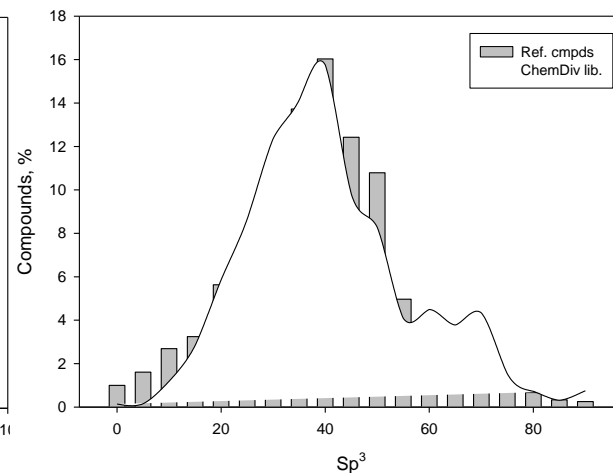
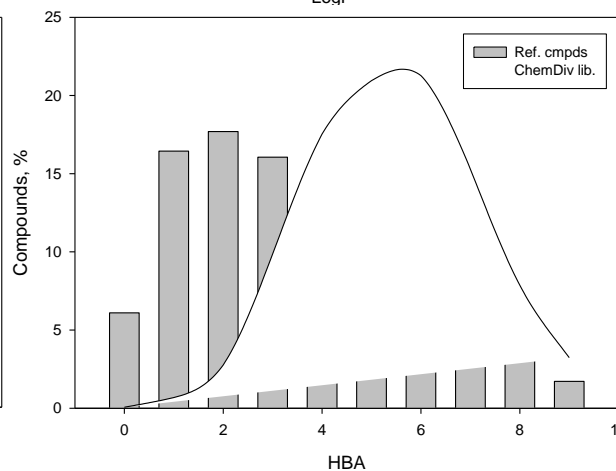
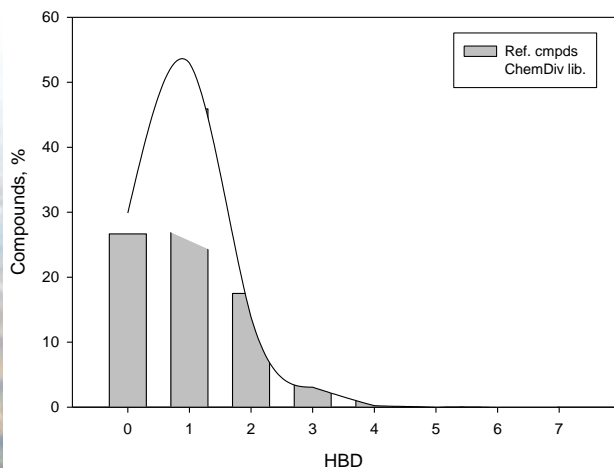
