

SBML to BioPAX

MIRIAM Annotations in use

Camille Laibe

CellML Workshop, New Zealand, April 2009



- MIRIAM
- SBML to BioPAX conversion



MIRIAM

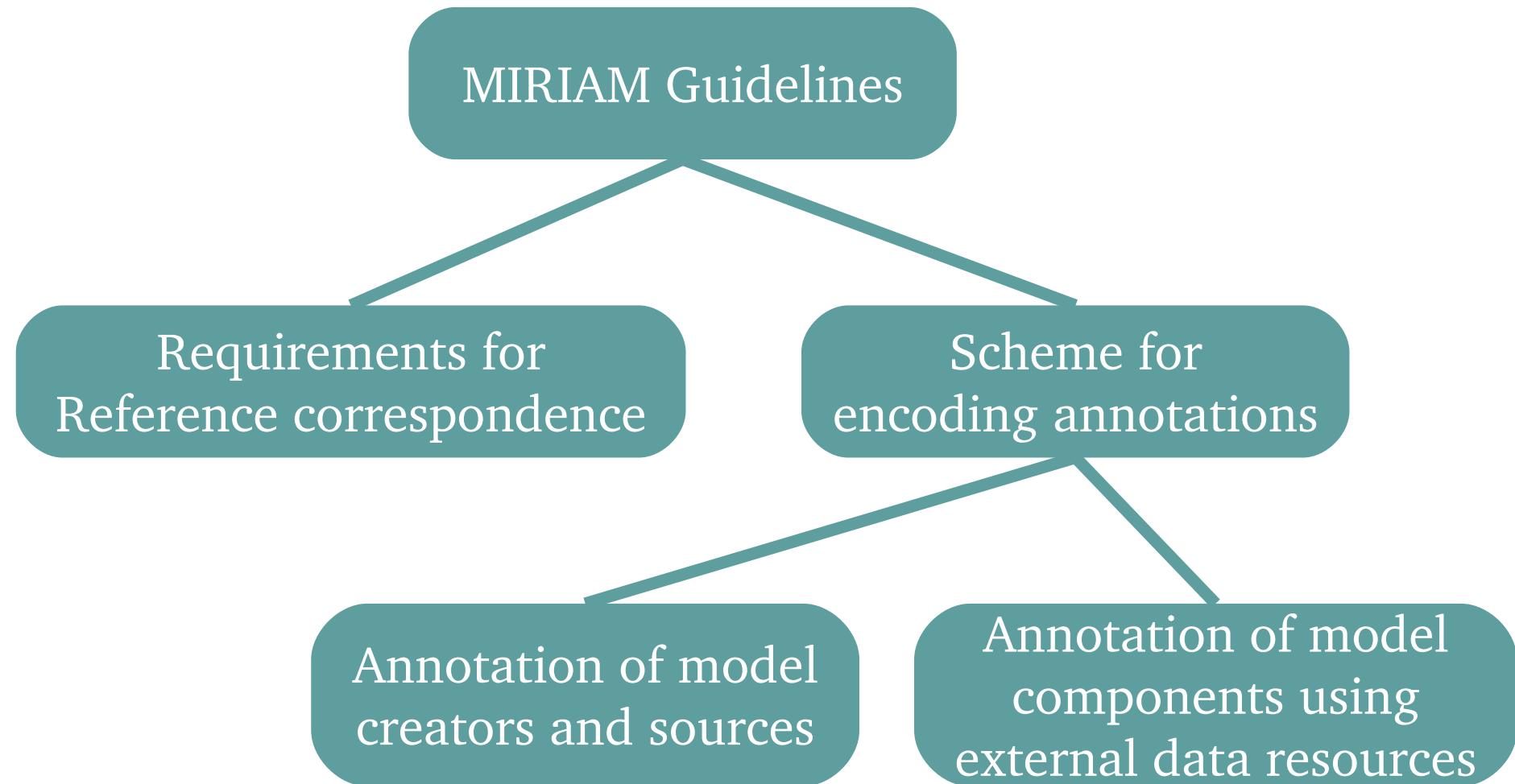
Minimum Information Requested In the
Annotation of (biochemical)
Models

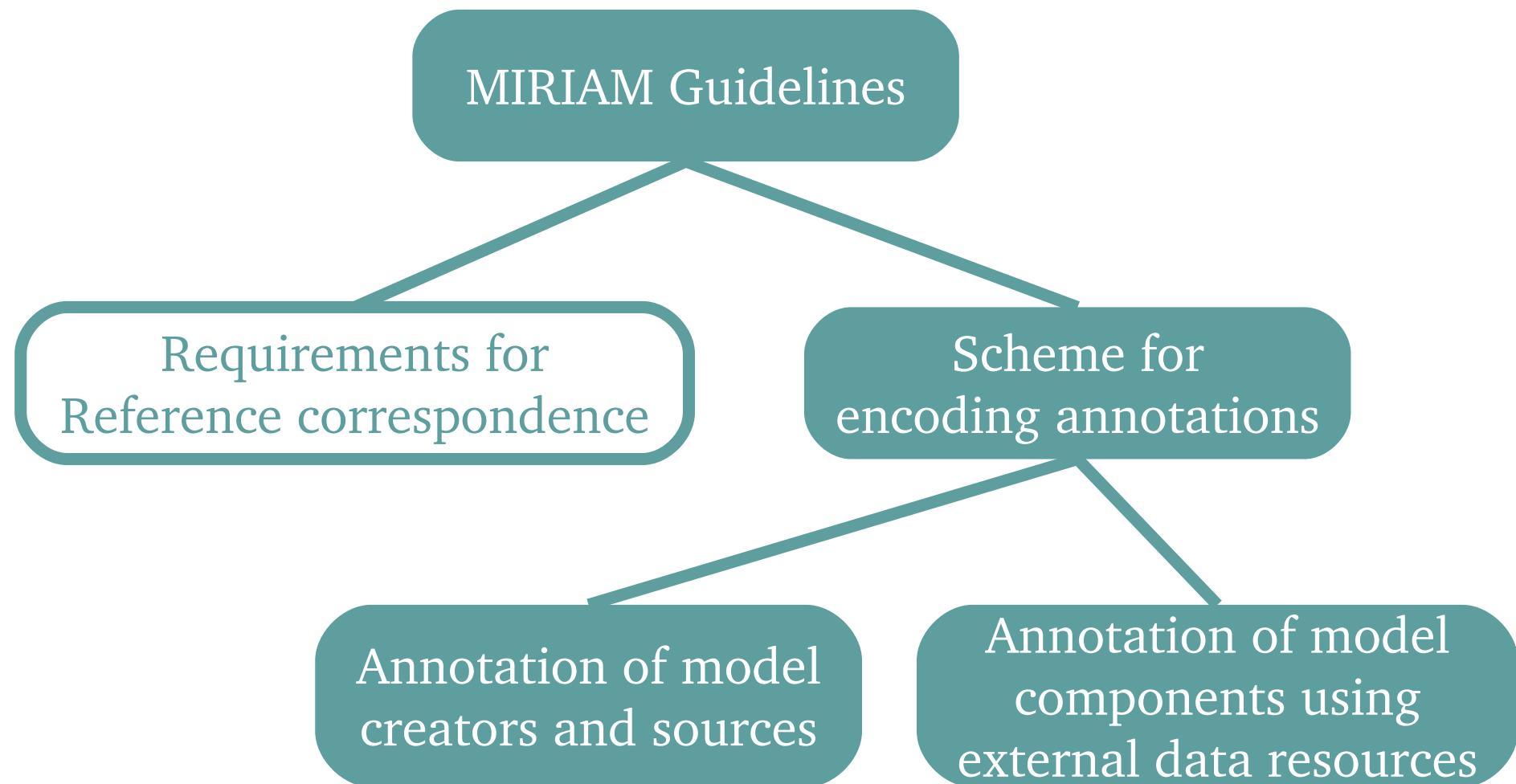


MIRIAM Standard: proposed guidelines for curation and annotation of quantitative models

cf. Nicolas Le Novère *et al.* **Minimum Information Requested in the Annotation of biochemical Models (MIRIAM).** *Nature Biotechnology*, 2005





