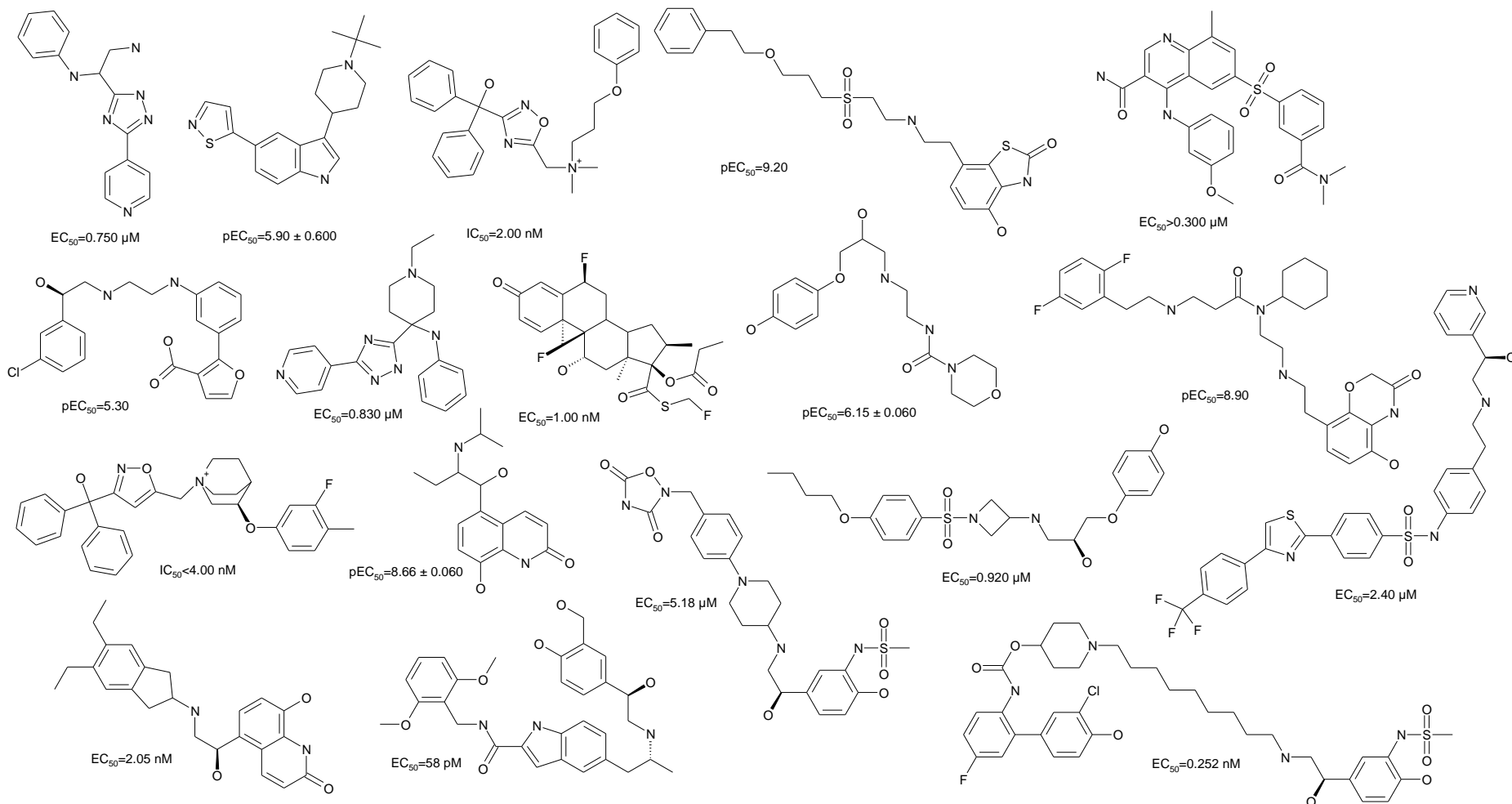


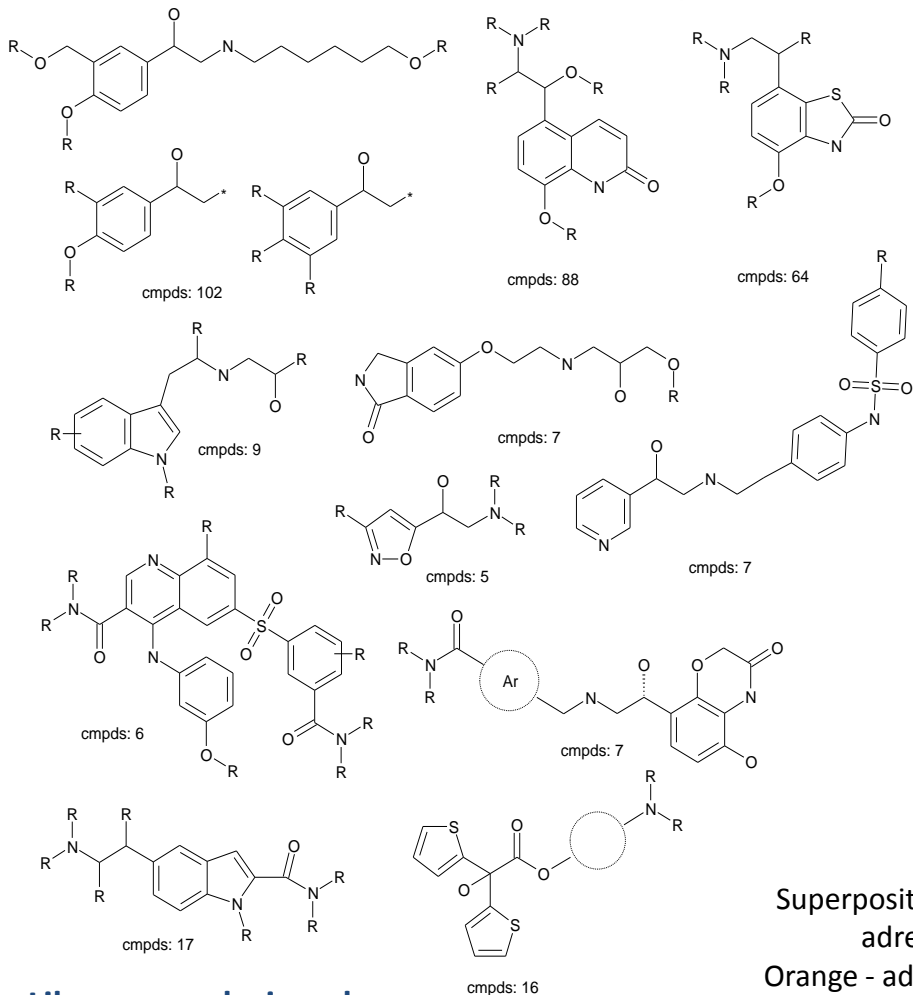
# Reference dataset: 1164 reported $\beta_2$ -adrenoceptor agonists/ligands

