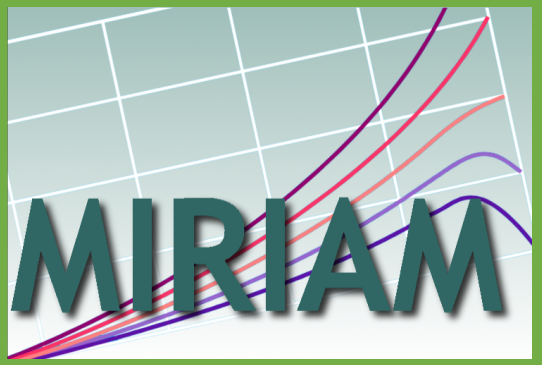
Identifiers.org MIRIAM Registry: annotation and cross-referencing framework



identifiers.org

Camille Laibe

EMBL-EBI

COMBINE 2011,
3-7 September 2011, Heidelberg, Germany

Background: MIRIAM

_computational BIOLOGY

PERSPECTIVE

Minimum information requested in the annotation of biochemical models (MIRIAM)

Nicolas Le Novère[1,15], Andrew Finney[2,15], Michael Hucka[3], Upinder S Bhalla[4], Fabien Campagne[5], Julio Collado-Vides[6], Edmund J Crampin[7], Matt Halstead[7], Edda Klipp[8], Pedro Mendes[9], Poul Nielsen[7], Herbert Sauro[10], Bruce Shapiro[11], Jacky L Snoep[12], Hugh D Spence[13] & Barry L Wanner[14]

Most of the published quantitative models in biology are lost for the community because they are either not made available or they are insufficiently characterized to allow them to be reused. The lack of a standard description format, lack of stringent reviewing and authors' carelessness are the main causes for incomplete model descriptions. With today's increased interest in detailed biochemical models, it is necessary to define a minimum quality standard for the encoding of those models. We propose a set of rules for curating quantitative models of biological systems. These rules define procedures for encoding and annotating models represented in machine-readable form. We believe their application will enable users to (i) have confidence that curated models are an accurate reflection of their associated reference descriptions, (ii) search collections of curated models with precision, (iii) quickly identify the biological phenomena that a given curated model or model constituent represents and (iv) facilitate model reuse and composition into large subcellular models.

[1]European Bioinformatics Institute, Hinxton, CB10 1SD, UK. [2]Physiomics PLC, Magdalen Centre, Oxford Science Park, Oxford, OX4 4GA,K. [3]Control and Dynamical Systems, California Institute of Technology,Pasadena, California 91125, USA. [4]National Centre for Biological Sciences, TIFR, UAS-GKVK Campus, Bangalore 560065, India. [5]Institute for Computational Biomedicine, Weill Medical College of Cornell University, New York, New York 10021, USA. [6]Center for Genomic Sciences, Universidad Nacional Autónoma de México, Av. Universidad s/n, Cuernavaca, Morelos, 62100, Mexico. [7]Bioengineering Institute and Department of Engineering Science, The University of Auckland, Private Bag 92019, Auckland, New Zealand. [8]Max-Planck Institute for Molecular Genetics, Berlin Center for Genome based Bioinformatics (BCB), Ihnestr. 73, 14195 Berlin, Germany. [9]Virginia Bioinformatics Institute, Virginia Tech, Washington St., Blacksburg, Virginia 24061-0477, USA. [10]Keck Graduate Institute, 535 Watson Drive, Claremont, California 91711, USA. [11]Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109, USA. [12]Triple-J Group for Molecular Cell Physiology, Department of Biochemistry, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa. [13]Department of Scientific Computing & Mathematical Modeling, GlaxoSmithKline Research & Development Limited, Medicines Research Centre, Gunnels Wood Road, Stevenage, Herts, SG1 2NY, UK. [14]Purdue University, Department of Biological Sciences, Lilly Hall of Life Sciences, 915 W. State Street, West Lafayette, Indiana 47907-2054, USA. [15]These authors have contributed equally to the work. Correspondence should be addressed to N.L.N. (e-mail: lenov@ebi.ac.uk).

Published online 6 December 2005; doi:10.1038/nbt1156

During the genomic era we have witnessed a vast increase in availability of large amounts of quantitative data. This is motivating a shift in the focus of molecular and cellular research from qualitative descriptions of biochemical interactions towards the quantification of such interactions and their dynamics. One of the tenets of systems biology is the use of quantitative models (see Box 1 for definitions) as a mechanism for capturing precise hypotheses and making predictions[1,2]. Many specialized models exist that attempt to explain aspects of the cellular machinery. However, as has happened with other types of biological information, such as sequences, macromolecular structures or

Box 1 Glossary

Some terms are used in a very specific way throughout the article. We provide here a precise definition of each one.

Quantitative biochemical model. A formal model of a biological system, based on the mathematical description of its molecular and cellular components, and the interactions between those components.

Encoded model. A mathematical model written in a formal machine-readable language, such that it can be systematically parsed and employed by simulation and analysis software without further human translation.

MIRIAM-compliant model. A model that passes all the tests and fulfills all the conditions listed in MIRIAM.

