRef="MS" accession="MS:1000886" name="protein name" value="Heat shock factor protein 1"/>
```

3.19 Element <cvParam>

Definition: Controlled vocabulary term adding information to the parent term

Type: cvParamType

Attributes:

Attribute Name	Data Type	Use	Definition
accession	xs:string	required	Accession number of the controlled vocabulary term referenced

cvRef	xs:IDREF	required	Reference to a controlled vocabulary for which this cvParam is
name	xs:string	required	Name of the controlled vocabulary term referenced
unitAccession	xs:string	optional	An optional CV accession number for the unit term associated with the value, if any (e.g., 'UO:0000266' for 'electron volt').
unitCvRef	xs:IDREF	optional	If a unit term is referenced, this attribute MUST refer to the CV 'id' attribute defined in the cvList in this mzML file.
unitName	xs:string	optional	An optional CV name for the unit accession number, if any (e.g., 'electron volt' for 'UO:0000266').
value	xs:string	optional	Scalar value qualifying the controlled vocabulary term referenced

Subelements: none

Example Context:

```
<cvParam cvRef="MS" accession="MS:1000042" name="peak intensity" value="4072" unitCvRef="MS" unitAccession="MS:1000905" unitName="percent of base peak times 100"/>
```

3.20 Element <userParam>

Definition: Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Type: UserParamType

Attributes:

Attribute Name	Data Type	Use	Definition
name	xs:string	required	The name for the parameter.
type	xs:string	optional	The datatype of the parameter, where appropriate (e.g.: xsd:float).
unitAccession	xs:string	optional	An optional CV accession number for the unit term associated with the value, if any (e.g., 'UO:0000266' for 'electron volt').
unitCvRef	xs:IDREF	optional	If a unit term is referenced, this attribute MUST refer to the CV 'id' attribute defined in the cvList in this mzML file.
unitName	xs:string	optional	An optional CV name for the unit accession number, if any (e.g., 'electron volt' for 'UO:0000266').
value	xs:string	optional	The value for the parameter, where appropriate.

Subelements: none

Example Context:

```
<userParam name="isomerization potential" value="0.583" type="xsd:float"/> <!-- Additional information may be added as a userParams if it is not possible and not appropriate to encode the information as a cvParam -->
```

3.21 Element <Peptide>

Definition: Peptide for which one or more transitions are intended to identify

Type: PeptideType

Attributes:

Attribute Name	Data Type	Use	Definition

id	xs:ID	required	Identifier for the peptide to be used for referencing within a document
sequence	xs:string	required	Amino acid sequence of the peptide being described

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
ProteinRef	0	unbounded	Reference to a protein which this peptide is intended to identify
Modification	0	unbounded	A molecule modification specification. If n modifications are present on the peptide, there should be n instances of the modification element. If multiple modifications are provided as cvParams, it is assumed the modification is ambiguous, i.e. one modification or the other. If no cvParams are provided it is assumed that the delta has not been matched to a known modification.
RetentionTimeList	0	1	List of retention time information entries
Evidence	0	1	Information about empirical mass spectrometer observations of the peptide

Example Context:

```
<Peptide id="ADTHFLLNIYDQLR-M1" sequence="ADTHFLLNIYDQLR">
  <cvParam cvRef="MS" accession="MS:1000891" name="heavy labeled peptide"/>
  <cvParam cvRef="MS" accession="MS:1000893" name="peptide group label" value="G1"/>
  <cvParam cvRef="MS" accession="MS:1000863" name="predicted isoelectric point"
value="5.22"/>
  <cvParam cvRef="MS" accession="MS:1001117" name="theoretical mass" value="1189.22"
unitCvRef="UO" unitAccession="UO:0000221" unitName="dalton"/>
  <userParam name="isomerization potential" value="0.583" type="xsd:float"/> <!-- Additional
information may be added as a userParams if it is not possible and not appropriate to encode
the information as a cvParam -->
  <ProteinRef ref="Q12149"/>
  ...
</Peptide>
```

cvParam Mapping Rules:

```
Path /TraML/CompoundList/Peptide
MAY supply term MS:1000863 (predicted isoelectric point) only once
MAY supply term MS:1000893 (peptide group label) only once
MAY supply term MS:1001117 (theoretical mass) only once
MAY supply a *child* term of MS:1000890 (peptide labeling state) one or more times
  e.g.: MS:1000891 (heavy labeled peptide)
  e.g.: MS:1000892 (unlabeled peptide)
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000891" name="heavy labeled peptide"/>
<cvParam cvRef="MS" accession="MS:1000893" name="peptide group label" value="G1"/>
<cvParam cvRef="MS" accession="MS:1000863" name="predicted isoelectric point" value="5.22"/>
<cvParam cvRef="MS" accession="MS:1001117" name="theoretical mass" value="1189.22"
unitCvRef="UO" unitAccession="UO:0000221" unitName="dalton"/>
```

3.22 Element <Compound>

Definition: Chemical compound other than a peptide for which one or more transitions

Type: CompoundType

Attributes:

Attribute Name	Data Type	Use	Definition
id	xs:ID	required	Identifier for the compound to be used for referencing within a document

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
RetentionTimeList	0	unbounded	List of retention time information entries

Example Context:

