BioModels, EMBL-EBI

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Abstract

Document contains details about the preferred annotation qualifiers and ontologies followed by BioModels for model annotation

Biomodels annotation Guidelines

SOP

**BioModels Annotation**

The process of annotating a model consists in identifying the model components. This is achieved by linking model components with terms from controlled vocabularies and entries in data resources. This is similar to attaching cross-references to the model with the addition of qualifiers, in order to explicitly define the relationship between the model component and the target element.

Other relevant information in annotation context can be found using links below:

* Basic annotation guideline at: <https://www.ebi.ac.uk/biomodels-main/annotation>
* Basic annotation tips: <http://www.ebi.ac.uk/biomodels-main/annotationtips>
* Basic qualifier usage: <http://co.mbine.org/standards/qualifiers>

**Model Annotation Levels**

1. High level model annotation
2. Model component level annotation
   1. Compartment
   2. Species
   3. Reaction
   4. Parameter
3. **Model level annotation:**

High level model annotation is done to provide details about overall model and its biological relevance dependent on model publication. Below are the details of preferred information, qualifiers and associated preferred ontologies:

|  |  |  |  |
| --- | --- | --- | --- |
| **Annotation Information** | **Qualifier/s** | **Preferred ontologies** | **Example set** |
| Taxonomy | hasTaxon | Taxonomy | (1) |
| Tissue/cell Type | occurs in | BTO | (2) |
| Modelling Approach | has Property / is Property Of | MAMO | (3) |
| Biological process explained by model (Ex. PDL-1 signaling) | has Property | GO / NCIT | (4) |
| Model relevance to a particular area (Ex. Immunotherapy) | has Property | GO / NCIT | (5) |
| Model dependency | is derived from | PMID/DOI | (6) |
| Model Reference | Is Described By | PMID/DOI/URLs | (7) |

Example set 1:

*<bqbiol:hasTaxon>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/taxonomy/9606"/>*

*</rdf:Bag>*

*</bqbiol:hasTaxon>*

Example set 2:

*<bqbiol:occursIn>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/bto/0000782"/>*

*</rdf:Bag>*

*</bqbiol:occursIn>*

Example set 3:

*<bqbiol:isPropertyOf>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/mamo/MAMO:0000046"/>*

*</rdf:Bag>*

*</bqbiol:isPropertyOf>*

Example set 4:

*<bqbiol:hasProperty>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/go/GO:0002840"/>*

*</rdf:Bag>*

*</bqbiol:hasProperty>*

Example set 5:

*<bqbiol:hasProperty>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/go/GO:0050852"/>*

*</rdf:Bag>*

*</bqbiol:hasProperty>*

Example set 6:

*<bqmodel:isDerivedFrom>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/pubmed/12871957"/>*

*<rdf:li rdf:resource="http://identifiers.org/pubmed/16314431"/>*

*</rdf:Bag>*

*</bqmodel:isDerivedFrom>*

Example set 7:

*<bqmodel:isDescribedBy>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/pubmed/30356330"/>*

*</rdf:Bag>*

*</bqmodel:isDescribedBy>*

1. **Model component level annotation:**

Model component level annotation are done to provide details about each component of the model using controlled vocabularies via known ontologies. Usually mechanistic models have 4 main components i.e. Compartment, Species, Reactions and Parameter.

* 1. Compartment annotation

Compartment represents the cellular localization at which the modelled process is happening. Same can be annotated as:

|  |  |  |  |
| --- | --- | --- | --- |
| **Annotation Information** | **Qualifier/s** | **Preferred ontologies** | **Example Set** |
| Compartment in which biological process is happening | is / has Property | GO / BTO / NCIT (for cellular/Tissue/organ annotation) | (8) |

Example set 8:

*<compartment constant="true" id="Cell" metaid="XYZ1" name="Cell" size="1" spatialDimensions="3">*

*<annotation>*

*<bqbiol:isVersionOf>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/ncit/NCIT:C28699"/>*

*</rdf:Bag>*

*</bqbiol:isVersionOf>*

*<bqbiol:isVersionOf>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/ncit/NCIT:C12546"/>*

*</rdf:Bag>*

*</bqbiol:isVersionOf>*

*</annotation>*

* 1. Species annotation

Species are basically the biological entities participating in a reaction as substrate / product / enzyme.

|  |  |  |  |
| --- | --- | --- | --- |
| **Annotation Information** | **Qualifier/s** | **Preferred ontologies** | **Example Set** |
| Biological entity (Proteins/mRNA/Metabolites etc.) | is / has Property / is Version of | Uniprot (Proteins)  ChEBI (Metabolites)  Ensembl (Gene) | (9) |
| Modifications (PTMs like phosphorylation/dephosphorylation etc.) | has Property | PATO / MOD / NCIT | (9) |
| Protein Complexes | has part | Uniprot id for both proteins | (10) |

