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Systems Biology Ontology: *Update*

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COMBINE 2010

Edinburgh, 6th - 9th October

Overview

- Brief introduction SBO
  - annotation layer issue
    - reiterate / clarify the problem
    - describe resolution process
- OBO Foundry Status
  - what it is, and how to get it
- Relationship between Systems Biology Graphical Notation (SBGN) with SBO
  - new glyphs

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What is SBO?

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http://www.ebi.ac.uk/sbo/

- Provide a strictly defined relational vocabulary of terms for use in Systems Biology
- A navigable structure of terms that has 'parents', 'children'

SBO structure

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6 orthogonal vocabularies:

- entity (macromolecule)
- interaction (transport, reactions)
- mathematical expression (mass action rate law)
- modelling framework (discrete)
- participant roles (S, P, M)
- quantitative parameters (Hill coefficient)

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```
<listOfCompartments>
  <compartment id="C" sboTerm="SBO:0000289">
</listOfCompartments>
<listOfSpecies>
  <species id="A" sboTerm="SBO:0000247" />
  <species id="B" sboTerm="SBO:0000247" /
  <species id="C" sboTerm="SBO:0000014" />
</listOfSpecies>
<listOfReactions>
  <reaction sboTerm="SBO:0000172">
    <listOfReactants>
      <speciesReference species="A" sboTerm="SBO:0000015"/>
    </listOfReactants>
    <listOfProducts>
      <speciesReference species="B" sboTerm="SBO:0000011"/>
    </listOfProducts>
    <listOfModifiers>
      <speciesReference species="C" sboTerm="SBO:0000014"/>
