SBML Level 3 Package Specification

PMF

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The latest release, past releases, and other materials related to this specification are available at
http://sbml.org/Documents/Specifications/PMF

This release of the specification is available at
http://sbml.org/Documents/Specifications/PMF_1_February_2017

Contents

1 Introduction

The encoding of predictive microbial models may require a significant amount of model meta data. SBML proves to be a major step in the right direction though it does not describe completely some models.

The SBML Level 3 PMF package addresses these shortcomings, extending SBML with extra classes and attributes in order to achieve a more meaningful and accurate description of the models.

1.1 Proposal corresponding to this package specification

This specification for PMF in SBML Level 3 Version 1 is based on the proposal located at the following URL:

https://sbml.svn.sf.net/svnroot/sbml/trunk/specifications/sbml-level-3/version-1/groups/proposal

The tracking number in the SBML issue tracking system (**?**) for Groups package activities is 2847474. The version of the proposal used as the starting point for this specification is the version of June, 2012 (**?**).

1.2 Package dependencies

The PMF package has no dependencies on other SBML Level 3 packages.

1.3 Document conventions

UML 1.0 (Unified Modeling Language; **??**) notation is used in this document to define the constructs provided by this package. Colors in the diagrams carry the following additional information for the benefit of those viewing the document on media that can display color:

■ *Black*: Items colored black in the UML diagrams are components taken unchanged from their definition in the SBML Level 3 Core specification document.

■ *Green*: Items colored green are components that exist in SBML Level 3 Core, but are extended by this package. Class boxes are also drawn with dashed lines to further distinguish them.

■ *Blue*: Items colored blue are new components introduced in this package specification. They have no equivalent in the SBML Level 3 Core specification.

The following typographical conventions distinguish the names of objects and data types from other entities; these conventions are identical to the conventions used in the SBML Level 3 Core specification document:

AbstractClass: Abstract classes are never instantiated directly, but rather serve as parents of other classes. Their names begin with a capital letter and they are printed in a slanted, bold, sans-serif typeface. In electronic document formats, the class names defined within this document are also hyperlinked to their definitions; clicking on these items will, given appropriate software, switch the view to the section in this document containing the definition of that class. (However, for classes that are unchanged from their definitions in SBML Level 3 Core, the class names are not hyperlinked because they are not defined within this document.)

Class: Names of ordinary (concrete) classes begin with a capital letter and are printed in an upright, bold, sans-serif typeface. In electronic document formats, the class names are also hyperlinked to their definitions in this specification document. (However, as in the previous case, class names are not hyperlinked if they are for classes that are unchanged from their definitions in the SBML Level 3 Core specification.)

`SomeThing`, `otherThing`: Attributes of classes, data type names, literal XML, and tokens *other* than SBML class names, are printed in an upright typewriter typeface.

For other matters involving the use of UML and XML, this document follows the conventions used in the SBML Level 3 Core specification document.

2 Background and context

The encoding of Quantitative Microbial Risk Assessment (QMRA) models requires special meta data that is not present in SBML. The Predictive Microbial Modelling in Food Markup Language (PMF-ML) addressed this challenge, extending SBML to describe more precisely QMRA models.

The strategy followed by PMF-ML was to further annotate SBML constructs such as Model and Rule with extra information carefully encoded within the annotation of this element.

While this strategy was relatively simple to implement its shortcomings eventually appeared, like difficult validation, hard maintenance or inability to supporting different implementations for different versions of SBML. This extension package aspires to address these issues.

3 Package syntax and semantics

This section contains a definition of the syntax and semantics of the PMF package for SBML Level 3 Version 1 Core. The PMF package involves the following new object classes:

- **CompartmentMetaData**
- **Correlation**
- **DataSource**
- **ListOfCorrelations**
- **ListOfDataSources**
- **ListOfModelVariables**
- **ListOfPrimaryModels**
- **ListOfReferences**
- **ModelVariable**
- **ParameterMetaData**
- **PrimaryModel**
- **Reference**
- **RuleMetaData**
- **SpeciesMetaData**
- **UnitTransformation**

?? on page ?? contains complete examples of using the constructs in SBML models.