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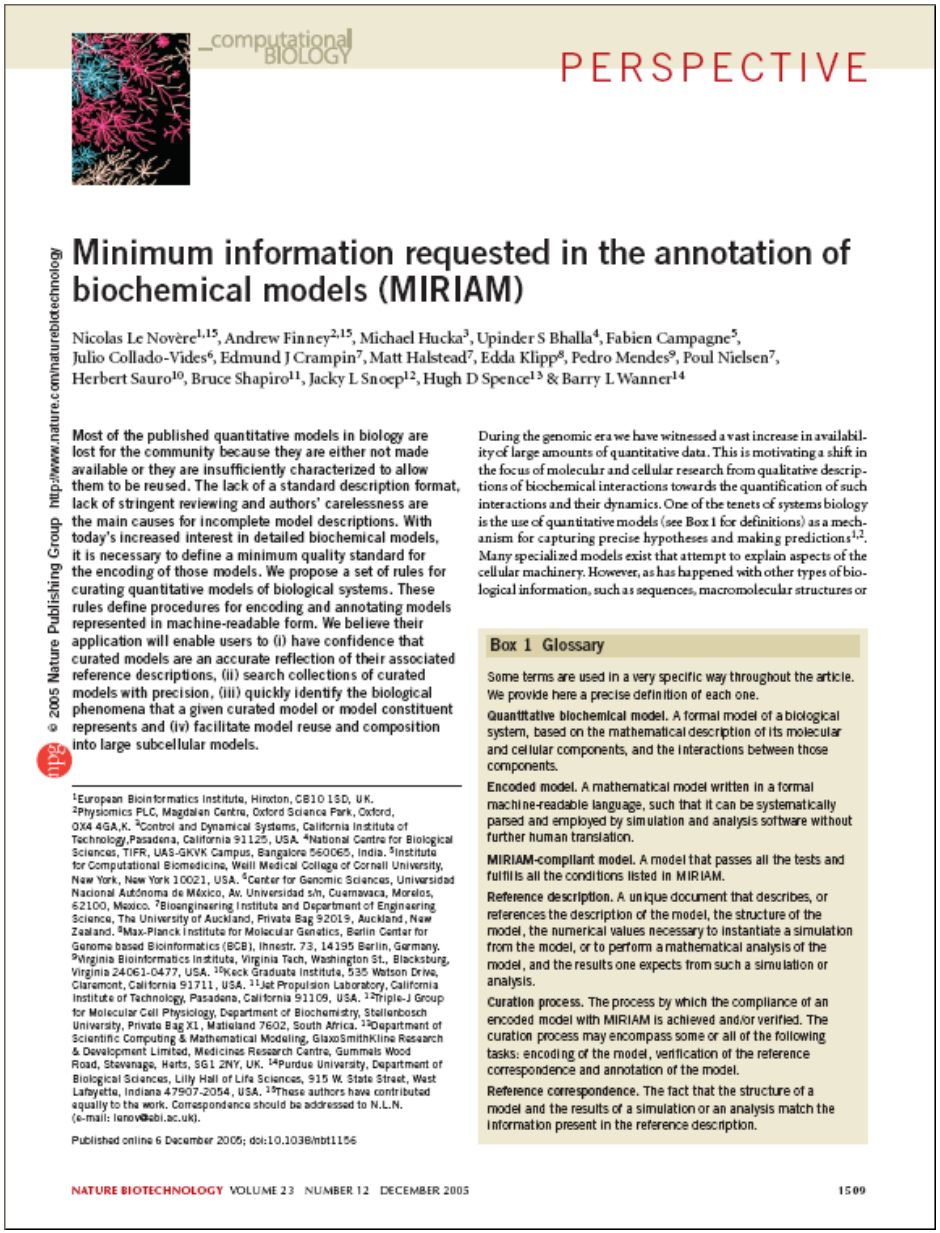

