



Annot package

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3 May 2010



Annot package

“SBML should not pre-emptively incorporate features that could be useful ‘at some point’”



Annot package

- Annot package workshop later this month...
 - http://sbml.org/Events/Other_Events/Annotation_package_workshop_2010
- Questions for today:
 - **why** we do / don't annotate models?
 - **what** we would like to do that we currently cannot, either due to lack of tools or more seriously, lack of support in SBML?
 - things that we would like to do that rely on annotations, but we **don't realise** it **yet**?
- Less fussed by “how”

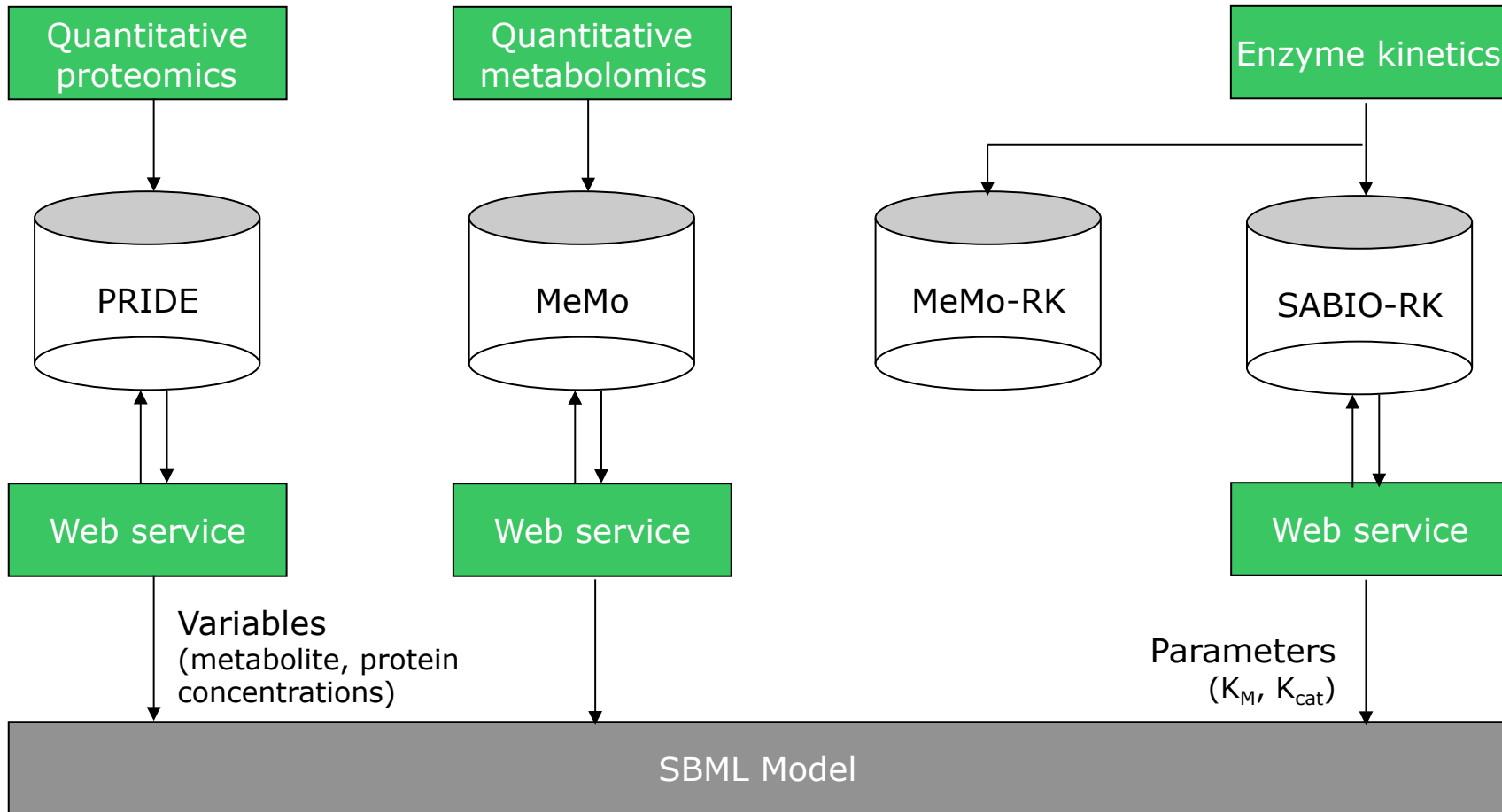


Why I annotate

- Provide **definitive, unique identifier** for “stuff”
 - One motivation: mapping experimental data to models
 - Need **annotated models AND annotated data**



