



Sanjeevini mobile application for Android devices

Supercomputing Facility for Bioinformatics & Computational Biology
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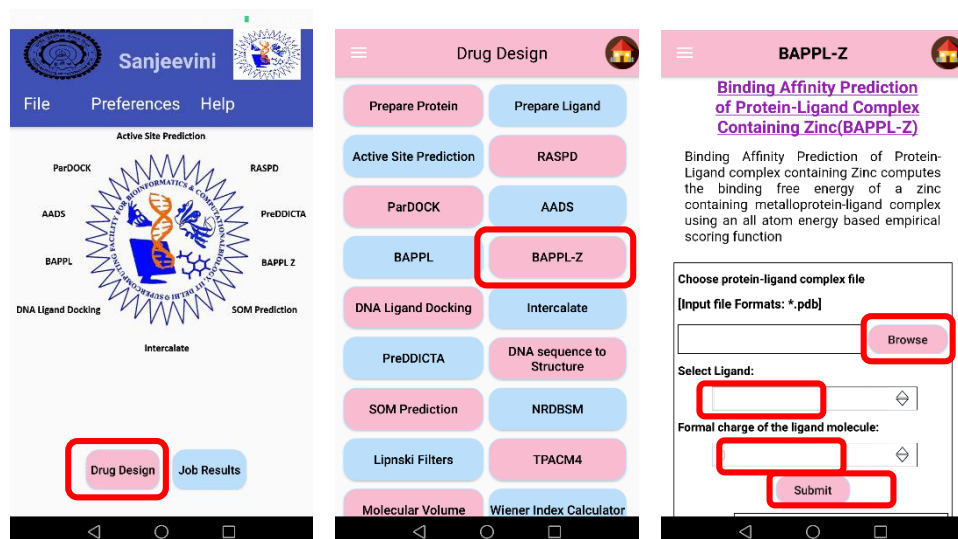
Tutorial Section

Module name: BAPPL-Z

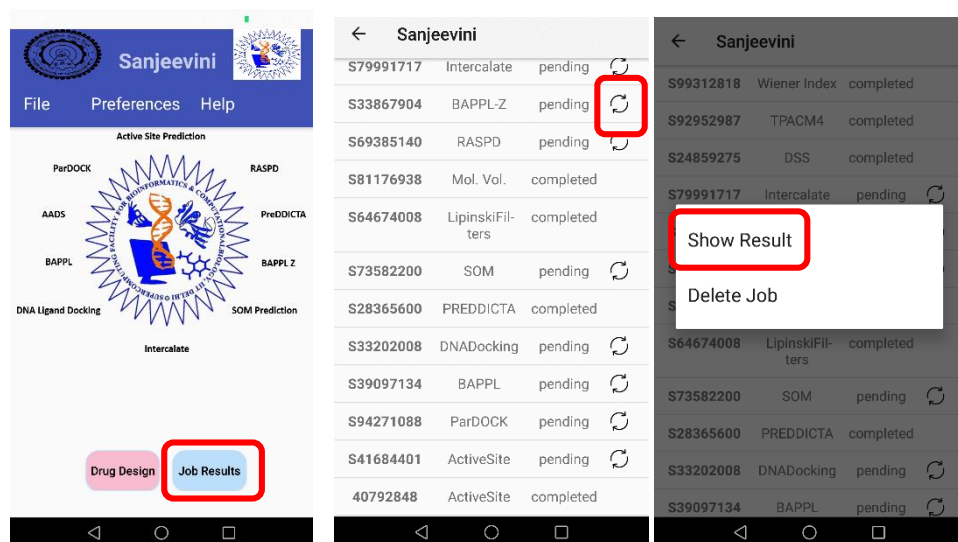
Description: Tool to predict the Gibbs free energy for Zinc-Protein-ligand complexes. It requires hydrogen added, energy minimized protein-ligand complex with zinc as input. The tool calculates formal charge using pre-calculated partial charges radius and epsilon on the input file Formal charge of candidate molecule is optional. File formats supported for zinc-protein-ligand complex: pdb.

Example usage: (Examples are provided at: /storage/emulated/0/Sanjeevini/Examples/BAPPLZ/)

Job Submission:



Results example:



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