nAPOLI: a web tool for protein-ligand interactions analysis

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Elucidating the mechanisms involved in the molecular recognition and which forces contribute to the recognition is a central problem in biology, since the interactions between two molecules are extremely important to biological systems as a whole and are very toilsome to be predicted even for small molecules. Nowadays, many interesting tools exist to analyze protein-ligand interactions, however, none of them presents large scale statistical, visual and interactive analysis. Thus, users must perform their comparison manually, that is completely infeasible. Therefore, we propose an easy and intuitive tool through visual strategies to depict the patterns and the types of interactions established between proteins and their ligands. In order to achieve it, we propose nAPOLI (Analysis of PrOtein Ligand Interactions), an interactive web tool to study the protein-ligand interactions in large scale by using visual strategies and statistical analysis. Since from the first version, many improvements were added to nAPOLI as well as new features. nAPOLI as a server allows users to submit their own dataset or to use PDB files from the PDB.org database. Moreover, many interactive functionalities were designed in this version like, for example, the 3D and 2D-view of protein-ligand complexes, comparison between clusters and download of data. Additionally, we performed improvements in the method used to calculate interactions which contributes to detect accurately such interactions. Some of them are: hydrogen bonds are now detected by using angle; atoms properties were better defined by using properties like pH and atoms charge; and the cutoff used to set interactions were also redefined to improve nAPOLI results; etc. Finally, we compared nAPOLI to other two tools that is CREDO and LIGPLOT. Through this comparison we could show that nAPOLI presents accurate results regarding to these tools. Thus, nAPOLI showed to be very accurate and useful as it shed some light on the problem of discovering what is conserved in a set of ligands and which interactions they establish with a receptor.

Supported by: Brazilian agencies Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG), Financiadora de Estudos e Projetos (FINEP) and Pró-Reitoria de Pesquisa da Universidade Federal de Minas Gerais.