

BRENDA

General facts &
Search types

Some general facts about BRENDA

- Largest enzyme information system worldwide
- Includes scientific data of all known enzymes, classified according to the EC system
- Information comprises not only kinetical, structural, stability and genome properties but also methods to isolate and analyze the enzyme
- Half-yearly update to assemble latest information extracted from primary literature
- The databases AMENDA (Automatic Mining of ENzyme DATA) and FRENDA (Full Reference ENzyme DATA) provide additional enzyme data , extracted by textmining procedures
- Maintained and developed at the Institute for Biochemistry and Bioinformatics at the Technical University of Braunschweig

Information in BRENDA #I

Enzyme classification

- EC number
- Pathway(s) involved
- Enzyme Name (recommended/systematic)
- Synonyms
- CAS Registry Number

Biochemical parameters

- K_M and K_i value
- Turnover number
- Specific activity
- Natural substrates & products
- Further substrates & products
- Pathway belonging
- Coenzymes & Cosubstrates
- Inhibitors & Activators
- Metals/Ions and ligands
- Renaturation
- Purification methods
- Posttranslational modifications
- IC_{50}

Information in BRENDA #II

Physicochemical parameters

- pI value
- pH and temperature optimum
- pH and temperature range
- Crystallization & 3D structure (PDB link)
- Stability concerning temperature, organic solvents, oxidation and storage
- Molecular weight & subunits

Genetic parameters

- Engineering
- Sequence
- Cloning

Information in BRENDA #III

Additional enzyme information concerning:

- Organism: organisms, from which the enzyme was extracted
- Source tissue: enzyme allocation within various tissues
- Localization: intracellular enzyme distribution
- Disease: enzyme association with disease patterns
- Application: enzyme usage for industrial purposes
- References: list of publications, including data from investigations of the certain enzyme

The different search types on *BRENDA*

OR:

How can you find information on
BRENDA?

Options for Enzyme categorization

Classification mode:

- Enzyme Name or Recommended Name: accepted enzyme name in the literature
- Systematic Name: provides a more chemically based name, dependent on the reactants of the catalyzed reaction
- Synonyms: other names and abbreviations used for the enzyme in literature
- EC Number: enzyme classification according to the EC system

example:

- Pyruvate decarboxylase
- 2-oxo-acid carboxy-lyase
- PDC, alpha-Keto acid carboxy-lase, alpha-Carboxylase ...
- 4.1.1.1

SEARCH-Navigator

close all open all

- Nomenclature
- Reaction & Specificity
- Functional Parameters
- Organism related Information
- Enzyme Structure
- Isolation & Preparation
- Stability
- Disease & References
- Application & Engineering

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Display entries

Latest BRENDA update: June 2008

Nomenclature	Reaction & Specificity	Functional Parameters
Enzyme Names EC Number Common/ Recommended Name Systematic Name Synonyms	Pathway Catalysed Reaction Reaction Type Natural Substrates and Products Substrates and Products	Km Value Ki Value IC50 Value pI Value Turnover Number
Purification Cloned Renatured Crystallization	Cofactors Metals/Ions Activating Compounds Ligands	Organism-related information Organism Source Tissue Localization Protein-Specific Search
Stability pH Stability Temperature Stability General Stability Organic Solvent Stability Oxidation Stability Storage Stability	Enzyme Structure Sequence/ SwissProt link 3D-Structure/ PDB link Molecular Weight Subunits Posttranslational Modification	Disease & References Disease References Application & Engineering Engineering Application

Here you can start different modes of search, depending on the information you need.

Webmaster: **Maurice Scheer**
 m.scheer@tu-bs.de

For access to all features of the website Javascript must be activated, frames enabled and Java (at least version 1.4) has to be installed

 Quick search

[EC-Number](#) | [Enzyme Name](#) | [Organism](#) | [Protein](#) | [Full text](#) | [Advanced Search](#)

Search Display **10** entries

10
 50
 100

Latest BRENDA update 12/2007

Here you can choose between the different search fields.

Enter your query text.

Select the amount of hits to be displayed.