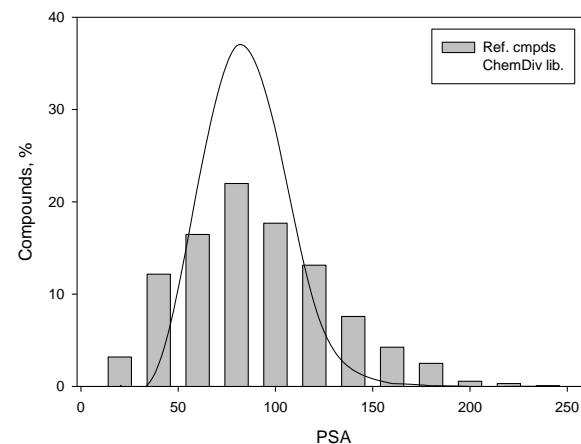
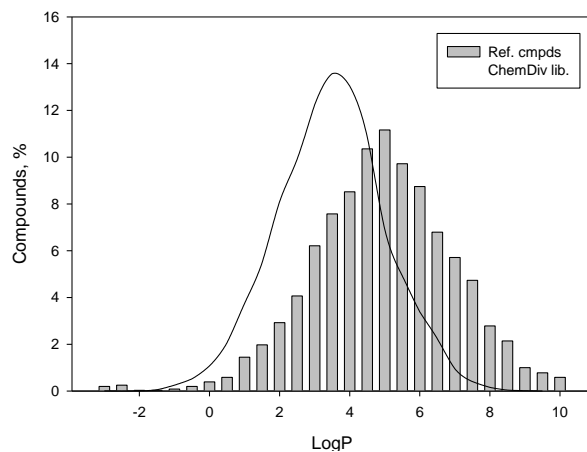
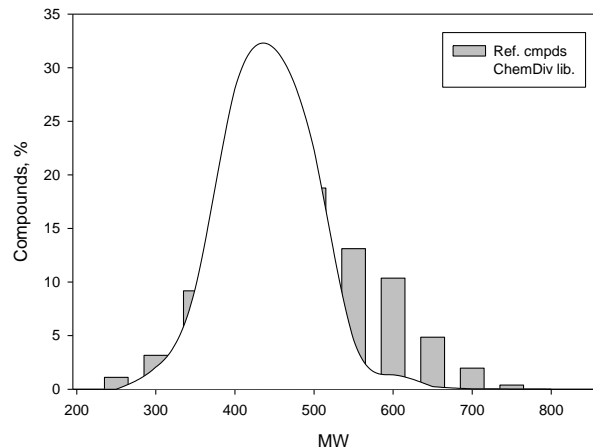