3.1 Namespace URI and other declarations necessary for using this package

Every SBML Level 3 package is identified uniquely by an XML namespace URI. For an SBML document to be able to use a given Level 3 package, it must declare the use of that package by referencing its URI. The following is the namespace URI for this version of the PMF package for SBML Level 3 Version 1 Core:

"`http://www.sbml.org/sbml/level3/version1/pmf/version1`"

In addition, SBML documents using a given packge must indicate whether the package can be used to change the mathematical interpretation of a model. This is done using the attribute `required` on the `<sbml>` element in the SBML document. For the PMF package, the value of this attribute must be "`false`", because the use of the PMF package cannot change the mathematical meaning of a model.

The following fragmen illustrates the beginning of a typical SBML model using SBML Level 3 Version 1 Core and this version of the PMF package.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http:/www.sbml.org/sbml/level3/version1/core" level="3" version="1"
  xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1"
  pmf:required="false">
```

"unknown"
"growth"
"inactivation"
"survival"
"growth/inactivation"
"inactivation/survival"
"growth/survival"
"growth/inactivation/survival"
"T"
"PH"
"aw"
"T/pH"
"T/aw"
"pH/aw"
"T/pH/aw"

Table 1: *Possible values for* `ModelClass`
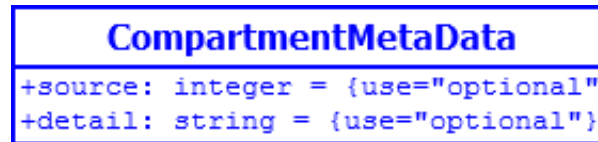
Figure 1: *Class diagram of CompartmentMetaData*

3.2 Primitive data types

The PMF package includes a new primitve data type, the `ModelClass`.

3.2.1 Type `ModelClass`

The `ModelClass` primitive data type is used in the deefinition of the **RuleMetaData** class. `ModelClass` is derived from type `string` and its values are restricted to being one of the possibilities listed in Table 1.

Attributes of type `ModelClass` cannot take on any other values. The meaning of these values is discussed in the context of the **RuleMetaData** class definition in Section 3.3.3 on the following page.

3.3 Meta data classes

The PMF package extends a number of classes from SBML Level 3 Version 1 with the addition of meta data classes. These classes act as place holders for extra meta data. The newly introduced meta data classes are:

■ **CompartmentMetaData**

■ **ParameterMetaData**

■ **RuleMetaData**

■ **SpeciesMetaData**

3.3.1 The CompartmentMetaData class

The **CompartmentMetaData** further describes a Compartment with two attributes: `source` and `detail`. Figure 1 provides the UML diagram of its definition.
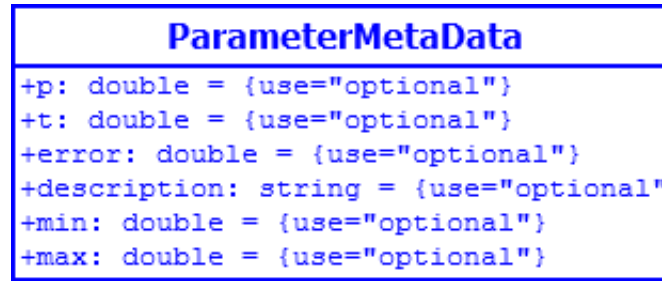
Figure 2: *Class diagram of ParameterMetaData*

The source attribute

The optional attribute `source` contains a signed integer refering to the PMF matrix vocabulary.

The detail attribute

The optional attribute `detail` contains a string with extra details of the **Compartment** object.

3.3.2 The ParameterMetaData class

The **ParameterMetaData** further describes a Parameter with the optional attributes: `p`, `t`, `error`, `description`, `min` and `max`. Figure 2 provides the UML diagram of its definition.

The `p` attribute

The optional attribute `p` contains a `double` with the partition coefficient (P) of the parameter.

The `t` attribute

The optional attribute `t` contains a `double` with the *t-statistic* of the parameter.

The `error` attribute

The optional attribute `error` contains a `double` with the *error* of the parameter.

The `description` attribute

The optional attribute `description` contains a `string` with the description of the parameter.

The `min` attribute

The optional attribute `min` contains a `double` with the minimum value of the parameter.

The `max` attribute

The optional attribute `max` contains a `double` with the maximum value of the parameter.

Figure 11 on page 12 features an example of **ParameterMetaData**.

3.3.3 The RuleMetaData class

The **RuleMetaData** further describes a **Rule** with the optional attributes: `formulaName`, `pmmLabId` and `modelClass`. Figure 3 on the following page provides the UML diagram of its definition.
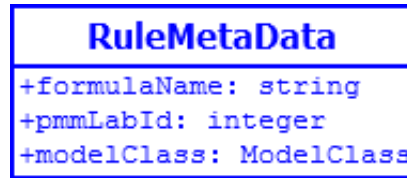
The `formulaName` attribute

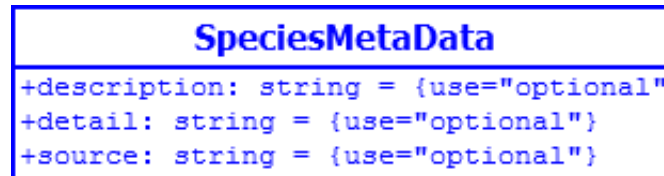The formulaName attribute

Figure 3: Class diagram of RuleMetaData

Figure 4: Class diagram of SpeciesMetaData

The `pmmLabId` *attribute*

Optional attribute of type `integer` with the PmmLab id.

The `modelClass` *attribute*

Optional attribute of type ModelClass with the class of the model.

3.3.4 The SpeciesMetaData class

The **SpeciesMetaData** further describes a **Species** with the optional attributes: `source`, `detail` and `description`. Figure 4 provides the UML diagram of its definition.

The `source` *attribute*

Optional attribute of type `string` with the source of the species

The `detail` *attribute*

Optional attribute of type `string` with the detail of the species

The `description` *attribute*

Optional attribute of type `ModelClass` with the class of the model.