Nomenclature	Reaction & Specificity	Functional Parameters
Enzyme Name EC Number Common/ Recommended Name Systematic Name Synonyms CAS Register	Pathway Catalysed Reaction Reaction Type Natural Substrates and Products Artificial Substrates and Products Natural Substrate Products	Km Value Ki Value pI Value Turnover Number Specific Activity pH Optimum pH Range Temperature Optimum Temperature Range
Isolation & Preparation	Inhibitors Cofactors Metals/Ions Activating Compounds Ligands	Organism-related information
Purification Cloned Renatured Crystallization		Organism Source Tissue Localization Protein-Specific Search
Stability	Enzyme Structure	Disease & References
pH Stability Temperature Stability General Stability Organic Solvent Stability Oxidation Stability Storage Stability	Sequence/ SwissProt link 3D-Structure/ PDB link Molecular Weight Subunits Posttranslational Modification	Disease References
		Application & Engineering
		Engineering Application

[EC-Number](#) | [Enzyme Name](#) | [Organism](#) | [Protein](#) | [Full text](#) | [Advanced Search](#)

Search Display **10** entries

10
 50
 100

Latest BRENDA update 12/2007

Nomenclature	Reaction & Specificity	Functional Parameters
Enzyme Names EC Number Common/ Recommended Name Systematic Name Synonyms CAS Registry Number	Pathway Catalysed Reaction Reaction Type Natural Substrates and Products Substrates and Products Substrates Natural Substrate Products Natural Product	Km Value Ki Value pl Value Turnover Number Specific Activity pH Optimum pH Range Temperature Optimum Temperature Range
Isolation & Preparation	Inhibitors Cofactors Metals/Ions Activating Compounds Ligands	Organism-related information
Purification Cloned Renatured Crystallization		Organism Source Tissue Localization Protein-Specific Search
Stability	Enzyme Structure	Disease & References
pH Stability Temperature Stability General Stability Organic Solvent Stability Oxidation Stability Storage Stability	Sequence/ SwissProt link 3D-Structure/ PDB link Molecular Weight Subunits Posttranslational Modification	Disease References
		Application & Engineering
		Engineering Application

You can also select one of the 52 search fields, which reflect all data fields of the database.

Enzyme Database - BRENDA - Mozilla Firefox

File Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe

http://www.brenda-enzymes.info/index.php4

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BRENDA
The Comprehensive Enzyme Information System

TU Braunschweig
Dept. of Bioinformatics

SEARCH-Navigator

close all open all

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EC-Number Enzyme Name Organism Protein Full text Advanced Search

Search Display 10 entries

SEARCH-Navigator

close all open all

Nomenclature

Reaction & Specificity

Functional Parameters

- KM Value
- Ki Value
- pI Value
- Turnover Number
- Specific Activity
- pH Optimum
- pH Range
- Temperature Optimum
- Temperature Range

Organism related Information

Enzyme Structure

Isolation & Preparation

Stability

Disease & References

Application & Engineering

...or you use the Search-Navigator on the left tool bar to choose one of the 52 search fields that are arranged in the nine topical subgroups.

http://www.brenda-enzymes.info/nav_main.php4?nav=,,1,,,,,

Start Enzyme Database - B... Tutorial BRENDA info - Open... DE 16:47

[EC-Number](#) | [Enzyme Name](#) | [Organism](#) | [Protein](#) | [Full text](#) | [Advanced Search](#)

Search Display **10** entries

10
 50
 100

Latest BRENDA update 12/2007

Nomenclature	Reaction & Specificity	Functional Parameters
Enzyme Names EC Number Common/ Recommended Name Systematic Name Synonyms CAS Registry Number	Pathway Catalysed Reaction Reaction Type Natural Substrates and Products Substrates and Products Substrates Natural Substrate Products Natural Product	Km Value Vmax Value pH Optimum Specific Activity pH Range Temperature Optimum Temperature Range
Isolation & Preparation	Inhibitors Cofactors Metals/Ions Activating Compounds Ligands	Organism-related information
Purification Cloned Renatured Crystallization		Organism Source Tissue Localization Protein-Specific Search
Stability	Enzyme Structure	Disease & References
pH Stability Temperature Stability General Stability Organic Solvent Stability Oxidation Stability Storage Stability	Sequence/ SwissProt link 3D-Structure/ PDB link Molecular Weight Subunits Posttranslational Modification	Disease References
		Application & Engineering
		Engineering Application