*The chemistry of cures<sup>SM</sup>*

# Calcium channels focused library

# A brief insight into the property space of the reported calcium channels binders and compounds from the Lib

- ▶ more than **3600** small-molecule calcium channels ligands (**MW<700**) have been reported to date

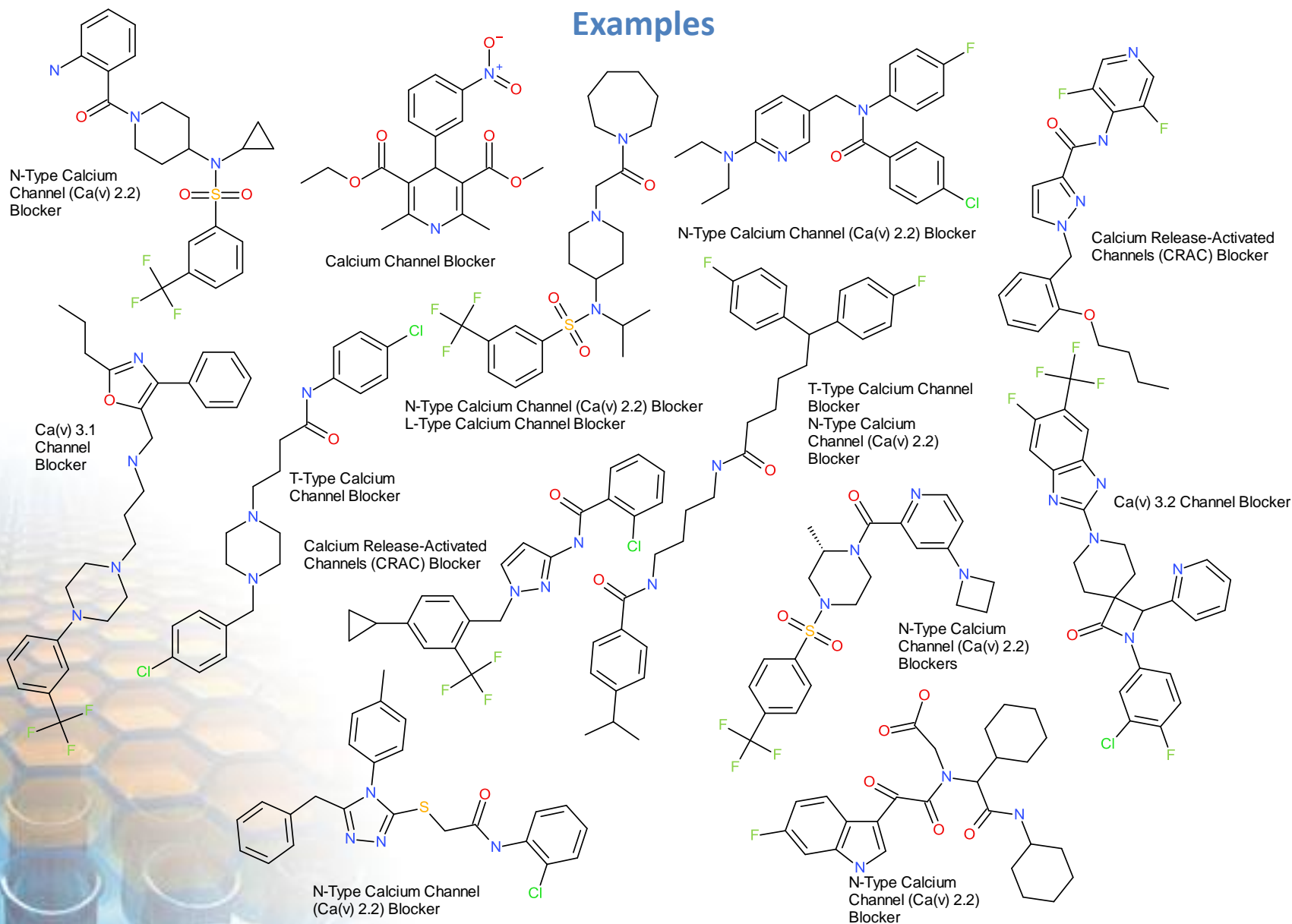


