OTAVA chemicals

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

# CALCIUM CHANNEL
## BLOCKERS LIBRARY

OTAVACHEMICALS.COM

OTAVA chemicals

OTAVA offers Calcium Channel Blockers Library. This library provides an excellent basis for drug discovery projects related with calcium channel.

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:

Our Calcium Channel Blocker library was designed as a special screening library containing compounds with predicted calcium channels blocking activity and selectivity. The compounds have been selected by pharmacophore screening of **OTAVAchemicals Drug-like Green Collection** against four ligand-based pharmacophore models. The models were built based on known calcium channel blockers.

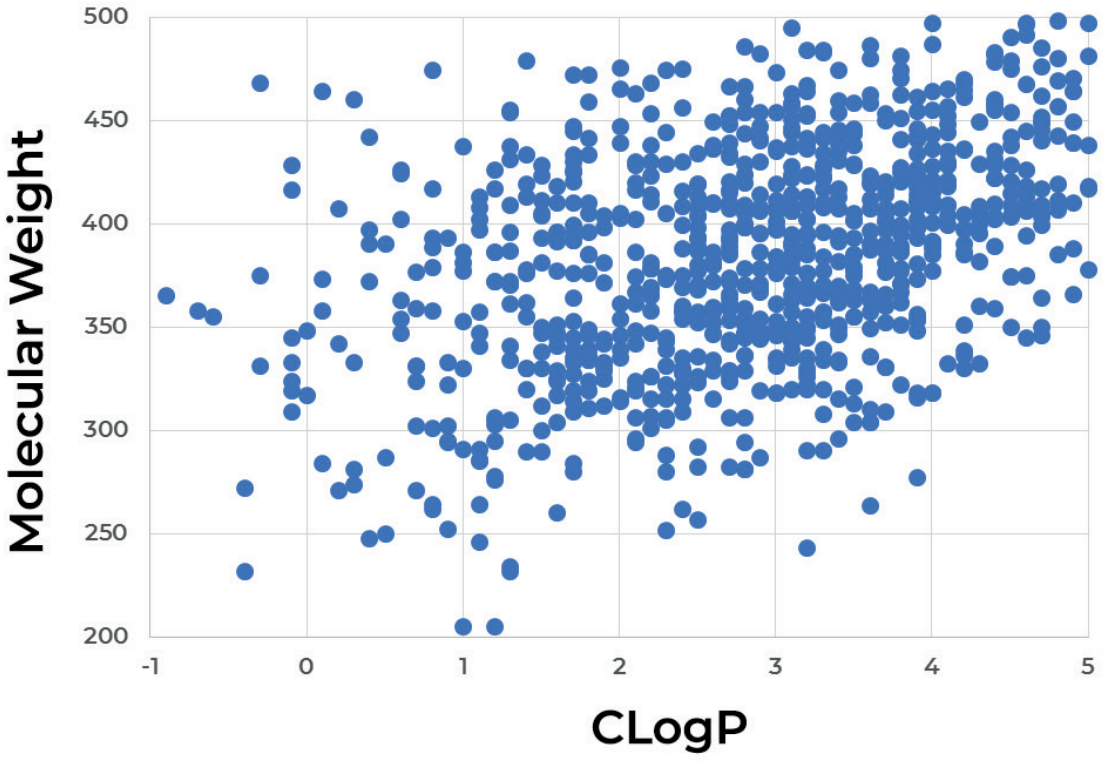
# The summary of the library characteristics:

| | Minimum | Maximum | Average value |
|---|---|---|---|
| **Molecular Weight** | 205.2 | 500.9 | 384.3 |
| **Number of Hydrogen Bond Donors** | 0 | 4 | 1.6 |
| **Number of Hydrogen Bond Aceptors** | 2 | 9 | 4.8 |
| **Number of Rotatable Bonds** | 0 | 11 | 5.6 |
| **CLogP** | -0.9 | 5 | 2.8 |
| **Number of Rings** | 2 | 5 | 3.2 |
| **Polar Surface Area** | 31.6 | 188.2 | 89.8 |