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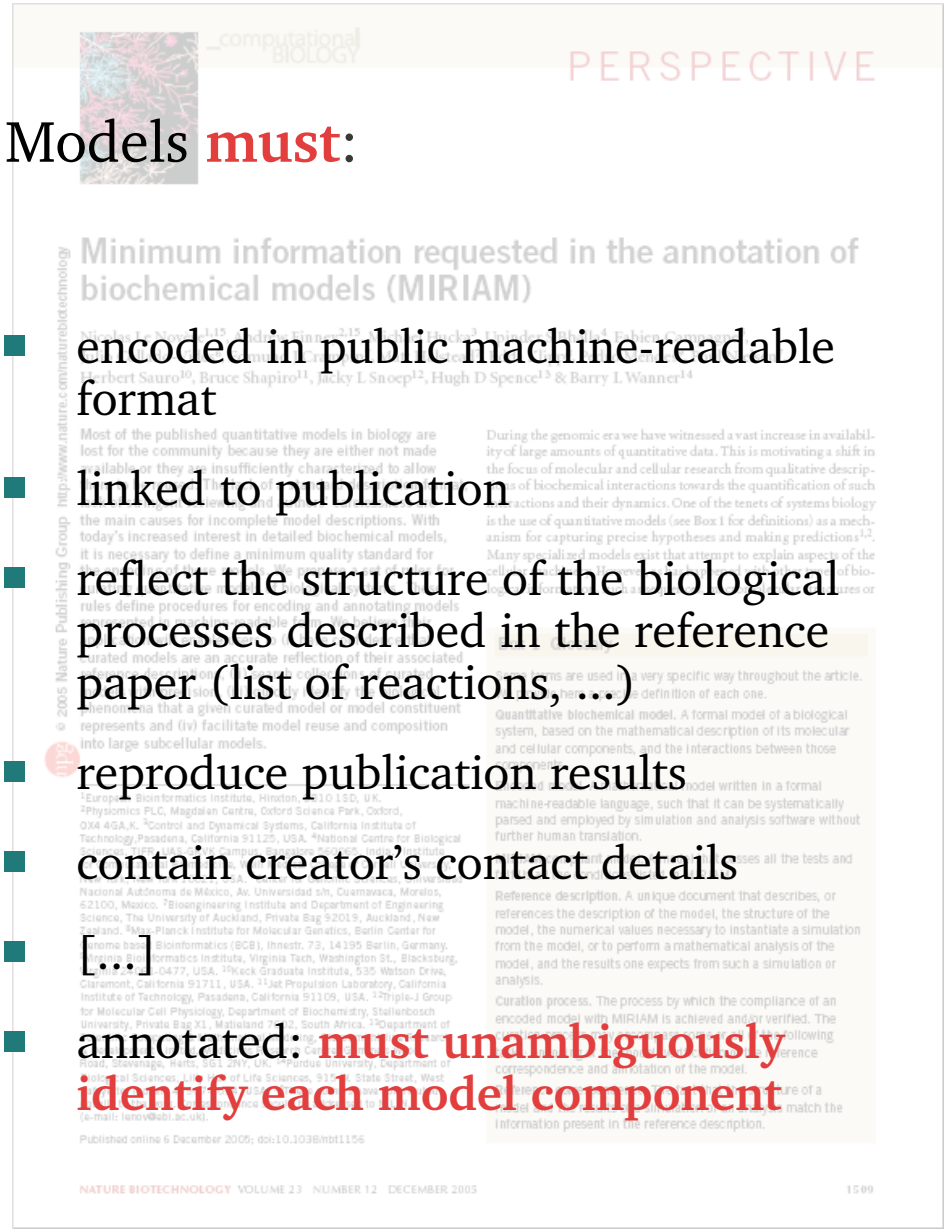
- proposed guidelines for curation and annotation of quantitative biological models
- applicable to any structured model format

http://biomodels.net/miriam/

MIRIAM guidelines



Models **must**:

- encoded in public machine-readable format
- linked to publication
- reflect the structure of the biological processes described in the reference paper (list of reactions, ...)
- reproduce publication results
- contain creator's contact details
- [...]
- annotated: **must unambiguously identify each model component**

- proposed guidelines for curation and annotation of quantitative biological models
- applicable to any structured model format

http://biomodels.net/miriam/

Why are annotations important?

Annotations (**unambiguously identify** entities) are essential for:

- understanding
- reuse
- comparison
- integration
- efficient search strategies
- conversion
- ...

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→ for any kind of data

Identifiers

603903

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In PubMed:

Specification of angulated projections in coronary arteriography

In OMIM:

Sickle cell anemia

In PubChem Compound:

3-([2-(4-Bromophenyl)-2-oxoethyl]sulfanyl)-6-methyl-1,2,4-triazin-5(4H)-one

…

Identifiers

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```
SWISS-PROT:P49581

UniProt/Swiss-Prot:P49581

UniProtKB/Swiss-Prot:P49581

...
```

Identifiers

- not unique
- ambiguous
- **not consistent**

```
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UniProt/Swiss-Prot:P49581

