Resource Summary Report

Generated by nidm-terms on Jul 28, 2026

SitesBase

RRID:SCR_007932
Type: Tool

Proper Citation

SitesBase (RRID:SCR_007932)

Resource Information

URL: http://www.modelling.leeds.ac.uk/sb/

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Description: THIS RESOURCE IS NO LONGER IN SERVICE, documented August 22, 2016. A database of known ligand binding sites within the PDB which is navigable by PDB identifier or ligand 3 letter code e.g. NAD. Each binding site has a frequently updated register of structurally similar binding sites sharing atomic similarity detected by geometric hashing. Multiple alignments, structural superpositions and links to other structural databases are also available enabling further analysis. The rapid expansion of structural information for protein-ligand binding sites is potentially an important source of information in structure-based drug design and in understanding ligand cross reactivity and toxicity. We have developed a large database of ligand binding sites extracted automatically from the Protein Data Bank. This has been combined with a method for calculating binding site similarity based on geometric hashing to create a relational database for the retrieval of site similarity and binding site superposition. It contains an all-against-all comparison of binding sites and holds known protein-ligand binding sites, which are made accessible to data mining. Here we demonstrate its utility in two structure-based applications: in determining site similarity and in aiding the derivation of a receptor-based pharmacophore model.

Synonyms: SitesBase

Resource Type: data or information resource, database

Availability: THIS RESOURCE IS NO LONGER IN SERVICE

Resource Name: SitesBase

Resource ID: SCR_007932

Record Creation Time: 20220129T080244+0000

Record Last Update: 20260729T044159+0000

Ratings and Alerts

No rating or validation information has been found for SitesBase.

No alerts have been found for SitesBase.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 3 mentions in open access literature.

Listed below are recent publications. The full list is available at nidm-terms .

Dalton JA, et al. (2010) Homology-modelling protein-ligand interactions: allowing for ligand-induced conformational change. Journal of molecular biology, 399(4), 645.

Defranchi E, et al. (2010) Binding of protein kinase inhibitors to synapsin I inferred from pair-wise binding site similarity measurements. PloS one, 5(8), e12214.

Yeturu K, et al. (2008) PocketMatch: a new algorithm to compare binding sites in protein structures. BMC bioinformatics, 9, 543.