

AutoQSAR is an advanced, rapid, intelligent and automated QSAR solution from VLife Sciences Technologies Pvt. Ltd. It empowers users by creating a knowledge base for designing new molecules.

AutoQSAR is particularly useful in cases involving analysis of a large amount of molecular structural data along with their experimental properties or activities. The smart AutoQSAR approach drastically reduces the time otherwise spent on iterative statistical model building and analysis thus helping users to generate a variety of models to screen molecular libraries.

AutoQSAR also provides an approach to build a consensus QSAR model by presenting the best possible statistical models with a 'single click', which in turn can provide clues for new molecule design.

AutoQSAR workflow:

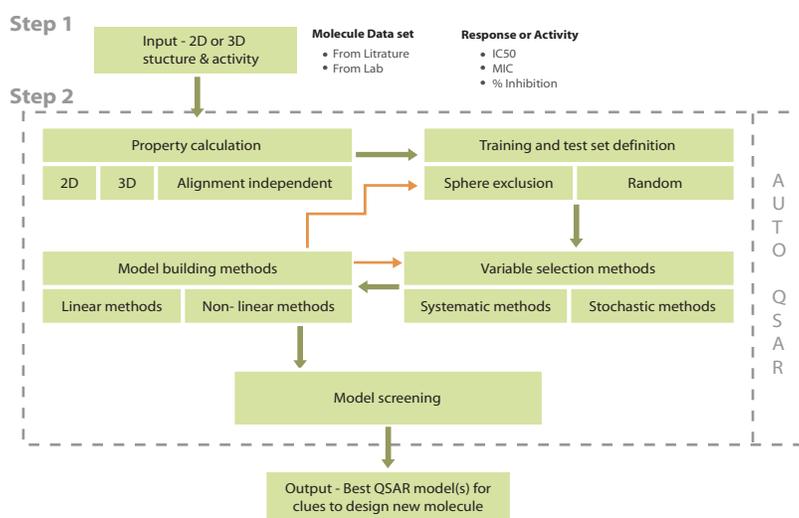
A typical approach using conventional QSAR requires significant statistical expertise and time as it involves a series of steps including property calculations, training and test set definition, variable selection and finally model generation. These steps usually have to be performed in several iterations before a 'good' QSAR model can be generated.

AutoQSAR simplifies this task by completely automating this procedure. AutoQSAR works in two simple steps:

Step 1. Input data set of molecules and their activity information

Step 2. Automatic QSAR process to produce the best model(s)

The AutoQSAR output is dictated by multiple options for variable selection and model building exercised by the user in one single instance.



AutoQSAR result:

- One single consolidated report of best QSAR model(s) that can be used to screen a library
- Contribution plot of descriptors in the final model(s) to decide their relative importance in design of new molecules
- Fitness plot to show the prediction accuracy of training and test set
- Statistical parameters like r^2 , pred r^2 , q^2 , Standard Error, F-test etc. to build a consensus model

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