

In-silico evaluation of new ligand against sur1 receptor

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Diabetes Mellitus is a metabolic disorder characterized by the hypoglycaemia, glycosuria, hyperlipaemia, negative nitrogen balance & sometimes ketonaemia. Type II Noninsulin-dependent diabetes mellitus (NIDDM), maturity onset diabetes mellitus:- Cause may be (a) Abnormality in glucose receptor of beta-cell so that they respond at high glucose concentration.(b) Reduced sensitivity of peripheral tissues to insulin, reduction in number of insulin receptor, 'down regulation of insulin receptors'. (c) Excess of hyperglycaemic hormone. Prepare a oral drugs an in-silico (Drug Designing) research has been worked-out which is based on some computational tools & on the principle of protein-protein & protein-ligands binding. Protein-protein and protein-ligand interactions are fundamental as many proteins mediate their biological function through these interactions. Many important applications follow directly from the identification of residues in the interfaces between protein-protein and protein-ligand interactions, such as drug design, protein mimetics engineering, elucidation of molecular pathways, and understanding of disease mechanisms. The identification of interface residues can also guide the docking process to build the structural model of protein-protein complexes. This dissertation focuses on developing computational approaches for protein-ligand and protein-protein binding site prediction and applying these predictions to improve protein-ligand docking. The Ligand could be developed with the help of some available software of Bioinformatics like ChemSketch of ACDLabs. The Ligand must follow the Lipinski Rule. After that a Docking procedure is performed with a specified Receptor of a Ligand prepared with the help of such software like Auto-Dock, Virtual Dock. A result that obtained when compared with the result of prescribed drug is lower, than this proved to proposed a more chance of better Ligand against that particular Protein (SUR1- NIDDM).

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