

Pharmacophore modeling:

Pharmacophore modeling based virtual screening of compounds is a ligand based approach and is useful when the 3D structure of the target is not available but a few known active compounds are known.

We use 'Catalyst under Discovery Studio 2.0' software for pharmacophore modeling and pharmacophore based screening of compounds. HipHop and HypoGen are the algorithms used. We have incorporated 15 databases comprising of 1079987 compounds into the Discovery Studio for virtual screening and identifying novel active compounds in specific cases.

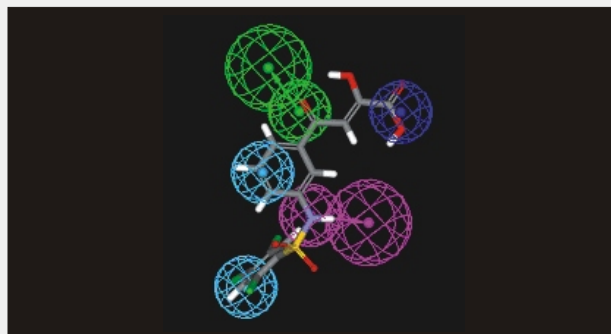
Data bases incorporated into Discovery Studio 2.0

No.	Database Name	Number of compounds	No.	Database Name	Number of compounds
1	Apollo Scientific	19558	9	Lopac	1416
2	Asinex	310697	10	Maybridge	64252
3	Bachem	2748	11	Microsource	2904
4	Chembridge	300718	12	Peakdale	7162
5	Chemstar	59869	13	Pharmek	138059
6	Comgenex	83537	14	Toslab	18180
7	Frinton	1119	15	Tyger	3097
8	IBScreen	66671			

The above databases also enable us to perform docking based virtual screening, using our in-house docking tool.

Example:

This is a pharmacophore model generated for representing the Hepatitis C Virus RNA-Dependent RNA Polymerase inhibitors. The hypothesis consists of five pharmacophoric features, one **H-Bond donor**, one **H-Bond acceptor**, one **negatively ionizable group** and two **hydrophobes**. One potent inhibitor (stick model) has been shown as superposed onto the hypothesis.



We have also developed an in-house tool where several global features of a known compound are used to perform compound screening.

Example:

