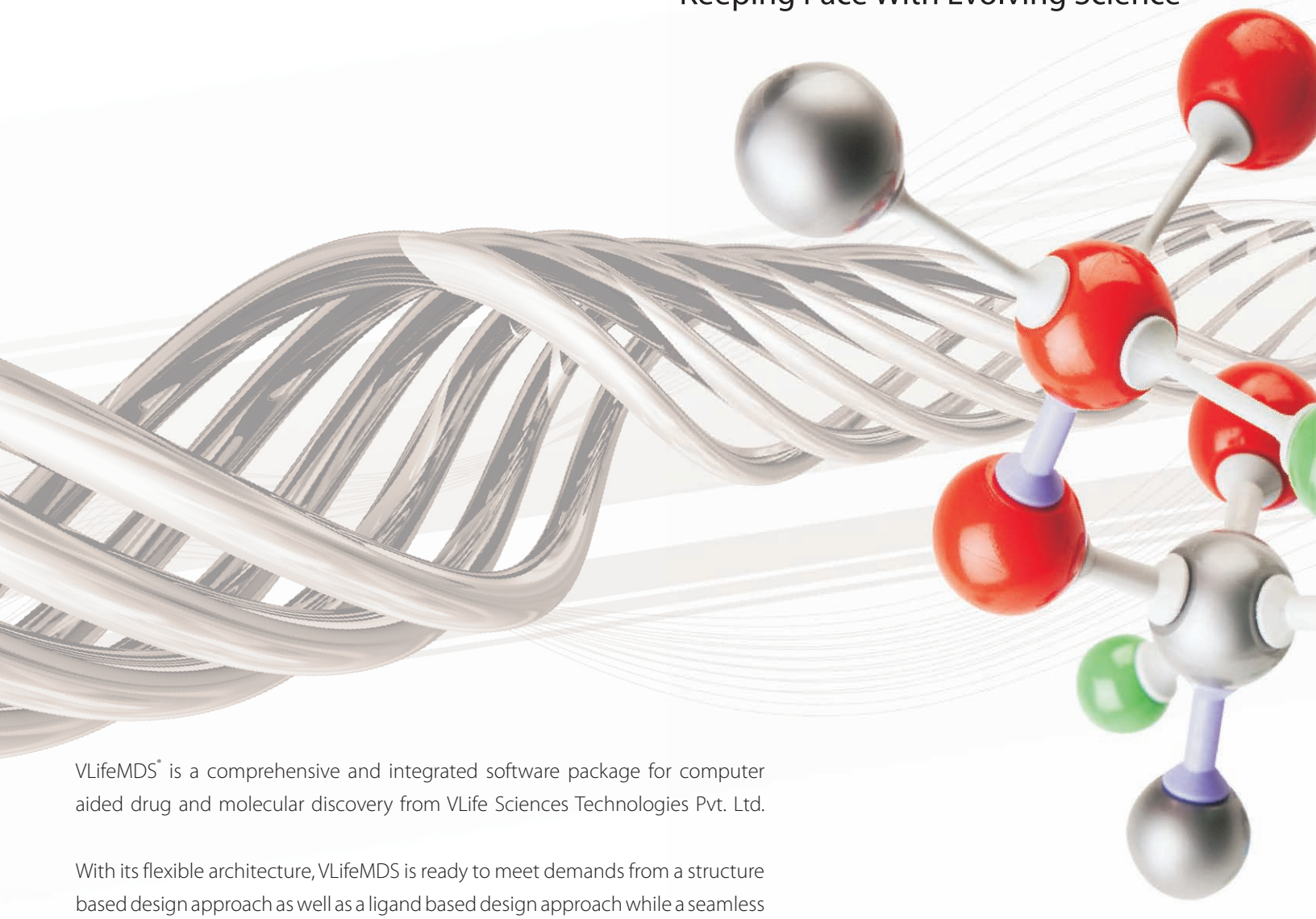
# VLifeMDS®

Keeping Pace With Evolving Science



VLifeMDS® is a comprehensive and integrated software package for computer aided drug and molecular discovery from VLife Sciences Technologies Pvt. Ltd.

With its flexible architecture, VLifeMDS is ready to meet demands from a structure based design approach as well as a ligand based design approach while a seamless integration between various modules within VLifeMDS allows a hybrid approach for discovery projects. With VLifeMDS users can access intuitive features for multiple activities within a discovery project.

