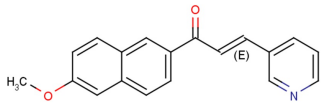
Data Sheet (Cat.No.T11066)

TargetMol
A DRUG SCREENING EXPERT

DMU2139

Chemical Properties



CAS No.:	1821143-80-9
Formula:	C19H15NO2
Molecular Weight:	289.33
Appearance:	N/A
Storage:	0-4℃ for short term (days to weeks), or -20℃ for long term (months).

Biological Description

Description	DMU2139 is a potent and specific CYP1B1 inhibitor with IC50s of 9 nM and 795 nM for CYP1B1 and CYP1A1, respectively.
Targets(IC_{50})	CYP1B1: 9 nM CYP1A1: 795 nM
In vitro	DMU2139 (6j) was more selective for CYP1B1 than CYP1A1 and CYP1A2, which were 88 times and 133 times respectively. In the presence of DMU2139, the EC50 reversed from 61 to 8.3 (visible in cells expressing cyp1b1 without any inhibitor). In the presence of DMU2139, the EC50 value was similar to that of cisplatin, that is, the EC50 value of 8.7°M was in cells transfected with an empty plasmid without the CYP1B1 gene. The empty plasmid cannot express the CYP1B1 protein.DMU2139 (6j) shows 88 and 133-fold selectivity for CYP1B1 over CYP1A1 and CYP1A2. In the presence of DMU2139, the EC50 is reversed back to 8.3 μM from 61 μM (seen in CYP1B1-expressing cells without any inhibitor). The EC50 value, in the presence of DMU2139, resembles the EC50 of cisplatin, 8.7μM, in cells transfected with the empty plasmid which has no CYP1B1 gene and therefore cannot express CYP1B1 protein[1].

Solubility Information

Solubility	DMSO: 77.5 mg/mL (267.86 mM) Ethanol: 5 mg/mL (17.28 mM) (< 1 mg/ml refers to the product slightly soluble or insoluble)

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	3.456 mL	17.281 mL	34.563 mL
5 mM	0.691 mL	3.456 mL	6.913 mL
10 mM	0.346 mL	1.728 mL	3.456 mL
50 mM	0.069 mL	0.346 mL	0.691 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. The storage conditions and period of the stock solution: - 80 ℃ for 6 months; - 20 ℃ for 1 month. Please use it as soon as possible.

Reference

1. Horley NJ, et al. Discovery and characterization of novel CYP1B1 inhibitors based on heterocyclic chalcones: Overcoming cisplatin resistance in CYP1B1-overexpressing lines. Eur J Med Chem. 2017 Mar 31;129:159-174.

Tel:781-999-4286 E-mail:info@targetmol.com Address:36 Washington Street,Wellesley Hills,MA 02481