3D-PP: A tool for discovering conserved three-dimensional protein patterns

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Discovering conserved three-dimensional (3D) patterns among protein structures may provide valuable insights into protein classification, functional annotations or the rational design of multi-target drugs. Thus, several computational tools have been developed to discover and compare protein 3D-patterns. However, most of them only consider previously known 3D-patterns such as orthosteric binding sites or structural motifs. This fact makes necessary the development of new methods for the identification of all possible 3D-patterns that exist in protein structures (allosteric sites, enzyme-cofactor interaction motifs, among others). In this work, we present 3D-PP, a new free access web server for the discovery and recognition all similar 3D amino acid patterns among a set of proteins structures (independent of their sequence similarity). This new tool does not require any previous structural knowledge about ligands, and all data are organized in a high-performance graph database. The input can be a text file with the PDB access codes or a zip file of PDB coordinates regardless of the origin of the structural data: X-ray crystallographic experiments or in silico homology modeling. The results are presented as lists of sequence patterns that can be further analyzed within the web page. We tested the accuracy and suitability of 3D-PP using two sets of proteins coming from the Protein Data Bank: (a) Zinc finger containing and (b) Serotonin target proteins. We also evaluated its usefulness for the discovering of new 3D-patterns, using a set of protein structures coming from in silico homology modeling methodologies, all of which are overexpressed in different types of cancer. Results indicate that 3D-PP is a reliable, flexible and friendly-user tool to identify conserved structural motifs, which could be relevant to improve the knowledge about protein function or classification. The web server can be freely utilized at https://appsbio.utalca.cl/3d-pp/.

3D-patterns

Conserved patterns

Similarity

zinc ion

algorithm

amino acid sequence

Article

binding site

computer model

cryoelectron microscopy

crystal structure

drug design

enzyme active site

hydrogen bond

molecular docking

protein analysis

Protein Data Bank

protein function

protein structure

protein synthesis

protein unfolding

sequence alignment

signal transduction

virtual reality

X ray crystallography

allosteric site

animal

conserved sequence

human

procedures

protein conformation

sequence analysis

software

Allosteric Site

Amino Acid Sequence

Animals

Conserved Sequence

Humans

Protein Conformation

Sequence Analysis, Protein

Software