- Active site analysis
- Homology modeling
- Pharmacophore identification
- Virtual Combinatorial library
- Docking
- QSAR analysis
- Database querying
- Virtual screening
- Automated Workflows
- Scripting Console

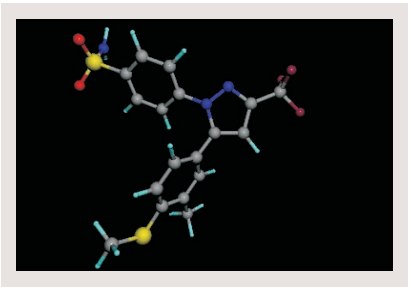
- Comprehensive functionality
- Modular and configurable architecture
- Practical and efficient methodologies
- Patent pending technologies
- Intuitive user interface
- Platform Independent
- Enhanced Graphics
- Multicore enabled
- Command line support

vLife
adding value to life

## **VLife Base-** Molecule visualization and editing

### Molecule building

- Plug-in for easy 2D sketching
- Extensive 3D editor and 2D to 3D batch converter



### Enhanced Graphics

- Stereo view for 3D Visualization
- Improved channel and cavity surfaces
- Switch Mode Graphics
- Export to Povary format for rendering Images

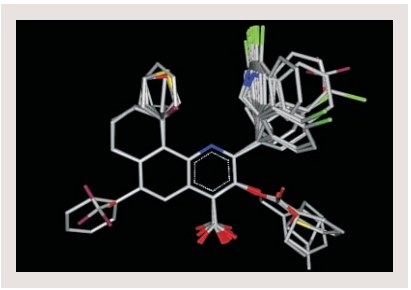
### Molecular alignment

- Template and atom based

## **VLife Engine®** - Essential molecular modeling functions

### Molecular Modeling Tools

- Energy calculation & minimization
- Multiple force fields: MMFF, MMFF94-S, UFF, Amber, Dreiding
- Charge calculation: Del Re, Gasteiger Marsilli, Modified Qeq, MMFF



### Comprehensive conformation generation

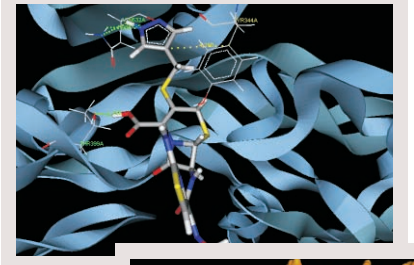
- Conformer generation: Systematic and Monte-Carlo methods
- Chirality & Non-aromatic ring considerations
- Diverse conformers using RMSD

### Scripting console

- Python Integration

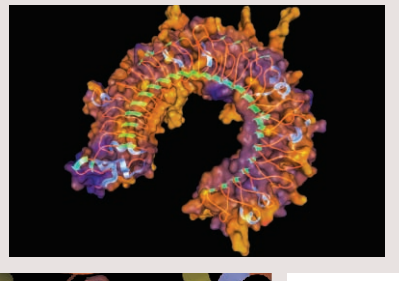
## **BioPredicta®** - Rapid and accurate protein studies

### Homology modeling facilities



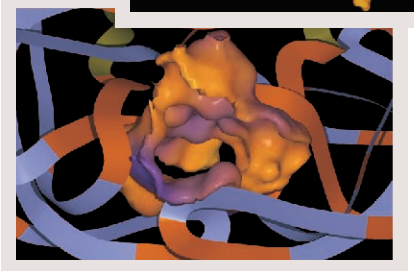
- BLAST interphase to perform sequence alignment and editing
- RMSD and similarity score based loop insertion
- Manual & automated model building with user selected template and alignment
- Multi template homology modeling for better consensus
- Rotamer library for side chain conformer exploration

### Extensive protein analysis



- Cavity & channel identification, property mapping, shape-size analysis
- Cavity ranking based on hydrophobic surface area of residues within cavity
- Protein cleaning, Ramachandran plot and local geometry analysis
- Secondary structure assignment based on atomic coordinates
- Structure based pharmacophore generation based on cavity or co-crystal ligand

