
ProBiS-ligands Server

2014

User's Guide

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Background

ProBiS-ligands web server predicts binding of ligands to a protein structure. Starting with a protein structure or binding site, ProBiS-ligands first identifies template proteins in the Protein Data Bank that share similar binding sites. Based on the superimpositions of the query protein and the similar binding sites found, the server then transposes the ligand structures from those sites to the query protein.

Software Requirement

ProBiS-ligands web server requires latest browsers that support HTML5 to use the Jsmol molecular viewer.

Input

The screenshot shows the ProBiS-ligands web server interface. The main heading is "ProBiS ligands" with a logo on the left and "Protein Binding Sites Detection" on the right. Below the heading, there is a search bar with the placeholder "e.g., PDB ID" and a "Search" button. The main content area is titled "Predict Ligands by Similarity in Binding Sites" and contains several input fields and checkboxes. The interface is annotated with six numbered steps: 1) PDB ID & Chain ID, 2) Select binding site (optional), 3) Change cutoff score for similar binding sites, 4) Search only for non-flexible similarities in binding sites, 5) Email (optional), and 6) Submit job. A yellow box highlights a pre-calculated local structural similarity profile for PDB entry 1azeA. A 3D molecular model of a protein is shown in the Jmol viewer, with a binding site highlighted in yellow. The right sidebar contains a "ProBiS-ligands in Brief" section with a 3D model and a "Contact" section with a form for user feedback.

1a) Get results from the ProBiS-Database

Predict Ligands by Similarity in Binding Sites

Pre-calculated local structural similarity profile is ready for a protein with >95% seq. id. Click here to show ProBiS-Database results for PDB entry 1azeA.

PDB ID: [1aze] Chain ID(s): [A]

Upload a PDB file

1) PDB ID & Chain ID

Select Binding Site (optional) 2) Select binding site (optional)

Loading of the protein in JSmol viewer may take a minute for the first time!

Binding site on chain A defined as a region within 3 Å of chain B (yellow)

3) Change cutoff score for similar binding sites

4) Search only for non-flexible similarities in binding sites

5) Email (optional)

6) Submit job

Figure 1. ProBiS-ligands input page. If the user checks the “Local Alignments Only” checkbox, ProBiS algorithm will run with the “-local” option, and will only find near perfect local structural alignments with about <2 Å root mean square deviation (RMSD) between the aligned residues. Otherwise, residues with up to 7 Å

RMSD will be considered in the alignments, which allows to find similar, but flexible residues in compared proteins.

Output

ProBiS-ligands output page is shown in Figure 2.

ProBiS ligands Protein Binding Sites Detection
As of Nov 30, 2013 your protein is compared with 37643 structures

e.g., PDB ID Search HOME | HELP

1D0C, Chain A : 100 similar structures

Click to view invariant binding site residues in JSmol viewer

Click to view 3D model of transposed ligand in JSmol viewer

Show conservation scores on the query protein

Change representation of the query protein (currently shown as green ribbons)

Structure	Cluster	Name	Source	BSite	Ligand
	1	N-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-amine	3b3p	Remove 3D	Remove 3D
	1	N-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-amine	3y5s	View 3D	View 3D
	1	2-[[2-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-yl]ethyl]pyridin-3-amine	3ynp	Remove 3D	Remove 3D
	1	6-[[[(3r,4s)-4-[(2-[[2-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-yl]ethyl]pyridin-3-yl]ethyl]amino]ethyl]pyridin-2-yl]pyridin-3-amine	3n1b	View 3D	View 3D
	1	6-[[[(3r,4s)-4-[(2-[[2-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-yl]ethyl]pyridin-3-yl]ethyl]amino]ethyl]pyridin-2-yl]pyridin-3-amine	3n1e	View 3D	View 3D
	1	6-[[[(3r,4r)-4-[(5-(6-aminopyridin-2-yl) pentyl)oxy]pyridin-2-yl]pyridin-3-amine	3u7v	View 3D	View 3D
	1	6,6'-[pyridine-2,6-diyldiethane-2,1-diylbis(4-methylpyridin-2-yl)]pyridin-3-amine	3n5y	View 3D	View 3D
	1	N-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-amine	3jvs	View 3D	View 3D
	1	6,6'-[[2-(2s,3s)-2-aminobutane-1,3-diyl]bis(oxymethone)]pyridin-2-amine	3nqn	View 3D	View 3D
	1	N-[(3s,4s)-4-[(6-amino-4-methylpyridin-2-yl) methyl]piperidin-3-yl]pyridin-2-amine	3jvw	View 3D	View 3D
	1	6,6'-[[2-(2s,3s)-2-aminobutane-1,3-diyl]bis(oxymethone)]pyridin-2-amine	4i5g	View 3D	View 3D

Toggle Labels Ligands Spacefill Spin Asymmetric Unit

Variable Structurally Conserved

Reset View Download PDB Download PNG Hide Query Black Background Conservation View

Figure 2. ProBiS-ligands output page. Left: Jsmol viewer. Right: predicted ligands (small molecule tab open).