```
<Compound id="glyoxylate">
  <cvParam cvRef="MS" accession="MS:1001117" name="theoretical mass" value="423.39"
unitCvRef="UO" unitAccession="UO:0000221" unitName="dalton"/>
  <cvParam cvRef="MS" accession="MS:1000866" name="molecular formula" value="C2HO3"/>
  <cvParam cvRef="MS" accession="MS:1000868" name="SMILES string"
value="[CH](=[O])[C](=[O])[O-]"/>
  <RetentionTimeList>
    <RetentionTime>
      <cvParam cvRef="MS" accession="MS:1000896" name="normalized retention time"
value="22.34" unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
  ...
</Compound>
```

cvParam Mapping Rules:

```
Path /TraML/CompoundList/Compound
MAY supply term MS:1000863 (predicted isoelectric point) only once
MAY supply a *child* term of MS:1000864 (chemical compound formula) one or more times
  e.g.: MS:1000865 (empirical formula)
  e.g.: MS:1000866 (molecular formula)
  e.g.: MS:1000867 (structural formula)
  e.g.: MS:1000868 (SMILES string)
MAY supply term MS:1001117 (theoretical mass) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1001117" name="theoretical mass" value="423.39"
unitCvRef="UO" unitAccession="UO:0000221" unitName="dalton"/>
<cvParam cvRef="MS" accession="MS:1000866" name="molecular formula" value="C2HO3"/>
<cvParam cvRef="MS" accession="MS:1000868" name="SMILES string"
value="[CH](=[O])[C](=[O])[O-]"/>
```

3.23 Element <Transition>

Definition: Information about a single transition for a peptide or other compound

Type: TransitionType

Attributes:

Attribute Name	Data Type	Use	Definition
compoundRef	xs:IDREF	optional	Reference to a compound for this transition
id	xs:string	required	String label for this transition
peptideRef	xs:IDREF	optional	Reference to a peptide which this transition is intended to identify

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Precursor	1	1	Precursor (Q1) of the transition or target
IntermediateProduct	0	unbounded	Intermediate product ion information of the transition when using MS3 or above
Product	1	1	Product (Q3) of the transition

RetentionTime	0	1	Information about predicted or calibrated retention time
Prediction	0	1	Information about a prediction for a suitable transition using some software
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Transition id="ADTHFLLNIYDQLR-M1-T2" peptideRef="ADTHFLLNIYDQLR-M1">
  <Precursor>
    <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
    <cvParam cvRef="MS" accession="MS:1000828" name="isolation window lower offset"
value="1.0" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
    <cvParam cvRef="MS" accession="MS:1000829" name="isolation window upper offset"
value="1.0" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
    <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
  </Precursor>
  ...
</Transition>
```

3.24 Element <TargetIncludeList>

Definition: List of precursor m/z targets to include

Type: TargetIncludeListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Target	1	unbounded	A peptide or compound that is to be included or excluded from a target list of precursor m/z values.

Example Context:

```
<TargetIncludeList>
  <Target id="PEPTIDEC2+" peptideRef="PEPTIDEC">
    <Precursor>
      <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
      <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
    </Precursor>
    <RetentionTime softwareRef="Skyline0.5">
  ...
</TargetIncludeList>
```

3.25 Element <TargetExcludeList>

Definition: List of precursor m/z targets to exclude

Type: TargetExcludeListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Target	1	unbounded	A peptide or compound that is to be included or excluded from a target list of precursor m/z values.

Example

```
<TargetExcludeList>
  <Target id="PEPTIDEM3+" peptideRef="PEPTIDEM">
```

Context:

```
      <Precursor>
        <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="698.3443" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
        <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="3"/>
      </Precursor>
    </Target>
    ...
</TargetExcludeList>
```

3.26 Element <Sequence>

Definition: Amino acid sequence of the protein

Type: SequenceType

Attributes: none

Subelements: none

Example Context:

```
<Sequence>MSTEMETKAEDVETFAFQAEIAQLMSLIINTFYSNKEIFLRELISNSSDALDKIRYESLTDPSKLDNGKEELISNSSDALDKI</Sequence>
```

3.27 Element <ProteinRef>

Definition: Reference to a protein which this peptide is intended to identify

Type: ProteinRefType

Attributes:

Attribute Name	Data Type	Use	Definition
ref	xs:IDREF	optional	Reference to a protein which this peptide is intended to identify

Subelements: none

Example Context:

```
<ProteinRef ref="ENSP00000332698"/>
```

3.28 Element <Modification>

Definition: A molecule modification specification. If n modifications are present on the peptide, there should be n instances of the modification element. If multiple modifications are provided as cvParams, it is assumed the modification is ambiguous, i.e. one modification or the other. If no cvParams are provided it is assumed that the delta has not been matched to a known modification.

Type: ModificationType

Attributes:

Attribute Name	Data Type	Use	Definition
averageMassDelta	xs:double	optional	Atomic mass delta when considering the natural distribution of isotopes in Daltons.
location	xs:int	required	Location of the modification within the peptide sequence, counted from the N-terminus, 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	xs:double	optional	Atomic mass delta when assuming only the most common isotope of elements in Daltons.

