OTAVA chemicals

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

GABA RECEPTORS

AGONIST LIBRARY

OTAVA chemicals

OTAVA offers GABA Agonist Library. This library provides an excellent basis for drug discovery projects related with GABA receptors.

The library consists of **664 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.

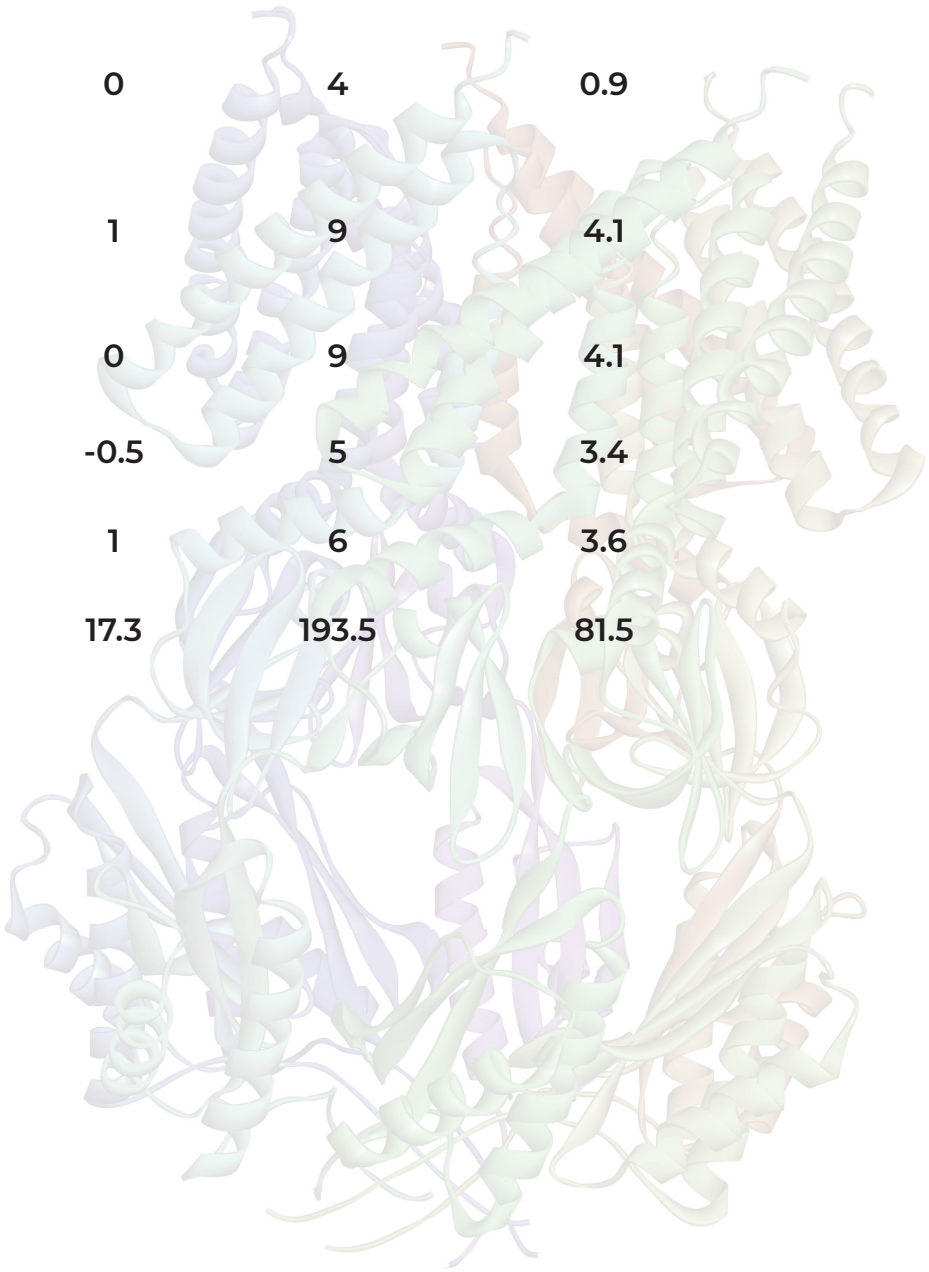
Design speciality:

These special sets of compounds have been carefully designed with powerful predictive tools - Bayesian and pharmacophore modeling combined with QSAR (See Appendix 1). Agonists of GABA were taken from ChEMBL database. Corresponding training sets were formed based on these compounds.

