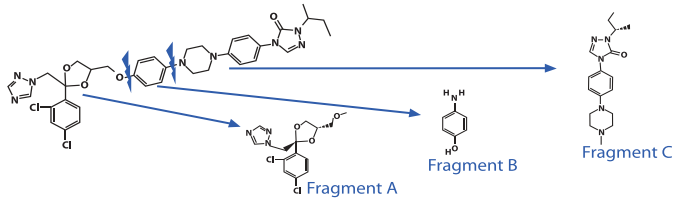
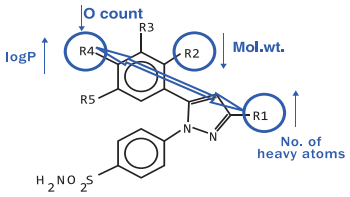
GQSAR

GQSAR is a novel group (fragment) based QSAR method developed by VLife Technologies Pvt. Ltd., which significantly enhances capability of conventional QSAR. 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 provides site specific clues for designing new molecules and quantitatively pre-dicting their activity.



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



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

Molecular fragmentation schemes

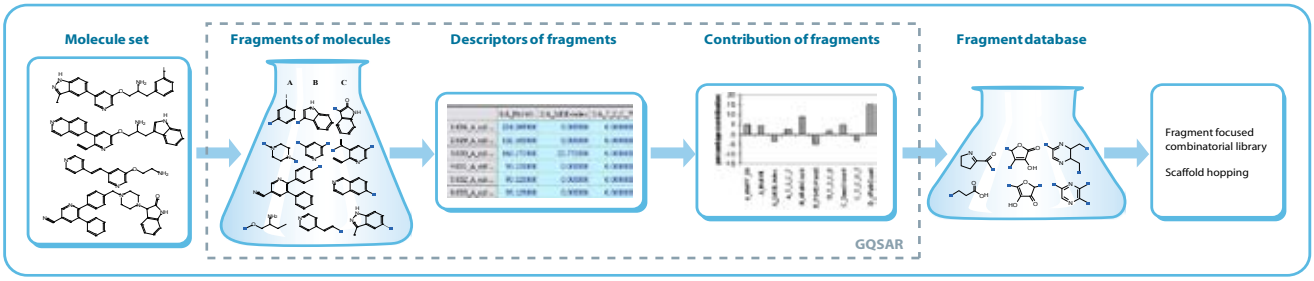
- Auto: Template based approach particularly for congeneric series of molecules
- Manual: User defined scheme particularly for non congeneric series of molecules

Fragments generated using these schemes inlude neighboring group participation

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	✗	✗	✓

Addressing the inverse QSAR problem through GQSAR



GQSAR works systematically to solve the inverse QSAR problem:

- Identifying important molecular sites and their corresponding properties (along with interaction terms)
- Deriving ranges of descriptors that are found to be important in GQSAR model(s)
- Searching for fragments that correspond to these ranges within fragment databases
- Generating new molecule designs by combining such fragments

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