UniProtKB/Swiss-Prot:P49581

...
```

Identifiers

- not unique
- ambiguous
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http://www.ebi.ac.uk/citexplore/citationDetails.do?dataSource=MED&externalId=16333295

http://www.ncbi.nlm.nih.gov/pubmed/16333295

http://www.hubmed.org/display.cgi?uids=16333295

http://srs.ebi.ac.uk/srsbin/cgi-bin/wgetz?-view+MedlineFull+[medline-PMID:16333295]

Identifiers

- not unique
- ambiguous
- not consistent
- **not perennial**

http://www.ebi.ac.uk/citexplore/citationDetails.do?dataSource=MED&externalId=16333295

http://www.ncbi.nlm.nih.gov/pubmed/16333295

http://www.hubmed.org/display.cgi?uids=16333295

http://srs.ebi.ac.uk/srsbin/cgi-bin/wgetz?-view+MedlineFull+[medline-PMID:16333295]

Identifiers

- not unique
- ambiguous
- not consistent
- **not perennial**
- **location dependent**

http://www.ebi.ac.uk/citexplore/citationDetails.do?dataSource=MED&externalId=16333295

http://www.ncbi.nlm.nih.gov/pubmed/16333295

http://www.hubmed.org/display.cgi?uids=16333295

http://srs.ebi.ac.uk/srsbin/cgi-bin/wgetz?-view+MedlineFull+[medline-PMID:16333295]

(MIRIAM) Identifiers / URIs

Namespace

Identifies a dataset

Entity identifier

Identifies a piece of data within the dataset

(MIRIAM) Identifiers / URIs

Namespace

Identifies a dataset

from a shared list of namespaces

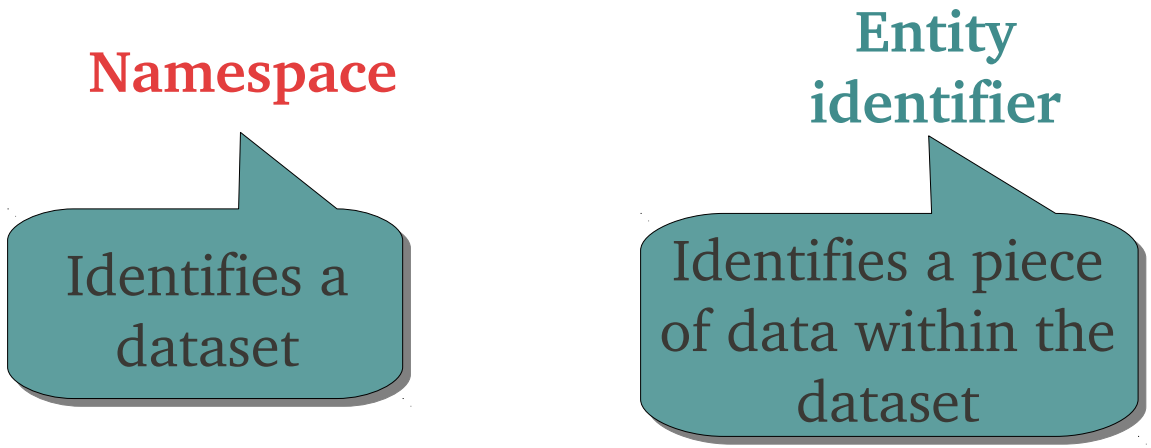
Entity identifier

Identifies a piece of data within the dataset

provided within the dataset

format defined by the dataset

MIRIAM URNs



Human calmodulin: P62158 in UniProt

↳ `urn:miriam:uniprot:P62158`

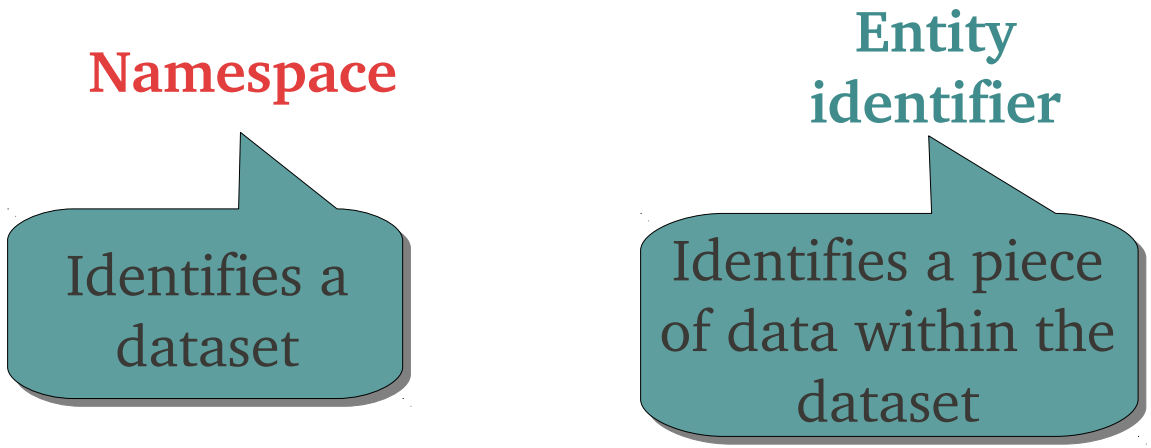
Alcohol dehydrogenase: 1.1.1.1 in EC code

↳ `urn:miriam:ec-code:1.1.1.1`

Activation of MAPKK activity: GO:0000186 in Gene Ontology

↳ `urn:miriam:obo.go:GO%3A0000186`

Identifiers.org URLs



Human calmodulin: P62158 in UniProt

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http://identifiers.org/uniprot/P62158

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urn:miriam:ec-code:1.1.1.1