Example set 9:

*<species boundaryCondition="false" compartment="Cell" constant="false" id="PD1" initialConcentration="500" metaid="ABC9" name="PD1">*

*<annotation>*

*<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:dc="http://purl.org/dc/elements/1.1/" xmlns:dcterms="http://purl.org/dc/terms/" xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/" xmlns:bqmodel="http://biomodels.net/model-qualifiers/">*

*<rdf:Description rdf:about="#ABC9">*

*<bqbiol:isVersionOf>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/uniprot/Q9NZQ7"/>*

*</rdf:Bag>*

*</bqbiol:isVersionOf>*

*<bqbiol:hasProperty>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/pato/0002355"/>*

*</rdf:Bag>*

*</bqbiol:hasProperty>*

*</rdf:Description>*

*</rdf:RDF>*

*</annotation>*

*</species>*

Example set 10:

*<species boundaryCondition="false" compartment="Cell" constant="false" id="CP1" initialConcentration="0" metaid="OPS2" name="CP1">*

*<annotation>*

*<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:dc="http://purl.org/dc/elements/1.1/" xmlns:dcterms="http://purl.org/dc/terms/" xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/" xmlns:bqmodel="http://biomodels.net/model-qualifiers/">*

*<rdf:Description rdf:about="#OPS12">*

*<bqbiol:hasPart>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/uniprot/Q06124"/>*

*</rdf:Bag>*

*</bqbiol:hasPart>*

*<bqbiol:hasPart>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/uniprot/Q9NZQ7"/>*

*</rdf:Bag>*

*</bqbiol:hasPart>*

*<bqbiol:hasProperty>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/pato/0002220"/>*

*</rdf:Bag>*

*</bqbiol:hasProperty>*

*</rdf:Description>*

*</rdf:RDF>*

*</annotation>*

* 1. Reaction annotation

Reaction represents the biochemical process in which different species are participating and/or getting produced. Reactions are governed by rate laws and their associated parameters.

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| --- | --- | --- | --- |
| **Annotation Information** | **Qualifier/s** | **Preferred ontologies** | **Example Set** |
| Biological process represented by Reaction (Binding, Phosphorylation, Inhibition etc.) | is / has Property / is Version of | SBO / GO / NCIT / Reactome | (11) |

Example set 11:

*<reaction id="LCKyi\_DP\_LCKi" metaid="KKT97" name="LCKyi\_DP\_LCKi" reversible="false">*

*<annotation>*

*<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:dc="http://purl.org/dc/elements/1.1/" xmlns:dcterms="http://purl.org/dc/terms/" xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/" xmlns:bqmodel="http://biomodels.net/model-qualifiers/">*

*<rdf:Description rdf:about="#KKT97">*

*<bqbiol:is>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/sbo/0000330"/>*

*</rdf:Bag>*

*</bqbiol:is>*

*</rdf:Description>*

*</rdf:RDF>*

*</annotation>*

*</reaction>*

* 1. Parameter annotation

Parameter values determines the rate of the reaction. Parameter can be local or global dependent on its usage in one or more reactions.

|  |  |  |  |
| --- | --- | --- | --- |
| **Annotation Information** | **Qualifier/s** | **Preferred ontologies** | **Example Set** |
| Parameter type (Ex. Forward Rate constant (Kf), Catalytic rate constant (Kcat ) | is / has Property/ is Homolog To | SBO | (12) |

Example set 12:

*<parameter metaid="MNO53" id="Ka\_shp" name="Ka,shp" value="0.0065" units="unit\_3" constant="true">*

*<annotation>*

*<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:dc="http://purl.org/dc/elements/1.1/" xmlns:dcterms="http://purl.org/dc/terms/" xmlns:vCard="http://www.w3.org/2001/vcard-rdf/3.0#" xmlns:bqbiol="http://biomodels.net/biology-qualifiers/" xmlns:bqmodel="http://biomodels.net/model-qualifiers/">*

*<rdf:Description rdf:about="#MNO53">*

*<bqbiol:isHomologTo>*

*<rdf:Bag>*

*<rdf:li rdf:resource="http://identifiers.org/sbo/SBO:0000363"/>*

*</rdf:Bag>*

*</bqbiol:isHomologTo>*

*</rdf:Description>*

*</rdf:RDF>*

*</annotation>*

*</parameter>*