In Silico Pharmacology for Drug discovery - Molecular Docking

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Abstract:

In silico means performed on computer or via computer simulation. In traditional pharmacological methods after performing the *In-vivo* experimentation than only the researchers know the activity of the ligand molecule. But now a days in advancement of computer simulation methods for identification and optimization of novel biological ligand is easy task before conducting the *In-vivo* experimentation. Molecular docking is a computational technique that helps in predict and understanding the interaction between the ligand and macro molecular target site. Several docking software's are available for visualization of molecule structure and docking score can also be analyzed with the help of machine tools. The major components in docking are representation of molecules, searching of molecules and scoring of potential solutions. The purpose of this review is to analyze current molecular docking strategies used in drug discovery and medicinal chemistry, exploring the advances in the field and the role played by the integration of structure- and ligand-based procedures.

Key words: Molecular docking, *In-silico*, Drug discovery, Ligand, macro molecule.