



# HIGH QUALITY LEAD-LIKE AND DRUG-LIKE Screening Compounds

## Highlights

- High quality, small molecule, lead-like and drug-like compounds
- More than 1.3 million in-stock compounds to select from
- New compounds based on novel, proprietary ChemBridge designs added each year
- Diverse chemotypes with structural analogs for SAR studies
- Available in DMSO and dry formats
- More than 2600 scientific articles cite the use of ChemBridge compounds

## Introduction

ChemBridge has been a provider of high quality screening compounds and libraries for hit identification for almost three decades and continues to produce novel, lead-like and drug-like small molecule screening compounds based on the evolving requirements of drug discovery and chemical biology researchers in industry and academia. We currently offer more than 1.3 million small molecule screening compounds that are readily available from stock that can be custom selected and formatted according to your requirements. Our stock is composed of two complementary parts with no overlap: The CORE Library Stock and the EXPRESS-Pick™ Stock.

## CORE Library Stock

Our in-house designed CORE Library Stock of lead-like, small molecule screening compounds with increased 3D character offers more than 830,000 compounds. These high quality compounds are designed and synthesized by ChemBridge and are based on more than 1,000 proprietary, synthetic schemes. To maximize novelty and diversity, our template and final compound designs draw from ChemBridge's internal Building Block Collection, from new reagents designed by ChemBridge and from external building block sources. New compounds based on novel designs are added to the CORE Library Stock each year.

These compounds are designed to cover unique chemical space not available from our EXPRESS-Pick Stock or other commercial sources. Final compound designs are assessed virtually prior to synthesis and only compounds with the most attractive physicochemical property profile and free of undesirable chemical functionalities are synthesized and added to the CORE Library Stock. Because of the lead-like properties of these compounds, more than half of all CORE Library Stock compounds are suitable for CNS focused research and are included in the CNS-MPO Library selection.

CORE Library Stock compounds have the following physicochemical and calculated property averages:

Molecular Weight Average = 344.9

Fsp3 Average = 0.5

clogP Average = 1.6

TPSA Average = 69.1

H-bond Donor Count Average = 1.1

H-bond Acceptor Count Average = 4.1

Rotatable Bond Count Average = 4.8

# EXPRESS-Pick Stock

The EXPRESS-Pick Stock contains over 500,000 small molecule screening compounds. Compounds were selected using novelty, diversity, drug-like property, and chemical structure analyses. Because chemical space covered by the EXPRESS-Pick Stock is different than the chemical space covered by the CORE Library Stock, the EXPRESS-Pick Stock provides access to additional chemotypes for hit finding. Both drug-like and lead-like compounds are represented in the EXPRESS-Pick Stock.

EXPRESS-Pick Stock compounds have the following physiochemical and calculated property averages:

Molecular Weight Average = 353.5

clogP Average = 3.4

TPSA Average = 66.8

H-bond Donor Count Average = 1.1

H-bond Acceptor Count Average = 3.8

Rotatable Bond Count Average = 3.8

## Format

- Custom select compounds according to your requirements
- Delivery in micromole or mg amounts
- Available as DMSO solutions or dry
- Formatted according to your requirements in standard or acoustic qualified plates, in 96-well format racks, or in customer specified materials

## Structure Files

- For files of CORE Library Stock and EXPRESS-Pick Stock structures, please email [sales@chembridge.com](mailto:sales@chembridge.com)
- ChemBridge can provide standard file versions or versions customized to the requirements of your project
- To search our stock online, visit ChemBridge's [www.hit2lead.com](http://www.hit2lead.com) online search and order site



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