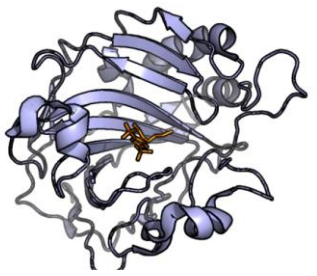
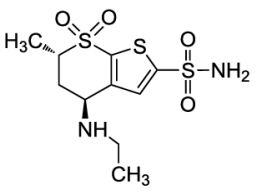
Computer Aided Drug Design Methods



Structure based methods
(The 3D structure of the target must be known)

Ligand based methods
(The 3D structure of the ligand must be known)



Docking

Pharmacophore Analyses
(structure based)

De Novo Analyses

QSAR

Pharmacophore Analyses
(ligand based)

Experimental studies
(*in-vitro, in-vivo*)

LEAD Compound

optimization

Drug Candidate