



# Voltage-Gated Sodium Channel Blockers Library from OTAVA

Andriy Petrenko

## ► To cite this version:

Andriy Petrenko. Voltage-Gated Sodium Channel Blockers Library from OTAVA. [Research Report] Otava. 2014. hal-01076470

**HAL Id: hal-01076470**

**<https://hal.science/hal-01076470>**

Submitted on 22 Oct 2014

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

## **Voltage-Gated Sodium Channel Blockers Library from OTAVA**

Voltage-gated sodium channels are a class of large integral membrane proteins, composed of a highly processed  $\alpha$  subunit and one or several smaller  $\beta$  subunits. The  $\alpha$ -subunit forms ion-conducting aqueous pore whereas auxiliary  $\beta$  subunits modify the kinetics and voltage-dependence of channel gating.

Voltage-gated ion channels are implicated in the regulation of synaptic transmission, muscle contraction and hormone secretion in response to membrane depolarization.

It was demonstrated that dysfunction of voltage-gated sodium channels led to the development of a wide range of human pathologies such as inherited epilepsy, migraine, periodic paralysis, cardiac arrhythmia, chronic pain syndromes and others. Therefore, the inhibition of voltage-gated sodium channels could be an effective strategy to prevent the development of these diseases.

OTAVA Ltd. offers new Voltage-gated sodium channel blockers library containing 1630 compounds. The library was designed as a special screening collection comprising compounds with predicted sodium channels blocking activity and selectivity. The compounds have been selected by pharmacophore screening of OTAVA Drug-like Green Collection toward three ligand-based pharmacophore models. The models were generated based on the known sodium channel blockers divided into three groups according to their structural features.

This library comprises drug-like compounds only and provides an excellent basis for drug discovery.