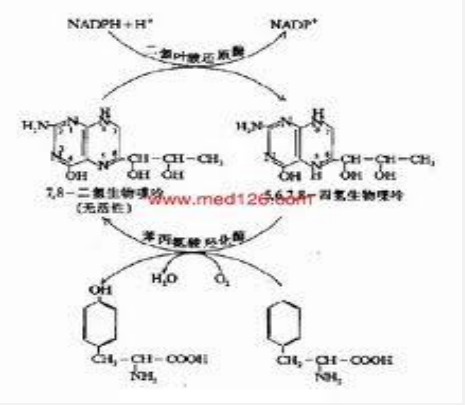
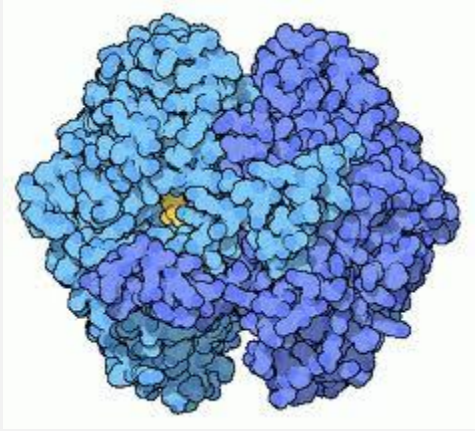
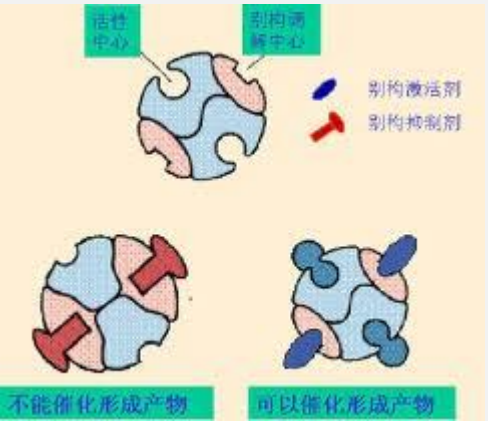


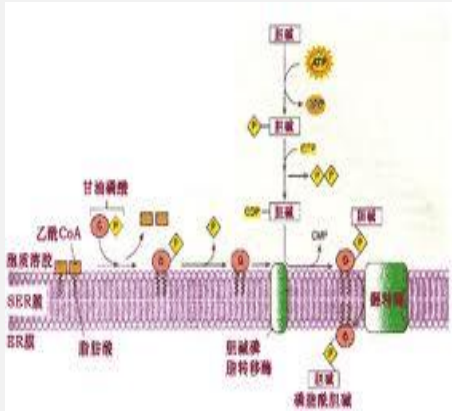


BRENDA

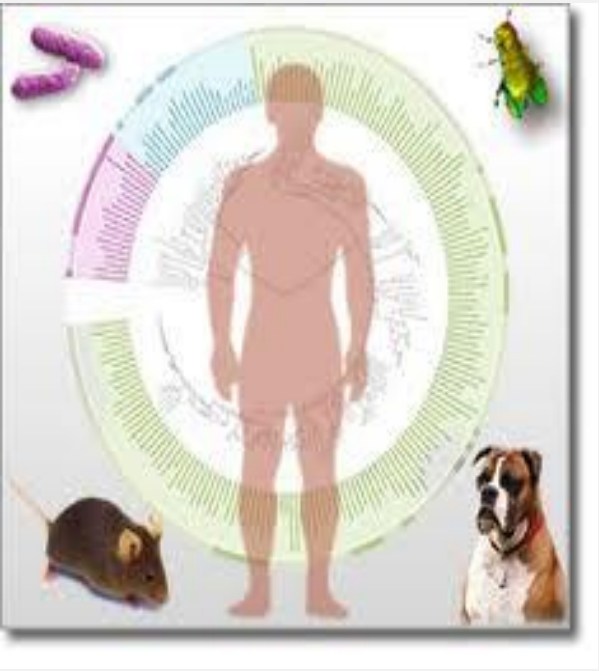
The Comprehensive Enzyme Information System



Reporter : Wang Cheng

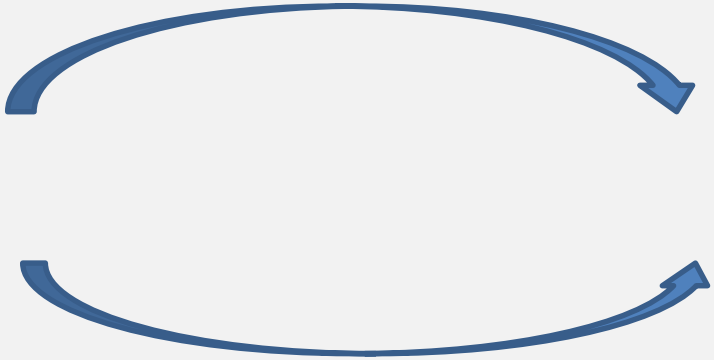


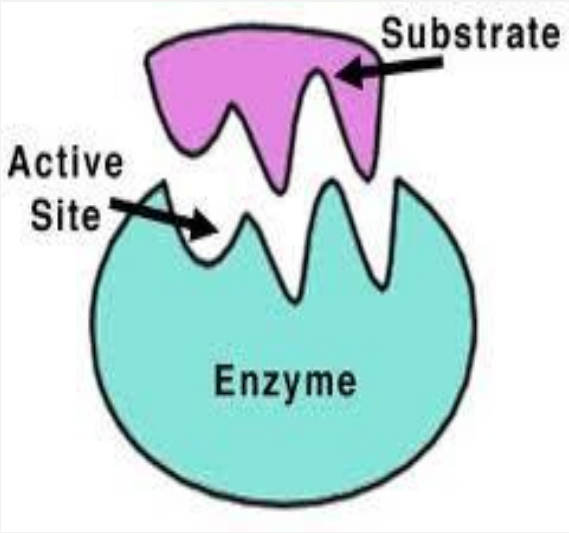
The background



huge sequence databases

a great amount of public attention





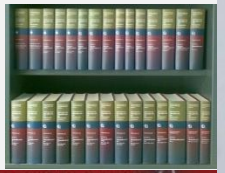
we are very limited in our ability to access **functional data** for the gene products – the proteins, **in particular for enzymes**

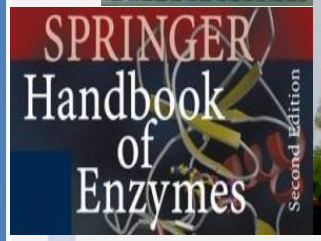
Compilation of Data

So we need a systematic collection

Project History

originally published as a series of books





started in 1987 at the German National Research Centre for Biotechnology in Braunschweig(GBF)

here BRENDA was further curated and transformed into a publicly available database

University of Cologne (1996)

MySQL DevConnect Member

continuous curation, technical improvement and further development

Technical University of Braunschweig (2007)

The BRENDA Enzyme Information System

- developed and maintained at Technische University Braunschweig, Germany
  Department of Bioinformatics and Biochemistry

Director of the department and
founder of BRENDA:
Prof. Dietmar Schomburg

Acknowledgements

- Financial support：

  FELICS & SLING & BMBF

- Team：

Dietmar Schomburg (Supervision)	
Ida Schomburg	Andreas Grote
Antje Chang	Carola Songen
Michael Rother	Cornelia Munaretto
Juliane Thiele	Maurice Scheer
... the external annotators	

