BAPPL

Binding Affinity Prediction of Protein-Ligand (BAPPL) server computes the binding free energy of a non-metallo protein-ligand complex using an all atom energy based empirical scoring function.

BAPPL server provides two methods as options:

Method 1 : Input should be an energy minimized protein-ligand complex with hydrogens added, protonation states, partial atomic charges and van der Waals parameters (R* and ε) assigned for each atom. The server directly computes the binding affinity of the complex using the assigned parameters.

Method 2 : Input should be an energy minimized protein-ligand complex with hydrogens added and protonation states assigned. The net charge on the ligand should be specified. The server derives the partial atomic charges of the ligand using the AM1-BCC procedure and GAFF force field for van der Waals parameters. Cornell et al. force field is used to assign partial atomic charges and van der Waals parameters for the proteins.

For the purpose of validation of the empirical scoring function a dataset of 161 non-metallo protein-ligand complexes has been prepared.