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

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urn:miriam:obo.go:GO%3A0000186

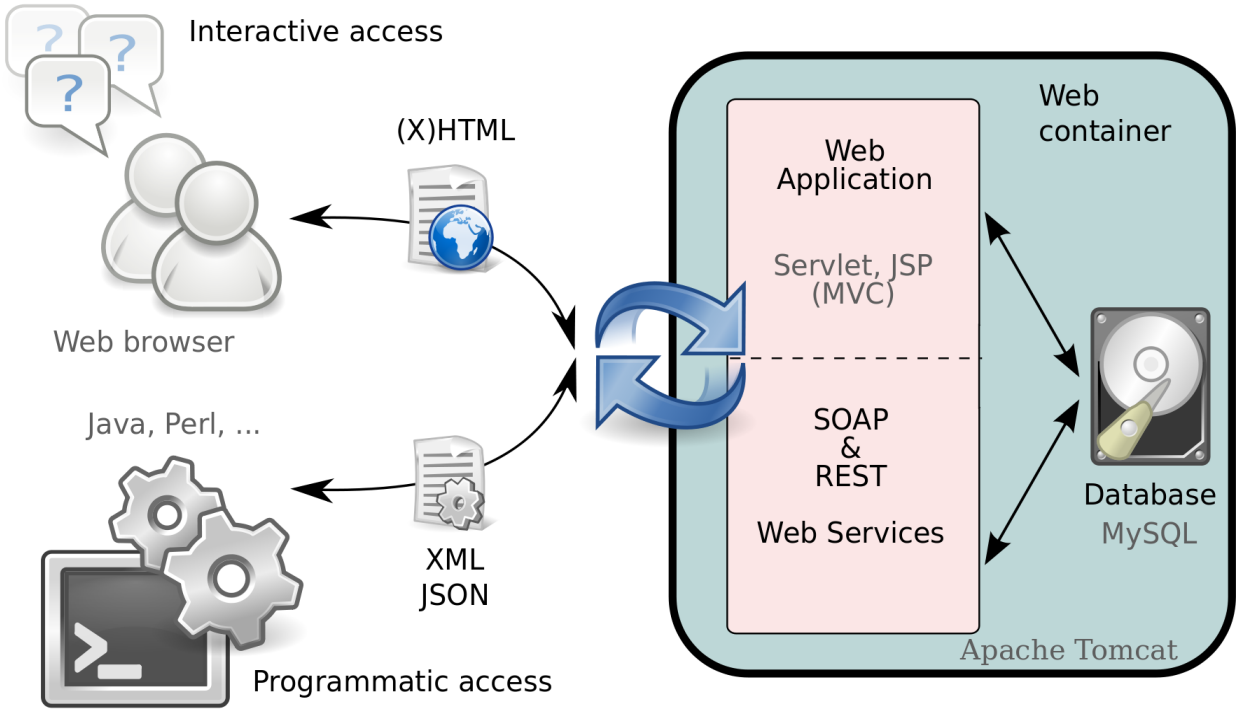
http://identifiers.org/obo.go/GO:0000186

Identifiers.org: summary

- **resolvable persistent identifiers** (URIs)
- identifiers available at **multiple levels** (dataset, provider and entity)
- **customisable** behaviours (formats available, preferred provider, ...)
- responses encoded in HTML and **RDF** (either requested explicitly in the URLs or via *content negotiation*)
- **community** driven
- **curated** resource (built on *MIRIAM Registry*)
- systems in place to **monitor** registered resources
- **unrestricted** scope (currently mainly focused on Life Sciences, but the scope is potentially unlimited)
- **free** to use

http://identifiers.org/

- Built upon the information stored in **MIRIAM Registry**:

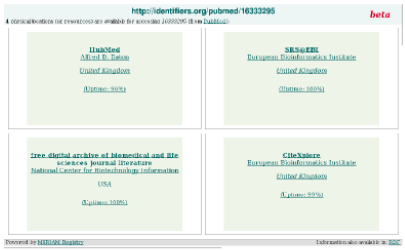


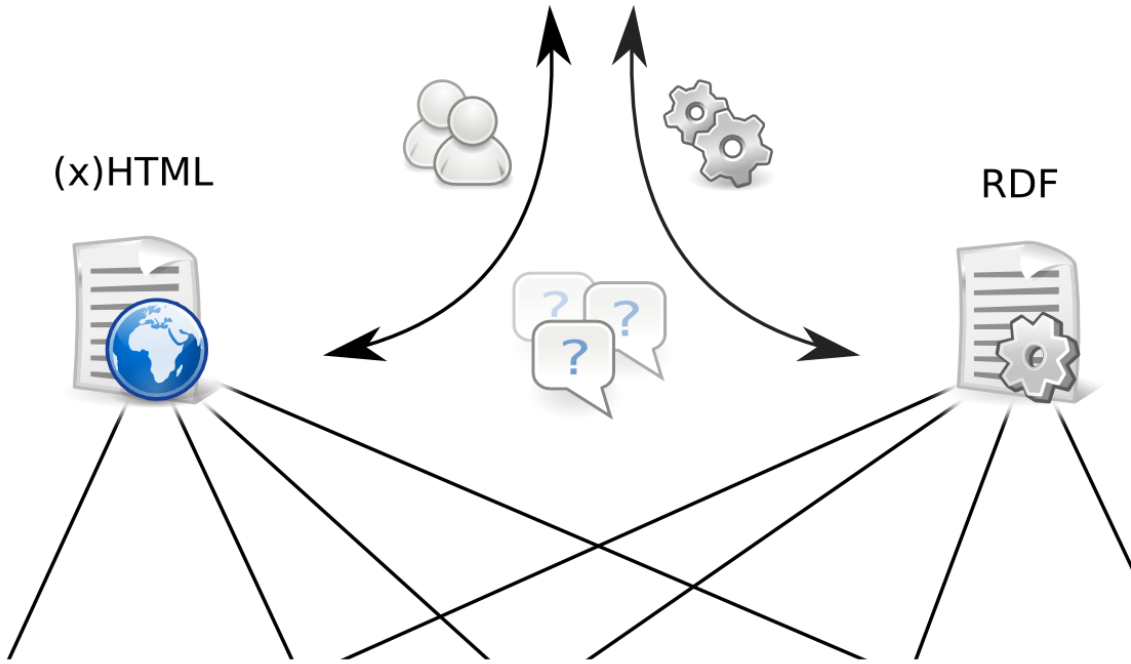
Camille Laibe and Nicolas Le Novère.
MIRIAM Resources: tools to generate and resolve robust cross-references in Systems Biology.
BMC Systems Biology, 2007

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

Identifiers.org: resolving

http://identifiers.org/pubmed/16333295





Identifiers.org: resolving

http://identifiers.org/pubmed/16333295

beta

4 physical locations (or resources) are available for accessing *16333295* (from PubMed):

CiteXplore
European Bioinformatics Institute

United King

Access to '16333295' via this resource (MIR:00100032)

(Uptime: 99%)

free digital archive of biomedical and life sciences journal literature
National Center for Biotechnology Information

USA

(Uptime: 100%)

SRS@EBI
European Bioinformatics Institute

United Kingdom

(Uptime: 100%)

HubMed
Alfred D. Eaton

United Kingdom

(Uptime: 97%)

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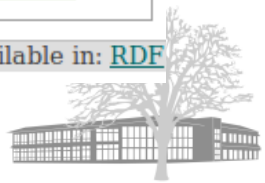
Information also available in: RDF



