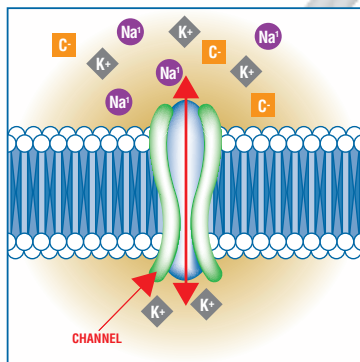


# Let ChemBridge help develop interesting leads for your Ion Channel Targets



## Introducing ChemBridge's NEW Ion Channel Set:

drug-like compounds containing known ion channel modulator pharmacophores.\*

The Ion Channel Set was rationally selected from our entire EXPRESS-Pick stock collection containing over 370,000 small molecules via a

### Pharmacophore Query Technique:

- Over 100 in-house drug-like/lead-like filters were applied to create a refined subset of the best drug-like molecules.
- From this highly filtered group, a conformational database with 1500 low energy conformers per compound was generated using MOE software (Chemical Computing Group).
- 10,000 compounds were finally selected after MOE analysis that matched these published ion-channel modulator pharmacophores.

### Targets Covered within the Ion Channel Set:

- **Ligand-gated:** 5-HT<sub>3</sub>, GABA, Glycine, nAChR, and PCP receptors
- **Voltage dependent ion channels:** (e.g. Na<sup>+</sup>, K<sup>+</sup>, Ca<sup>+</sup>)

## Working on Other Targets?

Then customize ChemBridge's computational expertise by tailoring our suite of tools to your specific targets.

### Computational Expertise:

- **Structure-based drug design:** including homology modeling, binding site characterization, and docking exercises.
- **Ligand-based modeling:** using 2D/3D descriptors or 3D pharmacophores; Library characterization, lead optimization, property optimization, and scaffold morphing.

### Software tools & resources:

- ICM-Pro, MOE, and Daylight program suites, providing tools in virtual ligand docking, homology modeling, protein modeling, pharmacophore modeling, flexible ligand alignment, molecular dynamics, and many others.

\* Li, 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.