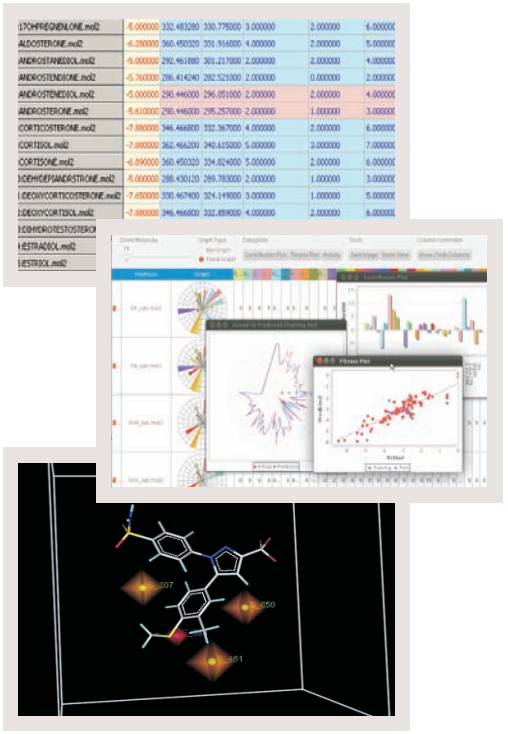
### Protein-ligand & Protein-Peptide* docking features



- User based active site modification based on size and residues
- GA based - Flexible docking and advanced GRIP based - Exhaustive docking
- Ample flexibility: Auto, batch and manual docking facilities
- Multiple scores: PLP with halogen bonding term, Dock Score, Electrostatic + Steric
- Comprehensive 2D & 3D visualizer for comparing protein-ligand interactions

* Efficient upto peptides of 20 amino acids

## **VLife QSARPlus –** QSAR modeling and data analysis facilities



### 2D QSAR

- Rapid calculation of 2000+ descriptors including 2D, 3D, alignment independent & interaction descriptors.
- Applicability domain check
- AutoQSAR for multiple model building

### 3D QSAR

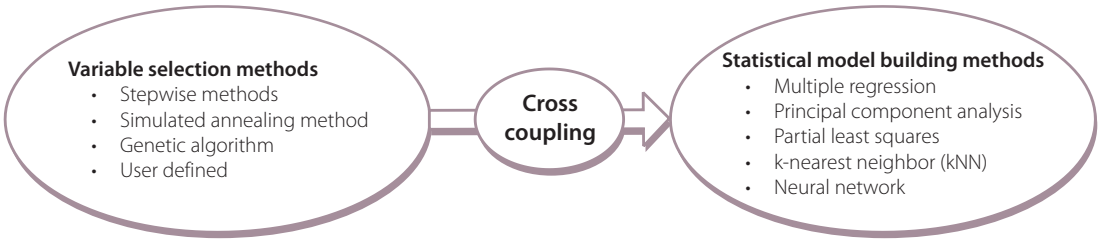
- Novel molecular field analysis based on kNN method (kNN MFA) to correlate molecular field descriptors with biological activity
- Consideration of non-linear relationships between activity and descriptors using kNN MFA
- Contour visualization with PLS MFA
- AutoQSAR for multiple model building

### Data preprocessing

- Graphical representation of relative distribution of descriptor values by distribution and pattern plot
- Univariate analysis of descriptors
- Cross correlation matrix to investigate the relationship between different descriptors

### Data processing

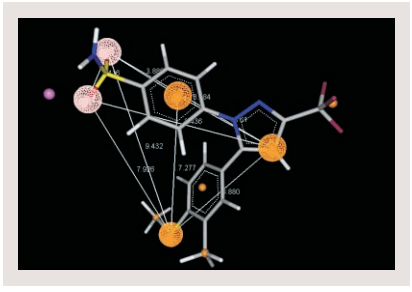
- Multiple response QSAR modeling
- Training and test set selection methods: Manual, Sphere Exclusion, Random




### Data Analysis

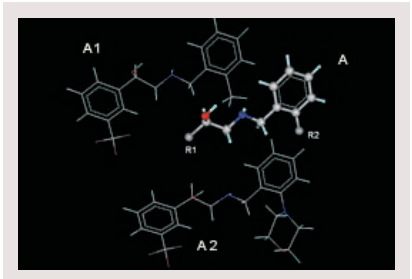
- Advanced Statistical and Graphical Analysis
- YY Randomization

