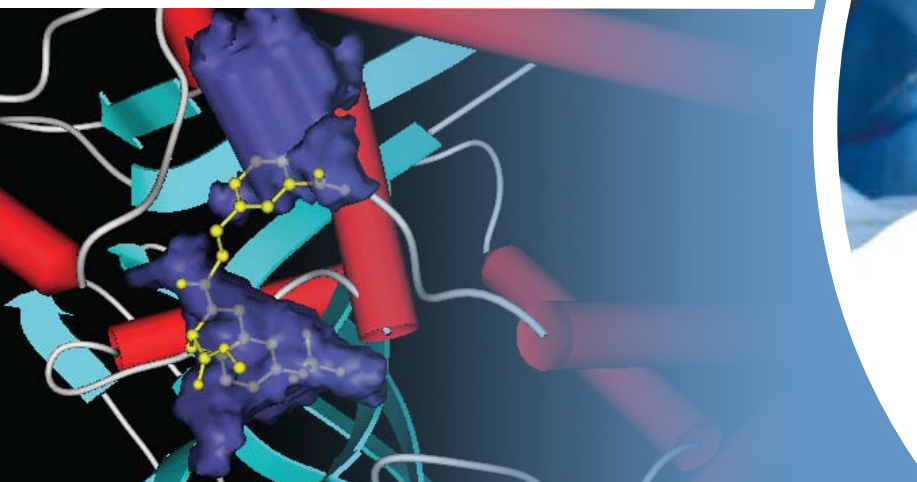




Keeping Pace With Evolving Science



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
- Conformer generation
- Combinatorial library
- Property visualization
- Docking
- QSAR analysis
- Database querying
- Virtual screening

- Comprehensive functionality
- Modular and configurable architecture
- Practical and efficient methodologies
- Patent pending technologies
- Intuitive user interface

VLife Engine[®] – Molecule visualization and optimization

Extensive features for performing fundamental molecular modeling functions

Molecule building and optimization

- Plug-in for easy 2D sketching
- 2D to 3D batch conversion
- Extensive 3D editor and 2D to 3D converter
- Multiple force fields: MMFF, MMFF94-S, UFF, Amber, Dreiding

Comprehensive conformation generation

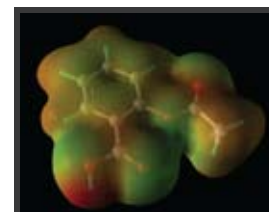
- Conformer generation: Systematic and Monte-Carlo methods
- Chirality consideration
- Non-aromatic ring conformers
- Diverse conformers using Torsion RMS

Molecular alignment

- Template and atom based
- Ease of alignment in active site with respect to co-crystallized ligand

Ligand preparation:

- Molecule builder
- Single click hydrogen addition
- Energy minimization
- Conformer analysis



BioPredicta[®] - Rapid and accurate protein studies

Advanced facilities for bio - molecule handling such as homology modeling, protein analysis and studying protein - ligand interactions

Protein-ligand docking features

BioPredicta features the innovative GRIP method for protein - ligand and protein - peptide docking. GRIP docking delivers superior results in terms of speed and accuracy. BioPredicta also provides other powerful features for protein – ligand docking.

- GA based - Flexible docking and grid based - Exhaustive rigid docking
- Interactive - manual docking for initial analysis
- Multiple scores: PLP, Dock Score, Steric + Electrostatic, Electrostatic
- Ample flexibility: Auto, batch and manual docking facilities
- Comprehensive visualizer for protein-ligand interactions

Homology modeling facilities

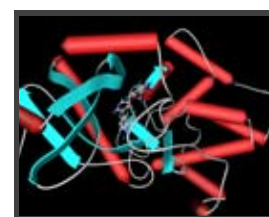
- BLAST link to perform sequence alignment and editing
- Manual mode for specific mutation, insertion, deletion and excision
- RMSD and similarity score based loop insertion
- Automated model building with user selected template and alignment
- Rotamer library for side chain conformer exploration

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

BioPredicta protein preparation:

- Auto water removal
- Single click hydrogen addition
- Check for incomplete residues
- Protein optimization by aggregate definitions



