Q. What is AADS?

AADS is an Automated Active site detection, Docking, and Scoring protocol for proteins with known 3D structure.

Q. How to site AADS?

Singh T, Biswas D,and Jayaram B. (2011) AADS-an automated active site identification, docking, and scoring protocol for protein targets based on physicochemical descriptors. J Chem Inf Model. 24;51(10):2515-27. doi: 10.1021/ci200193z.

Q. Does it also take the 2D structure of the protein as input?

No, AADS accept only 3D structure of protein in PDB format.

Q. What is the accepted format of input ligand in AADS?

AADS accept only hydrogen added ligand in PDB format.

Q. How are active sites sorted in AADS?

AADS sort active sites based on number of hydrogen-bond donor and acceptors, hydrophobic groups of the functional groups lining the active site and the volume of the cavity.

Q. Can I skip active site prediction and go straight to docking?

No, users can do docking only after active site prediction by AADS. Only docking is not allowed.

Q. How much time does AADS take to run a job?

AADS predicts active site in 3-4 seconds and performs docking with top-ten cavities in about 30 minutes.

Q. What is formal charge?

The formal charge is the difference in the number of valence electrons in the atom and the number of valence electrons in the Lewis structure.

Q. How can I resolve “error in input file”?

Please correct the format of input file according to the manual.