DOCKFACE: an easy to use application programming interface (API) for virtual ligand screening (VLS) using AUTODOCK software.

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Abstract:
Docking studies could be used as a useful method in order to decrease the expenses for the time consuming procedure of drug development. VLS based on docking simulation are widely used in many computational programs. The most cited application to perform docking studies is AUTODOCK software at the time being. An important issue with AUTODOCK is its limitations in virtual screening. The user is not therefore able to perform successive runs of docking in an automatic manner. For this purpose an easy to use interface was prepared for automatic docking of all ligands on the target. The interface is able to use all system resources to perform the screening task. The interface was prepared by means of batch scripting to make it compatible with all windows platforms (including XP, 7 and 8). In order to evaluate the efficiency of the prepared API, 3000 ligands of different targets were docked and the results revealed the efficiency of this application in VLS. An important advantage of this API is that, the preparation procedure for ligand and receptor is being done on the most used operating system (WINDOWS) while the time consuming procedure of docking is performable on both Linux and Windows operating systems. This feature permits the users to perform the screening task on both Linux and Windows servers.

Keyword: Docking, Virtual ligand screening, Application Programming Interface (API)