BioModels Database

Sharing and re-using computational models of biological processes

Nicolas Le Novère, Babraham Institute, EMBL-EBI

What is BioModels Database?

- Store and serve quantitative models of biological interest
- Models described in the peer-reviewed scientific literature + models automatically generated from pathway resources
- Models are curated: computer software check the syntax, while human curators check the semantics
- Models are simulated to ensure they provide the expected results
- Model components are annotated, to improve identification and retrieval
- Models are accepted in several formats, and served in several others

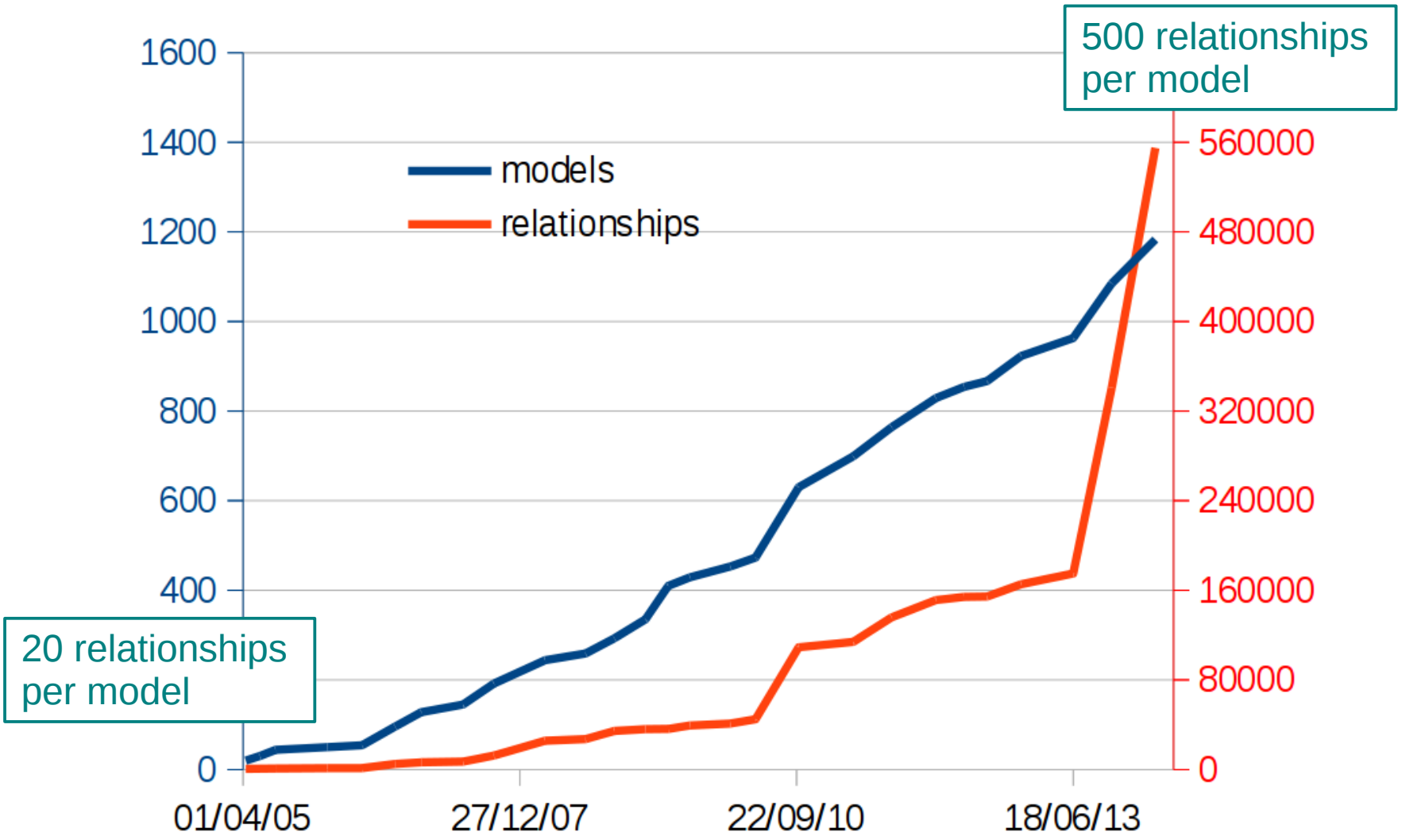
What can-we do with BioModels Database?

- Search and retrieve relevant quantitative or qualitative models
- Explore the variables and the structure of the model
- Run timecourse simulations of the model
- Download the model in many formats
- Do all the above via Web Services
- Learn about significant models using the Model of the Month

Where do models come from?

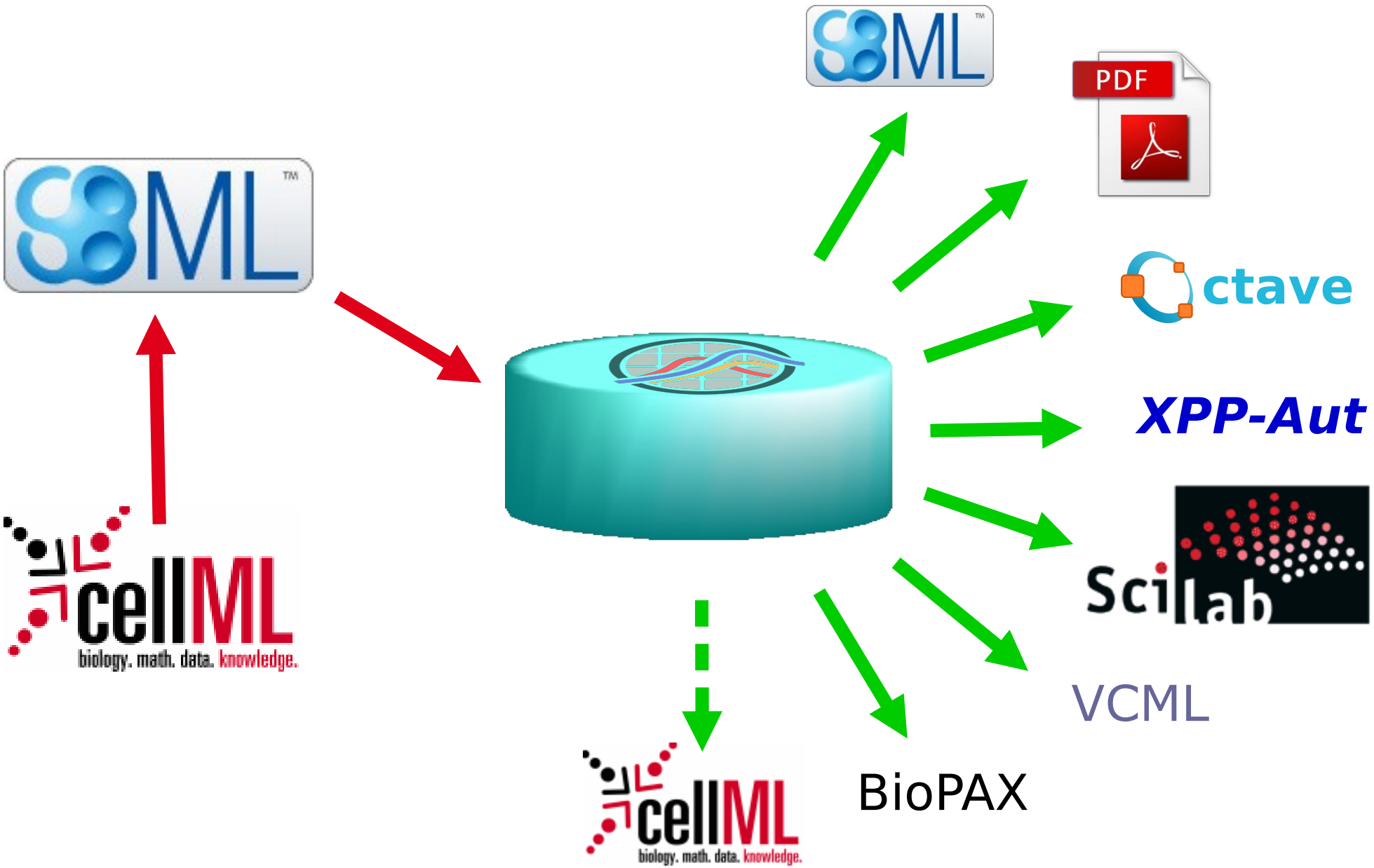
- From authors before grant applications or publications
- Over 300 scientific journals advise submission to BioModels Db:
  - Molecular Systems Biology
  - Public Library of Science journals
  - BioMedCentral journals
  - Royal Society of Chemistry journals
- Various people curated models out of interest.
- Submitted by curators
  - imported from other repositories (DOQCS, CellML)
  - reimplemented from literature

Computational models on the rise



BioModels Database growth (published models branch) since its creation

Input and output formats



Systems Biology Format Converter

Contents [hide]

The System Biology Format Converter

The System Biology Format Converter (SBFC) aims is to provide a generic framework that potentially allows any conversion between two formats. Interoperability between formats is a recurring issue in Systems Biology. Although there are various tools available to convert models from one format to another, most of them have been independently developed and cannot easily be combined, specially to provide support for more formats. The framework is written in Java and can be used as a standalone executable. This is a collaborative project and we hope that developers will provide support for more formats by creating new modules.SBFC allows anyone to easily add new converters and to integrate existing converters with a minimum of changes. We will also allow to combine several existing converters.

The SBFC framework currently supports conversion from SBML to BioPAX Level 2 and Level3, XPP, Octave and Dot.

Several others converters are in development:

- SBGN related:
  - SBML to SBGN-ML
  - SBGN-ML to an SBGN enriched graphical representation designed for use in a web browser

The main Sourceforge page for the SBFC project is http://sourceforge.net/projects/sbfc/

Converters

Here is a small description of all the conversions currently supported. You can access to a more detailed page by clicking on a converter name.

Step 1 : Choose your input format

The input format you choose should match the model(s) you will submit, otherwise you will get an error. We strongly advise you validate your model(s) before the conversion

At the moment only SBML files can be selected as input.

Model format : SBML

Step 2 : Choose your output format

The output format you choose will determine the converter to use, if the format you want doesn't appear here it means the converter is not implemented yet

Output format : Select the output format

- Select the output format
- BioPax Level 2
- BioPax level 3
- Octave
- XPP
- SBML_L3V1
- SBML_L2V4
- SBML_L2V1
- SBML_L1V2

Step 3 : Enter et a URL to your results (optional)

Step 4 : Choose the model(s) you want to convert

BioModels is not limited to biochemistry!

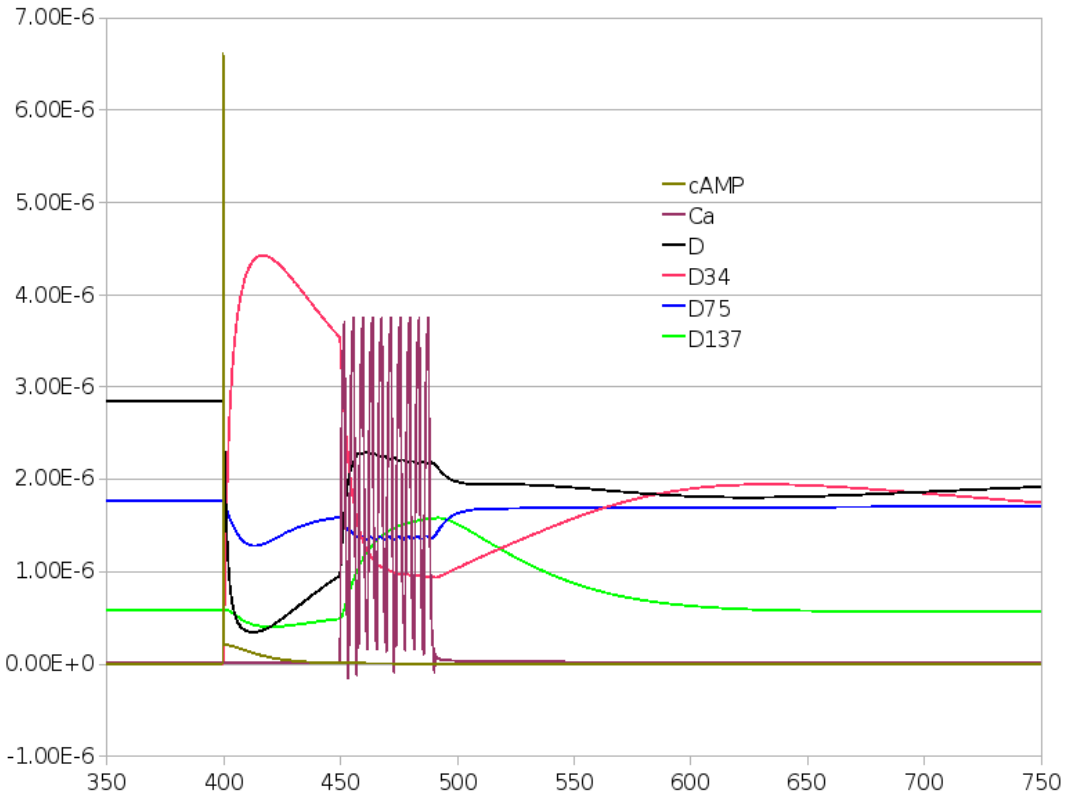
Is it about bio[logy|chemistry|medicine]?