Availability

- Web interface & SOAP interface : freely accessible
  Flat file: free download after registration on web site
- To obtain a *software package that enables a **local installation of BRENDA*** databases and query engine:

academic/non-profit institutions → Please contact

enzymeta GmbH

http://www.enzymeta.de

Companies/for-profit institutions → BIOBASE BIOLOGICAL DATABASES

http://www.biobase-international.com

Scope and content

Most comprehensive information systems on

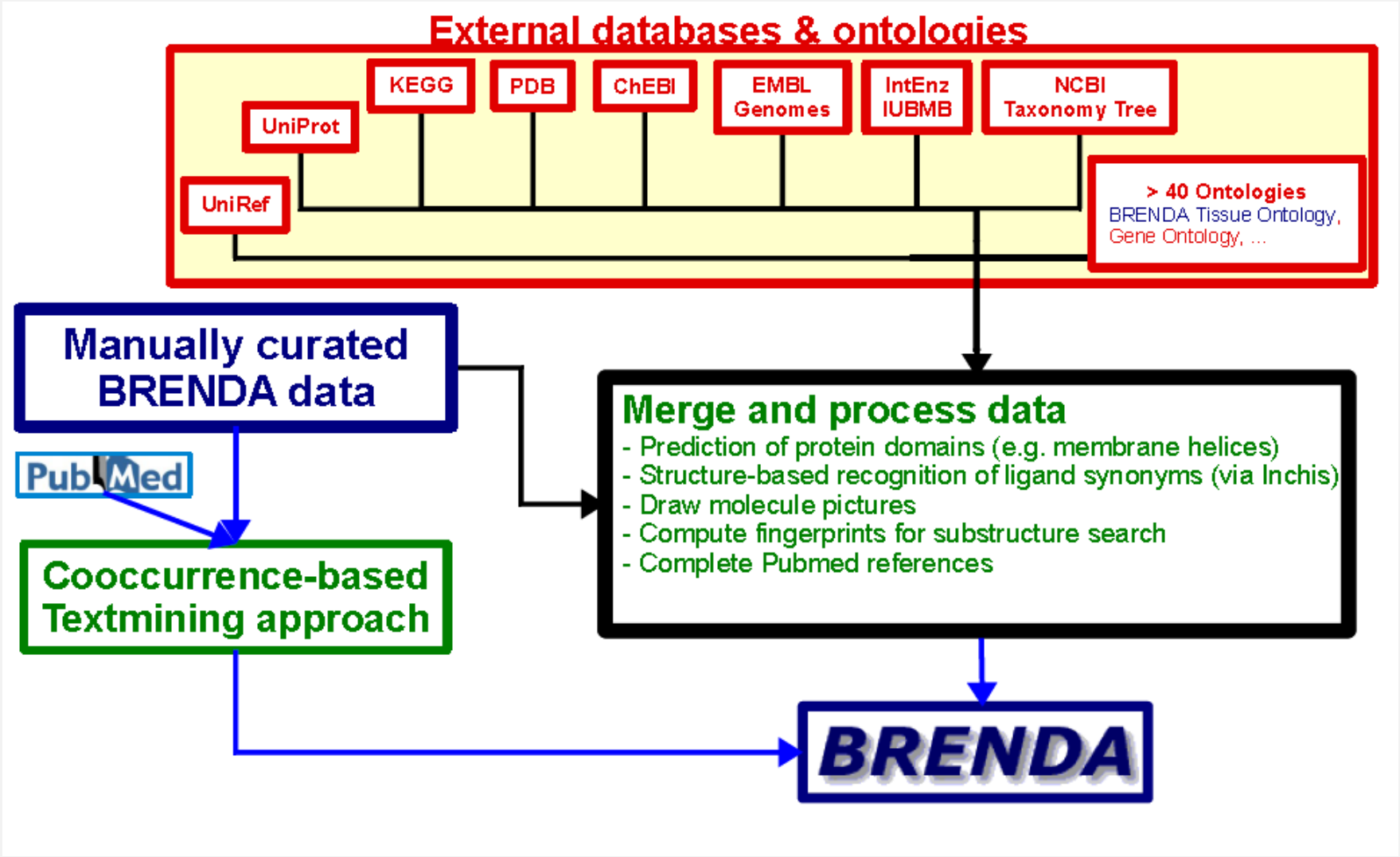
- **Enzymes** ⇒ > 500,000 different enzymes
  > 50,000 manually curated ones
  4,900 EC numbers