Identifiers.org: resolving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Identifiers.org: resolving to specific provider

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

Access to 1.1.1.1 (from Enzyme Nomenclature) using the resource MIR:00100001.
Entity available from **3** providers, for more information please refer to: http://identifiers.org/ec-code/1.1.1.1.

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EC 1 - Oxidoreductases

EC 1.1 - Acting on the CH-OH Group of Donors

EC 1.1.1 - With NAD^+ or $NADP^+$ as acceptor

EC 1.1.1.1 - Alcohol dehydrogenase

IntEnz view | ENZYME view

XML

IntEnz Enzyme Nomenclature

EC 1.1.1.1

Names

Accepted name: alcohol dehydrogenase

Other names: ADH
NAD-dependent alcohol dehydrogenase
NAD-specific aromatic alcohol dehydrogenase
NADH-alcohol dehydrogenase
NADH-aldehyde dehydrogenase
alcohol dehydrogenase (NAD)
aldehyde reductase
aliphatic alcohol dehydrogenase
ethanol dehydrogenase
primary alcohol dehydrogenase
yeast alcohol dehydrogenase

Systematic name: alcohol:NAD^+ oxidoreductase

Identifiers.org: resolving to specific provider

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

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EC 1 - Oxidoreductases

EC 1.1 - Acting on the CH-OH Group of Donors

EC 1.1.1 - With NAD+ or NADP+ as acceptor

EC 1.1.1.1 - Alcohol dehydrogenase

IntEnz view | ENZYME view

XML

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IntEnz Enzyme Nomenclature

EC 1.1.1.1

Names

Accepted name: alcohol dehydrogenase

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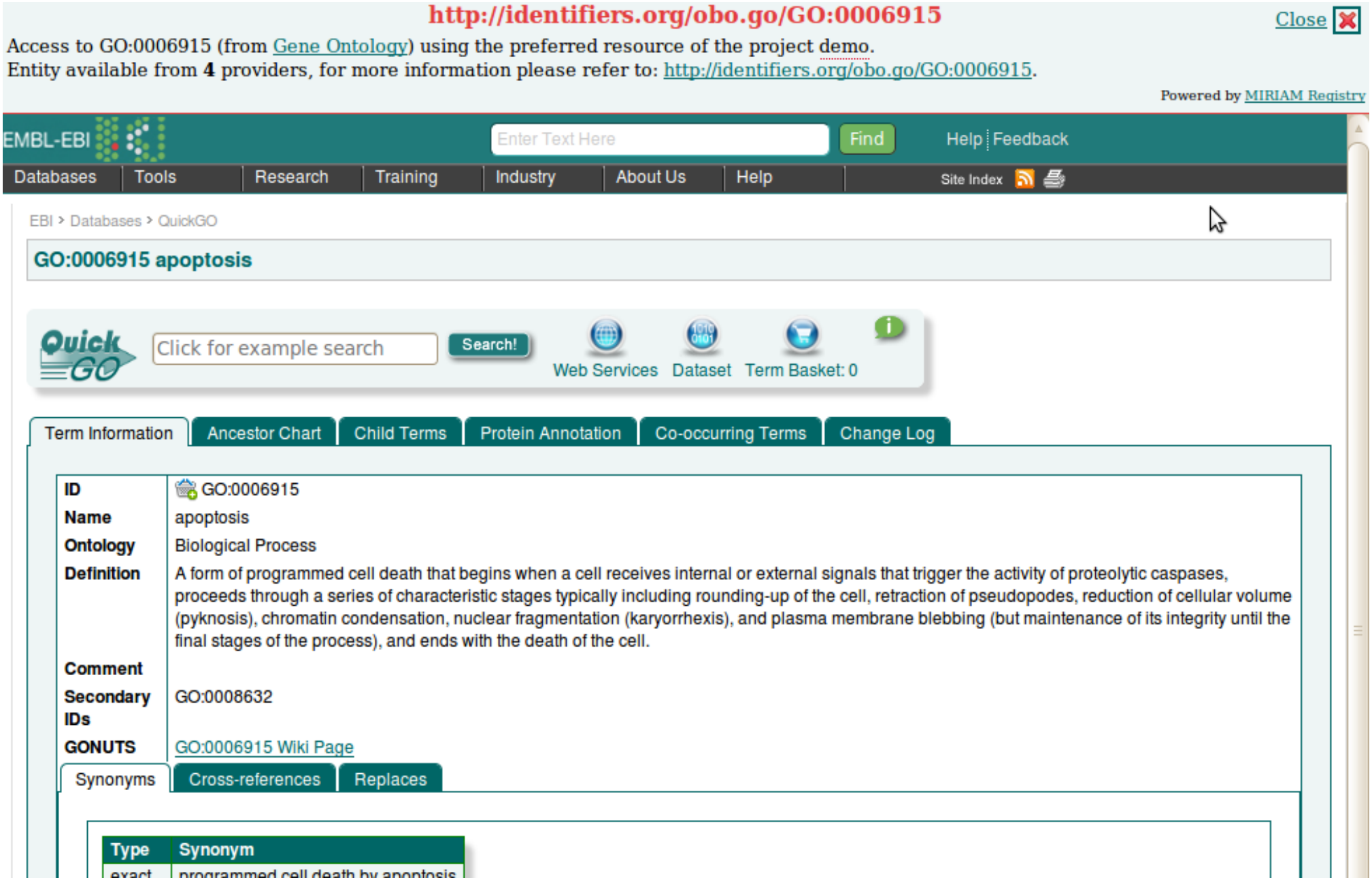
NAD-dependent alcohol dehydrogenase
NAD-specific aromatic alcohol dehydrogenase
NADH-alcohol dehydrogenase
NADH-aldehyde dehydrogenase
alcohol dehydrogenase (NAD)
aldehyde reductase
aliphatic alcohol dehydrogenase
ethanol dehydrogenase
primary alcohol dehydrogenase
yeast alcohol dehydrogenase

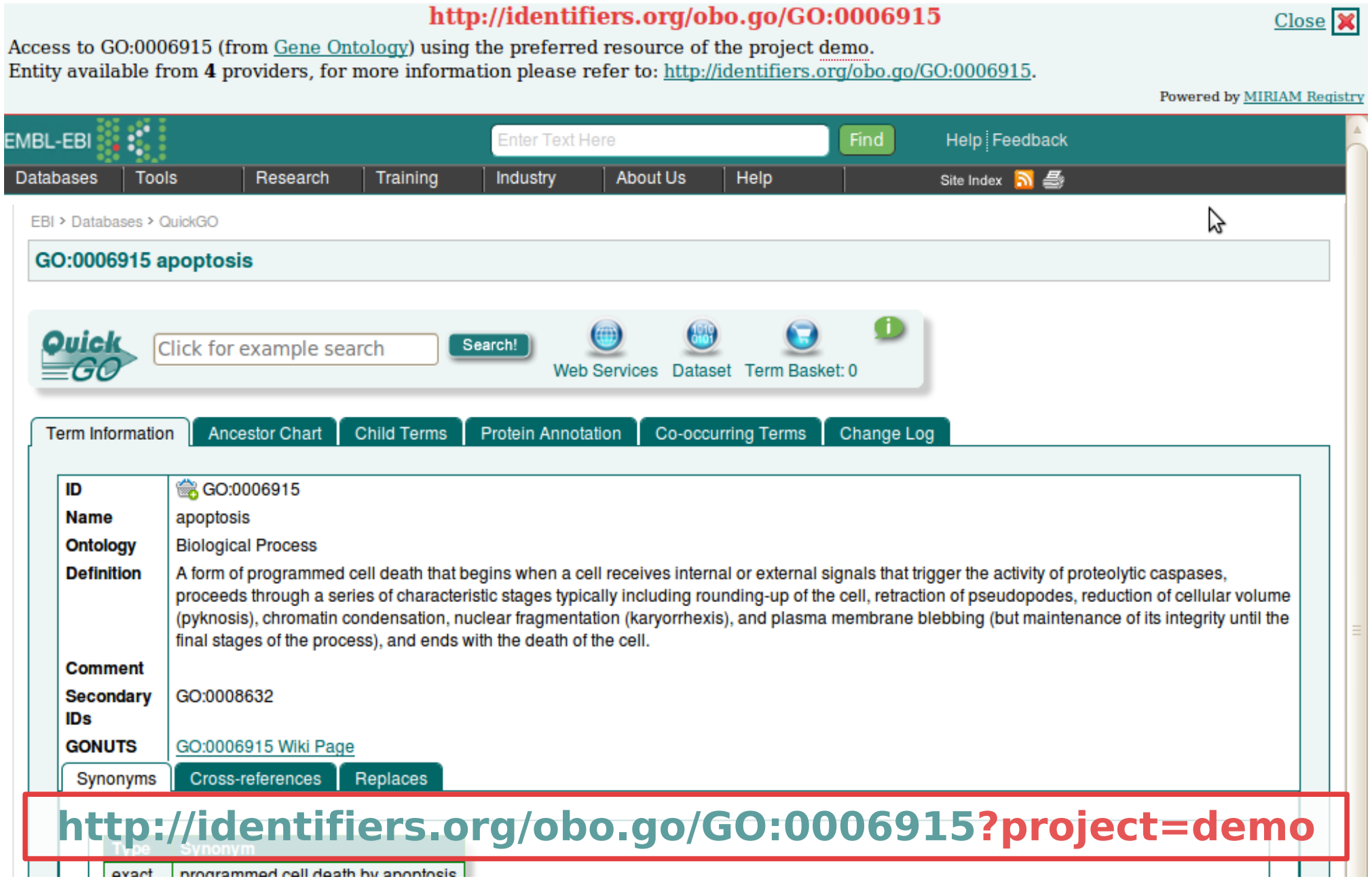
Systematic name: alcohol:NAD+ oxidoreductase