    </listOfModifiers>
    <kineticLaw sboTerm="SBO:0000031">
      <listOfParameters>
        <parameter id="U" sboTerm="SBO:0000027"/>
        <parameter id="V" sboTerm="SBO:0000025"/>
      </listOfParameters>
    </kineticLaw>
  </reaction>
</listOfReactions>
```

Semantics

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Semantic layer:

- link between models encoded in SBML and graphical notations (such as SBGN)
- conversion to semantically enriched computing formats (such as BioPAX)
- translation of models between *continuous deterministic frameworks* and *discrete stochastic framework*
- merging of models

SBO annotation I

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SBO annotation layer
(as it was):

SBML component	SBO branch
<speciesReference>	participant role
..	
<parameter>	quantitative parameter
..	
<kineticLaw>	rate law
..	
<Species>	entity
..	

SBO annotation II

SBO annotation layer
(as it was):

SBML component	EXAMPLE	SBO branch
<speciesReference>	substrate inhibitor	participant role
..		
<parameter>	kinetic constant time	quantitative parameter
..		
<kineticLaw>	mass action rate law	rate law
..		
<Species>	simple chemical enzyme	entity
..		

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Annotation issue

SBO annotation layer
(as it was):

SBML component	SBO branch
<speciesReference>	participant role
<kineticLaw>	rate law

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Annotation issue

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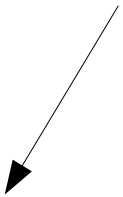
SBO annotation layer
(as it was):

SBML component	SBO branch
<speciesReference>	participant role
<kineticLaw>	rate law



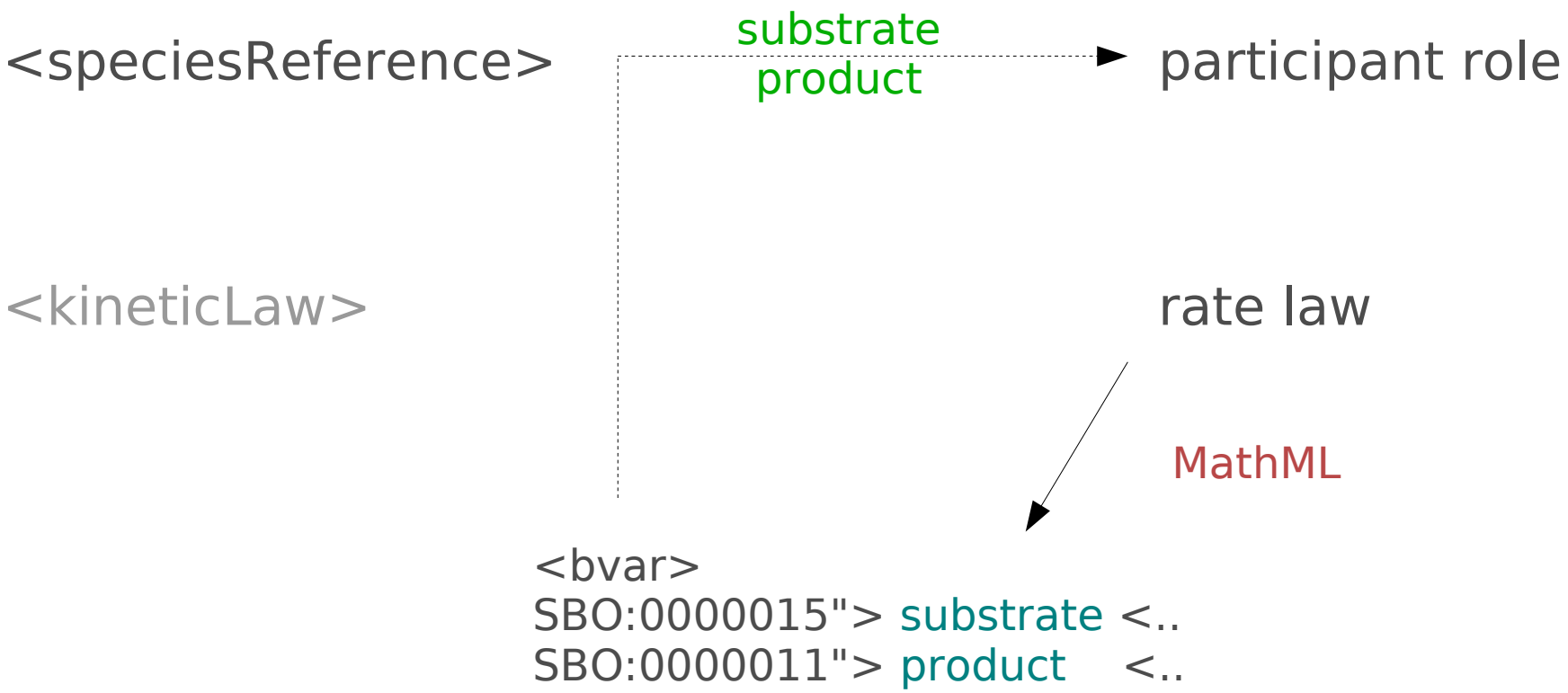
MathML

