



COMPOUNDS WITH NATURAL PRODUCT-LIKE FEATURES

Natural Product-like Library

Highlights

- Synthetic compounds with natural product-like features
- Custom select from more than 70,000 compounds based on your requirements

Introduction

Natural products provide a source of substructures found in synthetic, bioactive molecules. Early on, a number of substructures found in natural products occurred at low frequency in traditional, synthetic, drug-like compounds. The ChemBridge® lead-like and drug-like compound designs have continued to evolve to incorporate a range of new features, including substructure elements commonly seen in natural products. ChemBridge has employed a published scoring method designed to identify compounds with natural product-like features to create the Natural Product-like Library selection. The Natural Product-like Library contains approximately 70,000 compounds from ChemBridge's stock. These compounds provide a source of synthetic compounds with a high similarity to the structural space covered by natural products.

Method

A scoring method, published by Ertl et al¹, was applied to ChemBridge's stock of small molecule lead-like and drug-like compounds to identify a subset showing a higher natural product-likeness based on the presence of features more common to natural products than to traditional synthetic compounds. A cutoff of zero and higher for the natural product-likeness score was selected as the majority of the natural products used in the publication had scores of zero or higher (most coming within the range 0 to 4.0), while the majority of the 1 million traditional, synthetic compounds used in the analysis had scores of -1.0 or less (see Figure 3 in the article cited). Small percentages of both synthetic and natural product compounds scored in the -1.0 to 0 range, which indicates this range of scores was least able to discriminate between natural product and synthetic compounds.



Characteristics

Natural Product-like Library compounds are lead-like and drug-like and have the following physiochemical and calculated property averages:

Molecular Weight Average = 325.9

Fsp3 Average = 0.6

clogP Average = 2.4

TPSA Average = 62.4

H-bond Donor Count Average = 1.2

H-bond Acceptor Count Average = 3.9

Rotatable Bond Count Average = 4.0

Format

- Custom select from more than 70,000 Natural Product-like Library compound
- 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

References

1. Ertl P et al. Natural product-likeness score and its application for prioritization of compound libraries. J Chem Inf Model, 2008 48 (1), 68-74.



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