

# ASINEX ANTIBACTERIAL LIBRARY

5000 compounds

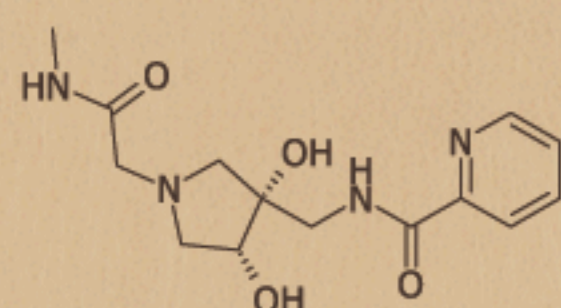
## Novel Chemistries to Address the Challenge of Antibacterial Drug Discovery

Among the many challenges facing drug discovery research in recent years, the search for new antibacterial agents has proved to be among the most unproductive. Many factors have contributed to this bottleneck, but one key area for improvement is the need to test compounds that are more relevant, as it has become apparent that the screening of randomly assembled, diverse compound libraries has resulted in extremely low hit rates [1]. Moreover, in-vitro screening often delivers non-drug like & non-target specific structures which tend to face serious efficacy issues in vivo.

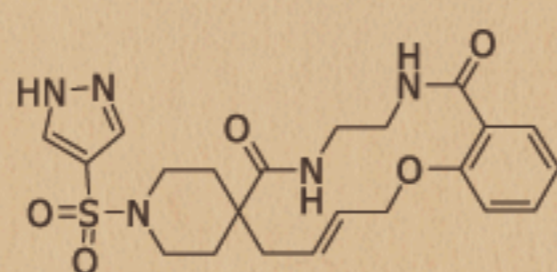
It is critical to access compounds which are capable of delivering excellent chemical starting points for completely new classes of antibacterials in order to address the major challenge of antibacterial drug discovery. A large proportion of known antibacterials have come from natural products & these compounds clearly have structures & properties which render them a particularly rich source.

ASINEX has developed an Antibacterial Compound Library based on unique **natural product-like scaffolds** which are **skeletally diverse** (saturated fused-, spiro- systems, macrocycles), enriched in **polar functionality** & which contain **multiple stereocenters**. The scaffolds & final compounds have been produced by utilizing **stereo-controlled transformations** & modern coupling reactions, generating specific structural elements inherent to antibacterials, but lacking in traditional screening libraries such as **cyclic polyethers**, **"sugar"-like compounds** & **macrolactams**. It is also significant that the library occupies the unique physicochemical space of known antibiotics which enhances the chances of finding high quality hits in both target-specific & whole cell assays [2].

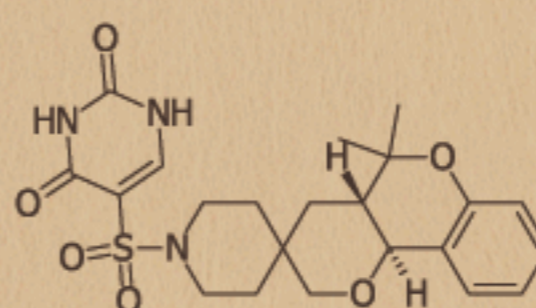
A wide range of chemical transformations were used for scaffold generation & scaffold decoration which has allowed the introduction of higher polarity into the final compounds & the optimization of their physico-chemical profile. Moreover, the wide use of **advanced stereocontrolled** reactions such as stereoselective epoxidation, tandem etherification & reductive etherification has enabled us to obtain target molecules containing multiple stereocenters with clearly defined stereo configuration.



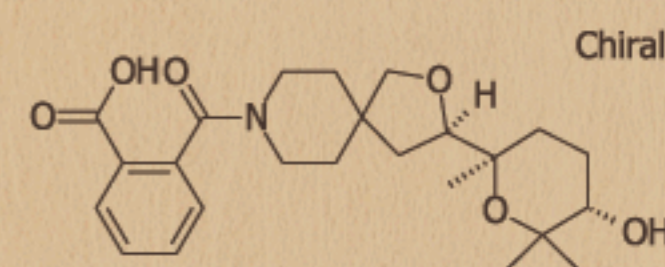
BDG 33208623  
MW 308  
cLogP -0.8



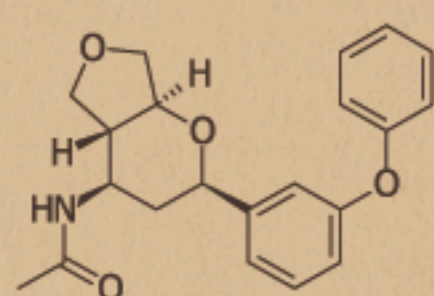
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cLogP 0.4



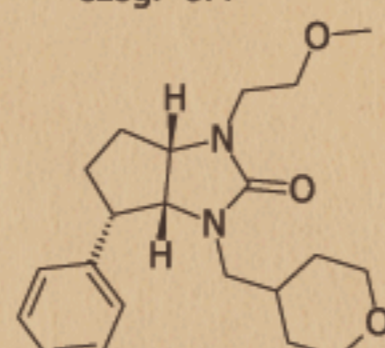
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cLogP 1.2



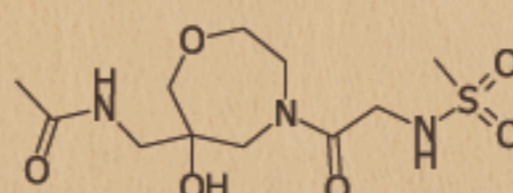
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MW 431  
cLogP 1.7



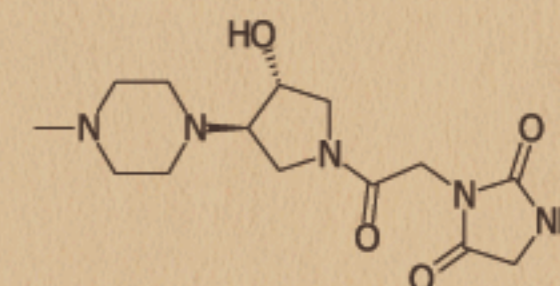
BDF 33664330  
MW 353  
cLogP 1.5



BDG 33257204  
MW 358  
cLogP 2.5



BDE 33199555  
MW 323  
cLogP -1.9



BDE 32163620  
MW 325  
cLogP -2.4

### Oxygen Enriched Compounds

- 3 or more O-atoms per molecule
- 2 or more O-atoms in cyclic systems

### Increased density of polar functionalities

- Poly OH, polar functionalities
- Cyclic Amides and Carbamates
- Chargeable moieties
- Capable to generate zwitterionic forms

**ClogP: -3.0 to 2.0**

**MW: ≤ 475**

**PSA: ≥ 80**

**HBD: ≥ 3**

**HBA: ≥ 5**

**MW/Ha+Hd: 20-60**

**Rot.Bonds: ≤ 10**

### Library specifics:

**Measured Solubility:** 100% of compounds are soluble in DMSO at 10 mM, and in PBS at 50 μM

**Quality:** min.purity of 90%, avg. of 95% (LC-MS, NMR), stored as dry powder

ASINEX's ANTIBACTERIAL LIBRARY is only available upon request, please contact us at:  
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