by their chemical names. Enzyme structures defined in the database are amino acid sequences and three-dimensional structures. LIGAND have neither sequence nor atomic coordinate, but actually has the entry names of PIR and PDB under the label of DBLINKS. DISEASE items in LIGAND contain MIM number by McKusick and name of the disease which is induced by the failure of enzymatic function.

Public service of LIGAND started through anonymous ftp (ftp.genome.ad.jp) on GenomeNet in 1990, then by gopher (gopher.genome.ad.jp) and WWW (http://www.genome.ad.jp) in June 1994. In the first WWW version, it was possible to look up PIR and PDB by clicking their entry names and to display the chemical structures of 842 substances by clicking their chemical names. We have stepwisely added WWW-LIGAND new figures of chemical structures and linkages with the reactions related by metabolic pathways. On July 1994, each enzyme was linked to other ligand-related enzymes which share a common chemical substance in their reactions. On November 1994, LIGAND was mutually linked with the structural databases on GenomeNet. In the latest version (October 1995), information on chemical substances was integrated into the COMPOUND dictionary which has 1400 CAS registry numbers and chemical formulae, 1990 figures of chemical structures, and EC numbers of ligand-related enzymes.

The main purpose of LIGAND is to serve for the retrieval of the structures and reactions of enzymes through graphical user interface. It is easy to collect the structural data of functionally related enzymes. For example, we collected the amino acid sequences of PLP-related enzymes, which use PLP as a cofactor in their reactions, and extracted sequence motifs, which are conserved in the sequences collected, by using an algorithm GAPE [2].

2 Future plan of LIGAND

LIGAND has a potential link between genes and their phenotypes. In cells, genetic information is first expressed as enzymes. Then they catalyze chemical reactions to produce chemical substances necessary for development and differentiation of a living organism. Finally these substances are integrated to express a destined phenotype. Therefore the next revision of LIGAND is going to provide links between enzyme and its location in metabolic pathways, and between ligand chemical and its location in metabolic pathways.

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LIGAND Chemical Database for Enzymatic Reactions: A Link between enzyme structures and chemical reactions

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Abstract

We have developed a database LIGAND Chemical Database for Enzymatic Reactions which is designed to link enzyme structures with enzyme-catalyzed chemical reactions. In the present paper, we report the present status of the database, WWW service on GenomeNet, and future plan.

1 WWW service of LIGAND on GenomeNet

LIGAND (ver. 12 released on October 1995) contains 3,489 entries for all the chemical reactions catalyzed by the enzymes which are biochemically characterized so far [1]. Each enzyme is uniquely identified not by its NAME(s) but by EC number which classifies enzymes based on the type of chemical reactions. Each entry links with chemical reaction, enzyme structure, and disease. Chemical REACTION items consist of a chemical equation, its reaction CLASS, and the names of the chemical substances called ligands. These are SUBSTRATEs and PRODUCTs which are the starting materials and the products of the reaction, INHIBITORs and EFFECTORs which modify the enzymatic activity, and COFACTORs which are the substances indispensable for the reaction. In LIGAND, 5118 chemical substances are registered

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