OTAVA chemicals

Compounds for HTS
Chemical building blocks
Fragment libraries
Targeted libraries
Drug discovery services

INSECTICIDES-LIKE LIBRARY

OTAVA chemicals

OTAVA offers Insecticides-Like Library - special screening library containing predicted insecticides. This library provides an excellent basis for insecticide discovery projects.

The library consists of **2,084 compounds***.

All compounds are:

- **in stock**; available amounts: 1 – 50 mg

QA/QC passed:

- minimal purity of compounds is **90%**;
- by **NMR** and/or **GC/LC/MS**
- **NMR spectra are available** upon request

Frendly packing services:

- **Cherry-picking is available**
- Supplied as dry powder or DMSO solution**
- Packaging in deep-well plates or barcoded vials***
- **Weighing out is free**

*Please note that the library does not contain known inhibitors. The compounds were selected with computational approach and are intended for screening projects

**there is additional fee for preparation of the solution

***4 ml amber glass vials or Deep-well plates: Matrix cat# 4247 (1.4 mL, Blank, Polypropylene, Round Bottom Tubes) w/CapMats. Or plates and vials provided by customer.

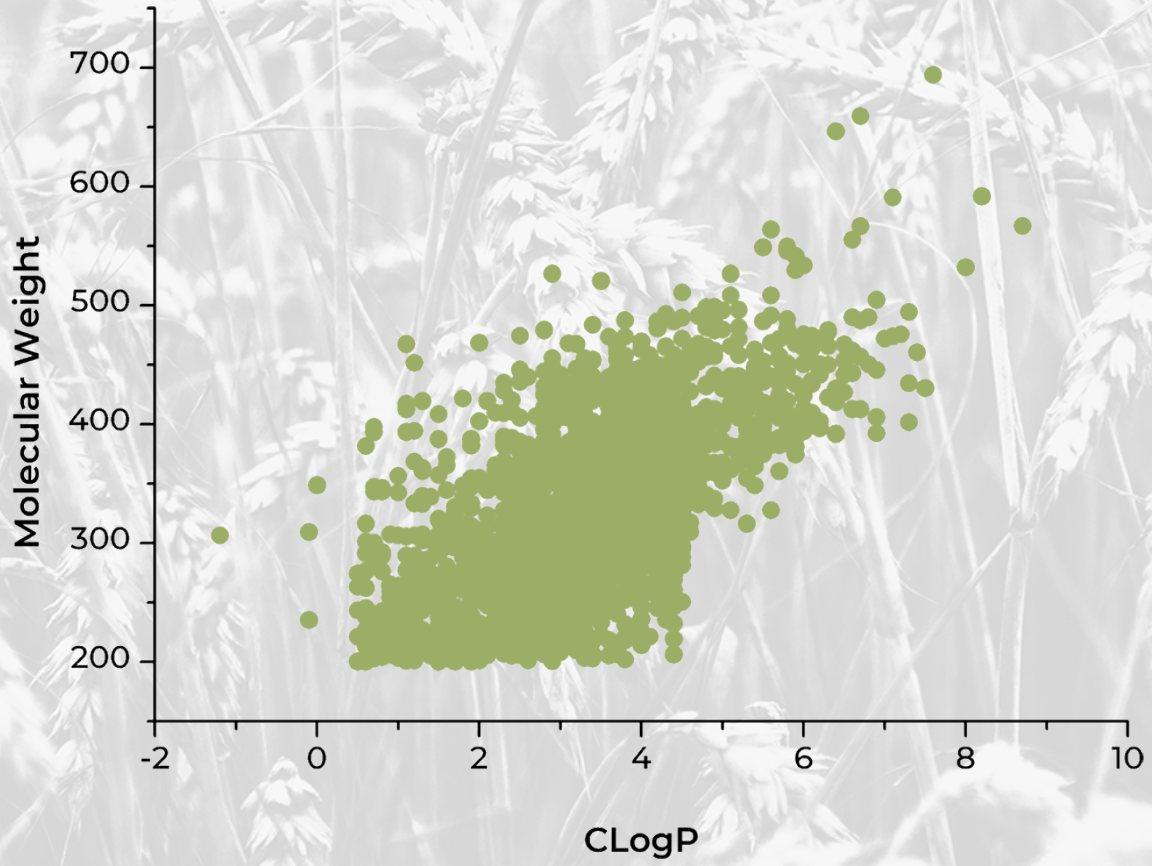
Target engagement:

Insecticide are chemicals used to kill insects. They are claimed to be a major factor behind the increase in the 20th century's agricultural productivity. At the same time almost everyone insecticides have the potential to significantly alter ecosystems. Many of them are toxic to humans, some concentrate along the food chain. So today it is need to develop new effective insecticides.

