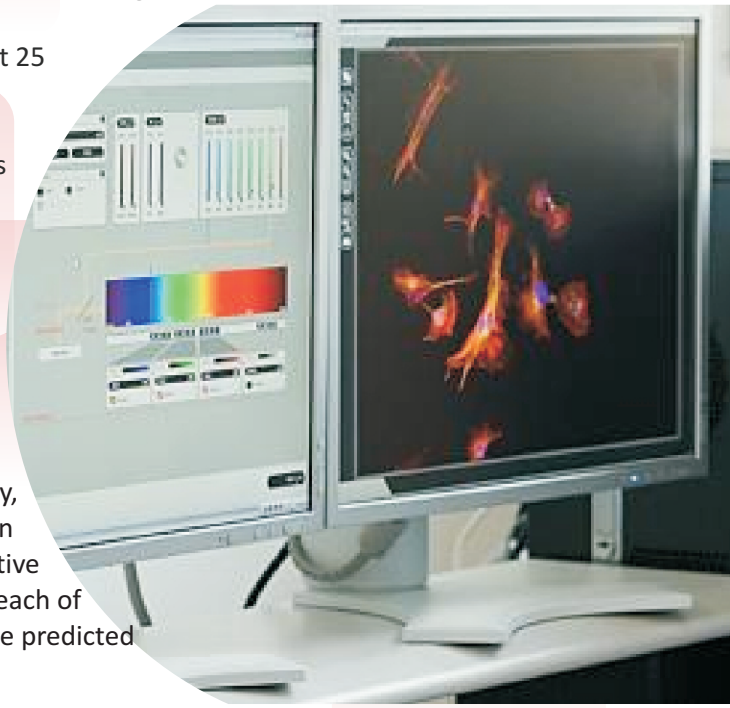
RASA™
LIFE SCIENCE INFORMATICS

ADMESpec™ Package

ADMESpec ™ package of RAASI ™ suite enables you to perform high-throughput screening of high dimension chemical compound database based on ADME (Adsorption, Distribution, Metabolism and Excretion) properties. Our ADMESpec ™ package currently provides you with following predictive values:

Intrinsic aqueous solubility of organic compounds predicted in **logS** (Aqueous Solubility), moles/L and grams/L units at 25 degree Celsius and pH 7

- **logP** (Partition Coefficient) of organic compounds predicted at 25 degree Celsius and pH 7
- **logD** (Distribution Coefficient)of organic compounds predicted at 25 degree Celsius and pH 7
- **pKa** - Ionization Constant of organic compounds predicted at 25 degree Celsius and pH 7



We have collected curated data from several thousands ofdrug-like diverse organic compounds, which is used to train the models. The training set molecules are diverse in functional group and molecular weight (16 to 1300).Custom tailored models can be implemented using customer in-house data.

Deliverables

A report highlighting important finding of ADME predictive study, detailed result in Excel format. Output will also be provided in an SDF format comprising structure of input molecules and predictive results. Quantitative and qualitative result will be provided for each of the ADME properties. ADME values of 10 000 compounds can be predicted per person-day.

Future Directions

ADME Physicochemical prediction package will have the following modules by last quarter of 2011.

- ADME profile in terms of varied pH and temperature
- Physicochemical models for cell permeability comprising blood brain barrier, Caco-2 cell channel, HERG ion channel

Required Input Data

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

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