```
<species compartment="Culture_medium" boundaryCondition="false" constant="false"
  id="some_species" hasOnlySubstanceUnits="true">
  <pmf:parameterMetaData xlmns:pmf="http://www.sbml.org/sbml3/version1/pmf/version1"
    description="bacterial_population_at_time-ln()" detail="Salmonella_spec"
    source="http://identifiers.org/ncim/C0036111" />
</species>
```

3.4 New classes

The PMF package also includes a number of new elements.

- **Correlation**

- **DataSource**

- **ModelVariable**
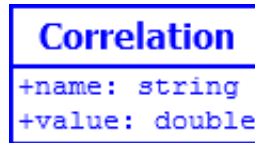
Figure 5: *Class diagram of Correlation*

Figure 6: *Class diagram of DataSource*

- **Reference**
- **UnitTransformation**

3.4.1 The Correlation class

The **Correlation** expresses the existing dependence between the current **Parameter** and a second **Parameter**. It involves two attributes: `name` and `value`. Figure 5 provides its UML diagram.

The name attribute

Mandatory attribute with the name of the second parameter.

The value attribute

Mandatory attribute with the value of the dependence with the second parameter.

3.4.2 The DataSource class

The **DataSource** is used to link to a separated file with numerical data associated to the model. Figure 6 provides its UML diagram.

3.4.3 The ModelVariable class

The **ModelVariable** is used to describe a variable of the model such as temperature, water activity, pH, etc. Figure 7 provides its UML diagram.

3.4.4 The PrimaryModel class

The **PrimaryModel** is used to link to a meta data file describing a primary model with current model. Figure 11 on page 12 provides its UML diagram.
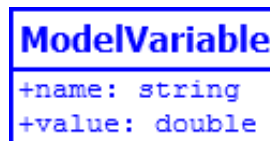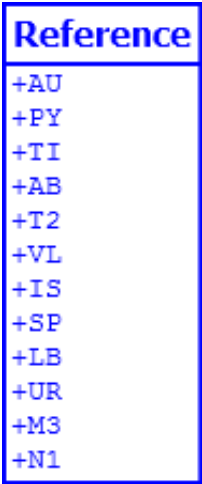

Figure 7: *Class diagram of ModelVariable*

Reference

