BRENDA Tutorial

Introduction to the Enzyme Information System
Facts about BRENDA

- BRENDA (BRaunschweig ENzyme DAtabase)
- one of the most comprehensive enzyme information repositories
- 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) in 1987
- BRENDA was originally published as a series of book
  - 2nd Edition 2001-...
- BRENDA moved to the University of Cologne
- 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 Department of Bioinformatics & Biochemistry at the 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 properties
BRENDA data and information fields „classic view“
BRENDA is the most comprehensive information system on:

- 6671 EC Numbers (January 2015)
- more than 1.9 Mill. different enzymes
- more than 3 Mill. enzyme data, manually annotated from more than 130,000 literature references

**Enzyme Commission numbers (EC Numbers) are defined according to the catalyzed reaction**

Enzyme nomenclature is defined by the IUBMB (International Union of Biochemistry and Molecular Biology)

**Format:** Four numbers separated by periods, e.g. 1.2.1.2

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

**EC 1.2.1.2** Formate + NAD\(^+\) = CO\(_2\) + NADH

- formate dehydrogenase
- with NAD\(^+\) or NADP\(^+\) as acceptor
- acting on the aldehyde or oxo group of donors
- oxidoreductase (main class)
Two main search options:
- quick access (A)
- and more specific queries (B)

...further details in the corresponding BRENDA tutorials
Data sources & updates: Merge and process of data

Text mining data
- **FREenda**: Enzyme name + organism
- **AMENDA**: Enzyme name + organism + occurrence
- **DREnda**: Disease-related enzyme data
- **KENDA**: Kinetic data

Manual annotation
- IUBMB enzyme classes

Literature
- PubMed

Literature annotation

External databases und ontologies

**Data sources & updates**: Merge and process of data