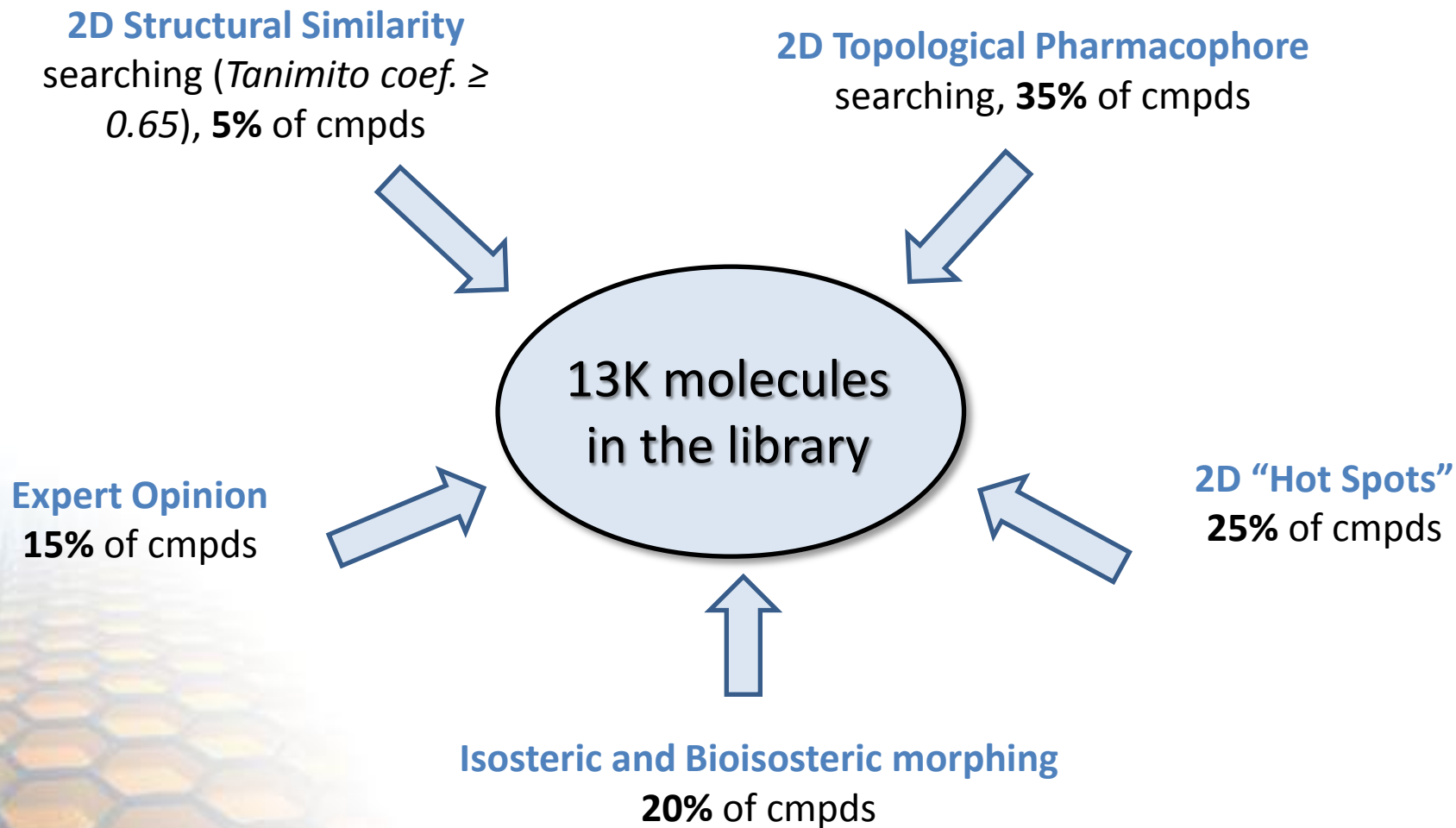
## ChemDiv calcium channels library

- ▶ Lower **LogP** values / Lipinski rule matched
- ▶ Optimal **PSA** for sufficient solubility
- ▶ Good **Sp<sup>3</sup>** cover (>90%)

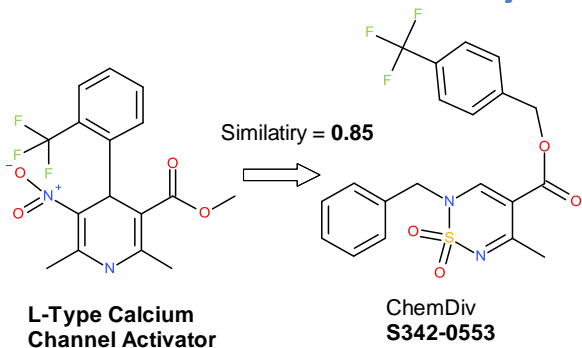
► More than **800** cmpds with  $IC_{50} < 10 \mu M$  were selected for the reference set