## Representative examples

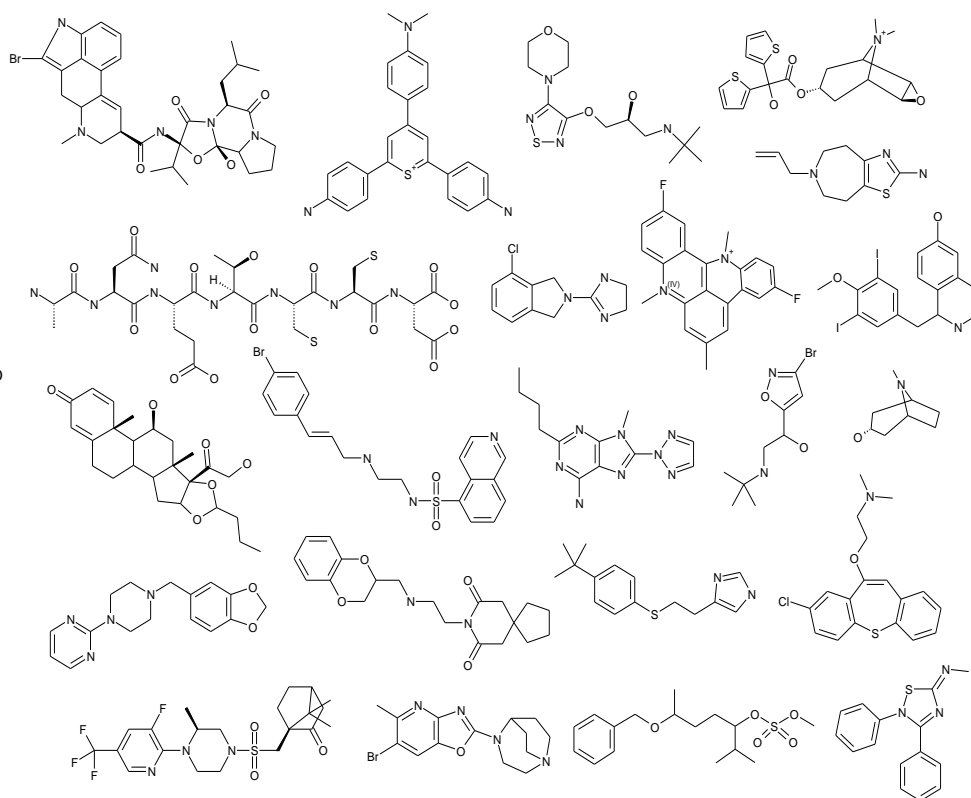


Diversity: 0.68

# Reference database clustering

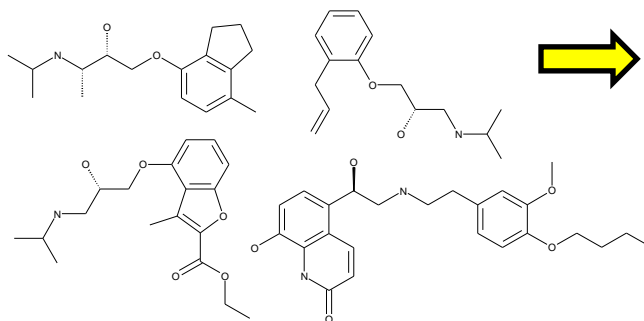


# Ref Divers set

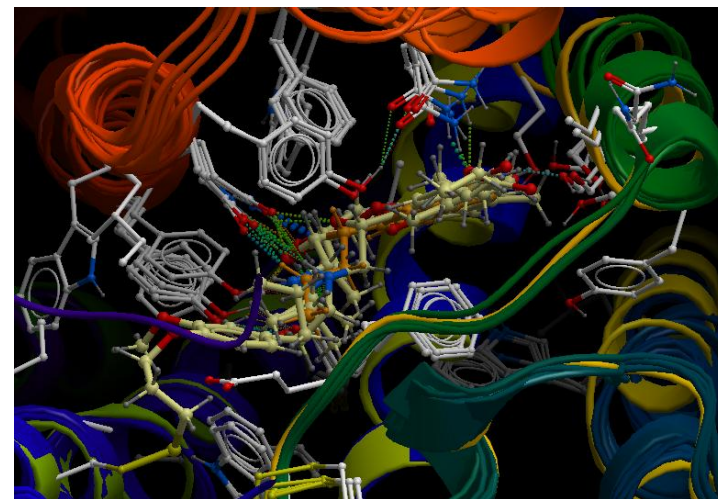


## Library was designed as:

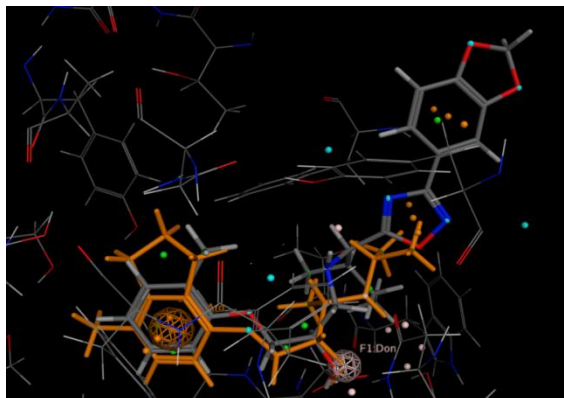
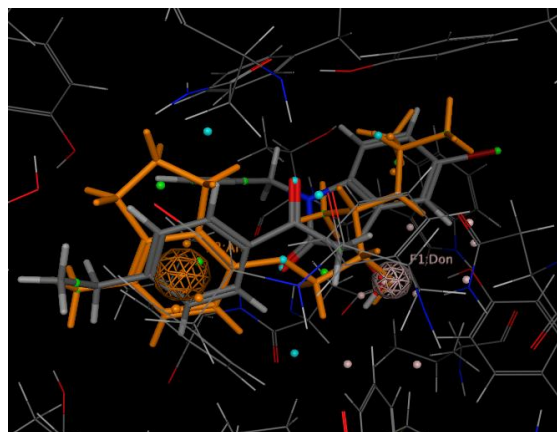
