3rd Brazil-France Symposium on Medicinal Chemistry
Maceió/AL | November 12 -14, 2024

DUNASCREEN: AN AUTOMATED TOOL FOR STRUCTURE-BASED VIRTUAL SCREENING

Rodrigo O. Lourenço (G)[1], Euzébio G. Barbosa (Prof)[1].

rodrigo.oliveira200310@gmail.com;

[1] *Laboratório de Química Farmacêutica Computacional – Universidade Federal do Rio Grande do Norte – UFRN – Rua General Gustavo Cordeiro de Faria, S/N, Petrópolis, CEP 59012-570, Natal – RN – Brasil.*

Keywords: Structure-Based Virtual Screening: Molecular Docking; Bioinformatics.

ABSTRACT

Background: Structure-Based Virtual Screening (SBVS) is a method for discovering bioactive compounds through in silico testing, which involves screening a library of ligands by evaluating their interaction with the target site of a specific receptor. This process is conducted through molecular docking using different types of scoring functions. Thus, the ligands with the best scores can be prioritized for possible modifications to their molecular structure or selected for further research stages. SBVS is applied in medicinal chemistry with the aid of computers; however, it is still a process that, in some cases, is performed manually, without automation. **Objectives:** This work aims to develop software to automate certain processes of SBVS, expedite steps in the discovery of bioactive molecules, and integrate knowledge between pharmacy and bioinformatics. **Methods:** The initial focus of this work is the development of software named DunaScreen, which is capable of automating docking processes with SBVS and managing the projects developed within a workspace. The program integrates two external molecular docking algorithms, Autodock Vina and Protein-Ligand ANTSystem (PLANTS), each with its own configurations defined by the user. The automation arises from the tool's ability to manage the input and output processes of the algorithms following the SBVS model; that is, when defining a ligand library and a receptor, the software is responsible for managing the preparation of 3D molecules, executing the dockings, and obtaining scores using the algorithms. Additionally, the work includes a quantitative approach to analyze the differences and similarities between the best scores, results from tests using the same ligand libraries and receptor, as well as measuring the processing time of the tests. **Results and Discussion:** Recent tests with the software demonstrate satisfactory integration with the docking algorithms, effective management and operation of the workspace, and adequate filtering of results through the scores. Furthermore, during the tests, a distinction was noted in the filtered scores obtained when applying a large number of ligands to the same target site while using both algorithms. Differences in the 3D anchoring conformations at the target site of the same ligand were also observed when using different algorithms. The execution time, in turn, is relative to the processing capabilities of the computer, the molecules used, and the algorithm, but has shown greater advantages compared to manual SBVS use. **Conclusion:** Therefore, the software, now operational for screening activities, has demonstrated significant advances in its development. In this regard, the program should be refined to incorporate new configuration possibilities and utility for the end user. Ultimately, it is intended that the tool be used for research purposes in molecule discovery by the study group.