- **Enzyme ligand data**

e.g. → catalyzed reactions → substrates, products, cofactors

→ enzyme ligands → activators, inhibitors

Data sources

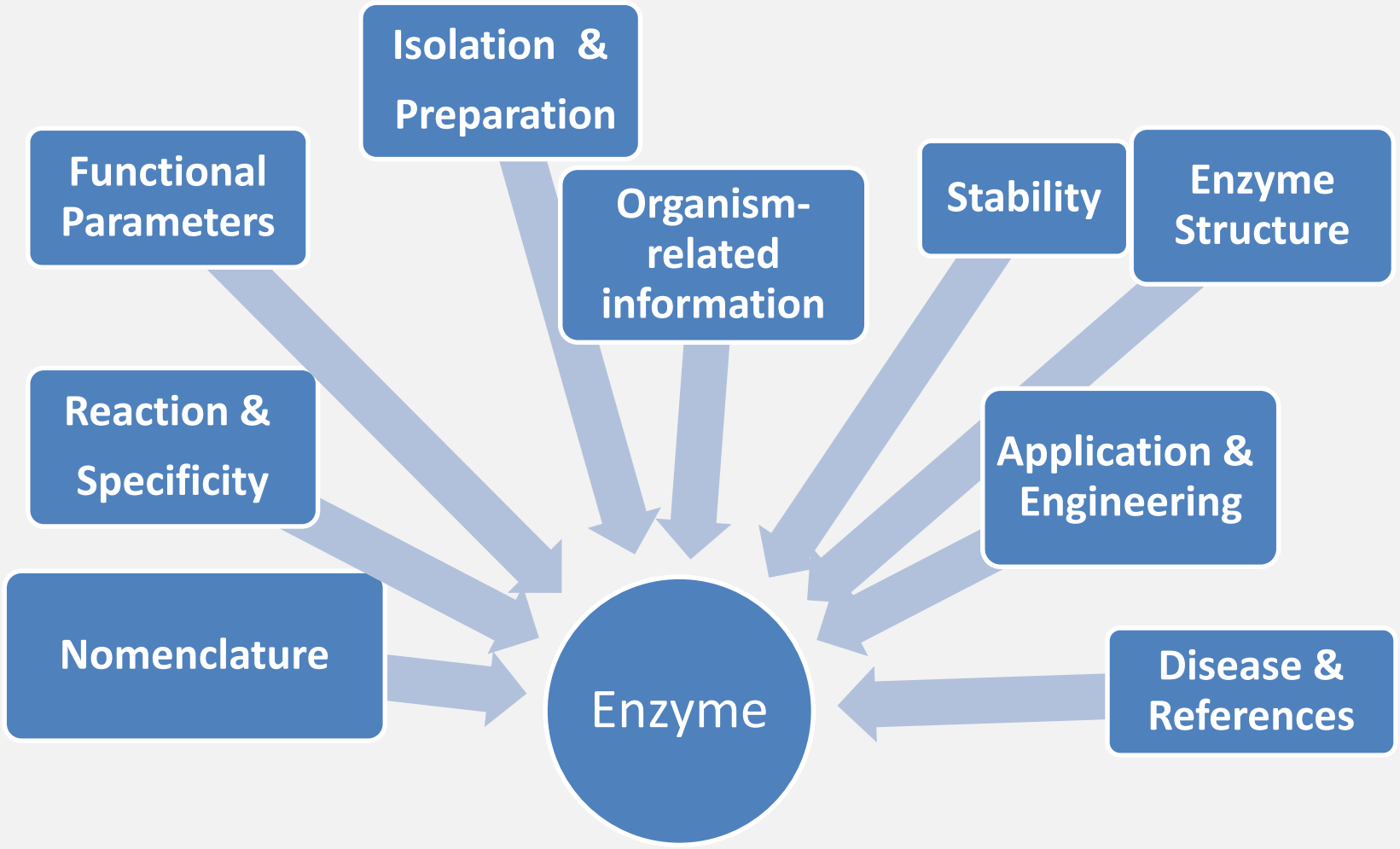


Introduction

- 【URL】:http://www.brenda-enzymes.org/
- 【分类依据】： the Enzyme Commission list of enzymes
- 【更新的频率】： **Half-yearly** update to assemble latest information extracted from primary literature (January and July)
- Information comprises not only kinetical, structural, stability and genome properties but also methods to isolate and analyze the enzyme

PS1:we need to go to the primary literature for more detailed information
PS2: B-enzymes, eg 3.2.1.B(about 200 EC classes)

Information in BRENDA



How can you find information on BRENDA?

Options for Enzyme categorization

Enzyme Name or Recommended Name	• Pyruvate decarboxylase
Systematic Name	• 2-oxo-acid carboxy-lyase
Synonyms	• PDC, alpha-Keto acid carboxylase, alpha-Carboxylase ...
EC Number	• 4.1.1.1

BRENDA

The Comprehensive Enzyme Information System

TU Braunschweig Dept. of Bioinformatics

EC-Number | Enzyme Name | Organism | Protein | Full text | Advanced Search

Search Display 10 entries

Meet Braunschweig Enzyme Database (BRENDA) at GCB 2010 in Braunschweig

How to cite BRENDA?

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 Inhibitors Cofactors Metals/Ions Activating Compounds Ligands Ligand Views NEW	Km Value Ki Value IC50 Value pI Value Turnover Number Specific Activity pH Optimum pH Range Temperature Optimum Temperature Range
Isolation & Preparation		**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	Sequence/ SwissProt link 3D-Structure/ PDB link Molecular Weight Subunits	Disease/ Diagnostics References
		Application & Engineering

最常用的搜索方式


BRENDA
The Comprehensive Enzyme Information System
EC-Number
Enzyme Name
Organism
Protein
Full text
Advanced Search
Search
Display 10 entries
Meet Braunschweig Enzyme Database (BRENDA) at GCB 2010 in Braunschweig
How to cite BRENDA?
Nomenclature
Enzyme Names
EC Number
Common/ Recommended Name
Systematic Name
Synonyms
CAS Registry Number
Isolation & Preparation
Purification
Cloned
Renatured
Crystallization
Stability
pH Stability
Temperature Stability
General Stability
Organic Solvent Stability
Oxidation Stability
Storage Stability
Reaction & Specificity
Pathway
Catalysed Reaction
Reaction Type
Natural Substrates and Products
Substrates and Products
Substrates
Natural Substrate
Products
Natural Product
Inhibitors
Cofactors
Metals/Ions
Activating Compounds
Ligands
Ligand Views NEW
Enzyme Structure
Sequence/ SwissProt link
3D-Structure/ PDB link
Molecular Weight
Subunits
Posttranslational Modification
Functional Parameters
Km Value
Ki Value
IC50 Value
pI Value
Turnover Number
Specific Activity
pH Optimum
pH Range
Temperature Optimum
Temperature Range
Organism-related information
Organism
Source Tissue
Localization
Protein-Specific Search
Disease & References
Disease/ Diagnostics
References
Application & Engineering
Engineering
Application

查询结果显示

Search Enzyme Names (Synonyms)

Pyruvate decarboxylase | contains | Search | show 10 results | clear

Recommended Name: | exact

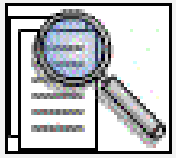
EC Number: | exact

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

Results **1** - **10** of **16**

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

EC Number	Recommended Name	Synonyms	Commentary
1.2.4.1	pyruvate dehydrogenase (acetyl-transferring)	pyruvate decarboxylase	-
4.1.1.1	Pyruvate decarboxylase	pyruvamide-activated yeast pyruvate decarboxylase	-
4.1.1.1	Pyruvate decarboxylase	pyruvate decarboxylase	-
4.1.1.1	Pyruvate decarboxylase	pyruvate decarboxylase 1	-
4.1.1.1	Pyruvate decarboxylase	yeast pyruvate decarboxylase	-
4.1.1.40	Hydroxypyruvate decarboxylase	Hydroxypyruvate decarboxylase	-
4.1.1.43	Phenylpyruvate decarboxylase	phenyl/indolepyruvate decarboxylase	-