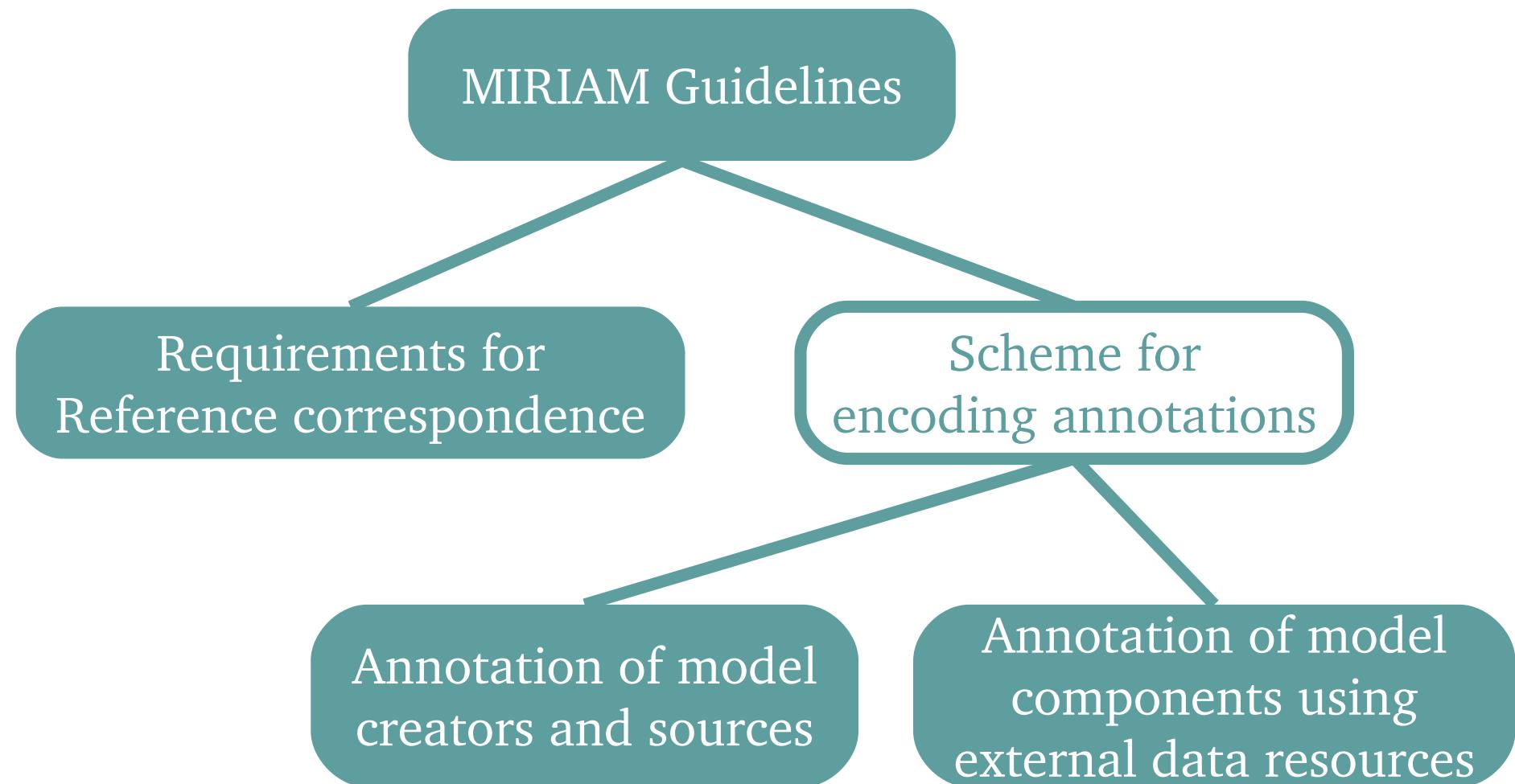


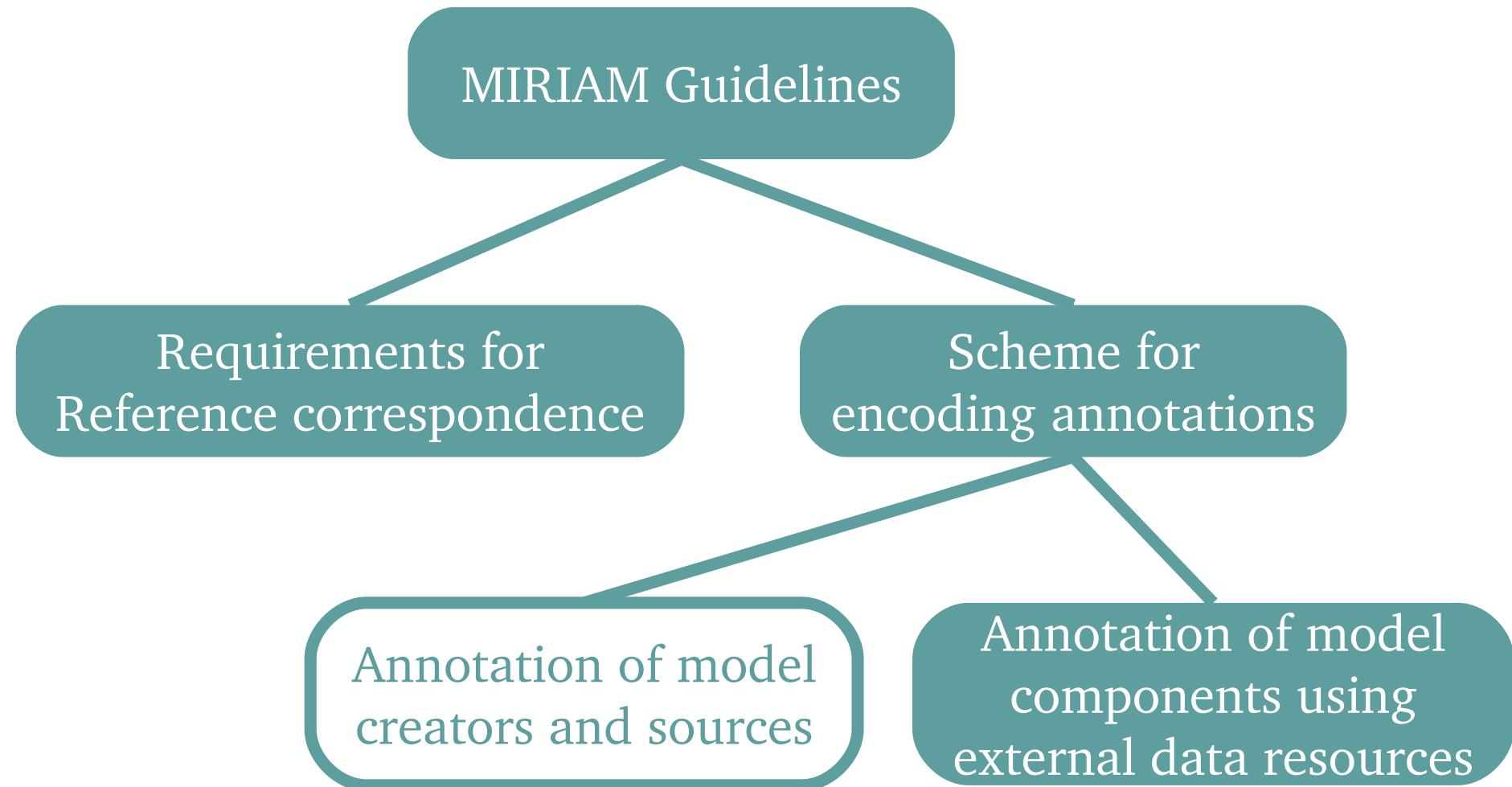
- model encoded in a public, standardised, **machine-readable format**
- model valid with the **standard** in which it is encoded
- model related to a single **reference description**



- encoded model structure must **reflect the biological processes** listed in the reference description
- model must be **instantiated in a simulation**: all quantitative attributes have to be defined, including initial conditions
- when instantiated, the model must be able to **reproduce all results** given in the reference description within an epsilon (algorithms, round-up errors)