Experimental project overview





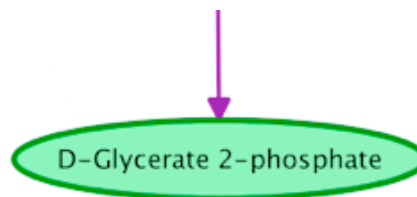
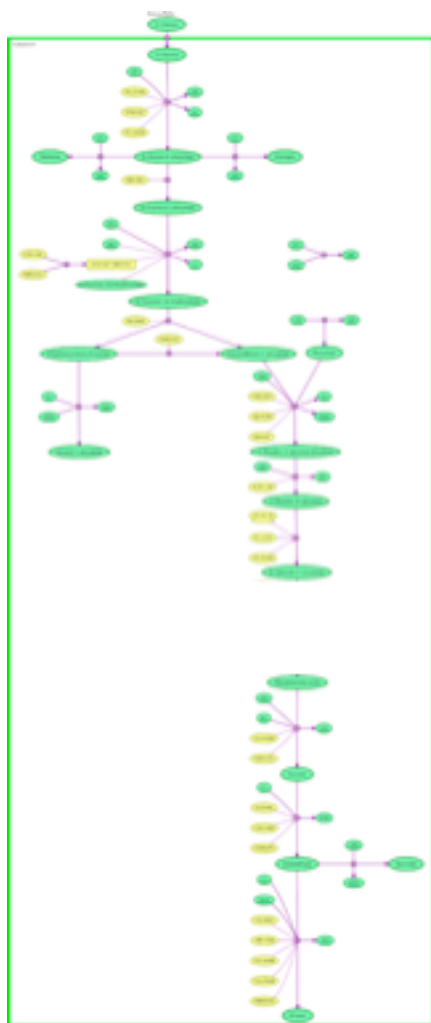
Genome-scale models

- **Ridiculous-ome** – Jim Schaff
- Genome-scale SBML model of metabolism
 - Requires annotation to understand / query (bloody huge)
 - Requires annotation to build (merged from smaller models)



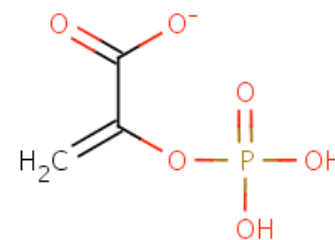
Purpose of annotations

- More interesting purpose...
 - Use the annotations to **reason** over the model
 - Does my model accurately reflect the biochemistry?
 - Do my reactions **elementally balance**? Are the **stoichiometries** correct?
 - Easy to determine if we “**deference**” ChEBI identifier (or whatever) to determine chemical formulae

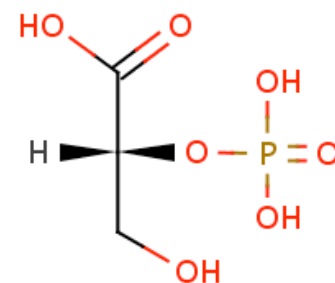
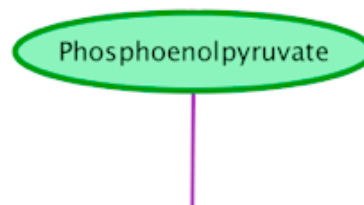


Gap-filling

CHEBI:17835



CHEBI:18021





Limitations

- We can only annotate **elements** not **attributes**...

A screenshot of an XML editor window titled 'BIOMD0000000003.xml'. The editor shows the following XML code:

```
1 <species metaid="_metal" id="id1" name="Lipopolysaccharide"  
2   initialConcentration="50.2" units="nM"  
3   compartment="EndoplasmicReticulum">  
4   <annotation>  
5     <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"  
6       xmlns:bqbiol="http://biomodels.net/biology-qualifiers/">  
7       <rdf:Description rdf:about="#_metal">  
8         <bqbiol:isDescribedBy>  
9           <rdf:Bag>  
10            <rdf:li rdf:resource="urn:miriam:obo.eco:ECO%3A0000123"/>  
11            <rdf:li rdf:resource="urn:miriam:pubmed:17882155"/>  
12          </rdf:Bag>  
13        </bqbiol:isDescribedBy>  
14      </rdf:Description>  
15    </rdf:RDF>  
16  </annotation>  
17 </species>
```



Limitations

- Who did what when?
 - Improved history
- Annotations of annotations
 - X was annotated with Y because of publication Z
- Examples being collected here...
- http://docs.google.com/View?id=dftdk3rc_58gvv857tg
- Speak to me...



Versioning?

- Species X in Model Y, version 1 was Species A in Model B, version 6
- Is this an annotation issue?



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