OTAVA chemicals

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

# VOLTAGE-GATED SODIUM CHANNEL BLOCKERS LIBRARY

OTAVA chemicals

OTAVA offers Voltage-Gated Sodium Channel Blockers Library. This is a special screening collection containing drug-like compounds with predicted affinity to voltage-gated sodium channel. This library provides an excellent basis for epigenetic drug discovery.

The library consists of **1,458 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 libraries.

## 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:

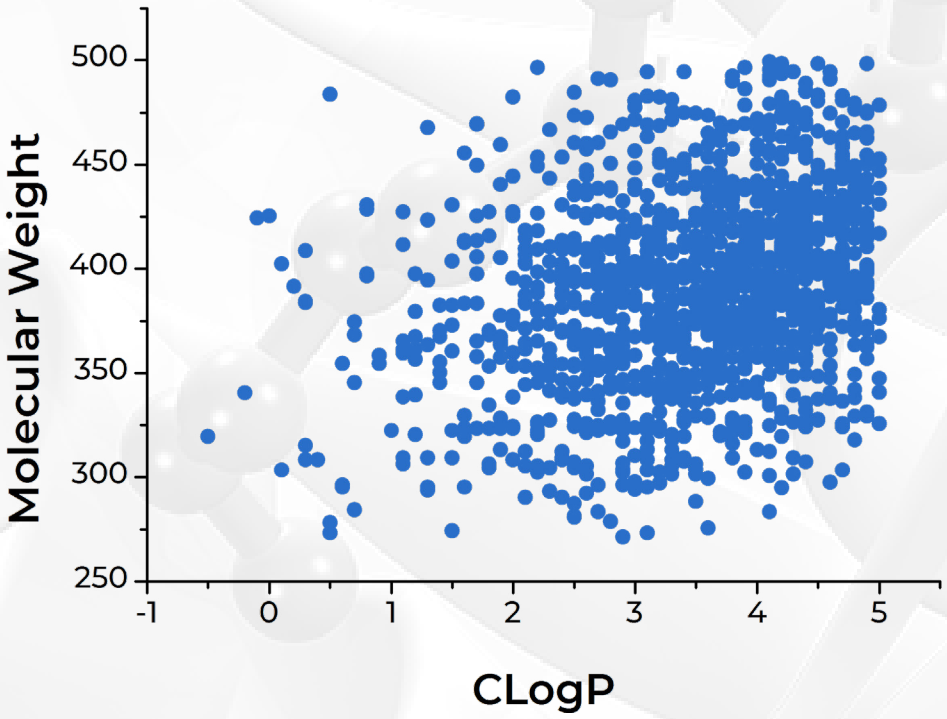
The voltage-gated sodium channels (VGSCs) are a family of membrane proteins forming a pore, through which they selectively conduct sodium ions inward and outward cell's plasma membranes in response to variations of membrane potentials.

Many of the most common neurological disorders, such as epilepsy, migraine, neurodegeneration, and chronic pain, involve abnormalities in neuronal excitability. VGSCs play a fundamental role in originating the rising phase of cell membrane action potential and many experimental data indicate that the functional VGSCs could be implicated in the pathogenesis and/or the progression of such disorders. VGSC-interfering drugs have been used for decades to treat epileptic seizures, the most common disease related to abnormal neuronal excitability, and it has become evident that VGSC blockers could also be beneficial in the therapy of a broad range of disorders.

