



# HIGHLY DIVERSE PRIMARY SCREENING TOOLS

# DIVERSet® Libraries

## Highlights

- High-quality, structurally diverse compounds
- Select from multiple 10,000-compound blocks to build a library of 10,000 to more than 100,000 compounds
- Option to expand as new DIVERSet Library blocks are released
- Economically priced, pre-plated diversity option

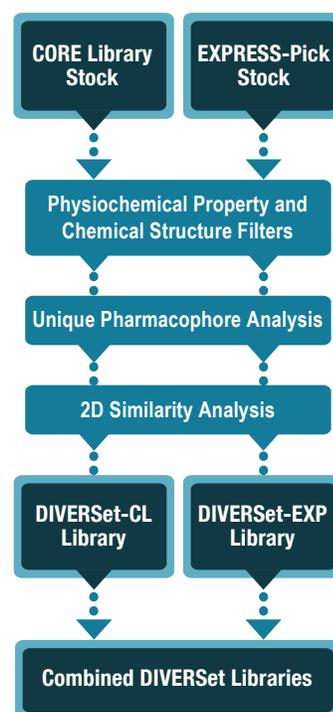
## Introduction

ChemBridge® offers two, complementary DIVERSet® Libraries. Both DIVERSet Libraries (the DIVERSet-CL and the DIVERSet-EXP) are designed to provide the greatest coverage of pharmacophore space within a fixed library size while maintaining structural diversity. The two DIVERSet Libraries have also been designed to be complementary so that they can be combined to create a small molecule diversity library of more than 100,000 compounds. ChemBridge continues to expand the DIVERSet Library offering as new compounds based on novel ChemBridge designs are added to our stock, which allows researchers to expand their DIVERSet Library over time. The DIVERSet Library approach has been applied successfully to multiple, different releases of the DIVERSet Libraries since the initial launch and has led to hundreds of citations in peer-reviewed scientific publications.

## Selection

Compounds represented in the DIVERSet Libraries are carefully selected to provide the broadest pharmacophore space coverage and chemical structure diversity within a fixed library size. Stringent drug-like and desirable chemical group filters coupled with a 3D conformer analysis and a 2D structure similarity analysis are used in selecting premium sets of diverse lead-like and drug-like compounds for each set with maximum pharmacophore coverage.

- The DIVERSet-CL Library represents diverse compounds from ChemBridge's CORE Library Stock, which currently offers than 830,000 ChemBridge proprietary compounds and increases in size each year with the addition of new compounds based on novel ChemBridge designs.
- The DIVERSet-EXP Library represents compounds from ChemBridge's EXPRESS-Pick Stock, which offers more than 500,000 handcrafted compounds.





The DIVERSet small molecule screening libraries allow clients to efficiently explore extensive lead-like, drug-like, and pharmacophore space with each unique 3-point pharmacophore representing a potential interaction between a compound and a biological target. The DIVERSet Libraries are ideal tools for screening programs that require high diversity and quality drug-like and lead-like compounds. The DIVERSet Libraries are well recognized and proven screening tools for a wide range of both validated and new biological targets.

## Filtering and Pharmacophore Analysis

To ensure a competent and diverse set of compounds within the DIVERSet Libraries, ChemBridge applies a range of filtering methods, including:

- Filtering for enhanced physicochemical properties while allowing exploration of available chemical space:  $MW \leq 500$ ,  $clogP \leq 5$ ,  $TPSA \leq 100$ , rotatable bonds  $\leq 8$ , hydrogen bond acceptors  $\leq 10$  and hydrogen bond donors  $\leq 5$
- Removal of non-drug like compounds and undesirable chemical groups (e.g. Michael acceptors, crown-ethers & analogs, disulfides, epoxides, etc.)

A full 3D conformational analysis method is then used to identify all 3-point pharmacophores presented within the subset of filtered compounds. The seven types of interaction centers used to create the 3-point pharmacophores are hydrogen bond donors, hydrogen bond acceptors, positive charge centers, aromatic ring centers, hydrophobic centers, acidic groups, and basic groups, and a structural diversity measure is applied to select a fixed size compound set that displays the largest coverage of pharmacophore space while maintaining a high level of structural diversity.

## Format

- Economically priced, pre-plated format
- Purchase a library of 10,000 to more than 100,000 compounds
- Delivery in micromole amounts as 10mM DMSO solutions or as dry film
- Formatted according to your requirements in standard or acoustic qualified plates, in 96-well format racks, or in customer specified materials

## Structures

- For files of DIVERSet Library structures, please email [sales@chembridge.com](mailto:sales@chembridge.com)



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