# Distribution of physicochemical properties of compounds in the library:

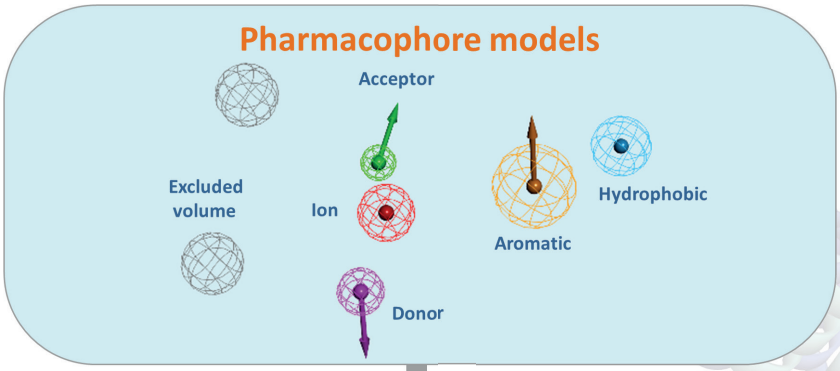
**100%** Drug-like

**54%** 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

# Our contacts:

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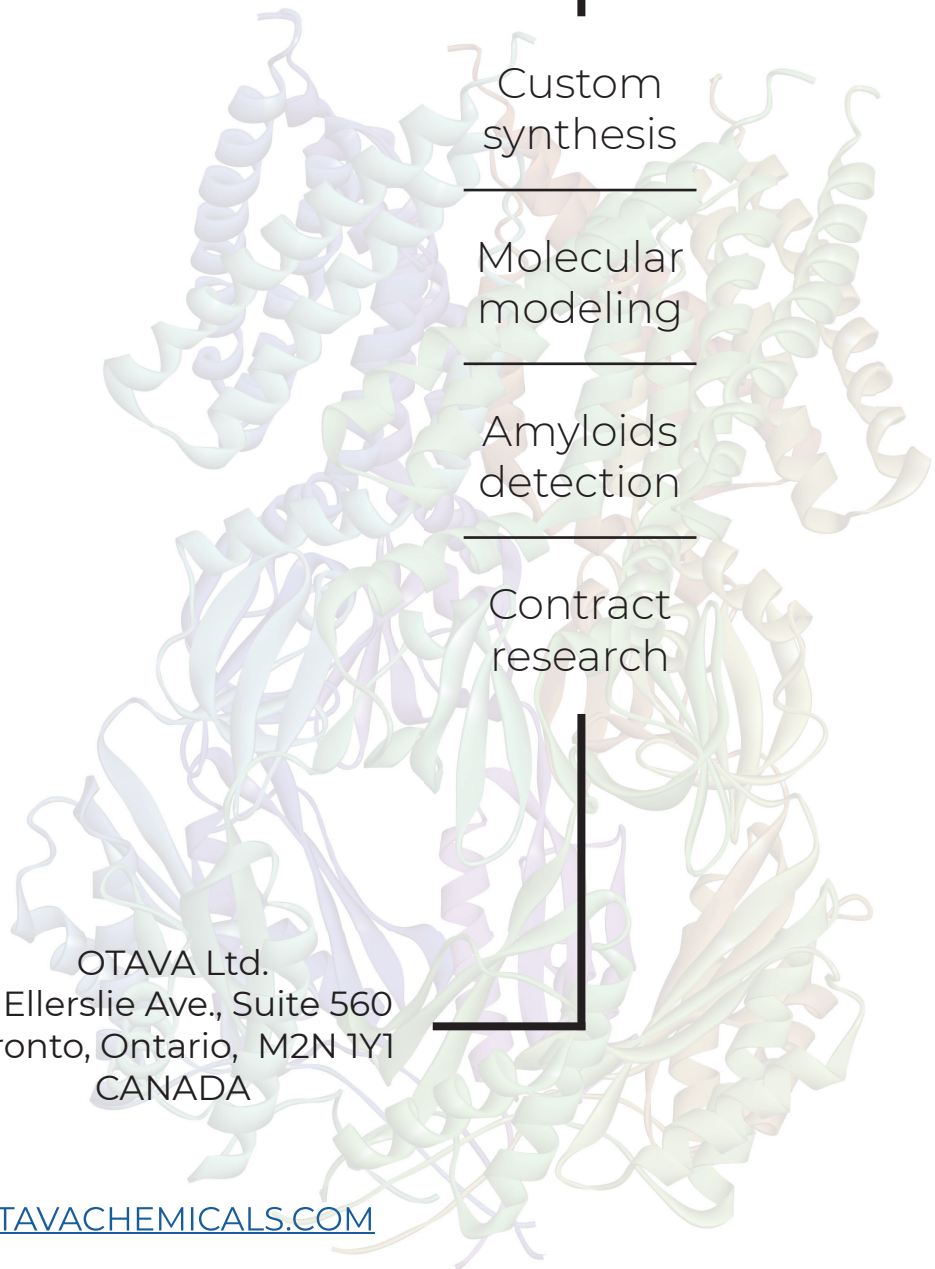
Custom synthesis

Molecular modeling

Amyloids detection

Contract research



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