http://identifiers.org/ec-code/1.1.1.1?resource=MIR:00100001

Identifiers.org: resolving using a profile



Identifiers.org: resolving using a profile



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

Close

Access to 1.1.1.1 (from Enzyme Nomenclature) using the preferred resource of the project most reliable.
Entity available from **3** providers, for more information please refer to: http://identifiers.org/ec-code/1.1.1.1.

Powered by: Identifiers.org & MIRIAM Registry

KEGG

ENZYME: 1.1.1.1

Help

Entry	EC 1.1.1.1 Enzyme
Name	alcohol dehydrogenase; aldehyde reductase; ADH; alcohol dehydrogenase (NAD); aliphatic alcohol dehydrogenase; ethanol dehydrogenase; NAD-dependent alcohol dehydrogenase; NAD-specific aromatic alcohol dehydrogenase; NADH-alcohol dehydrogenase; NADH-aldehyde dehydrogenase; primary alcohol dehydrogenase; yeast alcohol dehydrogenase
Class	Oxidoreductases; Acting on the CH-OH group of donors; With NAD+ or NADP+ as acceptor BRITE hierarchy
Sysname	alcohol:NAD+ oxidoreductase
Reaction(IUBMB)	(1) a primary alcohol + NAD+ = an aldehyde + NADH + H+ [RN:R07326]; (2) a secondary alcohol + NAD+ = a ketone + NADH + H+ [RN:R07327]
Reaction(KEGG)	R07326 > R00623 R00754 R02124 R04805 R04880 R05233 R05234 R06917 R06927 R08281 R08306 R08557 R08558; R07327 > R00624 R08310; (other) R07105 Show all
Substrate	primary alcohol [CPD:C00226];

All links

Ontology (6)
- KEGG BRITE (6)

Pathway (7924)
- KEGG PATHWAY (7915)
- KEGG MODULE (9)

Disease (4)
- OMIM (4)

Chemical substance (38)
- KEGG COMPOUND (38)

Chemical reaction (52)
- KEGG REACTION (21)
- KEGG RPAIR (18)
- KEGG RCLASS (13)

Genome (4)
- KEGG GENOME (4)

Gene (7537)
- KEGG ORTHOLOGY (9)
- KEGG GENES (3238)
- KEGG DGENES (121)
- KEGG EGENES (1663)
- KEGG MGENES (2506)

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- UniProt (3594)
- PRF (405)
- RefSeq(pep) (2305)
- PDBSTR (217)
- PMD (55)

DNA sequence (4640)
- RefSeq(nuc) (1494)
- GenBank (1571)

Identifiers.org: resolving to most reliable resource

