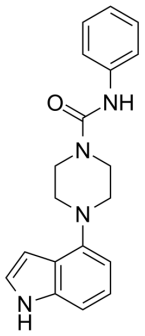
iGOT1-01

Cat. No.:	HY-124825		
CAS No.:	882256-55-5		
Molecular Formula:	$C_{19}H_{20}N_4O$		
Molecular Weight:	320.39		
Target:	Others		
Pathway:	Others		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (312.12 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.1212 mL	15.6060 mL	31.2120 mL
5 mM	0.6242 mL	3.1212 mL	6.2424 mL
10 mM	0.3121 mL	1.5606 mL	3.1212 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: ≥ 2.5 mg/mL (7.80 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (7.80 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (7.80 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

iGOT1-01 is a potent aspartate aminotransferase 1 (glutamate oxaloacetate transaminase 1; GOT1) inhibitor. iGOT1-01 has IC_{50}s of 85 μM and 11.3 μM in MDH coupled GOT1 enzymatic assay and GOT1/GLOX/HRP assay, respectively. iGOT1-01 has anti-cancer activity[1][2].

IC_{50} & Target

IC50: 85 μM (MDH coupled GOT1 enzymatic assay) and 11.3 μM (GOT1/GLOX/HRP assay)[1]

In Vitro

iGOT1-01 has an IC_{50} of 84.6 μM in the GOT1/MDH1 assay. No inhibitory activity is observed for iGOT1-01 against MDH1 alone

	at 100 μM[2]. iGOT1-01 (3.125-200 μM; for 3 h) reveals little to no toxicity using two readouts of cell viability in PaTu8902 pancreatic and DLD1 colon cancer cells[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	iGOT1-01 (compound 1a; 20 mg/kg; oral) has reasonable bioavailability and exposure properties ($t_{1/2}$=0.7 hours, C_{max}=4133 ng/mL, $AUC_{(0\text{-}24\ hours)}$=11734 hour•ng/mL)[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Female CD1 mice with 9 weeks old[1]
Dosage:	20 mg/kg (Pharmacokinetic Analysis)
Administration:	Oral
Result:	Has reasonable bioavailability and exposure properties ($t_{1/2}$=0.7 hours, C_{max}=4133 ng/mL, $AUC_{(0\text{-}24\ hours)}$=11734 hour•ng/mL).

REFERENCES

[1]. Justin Anglin, et al. Discovery and optimization of aspartate aminotransferase 1 inhibitors to target redox balance in pancreatic ductal adenocarcinoma. Bioorg Med Chem Lett. 2018 Sep 1;28(16):2675-2678.

[2]. Melissa C Holt, et al. Biochemical Characterization and Structure-Based Mutational Analysis Provide Insight into the Binding and Mechanism of Action of Novel Aspartate Aminotransferase Inhibitors. Biochemistry. 2018 Nov 27;57(47):6604-6614.

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