Frequently you will only type the enzyme name and start "search"

SEARCH-Navigator

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Any question? -> Use the BRENDA Discussion groups

Search Enzyme Names (Synonyms)

Pyruvate Decarboxylase contains Search show 10 results clear

Recommended Name: exact

EC Number: exact

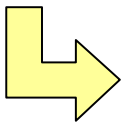
= amino acid sequences = comprehensive online version = show the catalyzed reaction

Results 1 - 10 of 11



download this result as tab stop separated values (Excel, OpenOffice) format

EC Number	Recommended Name	Synonyms
1.2.4.1	pyruvate dehydrogenase (acetyl-transferring)	pyruvate decarboxylase
4.1.1.1	Pyruvate decarboxylase	Pyruvate decarboxylase
4.1.1.40	Hydroxypyruvate decarboxylase	Hydroxypyruvate decarboxylase
4.1.1.43	Phenylpyruvate decarboxylase	Phenylpyruvate decarboxylase
4.1.1.74	Indolepyruvate decarboxylase	Indole-3-pyruvate decarboxylase
4.1.1.74	Indolepyruvate decarboxylase	Indolepyruvate decarboxylase
4.1.1.74	Indolepyruvate decarboxylase	Indolepyruvate decarboxylase (Enterobacter herbocola strain 299R clone pMB2 gene ipdC reduced)
4.1.1.79	sulfopyruvate decarboxylase	sulfopyruvate decarboxylase
4.1.1.80	4-hydroxyphenylpyruvate decarboxylase	4-hydroxyphenylpyruvate decarboxylase
4.1.1.80	4-hydroxyphenylpyruvate decarboxylase	p-hydroxyphenylpyruvate decarboxylase

 You receive the query results with all enzymes, which include the names you previously entered.

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Search Enzyme Names (Synonyms)

Pyruvate Decarboxylase contains Search show 10 results clear

Recommended Name: exact

EC Number: exact

= amino acid sequences = comprehensive online version = show the catalyzed reaction

Results 1 - 10 of 11



download this result as tab stop separated values (Excel, OpenOffice) format

EC Number	Recommended Name	Synonyms
1.2.4.1	pyruvate dehydrogenase (acetyl-transferring)	pyruvate decarboxylase
4.1.1.1	Pyruvate decarboxylase	Pyruvate decarboxylase
4.1.1.40	Hydroxypyruvate decarboxylase	Hydroxypyruvate decarboxylase
4.1.1.43	Phenylpyruvate decarboxylase	Phenylpyruvate decarboxylase
4.1.1.74	Indolepyruvate decarboxylase	Indole-3-pyruvate decarboxylase
4.1.1.74	Indolepyruvate decarboxylase	Indolepyruvate decarboxylase
4.1.1.74	Indolepyruvate decarboxylase (Enterobacter herbicola strain 299R clone pMB2 gene ipdC reduced)	Indolepyruvate decarboxylase (Enterobacter herbicola strain 299R clone pMB2 gene ipdC reduced)
4.1.1.79	sulfopyruvate decarboxylase	sulfopyruvate decarboxylase
4.1.1.80	4-hydroxyphenylpyruvate decarboxylase	4-hydroxyphenylpyruvate decarboxylase
4.1.1.80	4-hydroxyphenylpyruvate decarboxylase	4-hydroxyphenylpyruvate decarboxylase

You choose the enzyme of interest to get a comprehensive view of its dataset

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Fulltext search

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http://www.brenda-enzymes.info/

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Fulltext Search

Enter your searchterm (use **AND, OR, AND NOT** for simple Boolean queries)

alpha-D-Glucose contains Search

Search in the complete database

or search only in these fields

(hold the ctrl-key to select more than one field)

- Activating Compound
- Application
- CAS Registry Number
- Cloned(Commentary)
- Cofactor

Select categories you are interested in.

If you are not sure where to find the requested information, you may perform a fulltext search. This option searches the complete database.

