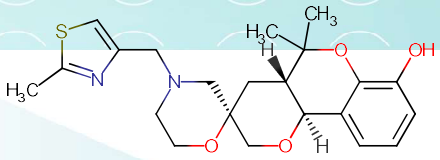
SL-76. OxyTerpenoids for CNS drug discovery

ASINEX
Signature Libraries

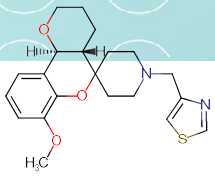
The historical success of Natural Products (NP) in drug discovery provides strong evidence that NP-like small molecules represent privileged chemical space for novel, biologically relevant starting points in pharmaceutical research. The structural diversity of terpene-derived natural products provides a very rich source of inspiration for medicinal chemists, helping them to design new drugs for the treatment of challenging human diseases. It is believed that small drug-like molecules containing a similar distribution of oxygen and nitrogen atoms within a polycyclic framework may demonstrate similar biological effect to their natural product prototypes, but with a greater efficacy and specificity to a certain molecular target.

ASINEX has developed a synthetic toolbox which has enabled us to generate a unique library of skeletally diverse terpenoid-like molecules.

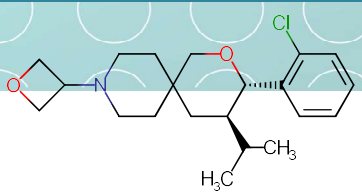
These molecules are particularly interesting for CNS-related research due to favorable CNS-likeness properties: CNS-MPO score >4 [1] and high PAMPA-BBB [2].



LAS 73704969
CNS MPO 4.8
PAMPA BBB 8 x10-6 cm/s



LAS 33900206
CNS MPO 5.1
PAMPA BBB 9.9x10-6 cm/s



LAS 73708654
CNS MPO 4.9
PAMPA BBB 7.9x10-6 cm/s

Signature Library 76

Formats	Supplementary Information
80 compounds per plate 0.1 mg; 1 mg; 2 mg dry film/powder 0.1 µmol; 1 µmolDMSO solutions	SL#76_OxyTerpenoid_for_CNS.sdf

References:

1. *ACS Chem.Neurosci.,* 2010 Jun 16; 1(6): 435–449. doi: 10.1021/cn100008c
2. *J Pharm Sci*., 2009 Jun;98(6):1980-91. doi: 10.1002/jps.21580

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