



DIRECTED SETS FOR ION CHANNEL SCREENING

IONCore/IONSet

Introduction

ChemBridge® offers two computationally selected sets of compounds for ion channel screening: The IONCore™ Library, selected from our CORE Library stock, and the IONSet™ Library, selected from our EXPRESS-Pick™ Collection stock. Both libraries are based on pharmacophores generated from compounds active against ion channel targets (voltage-dependent and ligand-gated). The libraries are non-overlapping, and clients can purchase the full sets or custom-select a subset of compounds from one or both libraries.

IONCore

The IONCore Library is a computationally selected library of more than 6,000 leadlike small molecules. IONCore compounds are part of ChemBridge's CORE Library stock and were selected for synthesis based on similarity to 3D pharmacophore fingerprints generated from published compounds with activity against ion channel targets. More than 320 novel scaffolds are represented in the IONCore Library, and in-stock analogs are available for any compound identified as a hit.

Compounds showing activity against ion channel targets were extracted from public, scientific databases. 3D conformers were generated for each agonist or antagonist compound, and 3D pharmacophore fingerprints were generated from the 3D conformers. These fingerprints were then compared to the 3D pharmacophore fingerprints generated for virtual compounds based on novel scaffolds designed by ChemBridge. Virtual compounds with a high similarity to a published active fingerprint were synthesized and included in the IONCore Library selection.

IONCore Library compounds may show the following type of activity based on the active molecules from which the 3D pharmacophore fingerprints were generated:

- Calcium Channel Activator
- Calcium Channel Agonist
- Calcium Channel Antagonist
- Calcium Channel Blocker
- Calcium Channel Inhibitor
- Calcium Channel Modulator
- Chloride Channel Blocker
- Potassium Channel Activator
- Potassium Channel Antagonist
- Potassium Channel Blocker
- Potassium Channel Disinactivator
- Potassium Channel Inhibitor
- Potassium Channel Modulator
- Potassium Channel Opener
- Sodium Channel Antagonist
- Sodium Channel Blocker
- Sodium Channel Closer
- Sodium Channel Inhibitor
- Sodium Channel Modulator

IONSet

The IONSet Library is a computationally selected library of more than 6,000 druglike small molecules. IONSet compounds are part of ChemBridge's EXPRESS-Pick Collection stock and contain pharmacophores matching pharmacophores from known ion channel modulators as published by Li and Harte¹. To ensure a high-quality set of compounds, ChemBridge applied a range of filtering, including filtering for enhanced physiochemical properties and removal of compounds with undesirable chemical groups (e.g. Michael acceptors, crown-ethers & analogs, disulfides, epoxides, etc.). A 3D conformational analysis was then used to identify all pharmacophores presented within the subset of filtered compounds (based on low-energy conformers). EXPRESS-Pick Collection stock compounds exhibiting pharmacophores matching those identified in Li and Harte were retained and included in the IONSet Library.

IONSet Library compounds may show activity against the following ion channel targets based on active molecules from which the pharmacophores were generated:

- Ligand-gated: 5-HT₃, GABA, glycine, nAChR, and PCP receptors
- Voltage-dependent: Sodium, potassium and calcium

¹Li, Y.; Harte, W. E. A review of molecular modeling approaches to pharmacophore models and structure-activity relationships of ion channel modulators in CNS. *Curr. Pharm. Des.* 2002, 8 (2), 99-110.

Format

- Download structures and custom select IONCore Library and/or IONSet Library compounds
- Compounds can be provided in 96-well or 384-well format
- Compounds are available dry or as DMSO solutions



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