IDO1/TDO-IN-4

Cat. No.: HY-151108

CAS No.: 461424-21-5

Molecular Formula: $C_{14}H_{10}N_4$

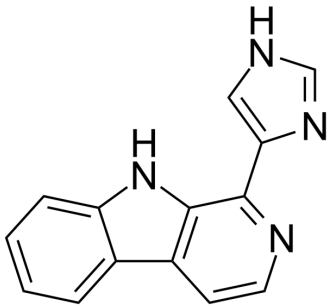
Molecular Weight: 234.26

Target: Indoleamine 2,3-Dioxygenase (IDO)

Pathway: Metabolic Enzyme/Protease

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 : 125 mg/mL (533.60 mM; ultrasonic and warming and heat to 60°C)

Methanol : 16.67 mg/mL (71.16 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	4.2688 mL	21.3438 mL	42.6876 mL
5 mM	0.8538 mL	4.2688 mL	8.5375 mL
10 mM	0.4269 mL	2.1344 mL	4.2688 mL

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

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (8.88 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

IDO1/TDO-IN-4 is a potent IDO1/TDO dual inhibitor, with IC_{50} values of 3.53 μM (IDO1) and 1.15 μM (TDO). IDO1/TDO-IN-4 forms hydrogen bond with IDO1, and π−π stacking interaction with TDO. IDO1/TDO-IN-4 can be used in the research of depression, and depression-induced infectious, metabolic, and autoimmune disorders[1].

IC_{50} & Target

IDO1

3.53 μM (IC_{50})

In Vitro

IDO1/TDO-IN-4 (compound 28, 0-2 μM, 1 h) inhibits the LPS-induced activation of BV2 microglial cells (determined by morphological changes)[1].

IDO1/TDO-IN-4 (0-2 μM, 1 h) inhibits the generation of pro-inflammatory factors and promotes the expression of IL-10[1].

IDO1/TDO-IN-4 (0-2 μM, 1 h) decreases the expression of IDO1 and prevents the excessive degradation of tryptophan via the

kynurenine pathway[1].

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

RT-PCR[1]

Cell Line:	100 ng/mL LPS-induced BV2 microglial cells
Concentration:	0, 0.25, 0.5, 1, 2 μM
Incubation Time:	1 h
Result:	Inhibited the generation of COX2, iNOS, TNF-α, and IL-1β. Increased the level of IL-10.

In Vivo

IDO1/TDO-IN-4 (compound 28, i.p., 20 mg/kg, at day 1, 2, 3) rescues LPS-induced neuroinflammation and depressive-like behavior in mice[1].

IDO1/TDO-IN-4 (I.p. or i.v., 20 mg/kg) displays high exposure and a high volume of distribution at the steady state in normal mice[1].

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

Animal Model:	2 mg/kg LPS-induced depressive mice[1]
Dosage:	20 mg/kg
Administration:	Intraperitoneal injection (i.p.), at day 1, 2, 3.
Result:	Attenuated microglial activation significantly. Decreased inflammatory factors in the hippocampus, such as TNF-α, IL-1β, and iNOS. Downregulated LPS-induced overexpression of IDO1.

Animal Model:	Male C57BL/6J mice (pharmacokinetic assay)[1]
Dosage:	20 mg/kg
Administration:	Intraperitoneal injection and intravenous injection
Result:	Pharmacokinetic profile of IDO1/TDO-IN-4 (compound 28)

pharmacokinetic property	$T_{1/2}$ (h)	T_{max} (h)	C_{max} (ng/mL)	bioavailability F (%)
i.v./i.p.	2.31/0.77	0.25	5543.99/3878	52.55

REFERENCES

[1]. Yu Zhang, et al. B Discovery of 1-(Hetero)aryl-β-carboline Derivatives as IDO1/TDO Dual Inhibitors with Antidepressant Activity. J Med Chem. 2022 Aug 7.

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

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