

Controlled Vocabularies in Systems Biology

Nicolas Le Novère, EMBL-EBI

- Controlled Vocabularies
- “Organized lists of words and phrases, or notation systems, that are used to initially tag content, and then to find it through navigation or search.” *Amy J. Warner. A Taxonomy Primer.*
<http://www.lexonomy.com/publications/aTaxonomyPrimer.html>
- “An indexed dictionary”. *Nicolas Le Novère. This presentation.*
- “A set of codes, managed by some authority (eg a person or an organisation), employing some mechanism”. Misha Wolf on *IPTC internal developer forum for the News Metadata Framework WG*
- Ontology
- “(Computers) A systematic arrangement of all of the important categories of objects or concepts which exist in some field of discourse, showing the relations between them. When complete, an ontology is a categorization of all of the concepts in some field of knowledge, including the objects and all of the properties, relations, and functions needed to define the objects and specify their actions. A simplified ontology may contain only a **hierarchical** classification (a **taxonomy**)” *The Collaborative International Dictionary of English v.0.48*
- A set of controlled vocabularies with defined relationships between terms. *Nicolas Le Novère. This presentation.*

- Each term is associated to a perennial identifier. Once created a term is never destroyed. It can be merged with other, or made obsolete, but it still exists.
- An ontology is an evolving structure: It can cope with an increase or refinement of knowledge. No need to reconstruct everything as with the taxonomies.
- An ontology is a Direct Acyclic Graph, and not a hierarchy. A term can possess more than one parent.
- Ontologies are stored in standard machine-readable formats. They can be subjected to automatic treatments.

Search GO

- ☐ Exact Match
☒ Terms
☐ Gene Symbol/Name

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Gene Product Filters

Species

-

Datasource

-

Evidence Code

-

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Last updated: 2005-08-21

- [-] all : all (218850)
 - [+] ① GO:0008150 : biological_process (145098)
 - [+] ① GO:0009987 : cellular process (91236)
 - [+] ① GO:0007154 : cell communication (15496)
 - [+] ① GO:0007267 : cell-cell signaling (1894)
 - [+] ① GO:0019226 : transmission of nerve impulse (1230)
 - [-] ② GO:0007268 : synaptic transmission (1124)
 - [+] ① GO:0007270 : nerve-nerve synaptic transmission (92)
 - ① GO:0007274 : neuromuscular synaptic transmission (33)
 - [+] ② GO:0045213 : neurotransmitter receptor metabolism (32)
 - [+] ② GO:0001505 : regulation of neurotransmitter levels (547)
 - [+] ② GO:0050803 : regulation of synapse structure and function (49)
 - [+] ① GO:0007582 : physiological process (96419)
 - [+] ① GO:0050874 : organismal physiological process (9314)
 - [+] ① GO:0050877 : neurophysiological process (4743)
 - [+] ② GO:0019226 : transmission of nerve impulse (1230)
 - [-] ② GO:0007268 : synaptic transmission (1124)
 - [+] ① GO:0007270 : nerve-nerve synaptic transmission (92)
 - ① GO:0007274 : neuromuscular synaptic transmission (33)
 - [+] ② GO:0045213 : neurotransmitter receptor metabolism (32)
 - [+] ② GO:0001505 : regulation of neurotransmitter levels (547)
 - [+] ② GO:0050803 : regulation of synapse structure and function (49)
 - [-] ① GO:0005575 : cellular_component (131714)
 - [-] ① GO:0005623 : cell (96196)
 - [+] ② GO:0045177 : apical part of cell (293)
 - [+] ② GO:0043190 : ATP-binding cassette (ABC) transporter complex (145)
 - [+] ② GO:0045178 : basal part of cell (38)
 - [+] ② GO:0005933 : bud (294)
 - [+] ② GO:0000267 : cell fraction (2094)
 - [-] ② GO:0042995 : cell projection (1119)
 - [+] ② GO:0005930 : axoneme (69)
 - ② GO:0005932 : basal body (29)
 - [+] ① GO:0005903 : brush border (72)
 - [+] ② GO:0031253 : cell projection membrane (0)
 - [+] ① GO:0005929 : cilium (91)
 - ① GO:0035230 : cytoneme (0)
 - [+] ① GO:0030175 : filopodium (34)
 - [+] ① GO:0019861 : flagellum (251)
 - [+] ① GO:0030027 : lamellipodium (197)
 - [+] ① GO:0005937 : mating projection (86)
 - [+] ① GO:0005902 : microvillus (40)
 - [-] ① GO:0043005 : neuron projection (236)
 - [+] ① GO:0030424 : axon (115)
 - [-] ① GO:0030425 : dendrite (106)
 - ② GO:0043198 : dendritic shaft (5)
 - ② GO:0043197 : dendritic spine (5)
 - [+] ① GO:0031143 : pseudopodium (20)
 - ① GO:0001726 : ruffle (76)



