GPCR Library

Designed for discovery of new GPCR ligands

54,077 compounds

G protein coupled-receptors (GPCRs) are to date the most successful family of druggable targets in modern Medicinal Chemistry. More than 1/3 of all approved drugs target GPCRs.

We have carefully selected 54,077 diverse compounds specifically targeting GPCR's. The library is available for cherry picking. All compounds are stored as dry materials and they can be acquired in diverse custom formats. Alternatively, we can promptly supply a copy of the **pre-plated GPCR Library** having 50,560 compounds, that can be also made in a customized ready-to-screen formats. Using our GPCR Library for hit discovery you receive multiple benefits allowing you to save on time and costs in lead generation:

- **Dry stock of over 2.6M compounds for hit resupply and hit expansion**.
- **Low-cost synthesis of analogues within only 3 weeks through our REAL Database technology**
- **Medicinal chemistry support enhanced with on-site broad ADME/T panel**

You have also an option to screen the librray directly at Enamine. In this case we will be happy to offer you discount on library cost depending on the collaboration scope.

Enamine's **GPCR Library** includes two sub-libraries focusing on *allosteric modulators* and *lipid GPCR*s.

- **Allosteric GPCR library** – 19,600 compounds
- **Lipid GPCR library** – 8,000 compounds

Most popular library formats available for immediate supply

Item	Catalog No.	No of compounds	No of plates	Amount	Plates and format
1	**GPR-50-Y-0**	50 560	158	Any applicable for 1 assay	384-well plates, 320 cpds per plate, first two and last two columns empty
2	**GPR-50-Y-10**	50 560	158	10 µL of 10mM DMSO stock solutions	384-well plates, 320 cpds per plate, first two and last two columns empty
3	**GPR-50-Y-50**	50 560	158	50 µL of 10mM DMSO solutions	384-well plates, 320 cpds per plate, first two and last two columns empty

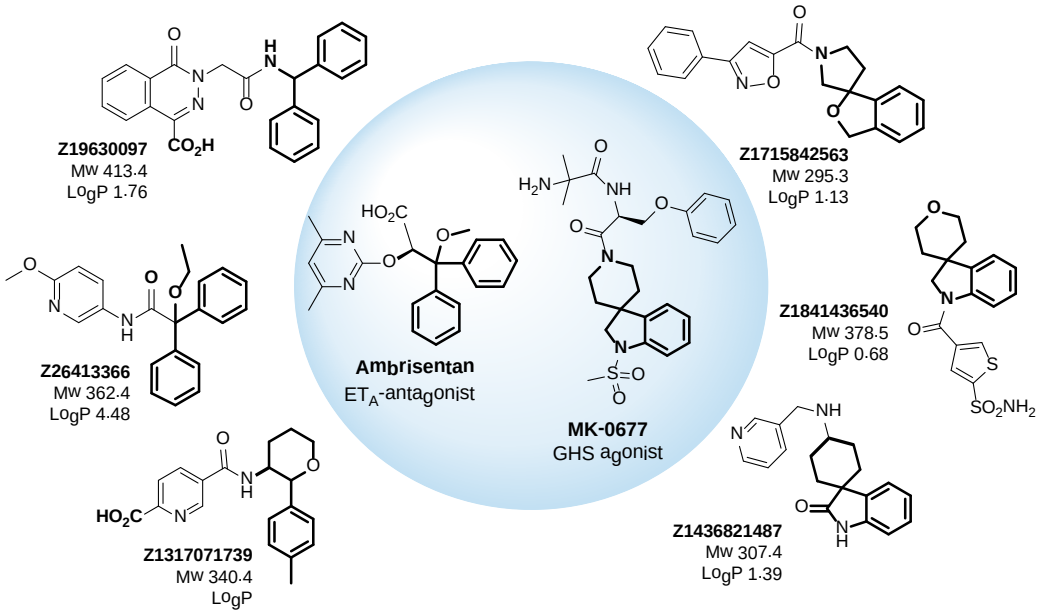
Library Design

We used combination of different *in silico* approaches to design our **GPCR Library**. The library covers a wide range of GPCR-targets and possesses most important features for initial Drug Discovery – *Novelty and High Diversity*. A combined approach, including framework 2D-fingerprint similarity search, careful selection of GPCR-privileged scaffolds and common structural motifs with extension by 3D pharmacophore searches, was used to search of potential actives. MedChem refinements were applied to the combined pool of compounds, resulting in a unique set of 54,000 high quality small molecules.

All compounds from Enamine's **GPCR Library** possess high chemical novelty and drug-like molecular properties with attractive structures.

The following molecular parameters were applied in construction of the library:
MW = 200...550, ClogP = -1.5… 5.5, TPSA ≤ 150 Å^2, RotBonds ≤ 9, HBD/HBA≤ 4 / 10

Examples of compounds from **GPCR Library** having pharmacophore similarity to Ambrisentan and bearing scaffolds that are bioisosteric to the spiro-piperidine-indane privileged fragment.



Novel sp^3-enriched scaffolds specifically designed as cores for Enamine's **GPCR Library**