```
+AU
+PY
+TI
+AB
+T2
+VL
+IS
+SP
+LB
+UR
+M3
+N1
```

Figure 8: *Class diagram of Reference*

Attribute	Description
AU	String with the author
PY	String with the publication year
TI	String with the title.
AB	String with the abstract.
T2	String with the journal.
VL	String with the volume.
IS	String with the issue.
SP	Integer with the page.
LB	Integer with the approval mode.
UR	String with the website.
M3	String with the type of literature.
N1	String with a comment.

Table 2: *Attributes of the **Reference** class*

3.4.5 The Reference class

The **Reference** class is used to annotate a literature reference associated to the model. It involves the following attributes. All the attributes of the **Reference** class are optional. The attributes are encoded using a subset of the RIS specification format as described in Table 2. Figure 8 provides its UML diagram.

```
<pmf:reference
  xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version"
  AU="Baranyi,_J" PY="1995" TI="Mathematics_of_predictive_food_microbiology"
  AB="Commonly_encountered_problems_related_to_..." VL="26" IS="2" SP="199" />
```

UnitTransformation

```
+name: string = {use="optional"}
```

Figure 9: *Class diagram of UnitTransformation*

ListOf_____ class	Contained class
ListOfCorrelations	**Correlation**
ListOfDataSources	**DataSource**
ListOfModelVariables	**ModelVariable**
ListOfPrimaryModels	**PrimaryModel**
ListOfReferences	**Reference**

*Table 3: New **ListOf**_____ classes*

3.4.6 The UnitTransformation class