Fulltext search

Fulltext Search

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

Pyruvate decarboxylase | contains | Search

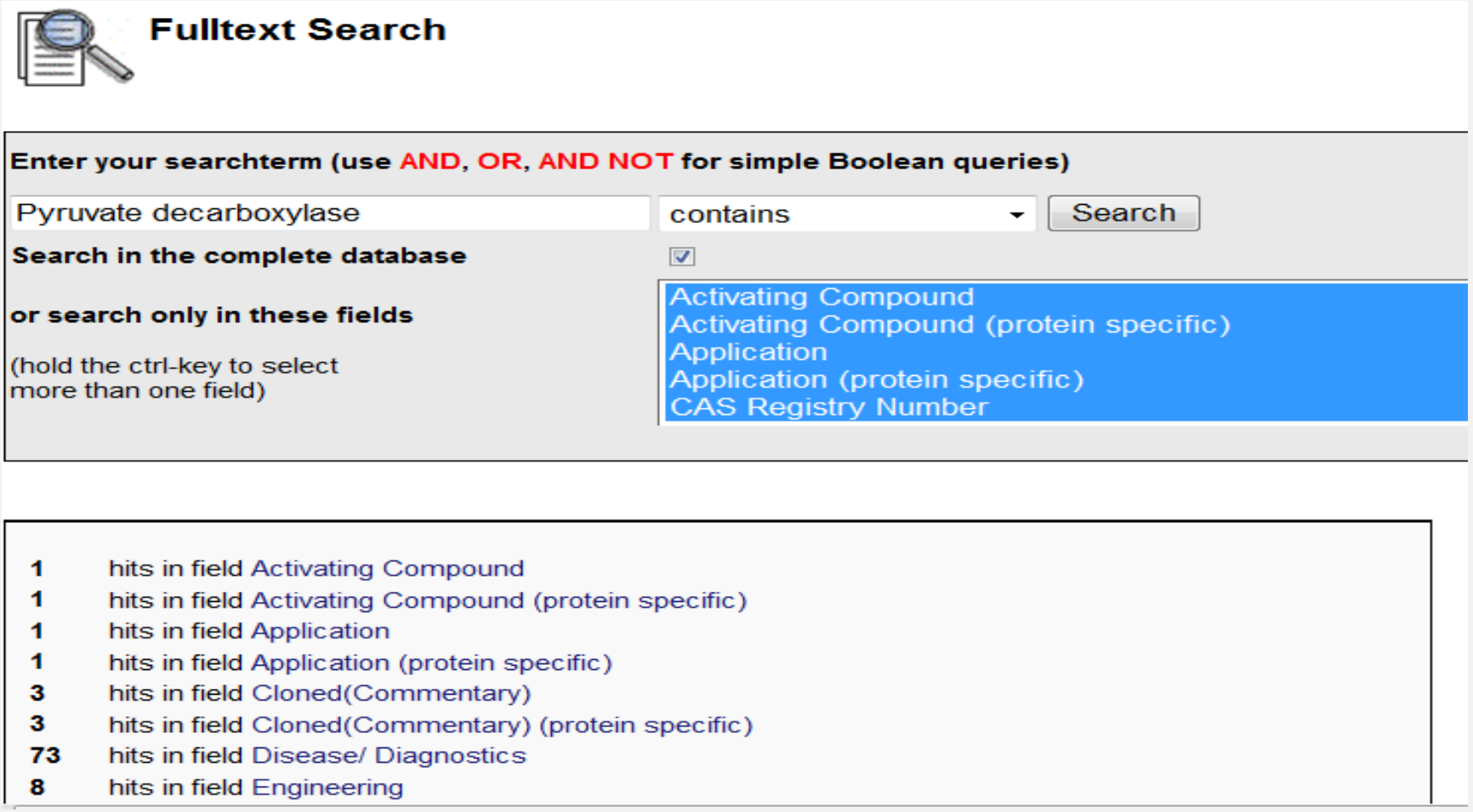
Search in the complete database ☑

or search only in these fields

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

- Activating Compound
- Activating Compound (protein specific)
- Application
- Application (protein specific)
- CAS Registry Number

查询结果


Fulltext Search
Enter your searchterm (use AND, OR, AND NOT for simple Boolean queries)
Pyruvate decarboxylase
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
Activating Compound (protein specific)
Application
Application (protein specific)
CAS Registry Number
1 hits in field Activating Compound
1 hits in field Activating Compound (protein specific)
1 hits in field Application
1 hits in field Application (protein specific)
3 hits in field Cloned(Commentary)
3 hits in field Cloned(Commentary) (protein specific)
73 hits in field Disease/ Diagnostics
8 hits in field Engineering

Advanced search

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

Enzyme Name: exact

1.use * as a wildcard
2. * in the beginning is very time consuming

Search in text fields

Choose a subitem | exact

add another search field

Search in numeric fields

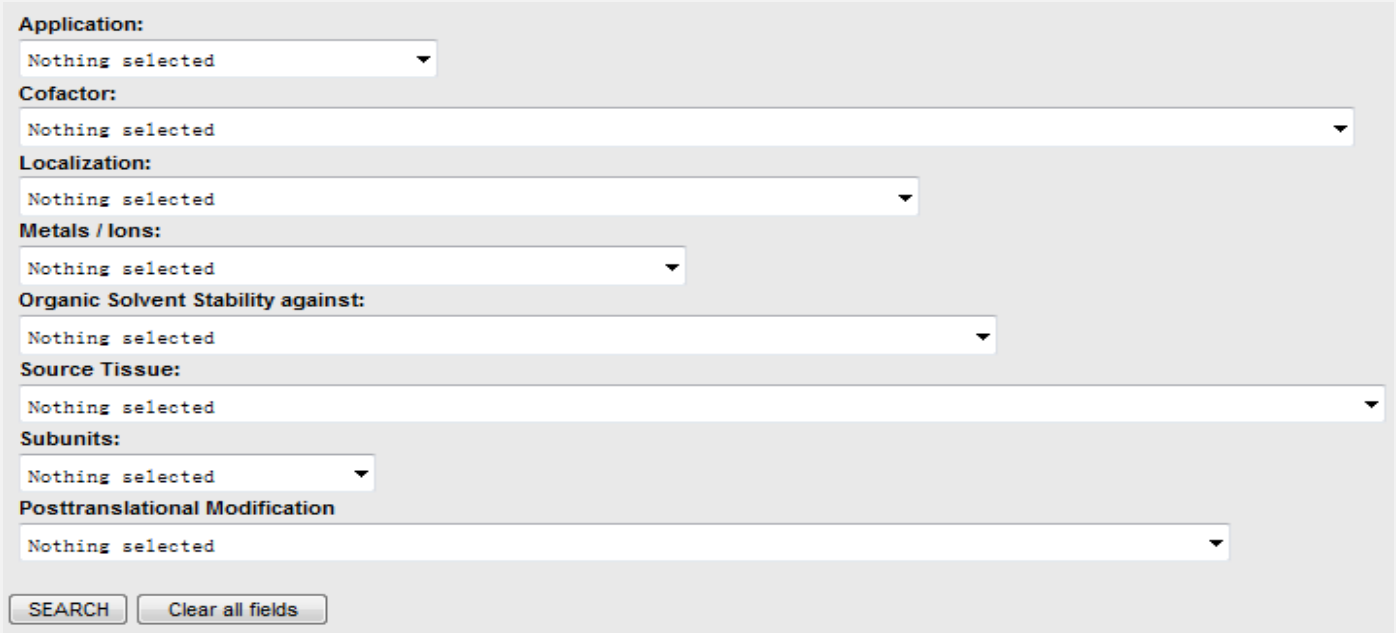
Choose a subitem | =

add another search field

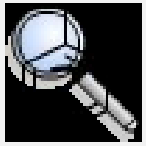
Search tip:

