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# Automated tool for virtual screening and pharmacology-based pathway prediction & analysis

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## Abstract

The virtual screening is an effective tool for the lead identification in drug discovery. However, there are limited numbers of crystal structures available as compared to the number of biological sequences which makes (Structure Based Drug Discovery) SBDD a difficult choice. The current tool is an attempt to automate the protein structure modelling and automatic virtual screening followed by pharmacology-based prediction and analysis. Starting from sequence(s), this tool automates protein structure modelling, binding site identification, automated docking, ligand preparation, post docking analysis and identification of hits in the biological pathways that can be modulated by a group of ligands. This automation helps in the characterization of ligands selectivity and action of ligands on a complex biological molecular network as well as on individual receptor. The judicial combination of the ligands binding different receptors can be used to inhibit selective biological pathways in a disease. This tool also allows the user to systemically investigate network-dependent effects of a drug or drug candidate.

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