```
<bvar>
 <ci definitionURL="http://biomodels.net/SBO/#SBO:0000015"> substrate <..
 <ci definitionURL="http://biomodels.net/SBO/#SBO:0000011"> product   <..
```

Annotation issue

SBO annotation layer
(as it was):

SBML component **SBO branch**



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Annotation solution

Problem: 'substrate' (participant role) = amount? concentration?

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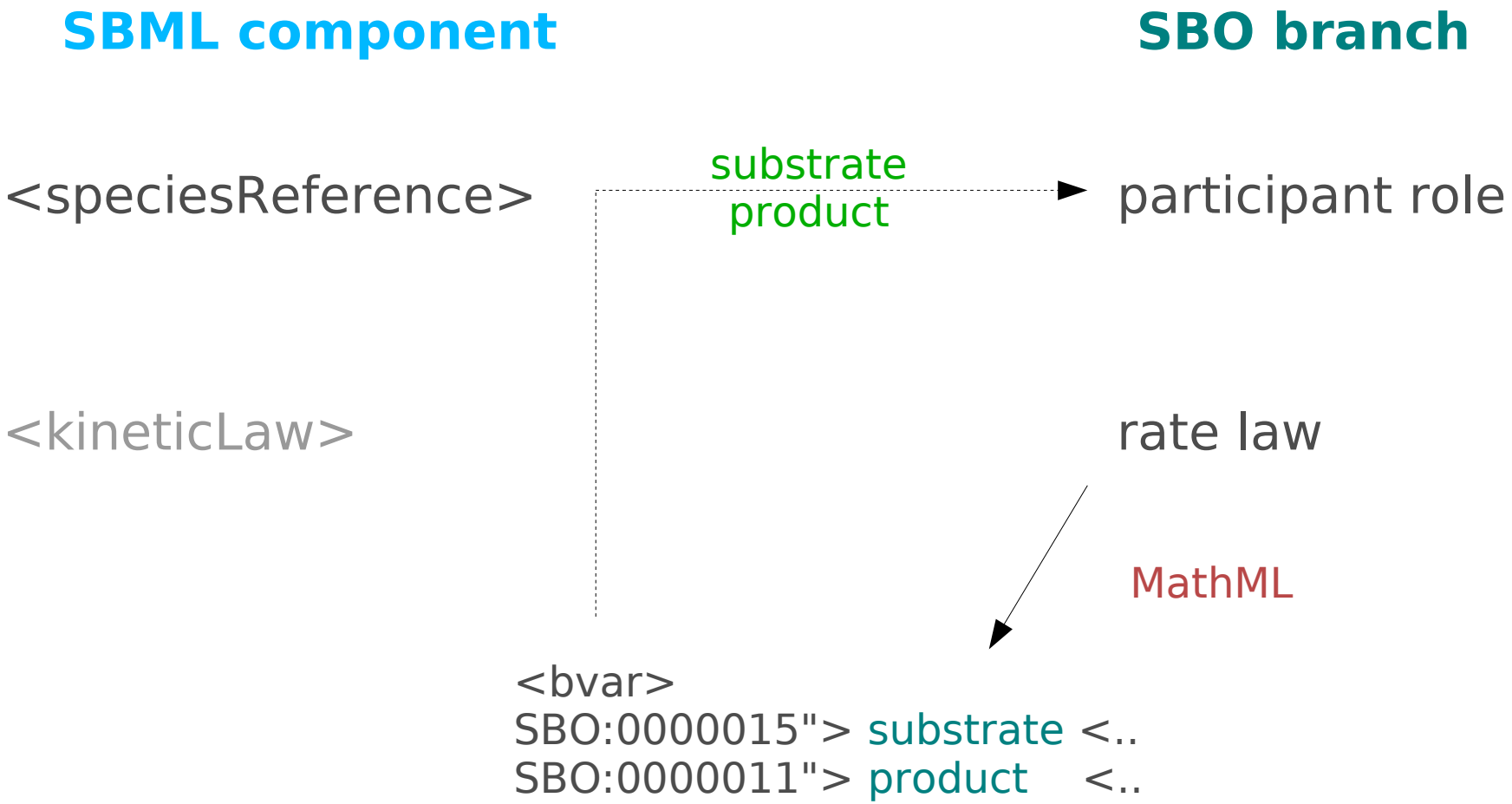

Annotation solution

Problem: 'substrate' (participant role) = amount? concentration?

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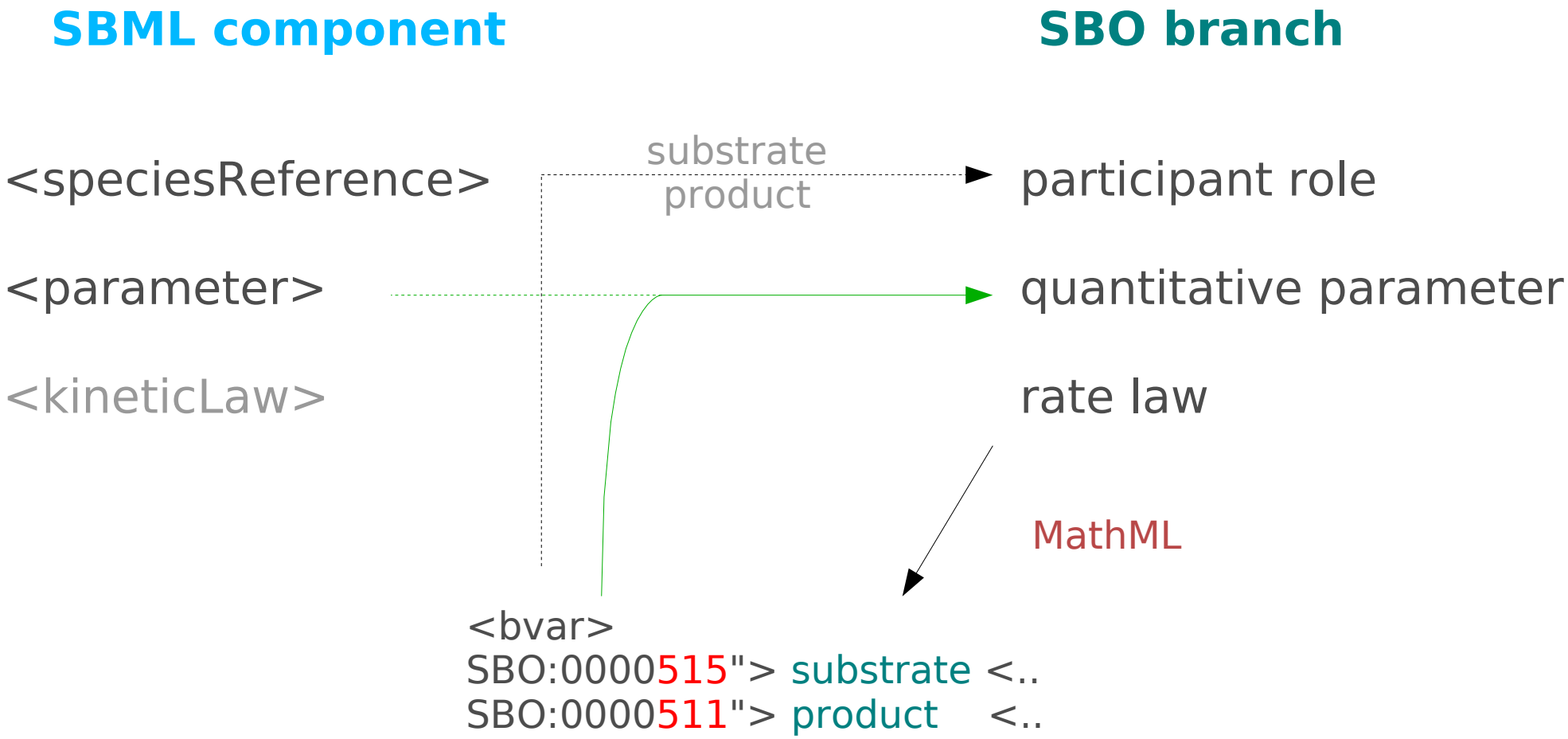
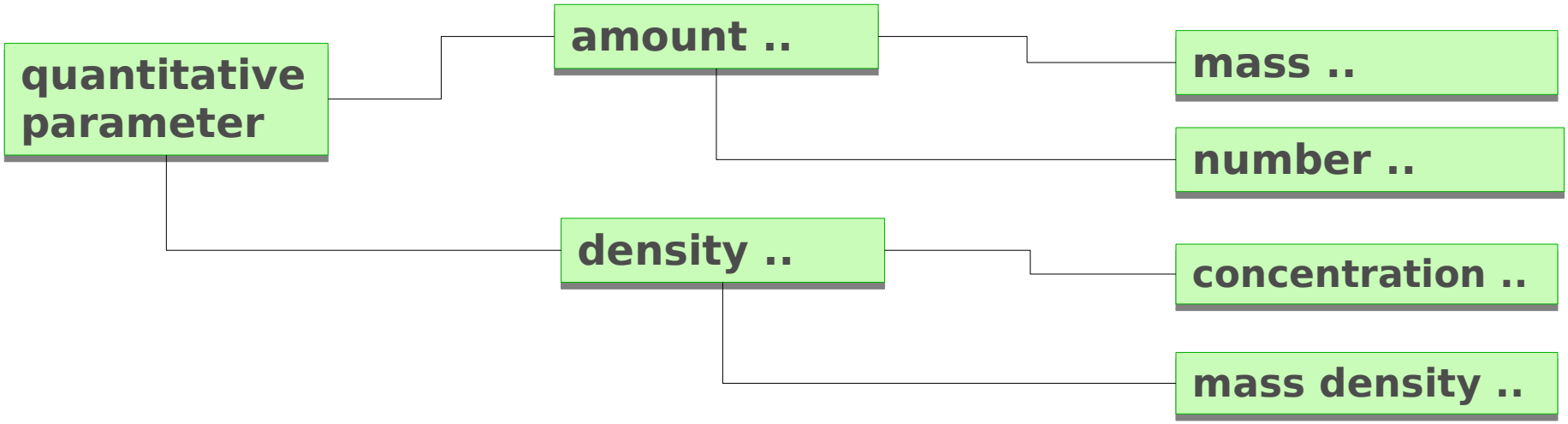


SBO branch changes

- Initial changes made on SBO 'demo'
- Introduce 'quantitative parameter's for 'participant role' terms



- Modify <bvar> links in all MathML - redirect to quantitative parameter branches
- Request feedback for selected users (validate)
- Move changes to SBO 'main' (implement → live version)

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OBO

- Open Biomedical ontologies – open community-level collaborative ontology development
- First Principles:
  - open - terms should be available for use without restriction
  - changeable – modified by community effort
  - orthogonal – additivity and modularity
  - machine friendly – interpretable and syntactically sound
  - identifiers – backward compatible