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Access to 1.1.1.1 (from Enzyme Nomenclature) using the preferred resource of the project most_reliable.
Entity available from **3** providers, for more information please refer to: http://identifiers.org/ec-code/1.1.1.1.

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KEGG

ENZYME: 1.1.1.1 Help

Entry	EC 1.1.1.1 Enzyme
Name	alcohol dehydrogenase; aldehyde reductase; ADH; alcohol dehydrogenase (NAD); aliphatic alcohol dehydrogenase; ethanol dehydrogenase; NAD-dependent alcohol dehydrogenase; NAD-specific aromatic alcohol dehydrogenase; NADH-alcohol dehydrogenase; NADH-aldehyde dehydrogenase; primary alcohol dehydrogenase; yeast alcohol dehydrogenase
Class	Oxidoreductases; Acting on the CH-OH group of donors; With NAD+ or NADP+ as acceptor BRITE hierarchy
Sysname	alcohol:NAD+ oxidoreductase
Reaction(IUBMB)	(1) a primary alcohol + NAD+ = an aldehyde + NADH + H+ [RN:R07326]; (2) a secondary alcohol + NAD+ = a ketone + NADH + H+ [RN:R07327]
Reaction(KEGG)	R07326 > R00623 R00754 R02124 R04805 R04880 R05233 R05234 R06917 R06927 R08281 R08306 R08557 R08558; R07327 > R00624 R08310; (other) R07105 Show all
Substrate	primary alcohol [CPD:C00226];

All links

- Ontology (6)
  - KEGG BRITE (6)
- Pathway (7924)
  - KEGG PATHWAY (7915)
  - KEGG MODULE (9)
- Disease (4)
  - OMIM (4)
- Chemical substance (38)
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- Chemical reaction (52)
  - KEGG REACTION (21)
  - KEGG RPAIR (18)
  - KEGG RCLASS (13)
- Genome (4)
  - KEGG GENOME (4)
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  - KEGG ORTHOLOGY (9)
  - KEGG GENES (3238)
  - KEGG DGENES (121)
  - KEGG EGENES (1663)
  - KEGG MGENES (2506)
- Protein sequence (6576)
  - UniProt (3594)
  - PRF (405)
  - RefSeq(pep) (2305)
  - PDBSTR (217)
  - PMD (55)
  - RefSeq(nuc) (7434)
  - GenBank (1571)

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Comments? Questions? Requests?

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