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



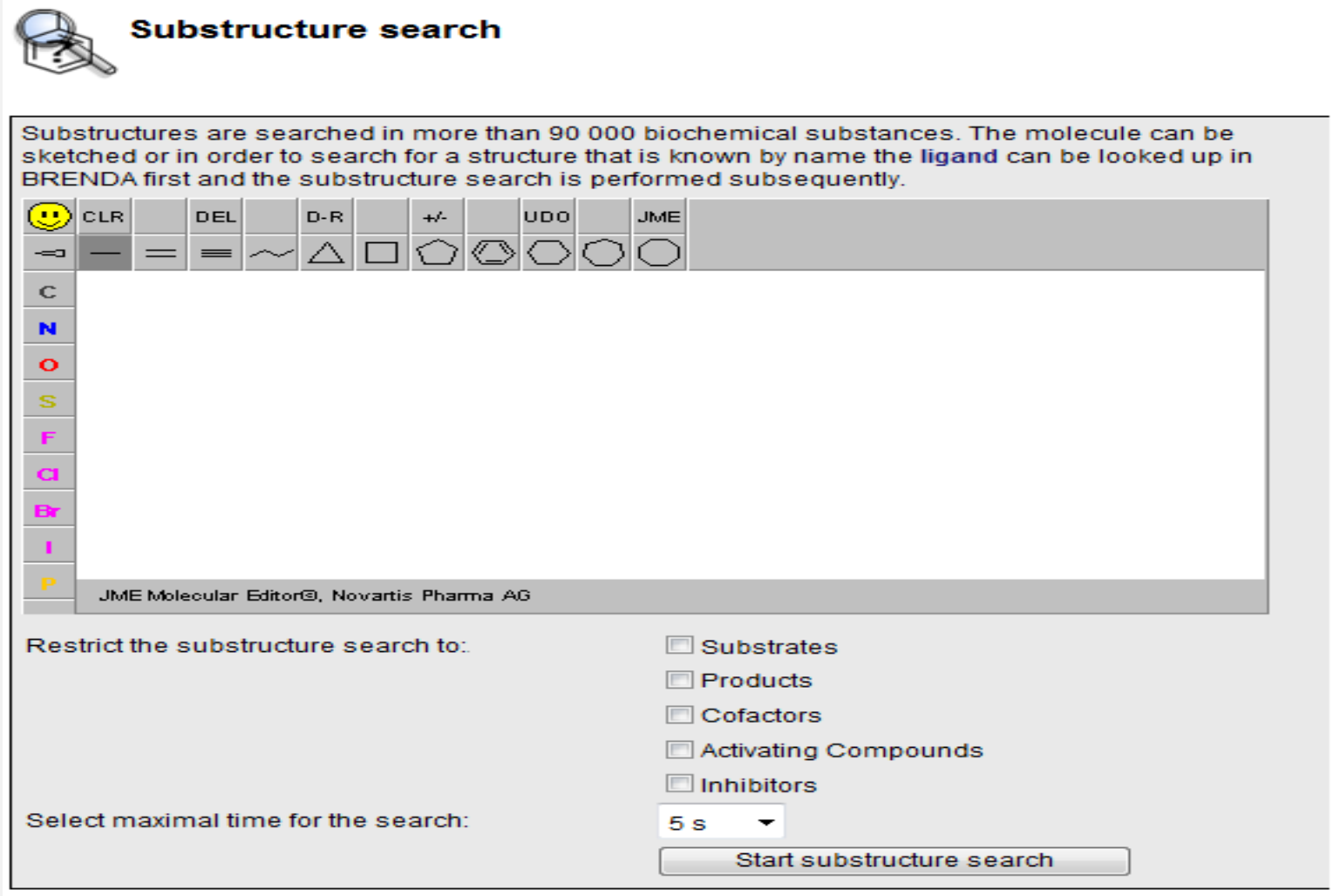
- in a combined search
- in addition you can search in text and numeric fields
- you can limit the request to your requirements (Cofactor, Subunits, Localization...)
- finally all selected datafields will be combined to an "AND"-query



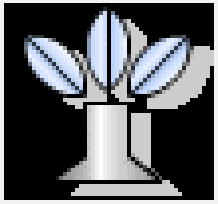
Substructure search

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

界面展示

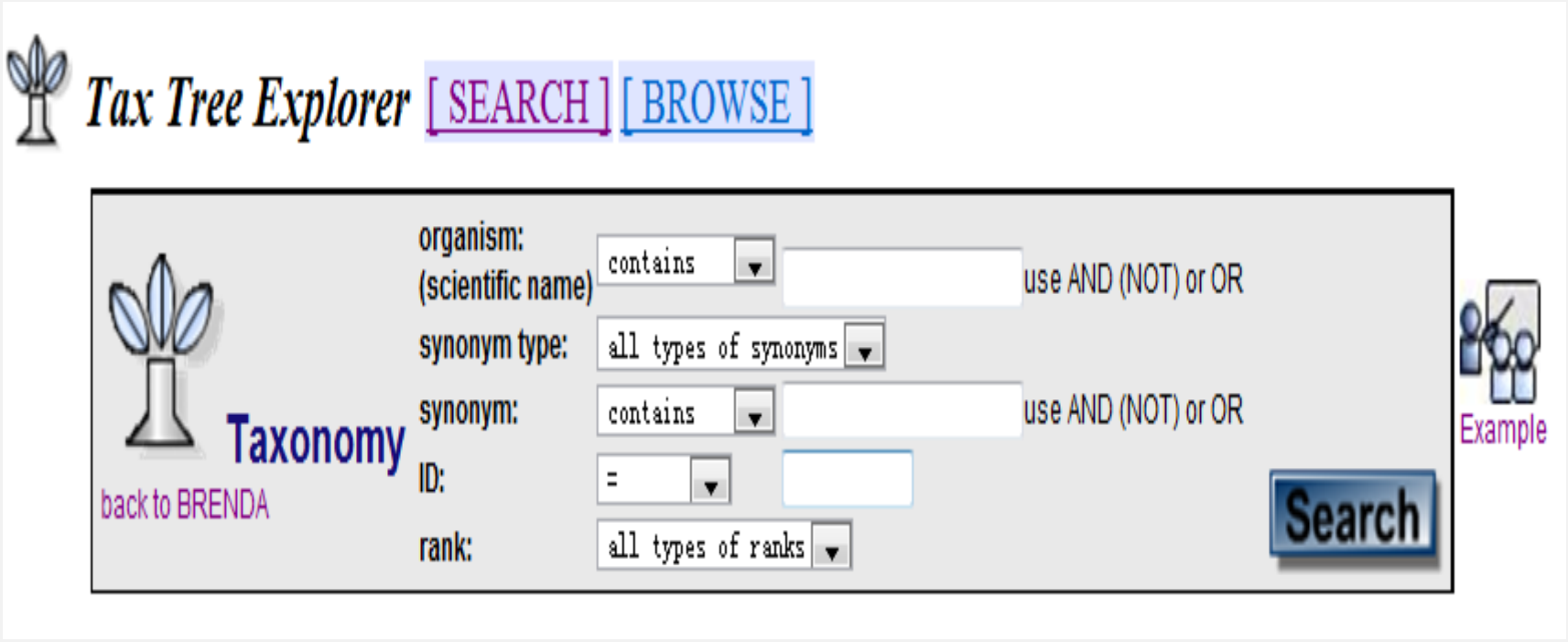

Substructure search
Substructures are searched in more than 90 000 biochemical substances. The molecule can be sketched or in order to search for a structure that is known by name the ligand can be looked up in BRENDA first and the substructure search is performed subsequently.
CLR
DEL
D-R
+/-
UDO
JME
C
N
O
S
F
Cl
Br
I
P
JME Molecular Editor©, Novartis Pharma AG
Restrict the substructure search to:
Substrates
Products
Cofactors
Activating Compounds
Inhibitors
Select maximal time for the search:
5 s
Start substructure search

Tax Tree Explorer
Taxonomy



Provides a template to search in the Taxonomy Tree database (NCBI) which contains the names of all organisms, that are represented in the genetic databases with at least one nucleotide or protein sequence.