The **UnitTransformation** further describes a **UnitDefinition** with the optional attribute transformation, of type `string`, which holds the transformation of the **UnitDefinition**. Figure 9 on the preceding page provides the UML diagram of its defintion. Figure 15 on page 14 sports an example of **UnitTransformation**.

3.5 New ListOf___ classes

The PMF package introduces new classes extending the **ListOf**_____ class. These classes are derived from *SBase* and inherit the attributes `metaid` and `sboTerm`, as well as the subcomponents for **Annotation** and **Notes**. There are not empty lists, the lists must contain at least one object. The list contain only one type of object.

3.6 Extended classes

- ■ **Compartment**

- ■ **Model**

- ■ **Parameter**

- ■ **Rule**

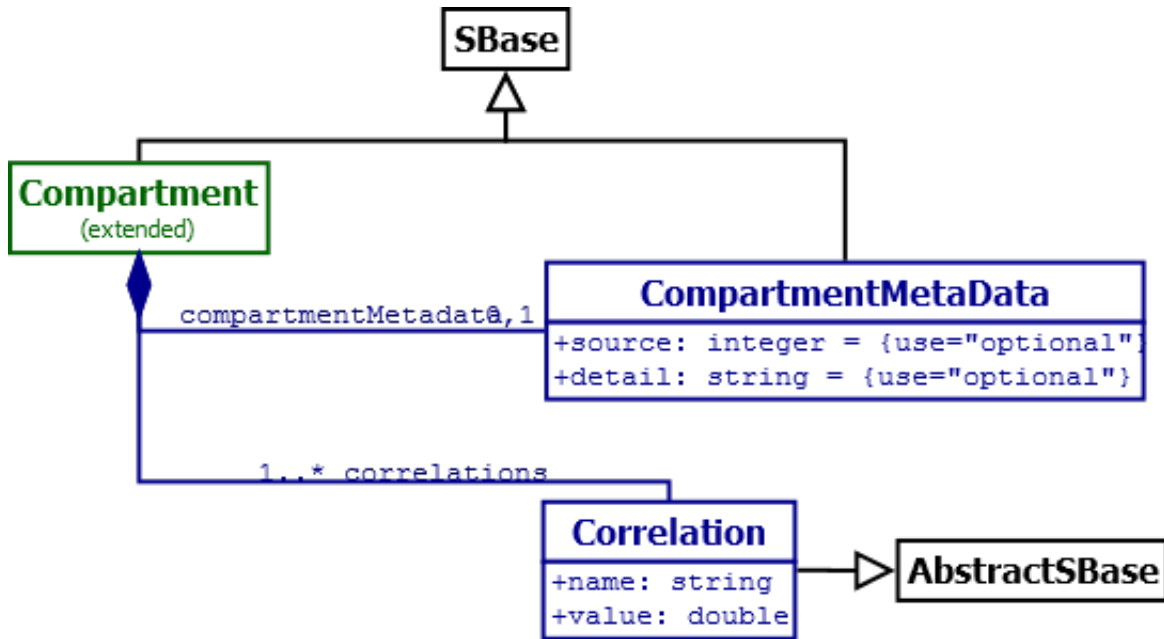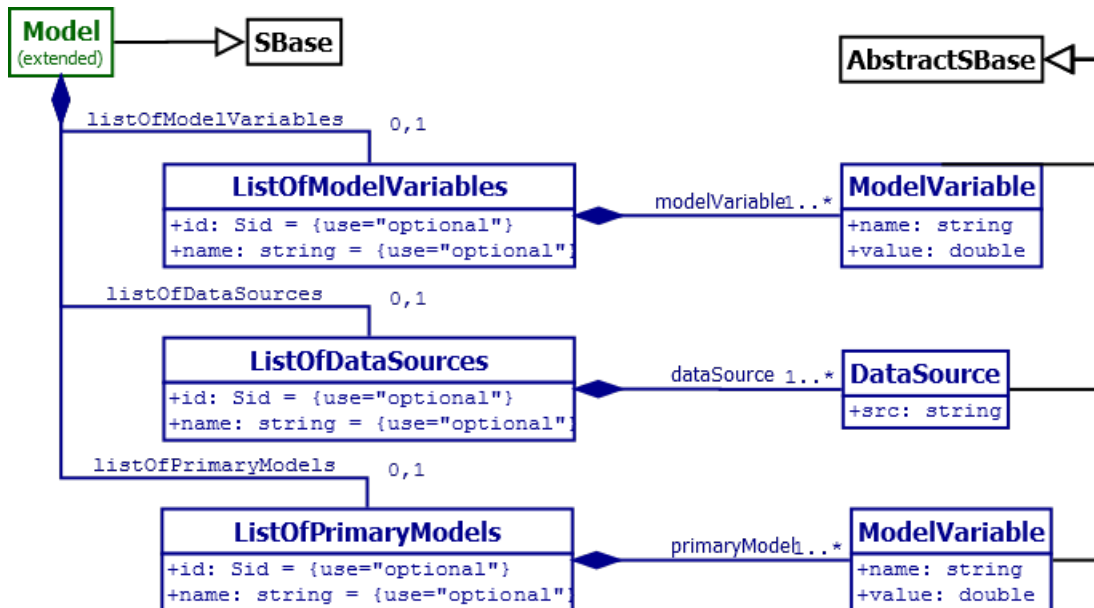- ■ **Species**

- ■ **UnitDefinition**

3.6.1 Compartment

The **Compartment** class is extended with one **CompartmentMetaData** to hold extra meta data related to the compartment. Figure 10 on the following page provides the UML diagram for the extension.

```
<compartment id="Culture_medium" name="Culture_medium" constant="true"
  <pmf:compartmentMetaData xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1"
    detail="broth" source="36">
</compartment>
```

3.6.2 Model

The **Model** class is extended with the optional lists **ListOfPrimaryModels**, **ListOfDataSources** and **ListOfPrimaryModels**. Figure 11 on the next page provides the UML diagram for the extension.