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition

cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Modification location="1" monoisotopicMassDelta="15.994919">
  <cvParam cvRef="UNIMOD" accession="UNIMOD:35" name="Oxidation"/>
</Modification>
```

cvParam Mapping Rules:

```
Path /TraML/CompoundList/Peptide/Modification
MAY supply a *child* term of UNIMOD:0 (unimod root node) one or more times
```

Example cvParams:

```
<cvParam cvRef="UNIMOD" accession="UNIMOD:29" name="SMA"/>
<cvParam cvRef="UNIMOD" accession="UNIMOD:35" name="Oxidation"/>
```

3.29 Element <RetentionTimeList>

Definition: List of retention time information entries

Type: RetentionTimeListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
RetentionTime	1	unbounded	Information about predicted or calibrated retention time

Example Context:

```
<RetentionTimeList>
  <RetentionTime softwareRef="SSRCalc3.0">
    <cvParam cvRef="MS" accession="MS:1000897" name="predicted retention time" value="44.07"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
  </RetentionTime>
  <RetentionTime>
    <cvParam cvRef="MS" accession="MS:1000896" name="normalized retention time" value="38.43"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
    <cvParam cvRef="MS" accession="MS:1000902" name="H-PINS retention time normalization
standard"/>
  ...
</RetentionTimeList>
```

3.30 Element <Evidence>

Definition: Information about empirical mass spectrometer observations of the peptide

Type: EvidenceType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Evidence>
  <cvParam cvRef="MS" accession="MS:1001100" name="confident peptide" value="6"/>
</Evidence>
```

cvParam

```
Path /TraML/CompoundList/Peptide/Evidence
```

Mapping Rules:
```
MAY supply term MS:1001100 (confident peptide) only once
```

Example cvParams:
```
<cvParam cvRef="MS" accession="MS:1001100" name="confident peptide" value="6"/>
```

3.31 Element <Precursor>

Definition: Precursor (Q1) of the transition or target

Type: PrecursorType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:
```
<Precursor>
  <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
  <cvParam cvRef="MS" accession="MS:1000828" name="isolation window lower offset"
value="1.0" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
  <cvParam cvRef="MS" accession="MS:1000829" name="isolation window upper offset"
value="1.0" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
  <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
</Precursor>
```

cvParam Mapping Rules:
```
Path /TraML/TargetExcludeList/Target/Precursor
MAY supply term MS:1000828 (isolation window lower offset) only once
MAY supply term MS:1000829 (isolation window upper offset) only once
Path /TraML/TransitionList/Transition/Precursor
MAY supply term MS:1000828 (isolation window lower offset) only once
MAY supply term MS:1000829 (isolation window upper offset) only once
MUST supply term MS:1000827 (isolation window target m/z) only once
MAY supply term MS:1000041 (charge state) only once
Path /TraML/TargetList/TargetIncludeList/Target/Precursor
MUST supply term MS:1000827 (isolation window target m/z) only once
MAY supply term MS:1000041 (charge state) only once
Path /TraML/TargetList/TargetExcludeList/Target/Precursor
MUST supply term MS:1000827 (isolation window target m/z) only once
MAY supply term MS:1000041 (charge state) only once
Path /TraML/TargetIncludeList/Target/Precursor
MAY supply term MS:1000828 (isolation window lower offset) only once
MAY supply term MS:1000829 (isolation window upper offset) only once
```

Example cvParams:
```
<cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
<cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
<cvParam cvRef="MS" accession="MS:1000828" name="isolation window lower offset" value="1.0"
unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
<cvParam cvRef="MS" accession="MS:1000829" name="isolation window upper offset" value="1.0"
unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
```

3.32 Element <IntermediateProduct>

Definition: Intermediate product ion information of the transition when using MS3 or above

Type: IntermediateProductType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially

			allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
InterpretationList	0	1	List of possible interprations of fragment ions for a transition
ConfigurationList	0	1	List of insutrument configurations used in the validation or optimization of the transitions

Example Context:

```
<IntermediateProduct>
  <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="1040.57" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
  <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="1"/>
  <InterpretationList>
    <Interpretation>
      <cvParam cvRef="MS" accession="MS:1000926" name="product interpretation rank"
value="1"/>
      <cvParam cvRef="MS" accession="MS:1001220" name="frag: y ion"/>
  ...
</IntermediateProduct>
```

cvParam Mapping Rules:

```
Path /TraML/TransitionList/Transition/IntermediateProduct
MAY supply term MS:1000828 (isolation window lower offset) only once
MAY supply term MS:1000829 (isolation window upper offset) only once
MUST supply term MS:1000827 (isolation window target m/z) only once
MAY supply term MS:1000041 (charge state) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="1040.57" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
<cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="1"/>
```

3.33 Element <Product>

Definition: Product (Q3) of the transition

Type: ProductType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
InterpretationList	0	1	List of possible interprations of fragment ions for a transition
ConfigurationList	0	1	List of insutrument configurations used in the validation or optimization of the transitions

