# The ENZYME data bank

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# INTRODUCTION

The ENZYME data bank is a repository of information relative to the nomenclature of enzymes. It is primarily based on the recommendations of the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (IUBMB) [1] and it contains the following data for each type of characterized enzyme for which an EC (Enzyme Commission) number has been provided:

EC number

Recommended name

Alternative names (if any)

Catalytic activity

Cofactors (if any)

Pointers to the SWISS-PROT [2] protein sequence entrie(s) that correspond to the enzyme (if any)

Pointers to human disease(s) associated with a deficiency of the enzyme (if any)

We believe that the ENZYME data bank can be useful to anybody working with enzymes and that it can be of help in the development of computer programs involved with the manipulation of metabolic pathways.

As stated above the main source for the data in the ENZYME data bank comes from the recommendations of the IUBMB, but additional information has been extracted from the literature. The information concerning human diseases originates from the MIM data base of Victor McKusick [3].

We do not assign EC numbers for newly characterized enzymes, this is the responsibility of the Nomenclature Committee of IUBMB (NC-IUBMB). To contact the committee one should write to:

Prof. K. Tipton
Department of Biochemistry

Trinity College

Dublin 2

Republic of Ireland

He can also be contacted by electronic mail at the following address:

ktipton@vax1.tcd.ie

And by fax at the number:

+353-16-77 24 00

In the near future the ENZYME data bank will be distributed with a form that can be used to fill in the information necessary for the NC-IUBMB to assign an EC number. The commission will regularly send us updates and additions to the nomenclature

so that they can be integrated into the data bank in a timely manner.

#### **FORMAT**

The entries in the database are structured so as to be usable by human readers as well as by computer programs. An entry in the database is composed of defined line types, each with its own format; they are used to record the various types of data which make up the entry. For standardization purposes the format of ENZYME follows as closely as possible that of the SWISS-PROT [2] protein and EMBL [4] nucleotide sequence databases. Two sample ENZYME entries are shown below:

ID 1.14.17.3

DE PEPTIDYLGLYCINE MONOOXYGENASE.

AN PEPTIDYL ALPHA-AMIDATING ENZYME.

AN PEPTIDYLGLYCINE 2-HYDROXYLASE.

CA PEPTIDYLGLYCINE + ASCORBATE + O(2) =

CA PEPTIDYL(2-HYDROXYGLYCINE) + DEHYDRO-

CA ASCORBATE + H(2)O.

CF COPPER.

CC -!- PEPTIDYLGLYCINES WITH A NEUTRAL AMINO ACID

CC RESIDUE IN THE PENULTIMATE POSITION ARE THE

CC BEST SUBSTRATES FOR THE ENZYME.

CC -!- THE ENZYME ALSO CATALYZES THE DISMUTATION

CC OF THE PRODUCT TO GLYOXYLATE AND THE

CC CORRESPONDING DESGLYCINE PEPTIDE AMIDE.

DR P10731, AMD\_BOVIN; P19021, AMD\_HUMAN; P14925,

DR AMD\_RAT; P08478, AMD1\_XENLA; P12890,

DR AMD2\_XENLA;

ID 2.3.1.43

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DE PHOSPHATIDYLCHOLINE--STEROL ACYLTRANS-FERASE.

AN LECITHIN-CHOLESTEROL ACYLTRANSFERASE.

AN LCAT

AN PHOSPHOLIPID-CHOLESTEROL ACYLTRANSFERASE.

CA PHOSPHATIDYLCHOLINE + STEROL = STEROL ESTER

CA + 1-ACYLGLYCEROPHOSPHOCHOLINE.

CC -!- PALMITOYL, OLEOYL, AND LINOLEOYL CAN BE

CC TRANSFERRED; A NUMBER OF STEROLS, INCLUDING

CC CHOLESTEROL, CAN ACT AS ACCEPTOR.

DI NORUM DISEASE; MIM:245900.

DI FISH-EYE DISEASE; MIM:136120.

DR P10480, GCAT\_AERHY; P04180, LCAT\_HUMAN;

DR P16301, LCAT\_MOUSE;

DR P18424, LCAT\_\_RAT;

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#### PRACTICAL INFORMATION

#### Content of the current release

Release 12.0 of ENZYME (April 1993) contains information relevant to 3489 enzymes. The data file (ENZYME.DAT) requires about 1 Mb of disk storage space. The database is distributed with a user's manual (ENZUSER.TXT); a file describing the various classes, subclasses and sub-subclasses of enzymes (ENZCLASS.TXT); and a file that describes how the database can be obtained (ENZYME.GET).

## How to obtain ENZYME

ENZYME is distributed on magnetic tape and on CD-ROM by the EMBL Data Library. For all enquiries regarding the subscription and distribution of ENZYME one should contact:

EMBL Data Library

European Molecular Biology Laboratory

Postfach 10.2209, Meyerhofstrasse 1

6900 Heidelberg, Germany

Telephone: (+49 6221) 387 258

Telefax: (+49 6221) 387 519 or 387 306

Electronic network address: datalib@EMBL-heidelberg.de ENZYME can be obtained from the EMBL File Server [5]. Detailed instructions on how to make the best use of this service, and in particular on how to obtain ENZYME, can be obtained by sending to the network address netserv@EMBL-heidelberg.de the following message:

# HELP ENZYME

If you have access to a computer system linked to the Internet you can obtain ENZYME using FTP (File Transfer Protocol), from the following file servers:

EMBL anonymous FTP server

Internet address: ftp. EMBL-heidelberg.de (or 192.54.41.33)

NCBI Repository (National Library of Medicine, NIH, Washington D.C., U.S.A.)

Internet address: ncbi.nlm.nih.gov (130.14.20.1)

Basel Biozentrum Biocomputing server (EMBnet SWISS node) Internet address: *bioftp.unibas.ch* (or 131.152.8.1)

ExPASy (Expert Protein Analysis System server, University of Geneva, Switzerland)

Internet address: expasy.hcuge.ch (129.195.254.61)

National Institute of Genetics (Japan) FTP server Internet address: ftp.nig.ac.jp (133.39.16.66)

A version of the database in the ASN.1 data exchange format compatible with the databases and software developed by the National Center for Biotechnology Information (NCBI) [6] is also available on some of the above servers.

You can also browse through ENZYME using various Internet Gopher servers that specialize in biosciences (biogophers) [7]. Gopher is a distributed document delivery service that allows a neophyte user to access various types of data residing on multiple hosts in a seamless fashion.

The present distribution frequency is four releases per year. No restrictions are placed on use or redistribution of the data.

#### REFERENCES

- Enzyme Nomenclature, Recommendations of the Nomenclature Committe
  of the International Union of Biochemistry and Molecular Biology on the
  Nomenclature and Classification of Enzymes, NC-IUBMB, Academic Press,
  New-York, (1992).
- 2. Bairoch A., Boeckmann B. Nucleic Acids Res. 20:2019-2022(1992).
- McKusick V.A. Mendelian Inheritance in Man. Catalogs of autosomal dominant, autosomal recessive, and X-linked phenotypes; Tenth edition; Johns Hopkins University Press, Baltimore, (1991).
- Higgins D.G., Fuchs R., Stoehr P.J., Cameron G.N. Nucleic Acids Res. 20:2071-2074(1992).
- 5. Stoehr P.J., Omond R.A. Nucleic Acids Res. 17:6763-6764(1989).
- 6. Benson D. CODATA Bulletin 23:76-78(1991).
- 7. Gilbert D. Trends Biochem. Sci. 18:107-108(1993).