Is it a computational model?

Is it published?

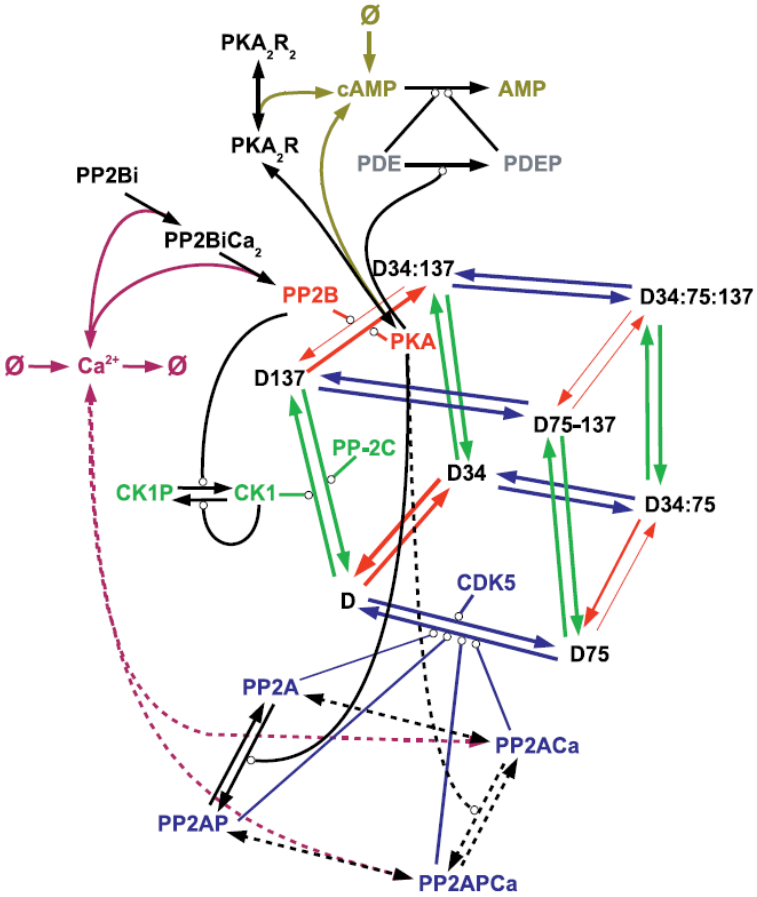
Then it should be in BioModels

Process based biochemical models



Fernandez et al. DARPP-32 is a robust integrator of dopamine and glutamate signals
PLoS Comput Biol (2006) 2: e176.

BIOMD0000000153

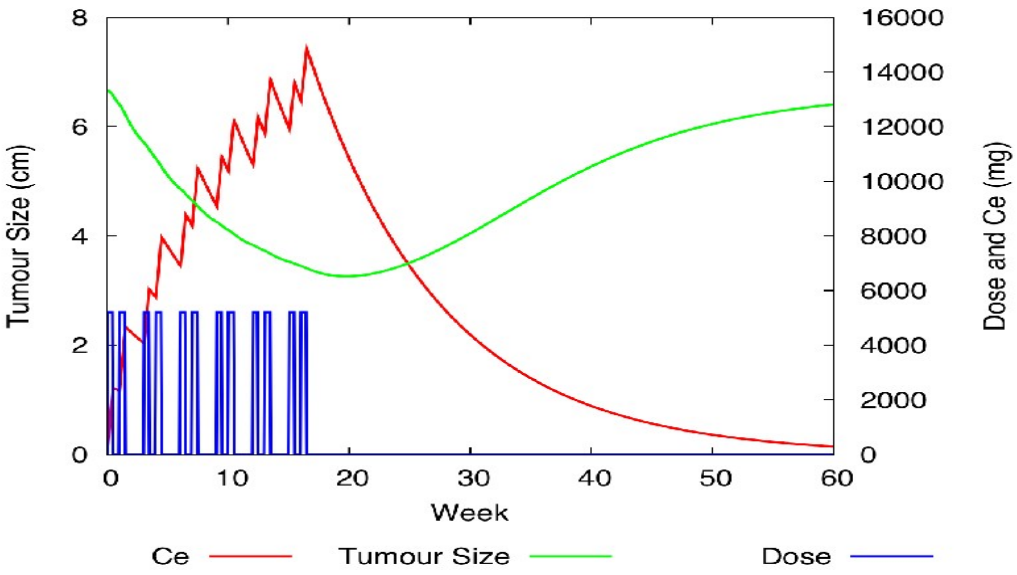


reaction:

$$v_{\text{on}} = k_{\text{on}} \times [\text{D}] \times [\text{CDK5}] \times \text{Vol}$$

EMBL-EBI

Pharmacometrics models



Tham et al (2008) A pharmacodynamic model for the time course of tumor shrinkage by gemcitabine + carboplatin in non-small cell lung cancer patients. *Clin Cancer Res*. 2008 14(13): 4213-8.

BIOMD0000000234

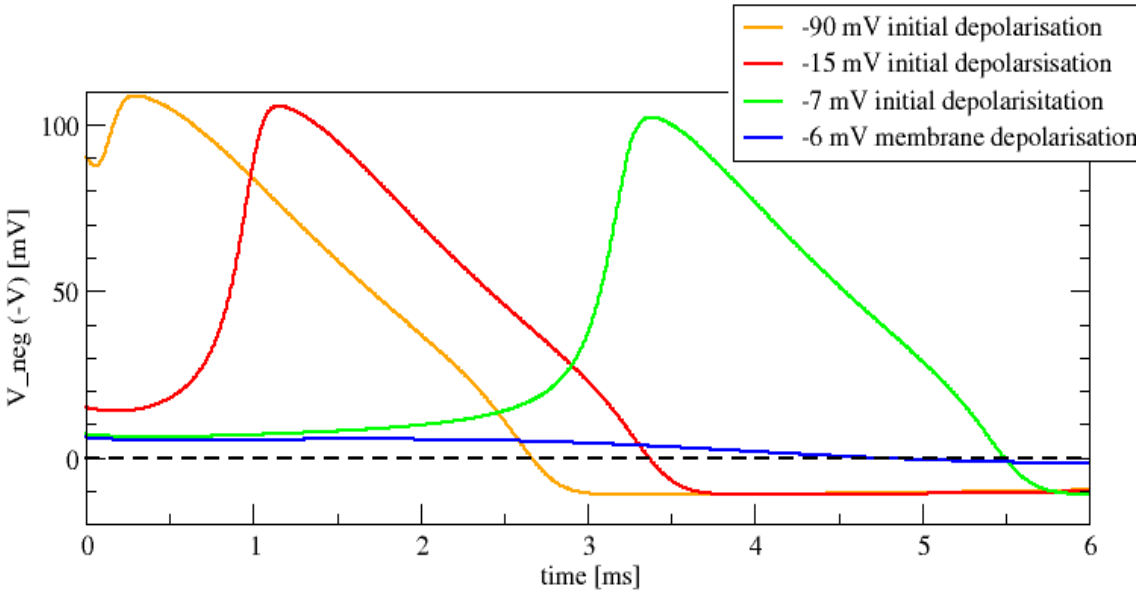
rate rule:

$$\frac{dSize}{dt} = (Rate_{in} \times Effect - K_{over} \times Size) \times Size$$

assignment rule:

$$Effect = 1 - \frac{E_{max} \times Ce}{Amt_{50} + Ce}$$

Conductance-based model



Hodgkin AL, Huxley AF.
A quantitative description of membrane current and its application to conduction and excitation in nerve.
J Physiol (1952) 117:500-544.

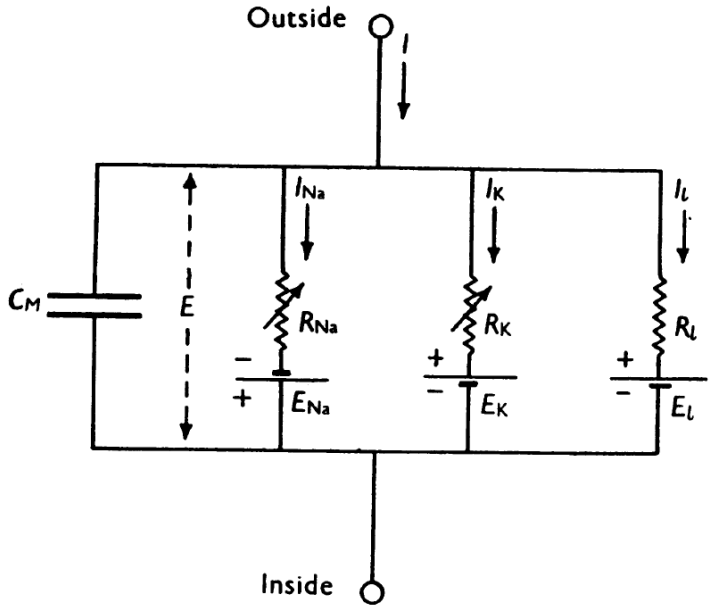
BIOMD0000000020

rate rule:

$$\frac{dv}{dt} = \frac{I - (i_{\mathrm{N\ a}} + i_{\mathrm{K}} + i_{\mathrm{L}})}{C_{\mathrm{m}}}$$

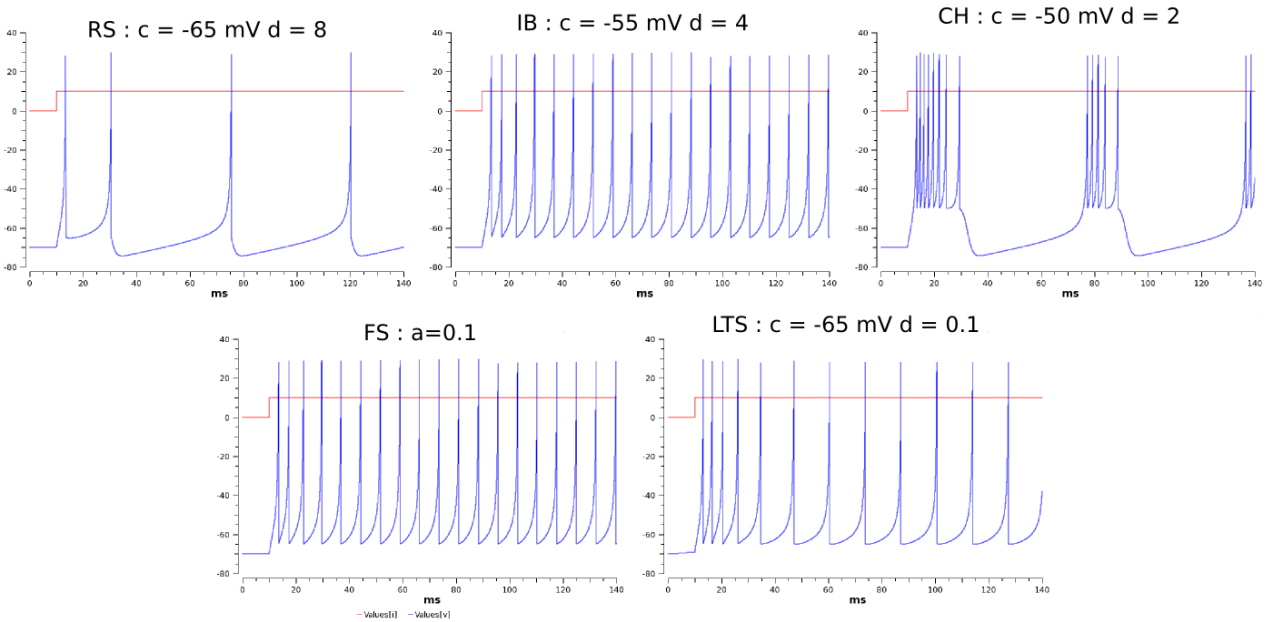
assignment rule:

$$i_{\mathrm{N\ a}} = g_{\mathrm{N\ a}} \times m^3 \times h \times (V - E_{\mathrm{N\ a}})$$



EMBL-EBI

Neuroscience models



Izhikevich EM. Simple model of spiking neurons. *IEEE Trans Neural Netw* (2003) 14(6):1569-1572.