Example Context:

```
<Product>
  <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="1040.57" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
  <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="1"/>
  <InterpretationList>
    <Interpretation>
      <cvParam cvRef="MS" accession="MS:1000926" name="product interpretation rank"
value="1"/>
      <cvParam cvRef="MS" accession="MS:1001220" name="frag: y ion"/>
  ...
</Product>
```

cvParam

```
Path /TraML/TransitionList/Transition/Product
```

Mapping Rules:

```
MAY supply term MS:1000828 (isolation window lower offset) only once
MAY supply term MS:1000829 (isolation window upper offset) only once
MUST supply term MS:1000827 (isolation window target m/z) only once
MAY supply term MS:1000041 (charge state) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="1040.57" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
<cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="1"/>
```

3.34 Element <RetentionTime>

Definition: Information about predicted or calibrated retention time

Type: RetentionTimeType

Attributes:

Attribute Name	Data Type	Use	Definition
softwareRef	xs:IDREF	optional	Software used to determine the retention time

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	1	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<RetentionTime softwareRef="Skyline0.5">
  <cvParam cvRef="MS" accession="MS:1000895" name="local retention time" value="40.02"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
  <cvParam cvRef="MS" accession="MS:1000916" name="retention time window lower offset"
value="3.0" unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
  <cvParam cvRef="MS" accession="MS:1000917" name="retention time window upper offset"
value="3.0" unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
</RetentionTime>
```

cvParam Mapping Rules:

```
Path /TraML/TransitionList/Transition/RetentionTime/RetentionTime
MAY supply a *child* term of MS:1000915 (retention time window attribute) one or more times
  e.g.: MS:1000916 (retention time window lower offset)
  e.g.: MS:1000917 (retention time window upper offset)
  e.g.: MS:1001907 (retention time window width)
MAY supply a *child* term of MS:1000901 (retention time normalization standard) only once
  e.g.: MS:1000902 (H-PINS retention time normalization standard)
MUST supply term MS:1000895 (local retention time) only once
Path /TraML/TargetList/Target/RetentionTime/RetentionTime
MAY supply a *child* term of MS:1000915 (retention time window attribute) one or more times
  e.g.: MS:1000916 (retention time window lower offset)
  e.g.: MS:1000917 (retention time window upper offset)
  e.g.: MS:1001907 (retention time window width)
MAY supply a *child* term of MS:1000901 (retention time normalization standard) only once
  e.g.: MS:1000902 (H-PINS retention time normalization standard)
MUST supply term MS:1000895 (local retention time) only once
Path /TraML/CompoundList/Peptide/RetentionTimeList/RetentionTime
MAY supply a *child* term of MS:1000915 (retention time window attribute) one or more times
  e.g.: MS:1000916 (retention time window lower offset)
  e.g.: MS:1000917 (retention time window upper offset)
  e.g.: MS:1001907 (retention time window width)
MAY supply a *child* term of MS:1000901 (retention time normalization standard) only once
  e.g.: MS:1000902 (H-PINS retention time normalization standard)
MAY supply a *child* term of MS:1000894 (retention time) one or more times
  e.g.: MS:1000895 (local retention time)
  e.g.: MS:1000896 (normalized retention time)
  e.g.: MS:1000897 (predicted retention time)
  e.g.: MS:1000916 (retention time window lower offset)
  e.g.: MS:1000917 (retention time window upper offset)
  e.g.: MS:1001907 (retention time window width)
Path /TraML/CompoundList/Compound/RetentionTimeList/RetentionTime
MAY supply a *child* term of MS:1000915 (retention time window attribute) one or more times
  e.g.: MS:1000916 (retention time window lower offset)
  e.g.: MS:1000917 (retention time window upper offset)
  e.g.: MS:1001907 (retention time window width)
MAY supply a *child* term of MS:1000901 (retention time normalization standard) only once
  e.g.: MS:1000902 (H-PINS retention time normalization standard)
MAY supply a *child* term of MS:1000894 (retention time) one or more times
```

```
  e.g.: MS:1000895 (local retention time)
  e.g.: MS:1000896 (normalized retention time)
  e.g.: MS:1000897 (predicted retention time)
  e.g.: MS:1000916 (retention time window lower offset)
  e.g.: MS:1000917 (retention time window upper offset)
  e.g.: MS:1001907 (retention time window width)
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000897" name="predicted retention time" value="44.07"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
<cvParam cvRef="MS" accession="MS:1000896" name="normalized retention time" value="38.43"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
<cvParam cvRef="MS" accession="MS:1000902" name="H-PINS retention time normalization
standard"/>
<cvParam cvRef="MS" accession="MS:1000895" name="local retention time" value="40.02"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
<cvParam cvRef="MS" accession="MS:1000916" name="retention time window lower offset"
value="3.0" unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
<cvParam cvRef="MS" accession="MS:1000917" name="retention time window upper offset"
value="3.0" unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
```

3.35 Element <Prediction>

Definition: Information about a prediction for a suitable transition using some software

Type: PredictionType

Attributes:

Attribute Name	Data Type	Use	Definition
contactRef	xs:IDREF	optional	Reference to a contact person that generated this prediction
softwareRef	xs:IDREF	required	Reference to a software package from which this prediction is derived

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Prediction softwareRef="MaRiMba" contactRef="CS">
  <cvParam cvRef="MS" accession="MS:1000912" name="transition purported from an MS/MS
spectrum on a different, specified instrument"/>
  <cvParam cvRef="MS" accession="MS:1000291" name="linear ion trap"/>
  <cvParam cvRef="MS" accession="MS:1000042" name="peak intensity" value="10000"
unitCvRef="MS" unitAccession="MS:1000905" unitName="percent of base peak times 100"/>
  <cvParam cvRef="MS" accession="MS:1000906" name="peak intensity rank" value="1"/>
  <cvParam cvRef="MS" accession="MS:1000907" name="peak targeting suitability rank"
value="1"/>
</Prediction>
```