SEARCH-Navigator

- close all open all
- Nomenclature
- Reaction & Specificity
- Functional Parameters
- Organism related Information
- Enzyme Structure
- Isolation & Preparation
- Stability
- Disease & References
- Application & Engineering

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alpha-D-Glucose contains Search

Search in the complete database

or search only in these fields

- Activating Compound
- Application
- CAS Registry Number
- Cloned(Commentary)
- Cofactor

(hold the ctrl-key to select more than one field)

25	hits in field Activating Compound
2	hits in field Application
2	hits in field Crystallization (Commentary)
2	hits in field Disease
9	hits in field Engineering
18	hits in field Enzyme Names (Synonyms)
2	hits in field General Stability
20	hits in field Inhibitors
8	hits in field Ki Value [mM]
152	hits in field KM Value [mM]
33	hits in field Natural Product
13	hits in field Natural Substrate
445	hits in field Natural Substrates/ Products (Substrates)
1	hits in field pH Optimum
2	hits in field Posttranslational Modification
199	hits in field Product
135	hits in field Reaction
30	hits in field Reference by Title
1	hits in field Specific Activity [micromol/min/mg]
1	hits in field Storage Stability
164	hits in field Substrate
2147	hits in field Substrates and Products (Substrate)
5	hits in field Synonyms

The results are grouped by the previously selected categories.



Advanced search

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- All enzymes



- SEARCH-Navigator**
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Advanced Search

SEARCH Clear all fields

Organism synonyms, domain, kingdom, phylum, class or order
 exact (e.g. eukarya, animals, chordata or primates)

EC Number: exact (use * as a wildcard)

Organism: exact (1.use * as a wildcard, 2. * in the beginning is very time consuming)

Enzyme Name: exact (very time consuming)

Search in text fields
 1 Choose a subitem exact
 + add another search field

Search in numeric fields
 1 Choose a subitem =
 + add another search field

Search tip:
 If you search a value between two limits write 'min-max' and choose between. Whereby min is the minimum value and max the maximum value.

Cloned
 Crystallized
 Engineering
 Purified
 Renatured
 PDB entry

Application: Nothing selected

Cofactor: Nothing selected

Localization: Nothing selected

Metals / Ions:



Advanced Search

SEARCH Clear all fields

Organism synonyms, domain, kingdom, phylum, class or order
exact (e.g. eukarya, animals, chordata or primates)

EC Number: exact 4.1.1.1 (use * as a wildcard)

Organism: exact Saccharomyces cerevisiae 1.use * as a wildcard
2. * in the beginning is very time consuming

Enzyme Name: exact

Search in text fields
1 Choose a subitem exact
+ add another search field

Search in numeric fields
1 Choose a subitem =
+ add another search field

Search tip:
If you search a value between two limits write 'min-max' and choose between.
Whereby min is the minimum value and max the maximum value.

Cloned
 Crystallized
 Engineering
 Purified
 Renatured
 PDB entry

Application:
Nothing selected

Cofactor:
Nothing selected

Localization:
Nothing selected

Metals / Ions:
Nothing selected

Organic Solvent Stability against:
Nothing selected

Source Tissue:
Nothing selected

Subunits:
Nothing selected

Posttranslational Modification
Nothing selected

SEARCH Clear all fields

The advanced search offers you the widest range of options to find specific information you need from the 52 data fields:

- in a combined search, e.g. via organism and EC-Number, you find scientific data much faster
- in addition you can search in text and numeric fields
- furthermore you can limit the request to your requirements (Cofactor, Subunits, Localization...)
- finally all selected datafields will be combined to an "AND"- query

SEARCH-Navigator

close all open all

- Nomenclature
- Reaction & Specificity
- Functional Parameters
- Organism related Information
- Enzyme Structure
- Isolation & Preparation
- Stability
- Disease & References
- Application & Engineering

Advanced Search results

Results 1 - 1 of 1

1. **Pyruvate decarboxylase** from *Saccharomyces cerevisiae*
(→ EC Number: 4.1.1.1)

Link to enzyme information.