BIOMD0000000127

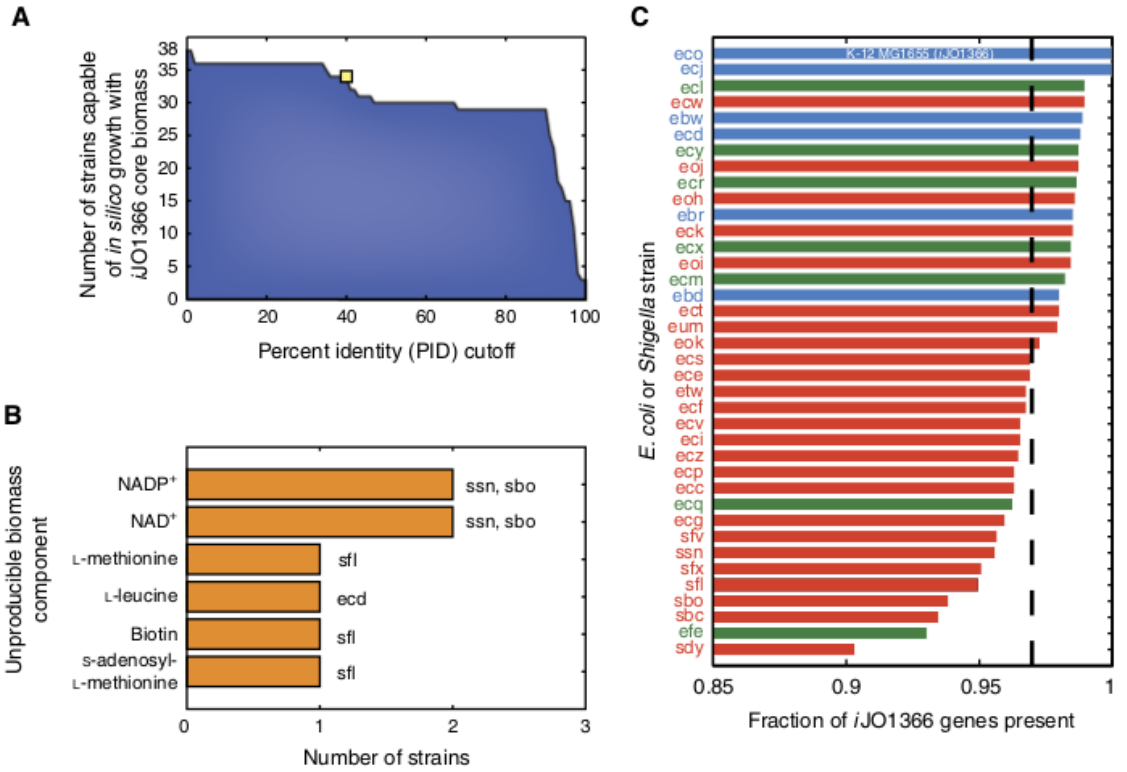
rate rule:

$$\frac{dv}{dt} = 0.04^2 + 5 \times V + 140 - U + i$$

event:

$$\text{when } v > V_{\text{thresh}} \begin{cases} v = c \\ U = U + d \end{cases}$$

Flux Balance Analysis models

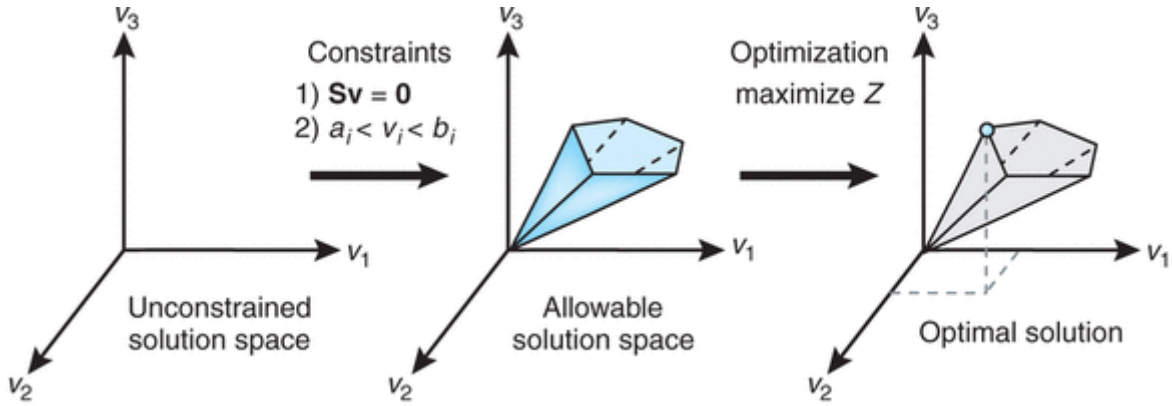


Orth et al. A comprehensive genome-scale reconstruction of Escherichia coli metabolism - 2011
Mol Syst Biol (2011);7:535

MODEL1108160000

reaction:

$$v_i = flux_i$$



BioModels Db does not belong to anyone!

CC0 1.0 Universal (CC0 1.0)
Public Domain Dedication

This is a human-readable summary of the **Legal Code (read the full text)**.

Disclaimer

No Copyright

The person who associated a work with this deed has **dedicated** the work to the public domain by waiving all of his or her rights to the work worldwide under copyright law, including all related and neighboring rights, to the extent allowed by law.

You can copy, modify, distribute and perform the work, even for commercial purposes, all without asking permission. See **Other Information** below.

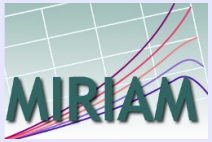
Minimal Information Required In the Annotation of Models

Reference correspondence

1. In a public, standardized, machine-readable format
2. Comply with the standard in which it is encoded
3. Clearly related to a single reference description
4. Reflect biological processes
5. Instantiable in a simulation all numbers provided
6. Able to reproduce results

Attribution

1. Has to be named
2. Citation must be provided
3. Model creators details
4. Date and time of creation and last modification
5. Link to precise statement about terms of distribution



External resources

1. Annotation unambiguously model constituent to data
2. Link to external information as a triplet {collection, identifier, qualifier}
3. Annotation written as a Uniform Resource Identifier
4. Identifier considered within framework of the collection.
5. Collection namespace and record identifier in one URI
6. Qualifiers to refine the link between model constituent and external knowledge
7. Standard set of valid URIs agreed upon by community

http://co.mbine.org/standards/miriam

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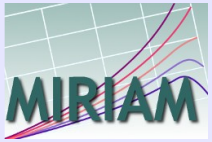

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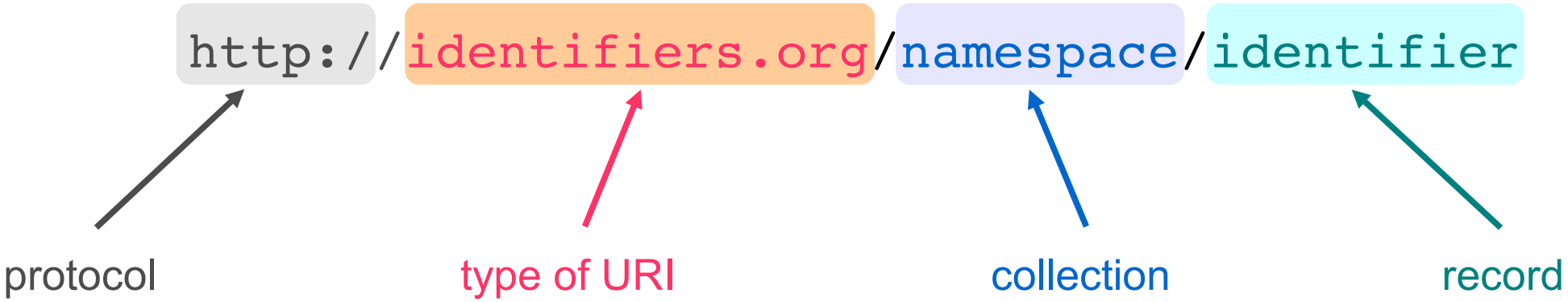
Why are annotations important?

Annotation of model components are essential to:

- allow efficient search strategies
- unambiguously identify model components
  - improve understanding the structure of the model
  - allow easier comparison of different models
  - ease the integration of models
- add a semantic layer to the model
  - improve understanding of the biology behind the model
  - allow conversion and reuse of the model
  - ease the integration of model and biological knowledge

Enters identifiers.org (aka new MIRIAM URIs)



http://identifiers.org/uniprot/P62158

http://identifiers.org/ec-code/1.1.1.1

http://identifiers.org/obo.go/GO:0000186

Curated and Non-curated Models

- Curated models – Comply with the MIRIAM guidelines
- Non-Curated models – valid SBML, not curated or annotated
  - Not MIRIAM compliant:

    cannot reproduce results published in the paper.