Quick Search

Example: water

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General Information

ChEBI Name	acetylcholine
ChEBI ID	CHEBI:15355

Ontology

CHEBI:23091 chemical_ontology

- △ CHEBI:24432 grouped_by_functions
 - △ CHEBI:25512 neurotransmitters
 - △ CHEBI:15355 acetylcholine
- △ CHEBI:24431 grouped_by_chemistry
 - △ CHEBI:25367 molecules
 - △ CHEBI:25700 organic molecules
 - △ CHEBI:32952 amines
 - △ CHEBI:22879 biogenic amines
 - △ CHEBI:22227 acylcholines
 - △ CHEBI:15355 acetylcholine

[Parents and children](#)

IUPAC Name

2-acetyloxy-*N,N,N*-trimethylethanaminium

Synonyms

acetylcholine
Acetylcholine
O-acetylcholine
<i>D</i> -acetylcholine
O-Acetylcholine

Sources

IntEnz
KEGG COMPOUND
ChEBI
IntEnz
KEGG COMPOUND

Database Link

[C01996](#)

Database

KEGG COMPOUND

Registry Number

51-84-3

Type

CAS Registry Number

Source

KEGG COMPOUND

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

IUBMB Enzyme Nomenclature

EC 3.1.1.7

Common name: acetylcholinesterase**Reaction:** acetylcholine + H₂O = choline + acetate**Other name(s):** AcCholE
acetyl-β-methylcholinesterase
acetylcholine hydrolase
acetylthiocholinesterase
choline esterase I
cholinesterase
true cholinesterase**Systematic name:** acetylcholine acetylhydrolase**Comments:** Acts on a variety of acetic esters; also catalyses transacetylations.**Links to other databases:** [BRENDA](#), [ERGO](#), [GO](#), [KEGG](#), [NIST 74](#)

CAS Registry Number: 9000-81-1

References:

1. Augustinsson, K.-B. Cholinesterases. A study in comparative enzymology. *Acta Physiol. Scand.* 15 (1948)
2. Bergmann, F., Rimon, S. and Segal, R. Effect of pH on the activity of eel esterase towards different substrates. *Biochem. J.* 68 (1958) 493-499.
3. Cilliv, G. and Ozand, P.T. Human erythrocyte acetylcholinesterase purification, properties and kinetic behavior. *Biochim. Biophys. Acta* 284 (1972) 136-156. [PMID: [5073758](#)]
4. Leuzinger, W., Baker, A.L. and Cauvin, E. Acetylcholinesterase. II. Crystallization, absorption spectra, isoionic point. *Proc. Natl. Acad. Sci. USA* 59 (1968) 620-623. [PMID: [5238989](#)]
5. Nachmansohn, D. and Wilson, I.B. The enzymic hydrolysis and synthesis of acetylcholine. *Adv. Enzymol. Relat. Subj. Biochem.* 12 (1951) 259-339.
6. Zittle, C.A., DellaMonica, E.S., Custer, J.H. and Krikorian, R. Purification of human red cell acetylcholinesterase by electrophoresis, ultracentrifugation and gradient extraction. *Arch. Biochem. Biophys.* 56 (1955) 469-475.

[EC 3.1.1.7 created 1961]

Please contact [EBI Support](#) with any problems or suggestions regarding this site.

