Cheminformatics and Metabolism

Chemical resources (structure, bioactivity and metabolomics): ChEBI, MetaboLights and the Enzyme Portal

SME Bioinformatics Forum, Barcelona 8-9 October 2012

Pablo Conesa
Overview

- ChEBI
- Enzyme Portal
- MetaboLights
ChEBI

dictionary of ‘small’ molecules

EBI is an Outstation of the European Molecular Biology Laboratory.
What is ChEBI?

- **Chemical Entities of Biological Interest**
- Freely available
- Focused on ‘small’ chemical entities (no proteins or nucleic acids)
- Illustrated dictionary of chemical nomenclature
- High quality, manually annotated database
- Provides chemical ontology

Access ChEBI at [http://www.ebi.ac.uk/chebi/](http://www.ebi.ac.uk/chebi/)
Chemicals - ChEBI

Nomenclature
caffeine
1,3,7-trimethylxanthine
methyltheobromine

Ontology
metabolite
CNS stimulant
trimethylxanthines

Chemical data
Formula: C8H10N4O2
Charge: 0
Mass: 194.19

Database Xrefs
MSDchem: CFF
KEGG DRUG: D00528

Chemical Informatics
InChI=1/C8H10N4O2/c1-10-4-9-6-5(10)7(13)12(3)8(14)11(6)2/h4H,1-3H3
SMILES CN1C(=O)N(C)c2ncn(C)c2C1=O

Visualisation
Small molecule annotations

- Often appear as free text in biological databases, in which they are not the core data
- Are frequently referred to by common names which may be chemically ambiguous
  - eg. adrenaline
    - = (S)-adrenaline ? (R)-adrenaline ?

- May be referred to by several different names
  - paracetamol, acetaminophen, 4-acetamidophenol, N-(4-hydroxyphenyl)acetamide, …
Chemical Entities of Biological Interest (ChEBI) is a freely available dictionary of molecular entities focused on 'small' chemical compounds.

Vitamin A deficiency is of public health significance in the developing world. Approximately half a million children in Africa and Asia go blind every year due to their diet being deficient in vitamin A, which is important for vision and the immune system. β-Carotene (CHEBI:17579), a red-orange pigment abundant in plants and fruit, is the primary dietary source of vitamin A worldwide. In the body, β-carotene is converted into vitamin A, which can exist in several forms (retinol, retinal, retinoic acid and retinyl esters). The role of vitamin A in the visual cycle is specifically related to the retinal form. Within the eye, 11-cis-retinal is bound to rhodopsin (rods) and iodopsin (cones) at conserved tryptophan residues. As light enters the eye, the 11-cis-retinal is isomerised to the all-trans form. This isomerisation induces a nervous signal along the optic nerve to the visual centre of the brain. The all-trans form is subsequently recycled via a series of enzymatic reactions.

Read more...
ChEBI entries contain

- A unique, unambiguous, recommended ChEBI name and an associated stable unique identifier
- An illustration where appropriate (compounds and groups, but generally not classes)
- A definition where appropriate (mostly classes)
- A collection of synonyms, including the IUPAC recommended name for the entity where appropriate
- A collection of cross-references to other databases

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<td>Definition</td>
<td>Aliphatic monocarboxylic acids derived from or contained in esterified form in an animal or vegetable fat, oil or wax. Natural fatty acids commonly have a chain of 4 to 28 carbons (usually unbranched and even-numbered), which may be saturated or unsaturated.</td>
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ChEBI entry view

[Image of ChEBI entry view]