JSmol Help

Some key tips on how the user can manipulate the 3D protein model in JSmol are presented in Figure 3.

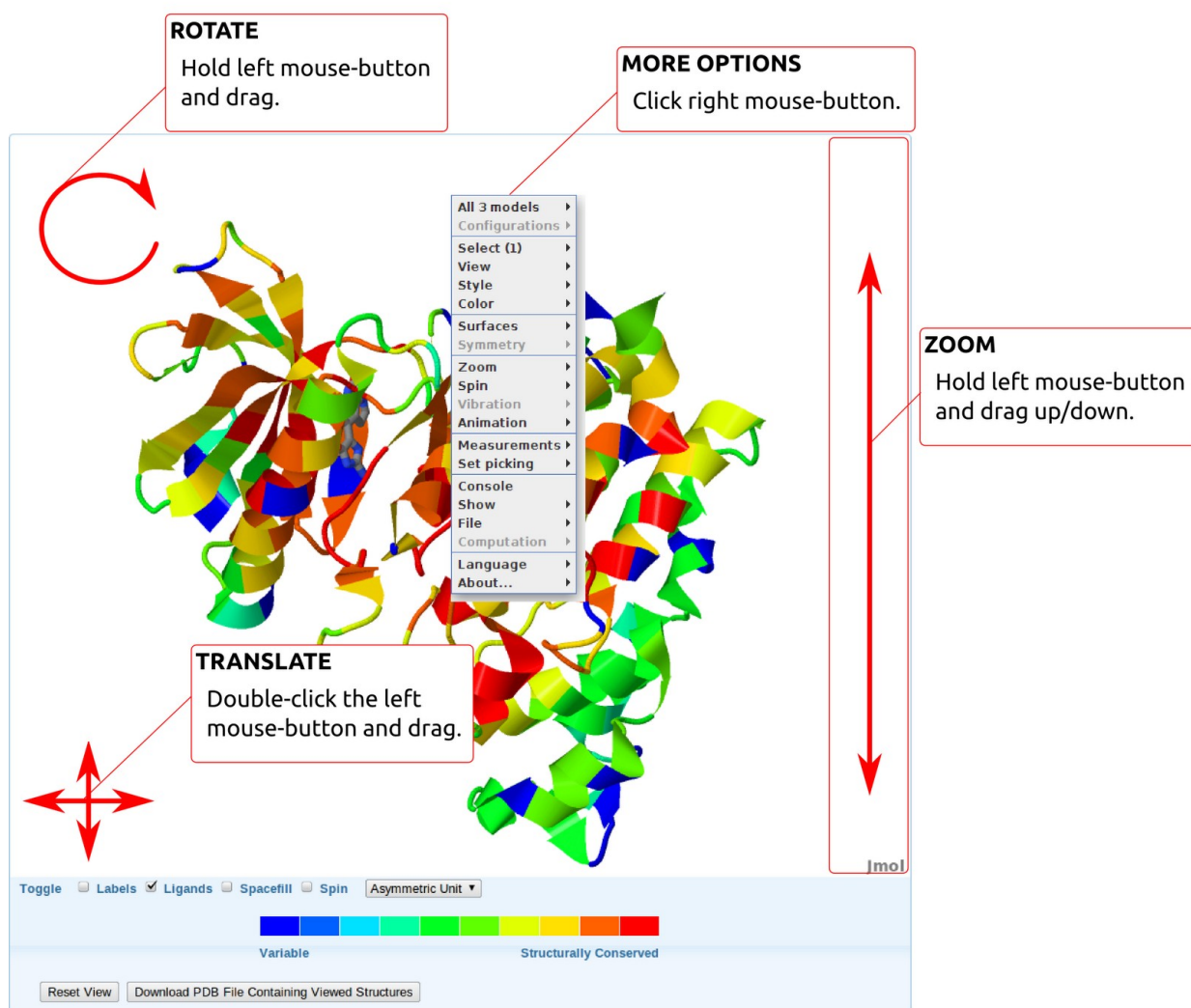


Figure 3. Mouse operations in JSmol.