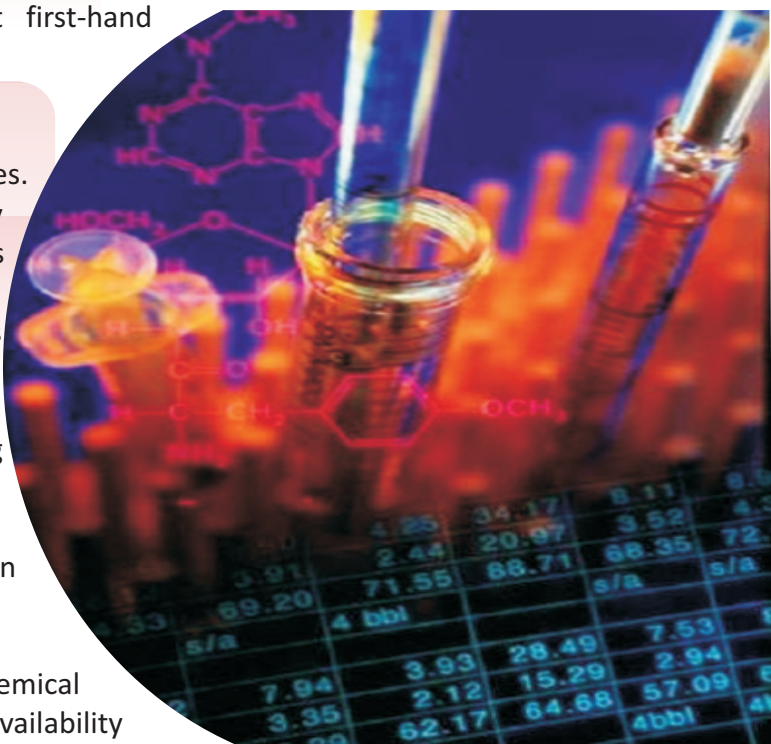


## Pharmacological Activity prediction

Each biologically active compound possesses a number of biological activities. Its specificity of action is always relative and is defined by the peculiarities of object, dose, route, etc. On the contrary, the biological potential of compound includes all activities, which can be discovered under some specific experimental conditions. We call such biological potential the biological activity spectrum. Biological activity spectrum of compound can be predicted on the basis of structure-activity relationships found by the analysis of the known data from the training set. This prediction in turn helps in finding of compounds with required properties, thus assisting chemists and medicinal scientists to get first-hand knowledge about the essential properties.

BioSpec<sup>TM</sup> of RAASI<sup>TM</sup> suite basically predicts the qualitative Biological Activity Spectrum of small molecules. BioSpec<sup>TM</sup> is designed to assist users to quickly understand the various drug targets, biological processes and therapeutic areas where a structure may be useful. The BioSpec<sup>TM</sup> Predictions can be applied in various areas like drug target identification, lead discovery and identification, compound selection for vHTS/ HTS. Besides, it also assists users in drug repositioning, buying chemical libraries, exploring in-house corporate molecular libraries.

BioSpec's prediction is based purely on correlation between a biological function and functionophore. The training data belonging to any spectrum or class are first clustered. The clustering is carried out on the basis of chemical intelligence and then rules are made depending on the availability of functionophore. BioSpec<sup>TM</sup> predictions can be warranted with literature references using LitSpec<sup>TM</sup>.



### Deliverables

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

### Required Input Data

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