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

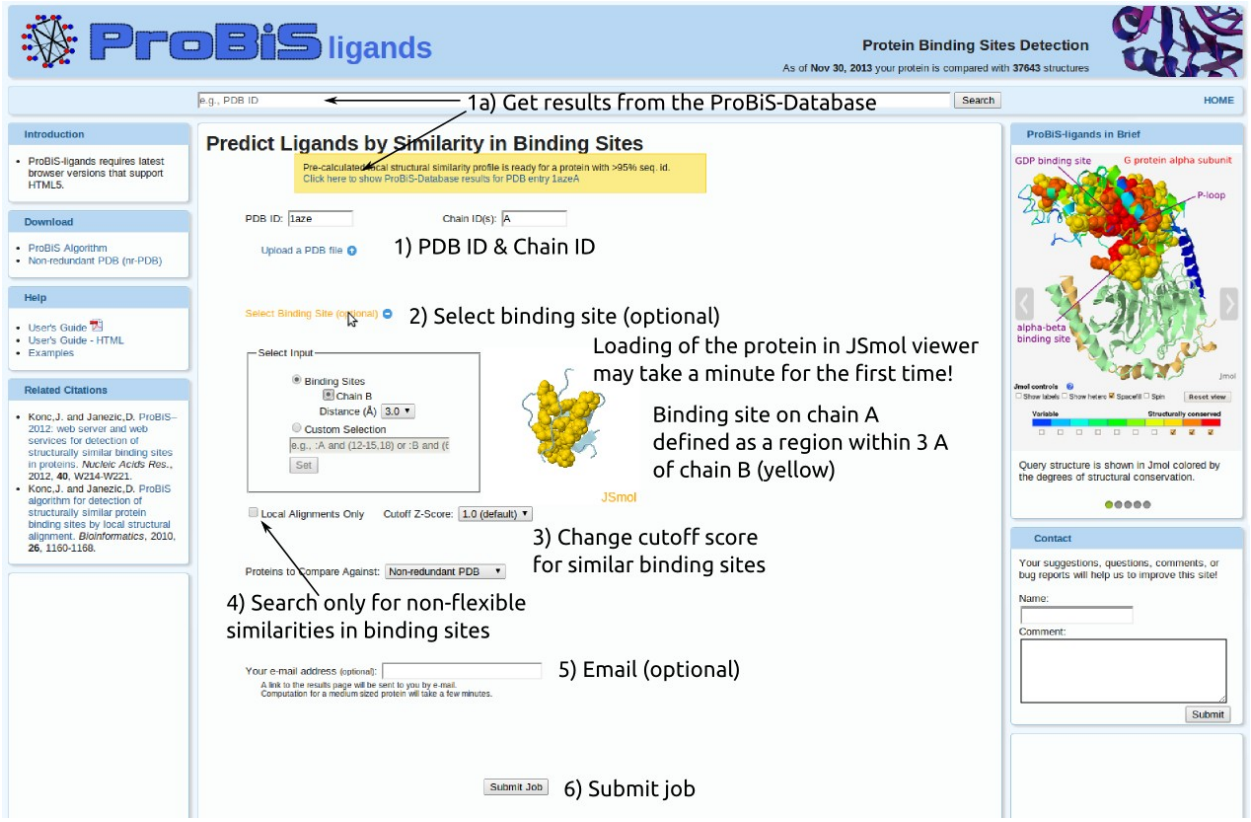

Figure 1. ProBiS-ligands input page. If the user checks the “Local Alignments Only” checkbox, ProBiS algorithm will run with the “-local” option, and will only find near perfect local structural alignments with about <2 Å root mean square deviation (RMSD) between the aligned residues. Otherwise, residues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

