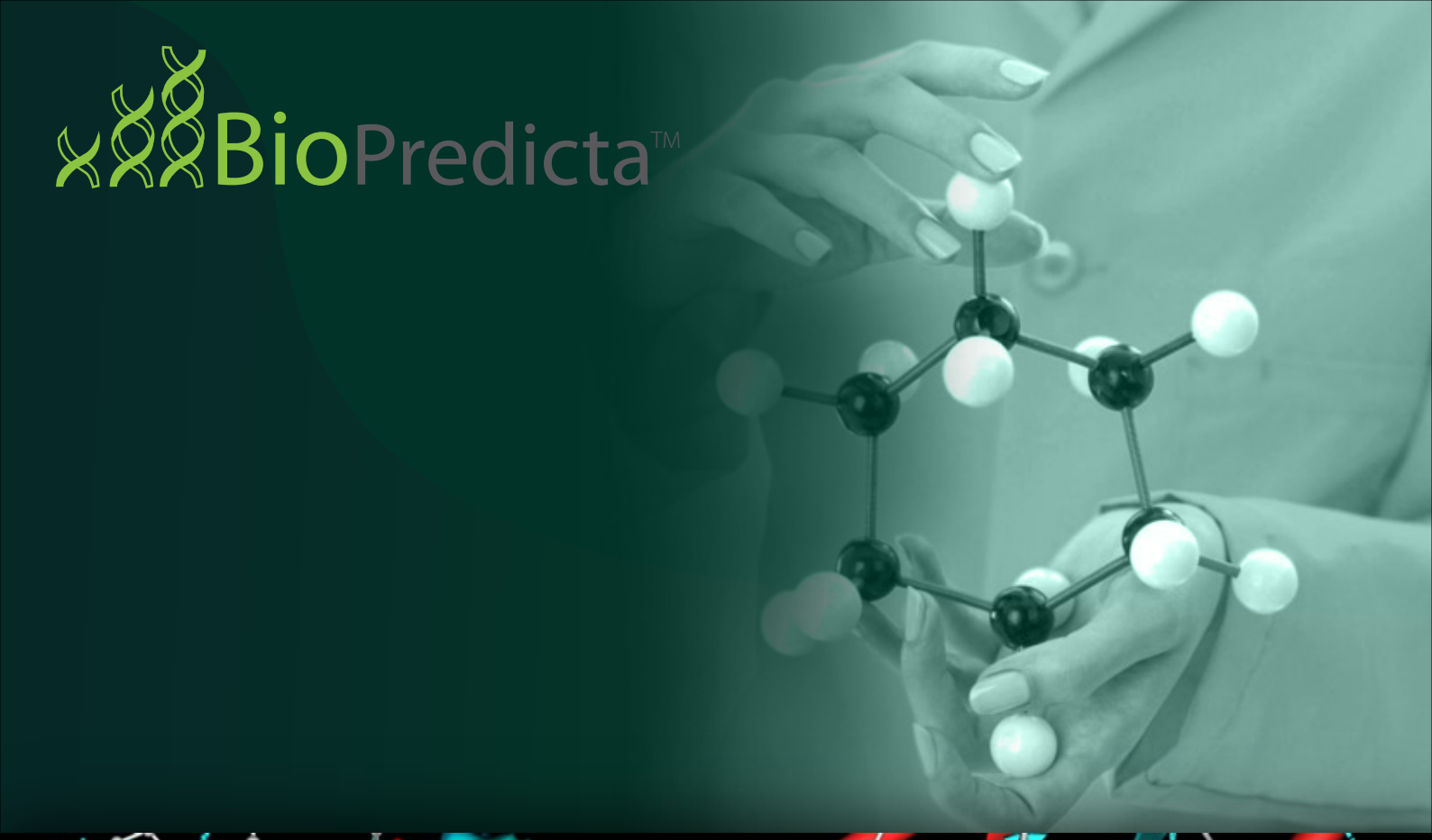
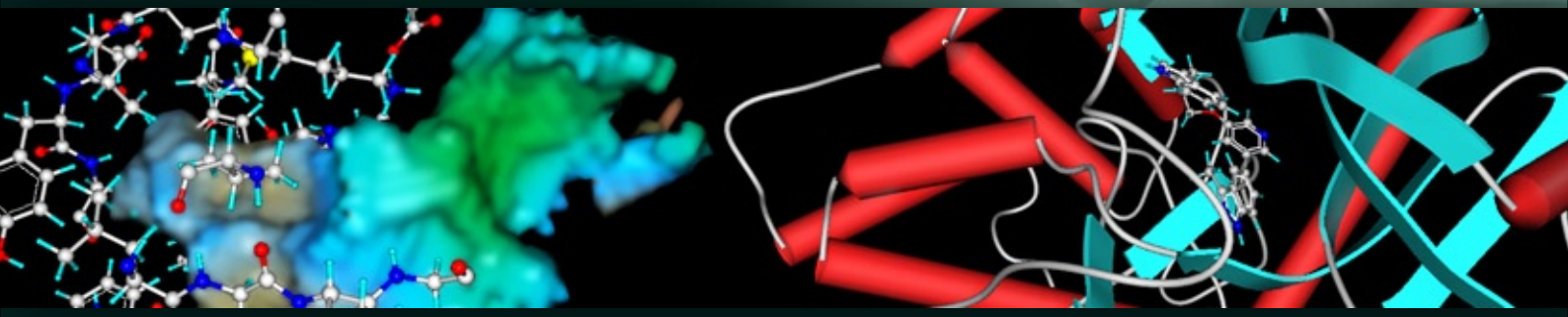
BioPredicta™