ChemDBS - Efficient searches for compound databases

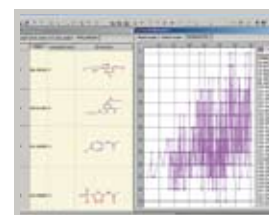
Advanced module for large size compound database creation and searches on single or multiple databases based on various criteria

Comprehensive search criteria

- 2D substructure, 3D substructure, similarity based or descriptor based searches
- Advanced molecular fingerprint based search
- Attribute definition for all atoms including dummy atoms
- Pharmacophore searches by considering conformations of hits

Extensive analysis of hits

- Scatter plot, distribution plot
- Diversity analysis using bar graph
- Descriptor calculator for property evaluation
- Results display in tabulated worksheets



VLife QSARPlus – QSAR modeling and data analysis facilities

Powerful facilities for quantitative structure activity relationship model building, its analysis and activity or property prediction

Data preprocessing

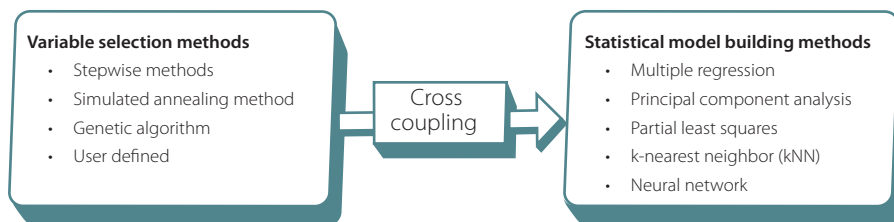
- Graphical representation of relative distribution of descriptor values by distribution and pattern plot
- Univariate analysis of descriptors
- Cross correlation matrix to investigate the relationship between different descriptors

Training and test set selection methods

- Manual
- Sphere exclusion
- Random selection

QSAR Model Building

- Choice of variable selection and model generation methods and the flexibility to combine any variable selection method with any model generation methods



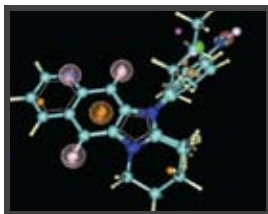
2D QSAR

- Rapid calculation of 1000+ descriptors including 2D, 3D, alignment independent etc.
- Applicability domain check

3D QSAR

- Novel molecular field analysis based on k-nearest neighbor method to correlate molecular field descriptors with biological activity
- Improved predictability due to consideration of non linear relationships between activity and descriptors using kNN MFA
- Automated generation of new molecules based on kNN MFA models through integration with LeadGrow

MolSign® - Pharmacophore identification and modeling



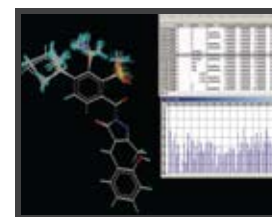
Identification of pharmacophore for a given dataset using features such as H-bond donor, H-bond acceptor, positive charge, negative charge and hydrophobe

- 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
- Classic depiction of pharmacophoric features with RMSD of alignment
- Generation of automated query for 3D database searches through integration with ChemDBS

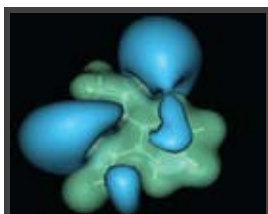
LeadGrow - Virtual combinatorial library generation

Focused and unbiased *in-silico* combinatorial library generation based on template

- Ability to define multiple sites for substitution
- Ability to define sites for bidentate 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