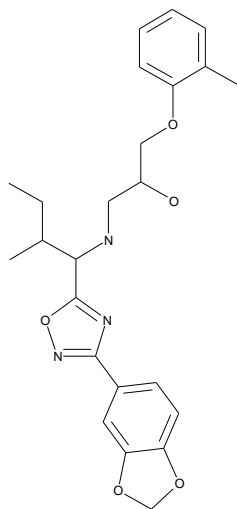
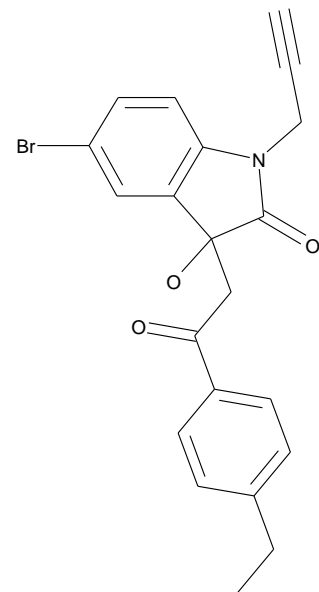
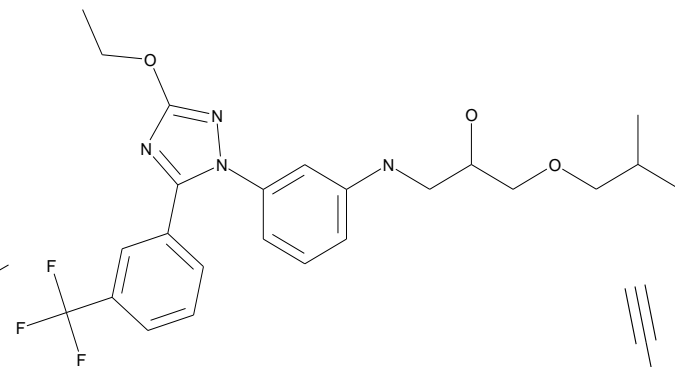
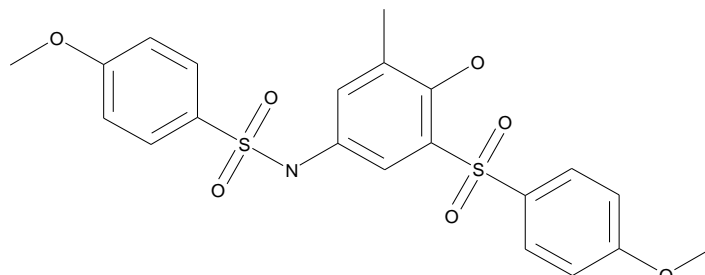
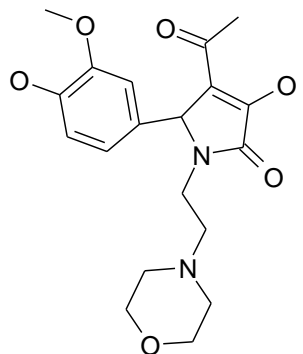
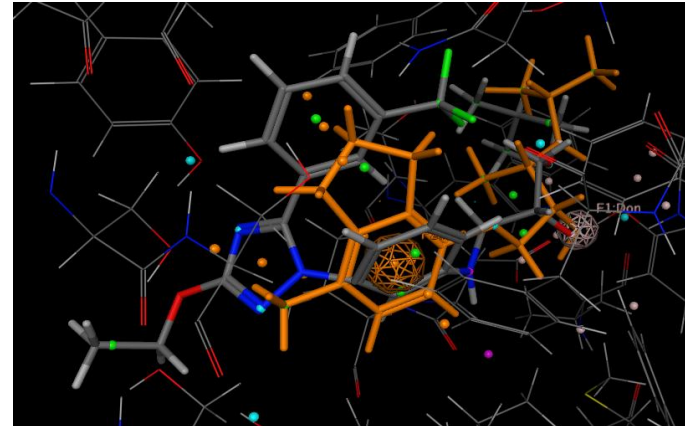
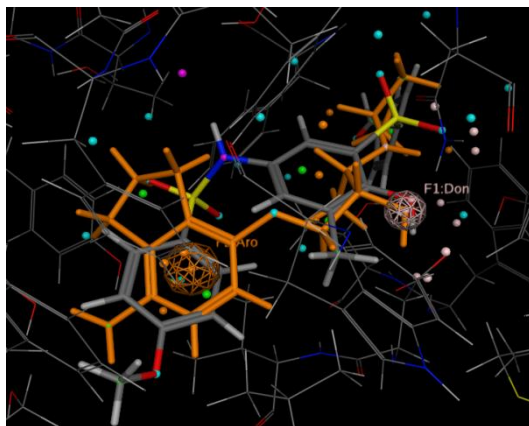
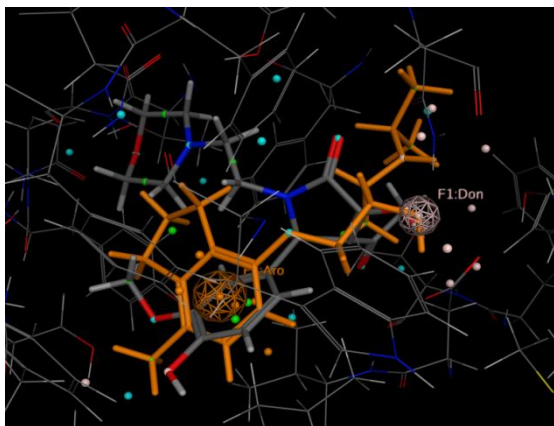
1. 2D similarity searching
2. 2D-topological analogues
3. "Hot-spot" recognition elements
4. 3D Docking / pharmacophore modeling  
(only for selected scaffolds)



Superposition of several  $\beta_2$ -adrenoceptor ligands  
Orange - adrenaline



# Representative examples of *in silico* hits



# Representative examples of compounds from the focused set