GRIP docking

Homology modeling

Protein analysis

Multiple scoring functions

Interaction visualizer

Molecule optimization

Conformation analysis

vLife Technologies

adding value to life

BioPredicta™

BioPredicta is an advanced tool for all bio - molecule related activities such as homology modeling, protein analysis and studying protein - ligand interactions. It includes GRIP™, a novel methodology for protein - peptide and protein - ligand docking. GRIP has demonstrated capabilities to deliver more accurate and fast docking results even for complex ligand chemistries.

From simple visualization to complex protein editing, BioPredicta facilitates all modeling activities like generation of homology model, model validation and analysis as well as molecular docking. BioPredicta enables analysis of protein cavities in terms of shape and electrostatic as well as hydrophobic properties, which provide critical clues for optimization of ligand design.

BioPredicta seamlessly interfaces with other VLife products like VLifeEngine™. This enables users to conveniently access supporting operations like molecule management, conformation analysis and geometry optimization.

Salient features

Homology modeling

BLAST link to perform sequence alignment and editing

Manual mode for specific mutation, insertion, deletion and excision

RMSD and similarity score based loop insertion

Auto mode for automatic model building with user selected template and alignment

Rotamer library for side chain conformer exploration

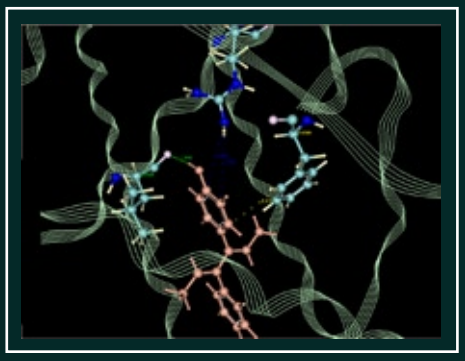
Protein analysis

Cavity and channel identification, property mapping, shape – size analysis

Cavity ranking based on hydrophobic surface area of residue within cavity

Protein cleaning, Ramchandran plot and local geometry analysis

Secondary structure assignment based on atomic coordinates



Docking

Stochastic: GA based for rapid flexible docking

Systematic: GRID based for exhaustive rigid docking

Manual: Interactive docking for precise analysis

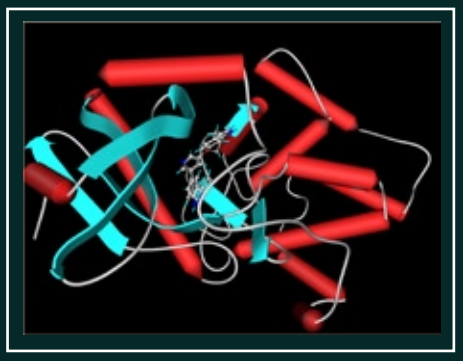
Multiple scores: PLP, DockScore, Steric + Electrostatic, Electrostatic

Docking flexibility: Auto, manual and batch docking facility

Comprehensive visualizer for protein – ligand interaction

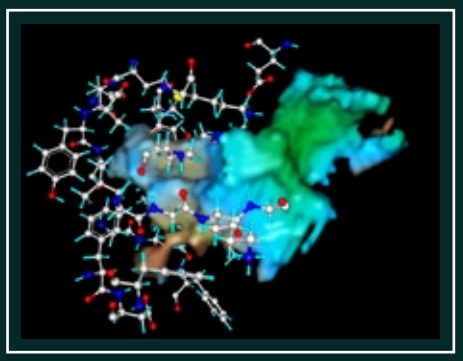
GRIP

GRIP is a rapid and accurate protein - ligand docking methodology, implemented innovatively in BioPredicta. GRIP has demonstrated superior results in terms of speed and accuracy in computational studies on variety of receptors and compound libraries.



Besides protein – ligand docking, GRIP is also useful for protein - peptide docking and interaction analysis. The GRIP scoring function is implemented in a novel way for fast but precise capturing of ligand – receptor interactions in the active site of proteins.

GRIP docking is available as rigid as well as flexible docking, where unique conformers of a set of ligands is taken as input.



