BRENDA Tutorial

Introduction to the Enzyme Information System
Facts about BRENDA (BRaunschweig ENzyme DAtabase)

• one of the most comprehensive enzyme information repositories

• BRENDA is a member of de.NBI (German Network for Bioinformatics Structure, since 2015)

• BRENDA is an ELIXIR Core Data Resource (since 2018)

• all enzymes, classified by the Enzyme Nomenclature (IUBMB)

• data of molecular biology, biochemistry, medical research, and biotechnology

• furthermore BRENDA includes data from interconnected databases containing results from text mining methods and bioinformatic approaches

• BRENDA is freely available to the scientific community

• more than 80,000 visits of the BRENDA website each month

• major updates of the data in BRENDA are performed twice a year
History and major developments of BRENDA

- BRENDA was created at the former German National Research Center for Biotechnology (GBF, now HZI, Helmholtz Zentrum für Infektionsforschung, Braunschweig, Germany) in 1987

- BRENDA was originally published as a series of book
  - 2nd Edition 2001-2013 (Handbook of Enzymes)

- BRENDA moved to the University of Cologne, Germany

- First online version in 1998 via the SRS system at the EBI

- First website of BRENDA in Cologne

- Transfer of BRENDA into a fully relational database system

- BRENDA moved back to Braunschweig in 2007

- BRENDA is now maintained and further developed at the BRICS - TU Braunschweig
Facts about BRENDA

The main categories are based on the **Enzymes** and the **Metabolites / Ligands**

Enzyme-related data encompasses information on:
- Enzyme and ligand nomenclature
- Organism
- Reaction and specificity
- Kinetic properties
- Structure and role of the ligands
- Stability information
- Ligand-enzyme information
- Enzyme sequence and structure
- Mutants and disease
- Occurrence, isolation, and preparation
- Pathways
BRENDA is the most comprehensive information system on:

- 8083 EC Numbers (Nov. 2020)
- more than 2 Mill. different enzymes
- more than 5 Mill. enzyme data, manually annotated from ~160,000 literature references

**Enzyme Commission numbers (EC Numbers) are defined according to the catalyzed reaction by the IUBMB (International Union of Biochemistry and Molecular Biology)**

**Format:** Four numbers separated by periods, e.g. 1.2.3.1

Numbers represent from left to right a progressively finer classification scheme

**Main Enzyme Classes:**
1. Oxidoreductases
2. Transferases
3. Hydrolases
4. Lyases
5. Isomerases
6. Ligases
7. Translocases

**EC 1.2.3.1**

- an aldehyde + H$_2$O + O$_2$ = a carboxylate + H$_2$O$_2$
  - aldehyde oxidase
  - with oxygen as acceptor
  - acting on the aldehyde or oxo group of donors
  - oxidoreductase (main class)
The main search options:

- Quick access (A)
- and more specific queries (B)
- Classic View (C)
- ...further details in the corresponding BRENDA tutorials
**BRENDA data and information fields „classic view“**

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NEWS will be announced in a new box, with all upcoming data and information, new developments and tools etc.
Data sources & updates: Merge and process of data

Text mining
Enzyme
Tissue
Disease

BRENDA
The Comprehensive Enzyme Information System

Manual annotation
Data selection

Literature annotation

High Quality Data
Data integration

Visualization

Manual annotation
Data selection

Literature annotation

High Quality Data
Data integration

BRENDA
BTO Tissue Ontology