



A HIGHLY DIVERSE PRIMARY SCREENING TOOL

DIVERSet™

Introduction

ChemBridge's DIVERSet™ library provides a highly diverse collection of 50,000+ compounds for primary screening. Stringent druglike and desirable chemical group filters, coupled with a 3D pharmacophore diversity analysis, are used in selecting a premium set of druglike compounds with maximum pharmacophore diversity. DIVERSet™ is selected from ChemBridge's main stock collection, the EXPRESS-Pick™ Collection of 450,000+ handcrafted compounds.

DIVERSet™ Selection

The DIVERSet™ library is carefully selected to provide the broadest pharmacophore coverage possible within a predetermined number of compounds. DIVERSet™ displays more than 260,000 unique 3-point pharmacophores, representing more than 60% of the total 3-point pharmacophore space covered by the entire EXPRESS-Pick™ Collection within only 12% of the compounds (50,000 compounds). This library efficiently allows clients to explore extensive druglike, pharmacophore space with each unique 3-point pharmacophore representing a potential interaction between a compound and a biological target.

The DIVERSet™ library is an ideal tool for initial screening programs that require high diversity and quality druglike and leadlike compounds. DIVERSet™ is a well recognized and proven primary screening tool for a wide range of both validated and new biological targets; please go to www.chembridge.com for a publication reference list.

Filtering and Pharmacophore Analysis

To ensure a competent and diverse set of compounds within the DIVERSet™, 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.)
- Removal of structural, salt, and tautomeric duplicates

A 3D pharmacophore analysis method is used to select the largest, most diverse set of unique 3-point pharmacophores presented within the subset of filtered compounds. A pharmacophore, as defined by Chem-X Software, is the essential requirement for activity between a molecule and a receptor needed to produce a biological response and is defined by three centers or atoms and the distances between them. The seven types of interaction centers used are hydrogen bond donors, hydrogen bond acceptors, positive charge centers, aromatic ring centers, hydrophobic centers, acidic groups, and basic groups. All 3-point pharmacophores present in the structure are calculated based on every possible combination of the seven center types contained within the three positions and their corresponding distances. The pharmacophore selection process is then used to identify the largest population of unique 3-point pharmacophores presented by a smaller compound subset.

Formats

- Download and individually select from the 50,000+ DIVERSet™ selection (SDfile and ISIS db files available). Individually selected compounds are available in powder form or dissolved in DMSO.
- Pre-plated sets in DMSO from 10,000 to 50,000 compounds are available.
- For libraries >50,000 compounds, DIVERSet™ can be supplemented using additional EXPRESS-Pick™ Collections (KINASet, Ion Channel Set, CNS-Set™, MicroFormats™) or ChemBridge diversity libraries (NOVACore, PHARMACophore).

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