Octopus: A Virtual High Throughput Screening Platform for Multi-Compounds and Targets

Alex G. Taranto[a](PQ), Bianca dos R. Santos[b] (IC), Marina S. Costa[b] (IC), Vinícius A. Campos[b] (IC), Iann G. Lima[b] (IC), Alisson M. da Silva[b] (PQ).

[a] *Universidade Federal de São João del-Rei - UFSJ, Campus Centro Oeste, Divinópolis- MG, Brazil.*
[b] *Centro Federal de Educação Tecnológica de Minas Gerais – CEFET-MG, Divinópolis-MG, Brazil.*

labqf_ufsj@ufsj.edu.br

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INTRODUCTION

Octopus is a software for virtual screening (VS) through AutoDock Vina. It can perform fast and friendly docking simulation. Differently from others VS platforms, *Octopus* can perform docking simulations of unlimited number of compounds into a set of molecular targets. In this work, we selected a successful case, which was addressed for biological assay.

METHODS

Octopus is able to integrate MOPAC2012 and AutoDock Vina. After the ligands generated in any draw package in protein data bank (PDB) format, the *Octopus* has carried out geometry refinement using the semi-empirical method PM7 implemented on MOPAC2012. Docking simulation was carried out on Our Own Molecular Targets (OOMT)[1] databank by AutoDock Vina. Finally, the proposed software compiles the best binding energy into standard table.

RESULTS AND DISCUSSION

A sets of compounds were generated and submitted on *Octopus*. As a result, the molecular target under code PDB 1GKC was found by VS process with -9.5 Kcal/mol binding energy, against -6.6 Kcal/mol of crystallographic ligand. Figure 1 summarizes the intermolecular interaction between 1GKC and ligand. This molecular target is a metalloprotease involved in cancer pathology. Following, all compounds were addressed for biological assay. As a result, the compound LE&007 was able to inhibit with 80% of enzymatic activity.

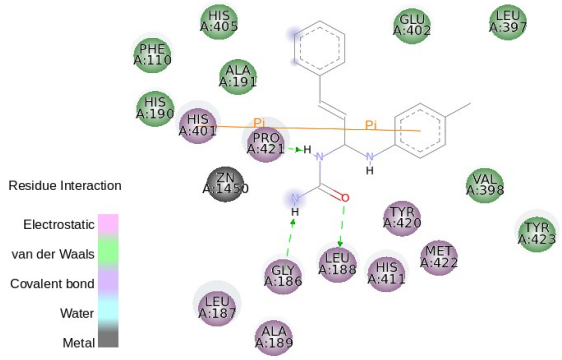

Figure 1. The intermolecular interaction LE&007 ligand in the binding site of 1GKC.

CONCLUSIONS

This successful example illustrated the performance of *Octopus* to find correct molecular targets. In other words, the software summarized the number of biological assay. Hence, it was able to find a new hit for lead compound optimization, that in this case, a new anti-neoplastic drug. Moreover, *Octopus* has a friendly gearing implemented on all Linux-based operation system for which MOPAC2012 and AutoDock Vina have been developed. Further development of molecular dynamics simulation routines are in progress.

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(1) A. P. Carregal, M. Comar Jr, A. G. Taranto. (2013) Our Own Molecular Targets Data Bank (OOMT). *BBR - Biochem. Biotechnol. Reports* 14–16.