- Provides option for ligand guided as well as cavity guided docking
- Available in manual, automated and batch mode
- Takes into consideration hydrogen bonding, repulsions and dispersion interactions
- Wide range of parameterizations available for better scanning of the placement space

Molecule builder/ analyzer

On-line 2D sketching utility

2D to 3D conversion

3D editor for various manipulations relating to chirality, charges, labeling etc.

Multiple force fields: UFF, MMFF, MMFF94, MMFF94-S etc.

Conformation analysis

Systematic method of conformation generation for an exhaustive conformation search

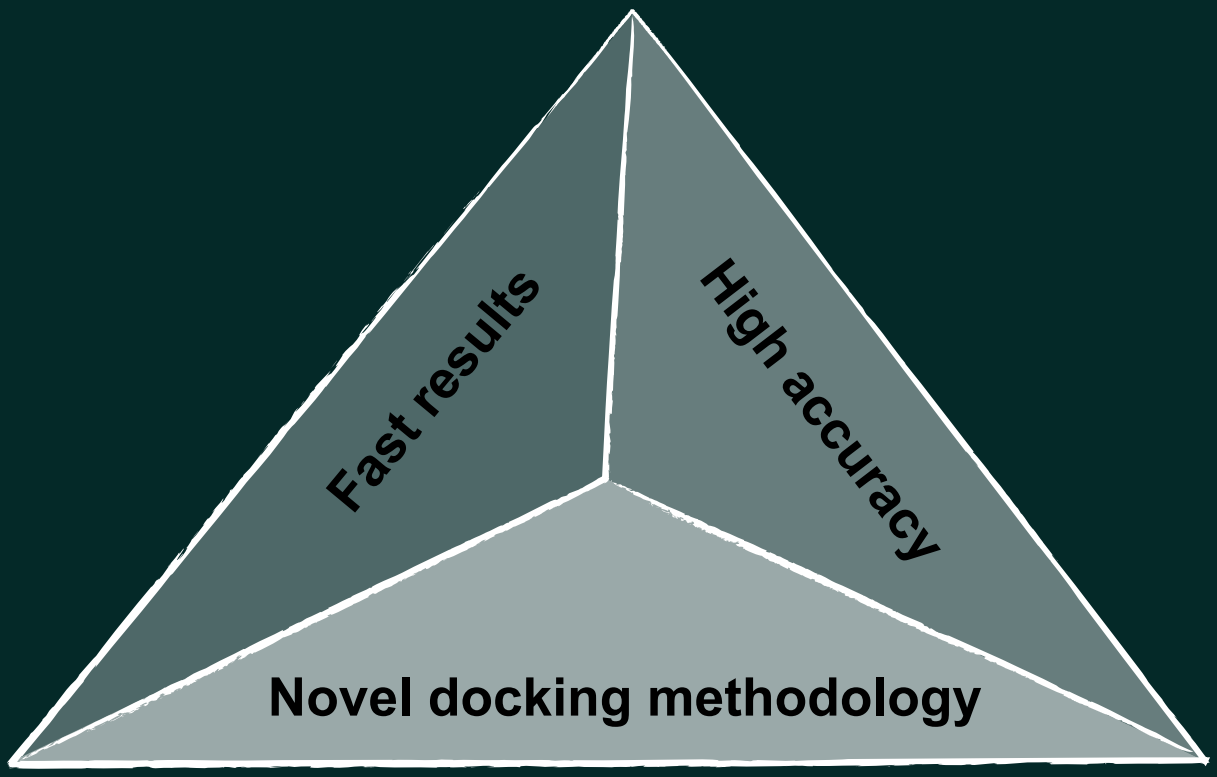
Consideration of chirality of atoms and facility to explore all possible chiralities

Conformer generation of non - aromatic rings via ring flip algorithm

Generation of diverse conformers using torsion RMS to span maximum conformational space

Generation of conformers using different seed numbers of Monte - Carlo method to exhaustively span the conformational space

Advantage GRIP



Technical features

- Completely designed by VLife's team of practicing scientists and technology experts
- Easily customizable and simple for integration

Recommended operating system:

Windows® XP

Optional operating system:

Windows Vista®

Recommended hardware:

Minimum free hard disk space : 1 GB

Minimum required memory : 1 GB (2 GB if operating with Windows Vista)

Graphic cards:

Standard graphic card (supporting OpenGL)

www.vlifesciences.com

vLife
adding value to life

VLife Sciences Technologies Pvt. Ltd.
Pride Purple Coronet, 1st Floor, Baner Road, Pune - 411 045, India
Tel.: + 91 20 2729 1590 **Fax**: + 91 20 2729 1591
Web: www.vlifesciences.com

Contact for DEMO

E-mail : products@vlifesciences.com
Phone : + 91 20 2729 1590