界面展示


Tax Tree Explorer
[SEARCH]
[BROWSE]
Taxonomy
back to BRENDA
organism:
(scientific name)
contains
use AND (NOT) or OR
synonym type:
all types of synonyms
synonym:
contains
use AND (NOT) or OR
ID:
=
rank:
all types of ranks
Search
Example

Tax Tree Explorer [SEARCH] [BROWSE]

Taxonomy

back to BRENDA

organism: (scientific name) contains Methanobacteria use AND (NOT) or OR

synonym type: all types of synonyms

synonym: contains use AND (NOT) or OR

ID: =

rank: all types of ranks

Search

Example

Details

Methanobacteria

1523 aa sequences of Methanobacteria

NCBI Taxonomy ID

183925

Links to enzymes in BRENDA

Found 309 enzymes (distinct EC numbers) linked to this organism:

1.1.1.1 Show enzyme data

Synonyms

1. Archaeobacteria
2. Archaeobacteria Murray 1988
3. Methanobacteria Boone 2002

Condensed Tree View

- cellular organisms
  - Archaea (superkingdom)
    - Euryarchaeota (phylum)
      - Methanobacteria (class)

Results

27 different results found

1. Methanobacteria
2. Methanobacteriaceae
3. Methanobacteriaceae archaeon 12aF
4. Methanobacteriaceae archaeon 14aZ
5. Methanobacteriaceae archaeon 15aZ
6. Methanobacteriaceae archaeon 1aR
7. Methanobacteriaceae archaeon 1aZ

EC Explorer

Introduction to the EC-system

- based on the chemical reactions they catalyze
- EC numbers VS enzymes

EC numbers  enzymes

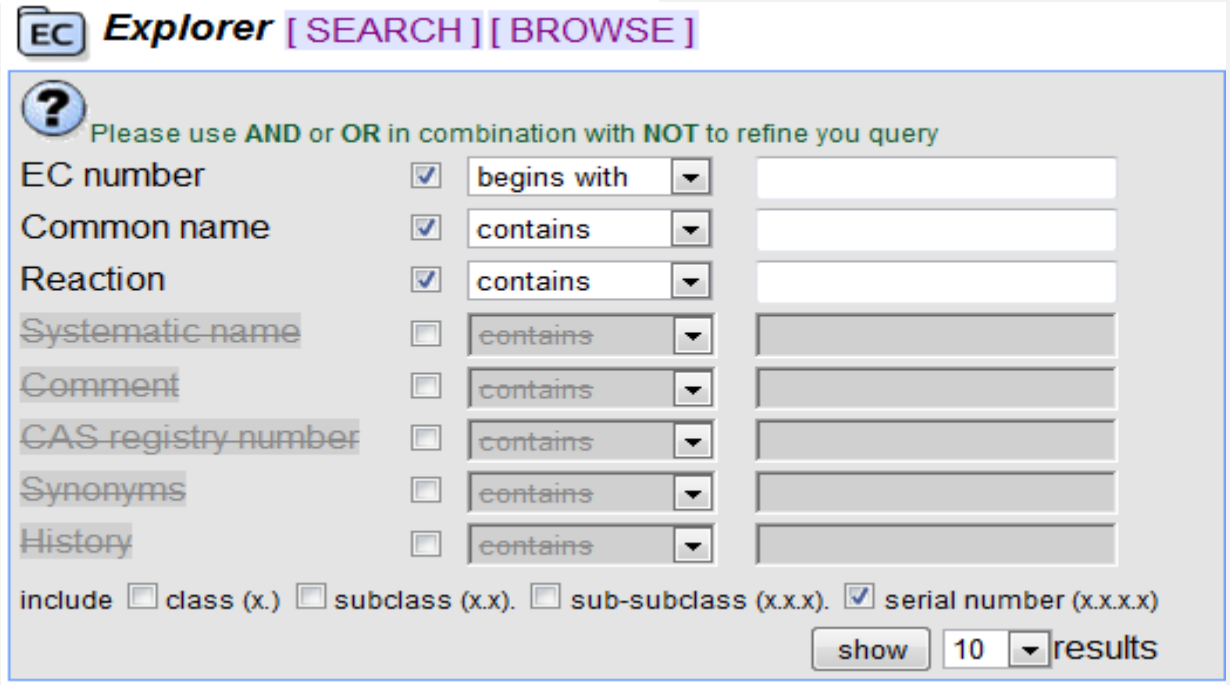
If different enzymes catalyze the same reaction, then they receive the same EC number

EC	1	2	3	4	5	6
classify	Oxidoreductases	Transferases	Hydrolases	Lyases	Isomerases	Ligases

界面展示

Browse界面

Search界面



Sequence Search

The Sequence Search is based on the Protein Knowledgebase(UniProt KB) www.uniprot.org

Sequence Search

Examples:	Example	Search
	sequences which contain "ikea"	start search
	sequences which begin with "mia"	start search
	sequences which end with "tkg"	start search
	1. sequences which contain "tkr" 2. followed by "mai" in a not defined distance	start search
	sequences with the consensus PROSITE pattern PDOC00952: GDA1/CD39 family of nucleoside phosphatases [LIVM]-x-G-x(2)-E-G-x-[FY]-x-[FW]-[LIVA]-[TAG]-x-N-[HY]	start search
	You have a DNA or RNA sequence and want to know if the translated sequence codes for an enzyme	start search

The database search is restricted to amino acid sequences of enzymes!

Amino acid Sequence

contains

No. of results: 10

Recommended name (of enzyme): contains

EC Number: contains

1st Accession Code (UniProt): contains

Organism: contains

Number of amino acids: =

Molecular weight [Da]: =

Transmembrane helices: = N-term inside outside

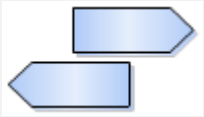
Source: SwissProt TREMBL

reset Search

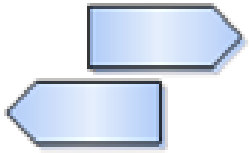
No.	EC Number	Recommended Name	1st Accession Code	Organism	No of Transm. helices	No aa	MW	Source	Tools/Links
1.	3.6.1.42	guanosine-diphosphatase	Q9UT35	Schizosaccharomyces pombe	1	556	61589	Swiss-Prot	
2.	3.6.1.5	apyrase	Q9USP2	Schizosaccharomyces pombe	1	572	64680	Swiss-Prot	

more than 3000
complete genomes, plasmids and
organelles for specific genes and
proteins

Genome Explorer



The Genome Explorer is a genome visualization tool for browsing and comparing **enzyme annotations** in full genomes. It closes the gap between **genomic and enzymatic data** and allows the alignment of genomes at a given enzyme-coding gene, thus allowing to **visually compare** the genomic environment of the gene in different organisms. The underlying genome database is compiled from EBI Genomes and ENSEMBL and supplemented by UniProt annotations.



Genome Explorer

Available genomes:

- *Archaea*
  - Acidianus ambivalens plasmid pDL10
  - Acidianus hospitalis strain W1 plasmid pAH1
  - Aciduliprofundum boonei T469
  - Aeropyrum pernix K1 DNA
  - Archaeoglobus fulgidus DSM 4304
  - Archaeoglobus profundus DSM 5631 plasmid pArcpr01
  - Archaeoglobus profundus DSM 5631

(Hold down CTRL or SHIFT to select multiple genomes)

Organism: exact [ ] Filter! Reset

Taxonomy: contains [ ]

EC Number: exact [ ]

UniProt Accession: exact [ ]

Protein Name: exact [ ]

Max. number of results: 50 ☑ Preview all results

Restrict your search: ☑ Search only in selected genomes

Extend your search: ☐ Display homolog proteins min. ○ 50% ○ 90% ○ 100% sequence identity

search/display

Ontology Explorer

Ontology

BTO (BRENDA Tissue Ontology)

GO (Gene Ontology project)

BTO (BRENDA Tissue Ontology)