- **Brand Name**: [Read full article at Wikipedia]
- **Formula**: C8H9NO2
- **Net Charge**: 0
- **Average Mass**: 151.16260
- **InChI**: InChI=1S/C8H9NO2/c1-6(10)9-7-2-4-8(11)5-3-7/h2-6,11H,1H3,(H,9,10)
- **InChIKey**: InChIKey=RIVAJINKMORJF-UHFFFAOYSA-N
- **SMILES**: CC(=O)Nc1ccc(O)cc1
- **ChEBI Ontology**: [Tree view]
  - **Outgoing**:
    - paracetamol (CHEBI:46195) has role cyclooxygenase 2 inhibitor (CHEBI:50629)
    - paracetamol (CHEBI:46195) has role cyclooxygenase 1 inhibitor (CHEBI:50630)
    - paracetamol (CHEBI:46195) has role non-narcotic analgesic (CHEBI:35481)
    - paracetamol (CHEBI:46195) has role antipyretic (CHEBI:35493)
    - paracetamol (CHEBI:46195) has role non-steroidal anti-inflammatory drug (CHEBI:35475)
    - paracetamol (CHEBI:46195) is a phenols (CHEBI:33853)
    - paracetamol (CHEBI:46195) is a acetamides (CHEBI:22183)
  - **Incoming**:
    - acetaminophen glutathione conjugate (CHEBI:32633) has functional parent paracetamol (CHEBI:46195)
    - paracetamol sulfate (CHEBI:32635) has functional parent paracetamol (CHEBI:46195)

**IUPAC Name**: N-[4-hydroxyphenyl]acetamide

[show Abstract]

**Last Modified**: [Source]
Automatic Cross-references

paracetamol (CHEBI:46185)

Main

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<td>Reactions &amp; Pathways</td>
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</tbody>
</table>

+ Genomes
  - PRIDE
    - Proteomics Identification Database
  - UniProt KB
    - UniProt Knowledge Base of protein sequences
    1. CP1A2_HUMAN
      - Cytochrome P450 1A2
    2. RR2A_ARATH
      - Ribonucleoside-diphosphate reductase small chain A
    3. RYBP_HUMAN
      - RING1 and YY1-binding protein
    4. SBP2_MOUSE
      - Selenium-binding protein 2

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+ Protein Sequences
  - 4

+ Molecular Interactions
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+ Reactions & Pathways
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+ Reactions & Pathways
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+ Genomes
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+ Nucleotide Sequences
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+ Protein Sequences
  - 4

+ Molecular Interactions
  - 0

+ Reactions & Pathways
  - 4
Chemical Structures

- Chemical structure may be interactively explored using MarvinView applet

- Available in formats
  - Image
  - Molfile
  - InChI and InChIKey
  - SMILES
How is ChEBI maintained?

• Automatic loading of preliminary data

• Automatic loading of data annotated elsewhere

• Manual annotation

• User requests via Submission Tool

• Public release: First Monday of every month.
For more information

- Email: chebi-help@ebi.ac.uk
- SourceForge: https://sourceforge.net/projects/chebi/
- User Manual: http://www.ebi.ac.uk/chebi/userManualForward.do
- RSS Feed
The EBI Enzyme Portal

Your portal to enzyme-related information at the EBI
The Enzyme Portal integrates EBI’s enzyme resources into a single access point.
Enzyme Portal home page

Enzyme Portal - Your portal to enzyme-related information at the EBI.

Welcome to the Enzyme Portal
The Enzyme Portal is for people who are interested in the biology of enzymes and proteins with enzymatic activity.

More about the enzyme portal...
Enzyme Portal Results Page

Search Filters

Species:
- Human [Homo sapiens]
- Mouse [Mus musculus]
- Rat [Rattus norvegicus]
- Fruit fly [Drosophila melanogaster]
- Baker's yeast [Saccharomyces cerevisiae [strain ATCC 204508 /S288c]]
- African clawed frog [Xenopus laevis]
- Anacystis nidulans R2 [Synechococcus elongatus [strain PCC 7942]]

Search here

Enzyme Portal - Your portal to enzyme-related information at the EBI.

-sildenafil

Example: sildenafil, Insulin receptor, Ceramide glucosyltransferase, Phenylalanine-4-hydroxylase, Cytochrome P450 3A4, CFTR, G13423, REACT_1400.4

44 results found for sildenafil, displaying 1 - 10

Page 1 of 5 Next

cGMP-specific 3',5'-cyclic phosphodiesterase [Human]

Function: Plays a role in signal transduction by regulating the intracellular concentration of cyclic nucleotides. This phosphodiesterase catalyzes the specific hydrolysis of cGMP to 5'-GMP.

