



MACROCYCLIC COMPOUNDS FOR CHALLENGING TARGETS

Macrocycle Library

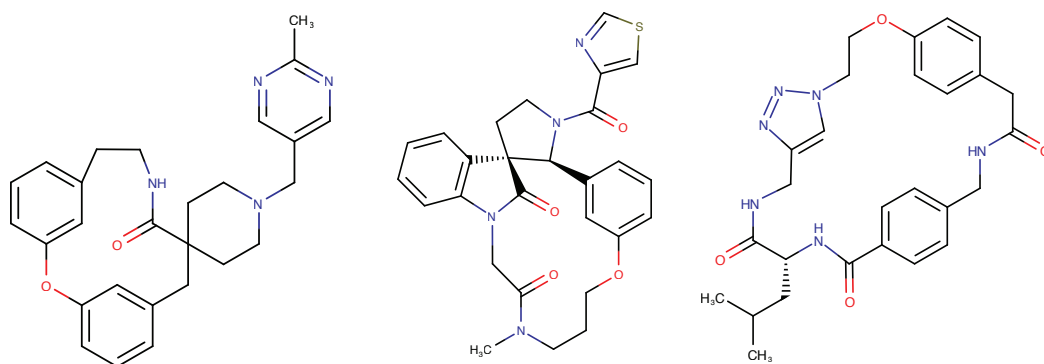
Introduction

Macrocycles offer a novel approach for low druggability targets such as antimicrobial, antiviral and protein-protein interaction. Topologically, macrocycles have the unique ability to span large surface areas while remaining conformationally restricted compared to acyclic molecules of equivalent molecular weight. Macrocyclization reduces overall polarity and enhances membrane penetration. Taken together these attributes make macrocycles a powerful approach for any lead discovery program against challenging targets. Macrocycles are typically defined as a carbo- or, more likely, a heterocycle comprising 12 or more heavy atoms and are often perceived as difficult to synthesize and challenging to incorporate chemical diversity. Through focusing on solutions to the synthetic challenges the chemists at ChemBridge® have produced a diverse library of more than 20,000 synthetic macrocycles that are in stock and available for purchase.

Characteristics

ChemBridge has developed a diverse collection of synthetic macrocycles intended to be accessible to both industry and academic researchers for use in hit generation. ChemBridge chemists have developed synthetic strategies for the synthesis and functionalization of macrocyclic compounds based on novel macrocyclic scaffolds. A first set of approximately 7,000 macrocycles was launched, and ChemBridge has continued to increase the size of the Macrocycle Library each year based on novel designs incorporating proprietary fragments into the macrocycle rings. Currently, the Macrocycle Library represents more than 20,000 synthetic macrocycles. Researchers have the option to custom select from the library or acquire the full library.

Example Macrocycle Library compounds include:

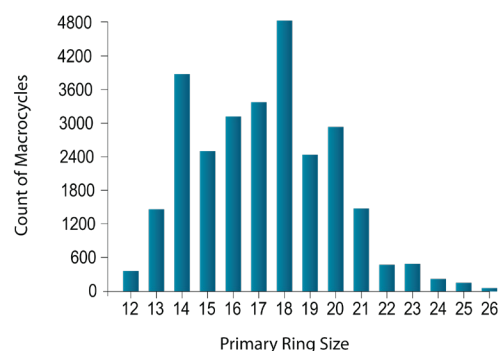
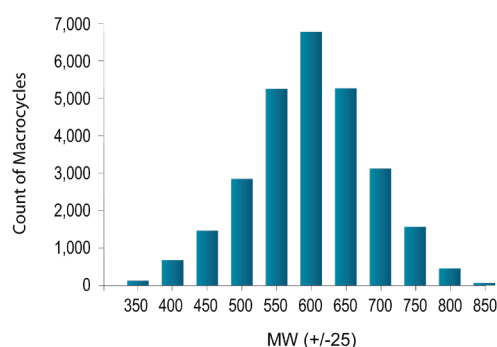


Characteristics

continued

General characteristics of compounds in the ChemBridge Macrocycle Library include:

- Molecular weight up to 850 with 90% having MW 450 to 750
- Primary ring size ranging from 12 to 26 atoms (based on shortest path / fewest bonds included in the primary ring) with 90% having primary ring size of 14 to 21 atoms
- Heterocyclic primary rings
- Scaffolds with and without peptidic backbone elements as part of the macrocyclic ring
- Scaffolds with and without fused rings as part of the primary macrocyclic ring



Macrocycle CNS Subset

An analysis of the initial 7,000 synthetic macrocycles produced by ChemBridge was performed to identify macrocycles that may be suitable for CNS research. A CNS MPO score approach was coupled with a detailed 3D conformational analysis (performed to examine the potential for formation of intramolecular hydrogen bonds). Data from the conformational analysis was used to adjust the HBD and TPSA values and resulting MPO score for each macrocycle to identify a subset with an “adjusted MPO” score ≥ 4.0 . See the Macrocycle CNS Subset product sheet for more details.

Format

- Custom select from more than 20,000 Macrocycle Library compounds
- Available in 384-well and 96-well formats including 384-well acoustic qualified plates
- Amounts as low as 0.25 micromole (25ul of 10mM DMSO solution) available
- Available as DMSO solutions or dry in micromole or mg amounts

Structure File

For a file of structures, please email sales@chembridge.com



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Rev. 20240130