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| 文章名 sc-PDB: an Annotated Database of Druggable Binding Sites from the Protein Data Bank | |
| 中文译名 | sc-PDB:蛋白质数据库中可药物结合位点的注释数据库 |
| 网址 | <http://bioinfo-pharma.u-strasbg.fr/scPDB/>. |
| 关键词 | **Druggable：可受到药物控制的。** |
| 摘要 | The sc-PDB is a collection of 6 415 three-dimensional structures of binding sites found in the Protein Data Bank (PDB). Binding sites were extracted from all high-resolution crystal structures in which a complex between a protein cavity and a small-molecular-weight ligand could be identified. Importantly, ligands are considered from a pharmacological and not a structural point of view. Therefore, ~~solvents, detergents, and most metal ions~~ are not stored in the sc-PDB. Ligands are classified into four main categories: nucleotides (< 4-mer), peptides (< 9-mer), cofactors, and organic compounds. The corresponding binding site is formed by all protein residues (including amino acids, cofactors, and important metal ions) with at least one atom within 6.5 Å of any ligand atom. The database was carefully annotated by browsing several protein databases (PDB, UniProt, and GO) and storing, for every sc-PDB entry, the following features: protein name, function, source, domain and mutations, ligand name, and structure. The repository of ligands has also been archived by diversity analysis of molecular scaffolds, and several chemoinformatics descriptors were computed to better understand the chemical space covered by stored ligands. The sc-PDB may be used for several purposes: (i) screening a collection of binding sites for predicting the most likely target(s) of any ligand, (ii) analyzing the molecular similarity between different cavities, and (iii) deriving rules that describe the relationship between ligand pharmacophoric points and active-site properties. The database is periodically updated and accessible on the web at <http://bioinfo-pharma.u-strasbg.fr/scPDB/>.  1找到蛋白质腔和小分子质量的基团的晶体结构。  2配合基被分为：核苷酸、多肽、辅酶因子、有机化合物。  3包含的特征有：蛋白质名字、功能、来源、域、变异、配合基名字、结构。  4该数据可以被用做这些：筛选结合位点；分析分子相似性；推导药物作用点和活性位点的关系。 |
| 启发 |  |
| 摘录 |  |
| 相关论文 |  |

INTRODUCTION

1

生物功能是大分子相互作用实现的，3D结构是有用的，在PDB里也是可以获得的。

PDBsite,4 Relibase,5 or the MSDsite part of the Macromolecular Structure Database.6等数据库可以获得ligand-protein binding sites.很多数据库都提供位点结合信息。但这些配合基的描述都是来自结构的。也就是说，这些基团不能区分有无作用效果：是包含激活或抑制这个靶点，或者是完全没有用的分子（比如金属离子，溶剂，清洗剂）

2

最近Carlson的团队建了个数据库。这个数据库和文献系统连接以确保确实有生物学功能的位点被收集。这项收集让分子识别和基于结构的药物发现技术受益。

3

逐步筛选获得数据库中的内容。