Synonyms: Cyclic 3,5-GMP phosphodiesterase; Cyclic GMP phosphodiesterase; Cyclic guanosine 3',5'-monophosphate phosphodiesterase; Cyclic guanosine 3',5'-phosphate phosphodiesterase; EC 3.1.4.35;

Species: [Human] [Bovine] [Dog] [Mouse] [Rat]

cAMP-specific 3',5'-cyclic phosphodiesterase 4B [Human]

Function: Hydrolyzes the second messenger cAMP, which is a key regulator of many important physiological processes. May be involved in mediating central nervous system effects of therapeutic agents ranging from antidepressants to anti-asthmatic and anti-inflammatory agents.

Synonyms: 3', 5'-cyclic nucleoside monophosphate phosphodiesterase; 3',5'-cyclic nucleotide phosphodiesterase; 3',5'-nucleotide phosphodiesterase; 3', 5'-monophosphate phosphodiesterase (cyclic CMP); 3',5'-cyclic nucleotide 3'-nucleotidohydrolase; Show more synonyms

Species: [Human] [Fruit fly] [Rat]

No structure available:

Rod cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha [Human]

Function: This protein participates in processes of transmission and amplification of the visual signal.

Synonyms: Cyclic 3,5-GMP phosphodiesterase; Cyclic GMP phosphodiesterase; Cyclic guanosine 3',5'-monophosphate phosphodiesterase; Cyclic guanosine 3',5'-phosphate phosphodiesterase; EC 3.1.4.36; Show more synonyms

Species: [Human] [Bovine] [Dog] [Mouse]
cGMP-specific 3',5'-cyclic phosphodiesterase

Function
Plays a role in signal transduction by regulating the intracellular concentration of cyclic nucleotides. This phosphodiesterase catalyzes the specific hydrolysis of cGMP to 5'-GMP.

EC Classification
Hydrolases > Acting on ester bonds > Phosphoric Diester Hydrolases > 3.1.4.35 - 3',5'-cyclic-GMP phosphodiesterase

Other names
cGMP-specific 3',5'-cyclic phosphodiesterase; EC 3.1.4.35; cGMP-binding cGMP-specific phosphodiesterase; cGMP phosphodiesterase; cGMP-PDE; Cyclic 3',5'-GMP phosphodiesterase; Cyclic GMP phosphodiesterase; Cyclic guanosine 3',5'-monophosphate phosphodiesterase; Cyclic guanosine 3',5'-phosphate phosphodiesterase; Guanosine cyclic 3',5'-phosphate phosphodiesterase;

Protein Sequence
This sequence has 875 amino acids

View Sequence in UniProt

Data Source: IntEnz & UniProt
IntEnz - (integrated relational Enzyme database) is a freely available resource focused on enzyme nomenclature.
UniProt - The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information.
cGMP-specific 3',5'-cyclic phosphodiesterase

27 protein structures available

Crystal structure of the PDE5A1 catalytic domain in complex with novel inhibitors

Description
Crystal structure of the PDE5A1 catalytic domain in complex with novel inhibitors

Description
HYDROLASE/HYDROLASE INHIBITOR

Method
x-ray diffraction

Experiment
Resolution: 2.647Å
R-Factor: 21.37%
Free R-Factor: 25.92%

Dates
Deposited: 17-06-2011
Released: 24-08-2011
Revised: 24-08-2011

Deposited by
These events initiate the clotting cascade (secondary hemostasis). Negatively-charged phospholipids exposed at the site of injury and on activated platelets interact with tissue factor, leading to a cascade of reactions that culminates with the formation of an insoluble fibrin clot.

**cGMP-specific 3′,5′-cyclic phosphodiesterase**

\[ 3',5'-cyclic \text{GMP} + H_2O \leftrightarrow \text{GMP} + H(+) \]

This reaction might be present in 2 pathway(s)

**Hemostasis**

Hemostasis is a physiological response that culminates in the arrest of bleeding from an injured vessel. Under normal conditions the vascular endothelium supports vasodilation, inhibits platelet adhesion and activation, suppresses coagulation, enhances fibrin cleavage and is anti-inflammatory in character. Under acute vascular trauma, vasoconstrictor mechanisms predominate and the endothelium becomes prothrombotic, procoagulatory and proinflammatory in nature. This is achieved by a reduction of endothelial dilating agents: adenosine, NO and prostacyclin; and by the direct action of ADP, serotonin and thromboxane on vascular smooth muscle cells to elicit their contraction (Becker et al., 2000). The chief trooper for the change in endothelial function that leads...
Enzyme Portal Small Molecules

**cGMP-specific 3',5'-cyclic phosphodiesterase**

Bioactive compounds that might bind to this enzyme

The following compound(s) have been classified as Bioactive compounds. They have been associated with this enzyme, but it is uncertain whether they bind to this enzyme.