Search:

Search Entries

Search InterPro

InterPro Parent-Child tree for InterPro Entry IPR006201

<http://www.ebi.ac.uk/interpro/>

InterPro entries can be related to each other in a parent-child relationship. See the [user manual](#) for more information.

Any domains (InterPro entries) in which an entry in this tree is found or contains is shown. Click on the accession number to go to the primary entry, click on the name to go to that entry's parent-child tree.



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Enter search term:

Match:

complete word

Query:

☐ Include all synonyms
and misspellings

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Homo sapiens (Human)

<http://www.ebi.ac.uk/newt/>

Lineage	Taxonomy identifier	9606	External information
Eukaryota Metazoa Chordata Craniata Vertebrata Euteleostomi Mammalia Eutheria Euarchontoglires Primates Catarrhini Hominidae Homo	Organism identification code	HUMAN	http://www.ebi.ac.uk/integr8/QuickSearch.do?action=doOrgSearch&organismName=homo+sapiens http://www.mnh.si.edu/anthro/humanorigins/ha/sap.htm
	Scientific name	Homo sapiens	
	Common name	Human	
	Synonym	-	
	Other NCBI synonyms	man	
	Rank	species	
	Number of UniProt/Swiss-Prot entries	12838	
	Number of UniProt/TrEMBL entries	57516	

Taxonomy navigation

Up taxonomy tree

Down taxonomy tree

[Homo](#)• [Homo sapiens neanderthalensis](#)Source of data : Swiss-Prot [NCBI taxonomy for this taxon](#)

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The PhyloCode is a formal set of rules governing phylogenetic nomenclature. It is designed to name the parts of the tree of life by explicit reference to phylogeny. The PhyloCode will go into operation in a few years, but the exact date has not yet been determined. It is designed so that it may be used concurrently with the existing codes based on rank-based nomenclature (ICBN, ICZN, etc.). We anticipate that many people whose research concerns phylogeny will find phylogenetic nomenclature advantageous.

The PhyloCode grew out of a workshop at Harvard University in August 1998, where decisions were made about its scope and content. Many of the workshop participants, together with several other people who subsequently joined the project, have served as an advisory group (see the PhyloCode preface for a list of the people involved). In April 2000, a draft was made public on this web site and comments were solicited from the scientific community. All comments were forwarded to the advisory group, and many of them elicited discussion.

A second workshop was held at Yale University in July 2002, at which some modifications were made in the rules and recommendations of the PhyloCode. An important decision made at the Yale workshop is that the rules governing clade names and those governing species names will be published in separate documents, and the timing of implementation of the two documents will be independent. The rules for clade names will almost certainly be implemented before those for species names because the latter have not yet been drafted. Only clade names are covered by the current version of the PhyloCode. As a result, the examples in the current version use binomials governed by the rank-based codes when species names are cited in the phylogenetic definitions of clade names.

The First International Phylogenetic Nomenclature Meeting, which took place July 6-9, 2004 in Paris, was attended by about 70 systematic and evolutionary biologists from 11 nations. The program can be downloaded from the left side of this page. The participants are grateful to the Organizing Committee, and particularly its Chair, Michel Laurin, for the care and effort that was devoted to making the meeting an enjoyable and stimulating event. This was the first open, multi-day conference that focused entirely on phylogenetic nomenclature. Papers presented at the meeting will form the core of a book whose publication, tentatively scheduled for 2006, will coincide with the implementation of the PhyloCode. This book will represent the official starting point of phylogenetic nomenclature as implemented in the PhyloCode. The Paris meeting also provided the venue for the inauguration of a new association, the International Society for Phylogenetic Nomenclature (ISPN). The ISPN membership will elect the Committee on Phylogenetic Nomenclature, the

OBO Ontology Browser

Browse the tree by clicking on the category names; click on an ontology name to view more information on it.

