BRENDA – A European Elixir Core Data Resource in de.NBI

Fkz 031A539D

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Short description of the project

BRENDA (www.brenda-enzymes.org), appointed Elixir Core Data Resource in 2018, is the world's largest and widely used information system for enzymes and enzyme ligands. Its manually curated 4.9 million data in 50 information fields make it absolutely unique world-wide. This manual information core is complemented by data obtained by text mining and calculations, e.g. genome annotation and enzyme localization. In order to provide a "one stop shopping" for enzyme information this is combined with data like sequences and 3D-structures from public-domain databases.

General information on the project

Three scientists are paid from the de.NBI grant. The PI, three further scientists and several external contributors are paid by the TU Braunschweig and commercial licensing.

de.NBI Training and education

Workshop:
Protein Structure Fundamentals, 23./24.09.2019 at the Center for Bioinformatics in Hamburg, topics related to:
ProteinsPlus, BRENDA and KNIME

Tutorials:
The BRENDA video and online training material was updated and supplemented!
BRENDA YouTube Channel

de.NBI services

Since the beginning of de.NBI:
- 2.8 million sessions
- 1.5 million different users
- 13.5 million page views

Since the appointment as an Elixir Core Data Resource:
- 21,000 downloads of the text file comprehending the BRENDA database

SOAP service
a simple and direct way to access data via almost 150 different methods without the requirement of parsing

Advanced Search
sophisticated queries in about 50 data categories by combining different search criteria

SBML output
the download of data in XML-based format for the construction of metabolic models from kinetic data

Text-based Queries

Functional Parameters
~456,000 manually annotated kinetic data and ~12,400 kinetic values from text mining methods

Sequence Search
a search for amino acid sequences in combination with a distribution of hits in the EC System

BRENDA 1987 2019 The Comprehensive Enzyme Information System

Ontology Explorer/BTO
a variety of about 40 biologically and biochemically relevant ontologies

Structure Search
a search for BRENDA ligands using a chemical structure (substructure) drawn with a molecule editor

Graphic-based Queries and Visualizations

Word Maps
graphical representations of enzyme- or organism-specific terms classified into different categories

Pathway Maps
interactive visualizations of BRENDA pathways linked to metabolites and enzymes

Genome Explorer
a genome visualization tool to compare enzyme locations and to show enzymes in their genomic context

Progress report

Enzyme summary page

BRENDA home
History

show all | hide all No of entries

- Enzyme Nomenclature 204
- Enzyme-Ligand Interactions 3052
  - Substrates/Products 494
  - Natural Substrates 120
  - Cofactors 0
  - Metals and Ions 20
  - Inhibitors 2351
  - Activating Compounds 67
- Diseases 5698
- Functional Parameters 2050
- Organism related Information 491
- General Information 55
- Enzyme Structure 823
- Molecular Properties 180
- Applications 33
- References 390
- External Links

Individual selection of categories and data fields, adaptable to the user's need

Information on EC 3.1.1.7 - acetylcholinesterase

for references in articles please use BRENDA:EC3.1.1.7

print visible entries
print all entries
show all entries

EC Tree
- 3 Hydrolases
  - 3.1 Acting on ester bonds
    - 3.1.1 Carboxylic-ester hydrolases
      - 3.1.1.7 acetylcholinesterase

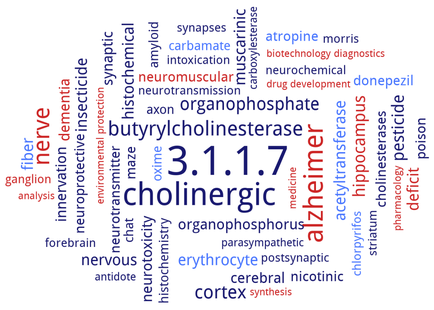
IUBMB Comments
Acts on a variety of acetic esters; also catalyses transacetylations.

Specify your search results

Mark a special word or phrase in this record: Mark!
Search Reference ID: Search
Search UniProt Accession: Search
Select one or more organisms in this record:
All organisms
Abelson murine leukemia virus
Ablabesmyia aspera
Abramis brama
Abrus precatorius
Submit

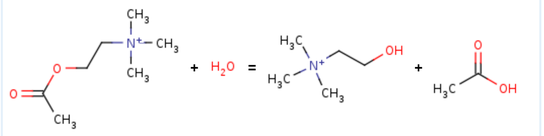
Show additional data
- Do not include text mining results
- Include AMENDA (text mining) results
- Include FRENDA results (AMENDA + additional results, but less precise)

Word Map hide



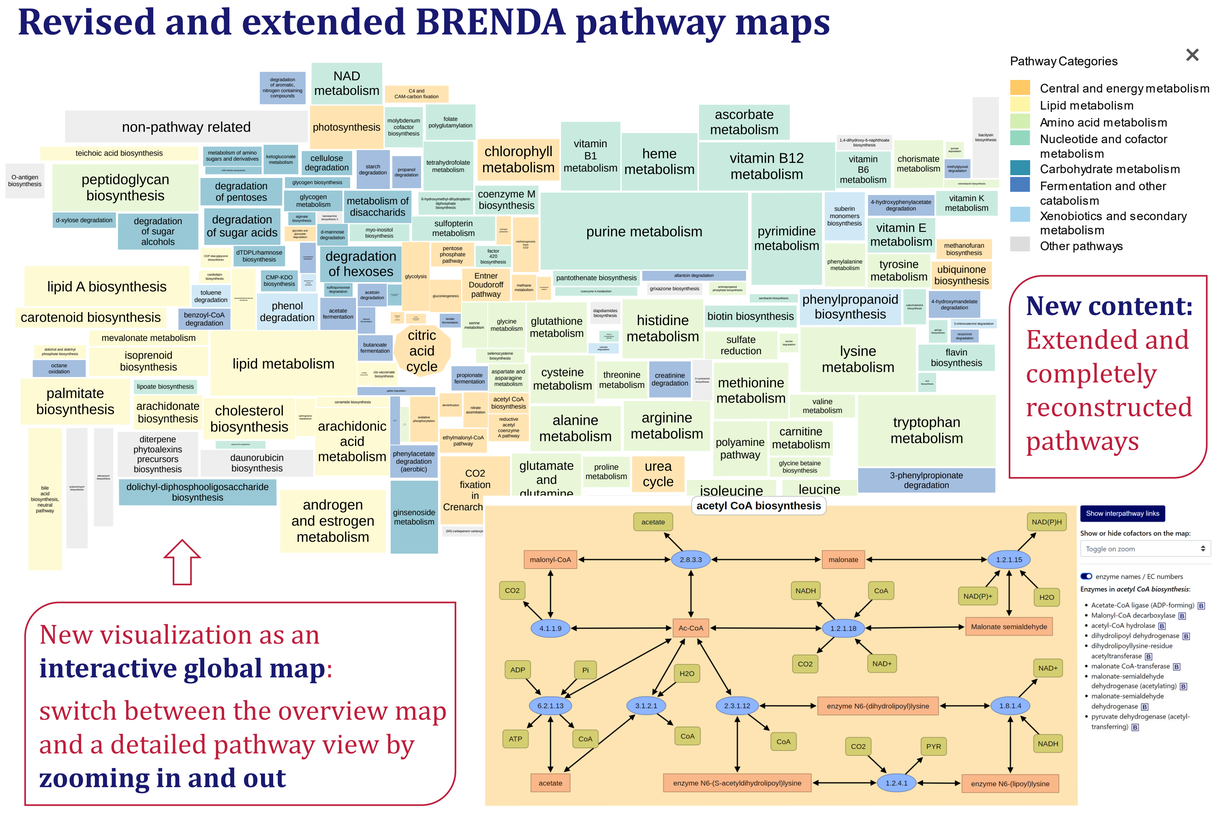
The enzyme appears in viruses and cellular organisms

Reaction Schemes hide



Improved usability: compact and clear initial view, **more flexible**, and accelerated loading time to access to the data

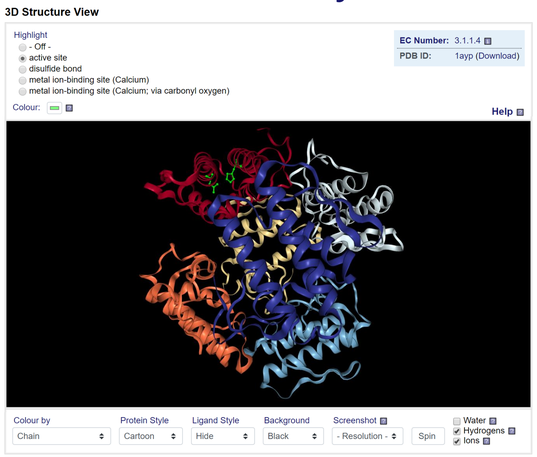
Revised and extended BRENDA pathway maps



New content: Extended and completely reconstructed pathways

New visualization as an **interactive global map**:
switch between the overview map and a detailed pathway view by **zooming in and out**

New viewer for enzyme 3D structures (NGL)



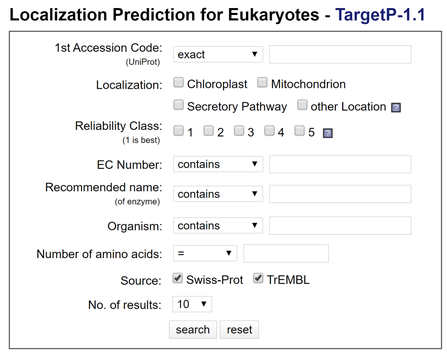
- Better resolution
- Colour selection for **highlighting details** of the structure
- Easy change between **different** colour schemes, protein and ligand **styles**

BRENDA MetaboMAPS

Data visualization in metabolic context & pathway sharing

Cellular localization prediction for eukaryotic enzymes

- Cellular localization prediction for eukaryotic enzymes based on the software **TargetP 1.1** (2)
- Prediction based on: N-terminal sequence motifs and other sequence properties
- **Reliability class** ranges from 1 (very reliable) to 5 (not reliable)



Publications / References

1. Jeske, L., Placzek, S., Schomburg, I., Chang, A., and Schomburg, D. (2019) BRENDA in 2019: A european ELIXIR Core Data Resource. Nucleic Acids Res. Nucleic Acids Res. 47:D542-D549.
2. Emanuelsson, O., Nielsen, H., Brunak, S. and von Heijne, G. (2000) Predicting subcellular localization of proteins based on their N-terminal amino acid sequence. J. Mol. Biol., 300: 1005-1016.

GEFÖRDERT VOM Bundesministerium für Bildung und Forschung
Projektträger Jülich Forschungszentrum Jülich