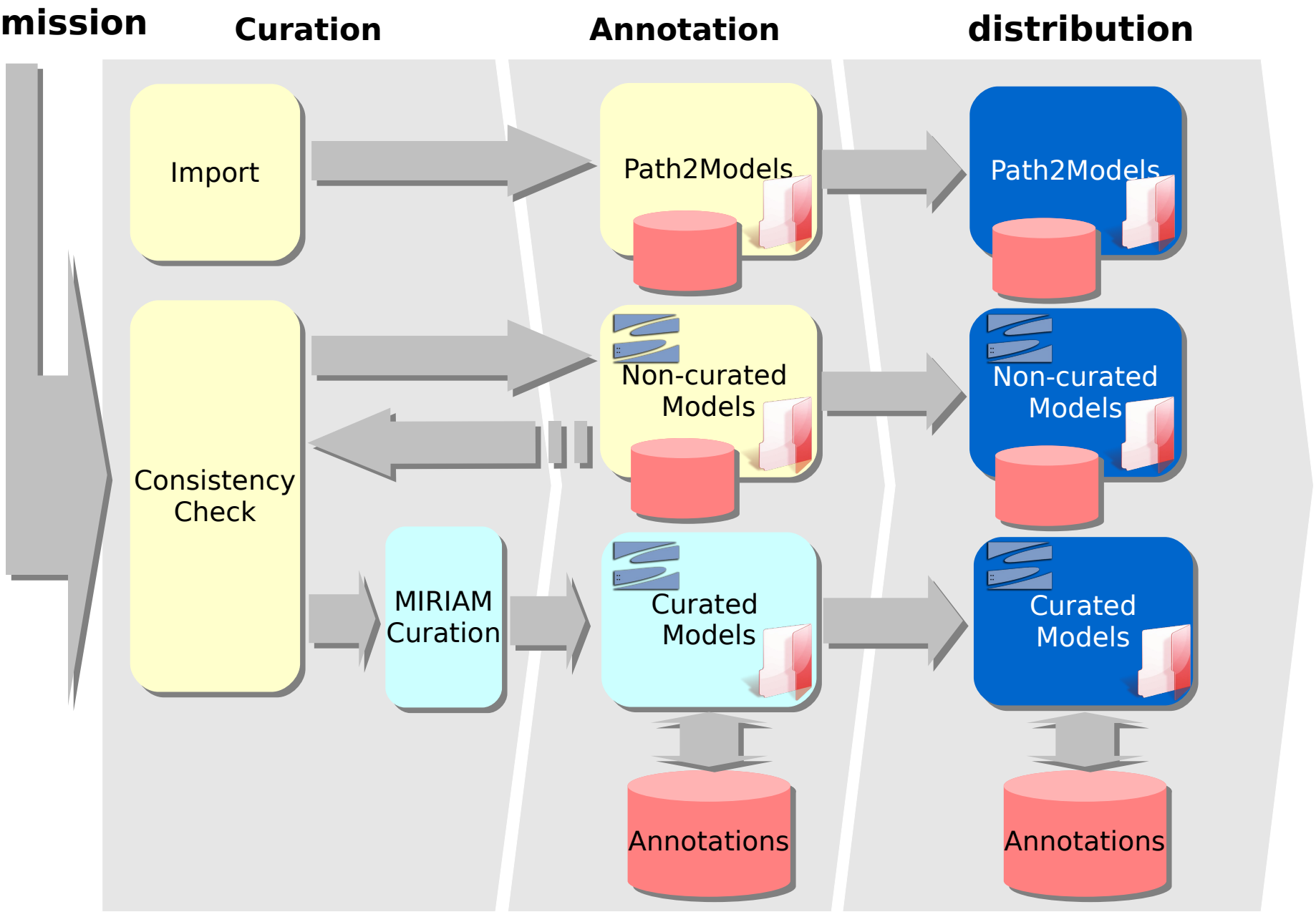
    differ in model structure

    non-kinetic models (eg. FBA, stoichiometric maps)
  - MIRIAM compliant:

    models contain kinetics that we cannot curate at present (e.g. reaction-diffusion models)

    models are yet to be curated

Current production pipeline



BioModels Database

Search
Advanced

BioModels Database is a repository of computational models of biological processes. Models described from literature are manually curated and enriched with cross-references. All models are provided in the Public Domain. More information about BioModels Database can be found in the FAQ.

Models published in the literature

Browse

Manually curated
(530 models)

Non curated
(655 models)

Alternative access

Gene Ontology classification (new)

Gene Ontology tree

Advanced search

Models automatically generated from pathway resources (Path2Models)

Browse

Metabolic (112,898 models)
Non-metabolic (27,531 models)
Whole genome metabolism (2,641 models)

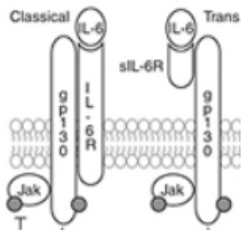
Alternative access

Taxonomy

Dedicated search

Model of the month

September, 2014



A mathematical model describing the inhibition of IL6 signalling in Crohn's Disease is presented here. Several antibody ligands were simulated with different targets and their varied effects upon IL6 signalling is observed.

Access this model of the month.

News

8 August 2014 Updated homepage, model access and display

BioModels' homepage has been updated to provide a clearer view of the content of the repository. Also, a GO classification is a new browsing tool for models from the literature. Finally, various updates have been implemented for non-curated models.

25 April 2014 Our recent diabetes review most downloaded in April on CPT:PSP

Our recent review "The impact of mathematical modeling on the understanding of diabetes and related complications" has been the most downloaded this month from the CPT: Pharmacometrics & Systems Pharmacology website!

BioModels Database

BioModels Home | Models | Submit | Support | About BioModels | Contact us

- Curated models
- Non-curated models
- Gene Ontology categories (*new*)
- Gene Ontology tree
- Taxonomy cloud
- Path2Models
- Advanced search
- Simulate in JWS (*ext*)
- Models of the Month
- Archives (*ext*)

BioModels … f computational models of biological processes. M… ture are manually curated and enriched with cross-r… rovided in the Public Domain. More information … can be found in the FAQ.

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BioModels Database

BioModels Home | Models | Submit | Support | About BioModels | Contact us

- Submit a new model
- Annotation information
- Curation guidelines
- Annotation guidelines

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Dedicated search

Main instance at EMBL-EBI, UK | Mirror at Caltech, USA | Model archives | Web

v.ebi.ac.uk/biomodels-main/#

Model

September, 2014

A mathematical
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8 August 201

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BioModels Home | Models | Submit | Support | About BioModels | Contact us

- FAQ
- Courses
- Converters (*ext*)
- Web Services
- SPARQL Endpoint
- Develop
- SourceForge (*ext*)

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- Terms of Use
- Citation
- News
- Acknowledgements
- Jobs
- Curator Sign in

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Submit - Step 1

You can submit here models to be included in BioModels Database.

The following formats are currently accepted:

- SBML Level 3: Version 1 (including any packages)
- SBML Level 2: Version 1, Version 2, Version 3 and Version 4
- SBML Level 1: Version 1 and Version 2
- CellML: 1.0 and 1.1

If you wish to submit a model under a different format, please contact us.

If you wish to provide additional files with your submission, please contact us.

The submitted model will not be publicly available from BioModels Database straightaway. If you wish to know more about the submission, curation and annotation pro sections of the Frequently Asked Questions.

To ensure a prompt processing of your model, please follow those simple guidelines:

- Check that your model is valid according to the format you chose. If your model is encoded in SBML, you can use the official online validator.
- Enter all relevant information which could help the work of our curators (relation between the model and publication, modifications or clarifications of the model example using the *notes* elements if your model is encoded in *SBML*), or in the *Comment* field provided in step 2 of this form.
- If you created the model (or collaborated to its creation) but are not an author of the associated publication, please add your personnal information (first and la in the model, so that your contribution can be acknowledged. If you used *SBML*, this can be done by adding to the *model* element a *dc:creator* annotation, as i the blue part if already present).
- Choose a meaningful name for your model. You can follow the pattern *AuthorNameYear - Topic, Method*, for example: *Levchenko2000 - MAPK, noScaffold* or

All models in BioModels Database are available under the terms of the Creative Commons CC0 1.0 (Public Domain Dedication). Therefore you need to agree to relea **Domain** before submitting it to BioModels Database.

Thank you for contributing to BioModels Database!

Please enter the identifier of the scientific publication associated with the model, and then click *Continue*. If the model has not been published, please select the 'Unpu

Publication Identifier:

Type of identifier: (•) PubMed ID (Search Medline) ( ) DOI (Resolve a DOI) ( ) URL ( ) Unpublished

publication. To actually facilitate this curation phase, prior to submitting a model, please do the following:

- Enter all the relevant information you believe is necessary for the curation (reference publication, modifications or clarifications of the model, etc.) either using the *notes* elements if your model is under one of the *SBML* formats), or into the *Curation comment* text field provided by the form below.
- If you created the model, or collaborated to its creation, and you are not an author of the reference publication, add to the *model* element a *dc:creator* ar name, organisation, email), so that your contribution can be acknowledged. Click here to view an example of a *dc:creator* annotation which you can re-us
- Choose a meaningful value for the attribute *name* of the *model* element. Examples of good model names are *NameAuthorYear_Topic_Method*, *Levcher Edelstein1996_EPSP_AChEvent*.
- Check the validity of the model (for example by using this online validator if your model is encoded in the *SBML* format). All the models undergo a primar and, as mentioned before, a more thorough testing during the curation phase, but an already valid model is of great help nevertheless!
- If the model was not created directly in SBML, or if it requires a specific software to be simulated adequately, please enter in the *Original Model* form a U repository. Refrain from entering a generic URL to the repository itself.

Please enter your personal details and any comment useful for the curation step (underlined fields are required), and then click *Submit*.

First name:

Last name:

Organisation:

Email:

Comment:

Original model:

Model file: Browse... No file selected.

Submit Reset

Browse - Curated models

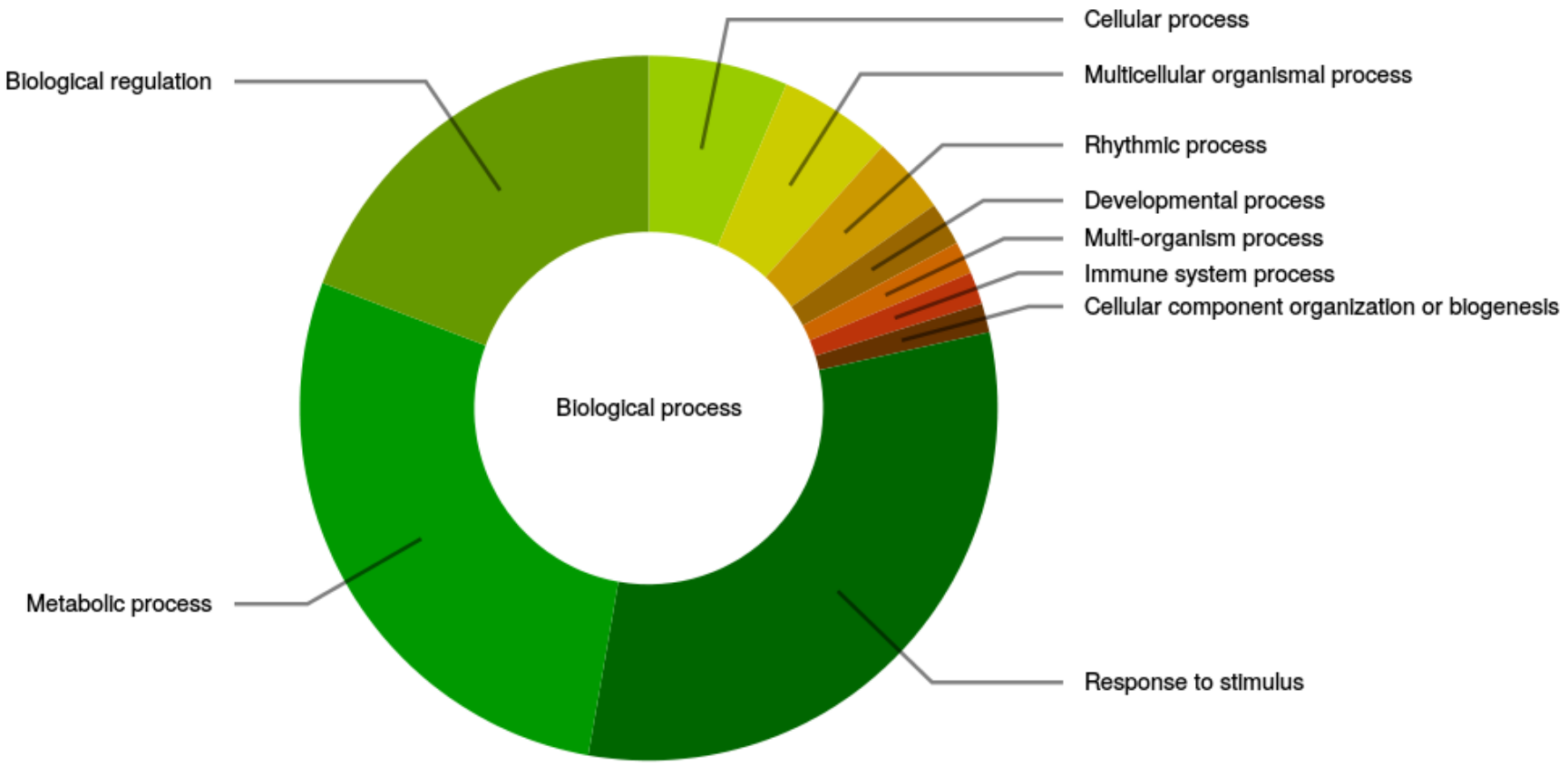
The following fields are used to describe a model: ...