- ☐ **anatomy**
 - ☐ cell type
 - ☐ **gross anatomy**
 - ☐ **animal gross anatomy**
 - ☐ C. elegans gross anatomy
 - ☐ Drosophila gross anatomy
 - ☐ eVoc (Expressed Sequence Annotation for Humans)
 - ☐ **human developmental anatomy**
 - ☐ Human developmental anatomy, timed
 - ☐ Human developmental anatomy, abstract
 - ☐ medaka fish anatomy and development
 - ☐ **mouse anatomy**
 - ☐ Mouse adult anatomy
 - ☐ Mouse anatomy and development
 - ☐ Zebrafish anatomy and development
 - ☐ **microbial anatomy**
 - ☐ Fungal anatomy
 - ☐ Dictyostelium anatomy
 - ☐ **plant anatomy**
 - ☐ Arabidopsis anatomy
 - ☐ Cereal anatomy
 - ☐ Maize anatomy
 - ☐ Plant anatomy
 - ☒ organ
 - ☐ BRENDA tissue / enzyme source
- ☐ animal natural history and life history
- ☐ **chemical**
 - ☐ chemical entities of biological interest
 - ☐ physico-chemical methods and properties
 - ☐ physico-chemical process
- ☐ **development**
 - ☐ **animal development**
 - ☐ C. elegans development
 - ☐ Drosophila development
 - ☐ eVOC (Expressed Sequence Annotation for Humans)
 - ☐ medaka fish anatomy and development

<http://obo.sourceforge.net/>

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DopaNet: The Meso-Telencephalic Dopamine Consortium

DopaNet aim is to investigate precisely and quantitatively all the aspects of neurotransmission - at the levels of the molecule, the supra-molecular assembly, the neuronal cell and the neuronal network - in a specific neuronal system, involved in many neuropathologies, such as Parkinson's disease, schizophrenia and drug abuse. The resulting integrated knowledge will not only provide relevant up-to-date information, methods and tools for the diagnosis and treatment of such pathologies, but will also form a firm substrate to link the function of the neurobiological structures with the implementation of cognitive and mental abilities.

News

NEW May 2005: The DopaNet Day took place at Lille on Tuesday May 17th, as a satellite of the 7th Congress of the French Society for Neurosciences. We enjoyed tremendously interesting presentations by various members. You can access some of the presentations online.

July 2004: The DopaNet Day will take place at Lille on Tuesday May 17th 2005, as a satellite of the 7th Congress of the French Society for Neurosciences. The meeting is open to everyone.

March 2004: The construction of the [Molecular Pages](#), aimed to store detailed functional information about molecules present in DopaNet target cells, has started. Everybody is invited to participate.

June 2003: The construction of an ontology of the neuronal cell has started. Everybody is invited to participate.

February 2003: The computing infrastructure of DopaNet will be hosted by the European Bioinformatics Institute (EBI), outstation of the European Molecular Biology Laboratory (EMBL).

December 2002: DopaNet is accepted as a Network of the European Science Foundation. A grant of 80 000 € is attributed for the period 2003-2005. (ESF Leaflet)

Search DopaNet


Google Search

DopaNet is supported by:



<http://www.dopanet.org/>



DopaNet Neuronal Ontology Browser

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The screenshot displays the DopaNet Ontology interface. On the left, a hierarchical tree shows the classification of 'sodium-dependent dopamine transporter' (DA:0000246) under 'cellular_component' and 'protein'. The right panel provides detailed information for this specific transporter, including its name, definition, date, and relationships.

DopaNet Ontology	
cellular_component	cell
cytoplasm	plasma membrane
neuron	molecule
molecular complex	protein
receptor tyrosine kinase	ligand-gated ion channel
neurotransmitter transmembrane transporter	sodium neurotransmitter symporter
serotonin transporter	noradrenaline transporter
GAT2 GABA transporter	dopamine transporter
sodium-dependent dopamine transporter	glycine transporter type 1
GAT1 GABA transporter	GAT3 GABA transporter
proton neurotransmitter exchanger	vesicular glutamate transporter
excitatory amino-acid transporter	serine/threonine protein phosphatase
neurotransmitter degradation enzyme	cytokine receptor
neurotrophin	

