

Proposals for extensions to SBML

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- 1) References to where the data originated. This could be a URL or reference to the original paper. We see these as being necessary for the reaction and parameters fields only.
- 2) A code for annotator's opinion as to reliability of the information. We use the Gene Ontology codes. IMP|IGI|IPI|ISS|IDA|IEP|IEA|NA|TAS|NAS|NR
- 3) A field <biospecies> to show in which species the parameter was measured. In a perfect world this would be unnecessary, but (as can be seen from our example) data is not always available for the species being studied.
- 4) Data for cofactors required by the reaction, inhibitors, and activators. These do not directly take part in the reactions (although it could be argued that they do by reacting with the enzymes to form more active, less active, or inactive forms)

Evidence
biospecies: string
anop: string {"IMP","IGI","IPI","ISS","IDA","IEP","IEA","NA","TAS","NAS","NR"}
reference: RefType

RefType
reference: string {minOccurs="0"}
referenceurl: string {minOccurs="0"}

below is an example of one reaction in E.coli as it would appear if our proposals were adopted.

```
<reaction name="ARGININE--TRNA LIGASE" reversible="false">
```

```
<evidence biospecies="e.coli" anop="IMP"  
referenceurl="http://www.genome.ad.jp/www.genome.ad.jp/dbget-  
bin/www_bget?E.coli+b1876"/>
```

<cofactor_required name="tRNA(Arg)">

<evidence biospecies="escherichia_coli" anop="ASS" reference="Biochemistry, 1988, 27(17), 6343-6348" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=PRO96327-02"/>

</cofactor_required>

<modulator name="spermine" modulation="eff">

<evidence biospecies="mycobacterium_smegmatis" anop="ASS" reference="The Journal of Biological Chemistry, 1976, 251(2), 414-423" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=NEN95062-03"/>

</modulator>

<modulator name="p-(hydroxymercuri)benzoate" modulation="inh">

<evidence biospecies="escherichia_coli" anop="ASS" reference="Biochemistry, 1979, 18(14), 3171-3178" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=TAT00338-01"/>

</modulator>

<listOfReactants>

<speciesReference specie="L-arginine" stoichiometry="1">

<speciesReference specie="ATP" stoichiometry="1">

<speciesReference specie="tRNA(Arg)" stoichiometry="1">

</listOfReactants>

<listOfProducts>

<speciesReference specie="AMP" stoichiometry="1">

<speciesReference specie="Pyrophosphate" stoichiometry="1">

<speciesReference specie="L-Arginyl-tRNA(Arg)" stoichiometry="1">

</listOfProducts>

<kineticLaw formula="to be advised">

<listOfParameters>

<parameter name="Vmax" value="0.475">

<evidence biospecies="ovis_aries" anop="ASS" reference="biochemistry, 1985, 24(19), 5099-5106" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=SEL89293-01"/>

</parameter>

<parameter name="Km" value="0.012">

<evidence biospecies="escherichia_coli" anop="ASS" reference="biochemistry, 1988, 27(17), 6343-6348" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=PRO96327-02"/>

</parameter>

<parameter name="temp" value="37">

<evidence biospecies="escherichia_coli" anop="ASS" reference="biochemistry, 1988, 27(17), 6343-6348" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=PRO96327-02"/>

</parameter>

<parameter name="pH" value="8.1...8.5">

<evidence biospecies="escherichia_coli" anop="ASS" reference="biochemistry, 1979, 18(14), 3171-3178" referenceurl="http://www.empproject.com/cgi-bin/rd_html.pl?id=TAT00338-01"/>

</parameter>

</listOfParameters>

</kineticLaw>

</reaction>