- **CHEMBL474226**
- **CHEMBL474227**
- **CHEMBL289047**

See all 1518 bioactive compounds in ChEMBL

Drugs that might interact with this enzyme

The following compound(s) have been classified as drugs. They have been associated with this enzyme, but it is uncertain whether they interact with this enzyme.

- dipyridamole
- DB00806
- sildenafil citrate
Enzyme Portal Small Molecules

Drugs that might interact with this enzyme

The following compound(s) have been classified as drugs. They have been associated with this enzyme, but it is uncertain whether they interact with this enzyme.

- **dipyridamole**
- **DB00806**
- **sildenafil citrate**

**Formula:** C24H40N8O4

See all 6 drugs in UniProt

No activators found for this enzyme!

Inhibitors that might inhibit this enzyme

The following compound(s) have been classified as inhibitors. They have been associated with this enzyme, but it is uncertain whether they inhibit this enzyme.

**ZAPRINAST**
Cystic fibrosis transmembrane conductance regulator

2 entries related to disease information found for this enzyme:

Defects in CFTR are the cause of cystic fibrosis (CF) [MIM:219700], also known as mucoviscidosis. CF is the most common genetic disease in the Caucasian population, with a prevalence of about 1 in 2,000 live births. Inheritance is autosomal recessive. CF is a common generalized disorder of exocrine gland function which impairs clearance of secretions in a variety of organs. It is characterized by the triad of chronic bronchopulmonary disease (with recurrent respiratory infections), pancreatic insufficiency (which leads to malabsorption and growth retardation) and elevated sweat electrolytes.

Defects in CFTR are the cause of congenital bilateral absence of the vas deferens (CBAVD) [MIM:277180]. CBAVD is an important cause of sterility in men and could represent an incomplete form of cystic fibrosis, as the majority of men suffering from cystic fibrosis lack the vas deferens.

Data Source: UniProt

UniProt - The mission of UniProt is to provide the scientific community with a comprehensive, high-quality and freely accessible resource of protein sequence and functional information
cGMP-specific 3',5'-cyclic phosphodiesterase

Filters:  Enzyme  Protein structure

Multiple cyclic nucleotide phosphodiesterases in human trabecular meshwork cells.
*Investigative ophthalmology & visual science* 40, 1745-52

The status, quality, and expansion of the NIH full-length cDNA project: the Mammalian Gene Collection (MGC).
Gerhard DS et al. (2004)
*Genome research* 14, 2121-7

Molecular cloning and expression of human cGMP-binding cGMP-specific phosphodiesterase (PDE5).
*Biochemical and biophysical research communications* 247, 249-54

Isolation and characterization of cDNAs encoding PDE5A, a human cGMP-binding, cGMP-specific 3',5'-cyclic nucleotide phosphodiesterase.
Loughney K et al. (1998)
*Gene* 216, 139-47

Regulation of cGMP-specific phosphodiesterase (PDE5) phosphorylation in smooth muscle cells.
*The Journal of biological chemistry* 277, 3310-7
Online training – Quick Tour

- http://www.ebi.ac.uk/training/online/course/enzyme-portal-quick-tour
MetaboLights

a repository for metabolomics experiments and derived information
MetaboLights - Goal

Create the first open cross-species, cross-platform metabolomics repository

http://www.ebi.ac.uk/metabolights
(metabolights.org, metabolights.eu)
MetaboLights – Main components

• Data Submission✔
  • ISA creator
  • Online data deposition

• Repository✔
  • Complete metabolomics experiments/studies
  • Sharing Experiments

• Reference Layer
  • Metabolite identification
  • Curated
MetaboLights – Data Submission Channels

