MPO-IN-1

Cat. No.: HY-139915

CAS No.: 2471981-21-0

Molecular Formula: $C_{24}H_{21}ClN_4$

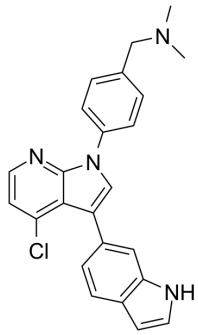
Molecular Weight: 400.9

Target: Glutathione Peroxidase

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 : 200 mg/mL (498.88 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4944 mL	12.4719 mL	24.9439 mL
	5 mM	0.4989 mL	2.4944 mL	4.9888 mL
	10 mM	0.2494 mL	1.2472 mL	2.4944 mL

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

BIOLOGICAL ACTIVITY

Description

MPO-IN-1 is a potent, orally active, and irreversible indole-containing inhibitor of myeloperoxidase (MPO). MPO-IN-1 has IC_{50}s of 2.6 μM and 5.3 μM for MPO and thyroid peroxidase (TPO), respectively. MPO-IN-1 inhibits MPO activity in an acute mouse model of inflammation[1].

IC_{50} & Target

2.6 μM (in plasma MPO assay); 0.12 μM (in fluorescent MPO peroxidation assay)[1]

In Vivo

MPO-IN-1 (compound 2) (5 and 90 mg/kg; p.o.; four hours post-Zymosan A administration) significantly reduces MPO activity in a mouse peritonitis model of acute inflammation[1].

Mouse pharmacokinetic parameter of MPO-IN-1[1].

Dose	V_{ss} (L/kg)	$T_{1/2}$ (h)	AUC_{inf} (nM•h) p.o.	C_{max} (nM) p.o.	PPB (%)	F (%)

1/10 mg/kg i.v./p.o.	9.8	2.6	2486	502	99.6	61

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

Animal Model:	Male C57BL/6J mice (mouse peritonitis model of acute inflammation)[1]
Dosage:	5 and 90 mg/kg
Administration:	p.o. (four hours post-Zymosan A administration)
Result:	Resulted in a ~50% reduction in the MPO activity at 90 mg/kg.

REFERENCES

[1]. Patnaik A, et al. Discovery of a novel indole pharmacophore for the irreversible inhibition of myeloperoxidase (MPO). Bioorg Med Chem. 2020;28(12):115548.

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