Training sets were used for optimization and validation of ligand-based pharmacophore models. Pharmacophore screenings were performed against best optimized pharmacophore models. 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. The training sets were also used for selection of compounds with Bayesian modeling. It was based on molecular descriptors, such as molecular polar surface area, LogP, molecular weight, number of hydrogen donors and acceptors, number of rotatable bonds, number of rings and fingerprints (ECFP4, FCFP4, ECFP6, FCFP6).

The summary of the library characteristics:

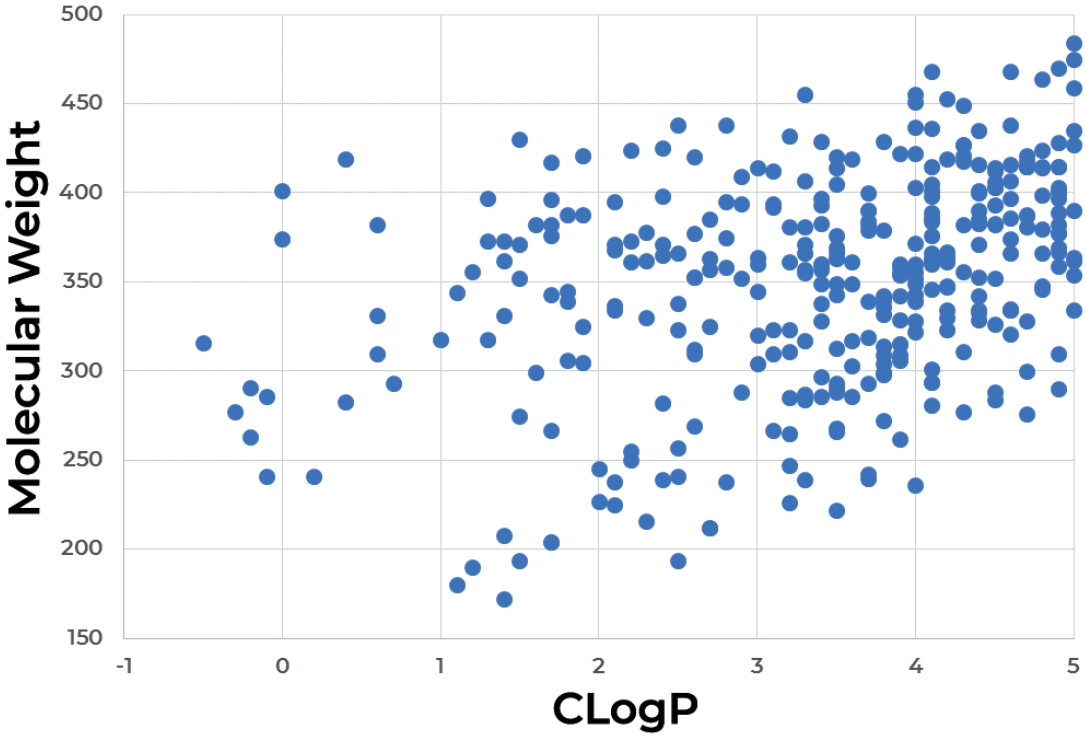
	Minimum	Maximum	Average value
Molecular Weight	172.3	483.6	350.5
Number of Hydrogen Bond Donors	0	4	0.9
Number of Hydrogen Bond Aceptors	1	9	4.1
Number of Rotatable Bonds	0	9	4.1
CLogP	-0.5	5	3.4
Number of Rings	1	6	3.6
Polar Surface Area	17.3	193.5	81.5



Distribution of physicochemical properties of compounds in the library:

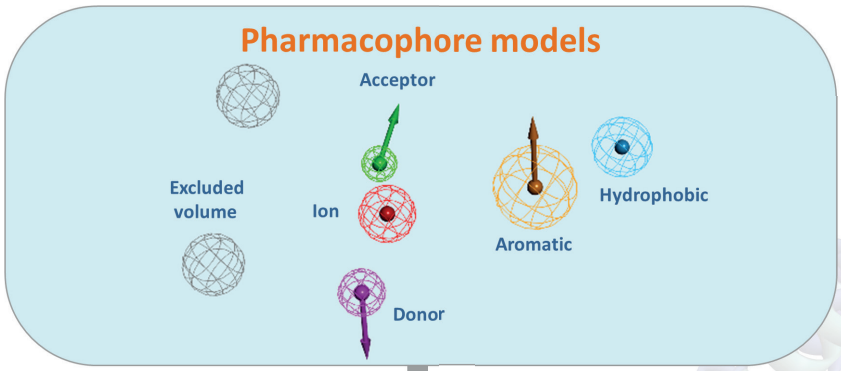
100% Drug-like

55% 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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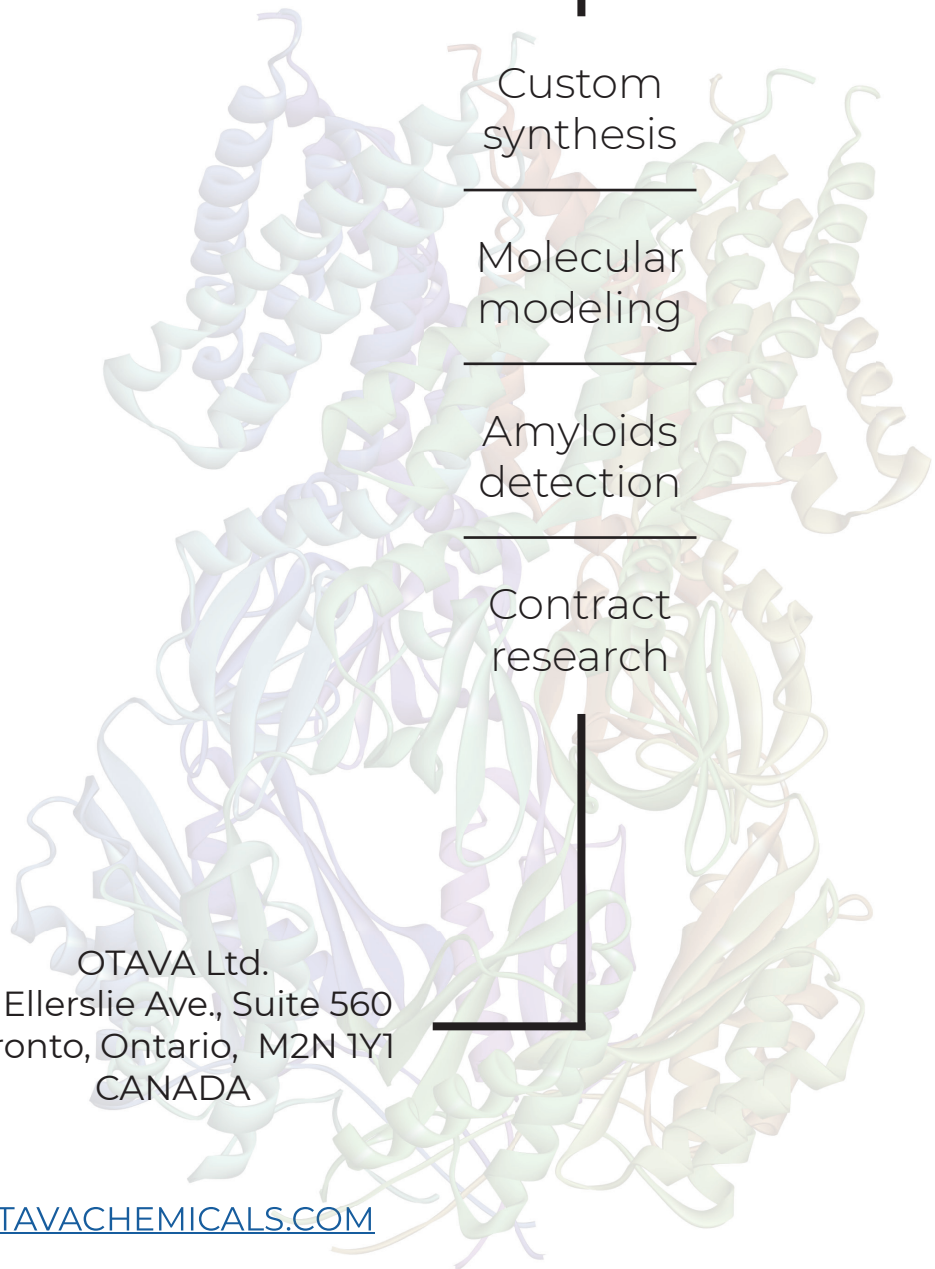

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