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	200.2	693.8	333.5
Number of Hydrogen Bond Donors	0	3	1
Number of Hydrogen Bond Aceptors	1	9	3.7
Number of Rotatable Bonds	0	12	4.5
CLogP	-1.2	8.7	3.4
Number of Rings	0	7	2.6
Polar Surface Area	12	201.9	75.7

Distribution of physicochemical properties of compounds in the library:



Design speciality:

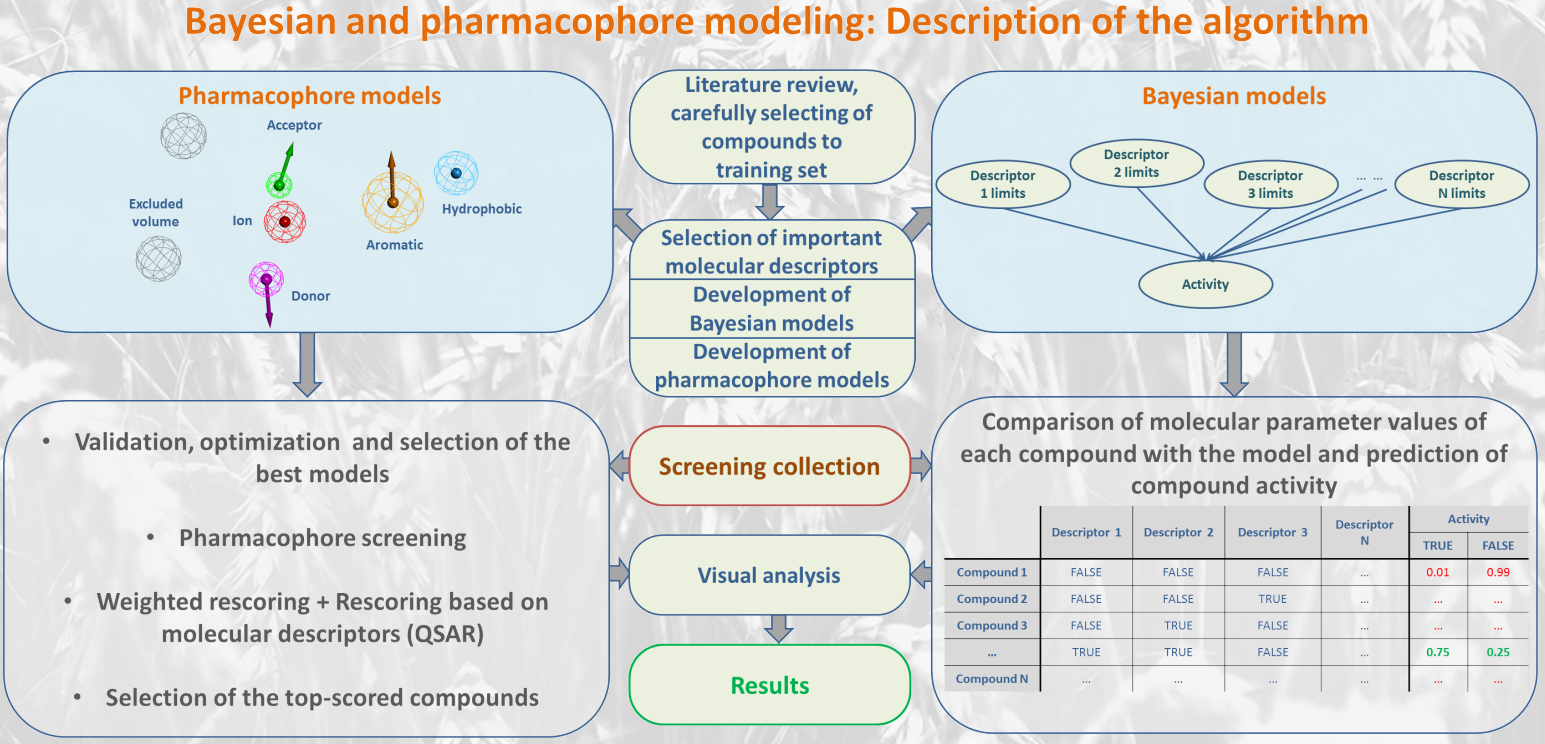
Bayesian and pharmacophore modeling combined with QSAR were used for design of this special screening library containing predicted insecticides.(See Scheme 1)

Known insecticides were clustered into four training sets which have been used for these modeling. The pharmacophore models with different pharmacophore features and excluded volumes were developed, optimized and validated using the training sets. OTAVA Screening Collection was screened against the best optimized pharmacophore models (from one to five models for each training set). Obtained results were rescored using two rescoring functions (first was based on pharmacophore feature weights and second was based on molecular descriptors (QSAR)), filtered on the basis of calculated scores and visually analyzed.

Also Bayesian models were constructed for the same training sets based on fingerprints (FCFP4, FCFP6, ECFP4, ECFP6) and different molecular descriptors (LogP, molecular weight, number of rotatable bonds, number of hydrogen acceptors and donors, number of rings and molecular polar surface area). OTAVA Screening Collection was screened against them and only top-scored compounds were selected.

The application of the combination of these methods and rescoring functions should allow increasing the number of active compounds identified during screening.

Scheme 1. Bayesian and pharmacophore modeling: Description of the algorithm



OTAVA chemicals

Custom synthesis

Molecular modeling

Amyloids detection

Contract research

OTAVA Ltd.
65 Ellerslie Ave., Suite 560
Toronto, Ontario, M2N 1Y1
CANADA

OTAVACHEMICALS.COM