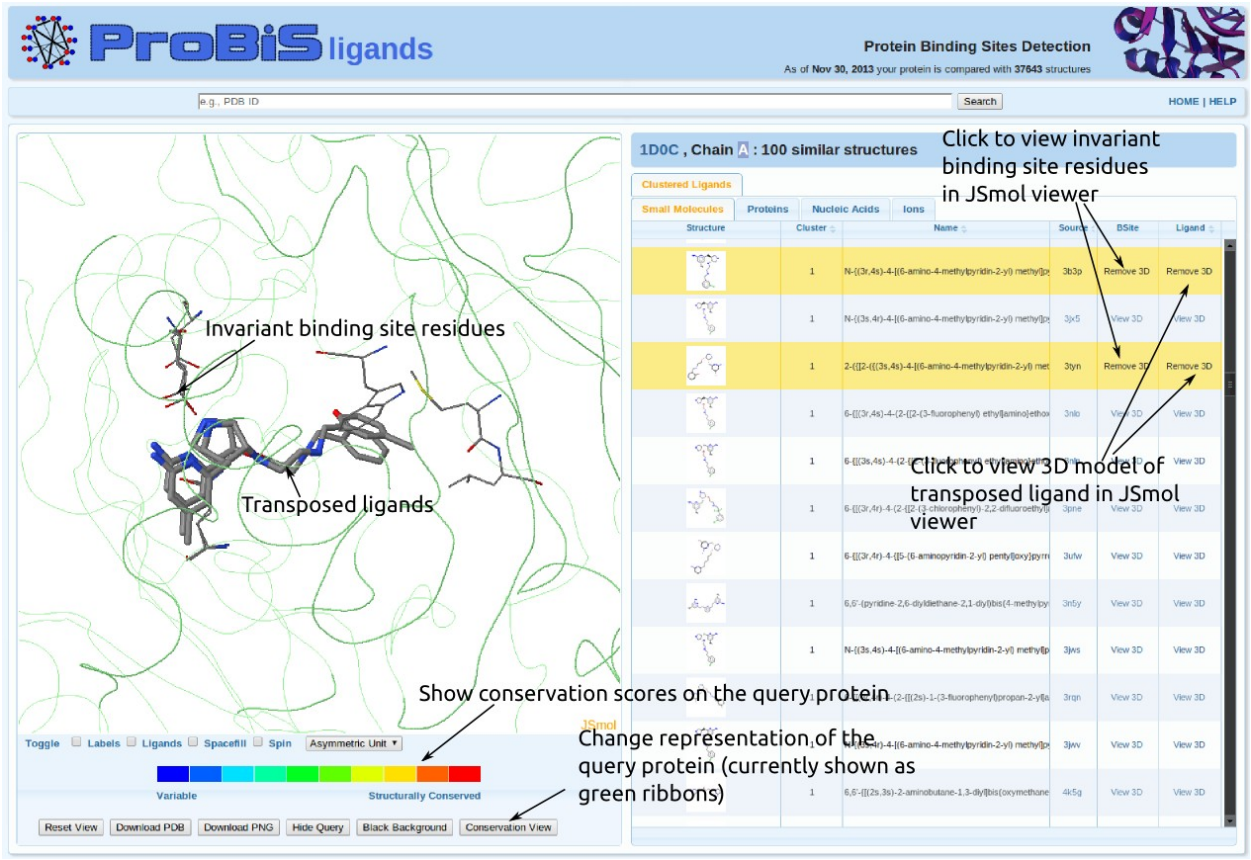

Figure 2. ProBiS-ligands output page. Left: Jsmol viewer. Right: predicted ligands (small molecule tab open).

JSmol Help

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

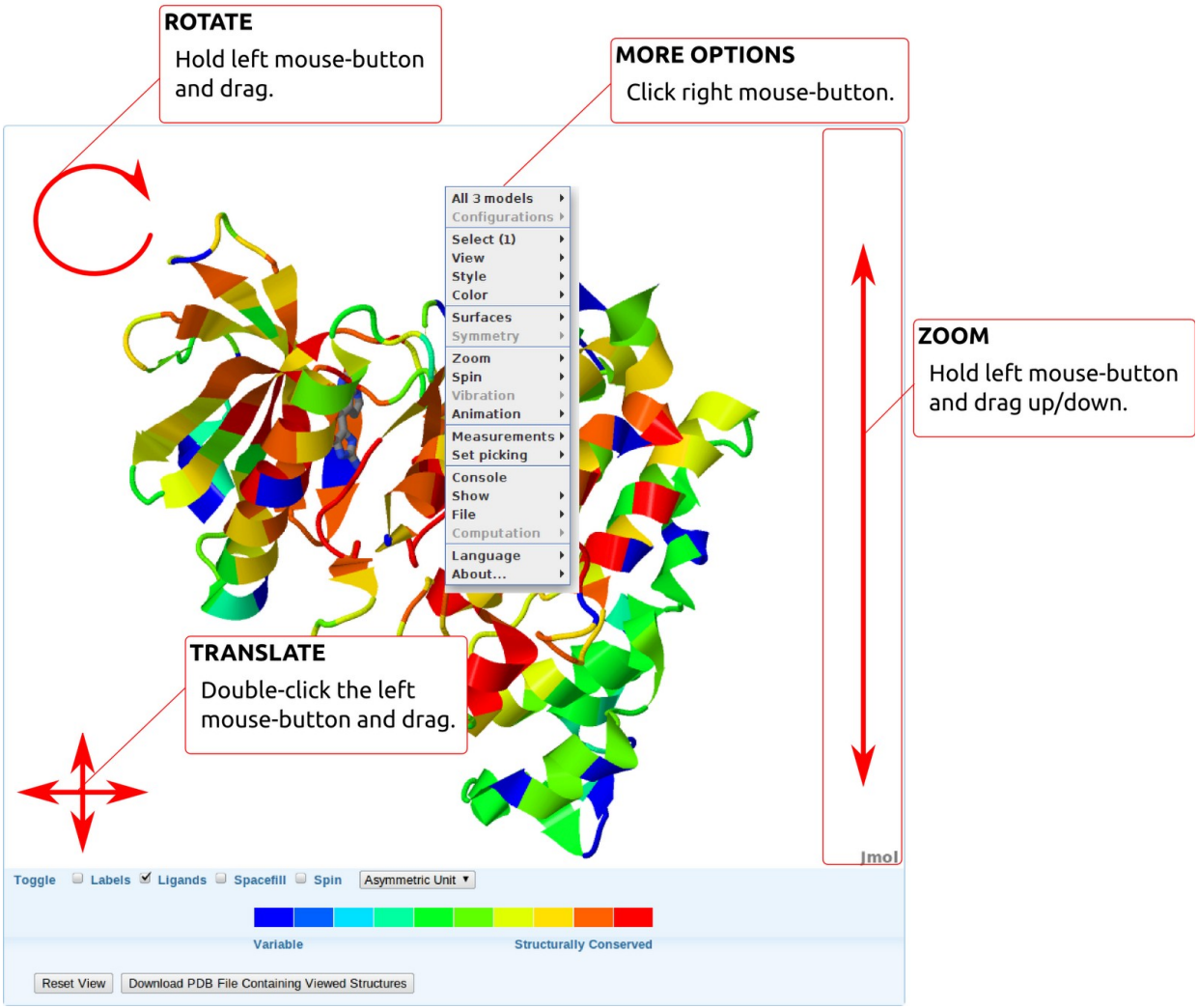

Figure 3. Mouse operations in JSmol.