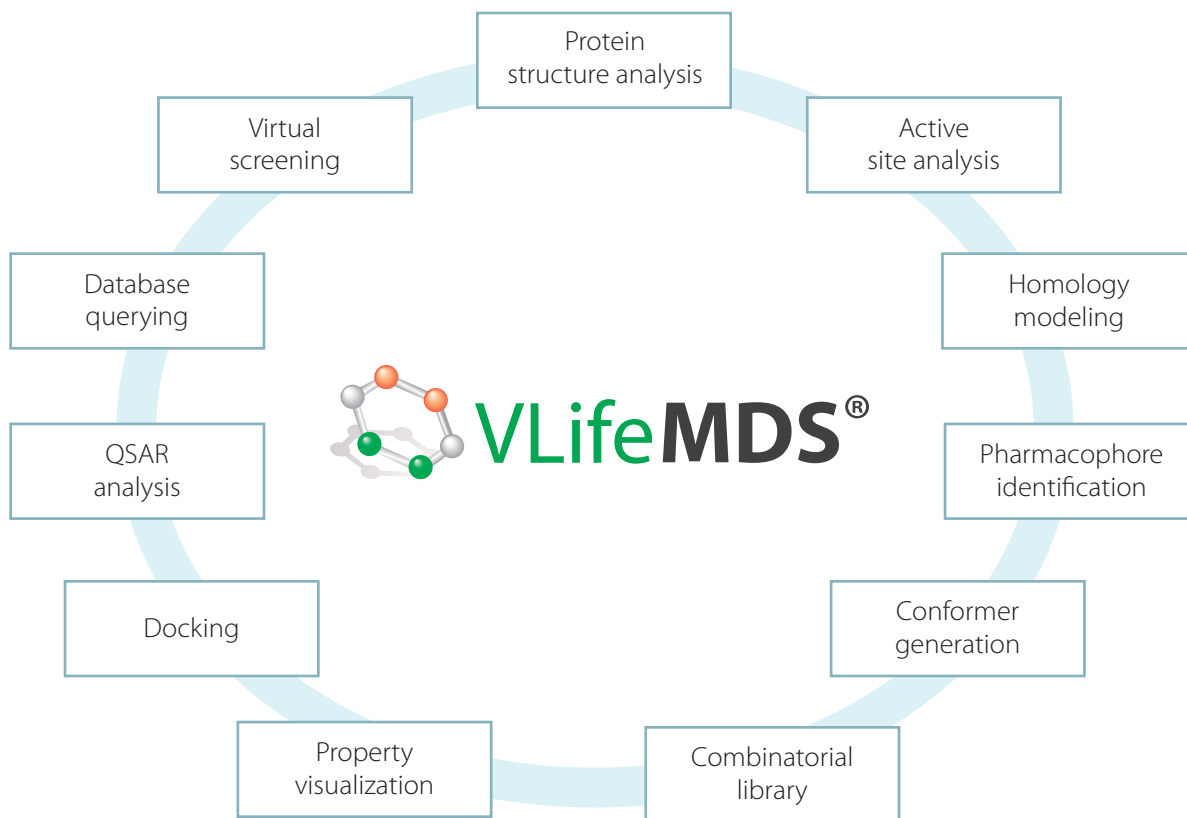
ProViz™ - 3D Property Visualization & Evaluation



Addresses the 'know-why' behind chemical interactions and stimulates special considerations on the structure and chemical bonding via molecular properties

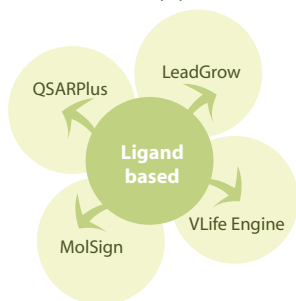
- Calculation and visualization of wide variety of Quantum Mechanical properties including ED, MESP, EMD, ELF, AIE, Moments of charge distribution, Mulliken population analysis, Molecular Orbitals (HOMO, LUMO)
- Calculation of molecular surface area, hydrophobicity, charge based ESP

VLifeMDS: End-to-end capabilities

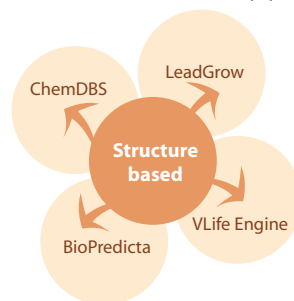


VLifeMDS: Customize your own molecular design suite

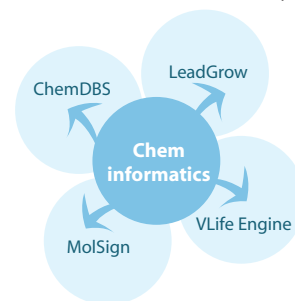
Ligand based approach



Structure based approach



Cheminformatics approach



System configuration

Operating systems:

Windows® XP, Windows Vista®, Windows 7, Linux (Fedora, Ubuntu, CentOS)

Recommended hardware:

Minimum free hard disk space: 1 GB

Minimum required memory: 2 GB

Graphic cards:

Standard graphic card (supporting OpenGL)

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