

## Toxicity prediction

The cost of drug designing increases because of drug failures due to toxicity being found in late development or even in clinical trials. We can minimize the expenditure by determining potential toxicity problems as early as possible. The use of predictive toxicology is very useful even before the synthesis of the chemical. This can help us screen molecules/chemicals and predict the unwanted properties, thus notifying us about the possible side-effects it is likely to cause. . Quantitative structure-activity relationships (QSARs), relating mostly to specific chemical classes, have long been used for this purpose, and exist for a wide range of toxicity endpoints.

We introduce ToxSpec<sup>TM</sup>, as a module in our RAASI<sup>TM</sup> suite, adapted for Toxicity and Side Effect alert based on 2D molecular structure. We advocate usage of ToxSpec<sup>TM</sup> as a tool to flag potential problems and not as something to help discard promising drug candidates. The situation is complicated by the fact that the toxicity that is present or absent in animal models may not always show up in human beings. Many a times, it is the metabolites and not the dosed molecules that are toxic. Hence, any toxicity prediction approach should flag the mechanistic reasons behind a prediction and not merely give a Boolean answer. A chemical compound becomes toxic due to the change in orientation of its functionophore. ToxSpec<sup>TM</sup> is well equipped to predict the changes in orientation of the functional groups and hence it can be used as a toxicity prediction tool. ToxSpec<sup>TM</sup> first clusters the data set on the basis of chemical intelligence and then rules are made depending on the orientation of functionophore.



### Deliverables

- A detailed report of the molecule's toxicity with graphical output.
- Report powered with extensive literature references.

### Required Input Data

- SDF
- SMILES
- Any Other format supported by Open Babel