- >80 library members, 8 Foundry

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EMBL-EBI

http://www.obofoundry.org/

The Open Biomedical Ontologies

Ontologies | Resources | Participate | About

The OBO Foundry is a collaborative experiment involving developers of science-based ontologies who are establishing a set of principles for ontology development with the goal of creating a suite of orthogonal interoperable reference ontologies in the biomedical domain. The groups developing ontologies who have expressed an interest in this goal are listed below, followed by other relevant efforts in this domain.

In addition to a listing of OBO ontologies, this site also provides a statement of the OBO Foundry principles, discussion fora, technical infrastructure, and other services to facilitate ontology development. We welcome feedback and encourage participation.

Click any column header to sort the table by that column. The 🐾s link to the term request trackers for the listed ontologies.

OBO Foundry candidate ontologies

Title	Domain	Prefix	File	Last changed
Amphibian gross anatomy	anatomy	AAO	amphibian_anatomy.obo	2008/06/19
Amphibian taxonomy	anatomy	ATO	amphibian_taxonomy.obo	
Ascomycete phenotype ontology	phenotype	APO	ascomycete_phenotype.obo	2009/07/10
Biological process	biological process	GO	gene_ontology_edit.obo 🐾	2009/08/21
C. elegans development	anatomy	WBls	worm_development.obo	2008/01/31
