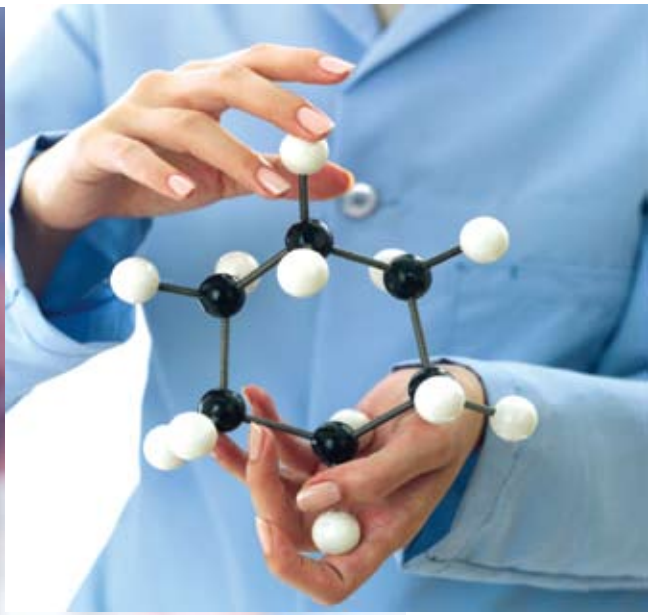
QSARpro®

Predict | Design | Discover



QSARpro® is an advanced software package from VLife Sciences Technologies Pvt. Ltd. for modeling the molecular activity or property with structural properties, analyzing such models and predicting activity of new molecules.

QSARpro incorporates the patented GQSAR technology that provides site specific clues for new molecule design by considering molecular fragment contributions and interaction between fragments in modeling. QSARpro also implements novel methodologies like kNN MFA for better predictability.

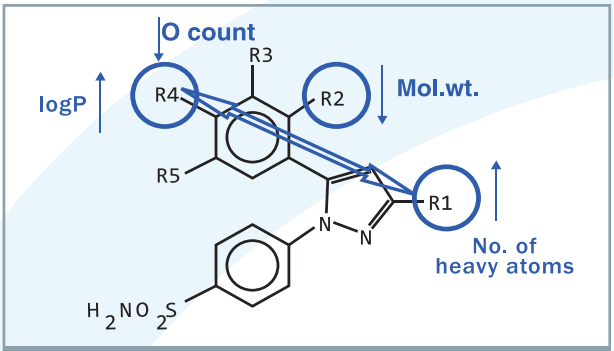
QSARpro seamlessly interfaces with VLife Engine thus enabling users to conveniently access supporting operations like molecule visualization, conformation analysis and geometry optimization.

- 2D and 3D QSAR
- Direct clues for new molecule design through GQSAR
- Better predictability due to inherent non-linearities in kNN MFA
- 1000 + descriptor types
- Applicability domain check
- Characterizing continuous as well as categorical biological response

vLife
adding value to life

GQSAR

GQSAR is a novel QSAR method developed by VLife and available within QSARpro. It studies relation of molecular fragments of interest and the variation in their biological response while considering interactions between fragments through cross-term fragment descriptors. GQSAR thus provides a focused direction for designing new molecules and quantitatively predict their activity.



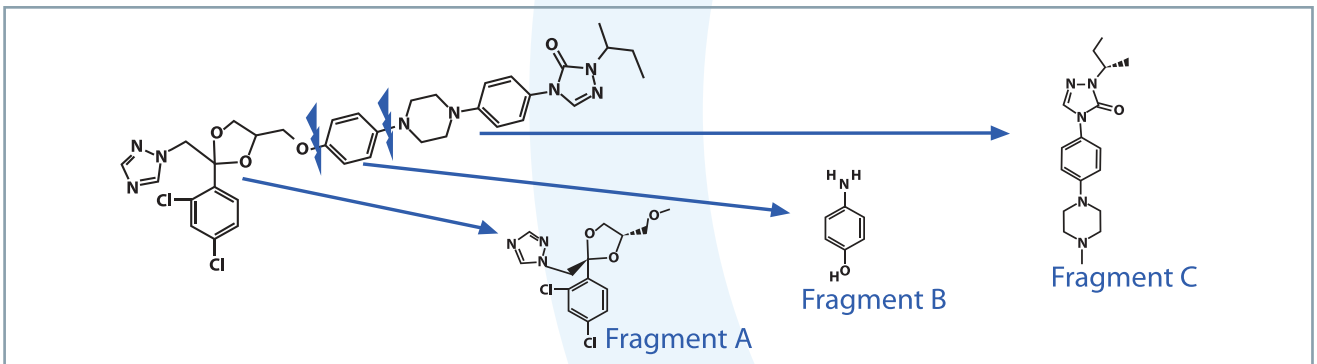
Site specific clues and direction of molecular descriptors for generated GQSAR model; includes interaction descriptors

Molecular fragmentation schemes

GQSAR provides two methods for molecular fragmentation.