A hierarchical ontology for enzyme sources or tissue

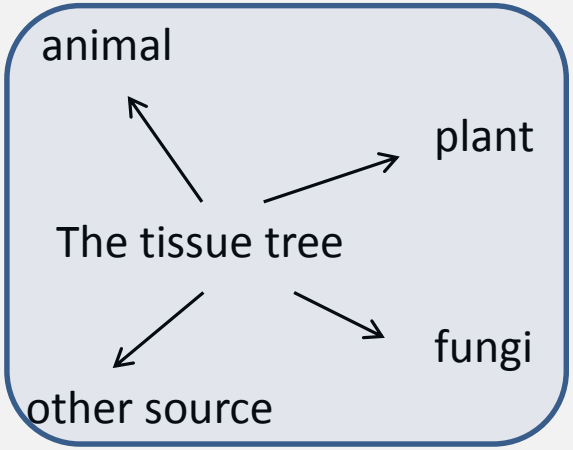
all parts of the body

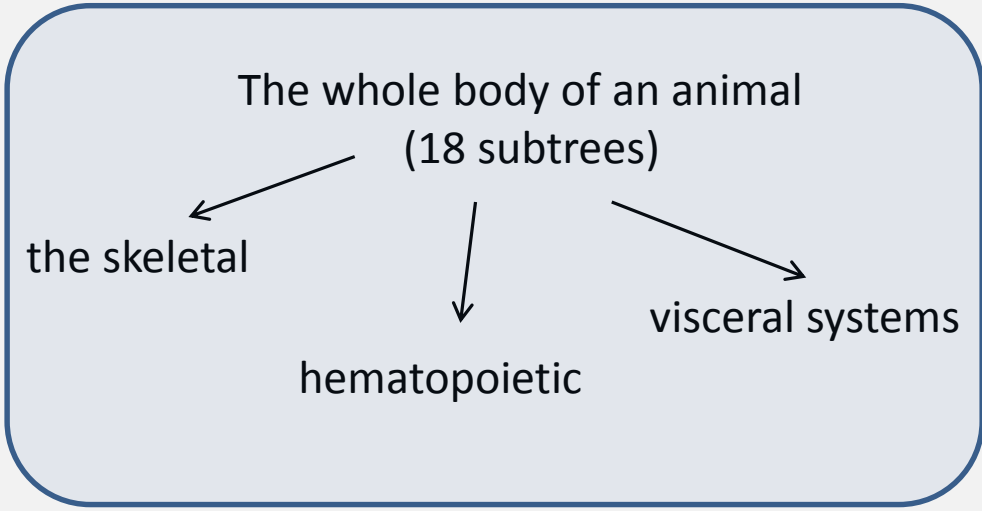
a single tissue

BRENDA`s own ontology

The same rules and formats

GO Consortium

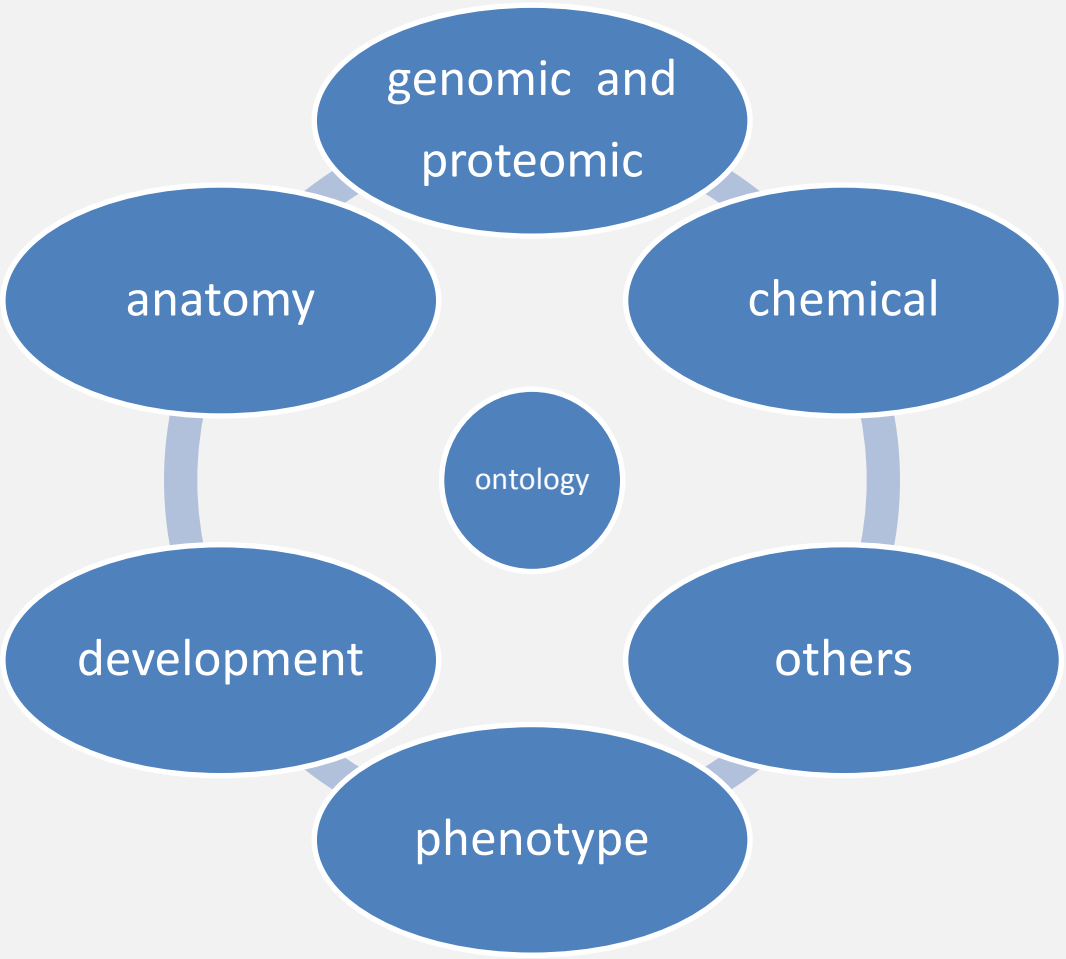




Each different cell type, cancer cell type or cell line is assigned to the tissue from which it has developed or to which it is related.