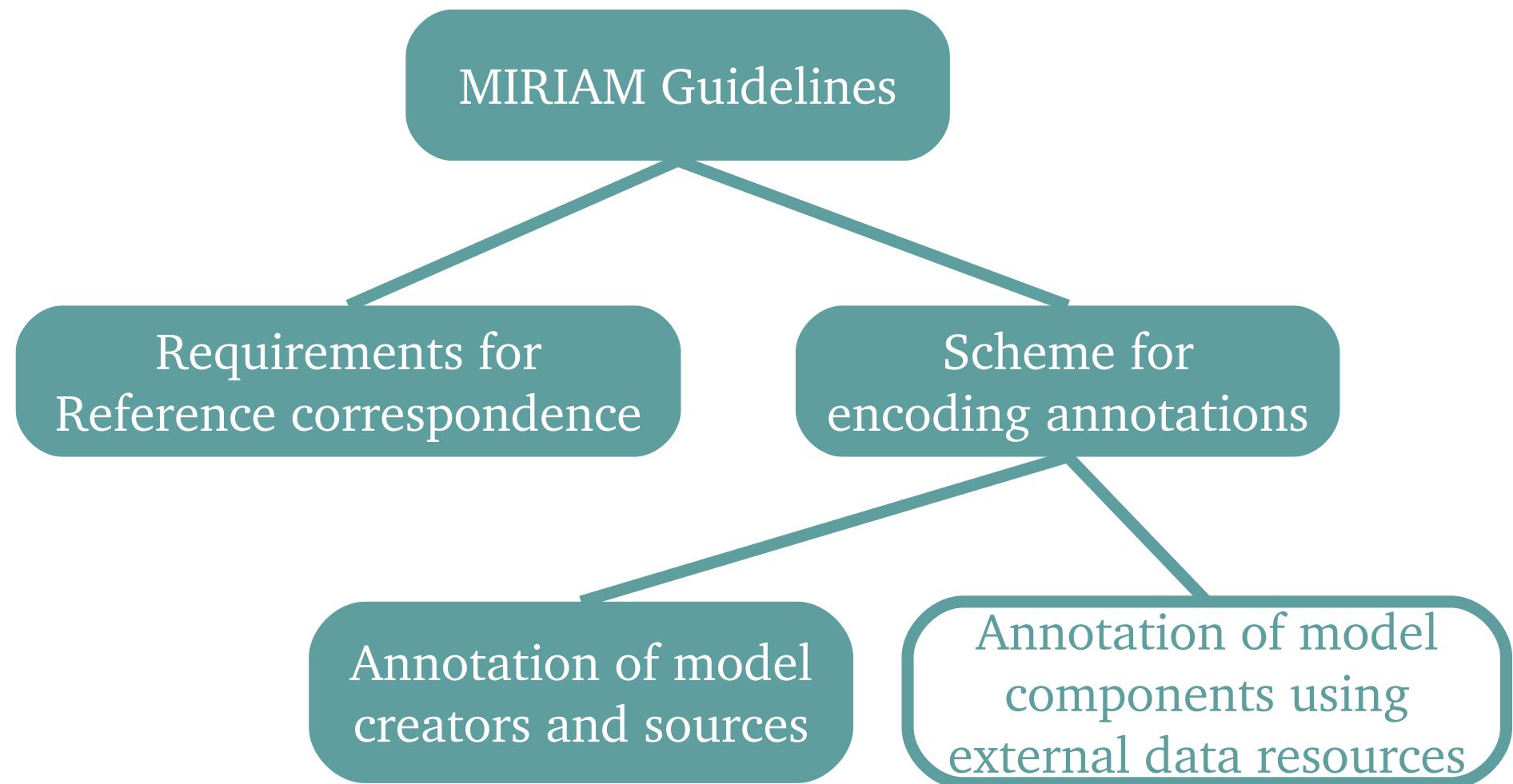






- The model has to be **named**
- A citation of the **reference description** must be given (complete citation, unique identifier, unambiguous URL). The citation should identify the authors of the model
- The name and contact of model **creators** must be stated
- The date and time of **creation** and **last modification** should be specified. A history is useful but not required
- The model should be linked to a precise statement about the **terms of distribution**. MIRIAM **does not** require “freedom of use” or “no cost”





**Unambiguously relate each model constituent
to a piece of knowledge**

triplet {**data type**, **identifier**, **qualifier**}

URI

Qualifiers (optional)

refine the link between the model constituent and the piece of knowledge



Epidermal growth factor receptor
Q9QX70



URLs (physical addresses):



<http://www.ebi.uniprot.org/entry/Q9QX70>



<http://us.expasy.org/uniprot/Q9QX70>



<http://www.pir.uniprot.org/cgi-bin/upEntry?id=Q9QX70>

Unique, perennial identifier: **MIRIAM URI**

urn:miriam:uniprot:Q9QX70



**Unambiguously relate each model constituents
to a piece of knowledge**

triplet {**data type**, **identifier**, **qualifier**}

MIRIAM URI

urn:miriam:uniprot:P12345

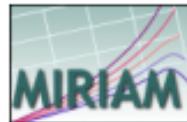
Qualifiers (optional)

refine the link between the model constituent and the piece of knowledge



```
[...]
<species metaid="metaid_0000006"
  id="L_EGFR"
  compartment="compartment"
  initialConcentration="0">
  <annotation>
    <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntaxns#"
      xmlns:bqbiol="http://biomodels.net/biologyqualifiers/">
      <rdf:Description rdf:about="#metaid_0000006">
        <bqbiol:hasPart>
          <rdf:Bag>
            <rdf:li rdf:resource="urn:miriam:uniprot:P07522" />
            <rdf:li rdf:resource="urn:miriam:uniprot:Q9QX70_RAT" />
          </rdf:Bag>
        </bqbiol:hasPart>
      </rdf:Description>
    </rdf:RDF>
  </annotation>
</species>
[...]
```





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 - MIRIAM Standard
 - FAQ
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- News 
- BioModels.net
- Qualifiers

- MIRIAM on SourceForge

- Support
- Contact

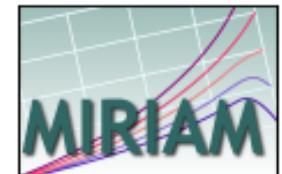


EBI > Groups > Computational Neurobiology > Research > MIRIAM Resources

MIRIAM Resources

MIRIAM Resources are a set of online services created to support [MIRIAM Standard](#).

The core of *MIRIAM Resources* is a catalogue of data types (these can be controlled vocabularies or databases), their URIs and the corresponding physical URLs or resources. Access to this data is made available via exports (XML) and Web Services (SOAP).



Quick links

Browse

- [by data type name](#)
- [by tags](#)

Web Services

- [services available](#)
- [usage of the services](#)
- [online demonstration](#)

Search

- [generic search](#)

Exports

- [XML](#)

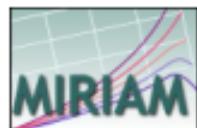
Resources

<http://www.ebi.ac.uk/miriam/>

Database

try and thi





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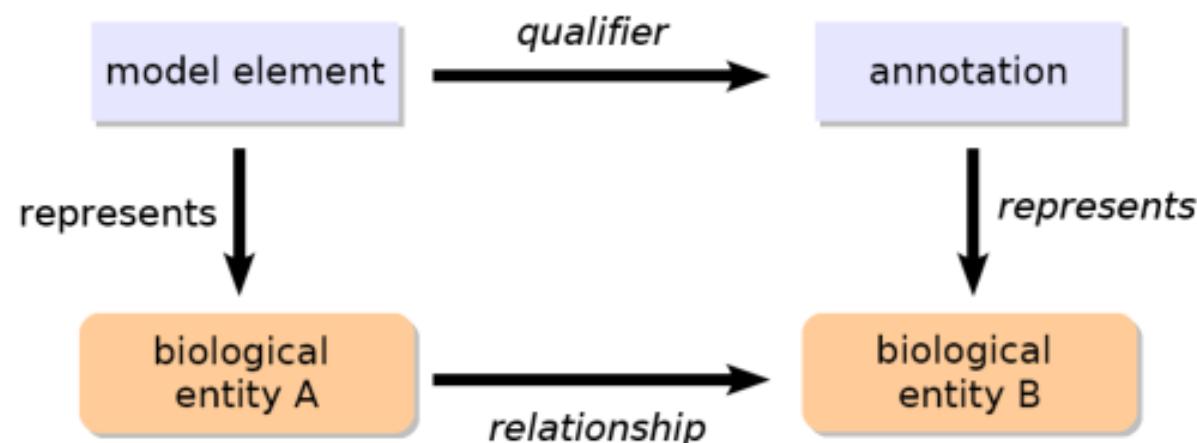
EBI > Groups > Computational Neurobiology > Research > MIRIAM Resources

MIRIAM Resources

BioModels.net qualifiers

The qualification of an annotation is important to grasp the relation between a model component and its annotation. The relationships is rarely one-to-one, and the information content of an annotation is greatly increased if one knows what it represents rather than to know it is "related to".

The qualifier of an annotation should reflect the relationships between the biological objects represented by the model element and the annotation:



The following is a list of the elements in the <http://biomodels.net/biology-qualifiers/> and <http://biomodels.net/model-qualifiers/> namespaces. These elements are used in the SBML standard RDF annotation format. This list may grow but no element will be removed.

In all cases using the biology qualifiers, the 'object' of the relation is the biological or biochemical object representing the model element. In the cases of the model qualifiers, the 'object' of the relation is the model component.

model-qualifiers





- is
- isDescribedBy
- hasPart
- isPartOf
- hasVersion
- isVersionOf
- isEncodedBy
- isHomologTo
- encodes
- ...