cvParam Mapping Rules:

```
Path /TraML/TransitionList/Transition/Prediction
MAY supply term MS:1000042 (peak intensity) only once
MAY supply a *child* term of MS:1000909 (transition validation method) only once
  e.g.: MS:1000910 (transition optimized on specified instrument)
  e.g.: MS:1000911 (transition validated with an MS/MS spectrum on specified instrument)
  e.g.: MS:1000912 (transition purported from an MS/MS spectrum on a different, specified
instrument)
  e.g.: MS:1000913 (transition predicted by informatic analysis)
MAY supply term MS:1000443 (mass analyzer type) or any of its children only once
  e.g.: MS:1000078 (axial ejection linear ion trap)
  e.g.: MS:1000079 (fourier transform ion cyclotron resonance mass spectrometer)
  e.g.: MS:1000080 (magnetic sector)
  e.g.: MS:1000081 (quadrupole)
  e.g.: MS:1000082 (quadrupole ion trap)
  e.g.: MS:1000083 (radial ejection linear ion trap)
  e.g.: MS:1000084 (time-of-flight)
  e.g.: MS:1000254 (electrostatic energy analyzer)
  e.g.: MS:1000284 (stored waveform inverse fourier transform)
```

```
    e.g.: MS:1000288 (cyclotron)
    et al.
  MAY supply term MS:1000906 (peak intensity rank) only once
  MAY supply term MS:1000907 (peak targeting suitability rank) only once
  MAY supply term MS:1000031 (instrument model) or any of its children only once
    e.g.: MS:1000139 (4000 QTRAP)
    e.g.: MS:1000140 (4700 Proteomics Analyzer)
    e.g.: MS:1000141 (apex IV)
    e.g.: MS:1000142 (apex Q)
    e.g.: MS:1000143 (API 150EX)
    e.g.: MS:1000144 (API 150EX Prep)
    e.g.: MS:1000145 (API 2000)
    e.g.: MS:1000146 (API 3000)
    e.g.: MS:1000147 (API 4000)
    e.g.: MS:1000148 (autoflex II)
    et al.
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000912" name="transition purported from an MS/MS spectrum
on a different, specified instrument"/>
<cvParam cvRef="MS" accession="MS:1000291" name="linear ion trap"/>
<cvParam cvRef="MS" accession="MS:1000042" name="peak intensity" value="10000"
unitCvRef="MS" unitAccession="MS:1000905" unitName="percent of base peak times 100"/>
<cvParam cvRef="MS" accession="MS:1000906" name="peak intensity rank" value="1"/>
<cvParam cvRef="MS" accession="MS:1000907" name="peak targeting suitability rank"
value="1"/>
```

3.36 Element <Target>

Definition: A peptide or compound that is to be included or excluded from a target list of precursor m/z values.

Type: TargetType

Attributes:

Attribute Name	Data Type	Use	Definition
compoundRef	xs:IDREF	optional	Reference to a compound for which this target is the trigger
id	xs:string	required	String label for this target
peptideRef	xs:IDREF	optional	Reference to a peptide for which this target is the trigger

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Precursor	1	1	Precursor (Q1) of the transition or target
RetentionTime	0	1	Information about predicted or calibrated retention time
ConfigurationList	0	1	List of insutrument configurations used in the validation or optimization of the transitions
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Target id="PEPTIDEC2+" peptideRef="PEPTIDEC">
  <Precursor>
    <cvParam cvRef="MS" accession="MS:1000827" name="isolation window target m/z"
value="862.9467" unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
    <cvParam cvRef="MS" accession="MS:1000041" name="charge state" value="2"/>
  </Precursor>
  <RetentionTime softwareRef="Skyline0.5">
    <cvParam cvRef="MS" accession="MS:1000895" name="local retention time" value="27.44"
unitCvRef="UO" unitAccession="UO:0000031" unitName="minute"/>
```

```
  ...
</Target>
```

3.37 Element <InterpretationList>

Definition: List of possible interprations of fragment ions for a transition

Type: InterpretationListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Interpretation	1	unbounded	A possible interpretation of the product ion for a transition

Example Context:

```
<InterpretationList>
  <Interpretation>
      <cvParam cvRef="MS" accession="MS:1000926" name="product interpretation rank"
value="1"/>
      <cvParam cvRef="MS" accession="MS:1001220" name="frag: y ion"/>
      <cvParam cvRef="MS" accession="MS:1000903" name="product ion series ordinal"
value="8"/>
      <cvParam cvRef="MS" accession="MS:1000904" name="product ion m/z delta" value="0.03"
unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
  </Interpretation>
  ...
</InterpretationList>
```

3.38 Element <ConfigurationList>

Definition: List of insutrument configurations used in the validation or optimization of the transitions

Type: ConfigurationListType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
Configuration	1	unbounded	Instrument configuration used in the testing, validation or optimization of the transitions

Example Context:

```
<ConfigurationList>
  <Configuration instrumentRef="QTRAP" contactRef="CS">
    <cvParam cvRef="MS" accession="MS:1000502" name="dwell time" value="0.12" unitCvRef="UO"
unitAccession="UO:0000010" unitName="second"/>
    <cvParam cvRef="MS" accession="MS:1000045" name="collision energy" value="26"
unitCvRef="UO" unitAccession="UO:0000266" unitName="electronvolt"/>
    <cvParam cvRef="MS" accession="MS:1000875" name="declustering potential" value="64"
unitCvRef="UO" unitAccession="UO:0000218" unitName="volt"/>
    <cvParam cvRef="MS" accession="MS:1000419" name="collision gas" value="argon"/>
    <cvParam cvRef="MS" accession="MS:1000869" name="collision gas pressure" value="12"
unitCvRef="UO" unitAccession="UO:0000110" unitName="pascal"/>
  ...
</ConfigurationList>
```

3.39 Element <Interpretation>

Definition: A possible interpretation of the product ion for a transition

Type: InterpretationType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one

			should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<Interpretation>
      <cvParam cvRef="MS" accession="MS:1000926" name="product interpretation rank"
value="2"/>
      <cvParam cvRef="MS" accession="MS:1001222" name="frag: b ion - H2O"/>
      <cvParam cvRef="MS" accession="MS:1000903" name="product ion series ordinal" value="9"/>
      <cvParam cvRef="MS" accession="MS:1000904" name="product ion m/z delta" value="-0.43"
unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
</Interpretation>
```

cvParam Mapping Rules:

```
Path /TraML/TransitionList/Transition/IntermediateProduct/InterpretationList/Interpretation
MUST 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:1001226 (product ion intensity)
  e.g.: MS:1001227 (product ion m/z error)
  et al.
MAY supply term MS:1000904 (product ion m/z delta) only once
MUST supply term MS:1000926 (product interpretation rank) only once
MUST supply term MS:1000903 (product ion series ordinal) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000926" name="product interpretation rank" value="1"/>
<cvParam cvRef="MS" accession="MS:1001220" name="frag: y ion"/>
<cvParam cvRef="MS" accession="MS:1000903" name="product ion series ordinal" value="8"/>
<cvParam cvRef="MS" accession="MS:1000904" name="product ion m/z delta" value="0.03"
unitCvRef="MS" unitAccession="MS:1000040" unitName="m/z"/>
<cvParam cvRef="MS" accession="MS:1001222" name="frag: b ion - H2O"/>
```

3.40 Element <Configuration>

Definition: Instrument configuration used in the testing, validation or optimization of the transitions

Type: ConfigurationType

Attributes:

Attribute Name	Data Type	Use	Definition
contactRef	xs:IDREF	optional	Reference to a contact person originating this information
instrumentRef	xs:IDREF	required	Reference to an instrument for which this configuration information is appropriate

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition
cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead
ValidationStatus	0	unbounded	Information about the state of validation of a transition on a given instrument model

Example Context:

```
<Configuration instrumentRef="QTRAP" contactRef="CS">
  <cvParam cvRef="MS" accession="MS:1000502" name="dwell time" value="0.12" unitCvRef="UO"
unitAccession="UO:0000010" unitName="second"/>
  <cvParam cvRef="MS" accession="MS:1000045" name="collision energy" value="26"
unitCvRef="UO" unitAccession="UO:0000266" unitName="electronvolt"/>
  <cvParam cvRef="MS" accession="MS:1000875" name="declustering potential" value="64"
unitCvRef="UO" unitAccession="UO:0000218" unitName="volt"/>
```

