Drug Designing Services Section Front Page

The fast isolation of particular ligands through phage display has a wide variety of applications like epitope mapping, analyzing different protein interactions, vaccine development, drug design, and therapeutic target validation. Phage display is also used to pick inhibitors for the active and allosteric sites of G-protein binding modulatory peptides, enzymes, and receptor antagonists and agonists. There are two major types of drug design: ligand-based drug design and structure-based drug design. In computer aided drug designing the most fundamental goal is to predict whether a given molecule will bind to a target and if so how strongly. Molecular mechanics or molecular dynamics are most often used to predict the conformation of the small molecule and to model conformational changes in the biological target that may occur when the small molecule binds to it.Molecular mechanics methods may also be used to provide semi-quantitative prediction of the binding affinity. The drug is an organic molecule, when it is bind to target site it can either inhibit or activate the function of a biomolecule which results in therapeutic benefit. The drug design involves the design of such molecules that are similar to the bio molecular target site in shape and charge in order to bind to it. Drug design relies on the knowledge of the three dimensional structure of bimolecular targets.