- set of valid and standard URIs for all the useful data types
- provide resolving services
- maintain and update the data



- Curator

From data type name + element identifier

generate MIRIAM URI

- Software developer

Resolve MIRIAM URI

into addresses (physical locations)



- browsing
- searching
- editing
- export (XML)
- **Web Services**
- documentation

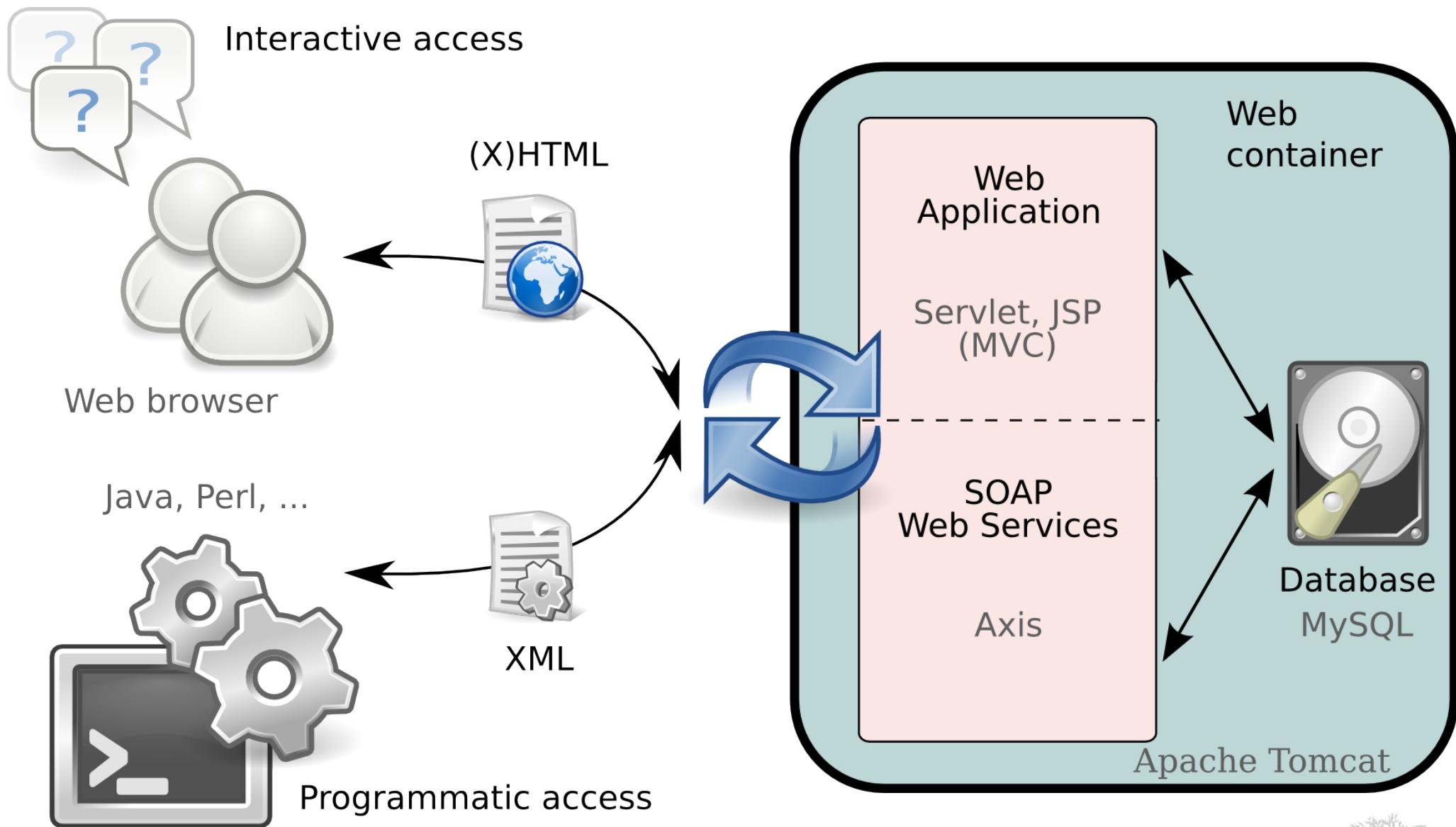
<http://www.ebi.ac.uk/miriam/>

Open Source:
available on
SourceForge.net

Camille Laibe and Nicolas Le Novère. **MIRIAM Resources: tools to generate and resolve robust cross-references in Systems Biology.**

BMC Systems Biology, 2007





4.10 Biological Entity

[...]

```
<cmeta:identifier rdf:parseType="Resource">  
    <cmeta:identifier_scheme>SWISS-PROT</cmeta:identifier_scheme>  
    <rdf:value>CALM_HUMAN</rdf:value>  
</cmeta:identifier>
```

[...]



4.10 Biological Entity

[...]

```
<cmeta:identifier rdf:parseType="Resource">  
    <cmeta:identifier_scheme>SWISS-PROT</cmeta:identifier_scheme>  
    <rdf:value>CALM_HUMAN</rdf:value>  
</cmeta:identifier>
```

[...]

```
[ ... ]  
<cmeta:identifier rdf:parseType="Resource">  
    <cmeta:ext_anno>urn:miriam:uniprot:P62158</cmeta:ext_anno>  
</cmeta:identifier>
```

[...]

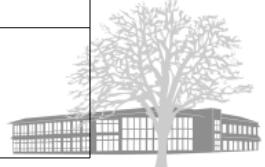


An example of the usage of MIRIAM Annotations

SBML to BioPAX conversion

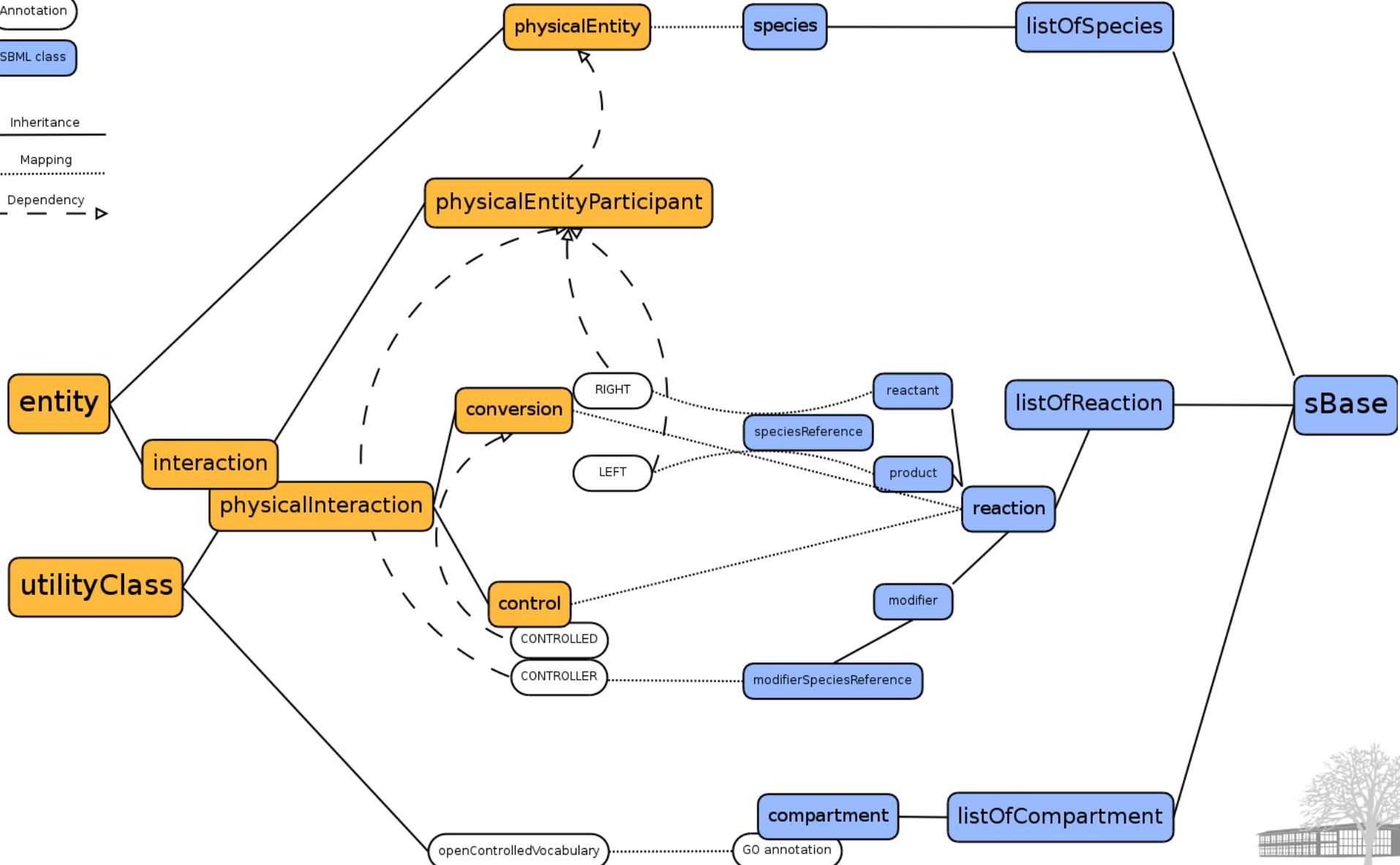
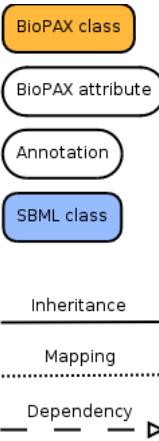


	SBML	BioPAX
file format	XML	OWL
kinetic laws	yes	no
molecules	<i>species</i>	<i>physicalEntity</i> + <i>subclasses</i>
biochemical reactions	<i>reactions</i>	<i>conversion</i> + <i>subclasses</i>
general annotations	<i>model</i>	<i>pathway</i>
...