# Distribution of physicochemical properties of compounds in the library:

**100%** Drug-like

**43%** Lead-like



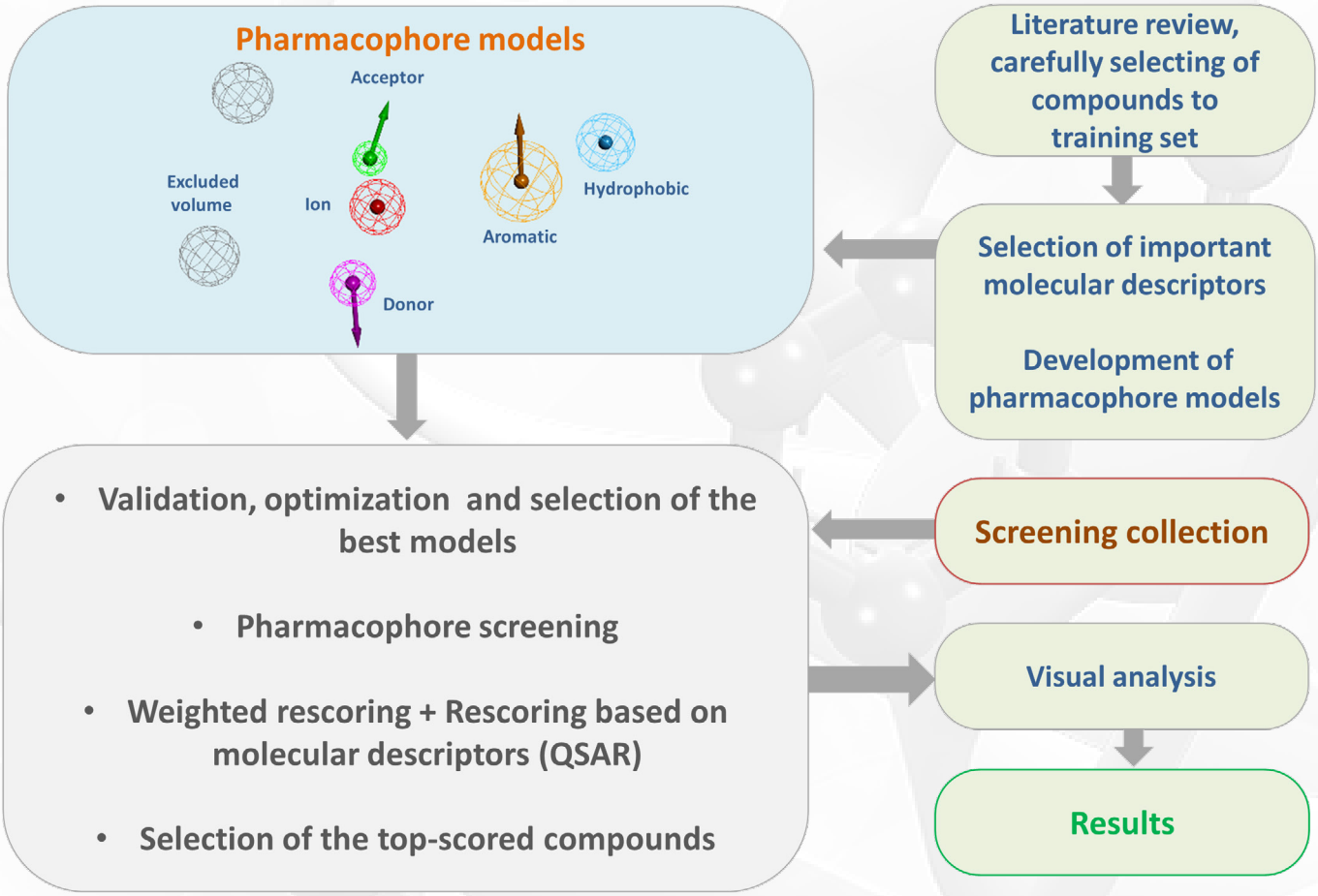
# The summary of the library characteristics:

| | Minimum | Maximum | Average value |
|---|---|---|---|
| **Molecular Weight** | 271.3 | 500 | 387.7 |
| **Number of Hydrogen Bond Donors** | 1 | 4 | 1.3 |
| **Number of Hydrogen Bond Aceptors** | 1 | 10 | 4.3 |
| **Number of Rotatable Bonds** | 3 | 16 | 6.4 |
| **CLogP** | -0.5 | 5 | 3.5 |
| **Number of Rings** | 1 | 5 | 3.1 |
| **Polar Surface Area** | 29.1 | 166.5 | 79.7 |

# Design speciality:

Voltage-Gated Sodium Channel Blockers Library was designed as a special screening library containing compounds with predicted sodium channels blocking activity and selectivity. The compounds have been selected by pharmacophore screening (Scheme 1) of OTAVAchemicals Drug-like Green Collection against three ligand-based pharmacophore models. The models were built based on the known sodium channel blockers divided into three groups according to their structural features.

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



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# OTAVA chemicals

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