Chem-informatics using structure-based approach

- **Drug Target Database Construction:** A small molecule database is acquired from DrugBank, PDB, and ChEMBL. The protein target database is also built from PDB. The active sites of drug targets will be annotated by defining the reference ligand or using site prediction tool in combination with literature findings. The active sites will be further clustered according to the structure similarity to facilitate a quick target finding.
- **Drug-likeness Filter:** Filtering attempts to eliminate inappropriate or undesirable compounds from a large set before beginning to use them in further studies. The goal is to remove all of the compounds that should not be suggested to a medicinal chemist as a potential hit.
- **Similarity Searching:** To identify the target of the drug-likeness compounds, a three-dimensional similarity searching is performed. The application of chemical similarity analysis in drug design is a commonly used and useful technique.
- **Reverse Docking:** It has been proved that docking has been successfully in identifying targets of given compound. A similar program has been developed by the applicant in MOE. The compound will be docked into the active sites of drug targets one by one and a consensus scoring method will be used to rank the most possible target interacted with given compounds.
- **Target similarity searching:** For given compound with complex structure, predict the interaction with other proteins based on the pocket similarity. Drugs can act on several protein targets, some of which can be unrelated by conventional molecular metrics. Predicting which molecules can bind to a given binding site of a protein with known 3D structure is important to decipher the protein function, and useful in drug design.