Current: DA:0000246 amine transporter polypeptide	
identifier:	DA:0000246
name:	sodium-dependent dopamine transporter polypeptide
definition:	Integral membrane protein with 12 transmembrane segments. Forms the sodium/dopamine symporter. TCDB: S6A3
date:	Tue Sep 7 17:30:00 2004
isa:	DA:0000320 ; sodium-neurotransmitter symporter polypeptide
part-of:	DA:0000092 ; dopamine transporter
children:	

Legend: : "isa" relationship | : "part-of" relationship

- The purpose of DopaNet Neuronal Ontology is to be the glue that will link all the data collected by the DopaNet project.
⇒ Must cover quite extensively the topics of Neurobiology
- Built from orthogonal ontologies
- Backbone: Gene Ontology
- Proteins: InterPro, completed by dedicated classifications, such as the Transport Classification Database.
- Small molecules: ChEBI

- “is-a” relationships
 - Sub-classing, refinement, subsumption, hyponymy
 - “nicotinic acetylcholine-gated receptor” (DA:000002)
is-a “ligand-gated ion channel” (DA:0000086)
- “part-of” relationships
 - Dissection, meronymy
 - “alpha6 nicotinic receptor subunit” (DA:0000186)
is part-of a “(alpha6)_2(beta2)_3 nAChR” (DA:0000031)
- Relationships are inherited!
 - “alpha6 nicotinic receptor subunit” (DA:0000186)
is also part-of a “nicotinic acetylcholine-gated receptor” (DA:000002)
and part-of a “ligand-gated ion channel” (DA:0000086)
and part-of a “protein” DA:0000260
and part-of a “molecular complex” DA:0000259
and part-of a “cellular component” DA:0000259
 - “plasma membrane” is part-of “yeast”
“post-synaptic membrane” is-a “plasma membrane”
then “post-synaptic membrane” is part-of “yeast” ...

- A taxonomy of the roles of reaction participants, including the following potential terms: “**substrate**”, “**catalyst**”, “**inhibitor**”, “**competitive inhibitor**”, “**non-competitive inhibitor**” etc.
- A CV for parameter roles in quantitative models. This CV will include terms like “**Hill coefficient**”, “**Michaelis constant**” etc.
- A classification of rate laws. This CV is a taxonomy of kinetic rate equations. Examples of potential terms in this CV are “**Mass action**”, “**Henri-Michaelis-Menten**”, “**Hill**” etc. Each term contains a precise mathematical expression stored as a MathML lambda function. The variable will refer to the CVs described above.

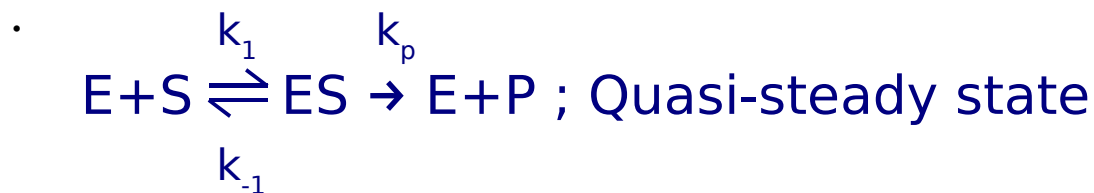
```
SBO:0000000 ; Systems Biology Ontology
% SBO:0000001 ; rate law
  % SBO:0000007 ; mass-action kinetics
  % SBO:0000011 ; kinetics of unireactant enzymes
    % SBO:0000012 ; Henri equation
    % SBO:0000013 ; Henri-Michaelis-Menten equation
    % SBO:0000014 ; Van Slyke equation
    % SBO:0000015 ; Briggs-Haldane equation
% SBO:0000002 ; quantitative parameter
  % SBO:0000018 ; kinetic constant
    % SBO:0000019 ; catalytic constant
    % SBO:0000008 ; Michaelis constant
% SBO:0000003 ; species role
  % SBO:0000004 ; reactant
  % SBO:0000005 ; product
  % SBO:0000006 ; modifier
    % SBO:0000016 ; activator
    % SBO:0000017 ; inhibitor
```



Henri-Michaelis-Menten:
$$v = \frac{E \cdot k_p \cdot [S]}{(K_m + [S])} ; K_m = \frac{k_{-1}}{k_1}$$