cvParam Mapping Rules:

```
  <cvParam cvRef="MS" accession="MS:1000419" name="collision gas" value="argon"/>
  <cvParam cvRef="MS" accession="MS:1000869" name="collision gas pressure" value="12"
unitCvRef="UO" unitAccession="UO:0000110" unitName="pascal"/>
  <cvParam cvRef="MS" accession="MS:1000876" name="cone voltage" value="1200" unitCvRef="UO"
unitAccession="UO:0000218" unitName="volt"/>
  ...
</Configuration>
Path /TraML/TargetList/TargetIncludeList/Target/ConfigurationList/Configuration
MAY supply a *child* term of MS:1000482 (source attribute) one or more times
  e.g.: MS:1000392 (ionization efficiency)
  e.g.: MS:1000486 (source potential)
  e.g.: MS:1000843 (wavelength)
  e.g.: MS:1000844 (focus diameter x)
  e.g.: MS:1000845 (focus diameter y)
  e.g.: MS:1000846 (pulse energy)
  e.g.: MS:1000847 (pulse duration)
  e.g.: MS:1000848 (attenuation)
  e.g.: MS:1000849 (impact angle)
  e.g.: MS:1000850 (gas laser)
  et al.
MAY supply a *child* term of MS:1000510 (precursor activation attribute) one or more times
  e.g.: MS:1000045 (collision energy)
  e.g.: MS:1000138 (percent collision energy)
  e.g.: MS:1000245 (charge stripping)
  e.g.: MS:1000412 (buffer gas)
  e.g.: MS:1000419 (collision gas)
  e.g.: MS:1000509 (activation energy)
  e.g.: MS:1000869 (collision gas pressure)
MAY supply term MS:1000502 (dwell time) only once
Path /TraML/TransitionList/Transition/Product/ConfigurationList/Configuration
MAY supply a *child* term of MS:1000482 (source attribute) one or more times
  e.g.: MS:1000392 (ionization efficiency)
  e.g.: MS:1000486 (source potential)
  e.g.: MS:1000843 (wavelength)
  e.g.: MS:1000844 (focus diameter x)
  e.g.: MS:1000845 (focus diameter y)
  e.g.: MS:1000846 (pulse energy)
  e.g.: MS:1000847 (pulse duration)
  e.g.: MS:1000848 (attenuation)
  e.g.: MS:1000849 (impact angle)
  e.g.: MS:1000850 (gas laser)
  et al.
MAY supply a *child* term of MS:1000510 (precursor activation attribute) one or more times
  e.g.: MS:1000045 (collision energy)
  e.g.: MS:1000138 (percent collision energy)
  e.g.: MS:1000245 (charge stripping)
  e.g.: MS:1000412 (buffer gas)
  e.g.: MS:1000419 (collision gas)
  e.g.: MS:1000509 (activation energy)
  e.g.: MS:1000869 (collision gas pressure)
MAY supply term MS:1000502 (dwell time) only once
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000502" name="dwell time" value="0.12" unitCvRef="UO"
unitAccession="UO:0000010" unitName="second"/>
<cvParam cvRef="MS" accession="MS:1000045" name="collision energy" value="26" unitCvRef="UO"
unitAccession="UO:0000266" unitName="electronvolt"/>
<cvParam cvRef="MS" accession="MS:1000875" name="declustering potential" value="64"
unitCvRef="UO" unitAccession="UO:0000218" unitName="volt"/>
<cvParam cvRef="MS" accession="MS:1000419" name="collision gas" value="argon"/>
<cvParam cvRef="MS" accession="MS:1000869" name="collision gas pressure" value="12"
unitCvRef="UO" unitAccession="UO:0000110" unitName="pascal"/>
<cvParam cvRef="MS" accession="MS:1000876" name="cone voltage" value="1200" unitCvRef="UO"
unitAccession="UO:0000218" unitName="volt"/>
<cvParam cvRef="MS" accession="MS:1000880" name="interchannel delay" value="0.01"
unitCvRef="UO" unitAccession="UO:0000010" unitName="second"/>
<cvParam cvRef="MS" accession="MS:1000877" name="tube lens voltage" value="23" unitCvRef="UO"
unitAccession="UO:0000218" unitName="volt"/>
```

3.41 Element <ValidationStatus>

Definition: Information about the state of validation of a transition on a given instrument model

Type: ValidationStatusType

Attributes: none

Subelements:

Subelement Name	minOccurs	maxOccurs	Definition

cvParam	0	unbounded	Controlled vocabulary term adding information to the parent term
userParam	0	unbounded	Uncontrolled user parameters (essentially allowing free text). Before using these, one should verify whether there is an appropriate CV term available, and if so, use the CV term instead

Example Context:

```
<ValidationStatus>
        <cvParam cvRef="MS" accession="MS:1000910" name="transition optimized on specified
instrument"/>
        <cvParam cvRef="MS" accession="MS:1000139" name="4000 QTRAP"/>
        <cvParam cvRef="MS" accession="MS:1000042" name="peak intensity" value="4072"
unitCvRef="MS" unitAccession="MS:1000905" unitName="percent of base peak times 100"/>
        <cvParam cvRef="MS" accession="MS:1000906" name="peak intensity rank" value="2"/>
        <cvParam cvRef="MS" accession="MS:1000907" name="peak targeting suitability rank"
value="1"/>
</ValidationStatus>
```

cvParam Mapping Rules:

```
Path /TraML/TransitionList/Transition/ConfigurationList/Configuration/ValidationStatus
MAY supply term MS:1000042 (peak intensity) only once
MAY supply a *child* term of MS:1000909 (transition validation method) only once
  e.g.: MS:1000910 (transition optimized on specified instrument)
  e.g.: MS:1000911 (transition validated with an MS/MS spectrum on specified instrument)
  e.g.: MS:1000912 (transition purported from an MS/MS spectrum on a different, specified
instrument)
  e.g.: MS:1000913 (transition predicted by informatic analysis)
MAY supply term MS:1000906 (peak intensity rank) only once
MAY supply term MS:1000907 (peak targeting suitability rank) only once
MAY supply term MS:1000031 (instrument model) or any of its children only once
  e.g.: MS:1000139 (4000 QTRAP)
  e.g.: MS:1000140 (4700 Proteomics Analyzer)
  e.g.: MS:1000141 (apex IV)
  e.g.: MS:1000142 (apex Q)
  e.g.: MS:1000143 (API 150EX)
  e.g.: MS:1000144 (API 150EX Prep)
  e.g.: MS:1000145 (API 2000)
  e.g.: MS:1000146 (API 3000)
  e.g.: MS:1000147 (API 4000)
  e.g.: MS:1000148 (autoflex II)
  et al.
```