## **MolSign®** - Pharmacophore identification and modeling



- Features such as H-bond donor, H-bond acceptor, positive charge, negative charge and hydrophobe
- Application of conformer flexibility of molecules for generation of several pharmacophore hypotheses
- Pattern search for 3 point, 4 point, 5 point and upto n-point pharmacophore identification with RMSD & distance
- Generation of automated query for 3D database searches through integration with ChemDBS

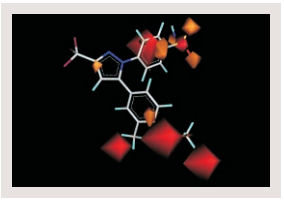
## **LeadGrow** - Virtual combinatorial library generation




- Ability to define multiple sites for substitution
- ADME screen based on extended Lipinski's rule
- Predicting activity of virtually generated library of molecules through QSARPlus
- Applicability domain check on generated library model
- GRIP docking based screening
- kNN MFA model based optimization and screening

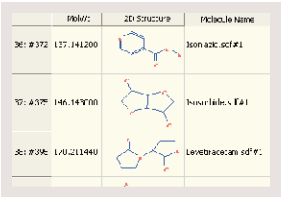
## ProViz™ - 3D Property Visualization & Evaluation

- Calculation and visualization of wide variety of Quantum Mechanical? properties including ED, MESP, EMD, ELF, AIE
- Moments of charge distribution, Mulliken population analysis, HOMO, LUMO
- Calculation of molecular surface area , hydrophobicity, charge based ESP



## ChemDBS - Efficient searches for compound databases

- Comprehensive Database Creation and Management
- Comprehensive search criteria: 2D/3D substructure, similarity or descriptor based
- Advanced molecular fingerprint and Pharmacophore based searches
- Comprehensive search criteria



## VLifeMDS: Add-on Modules

**GQSAR:** A Fragment Based QSAR method

**VLifeSCOPE:** Structure Based Compound Optimization, Prioritization & Evolution

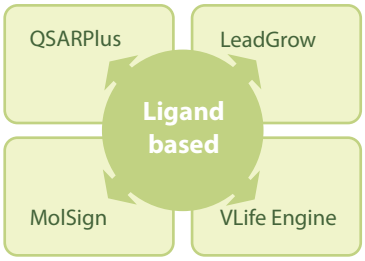
**LeadGrow+:** Scaffold hopping & Lead Optimization

**Aakar:** Shape Based Screening

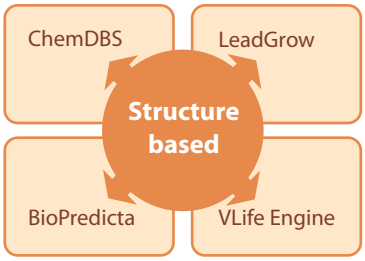
**VLifeWorkFlow:** Customized workflows for research protocols

## VLifeMDS: Customize your own molecular design suite

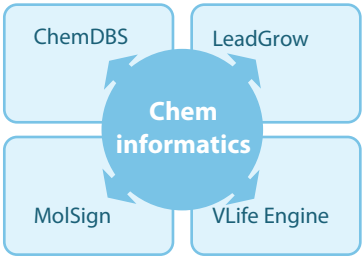
Ligand based approach




Structure based approach




Cheminformatics approach




## VLifeMDS: Customize your own molecular design suite

**Operating systems:**
Windows® XP, Windows Vista®, Windows 7, Windows 8, Linux (Fedora, Ubuntu, CentOS), Mac OSX 10.6

**Recommended hardware:**
Minimum free hard disk space: 1 GB
Minimum required memory: 2 GB
Processor: Intel P4 or equivalent CPU

**Graphic cards:**
Standard graphic card (supporting OpenGL)



vLife
adding value to life

**VLife Sciences Technologies Pvt. Ltd.**
2nd Floor, Plot No-05, Next to Sapling Nursery, Ram Indu Park,
Survey No-131/1b/2/11, Baner Road, Pune 411045, India
Tel.: + 91 20 6410 0335 Fax: + 91 20 2729 1591
Web: www.vlifesciences.com Portal: https://portal.vlifesciences.com

**Contact for DEMO**

E-mail: vlifemds@vlifesciences.com