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54

10 | 50 | 100 | All

BioModels ID	Name	Publication ID	Last Modified
BIOMD0000000355	Abell2011_CalciumSignaling_WithAdaptation	21844332	2011-09-08T12:03:57+00:00
BIOMD0000000354	Abell2011_CalciumSignaling_WithoutAdaptation	21844332	2011-09-08T12:16:51+00:00
BIOMD0000000428	Achcar2012 - Glycolysis in bloodstream form T. brucei	22379410	2013-06-10T13:41:07+00:00
BIOMD0000000476	Adams2012 - Locke2006 Circadian Rhythm model refined with Input Signal Light Function	22855577	2013-09-11T15:39:47+00:00
BIOMD0000000169	Aguda1999_CellCycle	10619492	2012-07-05T14:42:01+00:00
BIOMD0000000295	Akman2008_Circadian_Clock_Model1	18277380	2014-05-28T01:56:26+00:00
BIOMD0000000214	Akman2008_Circadian_Clock_Model2	18277380	2014-05-28T01:57:42+00:00
BIOMD0000000220	Albeck2008_extrinsic_apoptosis	18406323	2012-07-05T14:42:40+00:00
BIOMD0000000211	Albert2005_Glycolysis	15955817	2014-05-27T23:52:38+00:00
BIOMD0000000289	Alexander2010_Tcell_Regulation_Sys1	20195912	2014-03-11T13:38:50+00:00

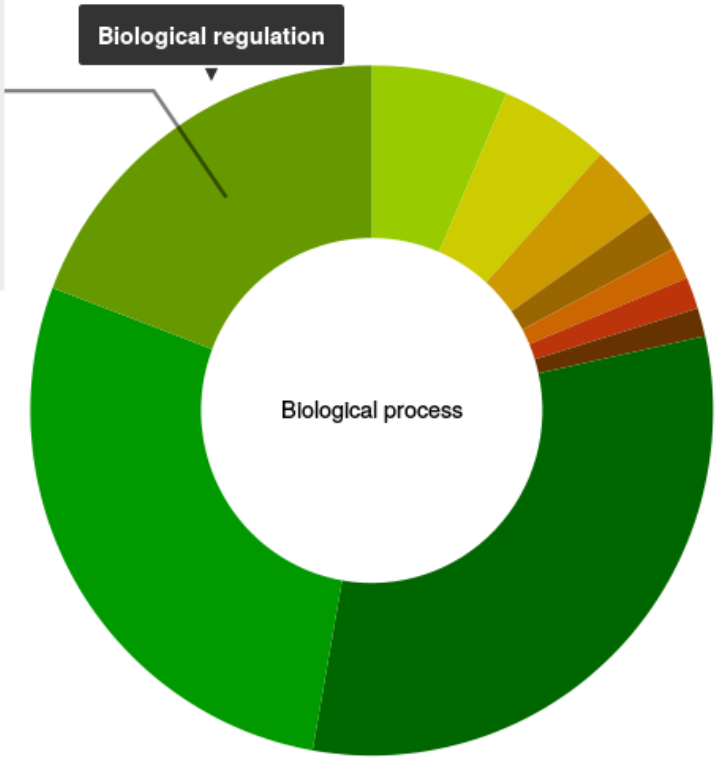
Classification of models published in the literature, based on GO



Clas…e literature, based on GO

Biological regulation (232)

- Regulation of biological process (109)
- Regulation of membrane potential (65)
- Homeostatic process (27)
- Regulation of localization (21)
- Regulation of molecular function (10)



Selected GO term: Regulation of biological process

Curated Models

BioModels ID	Name	Publication ID	Last Modified
BIOMD0000000012	Elowitz2000 - Repressilator	10659856	2013-07-10
BIOMD0000000065	Yildirim2003_Lac_Operon	12719218	2014-02-12
BIOMD0000000067	Fung2005_Metabolic_Oscillator	15875027	2012-05-16
BIOMD0000000079	Goldbeter2006_weightCycling	16595882	2012-07-05
BIOMD0000000080	Thomson1989_AdenylateCyclase	2574993	2014-02-12

BioModels Database: GO tree

This is a tree view of the curated models based on their Gene Ontology annotation.

To browse the models, please click the ▶ icon on the left of the term to expand the related branch and similarly click on the ▼ icon to collapse an already opened branch. By clicking on a term's name, the list of models annotated with this term (or one of its descendant) will be displayed on the right panel.

- ▼ GO:0008150 - biological_process (529)
  - ▶ GO:0022610 - biological adhesion (1)
  - ▼ GO:0065007 - biological regulation (373)
    - ▼ GO:0050789 - regulation of biological process (316)
      - ▼ GO:0048519 - negative regulation of biological process (77)
        - ▼ GO:0051129 - negative regulation of cellular component organization (5)
          - ▼ GO:0010639 - negative regulation of organelle organization (5)
            - ▼ GO:0051784 - negative regulation of nuclear division (5)
              - ▼ GO:0045839 - negative regulation of mitosis (5)
                - ▼ GO:0045841 - negative regulation of mitotic metaphase/anaphase transition (5)
                  - GO:0007094 - mitotic spindle assembly checkpoint (5)
        - ▶ GO:0048523 - negative regulation of cellular process (71)
        - ▶ GO:0051093 - negative regulation of developmental process (1)
        - ▶ GO:0045926 - negative regulation of growth (1)
        - ▶ GO:0002683 - negative regulation of immune system process (1)
        - ▶ GO:0009892 - negative regulation of metabolic process (54)
        - ▶ GO:0043901 - negative regulation of multi-organism process (5)
        - ▶ GO:0051241 - negative regulation of multicellular organismal process (1)
        - ▶ GO:0048585 - negative regulation of response to stimulus (32)
        - ▶ GO:0051283 - negative regulation of sequestering of calcium ion (7)
        - ▶ GO:0023057 - negative regulation of signaling (33)
        - ▶ GO:0051051 - negative regulation of transport (8)
      - ▶ GO:0048518 - positive regulation of biological process (91)
      - ▶ GO:0044087 - regulation of cellular component biogenesis (2)
      - ▶ GO:0051128 - regulation of cellular component organization (12)
      - ▶ GO:0050794 - regulation of cellular process (274)

Model(s) annotated with the GO term GO:0007094 or one of its descendant(s):

- Chen2004 - Cell Cycle Regulation (BIOMD0000000056)
- Ibrahim2008 - Mitotic Spindle Assembly Checkpoint - Convey variant (BIOMD0000000187)
- Ibrahim2008 - Mitotic Spindle Assembly Checkpoint - Dissociation variant (BIOMD0000000186)
- Ibrahim2008_Cdc20_Sequestring_Template_Model (BIOMD0000000194)
- Ibrahim2008_MCC_assembly_model_KDM (BIOMD0000000193)

- *Person* → Search BioModels Database for model submitter and/or creator(s) names, or model reference publication author(s) names (for example *Nicolas L Bruce Shapiro* or *Shapiro*, *Edelstein* or *Novak*).
- *SBML elements* → Search BioModels Database using the content of either "name" or "*notes*" SBML elements (for example *Edelstein* or *nicotinic*). Select the you want to find documents which matches the exact phrase; otherwise, all words will be searched as default.
- *Annotation (full text)* → Search BioModels Database for related information found in the models reference publication or third-party resources, by either publi identifier or text (for example *9256450* or *cyclin* for publication, *GO:0000278* or *cell cycle* for Gene Ontology, *P04551* or *cell division* for UniProt).
- *Annotation (identifier)* → Search BioModels Database for annotations, by third-party resource identifiers (for example *IPR002394* for InterPro, *hsa04080* for *68910* for Reactome).

A part from the *BioModels Identifier* -based search, for every other criteria the search operates on a *contains the entered string basis*, case-insensitive *Person* for *Shapl* or *shapl* will return the same results as searching for *Shapiro* or *shapiro*. In addition, since search strings are treated as words, do n expressions.

Multiple criteria can be combined with either *and* or *or*. If *and* is selected, only those models satisfying all the criteria will be returned. If instead *or* is s models satisfying at least one of the criteria will be returned.

BioModels identifier:

Person:

SBML elements: match the **exact phrase**

Annotation (full text): UniProt Knowledgebase

Annotation (full text): Publication — cell cycle

Annotation (full text): Gene Ontology

Annotation (identifier): PubChem-compound

Annotation (identifier): KEGG Reaction

Annotation (identifier): Enzyme Nomenclature

Compose by: and or

Search Reset

Search - Models

Query: *Publication* **cell cycle** [resources]

The search returned **44** models.

New Search

33 Curated models returned:

BioModels ID	Name	Publication ID	Last Modified
BIOMD0000000003	Goldbeter1991 - Min Mit Oscil	1833774	2013-05-16T14:38:01+00:00
BIOMD0000000004	Goldbeter1991 - Min Mit Oscil, Expl Inact	1833774	2012-12-11T15:30:15+00:00
BIOMD0000000005	Tyson1991 - Cell Cycle 6 var	1831270	2013-05-16T14:40:43+00:00
BIOMD0000000006	Tyson1991 - Cell Cycle 2 var	1831270	2013-05-16T14:38:56+00:00
BIOMD0000000007	Novak1997 - Cell Cycle	9256450	2014-03-26T14:20:21+00:00
BIOMD0000000008	Gardner1998 - Cell Cycle Goldbeter	9826676	2014-07-24T10:59:34+00:00
BIOMD0000000018	Morrison1989_FolateCycle	2732237	2012-07-05T14:40:37+00:00
BIOMD0000000056	Chen2004 - Cell Cycle Regulation	15169868	2013-06-07T10:59:38+00:00
BIOMD0000000109	Haberichter2007_cellcycle	17299420	2012-07-05T14:49:20+00:00
BIOMD0000000110	Qu2003_CellCycle	14645053	2012-05-16T10:13:14+00:00
BIOMD0000000111	Novak2001_FissionYeast_CellCycle	12779461	2012-07-05T16:47:55+00:00
BIOMD0000000150	Morris2002_CellCycle_CDK2Cyclin	11959850	2010-12-01T22:10:11+00:00

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

Download SBML | Other formats (auto-generated) | Actions | Send feedback

Model | Overview | Math | Physical entities | Parameters | Curation

Reference Publication

Publication ID: 1831270

Tyson JJ.
Modeling the cell division cycle: cdc2 and cyclin interactions.
Proc. Natl. Acad. Sci. U.S.A. 1991 Aug; 88(16): 7328-7332
Department of Biology, Virginia Polytechnic Institute and State University, Blacksburg 24061. [more]

Model

Original Model: *BIOMD0000000005.xml.origin*

Submitter: Nicolas Le Novère

Submission ID: MODEL6614644188

Submission Date: 13 Sep 2005 12:31:08 UTC

Last Modification Date: 16 May 2013 14:40:43 UTC

Creation Date: 08 Feb 2005 18:28:27 UTC

Encoders: Bruce Shapiro
Vijayalakshmi Chelliah

set #1	bqbiol:hasVersion	**Reactome** REACT_152
set #2	bqbiol:isVersionOf	**KEGG Pathway** sce04111 **Gene Ontology** mitotic cell cycle
	bqbiol:occursIn	**Taxonomy** Opisthokonta

Notes

Tyson1991 - Cell Cycle 6 var

Mathematical model of the interactions of cdc2 and cyclin.