Van Slyke:
$$v = \frac{E \cdot k_p \cdot [S]}{(K_m + [S])} ; K_m = \frac{k_p}{k_1}$$



Briggs-Haldane:
$$v = \frac{E \cdot k_p \cdot [S]}{(K_m + [S])} ; K_m = \frac{(k_{-1} + k_p)}{k_1}$$

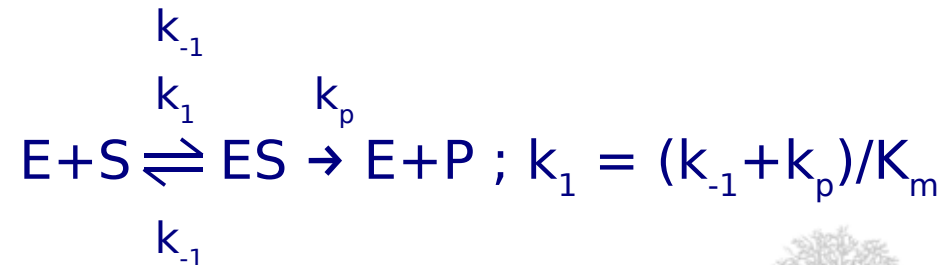
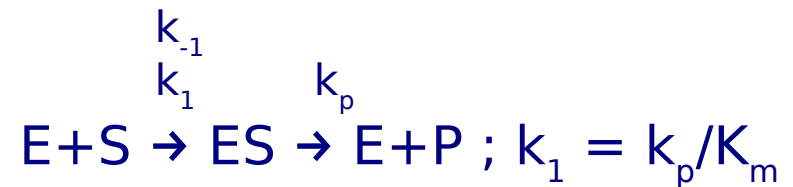
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  </listOfProducts>
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      <parameter id="kp" />
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          <ci>kp</ci>
          <ci>S</ci>
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      </apply>
    </math>
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Import in a discrete simulator



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      <parameter id="kp" />
    </listOfParameters>
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        <divide/><apply>
          <times/><ci>E</ci>
          <ci>kp</ci>
          <ci>S</ci>
        </apply>
        <apply>
          <plus/><ci>Km</ci>
          <ci>S</ci>
        </apply>
      </apply>
    </math>
  </kineticLaw>
</reaction>
```

```

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  </listOfReactants>
  <listOfProducts>
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  </listOfProducts>
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          <ci>kp</ci>
          <ci>S</ci>
        </apply>
        <apply>
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          <ci>S</ci>
        </apply>
      </apply>
    </math>
  </kineticLaw>
</reaction>

```

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def: "Rate-law presented in G. E. Briggs and J. B. S. Haldane (1925) A note on the
kinetics of enzyme action, Biochem. J., 19, 339-339. It is a general rate equation
that does not require the restriction of equilibrium of Michaelis-Menten or irreversible
reactions of Van Slyke, but instead make the hypothesis that the complex enzyme-substrate
is in steady-state. Although of the same form than the Henri-Michaelis-Menten equation,
it is semantically different since Km now represents a pseudo-equilibrium constant, and
is equal to the ratio between the rate of consumption of the complex (sum of dissociation
of substrate and generation of product) and the association rate of the enzyme and the
substrate.
is_a: SBO:0000011 ; kinetics of unireactant enzymes
math: <math xmlns="http://www.w3.org/1998/Math/MathML">
  <lambda>
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</math>
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  <listOfModifiers>
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  </listOfModifiers>
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      <parameter id="V" definitionURL="http://www.biomodels.net/SBO/#SBO:0000019"/>
    </listOfParameters>
  </kineticLaw>
</reaction>
```