Example cvParams:

```
<cvParam cvRef="MS" accession="MS:1000910" name="transition optimized on specified
instrument"/>
<cvParam cvRef="MS" accession="MS:1000139" name="4000 QTRAP"/>
<cvParam cvRef="MS" accession="MS:1000042" name="peak intensity" value="4072" unitCvRef="MS"
unitAccession="MS:1000905" unitName="percent of base peak times 100"/>
<cvParam cvRef="MS" accession="MS:1000906" name="peak intensity rank" value="2"/>
<cvParam cvRef="MS" accession="MS:1000907" name="peak targeting suitability rank" value="1"/>
```

Notes and Constraints:

If the "peak intensity" cvParam is used, its absolute units is not important. However, it MUST be proportional to other fragment ions from the same precursor. Ideally it will also be proportional to the intensities for other peptide ions from the same protein.

4. Conclusions

This document contains the specifications for using the TraML format to represent SRM transitions for monitoring biomolecular compounds via mass spectrometry. This specification, in conjunction with the XML schema, controlled vocabulary, and mapping file, 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 the PSI.

5. Authors and Contributors

Eric W. Deutsch

Institute for Systems Biology
1441 N 34th St,
Seattle WA 98103-8904
United States of America
edeutsch@systemsbiology.org

Matthew Chambers
Department of Biomedical Informatics
465 21st Ave S. Room 9160, Medical Research Building III
Vanderbilt University
Nashville, TN 37232
United States of America
matthew.chambers@vanderbilt.edu

Steffen Neumann
Leibniz Institute of Plant Biochemistry
Halle
Germany

Andreas Bertsch
Center for Bioinformatics
Eberhard Karls University Tübingen
Sand 14
72076 Tübingen
Germany
bertsch@informatik.uni-tuebingen.de

Fredrik Levander
Department of Immunotechnology
Lund University
Biomedical Centre D13, S-221
84 Lund
Sweden
Fredrik.Levander@immun.lth.se

Jim Shofsthal
Thermo Fisher Scientific
San Jose, CA
United States of America

Pierre-Alain Binz
Swiss Institute of Bioinformatics
Proteome Informatics Group
1, Rue Michel Servet
CH-1211 Geneve 4
Switzerland
Pierre-Alain.Binz@isb-sib.ch

Mi-Youn Brusniak
Institute for Systems Biology
1441 N 34th St,
Seattle WA 98103-8904
United States of America
mbrusniak@systemsbiology.org

The following people contributed to the model development, controlled vocabulary development, gave feedback or tested TraML or assisted with the manuscript:

- Mark Christiansen (Institute for Systems Biology)
- David Campbell (Institute for Systems Biology)
- Luis Mendoza (Institute for Systems Biology)
- Robert L. Moritz (Institute for Systems Biology)
- David Ovelleiro (European Bioinformatics Institute)
- Kenny Helsens (University of Gent)
- Lennart Martens (University of Gent)
- Ruedi Aebersold (Institute of Molecular Systems Biology, ETH Zurich)

6. References

Bradner, S. (1997). "Key words for use in RFCs to Indicate Requirement Levels, Internet Engineering Task Force, RFC 2119, http://www.ietf.org/rfc/rfc2119.txt."

Jones, A. R., M. Miller, et al. (2007). "The Functional Genomics Experiment model (FuGE): an extensible framework for standards in functional genomics." Nat Biotechnol **25**(10): 1127-1133.

7. Intellectual Property Statement

The PSI takes no position regarding the validity or scope of any intellectual property or other rights that might be claimed to pertain to the implementation or use of the technology described in this document or the extent to which any license under such rights might or might not be available; neither does it represent that it has made any effort to identify any such rights. Copies of claims of rights made available for publication and any assurances of licenses to be made available, or the result of an attempt made to obtain a general license or permission for the use of such proprietary rights by implementers or users of this specification can be obtained from the PSI Chair.

The PSI invites any interested party to bring to its attention any copyrights, patents or patent applications, or other proprietary rights which may cover technology that may be required to practice this recommendation. Please address the information to the PSI Chair (see contacts information at PSI website).

8. Appendix A: Using TraML as a subschema in mzML

It is currently envisioned that one might be able to use the TraML schema as a subschema in mzML. It is not known how this might be done exactly, but this section will explain it once we figure it out.

Copyright Notice

other organizations, except as needed for the purpose of developing Proteomics Recommendations in which case the procedures for copyrights defined in the PSI Document process must be followed, or as required to translate it into languages other than English.

The limited permissions granted above are perpetual and will not be revoked by the PSI or its successors or assigns.

This document and the information contained herein is provided on an "AS IS" basis and THE PROTEOMICS STANDARDS INITIATIVE DISCLAIMS ALL WARRANTIES, EXPRESS OR IMPLIED, INCLUDING BUT NOT LIMITED TO ANY WARRANTY THAT THE USE OF THE INFORMATION HEREIN WILL NOT INFRINGE ANY RIGHTS OR ANY IMPLIED WARRANTIES OF MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE."