BHARATHIDASAN UNIVERSITY

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Tamil Nadu, India.

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Unit-II
TOPIC: BIOLOGICAL DATABASES: BRENDA

Dr. P. JEGANATHAN
Guest Lecturer
Department of Biomedical Science

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INTRODUCTION

- BRENDA (BRaunschweig ENzyme DAtabase) was created in 1987 at the German National Research Center for Biotechnology in Braunschweig (GBF) and is now continued at the University of Cologne, Institute of Biochemistry. This enzyme information system was developed to collect and store enzyme functional data and has been an ongoing effort for >10 years. It was first published as a series of books [Enzyme Handbook, Springer (1)] with the intention from the very beginning to provide the data in a database as a retrieval system.

DEFINITION OF BRENDA

- BRENDA is an important tool for biochemical and medical research covering information on properties of all classified enzymes, including data on the occurrence, catalyzed reaction, kinetics, substrates/products, inhibitors, cofactors, activators, structure and stability.

➢Enzymes, the largest and most diverse group among the proteins, play an essential role in the metabolism of each organism. All chemical reactions and metabolic steps within the cell are catalyzed and regulated by enzymes.

➢ The development and progress of projects on structural and functional genomics suggest that the systematic collection and accessibility of functional information of gene products are indispensable to understanding biological functions and the correlation between phenotype and genotype.

➢BRENDA represents a protein function database, containing comprehensive enzymatic and metabolic data, extracted, continuously updated and evaluated from the primary literature.

➢ The key developments in the last few years were the conversion of the database to an organism-specific information system and the improvement of the validation and the correction of data and the standardization of the entries to create prerequisites for a systematic access and analysis.

CONTENTS OF BRENDA

➢BRENDA contains all enzymes classified according to the system of the EC numbers, which was implemented in 1955 by the International Commission of Enzymes [now the International Union of Biochemistry and Molecular Biology, IUBMB (2)].

➢ This nomenclature is based on the reaction the enzymes catalyzes and not on the individual enzyme molecule. Presently BRENDA contains data of approximately 3900 EC numbers, which represent more than 40 000 different protein molecules, given by the combination of EC number and organism

➢The database covers organism-specific information on functional and molecular properties, in detail on the nomenclature, reaction and specificity, enzyme structure, stability, application and engineering, organism, ligands, literature references and links to other databases

LIGANDS

➢ A major part in BRENDA is the information of ligands, which function as natural or *in vitro* substrates/products, inhibitors, activating compounds, cofactors, bound metals, etc. Altogether, approximately 320 000 enzyme–ligand relationships are stored with more than 33 000 different chemical compounds functioning as 'ligand'.

➢ In BRENDA the ligands are stored as compound names, SMILES ([4](#)) strings and as Molfiles. The latter two forms are interchangeable with respect to the connectivity information. The two-dimensional chemical structures of these compounds can be displayed as images.

METABOLISM

➢The data in BRENDA allow the calculation or simulation of metabolic pathways by extracting the information of substrate/product chains and the corresponding kinetic data of the preceding and following enzymes in the Boehringer and KEGG metabolism (with the risk of including 'pathways' with non-natural compounds).

➢Based on the representation of metabolic networks as directed graphs, navigation operation will be made possible. This will give answers to questions on the structure of the metabolic paths, e.g. on shortest or alternate paths for different organisms.

ENZYME AND DISEASE INFORMATION

➢ In order to keep up with the quickly growing scientific literature, automatic information extraction techniques were tested to include disease-related knowledge to BRENDA.

➢ References in electronic format are taken from the PubMed database, parsed for relevant key phrases and associated with correlated enzymes. Information on 789 enzymes and their associated human diseases has been included into the BRENDA database

REFERENCES

- HTTPS://WWW.GENOME.JP/TOOLS/MOTIF/

- HTTPS://WWW.GOOGLE.COM/URL?SA=T&SOURCE=WEB&RCT=J&URL=HTTPS://PROSITE.EXPASY.ORG/&VED=2AHUKEWIK7OG4H-Z9AHWXS2WGHWPWCAWQFNOECAUQAQ&USG=AOVVAW2YSYV7B25SZFM7D4PADBFC

THANK YOU !!