- XSLT
- generation of valid BioPAX
- no usage of MIRIAM Annotations





only high level (not specialised) classes instantiated

e.g. every SBML *species*

transformed into *physicalEntity* BioPAX class

→ converted BioPAX not very informative

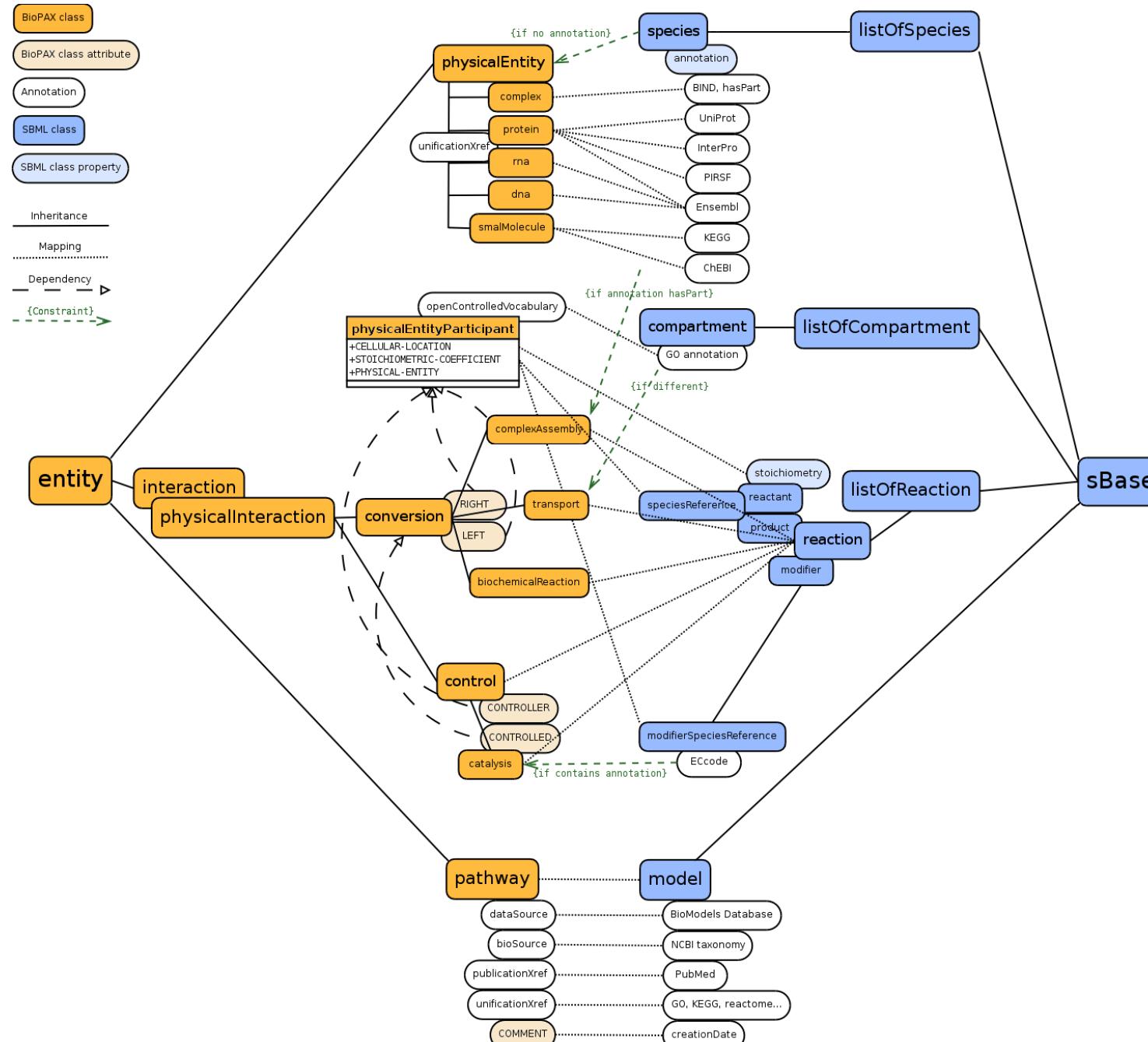


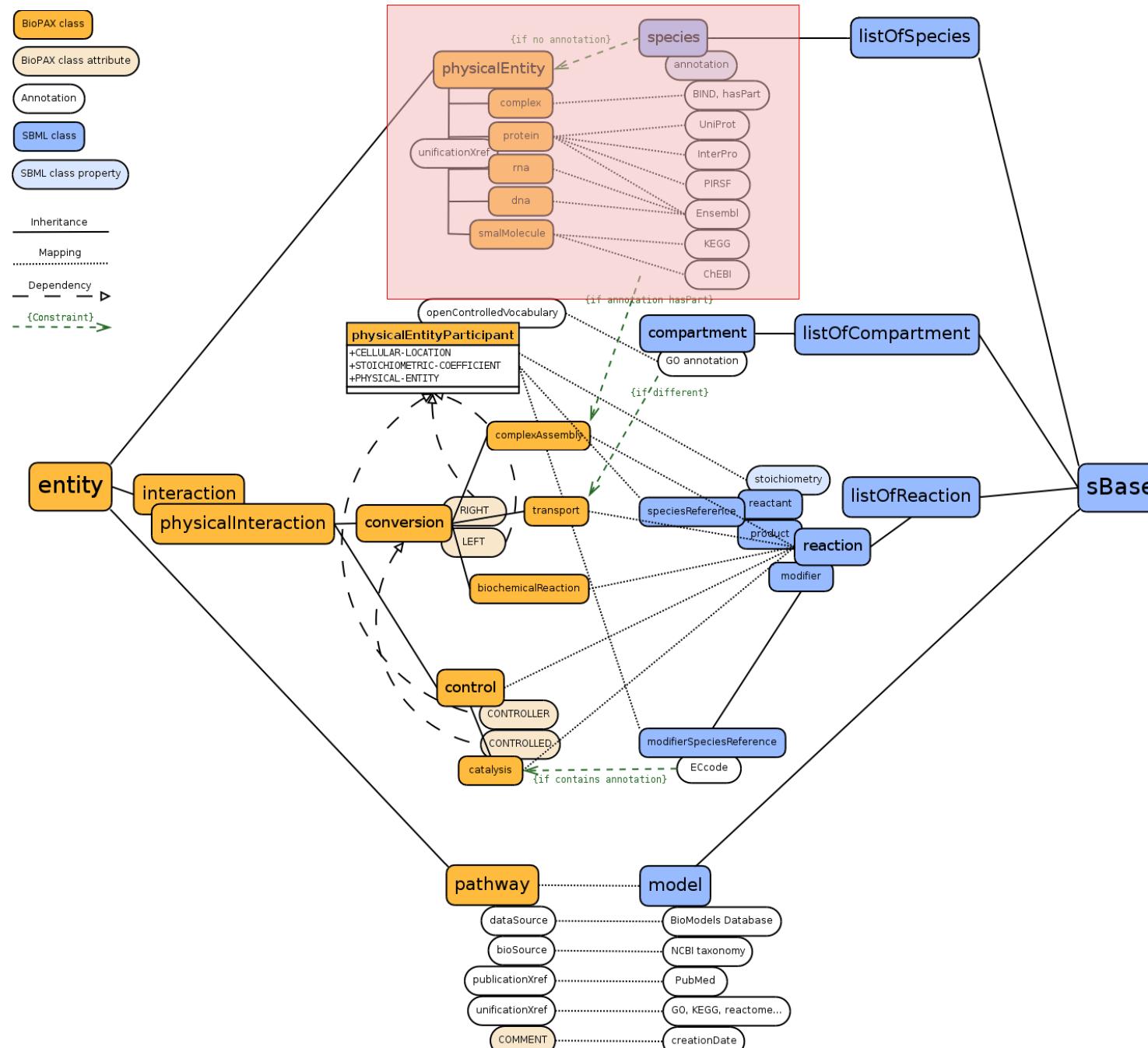
- Java

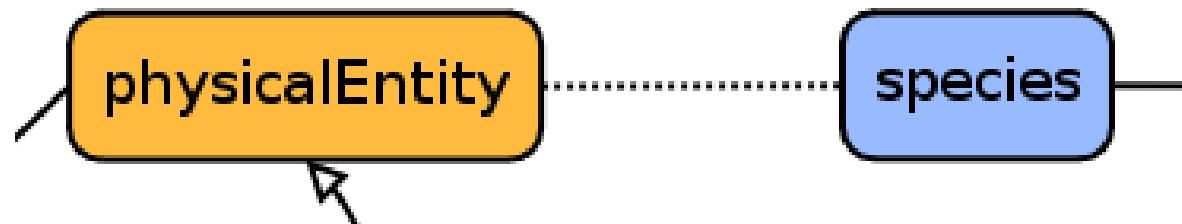


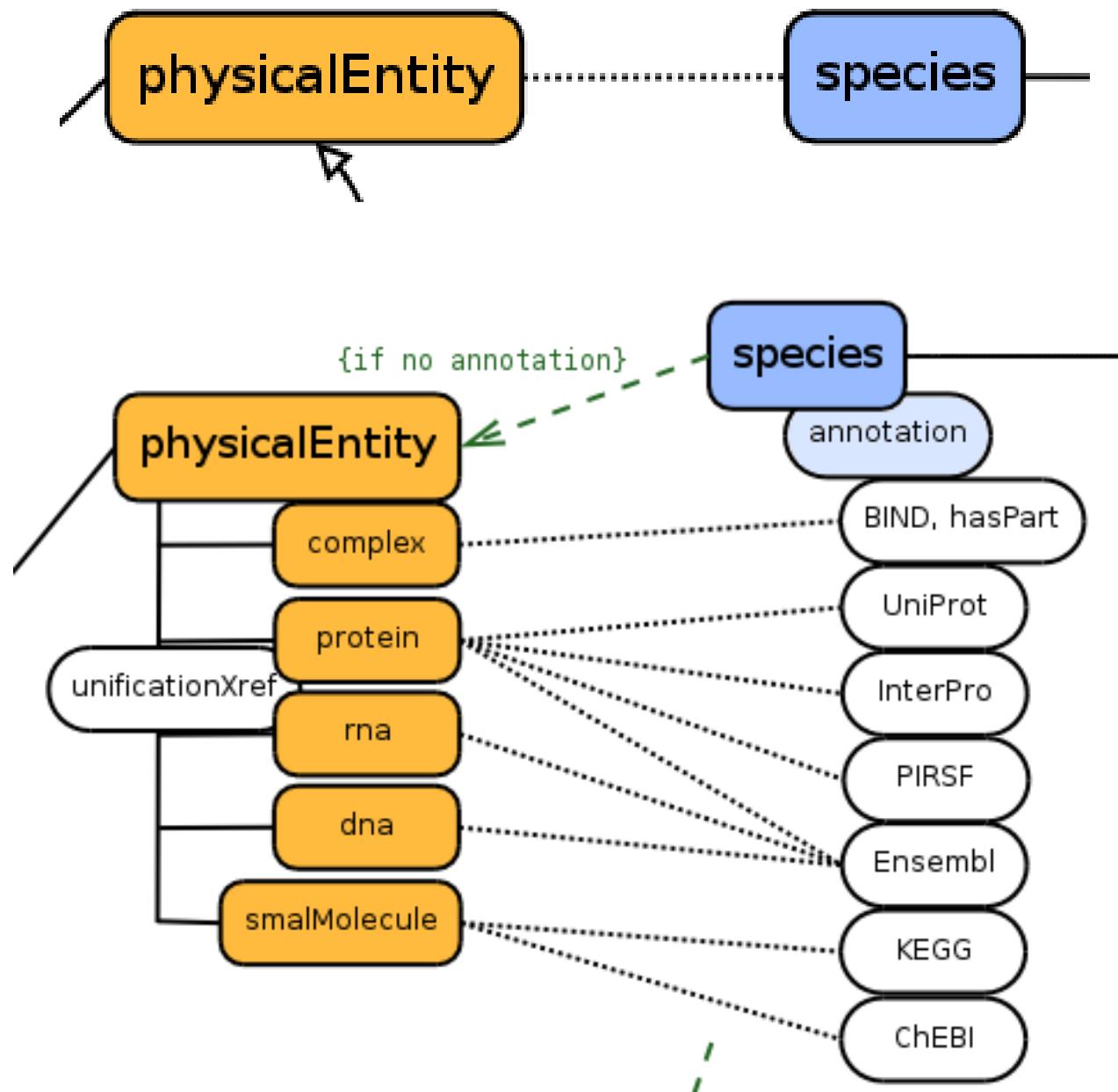
- generation of valid BioPAX
- Handles MIRIAM Annotations
(via MIRIAM Resources Web Services)

