

The BRENDA enzyme information resource in 2011

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BRENDA (BRaunschweig ENzyme DAtabase, <http://www.brenda-enzymes.org>) is the most comprehensive enzyme information system in the world and offers free web-based access to enzyme-relevant information to academic users (SGCS11).

BRENDA provides data on the biological function, tissue-specific appearance, preparation and purification, 3D structure, application, biophysical properties, mutations and medical aspects of enzymes. Information on the more than 5,000 different enzyme classes, as classified by the IUBMB, are available.

The content of BRENDA is based on data manually extracted from almost 115,000 literature references which constitutes an increase of nearly 10% during the last 15 months. In the same period the number of enzyme ligands - small biochemically active molecules acting as substrates or products of enzyme-catalyzed reactions or enzyme inhibitors/activators - has increased by more than 10%: Now, more than 115,000 structures/distinct ligand names are available that represent more than 80,000 different chemical structures.

Special effort was put into the inclusion of metabolite names and biochemical reactions that are relevant to metabolic models in order to facilitate their reconstruction. In this context, BRENDA was the main resource for the creation of an integrated database of biochemical reactions (BKM-react, LSS11) and a web-based tool for the visualization of metabolic models and validation of reconstructed networks (BRIME, see extra poster). A single, integrated web search form for enzyme ligands was implemented.

Furthermore, the textmining procedures which complement the manually annotated data of BRENDA were enhanced. The organism-, tissue- and cellular location-specific text mining approach (AMENDA and FRENDA, see CSGS09) is currently based on almost 21 million PubMed entries. The disease-specific text mining and classification was fundamentally reworked and optimized (DRENDA, SCS11) and provides more than 800,000 enzyme-specific, classified disease hits (distinct EC number, Disease, PubMed ID combinations) for BRENDA.

References

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