This model is described in the article:

Modeling the cell division cycle: cdc2 and cyclin interactions.
Tyson JJ.
Proc. Natl. Acad. Sci. U.S.A. 1991; 88(16); 7328-32

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

Download SBML | Other formats (auto-generated) | Actions | Send feedback

Model | Overview | Math | **Physical entities** | Parameters | Curation

⊞	Spatial dimensions: 3.0 Compartment size: 1.0
EmptySet *Compartment: cell*	Initial amount: 0.0
⊞ **cdc2k** *Compartment: cell*	Initial amount: 0.0
⊞ **cdc2k-P** *Compartment: cell*	Initial amount: 0.75
⊟ **p-cyclin_cdc2** *Compartment: cell*	Initial amount: 0.0
Annotations:	set #1 bqbiol:hasPart **UniProt Knowledgebase** CDK1_SCHPO **InterPro** IPR006670
⊞ **p-cyclin_cdc2-p** *Compartment: cell*	Initial amount: 0.25
⊞ **cyclin** *Compartment: cell*	Initial amount: 0.0
⊞ **p-cyclin** *Compartment: cell*	Initial amount: 0.0

Download SBML | Other formats (auto-generated) | Actions | Send feedback

Model | Overview | **Math** | Physical entities | Parameters | Curation

Reactions (9)

⊞ **cyclin_cdc2k dissociation**	[p-cyclin_cdc2] → [cdc2k] + [p-cyclin];
⊞ **cdc2k phosphorylation**	[cdc2k] → [cdc2k-P];
⊞ **cdc2k dephosphorylation**	[cdc2k-P] → [cdc2k];
⊞ **cyclin cdc2k-p association**	[cdc2k-P] + [cyclin] → [p-cyclin_cdc2-p];
⊟ **deactivation of cdc2 kinase**	[p-cyclin_cdc2] → [p-cyclin_cdc2-p];
Math:	$cell \times k5notP \times M$ *(Details:)*

Annotations:

set #1	bqbiol:hasVersion	**Reactome** REACT_6327 **Reactome** REACT_3178
	bqbiol:isVersionOf	**Enzyme Nomenclature** 2.7.10.2 **Gene Ontology** negative regulation of cyclin-dependent protein serine/threonine kinase activity **Gene Ontology** protein phosphorylation

⊞ **cyclin biosynthesis**	[EmptySet] → [cyclin];
⊞ **default degradation of cyclin**	[cyclin] → [EmptySet];
⊞ **cdc2 kinase triggered degration of cyclin**	[p-cyclin] → [EmptySet];
⊞ **activation of cdc2 kinase**	[p-cyclin_cdc2-p] → [p-cyclin_cdc2]; *{total_cdc2}*

Rules (2)

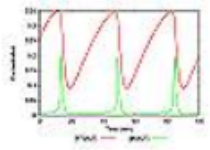
⊞ **Assignment Rule (*name: YT*)**	total_cyclin = Y+YP+M+pM
⊞ **Assignment Rule (*name: CT*)**	total_cdc2 = C2+CP+M+pM

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

Download SBML | Other formats (auto-generated) | Actions | Send feedback

Model | Overview | Math | Physical entities | Parameters | **Curation**

Representative curation result(s)



Curator's comment: (*updated:* 08 Feb 2010 10:29:04 GMT)

The model reproduces figure 3A of the reference publication. The model was integrated and simulated using Copasi v4.5 (Build 30).

Additional file(s)

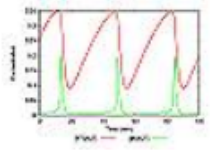
- **Simulation experiment description:**
  This SED-ML file allows you to reproduce the curation result (Fig 3a), for example, by loading it into SED-ML Web Tools (http://sysbioapps.dyndns.org/SED-ML_Web_Tools/).
  [BIOMD0000000005_SED-ML.xml]

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

Download SBML | Other formats (auto-generated) | Actions | Send feedback

Model | Overview | Math | Physical entities | Parameters | **Curation**

Representative curation result(s)



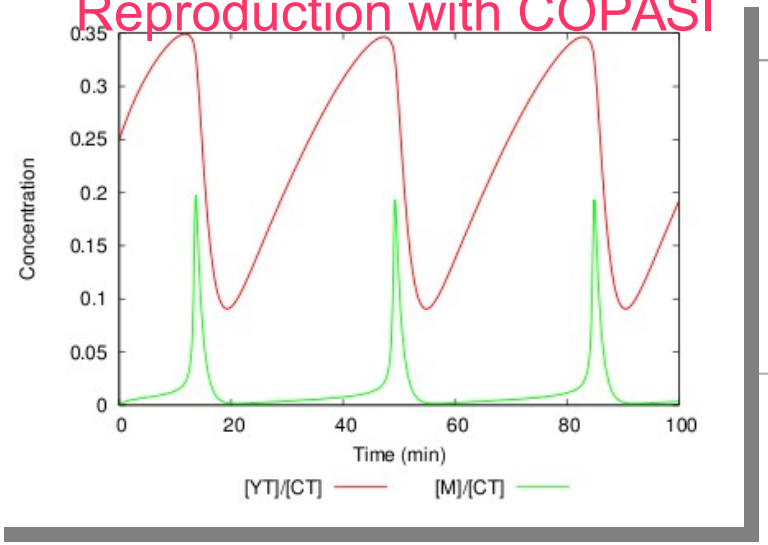
Curator's comment: (*updated:* 08 Feb 2010 10:29:04 GMT)

The model reproduces figure 3A of the reference publication. The model was integrated and simulated using Copasi v4.5 (Build 30).

Additional file(s)

- **Simulation experiment description:**
  This SED-ML file allows you to reproduce the curation result (Fig 3a), for example, by loading it into SED-ML Web Tools (http://sysbioapps.dyndns.org/SED-ML_Web_Tools/)
  [BIOMD...]

Reproduction with COPASI



original article

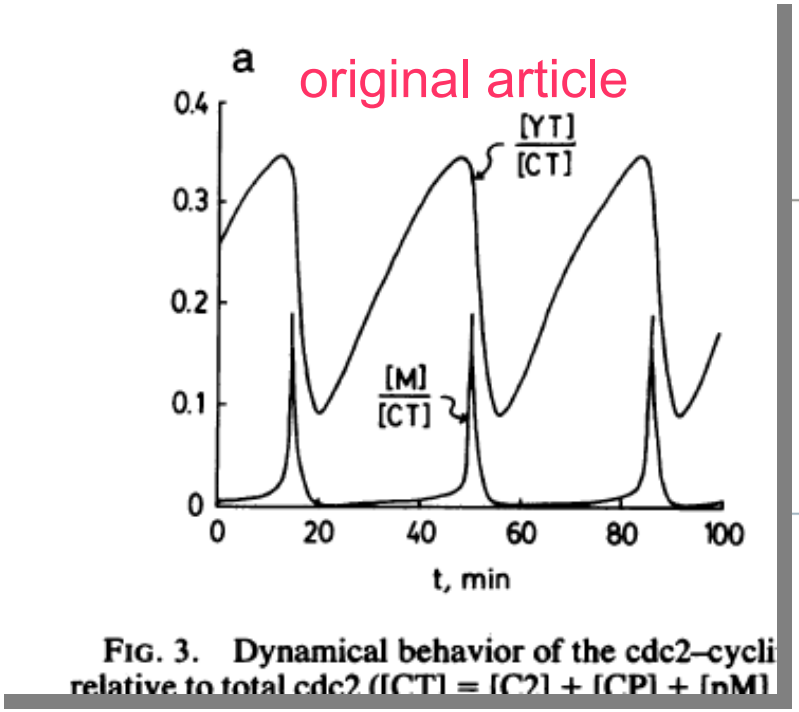


FIG. 3. Dynamical behavior of the cdc2–cycli
relative to total cdc2 ([CT] = [C2] + [CP] + [pM]

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

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Model | **Overview** | Math | Physical entities | Parameters | Curation

Create a submodel with selected elements — Deselect All

Model

Publication ID: 1831270 **Submission Date:** 13 Sep 2005 12:31:08 UTC **Last Modification Date:** 16 May 2013 14:40:43 UTC **Creation Date:** 08 Feb 2005 18:28:27 UTC

Mathematical expressions

Reactions

cyclin_cdc2k dissociation	cdc2k phosphorylation	cdc2k dephosphorylation	cyclin cdc2k-p association
deactivation of cdc2 kinase	cyclin biosynthesis	default degradation of cyclin	cdc2 kinase triggered degration of cyclin
activation of cdc2 kinase			

Rules

Assignment Rule (variable: total_cyclin)	Assignment Rule (variable: total_cdc2)

Physical entities

Compartments	Species		
cell	EmptySet	cdc2k	cdc2k-P
	p-cyclin_cdc2	p-cyclin_cdc2-p	cyclin
	p-cyclin	total_cyclin	total_cdc2

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

Download SBML | Other formats (auto-generated) | Actions | Send feedback

Model | Overview | Math | Physical entities | Parameters | Curation | Submodel1

Create a submodel with selected elements

Deselect All

Model

Publication ID: 1831270 **Submission Date:** 13 Sep 2005 12:31:08 UTC **Last Modification Date:** 16 May 2013 14:40:43 UTC **Creation Date:** 08 Feb 2005 18:28:27 UTC

Mathematical expressions

Reactions

cyclin_cdc2k dissociation	cdc2k phosphorylation	✓ cdc2k dephosphorylation	cyclin cdc2k-p association
deactivation of cdc2 kinase	cyclin biosynthesis	default degradation of cyclin	cdc2 kinase triggered degration of cyclin
activation of cdc2 kinase			

Rules

Assignment Rule (variable: total_cyclin)	Assignment Rule (variable: total_cdc2)

Physical entities

Compartments	Species		
cell	EmptySet	cdc2k	cdc2k-P
	p-cyclin_cdc2	p-cyclin_cdc2-p	cyclin
	p-cyclin	total_cyclin	total_cdc2

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

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Model | Overview | Math | Physical entities | Parameters | Curation | **Submodel1**

View the submodel in SBML

Reactions (1)	
⊞ **cdc2k dephosphorylation**	[cdc2k-P] → [cdc2k];

Compartments (1)			
cell	set #1	bqbiol:is	Gene Ontology cell
Referred to as: cell			

Species (2)	
⊞ **cdc2k** *Compartment: cell*	Initial amount: 0.0
⊞ **cdc2k-P** *Compartment: cell*	Initial amount: 0.75

Fully valid SBML model containing only the dephosphorylation of cdc2k

BIOMD0000000005 - Tyson1991 - Cell Cycle 6 var

Download SBML | Oth ... lback

SBML L2 V1 (auto-generated)
SBML L2 V3 (auto-generated)
SBML L2 V4 (curated)
SBML L3 V1 (auto-generated)
SBML L2 V4 (curated with URNs)

Automatically generated using libsbml (http://sbml.org/Software/libSBML)

Curated version of the model

... meters | Curation

Reference Publication

Publication ID: 1831270

... ate University, Blacksburg 24061. [more]

Model

Original Model: *BIOMD0000000005.xml.origin*

Submitter: Nicolas Le Novère

Submission ID: MODEL6614644188

Submission Date: 13 Sep 2005 12:31:08 UTC

Last Modification Date: 16 May 2013 14:40:43 UTC

Creation Date: 08 Feb 2005 18:28:27 UTC

Encoders: Bruce Shapiro
Vijayalakshmi Chelliah

set #1	bqbiol:hasVersion	**Reactome** REACT_152
set #2	bqbiol:isVersionOf	**KEGG Pathway** sce04111 **Gene Ontology** mitotic cell cycle
	bqbiol:occursIn	**Taxonomy** Opisthokonta

Notes

Tyson1991 - Cell Cycle 6 var

Mathematical model of the interactions of cdc2 and cyclin.