continuous simulator

$$v = \frac{C \cdot V \cdot [A]}{(U + [A])}$$

discrete simulator

$$v1 = \frac{(k_{-1} + V)}{U} \cdot [A] \cdot [C]$$

$$v2 = k_{-1} \cdot [D]$$

$$v3 = V \cdot [D]$$

- Shankar Subramaniam – Saturday 9:50

SBML development

- Michael Hucka
- Andrew Finney
- Herbert Sauro
- Hamid Bolouri
- Ben Bornstein
- Nicolas Le Novère
- Pedro Mendes
- Martin Ginkel
- Kouichi Takahashi
- Takeshi Sakurada
- Jim Schaff
- John Wagner
- Jorg Stelling
- Poul Nielsen
- Hiroaki Kitano
- Bruce Shapiro
- Eric Mjolness
- Victoria Gor
- Jonathan Webb
- Colin Gillespie
- Igor Goryanin
- Jorg Weimar
- Stefan Hoops
- Akira Funahashi
- Sven Sahle
- Ralf Gauges
- Hugh Spencer
- Wayne Rindone
- Fabien Campagne
- Maria Schilstra
- Vijay Saraswat
- Ed Frank
- Ben Kovitz
- Jeremy Zucker
- ...
- ...

BioModels.net

EBI

- Nicolas Le Novère
- Marco Donizelli
- Mélanie Courtot
- Lu Li
- Alexander Broicher

External contributors

- Upinder Bhalla
- Christoph Flamm
- Ryan Gutenkunst
- Adam Halasz
- Rainer Machné
- Marc Poolman
- Tomas Radivoyevitch
- Oleg Sokolsy
- Joanne Matthews
- Les Grivell
- Boris Kholodenko
- Tjeerd olde Scheper
- Paul Smolen
- Yukiko Matsuoka

SBML team

- Michael Hucka
- Andrew Finney
- Bruce Shapiro
- Benjamin Borstein
- Maria Schilstra
- Sarah Keating

Keck Graduate Institute

- Herbert Sauro
- Harish Dharuri

Systems Biology Institute

- Hiroaki Kitano
- Akira Funahashi

Stellenbosch University

- Jacky Snoep





<compneur>

<member name="Nicolas Le Novère" role="leader"/>

<member name="Alexander Broicher" role="trainee"/>

<member name="Mélanie Courtot" role="developer"/>

<member name="Marie-Ange Djite" role="trainee"/>

<member name="Marco Donizelli" role="developer">

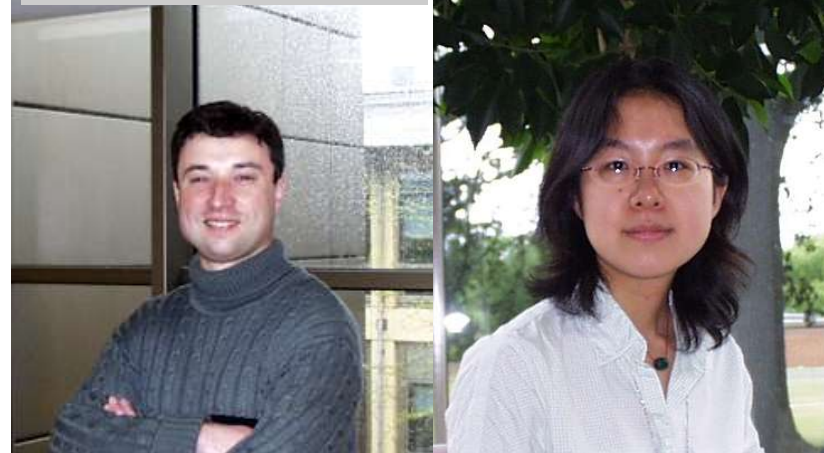
<member name="Éric Fernandez" role="post-doc"/>

<member name="Lu Li" role="trainee"/>

<member name="Nicolas Rodriguez" role="developer"/>

<member name="Dominic Tölle" role="PhD student"/>

</compneur>



British outstation of the European Molecular Biology Laboratory

- Databases

- Sequences, structures
- Transcriptomics, Proteomics pathways, models
- Controlled vocabularies and dictionaries



- Research groups

- Comparative genomics (Ouzounis)
Structural Genomics (Thornton)
Molecular Evolution (Goldman)
- Text-Mining (Rebholz-Schumman)
Computational Systems Biology (Le Novère)
Statistical array analysis (Huber)
Genomic analysis of regulatory systems (Luscombe)

Marie Curie Training site Fellowships: 3-6 months. Fully funded.