DockThor Web Server

The DockThor receptor-ligand docking program and the respective web server were developed by the GMMSB-LNCC (Molecular Modeling of Biological Systems) research group, member of INCT-INOFAR.

The DockThor web server (www.dockthor.lncc.br) was released during the 65 SBPC (Recife-PE, 2013). The use of the web server is free for the international academic community. DockThor constitutes the first brazilian docking program (and possibly the first docking program for the entire southern hemisphere). The web server uses the computational facilities provided by the Brazilian high performance platform (SINAPAD - https://www.lncc.br/sinapad/) and its development is also supported by INCT-INOFAR. The DockThor performance was evaluated through a comparative analysis of redocking experiments with three of the most widely used docking programs (i.e., Glide, GOLD and Autodock Vina). These comparative studies indicate that the program is very competitive in the capacity to predict the correct receptor-ligand binding modes and has a great potential to be widely used by the scientific community in real rational drug design projects.

Since its release the DockThor web server was accessed by more than 1330 unique visitors. In Brasil only the Acre and Tocantins states had no researches accesing the portal. About 30% of accesses are from foreign researches (23% from EUA and 7% from more than 20 countries). In the first half of the year the web server had ~1000 jobs submitted.

Currently are in development free energy empirical functions to predict protein-ligand binding affinities and one methodology based on the ensemble docking approach to incorporate the receptor flexibility. These developments will be integrated into a future web server version DockThor-VS for high throughput ligand virtual screening. This version will be integrated to the INCT-INOFAR projects (use of ligand libraries and specific molecular targets studies) and will use the SINAPAD computational platform. In the begining of 2105 is expected the arrival of a super-computer with 1,2 petaflops (expected to double in 2016). With the implementation of this super-computing platform it will be possible to provide the free use of the DockThor-VS web server to a wide variety of Brazilian research groups conducting studies in the rational drug design research field.