OTAVA chemicals

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

POTASSIUM CHANNEL
BLOCKER LIBRARY

OTAVACHEMICALS.COM

OTAVA chemicals

OTAVA offers Kv1.5 Potassium Channel Targeted Library This library provides an excellent basis for antianginal, antiarrhythmic, neuropathic research and drug discovery projects.

The library consists of **901 compounds***.

All compounds are:

- **in stock**; available amounts: 1 – 50 mg
- **Drug-like only**; reactive, pan-assay interference (PAINS), redox-active and aggregator compounds were removed from the library.

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.

Design speciality:

The Kv1.5 Potassium Channel Targeted Library has been designed as a special screening library containing compounds with predicted Kv1.5 blocking activity and selectivity. A four-center pharmacophore model developed by Yang et al which includes one aromatic ring, two hydrophobic points, and a hydrogen-bond acceptor has been used for the library design. The model was derived from forty Kv1.5 blocker compounds with distinct chemical structure types. We opted this pharmacophore model for virtual screening (See Appendix 1) of OTAVAchemicals Drug-like Green Collection.

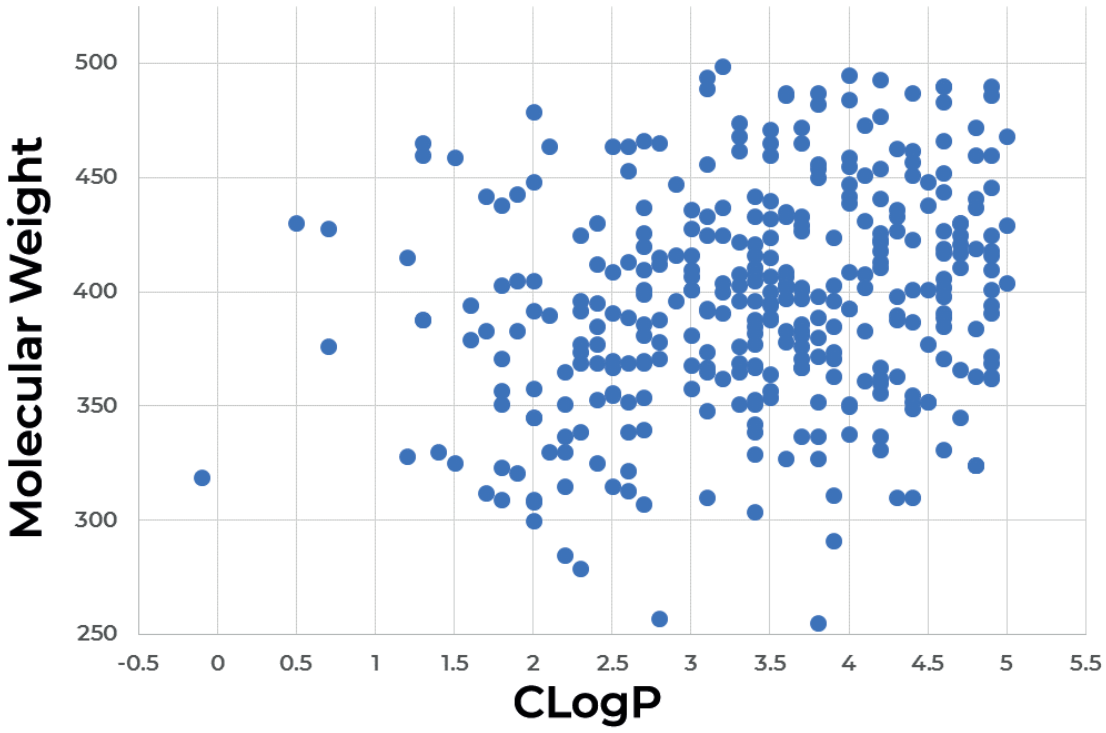
The summary of the library characteristics:

	Minimum	Maximum	Average value
Molecular Weight	255.3	499	400.5
Number of Hydrogen Bond Donors	0	4	1.1
Number of Hydrogen Bond Aceptors	2	8	4.8
Number of Rotatable Bonds	2	11	6.1
CLogP	-0.9	5	3.1
Number of Rings	2	6	3.3
Polar Surface Area	35.5	169.5	89.5

Distribution of physicochemical properties of compounds in the library:

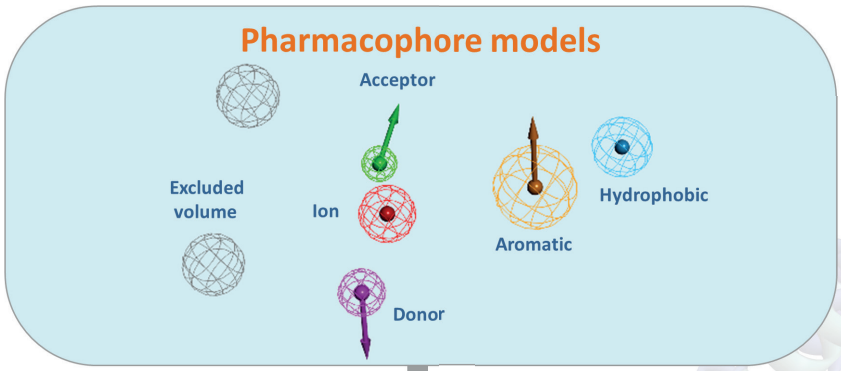
100% Drug-like

42% Lead-like



Appendix 1

Scheme 1. Application of ligand-based pharmacophore modeling for targeted library:



Literature review, carefully selecting of compounds to training set

Selection of important molecular descriptors

Development of pharmacophore models

- Validation, optimization and selection of the best models
- Pharmacophore screening
- Weighted rescoring + Rescoring based on molecular descriptors (QSAR)
- Selection of the top-scored compounds

Screening collection

Visual analysis

Results

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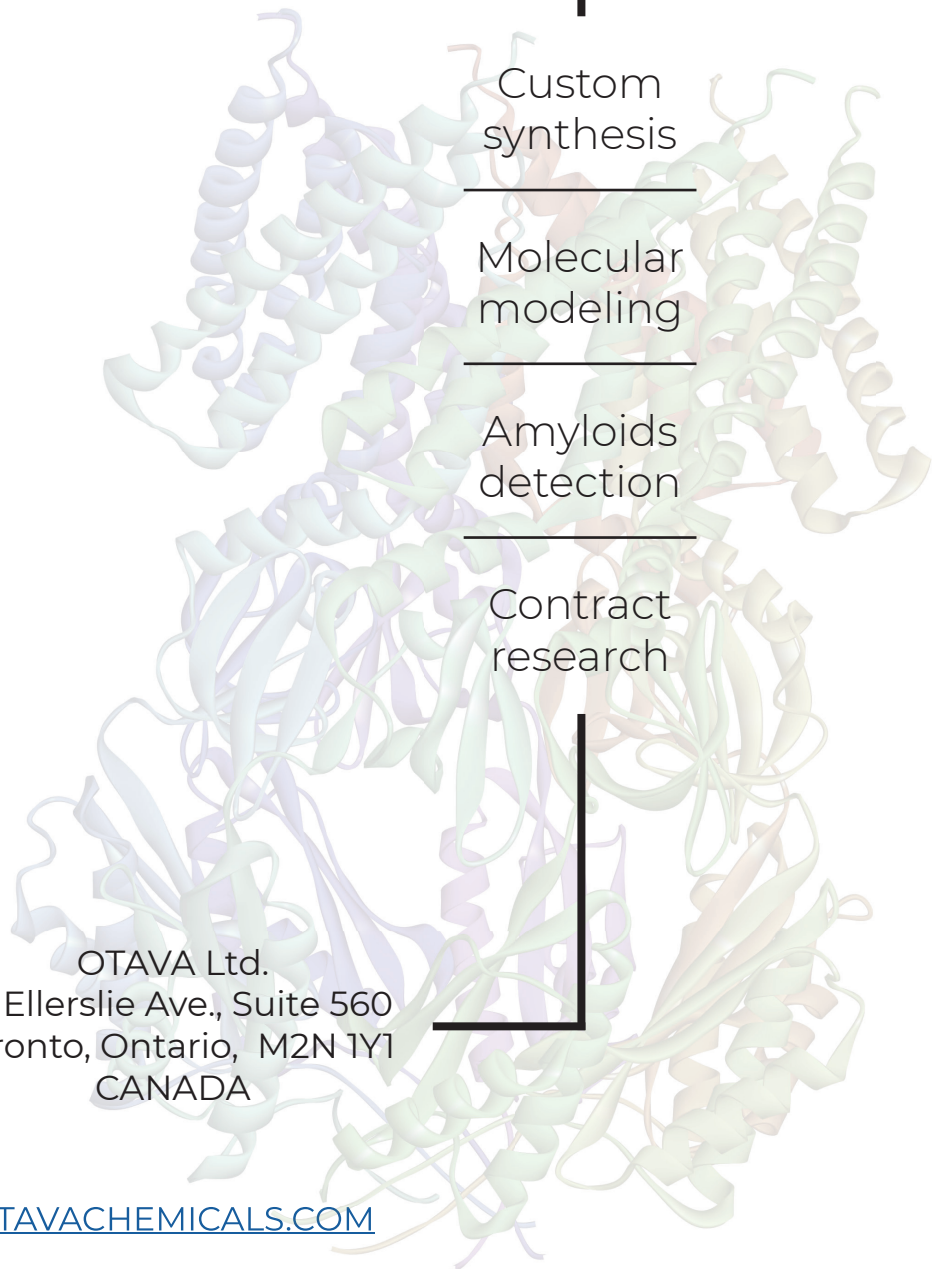

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