This model is described in the article:

Modeling the cell division cycle: cdc2 and cyclin interactions.
Tyson JJ.
Proc. Natl. Acad. Sci. U.S.A. 1991; 88(16): 7328-32

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BIOMD0000000005 - Tyson1991_CellCycle_6var

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- BioPAX (Level 3)
- Octave
- PDF
- SciLab
- VCML (VCell)
- XPP

Model | ath | Physica

Reference Publica

Publication ID: 1831270

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SBML Model Report

Model name: "Tyson1991_CellCycle_6var"

SBML2LaTeX

9th February 2009

1 General Overview

This is a document in SBML Level 2 Version 3 format. This model was created by the following two authors: Bruce Shapiro[1] and Vijayalakshmi Chelliah[2] at February eighth 2005 at 6:28 p.m. and last modified at August 21st 2008 at 11:31 a.m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: The SBML components in this model.
All components are described in more detail in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	1
species types	0	species	9
events	0	constraints	0
reactions	9	function definitions	0
global parameters	0	unit definitions	5
rules	2	initial assignments	0

Model Notes

Cell Cycle Model; Tyson (1991, 6 variables)

Description

[1]NASA Jet Propulsion Laboratory, bshapiro@jpl.nasa.gov
[2]EMBL-EBI, vijik@ebi.ac.uk

Produced by SBML2LaTeX 1

BioPAX versions of the model generated from SBML+MIRIAM

```
<?xml version="1.0" encoding="UTF-8"?>
<rdf:RDF xmlns:bp="http://www.biopax.org/release/biopax-level2.owl#"
xmlns:xsd="http://www.w3.org/2001/XMLSchema#"
xmlns:owl="http://www.w3.org/2002/07/owl#"
xmlns:base="http://www.ebi.ac.uk/biomodels/biopax.owl#"
xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#">
<owl:Ontology rdf:about="">
 <owl:imports rdf:resource="http://www.biopax.org/release/biopax-
level2.owl#"/>
</owl:Ontology>

<bp:physicalEntity rdf:about="EmptySet">
 <bp:NAME rdf:datatype="xsd:string">EmptySet</bp:NAME>
</bp:physicalEntity>

<bp:physicalEntityParticipant rdf:about="RIGHT_conversion_Reaction1_C2">
 <bp:PHYSICAL-ENTITY rdf:resource="C2"/>
 <bp:CELLULAR-LOCATION rdf:resource="cell"/>
 <bp:STOICHIOMETRIC-COEFFICIENT
rdf:datatype="xsd:double">1.0</bp:STOICHIOMETRIC-COEFFICIENT>
</bp:physicalEntityParticipant>

<bp:physicalEntityParticipant rdf:about="LEFT_conversion_Reaction4_CP">
 <bp:PHYSICAL-ENTITY rdf:resource="CP"/>
 <bp:CELLULAR-LOCATION rdf:resource="cell"/>
 <bp:STOICHIOMETRIC-COEFFICIENT
rdf:datatype="xsd:double">1.0</bp:STOICHIOMETRIC-COEFFICIENT>
</bp:physicalEntityParticipant>

<bp:physicalEntityParticipant rdf:about="LEFT_conversion_Reaction1_M">
 <bp:PHYSICAL-ENTITY rdf:resource="M"/>
 <bp:CELLULAR-LOCATION rdf:resource="cell"/>
 <bp:STOICHIOMETRIC-COEFFICIENT
rdf:datatype="xsd:double">1.0</bp:STOICHIOMETRIC-COEFFICIENT>
</bp:physicalEntityParticipant>
```

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BIOMD0000000005 - Tyson1991_CellCycle_6var

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- View Bitmap Reaction Graph
- View SVG Reaction Graph
- View Dynamic Reaction Graph
- View Model of Month
- JWS Online Simulation
- BioModels Online Simulation

Model | Overview | Math | Parameters | Curation

Publication ID: 1831270

Proc Natl Acad Sci
Modeling the cell di
Tyson JJ.
Department of Biology, Virginia Polytechnic Institute and St

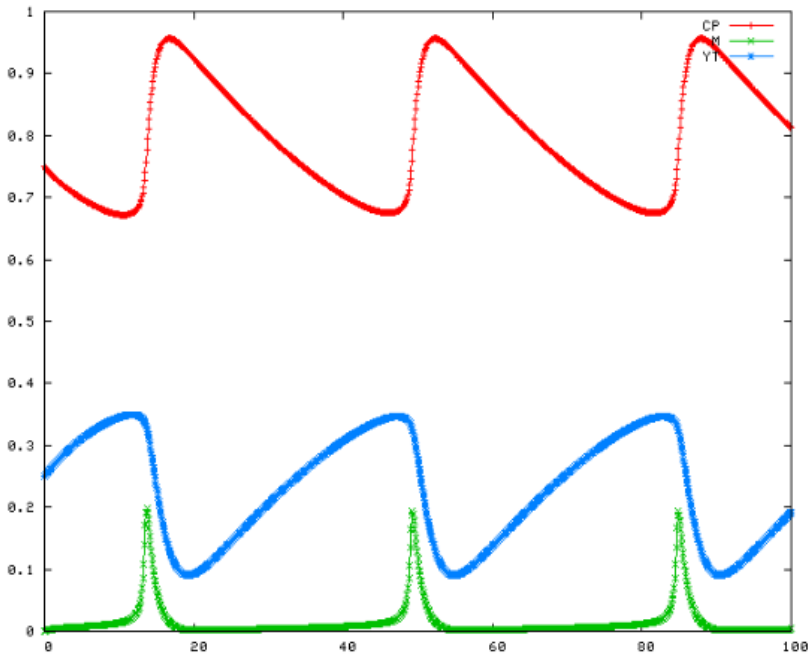
http://www.ebi.ac.uk/biomodels-main/publ-model-tab.do?cmd=MODEL:SIMU:RESULT

The simulation request has been submitted to the queue of our server cluster.

You could save following links and retrieve your simulation result later.

Link of simulation result:

http://www.ebi.ac.uk/biomodels-main/publ-model.do?cmd=SIMU:RETRIEVE&simuid=SIMU1234453623040



Close

http://www.ebi.ac.uk/biomodels/models-main/ode_simu/SIMU1234453623... zotero

Model

Reactome REACT_152

KEGG Pathway sce04111
Gene Ontology mitotic cell cycl

Taxonomy Fungi/Metazoa grou

Notes

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http://www.ebi.ac.uk/biomodels-main/publ-model-tab.do?cmd=MODEL:SIMU

Model - Simulation

For doing an online simulation, please select the species below. After specifying the *simulation time* and *print step*, and then click *Submit* to submit simulation job to our research cluster.

Click *Cancel* to close the window.

Cancel

Species

☐ EmptySet	☐ cdc2k	☑ cdc2k-P	☑ p-cyclin_cdc2
☐ p-cyclin_cdc2-p	☐ cyclin	☐ p-cyclin	☑ total_cyclin
☐ total_cdc2			

Simulation Time (use scientific notation e.g. 1e7 for 10000000): 100

Print step: 1000

Submit

Done zotero

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BIOMD0000000005 - Tyson1991_CellCycle_6var

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- View SVG Reaction Graph
- View Dynamic Reaction Graph
- View Model of Month
- JWS Online Simulation
- BioModels Online Simulation

Model | Overview | Math

Publication ID: 1831270

Proc Natl Acad Sci
Modeling the cell di
Tyson JJ.
Department of Biology, Virginia Polytechnic Institute

Model

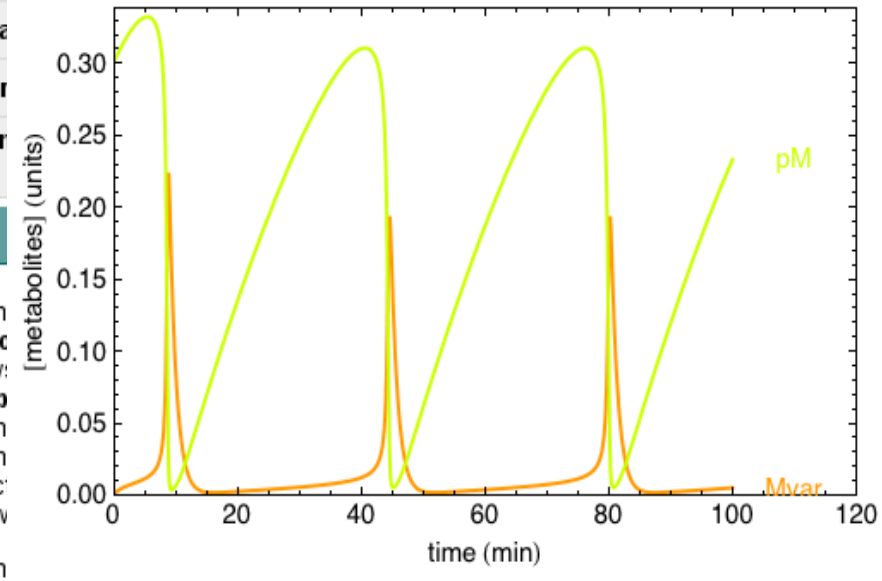
Original Model: *BIOMD0000000005.xml.origin*

Submitter: Nicolas Le Novère

Submission ID: MODEL6614644188

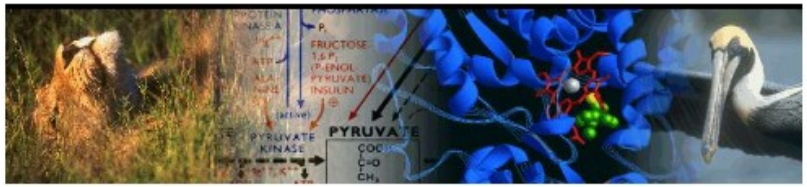
set #1	bqbiol:hasVersion	Reactome REACT_152
	bqbiol:isVersionOf	KEGG Pathway sce0411
		Gene Ontology mitotic ce
	bqbiol:occursIn	Taxonomy Fungi/Metazo

http://jjj.mib.ac.uk/webMathematica/Examples/PlotScript11.jsp?fun="JWS`Tyson199



Download the results in text or comma separated value format (e.g. for Excel import):

http://jjj.mib.ac.uk/biomodels/Tyson1991/index.html



Biomodels Home | Index | JWS Online

Biomodels: BIOMD0000000005

Tyson1991

Powered by JWS Online

JWSApplet – ver 5.0.3 Tyson1991

	Parameter	Value
P1_v1	cell	1
P2_v1	k6	1
P3_v1	k8notP	1.0e6
P4_v1	k9	1000
P5_v1	k3	200
P6_v1	k5notP	0.
P7_v1	k1aa	0.015
P8_v1	k2	0.
P9_v1	k7	0.6
P10_v1	k4	180
P11_v1	k4prime	0.018
E1	EmptySet	0.
I1	C2[0]	0.
I2	CP[0]	1
I3	Mvar[0]	0.
I4	Y[0]	0.
I5	YP[0]	0.
I6	pM[0]	0.3

Evaluate Model

Sim | State

StartTime 0 EndTime 100

Rates | Metabolites

Type	Output	Plot
M1	C2	
M2	CP	
M3	Mvar	✔
M4	Y	
M5	YP	
M6	pM	✔
F1	v[Rea...	
F2	v[Rea...	
F3	v[Rea...	
F4	v[Rea...	
F5	v[Rea...	
F6	v[Rea...	
F7	v[Rea...	

POWERED BY webMATHEMATICA2

Reset

Applet jjjApplet started

zotero

Chelliah V, L
uantitative kinetic models. BMC Syst Biol., 4:92.

From pathways to models … Path2Models

Signalling Pathways

+

Logical models
of individual signalling pathways

Metabolic Networks

Chemical kinetics models
of individual metabolic pathways

Metabolic Networks

+

Flux Balance Analysis
of whole genome reconstructions

Path2Models

Path2Models is a branch of BioModels Database dedicated to hosting models automatically generated from pathway resources, such as KEGG, BioCarta, MetaCyc, PID and SABIO-RK.

Browse models

Models from this branch are classified in 3 distinct categories:

- metabolic models
- non-metabolic models
- whole genome metabolism models

One can also browse those models by organism:

- list of all organisms

Search models

The following search will only look for models coming from the path2models project:

Search

Help about the search

- The keywords *AND* or *OR* (in upper cases) are available to refine the search. By default, if more than one word is present in a query, *OR* will be used to combine them.
- Double quotes (") can be used to force the search engine to match a whole expression containing several words.
- The colon character (:) must be escaped in the queries; one can use a backslash for this purpose (\:).

