# Focused Libraries

The selection process for our Focused Libraries sets involves identifying active ligands/inhibitors as prototypes existing in the patent and research literature or databases and performing bioisosteric replacement strategies, e.g. a known peptide ligand may be substituted with a small non-peptide peptidomimetic.

Using “privileged” scaffolds as building blocks is advantageous in synthesis of derivatives for discovery libraries, particularly in the cases when no small molecule ligands known for the target and no structural information is available. Privileged structures are defined as chemical scaffolds present in many biologically active ligands and determining the molecule’s specificity (Evans et al., 1988). For enriching IP potential of these libraries, we have applied the privileged scaffolds approach and implemented structural morphing of privileged structures based on functional equivalents of their constituent hetero atoms. Then a similarity search based on these strategies is conducted within ChemDiv’s collection for possible augmentation of the rational set.

Other techniques include computer-assisted 3-D pharmacophore matching and when possible, in silico docking experiments. The directed synthesis of new chemotypes with functionality mimicking recognition elements (shapes, “warheads”) of known active ligands/inhibitors has also been performed. In some cases, proof of concept has been established with in-house biological data.

A special effort has been made to select respective compounds and synthetic templates with good IP potential, as deduced from Beilstein, SciFinder and Markush sub-structure searches. The special rules of ChemDiv’s medchem filters (MCF) ensure the high quality and drug-like properties of selected

molecules.

Our Focused Libraries are montly updated with novel proprietary compounds that provide our valuable clients with unique approach to establish partnership in the file enrichment and special discovery projects.

Request more info about our **Focused Libraries**:

AKT target library – 13650 compounds

Aurora A-B Kinases library – 5507 compounds

C-Met library – 17130 compounds

CXCR4 antagonists library – 11524 compounds

Lysine Me-transferase G9a inhibitors library – 13319 compounds

GSK3b inhibitors library – 4991 compounds

Hsp70_90 targeted library – 14225 compounds

KRAS targeted library – 11316 compounds

MDM2 targeted library – 22319 compounds

NFkb regulators library – 3104 compounds

P2RX7 antagonists library – 13708 compounds

PI3K inhibitors library – 15683 compounds

**New**

Bcl2 PPI inhibitors library – 14433 compounds

Library of small molecule inhibitors of beta-Catenin signaling – 10132 compounds.

Bromodomains (library of small molecule modulators &

inhibitors of Bromodomains) – 6912 compounds.;

MDM2-p53 interaction inhibitors library – 7555 compounds;

Library of MEF2-HDAC (class II) modulators – 6400 compounds.

SH2 PTB focused library – 8040 compounds