```
<model id="model">
  <pmf:listOfModelVariables xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1">
    <pmf:modelVariable name="pH" value="5.0" />
    <pmf:modelVariable name="T" value="20.0" />
  </pmf:listOfModelVariables>
  <pmf:listOfPrimaryModels xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1">
    <pmf:primaryModel src="someModel.sbml" />
  </pmf:listOfPrimaryModels>
```

Figure 10: *Class diagram of extended* **Compartment**

Figure 11: *Class diagram of extended* **Model**

```
  <pmf:listOfDataSources                                                                      1
    xlmns:pmf="xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1">             2
    <pmf:dataSource src="someData.numl" />                                                    3
  </pmf:listOfDataSources>                                                                    4
</model>                                                                                      5
                                                                                             6
```
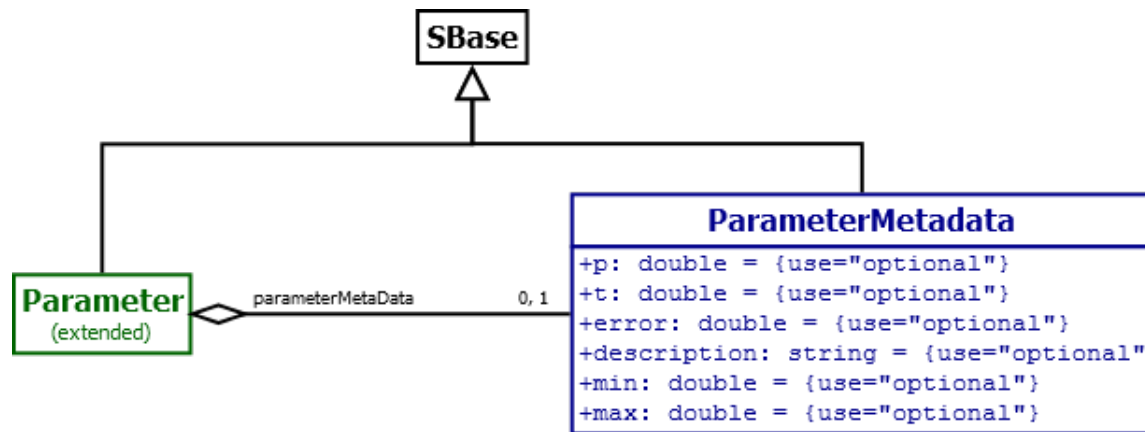
3.6.3 Parameter   7

The **Parameter** class is extended with one **ListOfCorrelations** and one optional **ParameterMetaData**.   8

Figure 12: *Class diagram of extended* **Parameter**

```
<parameter constant="false" id="p" value="0">
  <pmf:parameterMetaData xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1">
  <pmf:listOfCorrelations xlmns:pmf="http://wwww.sbml.org/sbml/level3/version1/pmf/version1">
    <pmf:correlation name="a" value="1" />
    <pmf:correlation name="b" value="2" />
  </pmf:listOfCorrelations>
</parameter>
```

3.6.4 Rule

The **Rule** class is extended with a **ListOfReferences** and one optional **RuleMetaData**.

```
<algebraicRule>
  <math xmlns="http://www.w3.org/1998/Math/MathML">
    <plus/>
    <cn>2</cn>
    <cn>2</cn>
  </math>
  <pmf:ruleMetaData xmlns:pmf="https://www.sbml.org/sbml/level3/version1/pmf/version1"
    formulaName="2_plus_2" ruleClass="growth" pmmLabID="1" />
</algebraicRule>
```

3.6.5 Species

The **Species** class is extended with one optional **SpeciesMetaData**.

```
<species compartment="Culture_medium" boundaryCondition="false" constant="false"
  id="some_species" hasOnlySubstanceUnits="true">
  <pmf:speciesMetaData xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1"
    description="bacterial_population_at_time_t-ln()" detail="Salmonella_spec"
    source="http://identifiers.org/ncim/C0036111" />
</species>
```

3.6.6 UnitDefinition

The **UnitTransformation** class is extended with an optional **UnitTransformation**.

