Lipid GPCR Library

7,512 compounds

Enamine Lipid GPCRs focused Library has been designed in collaboration with **NQuiX**. Over **7,000** compounds have been selected from Enamine ***Screening Collection*** and ***REAL Database***. They target the family of 8 EDG receptors (S1P1-5 and LPA1-3). The compounds may also be appropriate for screening at GPR3, GPR6 and GPR12 orphan receptors given some TM bundle binding site similarity and/or GPR23, GPR92 and P2Y5 given their more recent classification as additional, albeit distinct, LPA receptors. The compounds have been selected using a combination of ligand-based methods including chemical fingerprints, 2D pharmacophores and 3D shape/feature matches. They represent a combination of compounds for expanding SAR around known chemotypes and scaffold hops seeking novelty. The current set of compounds covers the non-acidic classes of ligand, with acidic compounds being designed *via* a different procedure and offered separately.

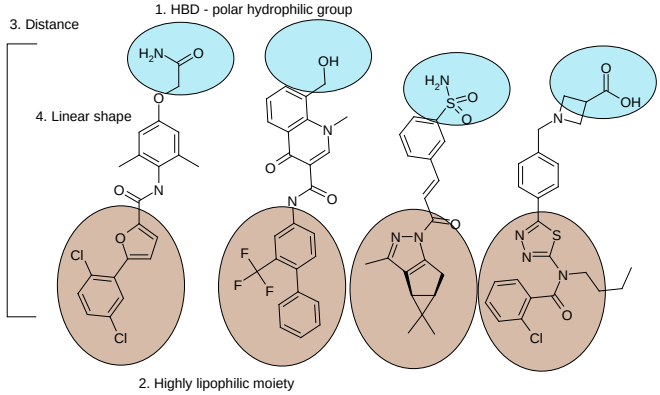

Fig. 6. *General scheme of dedicated design of compound structures included in the Library.*

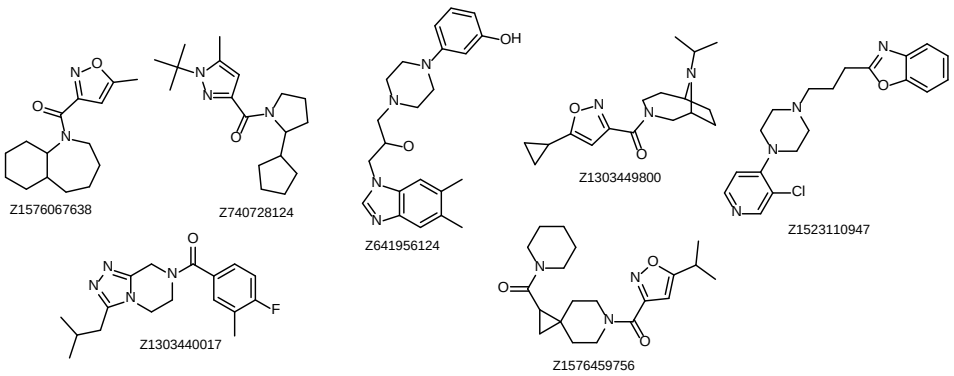

Fig.7. *Examples of non-acidic compounds in the Lipid GPCRs Library.*

The total number of unique compounds with activity (collected across 73 papers) is 1 393 of which 870 are acidic and 523 are non-acidic. The non-acidic ligands formed the basis for the library design via a combination of ligand-based selection methods.

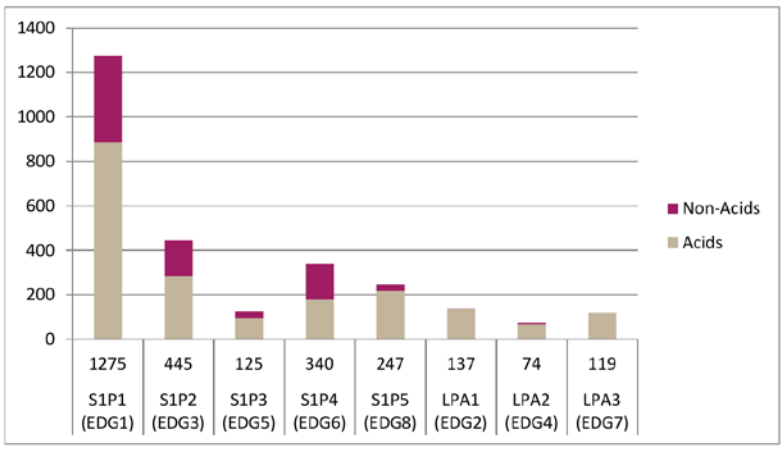

Fig. 8. Activity distribution of the training active compound set