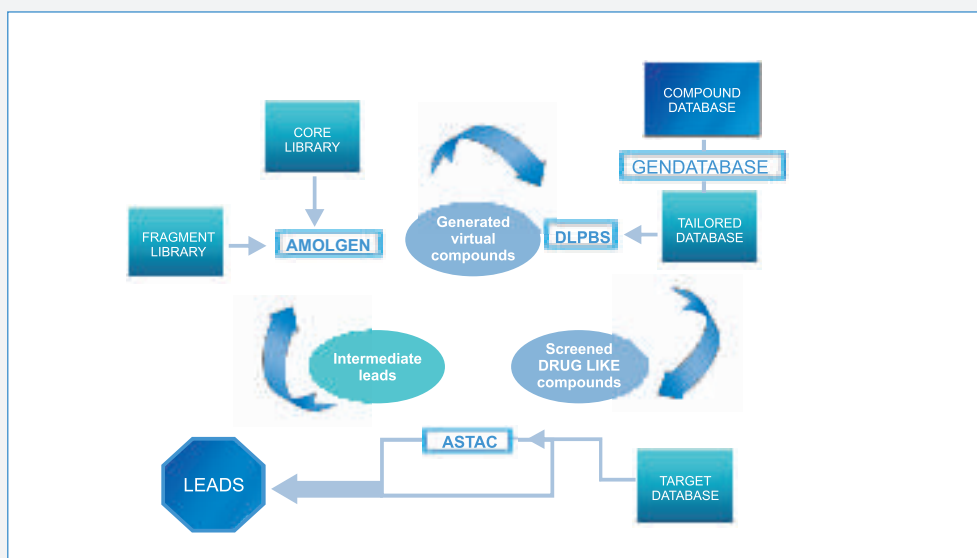


Docking

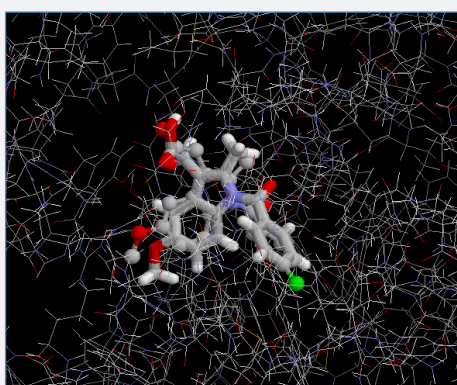
a. Molecular docking:

Chembiotek has developed proprietary (in-house) computational tool for molecular docking based virtual screening of compounds against the 3D model of a desired target, where the interaction energies between the ligand and the target is monitored in terms of electrostatic, van der Waal and solvent contributions. Full flexibility of the ligand is considered and the lowest energy pose is compared to the crystal structure pose for validating the method or ranked to perform virtual screening of compounds against a target. The overall scheme for the docking-based virtual screening is presented below.



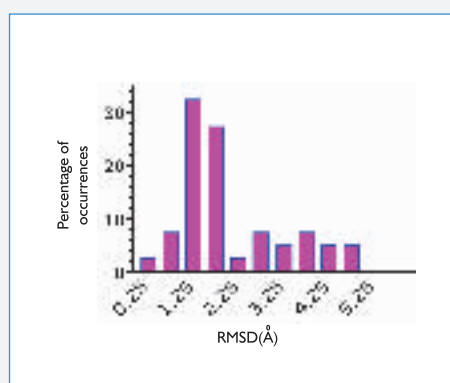
b. Validation of Docking tool:

Validation of our docking tool was done by performing the re-docking experiments using our docking tool for a number of ligand-protein crystal structures. Some signatures of its performance are shown below.



The crystal structure pose is shown by ball and stick model and the docked pose is shown by stick model.

rmsd =0.96Å PDB ID : 4cox.pdb



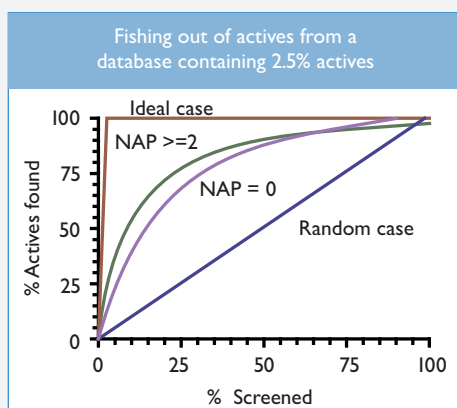
Distribution of the RMSD values between the configurations generated by our docking tool and the respective crystal structure configuration for 40 protein-ligand complexes randomly chosen from RCSB database.

c. Case study of virtual screening of known COX2 inhibitors against COX2.

25 known inhibitors were mixed with 975 randomly chosen compounds from the NCI database and screened against Cox-2 binding site.

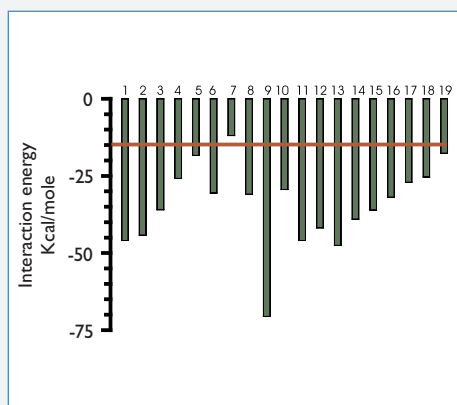
The plot shows the ability of our software to identify known active compounds from the total set.

NAP refers to the number of anchoring points used in the calculation. An anchoring point is defined as having an interaction energy less than -10Kcal/mol . The enhancement factor defined as the ability to enrich for actives increases with NAP.



d. *In Silico* compound profiling:

In Silico profiling of compounds against a panel of target proteins, say a protein family, can be quite useful in developing insight about the potential of the compound to exhibit cross-reactivity. An example is given below considering Staurosporin as the compound profiled against a kinase panel.



A panel of human Kinases was docked with staurosporine to generate an interaction profile.