```
<unitDefinition id="ln_count_g" name="ln(count/g)">
  <pmf:unitTransformation xmlns:pmf="http://www.sbml.org/sbml/level3/version1/pmf/version1"
    name="ln" />
```
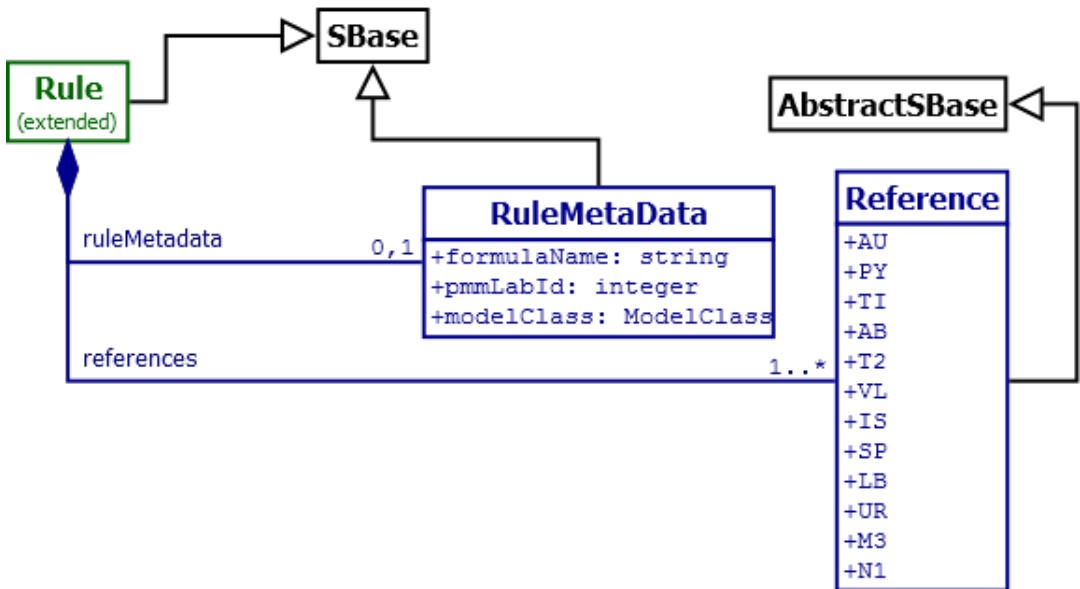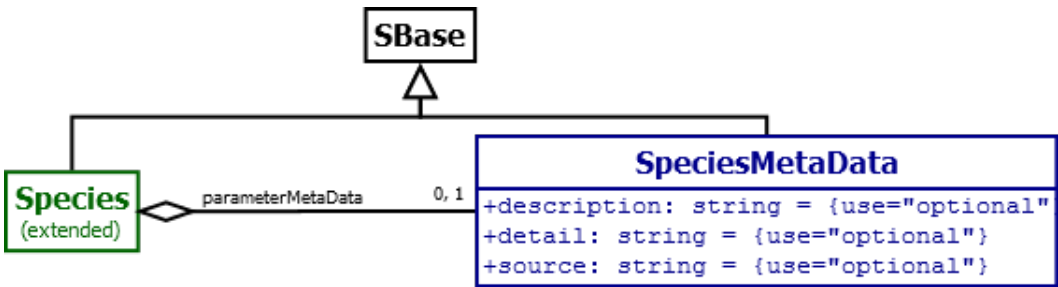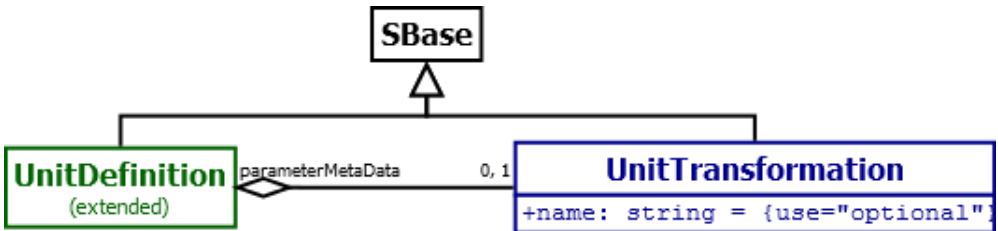
Figure 13: Class diagram of extended **Rule**

Figure 14: Class diagram of extended **Species**

```
</unitDefinition>
```


Figure 15: Class diagram of extended **UnitDefinition**

4 Examples

...