- ISAcreator
- Bulk submission pipeline
ISAcreator

investigation
high level concept to link related studies

study
the central unit, containing information on the subject under study, its characteristics and any treatments applied.

a study has associated assays

assay
test performed either on material taken from the subject or on the whole initial subject, which produce qualitative or quantitative measurements (data)

Nature Genetics
doi:10.1038/ng.1054
Susanna-Assunta Sansone,...... Haug, Neumann, de Matos, Griffin, Steinbeck, ..... and Hide
### ISACreator - Study

#### STUDY PUBLICATIONS

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<td>2:1 urine/deuterated 0.2 M phosphate buffer</td>
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MetaboLights – Repository Website

MetaboLights: a database for metabolomics experiments and derived information

http://www.ebi.ac.uk/metabolights (metabolights.org, metabolights.eu)
MetaboLights – Private data

A metabolomic strategy defines the regulation of lipid content and global metabolism in Caenorhabditis elegans

Study Public Release Date: 31-Dec-2012

Organism
- Caenorhabditis elegans

Study Factors
- gene knockout: [wild-type generic:Delta 9 fat 5:Delta 9 fat 5 fat 7:Delta 9 fat 7:Delta 9 fat 5 fat 6:Delta 9 fat 6, wild-type generic:Delta 9 fat 5:Delta 9 fat 7:Delta 9 fat 5 fat 6:Delta 9 fat 6, wild-type generic:Delta 9 fat 5:Delta 9 fat 5 fat 7:Delta 9 fat 7:Delta 9 fat 5 fat 6:Delta 9 fat 6, wild-type generic:Delta 9 fat 5:Delta 9 fat 5 fat 7:Delta 9 fat 7:Delta 9 fat 5 fat 6:Delta 9 fat 6]

Assays
- mass spectrometry (1)
MetaboLights – Study Details

MTBLS3: A metabolomic strategy defines the regulation of lipid content and global metabolism by delta 9 desaturases in Caenorhabditis elegans

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<th>Cecilia_AA_rerun08</th>
<th>Cecilia_AA_rerun10</th>
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**Name**: glycine

**Identifier**: CHEBI:15428

**Definition**: The simplest (and the only achiral) proteinogenic amino acid, with a hydrogen atom as its side chain.

**Other Identifiers**: CHEBI:5460CHEBI:10792CHEBI:14344CHEBI:42964CHEBI:144010CHEBI:24368

Cecilia_AA_rerun05: mass spectrometry - metabolite profiling - DSQ II Single Quadrupole GC/MS (Thermo Scientific) Delta 9 fat 5
MetaboLights – Download page

**Pre-packaged ISACreator download.** To make it easy for new users, please download our pre-packaged ISACreator with plugin and configurations [here](#). The latest version of the metabolite identification plugin for ISACreator can be downloaded [here](#). Please remember to place this in the "/Plugins" folder in your local ISACreator installation.

**Experiments.** All public MetaboLights experiments can be downloaded from our public [ftp archive](#). Please find zip archives under the "studies" folder. Each public study can be found in the corresponding MTBLS-id zip-archive. Complete experiments can be opened with [ISACreator](#) or you can extract the archives using your normal unzip program.

MetaboLights submissions are powered by the ISA software suite, so experimental data gets submitted in ISA-Tab format. The Investigation/Study/Assay (ISA) infrastructure is the first general-purpose format and freely available desktop software suite targeted to experimentalists, curators and developers and that assists in the reporting and local management of experimental metadata (i.e. sample characteristics, technology and measurement types, sample-to-data relationships) from studies employing one or a combination of technologies.
MetaboLights - Curation

Reference Spectroscopy
Reference Chemistry
Reference Biology

Publication

Experimental Repository

MetaboLights

NMR
GC
MS
LC

Structure
Crossrefs
Identifier

Species
Disease
Organs
Tissues
Pathways
Cell Types

Nomenclature

Beta-Jan-2012
Prod NOW!
MetaboLights – The way forward

- Standards, MSI compliance
- Filling a gap, “First of a kind”
- Journals
- Stable identifiers
- High demand
- High quality curated data
- Listening to our users
- Open Data Access
Thank you

Any questions?