## Examples

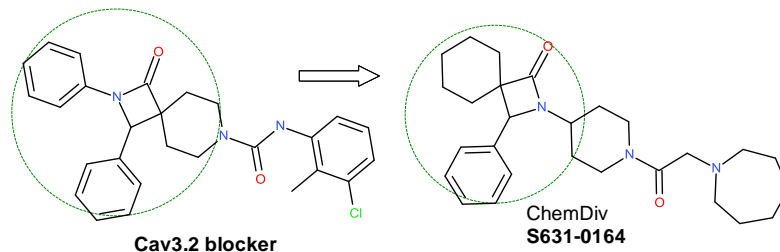




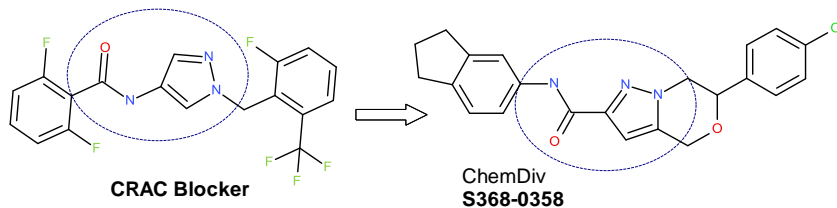
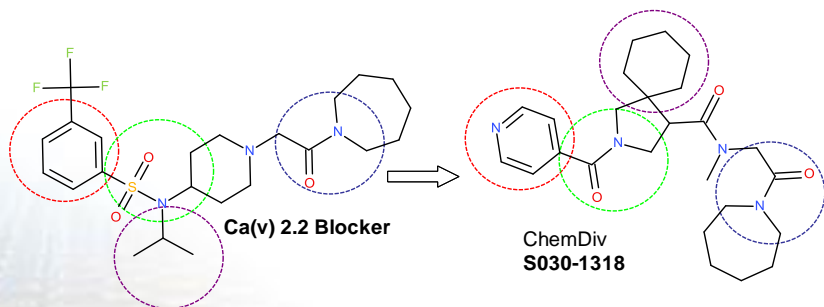
## 2D Structural Similarity



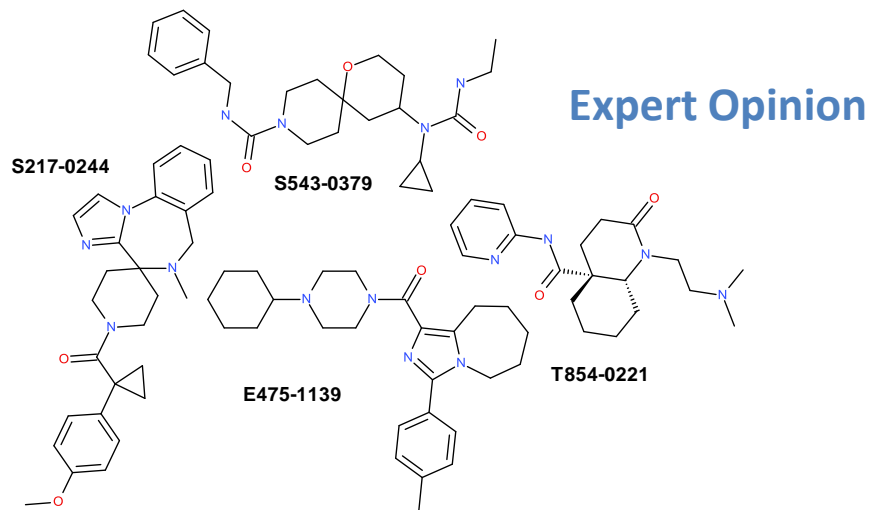
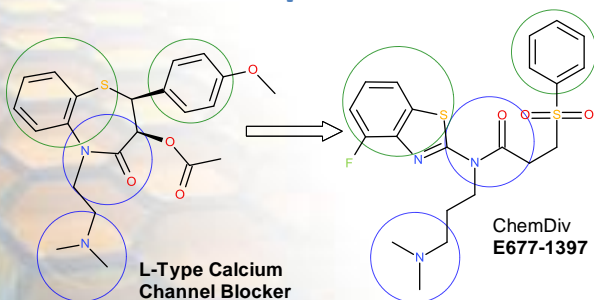
## Isosteric and Bioisosteric morphing