C. elegans gross anatomy	anatomy	WBbt	WBbt.obo 🐾	2009/08/19
C. elegans phenotype	phenotype	WBPhenotype	worm_phenotype.obo	2009/08/19
Systems Biology	biochemistry	SBO	SBO_OBO.obo 🐾	

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SBO OBO Status

- SBO is an OBO candidate ontology
  - Review 15th Feb 2010
  - Issues to address include:
    - Expose MathML terms (hidden relationships)
    - Versioning
    - Uniqueness/orthogonality
      - MIREOT (direct import)
      - Cross reference
      - Cross products
- Interface:
    - References for term (creation)
    - Cross references (relationships to other ontologies)

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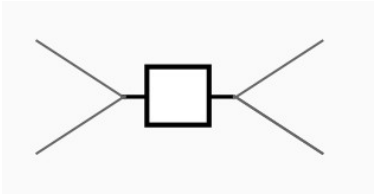
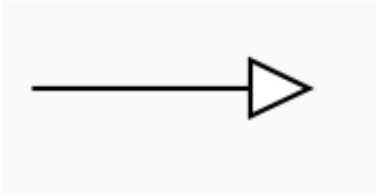
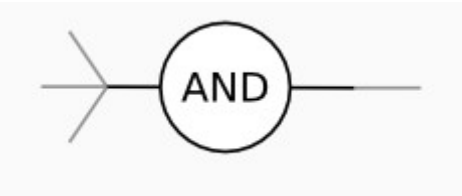
SBO / SBGN relationship

SBGN	<---------->	SBO
	Process (PD)	SBO:0000375
	Stimulation (ER)	SBO:0000170
	And (AF)	SBO:0000173

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SBO / SBGN metadata

SBGN	<---------->	SBO
	Annotation (ER)	?

- Do we need a 7th branch in SBO to accommodate:
  - Annotation,
  - cross-references,
  - metadata

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Sarah Keating

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The community of Systems Biology for their contributions, their software support and their comments.

https://sourceforge.net/projects/sbo

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