OTAVA chemicals

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

HERBICIDES-LIKE LIBRARY

OTAVA chemicals

OTAVA offers Herbicides-Like Library - special screening library containing predicted herbicides. This library provides an excellent basis for herbicide discovery projects.

The library consists of **2,017 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.

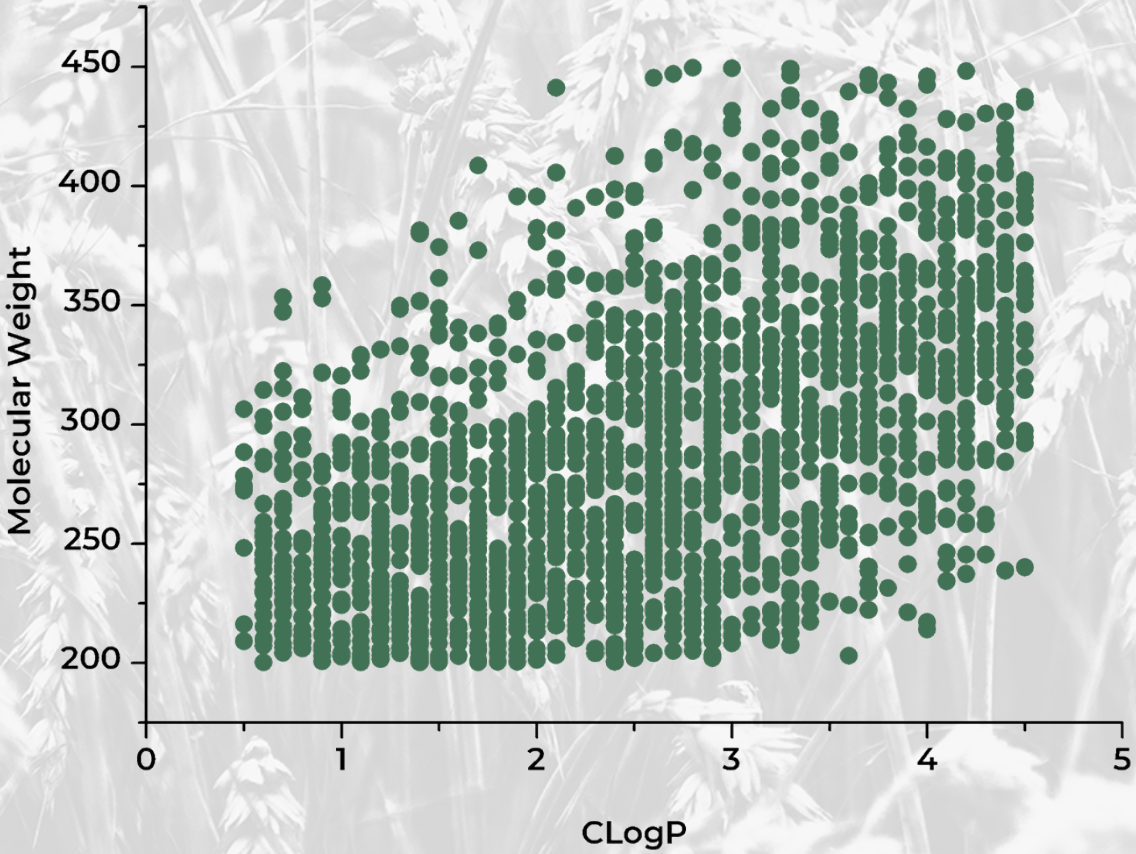
Target engagement:

Weed control is essential in agriculture. Many strategies have been developed to control these unwanted plants which can bring a lot of damage to the crops. Chemical attack with herbicides (weed killers) is one of the leading directions of struggle with weeds. Taking into account the occurrence of resistance in plants and also the negative impact on the environment of some herbicides, the development of new weedkillers is an urgent problem.

The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	200.2	44 9.6	289.9
Number of Hydrogen Bond Donors	0	2	1
Number of Hydrogen Bond Aceptors	1	5	3.8
Number of Rotatable Bonds	0	7	4.1
CLogP	0.5	4.5	2.6
Number of Rings	0	5	1.8
Polar Surface Area	9.2	150.2	72.1

Distribution of physicochemical properties of compounds in the library:



Design speciality:

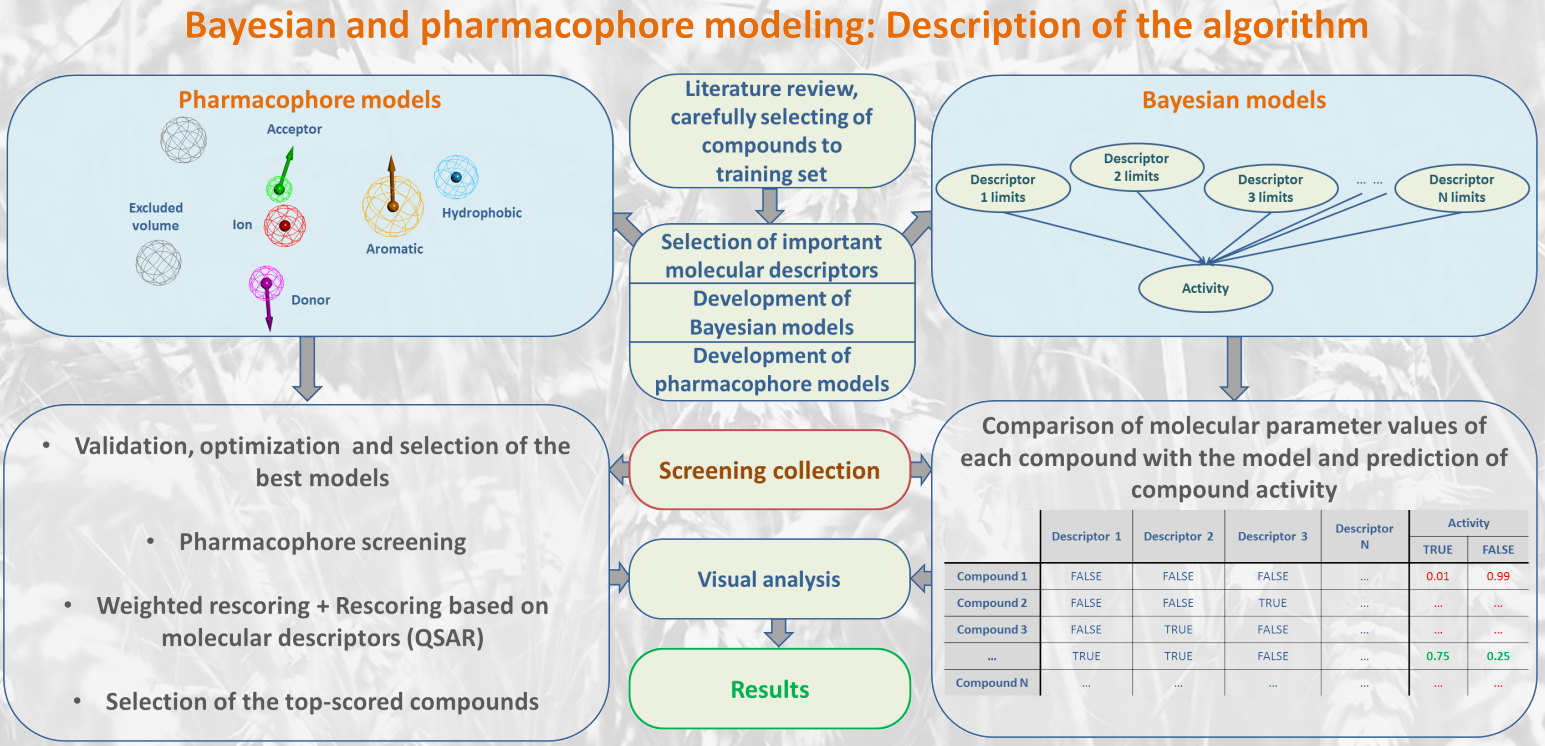
Bayesian statistics and pharmacophore modeling were used for the design of this unique screening collection containing predicted weedkillers. (See Scheme 1)

Known herbicides were clustered into five training sets which have been used for pharmacophore and Bayesian modeling.

Based on FCFP4, FCFP6, ECFP4 and ECFP6 fingerprints and different molecular descriptors (such as LogP, molecular weight, number of rings, number of rotatable bonds, number of hydrogen acceptors and donors and molecular polar surface area) individual Bayesian models were developed for each training set. Then OTAVA Screening Collection was screened against them. All probabilities of compounds activity were calculated with special mathematical apparatus. Thus Bayesian models estimated how physicochemical parameters, including structural (fingerprints) of the compounds were similar to the template herbicides. Only top-scored compounds were selected.

Also pharmacophore models with different combinations of pharmacophore features and excluded volumes were constructed, optimized and validated using the same training sets. OTAVA Screening Collection was screened against the best optimized pharmacophore models (from two to six models for each training set). Results were rescored using combination of special rescoring functions, based on pharmacophore feature weights and molecular descriptors (QSAR). The application of the rescoring should allow increasing the number of active compounds identified during screening. Top-scored compounds were selected and visually analyzed.

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



OTAVA chemicals

Custom synthesis

Molecular modeling

Amyloids detection

Contract research

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