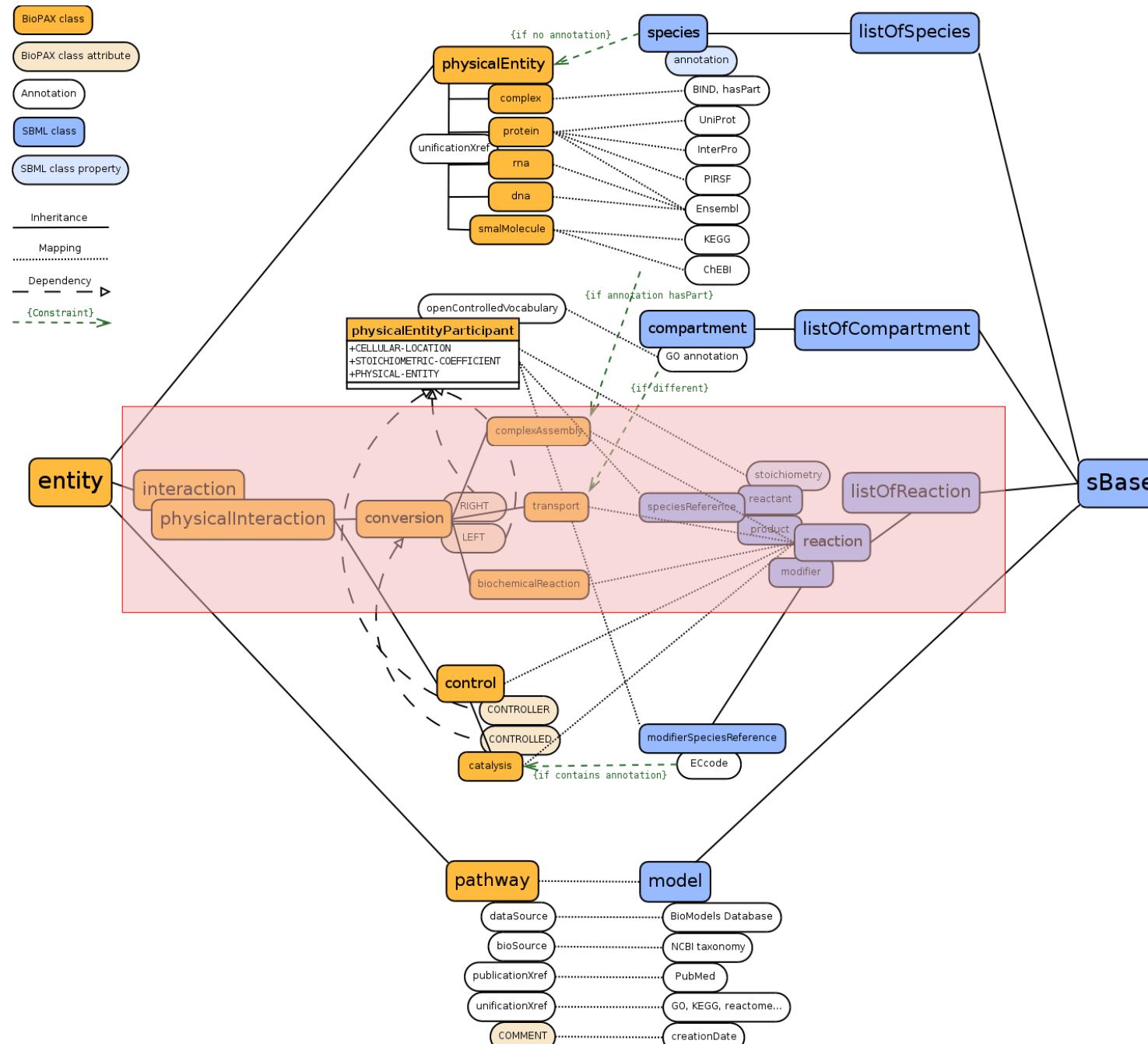


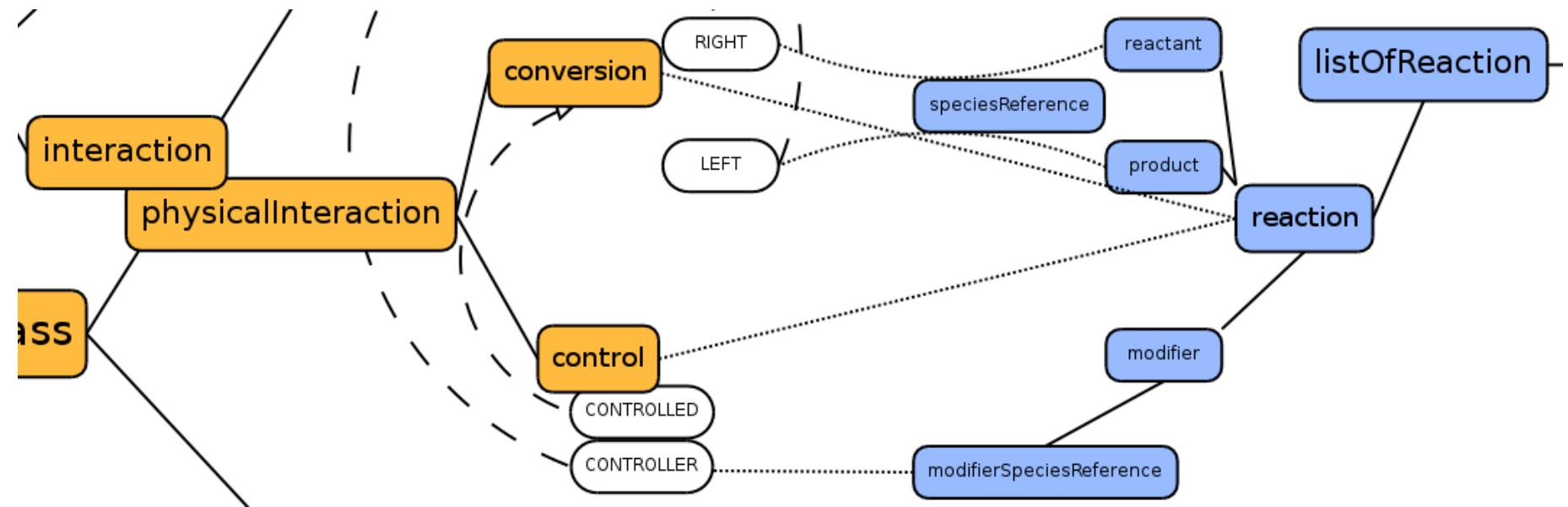


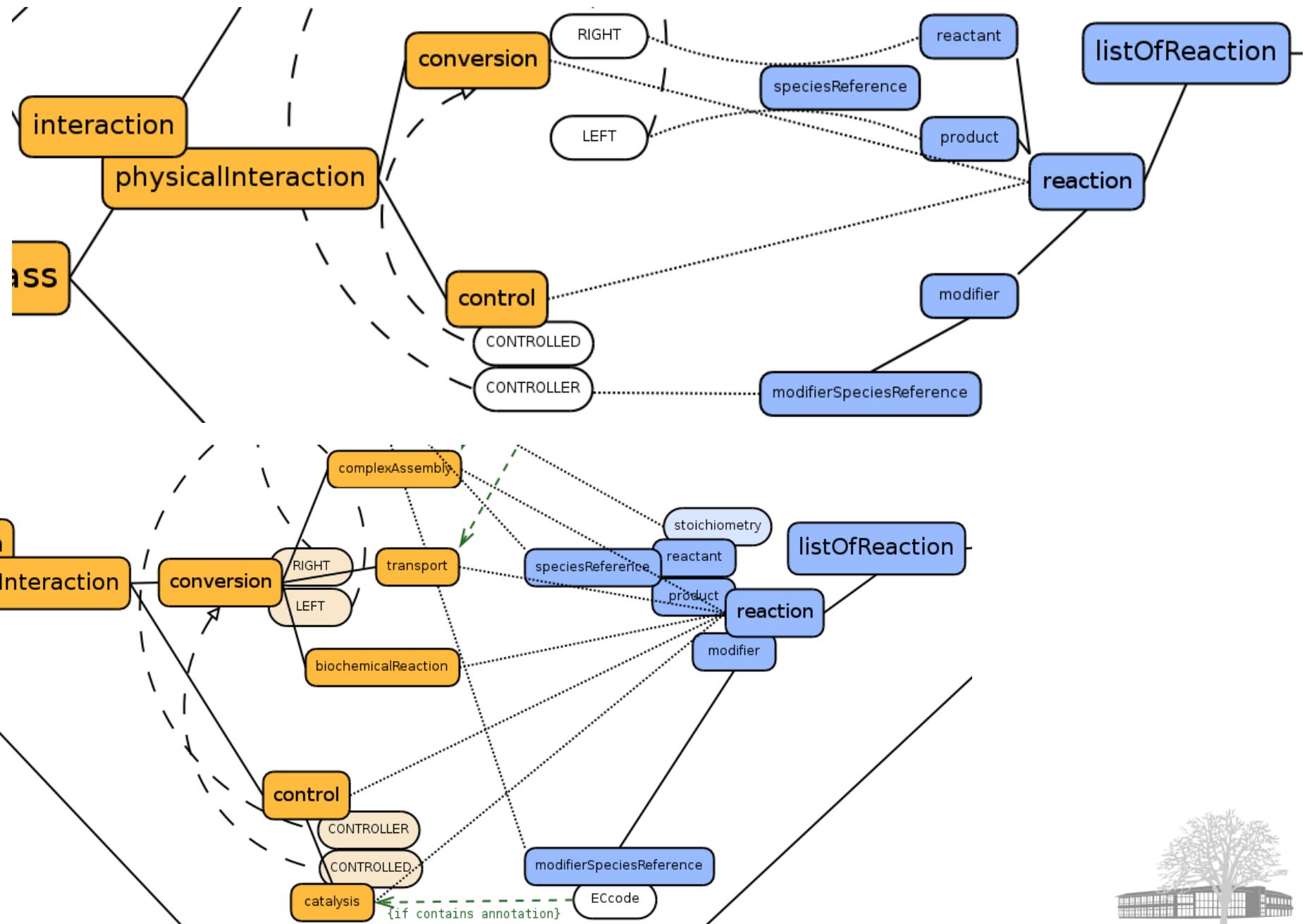


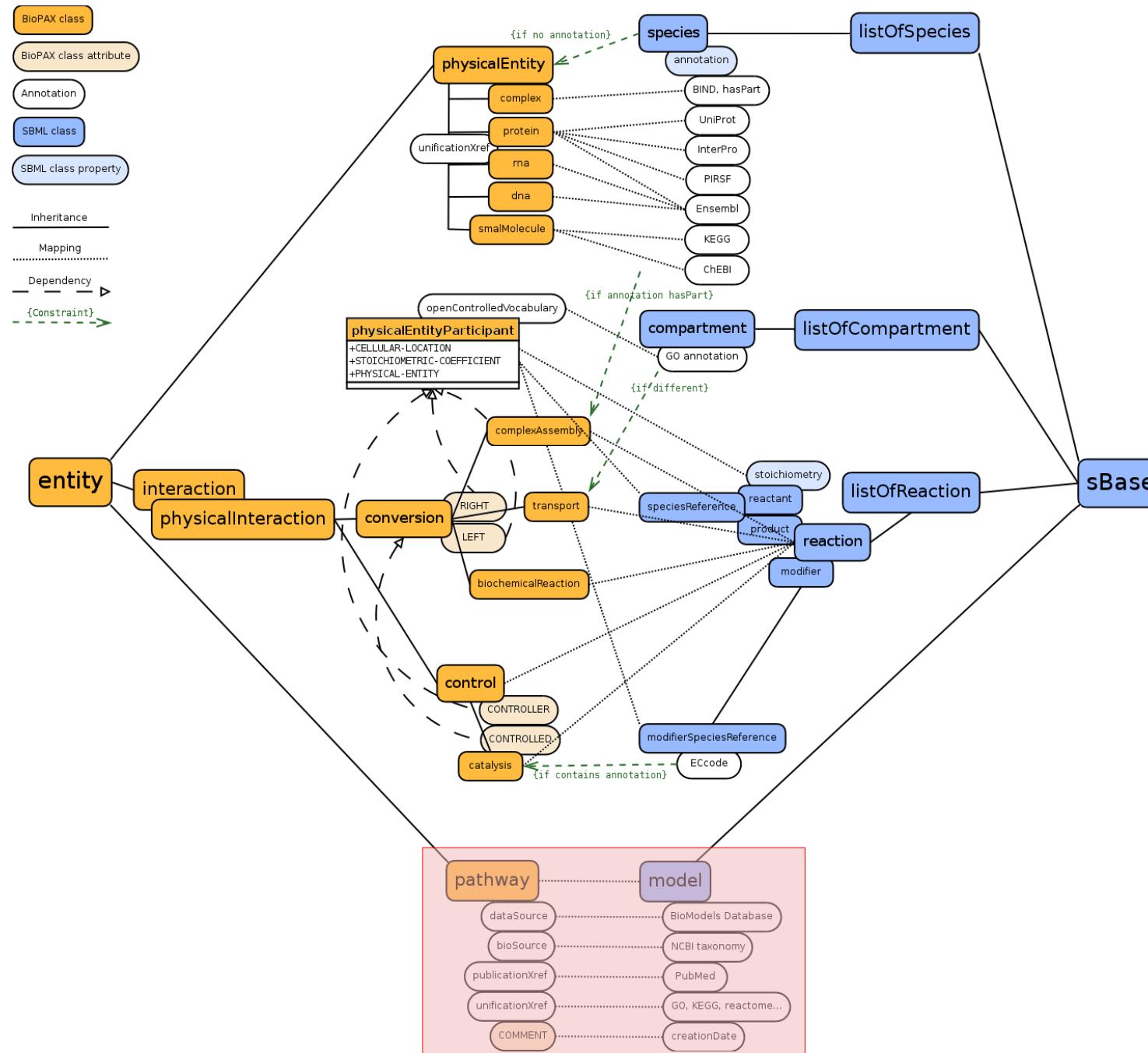


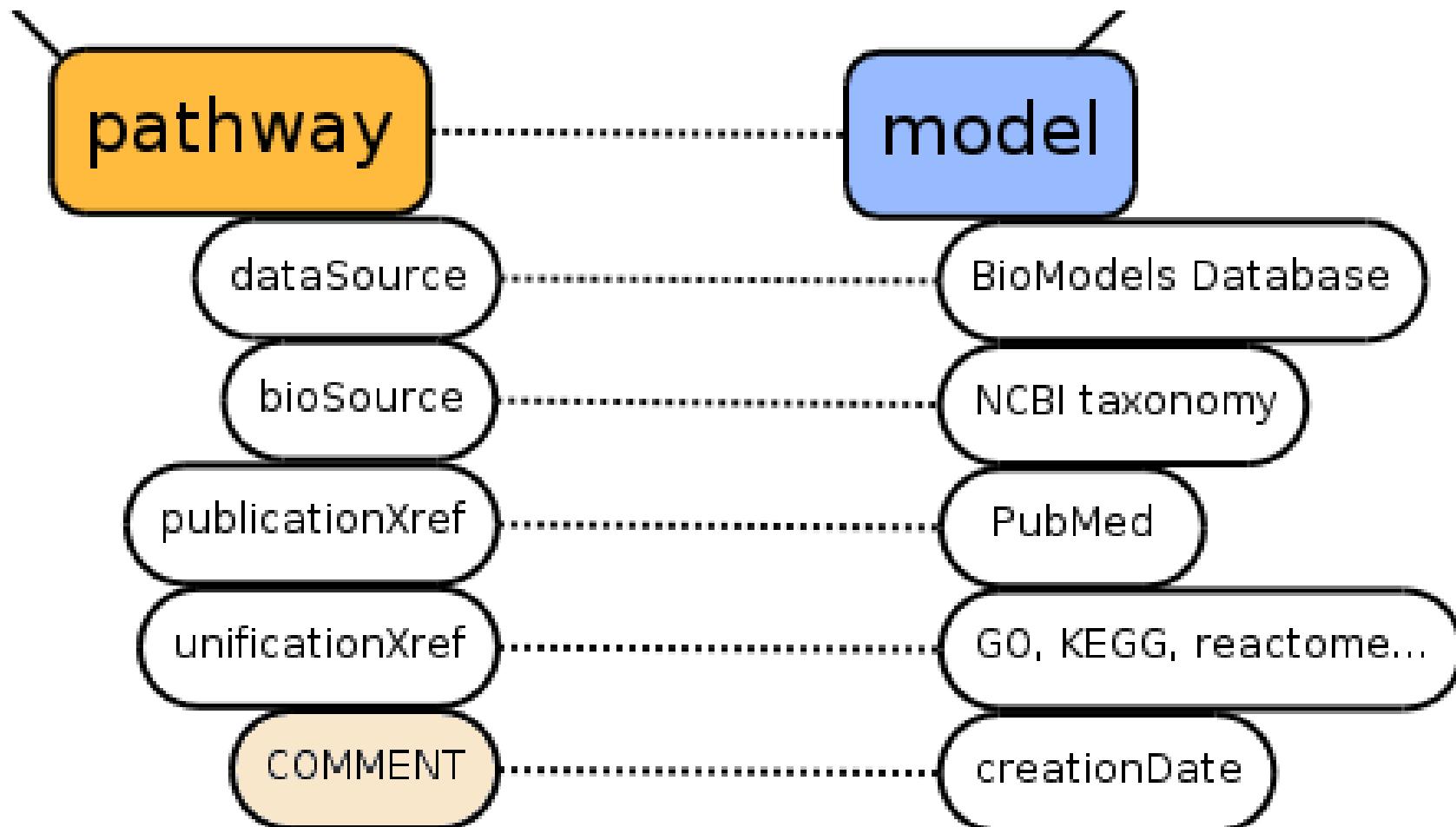












- annotation is kept (format converted)
- maintain mapping with the evolutions of the formats
 - ChEBI → smallMolecule
 - Ensembl → dna, rna, protein
- XML file
- in case of uncertainty
 - the top level class is used
- ...



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BIOMD0000000049 - Sasagawa2005_MAPK

[SBML L2 V1](#)[Other formats](#)[Actions](#)[Submit Model Comment/Bug](#)**Mod**[Other formats](#)[CellML](#)[SciLab](#)[XPP](#)[BioPAX](#)[VCell](#)[PDF](#)**Publication ID:**[Math](#)[Physical entities](#)[I](#)[Nat Cell Biol 2005 Apr;7\(4\):365-73.](#)[Prediction and validation of the distinct dynamics of transient and sustained MAPK activation in fibroblasts](#)[Sasagawa S, Ozaki Y, Fujita