HIGHLY DIVERSE PRIMARY SCREENING TOOLS
DIVERSet® Libraries

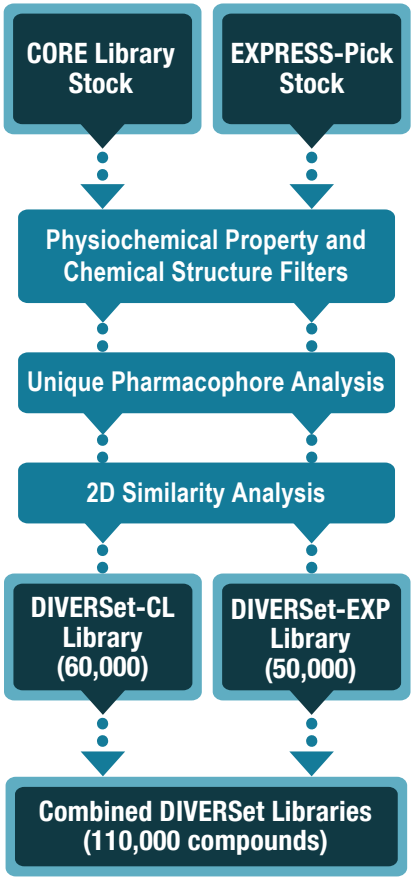
Introduction

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 100,000 or more compounds. 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.

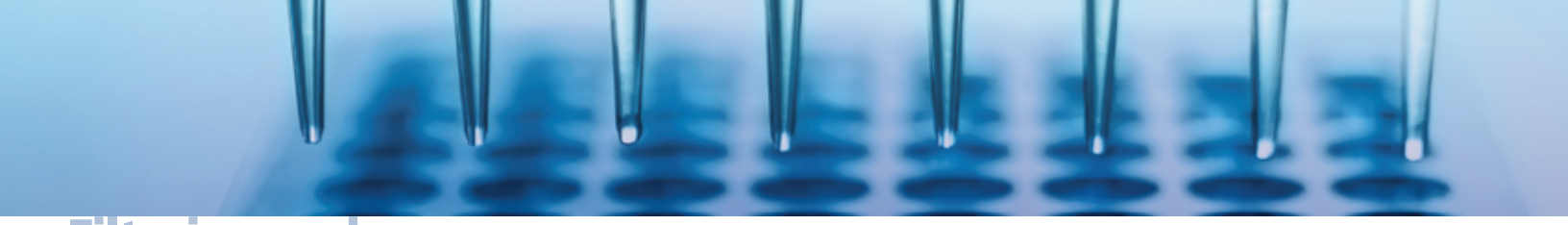
Selection

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 (the DIVERSet-CL Library is currently 60,000 compounds and the DIVERSet-EXP Library is currently 50,000 compounds). Stringent druglike 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 leadlike and druglike compounds for each set with maximum pharmacophore coverage.

- The 60,000 compound DIVERSet-CL Library is selected from ChemBridge's CORE Library stock of more than 670,000 leadlike and druglike compounds based on novel scaffolds designed by ChemBridge.
- The 50,000 compound DIVERSet-EXP Library is selected from ChemBridge's EXPRESS-Pick Collection stock of more than 480,000 handcrafted compounds.



The DIVERSet small molecule screening libraries allow clients to efficiently explore extensive leadlike, druglike, 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 druglike and leadlike 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 physiochemical properties while allowing exploration of available chemical space: MW ≤ 500, clogP ≤ 5, TPSA ≤ 100, rotatable bonds ≤ 8, hydrogen bond acceptors ≤ 10 and hydrogen bond donors ≤ 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 sets
- Available in 96-well or 384-well format
- Available as 10mM DMSO solutions or as dry film
- Amounts of 0.25umol and higher available (25ul and higher for DMSO solutions)
- Purchase the full library or partial sets (minimum purchase of 5,000 compounds)
- Plates from the two DIVERSet Libraries can be combined to create larger diversity libraries

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