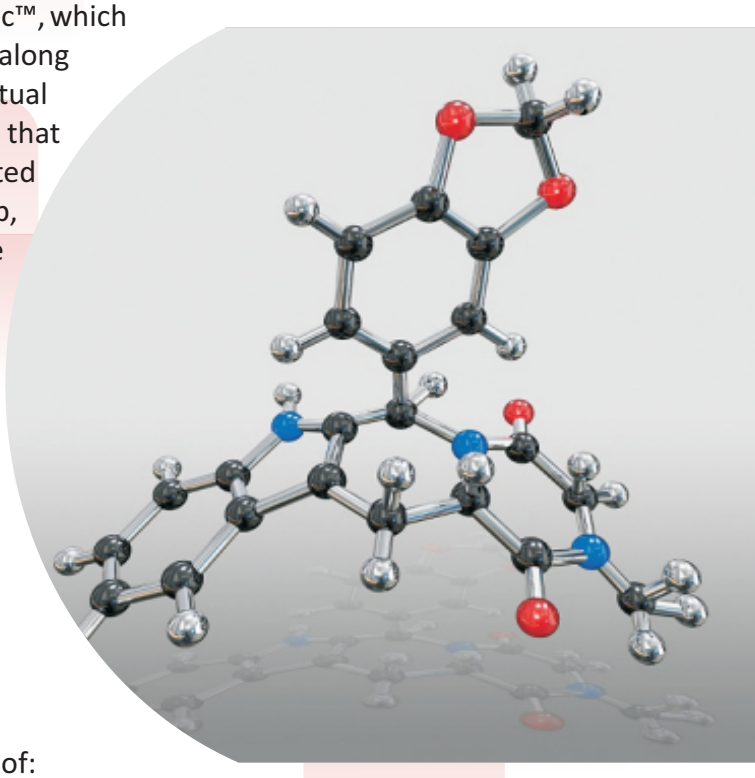
RASA™
LIFE SCIENCE INFORMATICS

vHTS & Scaffold Hopping Package

VirtuoSpec™ of RAASI™ suite designs virtual library based on Pharmacophore, Functionophore and customized scaffolds. Virtual library designing helps in creating an array of chemical structures which can be used in ligand-based or target-based in-silico Drug Designing. We use descriptors and fingerprints to create the desired virtual library

We perform Virtual Library design with the help of VituoSpec™, which is our in-house proprietary platform independent software along with standard tools and algorithms for virtual screening. Virtual library design by VirtuoSpec™ is based on principle that biological, Physical and chemical activity is strongly associated with Chemical intelligent Fingerprints (Functional group, ionic and non-ionic group, donor, Accepter, etc) irrespective of scaffold conservation. Potential hits will be validated through DockSpec™. VirtuoSpec™ 1.0 holds an advantage because it not only relies on scaffolds or Pharmacophore but also on Chemical intelligent Fingerprints information. No distinction is made between a scaffold and the pendant groups, while deriving the conserved Chemical intelligent Fingerprints. Thus by its very nature, the algorithm does not care for the scaffold conservation.



Deliverables

A detailed delivery report for Virtual Library Design consists of:

- VituoSpec™ Categorized Library depending upon Algorithm selected(Pharmacophore, Functionophore and customized scaffolds)
- Molecular scaffold similarity and dissimilarity analysis with the trained molecules in case of Pharmacophore and Functionophore (as Excel file)
- DockSpec™ Giving more weight age to analyzed hits by providing which molecules can be dock for further enhance that analyzed hits are highly believable (as Text file)
- Bioassay and Bio activity analysis (as Text file)
- Extensive literature study (as Document file)

RASA's USP

- SDF
- SMILES
- Any Other format supported by Open Babel

301 Dhanashree Construction, Opp. Chitaranjan Vatika, Model Colony, Shivaji Nagar, Pune. - 411 016.
Tel: 020-65600 408. E-mail: info@rasalsi.com