Resource Summary Report

Generated by NIF on Apr 9, 2025

Protein Data Bank Site

RRID:SCR_008227
Type: Tool

Proper Citation

Protein Data Bank Site (RRID:SCR_008227)

Resource Information

URL: http://wwwmgs.bionet.nsc.ru/mgs/gnw/pdbsite/

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Description: THIS RESOURCE IS NO LONGER IN SERVICE, documented on August 18, 2014. A database for structural and functional information on various protein sites (post-translational modification, catalytic active, organic and inorganic ligand binding, protein-protein, protein-DNA and protein-RNA interactions) in the Protein Data Bank (PDB). It was developed as a daughter database accumulating the data on functional and structural characteristics of functional sites stored in PDB, as well as their spatial surroundings. It consists of functional sites extracted from PDB using the SITE records and of an additional set containing the protein interaction sites inferred from the contact residues in heterocomplexes. The PDBSite was set up by automated processing of the PDB. The PDBSite database can be queried through the functional description and the structural characteristics of the site and its environment. The PDBSite is integrated with the PDBSiteScan tool allowing structural comparisons of a protein against the functional sites. The PDBSite enables the recognition of functional sites in protein tertiary structures, providing annotation of function through structure. The Protein Data Bank (PDB) contains data on the spatial protein structures and their biologically active sites (i.e., ligand binding regions, enzyme catalytic centers, regions subjected to biochemical modifications, etc.). However, neither of the well known systems searching PDB does not provide the user with possibility to make the queries related with the active sites. A database PDBSITE storing the data on biologically active sites contained in the PDB database has been developed. PDBSITE accumulates amino acid content, structure features calculated by spatial protein structures, and physicochemical properties of sites and their spatial surroundings. The data on biologically active protein sites are of extreme importance for solving many problems in molecular biology, biotechnology, and medicine. High specificity of biological activity in proteins is produced by unique structure of active sites that are often organized by a very complicate pattern. In particular, biologically active sites in proteins are often compiled out of remote by primary structure amino acid residues, which form compact clusters in the spatial structure with strictly ordered conformation. Specific structure and conformational parameters of these sites are determined by the structure of their spatial amino acid surroundings. For example, spatial amino acid surroundings of enzyme catalytic centres determine the relief of hollows in catalytic centres of enzymes in a substrate binding regions, whereas the residues of antigen determinants of proteins determine their structure by organizing prominent parts at the protein surface. For many natural and mutant proteins, the relationships were found between protein activity and physico-chemical properties of amino acid residues composing the local surroundings of a functional site. The spatial surroundings of biologically active sites may be detected only if the data on tertiary protein structures are available. The Protein Data Bank (PDB) contains data on the spatial protein structures and their biologically active sites. However, neither of the well-known systems searching PDB does not provide the user with possibility to make the queries related with the active sites. Sponsor: This site is funded by GeneNetWorks.

Abbreviations: PDBSITE

Resource Type: database, data or information resource

Defining Citation: PMID:15608173

Keywords: enzyme, functional, active, activity, amino acid, binding, biochemical, biological, biologically, biology, biotechnology, catalytic, dna, heterocomplex, inorganic, interaction, ligand, medicine, modification, molecular, organic, pattern, physiochemical, post-translational, primary, protein, protein sequence motifs and active sites databases, residue, rna, site, spatial, specificity, structural, structure, tertiary

Funding:

Availability: THIS RESOURCE IS NO LONGER IN SERVICE

Resource Name: Protein Data Bank Site

Resource ID: SCR_008227

Alternate IDs: nif-0000-21317

Record Creation Time: 20220129T080246+0000

Record Last Update: 20250409T060727+0000

Ratings and Alerts

No rating or validation information has been found for Protein Data Bank Site.

No alerts have been found for Protein Data Bank Site.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 1 mentions in open access literature.

Listed below are recent publications. The full list is available at NIF.

Hira D, et al. (2020) Structural basis for the core-mannan biosynthesis of cell wall fungal-type galactomannan in Aspergillus fumigatus. The Journal of biological chemistry, 295(45), 15407.