K, Kuroda S.](#)[Undergraduate Program for Bioinformatics and Systems Biology, Kyoto University](#)**Original Model:** *Unspecified*set#1 bqbiol:is [Taxonomy](#) *Rattus***Submitter:** [Shinya Kuroda](#)[Gene Ontology](#) *MAPKKK cascade***Submission Date:** 2006-01-12T13:42:52+00:00[Gene Ontology](#) *neurotrophin receptor signaling pathway***Last Modification Date:** 2008-08-21T11:55:50+00:00[Gene Ontology](#) *Ras protein signal transduction***Creation Date:** 2005-12-21T10:59:39+00:00[Gene Ontology](#) *epidermal growth factor receptor signaling pathway***Creators:** [Lu Li](#)
[Shinya Kuroda](#)

- Improvements
 - use of BioPAX *openControlledVocabulary* for SBO Terms
- BioPAX
 - level 3 version 1
- Paxtools
- SBML
 - support all new versions
- ...





Arnaud Henry



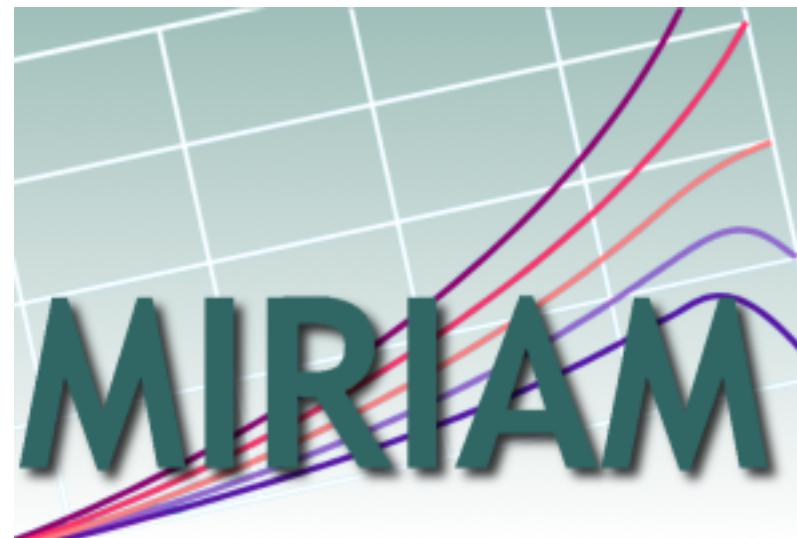
Nicolas Rodriguez



Do use MIRIAM Annotations!



Thank you



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