The BTO numbers are unique for each term

Categories for specific ontology



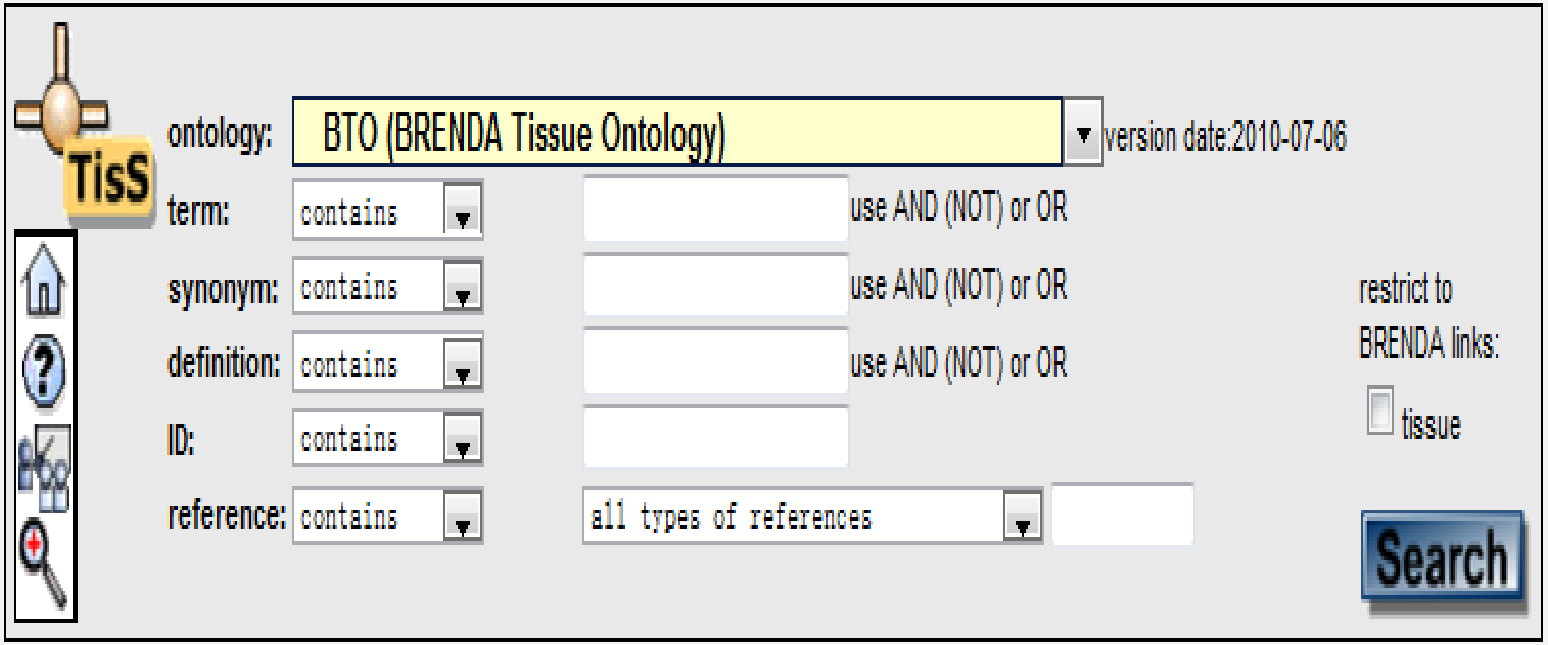
Ontology explorer

Fulltext Search

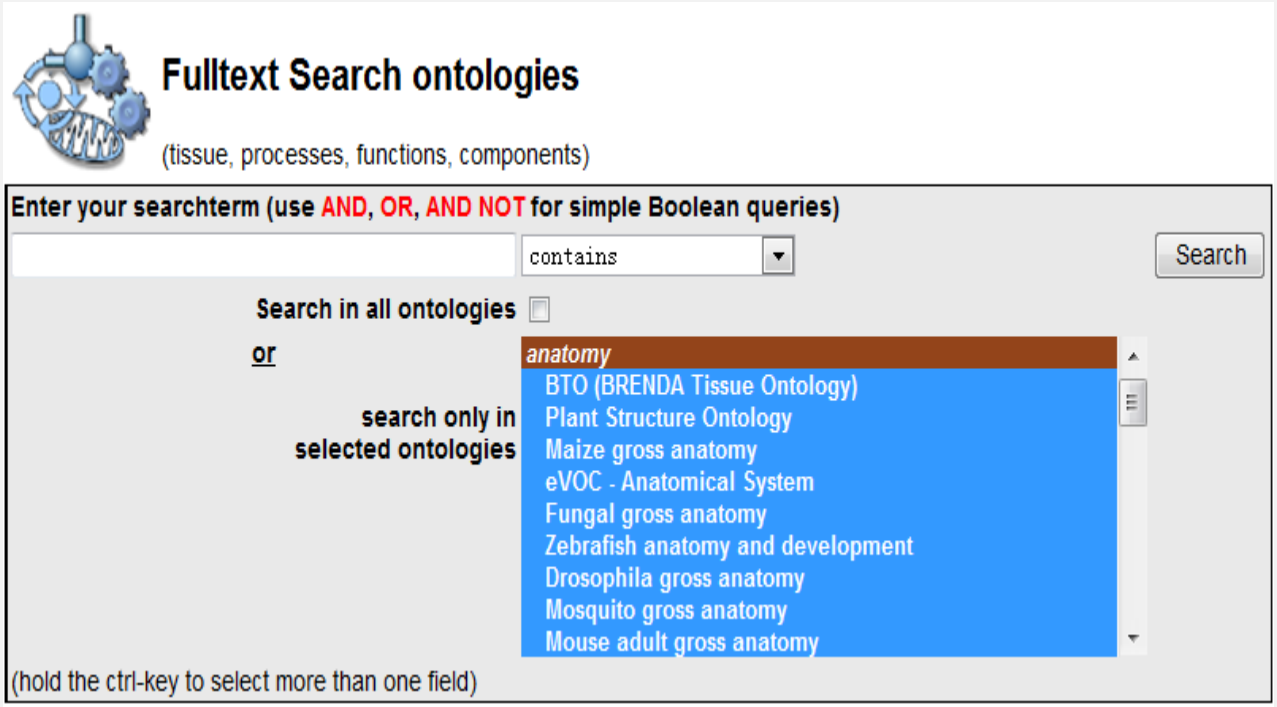
offers an easy access to the different ontologies (tissues, processes, components, functions, ...)

Search in a specific ontology

Ontology	status	version	terms	in tree	synonyms	definitions	contact	home	doc	source
anatomy										
BTO (BRENDA Tissue Ontology)	online	2010-07-06	4724	4724	3563	3875				
Plant Structure Ontology	online	2010-05-19	810	810	282	864				
Maize gross anatomy	online	2005-08-09	180	180	51	136				
eVOC - Anatomical System	online	2007-03-30	516	516	0	75				
Fungal gross anatomy	online	2009-11-17	74	74	19	72				
Zebrafish anatomy and development	online	2010-06-08	2552	2552	2292	1538				
Drosophila gross anatomy	online	2010-05-23	6718	6718	3801	2584				
Mosquito gross anatomy	online	2009-02-04	1862	1862	5178	1861				
Mouse adult gross anatomy	online	2010-04-02	2957	2957	478	0				
Dictyostelium discoideum anatomy	online	2010-03-15	138	138	114	138				
Arabidopsis gross anatomy	online	2010-05-19	1	1	282	864				
eVOC - Cell type	online	2007-03-04	189	189	0	10				
others										
Gene ontology	online	2010-07-07	30560	30560	0	31772				



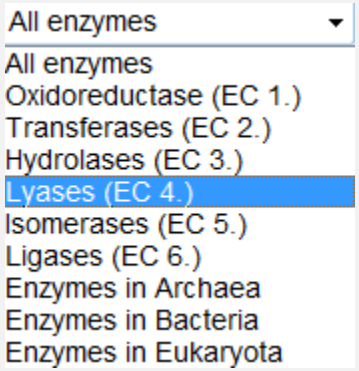
Full Search ontologies



Supplementary projects

- Functional Enzyme parameters

  BRENDA statistics：Distribution of KM_Value,KI_Value,PI_Value,IC50_Value, Turnover_Number, Specific_Activity, pH_Optimum, pH_Range, Temperature_Optimum, Temperature_Range



Currently statistics for enzymes in BRENDA will showing for you

- SBML Output
- Download

Computer-based access

- SOAP http://www.brenda-enzymes.org/soap2
- Textfile with BRENDA core data
- SBML output


Thank you
for
your intention