- Auto: Template based approach particularly for congeneric series of molecules
- Manual: User defined scheme particularly for non-congeneric series of molecules

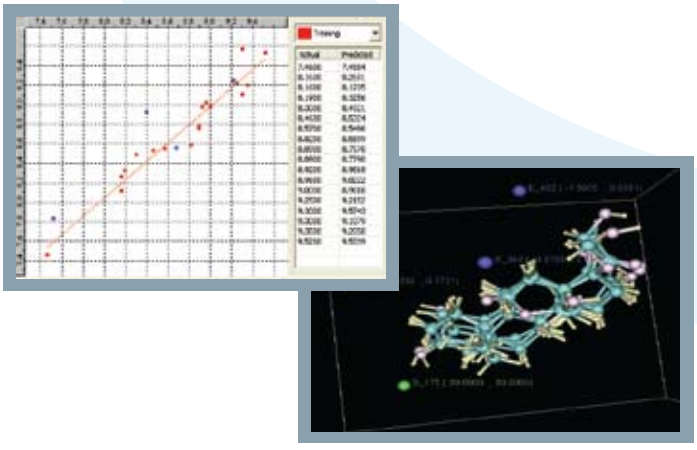
Fragments generated using these schemes inlude neighboring group participation



Simple fragmentation schemes: GQSAR comes with Auto and Manual molecule fragmentation methods

kNN MFA

kNN MFA (k Nearest Neighbor Molecular Field Analysis) is a novel methodology for correlating molecular field descriptors with biological activity that has been implemented within QSARpro. Conventional correlation methods try to generate linear relationship of the descriptors with activity however in many practical situations this relation is not linear. QSARpro delivers better predictability due to non linearities inherent in kNN MFA.



Data processing

Data preprocessing

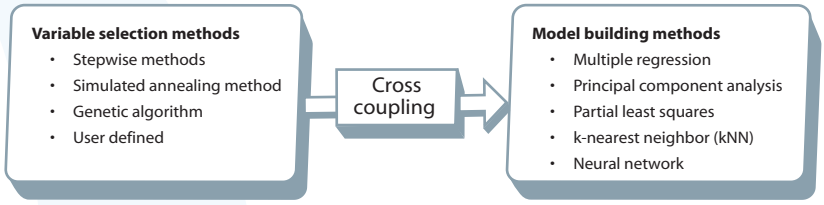
- Graphical representation of relative distribution of descriptor values by distribution and pattern plot
- Univariate analysis of descriptors
- Cross correlation matrix to investigate the relationship between different descriptors

Training and test set selection methods

- Manual
- Sphere exclusion
- Random selection

QSAR model generation

QSARpro provides users a choice of variable selection methods and model generation methods plus the flexibility to combine any variable selection method with any of the model generation methods.



QSARpro handles continuous (e.g. IC50, MIC, % inhibition etc.) as well as categorical (e.g. active/ inactive, low/ moderate/ high active, etc.) response

2D QSAR

- Rapid calculation of 1000+ descriptors including 2D, 3D, alignment independent etc.
- Applicability domain check for effectively verifying that the models generated are within their domain of application.

3D QSAR

- kNN Molecular Field Analysis based on k-nearest neighbor method to correlate molecular field descriptors with biological activity
- Unbiased results due to inherent non linear consideration between activity and descriptors

Model analysis

- Validating QSAR model using a host of validation parameters
- Analyzing the model with Contribution plot and Fitness plot
- Saving the QSAR model to screen molecules

Graphical visualization

- Pattern plot
- Bar graph
- 2D scatter plot, activity distribution plot
- Intuitive data manager with graphical interfaces
- Worksheet having mathematical and table manipulation functions

Other features

- Wide range of facilities for molecule visualization, force field analysis and geometry optimization
- Exhaustive conformation search using Systematic and Monte-Carlo methods
- Multiple methods for molecular alignment including template based and atom based

Advantage GQSAR:

Description	2D QSAR	3D QSAR	GQSAR
Conformation independent	✓	✗	✓
Alignment independent	✓	✗	✓
Fast descriptor calculation	✓	✓	✓
Interaction descriptors	✗	✗	✓
Clues for NCE design	✗	✓	✓
Site specific clues for NCE design	✗	✗	✓
Screening of fragment databases	✗	✗	✓
Generating NCE Library	✗	✗	✓

System configuration

Operating systems

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

Recommended hardware

Minimum free hard disk space: 1 GB
Minimum required memory: 2 GB

Graphic cards

Standard graphic card (supporting OpenGL)

vLife
adding value to life

VLife Sciences Technologies Pvt. Ltd.
1st Floor, Pride Purple Coronet, S. No. 287, 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: qsarpro@vlifesciences.com