Download all models

- Archives of all models (from the latest release)

Additional information

Those automatically generated models are only partially parameterized. In the case of KEGG signaling pathways for which no mechanistic details are provided, the models (with qual constructs) contain only topological relationships together with interaction signs. No logical rules specify the effects of (combined) interactions, and these models should be seen as scaffolds to be further parameterized before use in simulation. This can be done either by considering default, yet biologically meaningful, logical functions

Path2Models:

Here are all the whole genome metabolism models available:

- [Eubacterium] cylindroides T2-87
- Acaryochloris marina (strain MBIC 11017)
- Accumulibacter phosphatis (strain UW-1)
- Acetobacter pasteurianus (strain NBRC 3283 / LMG 1513 / CCTM 1153)
- Acetobacter pasteurianus IFO 3283-01-42C
- Acetobacter pasteurianus IFO 3283-03
- Acetobacter pasteurianus IFO 3283-07
- Acetobacter pasteurianus IFO 3283-12
- Acetobacter pasteurianus IFO 3283-22
- Acetobacter pasteurianus IFO 3283-26
- Acetobacter pasteurianus IFO 3283-32
- Acetobacterium woodii (strain ATCC 29683 / DSM 1030 / JCM 2381 / KCTC 1655)
- Acetohalobium arabaticum (strain ATCC 49924 / DSM 5501 / Z-7288)
- Acholeplasma laidlawii (strain PG-8A)
- Achromobacter xylosoxidans (strain A8)
- Acidaminococcus fermentans (strain ATCC 25085 / DSM 20731 / VR4)
- Acidaminococcus intestini (strain RyC-MR95)
- Acidianus hospitalis (strain W1)
- Acidilobus saccharovorans (strain DSM 16705 / VKM B-2471 / 345-15)
- Acidimicrobium ferrooxidans (strain DSM 10331 / JCM 15462 / NBRC 103882 / ICP)
- Acidiphilium cryptum (strain JF-5)
- Acidiphilium multivorum (strain DSM 11245 / JCM 8867 / AIU301)
- Acidithiobacillus caldus (strain SM-1)
- Acidithiobacillus ferrivorans SS3
- Acidithiobacillus ferrooxidans (strain ATCC 23270 / DSM 14882 / NCIB 8455)
- Acidithiobacillus ferrooxidans (strain ATCC 53993)
- Acidobacterium capsulatum (strain ATCC 51196 / DSM 11244 / JCM 7670)
- Acidothermus cellulolyticus (strain ATCC 43068 / 11B)
- Acidovorax avenae (strain ATCC 19860 / DSM 7227 / JCM 20985 / NCPPB 1011)
- Acidovorax citrulli (strain AAC00-1)
- Acidovorax ebreus (strain TPSY)
- Acidovorax sp. (strain JS42)

Whole Genome Metabolism - Homo sapiens

Download SBML
SBML L2 V4
SBML L2 V4 (with Identifiers.org URLs)

Send feedback

Model information

Identifier: BMID000000140905
Format: SBML L2 V4
Project: path2models
Categories: genome-scale
Submission: 19 May 2012 15:48:00 UTC
Last modified: 04 Oct 2013 04:05:27 UTC
Published: 19 May 2012 23:49:21 UTC

Annotations

occursIn	Homo sapiens	*Taxonomy*
isDerivedFrom	Homo sapiens (human)	*KEGG Genome*
isDescribedBy	Initial sequencing and analysis of the human genome.	*PubMed*
isDescribedBy	The sequence of the human genome.	*PubMed*
isDescribedBy	Finishing the euchromatic sequence of the human genome.	*PubMed*
isDescribedBy	The DNA sequence and biological annotation of human chromosome 1.	*PubMed*
isDescribedBy	Generation and annotation of the DNA sequences of human chromosomes 2 and 4.	*PubMed*
isDescribedBy	The DNA sequence, annotation and analysis of human chromosome 3.	*PubMed*
isDescribedBy	The DNA sequence and comparative analysis of human chromosome 5.	*PubMed*
isDescribedBy	The DNA sequence and analysis of human chromosome 6.	*PubMed*
isDescribedBy	Human chromosome 7: DNA sequence and biology.	*PubMed*
isDescribedBy	The DNA sequence of human chromosome 7.	*PubMed*
isDescribedBy	DNA sequence and analysis of human chromosome 8.	*PubMed*
isDescribedBy	DNA sequence and analysis of human chromosome 9.	*PubMed*
isDescribedBy	The DNA sequence and comparative analysis of human chromosome 10.	*PubMed*
isDescribedBy	Human chromosome 11 DNA sequence and analysis including novel gene identification.	*PubMed*
isDescribedBy	The finished DNA sequence of human chromosome 12.	*PubMed*
isDescribedBy	The DNA sequence and analysis of human chromosome 13.	*PubMed*
isDescribedBy	The DNA sequence and analysis of human chromosome 14.	*PubMed*
isDescribedBy	Analysis of the DNA sequence and duplication history of human chromosome 15.	*PubMed*
isDescribedBy	The sequence and analysis of duplication-rich human chromosome 16.	*PubMed*

BioModels Web Services

With BioModels Web Services, users can programmatically access up-to-date information from BioModels Database without installing a local copy of the database. They provide a wide range of features for searching and retrieving models. Furthermore, some features can help users to extract interesting parts from a large model and assemble them into a fully valid submodel. For any comments or new feature enquiries, please feel free to contact us.

Available features

- Available features
- WSDL

The list of available features's page describes all the available services in a nice human readable way, included a detailed description of all methods. The WSDL (Web Services Description Language) defines the provided services in an XML format file. This enables third-party software to automatically generate clients for accessing the services.

Java library

The Java library provides a very convenient way to use the web services. It gives access to improved methods (for example giving access to 'SimpleModel' objects rather than raw XML) in order to make the use of the web services easier.

Documentation

The library documentation gives information for developers wishing to use the API:

- Java library documentation (Javadoc)

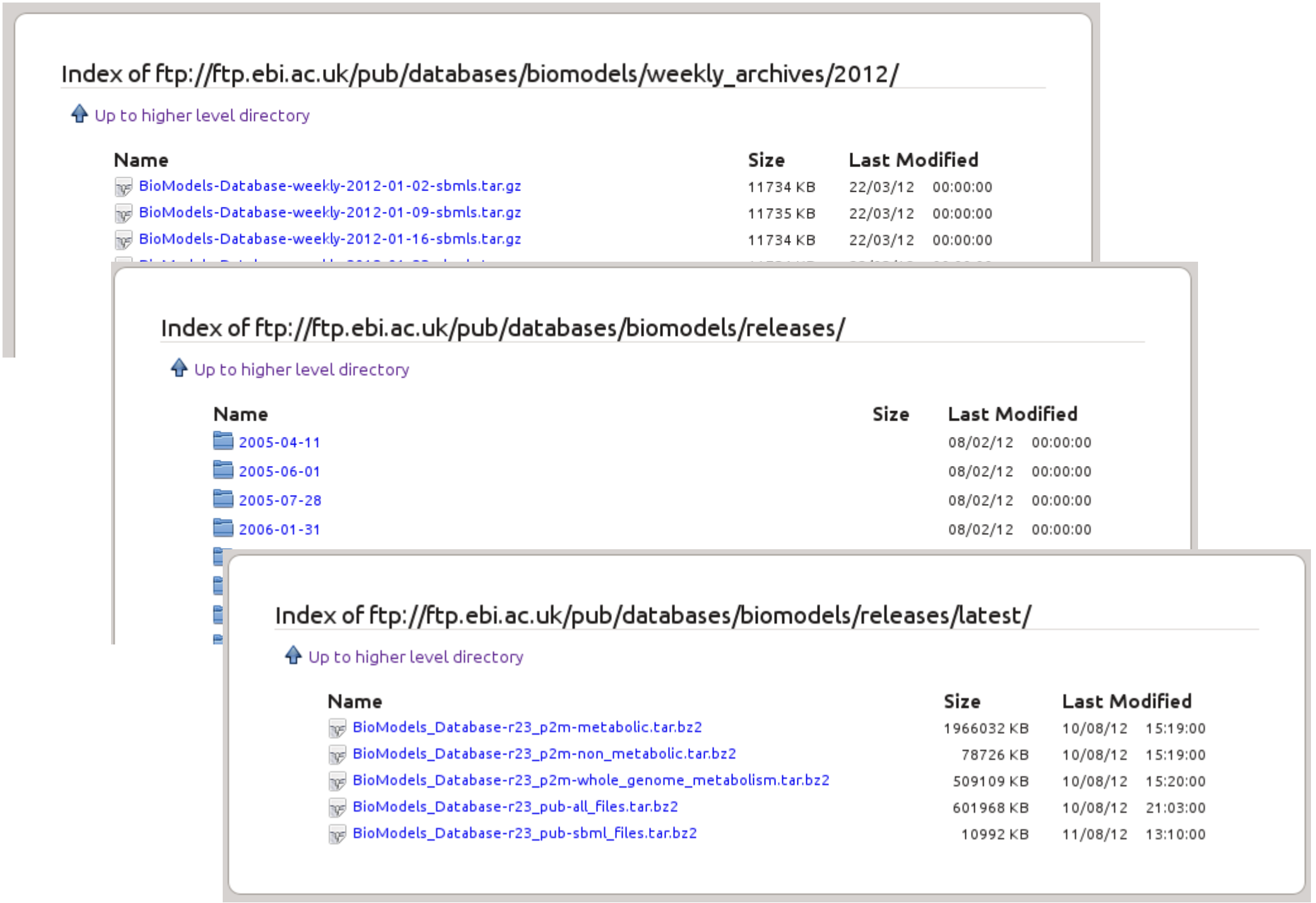
Get the library via Maven

The library is available from the EBI Maven repository.

You just need to add the following to your pom.xml to get it and all its dependencies:

```
<dependencies>
  <dependency>
    <groupId>uk.ac.ebi.biomodels</groupId>
    <artifactId>biomodels-wslib</artifactId>
    <version>1.21</version>
  </dependency>
</dependencies>

<repositories>
<repository>
  <id>ebi-repo</id>
  <name>The EBI internal repository</name>
  <url>http://www.ebi.ac.uk/~maven/m2repo</url>
  <releases>
    <enabled>true</enabled>
  </releases>
```



Index of ftp://ftp.ebi.ac.uk/pub/databases/biomodels/weekly_archives/2012/

Up to higher level directory

Name	Size	Last Modified
BioModels-Database-weekly-2012-01-02-sbmls.tar.gz	11734 KB	22/03/12 00:00:00
BioModels-Database-weekly-2012-01-09-sbmls.tar.gz	11735 KB	22/03/12 00:00:00
BioModels-Database-weekly-2012-01-16-sbmls.tar.gz	11734 KB	22/03/12 00:00:00

Index of ftp://ftp.ebi.ac.uk/pub/databases/biomodels/releases/

Up to higher level directory

Name	Size	Last Modified
2005-04-11		08/02/12 00:00:00
2005-06-01		08/02/12 00:00:00
2005-07-28		08/02/12 00:00:00
2006-01-31		08/02/12 00:00:00

Index of ftp://ftp.ebi.ac.uk/pub/databases/biomodels/releases/latest/

Up to higher level directory

Name	Size	Last Modified
BioModels_Database-r23_p2m-metabolic.tar.bz2	1966032 KB	10/08/12 15:19:00
BioModels_Database-r23_p2m-non_metabolic.tar.bz2	78726 KB	10/08/12 15:19:00
BioModels_Database-r23_p2m-whole_genome_metabolism.tar.bz2	509109 KB	10/08/12 15:20:00
BioModels_Database-r23_pub-all_files.tar.bz2	601968 KB	10/08/12 21:03:00
BioModels_Database-r23_pub-sbml_files.tar.bz2	10992 KB	11/08/12 13:10:00

EMBL-EBI

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- Henning Hermjakob, Janet Thornton

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- All the computational systems Biology community, in particular: Rainer Machne, Bruce Shapiro, Kieran Smallbone

Current member coordinator

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