DockBench: A useful tool to compare performances of docking protocols.

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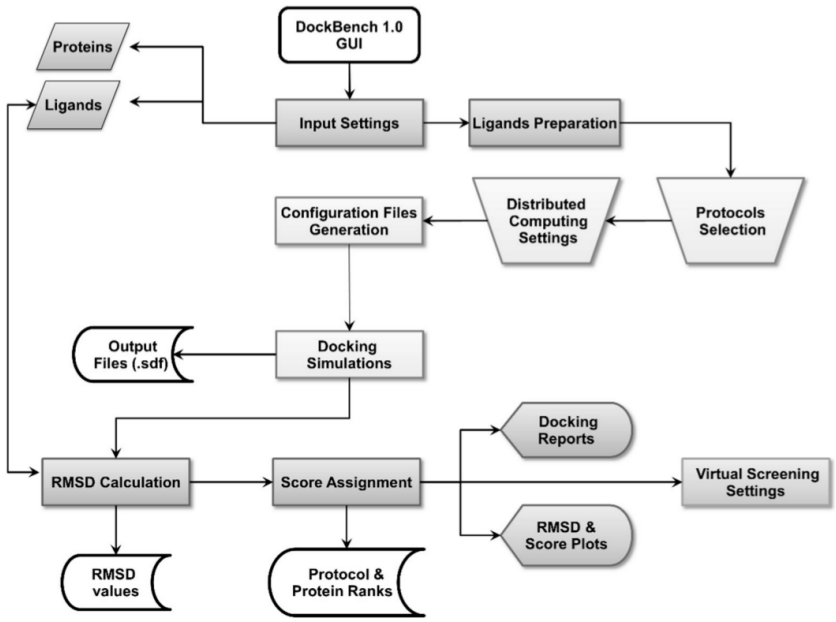
Nowadays, computational chemistry is a useful tool to identify and/or optimize novel and selective ligands for a particular protein. Docking programs are usually successful in reproduce the crystallographic binding mode, whereas scoring functions are much less successful to identify the corresponding “bioactive” binding mode. Therefore, it is important to determine which is the best docking protocol for the studied protein before performing computational simulations.[1]

In this work we present DockBench,[2] a useful tool to compare the performances of different docking/scoring combinations (Figure 1). To evaluate the performance of each protocol, the presented tool uses a novel consensus-based function defined as “Protocol Score” based on RMSD average value and the number of conformations generated by docking algorithm having a RMSD lower than the crystal structure resolution (R). The best 20 crystal structures of the protein Chk1 in complex with inhibitors were used as a case study.[3]

Figure 1. DockBech 1.0 workflow. The platform is accessed through a GUI.



References

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