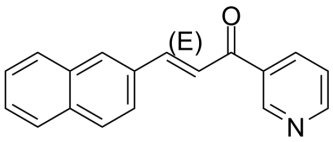
DMU2105

Cat. No.:	HY-101284
CAS No.:	1821143-79-6
Molecular Formula:	$C_{18}H_{13}NO$
Molecular Weight:	259.3
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 : 33.33 mg/mL (128.54 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.8565 mL	19.2827 mL	38.5654 mL
	5 mM	0.7713 mL	3.8565 mL	7.7131 mL
	10 mM	0.3857 mL	1.9283 mL	3.8565 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 3.33 mg/mL (12.84 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: 2.67 mg/mL (10.30 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

DMU2105 is a potent and specific CYP1B1 inhibitor, with IC_{50}s of 10 nM and 742 nM for CYP1B1 and CYP1A1, respectively.

IC_{50} & Target

CYP1B1	CYP1A1
10 nM (IC_{50})	742 nM (IC_{50})

In Vitro

DMU2105 (Compound 7k) shows 74 and 120-fold selectivity for CYP1B1 over CYP1A1 and CYP1A2. In the presence of DMU2105 however, the EC_{50} goes down to 1 μM indicating that the cells have suffered from toxicity which may have been mediated by CYP1B1 inhibition. Un-transfected cells (HEK293: pcDNA3.1), when treated with cisplatin and DMU2105 (10×IC_{50}) do not show any perceptible decrease of cisplatin EC_{50} (8.5 μM ± 0.9)[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.

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