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EC Explorer

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Genome Explorer

Ontology Explorer

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●Organism

Primary Accession No. (UniProt) Commentary Reference Textmining

●Cloned(Commentary)

Commentary	Reference
expression in Escherichia coli BL21(DE3)	650152
expression of W412F and W412A mutant PDC in Escherichia coli BL21(DE3)	649851
expression of wild-type, E91A, E91D and E91Q mutant PDC in Escherichia coli BL21(DE3)	649910
overexpression of wild-type and mutant YPDC in Escherichia coli BL21	650079

●Crystallization (Commentary)

Crystallization	Reference
-	114294 , 649851 , 650577
PDC complex with pyruvamide	651089
X-ray crystallography structure	651094

You get an information sheet with reference-specific data

●Purification (Commentary)

Commentary	Reference
-	114288 , 114301 , 650080 , 651089 , 651094
2 isoenzymes: I and II	114284
recombinant homomeric, alpha-only, PDC1	650577
W412F and W412A mutant PDC, expressed in Escherichia coli, W412A is purified as apoenzyme	649851
wild-type and D28A, D28N, E477Q mutant YPDC	650161
wild-type PDC and C221A/C222A double mutant	650049
wild-type, C221E/C222A and C221A/C222A double mutant YPDC	650152



Substructure search


--> Allows you to gain access to a large number of enzymic ligands.

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 **Substructure search**

i In order for the substructure search to work properly, you might need to enable cookies in your browser!

Search your structure in more than 50 000 biochemical substances. Sketch the molecule you want to search for. To search for a structure which you only know by name, you can search for this **ligand** first in BRENDA and perform a subsequent substructure search.

CLR DEL D-R +/- UDD JME

C

N

O

S

F

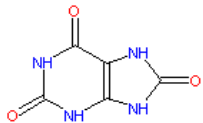
Cl

Br

I

P

X



Restrict the substructure search to:

- Substrates
- Products
- Cofactors
- Activating Compounds
- Inhibitors

Select the max-searchtime:

JME Editor courtesy of Peter Ertl, Novartis JME help

Here you can draw your molecule of interest...

...and here you are able to refine your search and to define the maximal search time.

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Substructure search

Edit your searchstructure:

☺ CLR DEL D-R +/- UDO

← = ≡ ~ △ □ ◊ ○

C

N

O

S

F

Cl

Br

I

P

X

JME Molecular Editor®, Novartis Pharma AG

Restrict the substructure search to:

- Substrates (S)
- Products (P)
- Cofactors (C)
- Activating Compounds (A)
- Inhibitors (I)

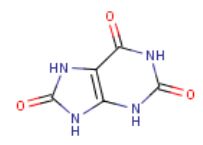
Select the max-searchtime: 5 s

Start substructure search

JME Editor courtesy of P. Ertl, Novartis JME help

Number of hits: 6

1. Uric acid, Urate
Role : S / P / I / A



start BRENDA search

2. 7-Methyluric acid
Role : I



start BRENDA search

You get all molecules with the desired structural elements and their course of action (S - Substrate, P - Product, A - Activator, I - Inhibitor, C - Cofactor)

You can also edit your structure and start a new query.

Enzyme Database - BRENDA - Mozilla Firefox

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http://134.169.106.62/index.php4

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Any question? -> Use the BRENDA Discussion groups

Search Ligands

Uric acid exact Search show 10 results clear

Don't show organism specific information (fast!)
 Search organism in taxonomic tree (slow, e.g. "mammalia" for rat,human,monkey,...)
 (Not possible to combine with the first option)

Recommended Name: contains
 EC Number: contains
 Role: contains
 Organism: contains
 Image of 2D Structure
 Search for synonyms (with exact matching searchword)

The synonyms for 'Uric acid' are:
 Urate, Uric acid
 ⓘ = amino acid sequences ⓘ = comprehensive online version ⓘ = show the catalyzed reaction

Results 1 - 10 of 33

EC Number	Recommended Name	Role	Ligand	Structure
1.2.3.11	retinal oxidase	Natural Product	urate	
1.2.3.11	retinal oxidase	Product	urate	
1.7.3.3	urate oxidase	Inhibitor	Urate	
1.7.3.3	urate oxidase	KM Value	Urate	
1.7.3.3	urate oxidase	Natural Substrate	urate	
1.7.3.3	urate oxidase	Substrate	urate	
1.7.3.3	urate oxidase	Turnover Number	Urate	
1.7.3.3	urate oxidase	Reaction	urate	

Fertig

Start Enzyme Database - B... LEO Ergebnisse für "h... BRENDA Info - Open... Unbenannt - Paint DE 13:32

And with "start BRENDA search" you obtain all enzymes which are linked to the selected compound.

Ideas for *BRENDA's*
improvement welcome !!!