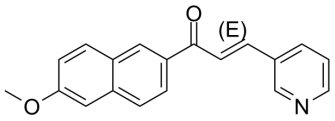
DMU2139

Cat. No.:	HY-101285
CAS No.:	1821143-80-9
Molecular Formula:	$C_{19}H_{15}NO_2$
Molecular Weight:	289.33
Target:	Cytochrome P450
Pathway:	Metabolic Enzyme/Protease
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 2 years -20°C 1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 77.5 mg/mL (267.86 mM; Need ultrasonic)
Ethanol : 5 mg/mL (17.28 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.4563 mL	17.2813 mL	34.5626 mL
	5 mM	0.6913 mL	3.4563 mL	6.9125 mL
	10 mM	0.3456 mL	1.7281 mL	3.4563 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.58 mg/mL (8.92 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.58 mg/mL (8.92 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

DMU2139 is a potent and specific CYP1B1 inhibitor, with IC_{50}s of 9 nM and 795 nM for CYP1B1 and CYP1A1, respectively.

IC_{50} & Target

CYP1B1	CYP1A1
9 nM (IC_{50})	795 nM (IC_{50})

In Vitro

DMU2139 (6j) shows 88 and 133-fold selectivity for CYP1B1 over CYP1A1 and CYP1A2. In the presence of DMU2139, the EC_{50} is reversed back to 8.3 μM from 61 μM (seen in CYP1B1-expressing cells without any inhibitor). The EC_{50} value, in the presence of DMU2139, resembles the EC_{50} of cisplatin, 8.7μM, in cells transfected with the empty plasmid which has no CYP1B1 gene and therefore cannot express CYP1B1 protein[1].

MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[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.

Caution: Product has not been fully validated for medical applications. For research use only.

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