BINF 731

Protein Structure Analysis

Iosif Vaisman

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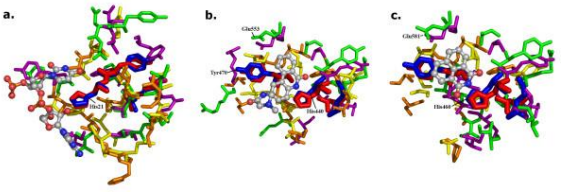
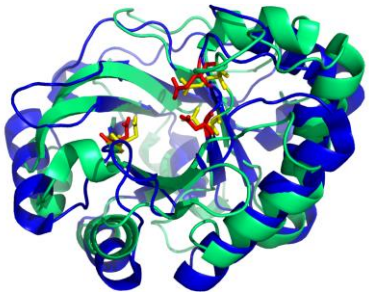


Prediction of function from structure using ProFunc.

Three reverse template matches for PDB entry 2aua, a protein of unknown function from Bacillus cereus. The matches are to the catalytic domains of three toxins: a) diphtheria toxin from *Corynebacterium diphtheriae* (PDB code 1f0l), b) exotoxin A from Pseudomonas aeruginosa (PDB code 1 × k9) and c) cholix toxin from Vibrio cholera (PDB entry 3ess). In each case, the template residues from the 2aua query structure are shown in thick, red sticks while the corresponding residues in the target structure are shown as thick, blue sticks. Neighbouring identical residues, in equivalent 3D positions, are shown in purple for 2aua and green for the target, while similar residues are shown in orange for 2aua and yellow for the target. The inhibitor molecules bound in the target structures are shown in ball-and-stick representation and are: a) adenylyl-3'-5'-phospho-uridine-3'-monophosphate, b) N-(6-oxo-5,6-dihydro-phenanthridin-2-yl)-N,N-dimethylacetamide and c) 1,8-naphthalimide. Catalytic residues are labelled using the residue numbering of the corresponding PDB entries.

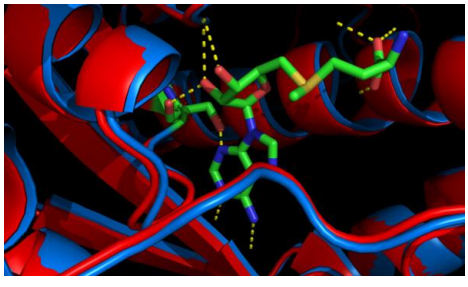
D.Lee et al., 2011



Refining function prediction using ProFunc.

Structural superposition of an uncharacterised protein with a possible functional annotation following sequence analysis (PDB entry 1sfs, in blue) and its top reverse template match, a bacterial muramidase (PDB entry 1jfx, in green). The folds of the two proteins are similar. The residues depicted by yellow sticks are the known catalytic residues in 1jfx (Asp9, Asp98 and Glu100), while the red sticks show the equivalenced residues in 1sfs (Asp9, Asn102 and Glu104).

D.Lee et al., 2011



Explaining the effect of an nsSNP using a homology model based on a MCSG structure.

The interaction between S-adenosyl methionine (SAM) and mitochondrial tRNA-specific 2-thiouridylase 1. The Ala10Ser variant probably introduces a hydrogen bond between SAM and the enzyme that increases binding affinity and thus slows down SAM release hence reducing activity. The wild type model is shown in red and the Ala10Ser variant is shown in blue. The variant residue and SAM are coloured according to their atom types and potential hydrogen bonds are shown in yellow.

D.Lee et al., 2011

STRING is a database of known and predicted protein interactions. The interactions include direct (physical) and indirect (functional) associations; they are derived from four sources:

Genomic Context	High-throughput Experiments	(Conserved) Coexpression	Previous Knowledge

STRING quantitatively integrates interaction data from these sources for a large number of organisms, and transfers information between these organisms where applicable. The database currently covers 9'643'763 proteins from 2'031 organisms.

http://string-db.org/