Pharma-Dock, another docking server based on free software

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Molecular docking algorithms have been used as a tool to test a hypothesis about the binding affinity of small ligands to pharmaceutical targets. Unfortunately, user accessibility to this kind of software made them very popular among users that require a fast explanation for some experiments. There exist any kind of online tutorials to learn how to use docking software without any recommendation about statistical considerations or cautions that as user must have to use them.

Here, we present a web server that will try to correct this issue. Pharma-dock is a web server based on free software that makes use of molecular dynamics simulations to improve the statistical results. Users may choose to use crystallographic coordinates, minimized structures, last structure or center-cluster structure based on clustering analysis from the molecular simulation as receptor structure and if they will like to use the entire protein (blind docking) or binding site coordinates (directed docking). Also, to estimate the statistical error associated with individual docking runs any docking submitted may report at least 3 (3, 10, 100 and 1000) independent docking experiments. Documentation associated with Pharma-dock gives a detailed explanation about the advantage to use these parameters.