## 2D Topological Pharmacophore

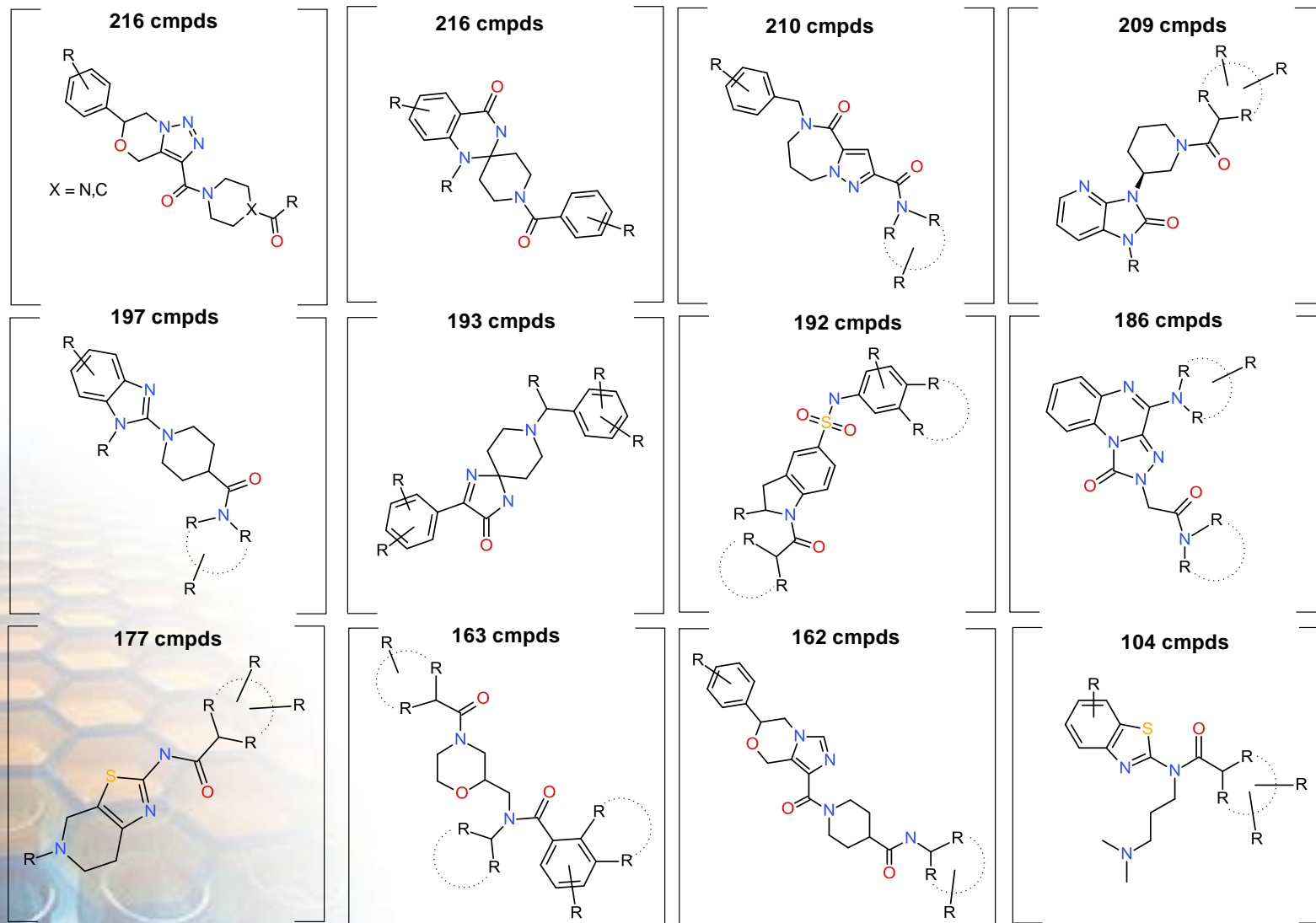


## 2D "Hot Spots"



## Key Properties

► cmpds, of total: **12814** ► clusters, total amount: **321** ► similarity threshold: **0.6** per cluster (*Tanimoto*) ► singeltones: **440** ► minimal cluster size: **5** ► Diversity: **0.793** ► Screens: **4435**





# Representative examples

