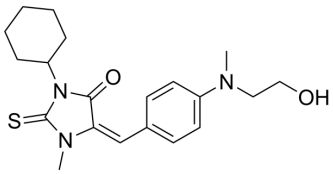
NADPH oxidase-IN-1

Cat. No.:	HY-152026
CAS No.:	2762405-17-2
Molecular Formula:	$C_{20}H_{27}N_3O_2S$
Molecular Weight:	373.51
Target:	NADPH Oxidase
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 : 62.5 mg/mL (167.33 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.6773 mL	13.3865 mL	26.7730 mL
	5 mM	0.5355 mL	2.6773 mL	5.3546 mL
	10 mM	0.2677 mL	1.3387 mL	2.6773 mL

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

BIOLOGICAL ACTIVITY

Description

NADPH oxidase-IN-1 is an orally active NADPH oxidase (Nox) inhibitor, related with neuronal inflammation. NADPH oxidase-IN-1 can cross the blood-brain barrier (BBB), inhibits Nox2 and Nox4 with IC_{50}s of 1.9 μM and 2.47 μM, respectively. NADPH oxidase-IN-1 suppresses pro-inflammatory cytokines production and LPS-mediated microglial migration, also has in vivo efficacy[1].

IC_{50} & Target

NOX2	NOX4
1.9 μM (IC_{50})	2.47 μM (IC_{50})

In Vitro

NADPH oxidase-IN-1 (compound 11) can cross cross the blood-brain barrier (BBB) with P_e value of 13.6 (10^{-6} cm/s), determined by parallel artificial membrane permeability assay (PAMPA assay)[1].

NADPH oxidase-IN-1 (1 nM-10 mM; 30 min) LPS-induced ROS generation in BV2 microglial cells in a dose-dependent manner [1].

NADPH oxidase-IN-1 (10 μM; 24 h) inhibits the mRNA expression of pro-inflammatory cytokines in BV2 cells[1].

NADPH oxidase-IN-1 (1 nM-10 mM; 24 h) also inhibits activation and migration of BV2 cells[1].

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

RT-PCR[1]

Cell Line:	BV2 microglial cells
Concentration:	10 μM
Incubation Time:	24 hours
Result:	Inhibited the mRNA expression of pro-inflammatory cytokines (iNOS, IL-1β, TNFα) in BV2 cells.

Cell Migration Assay [1]

Cell Line:	BV2 microglial cells
Concentration:	10 μM
Incubation Time:	24 hours
Result:	Ameliorated inflammatory response and migration of microglia.

In Vivo

NADPH oxidase-IN-1 (compound 11) (30 mg/kg; p.o.; daily for 4 wk) attenuates MPTP induced microglia activation and diminishes dopaminergic neuronal damage in Parkinson's disease (PD) mice model[1].
NADPH oxidase-IN-1 is safe in both male and female mice following IV injection (10-300 mg/kg; single dose) and oral gavage (10-1000 mg/kg; single dose), respectively[1].

Pharmacokinetic profile in rats

Parameters	C_0 (μg/mL)	C_{max} (μg/mL)	$t_{1/2}$ (h)	T_{max} (h)	AUC_{last} (μg/h/mL)	k_e (1/h)	V_d (L)	V_d/F (L)	Cl (L/h)	Cl/F (L/h)	F (%)
IV (2 mg/kg)	1.70		0.79		0.468	1.32	0.211		0.217		
PO (10 mg/kg)		0.609	5.01	[0.083-2]	1.31	0.170		1.99		0.341	56.0
PO (20 mg/kg)		0.783	6.13	[0.67-2]	4.16	0.159		1.82		0.217	88.9

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

REFERENCES

[1]. Shim S, et al. Discovery of a NADPH oxidase inhibitor,(E)-3-cyclohexyl-5-(4-((2-hydroxyethyl)(methyl) amino) benzylidene)-1-methyl-2-thioxoimidazolidin-4-oneone, as a novel therapeutic for Parkinson's disease[J]. European Journal of Medicinal Chemistry, 2022, 244: 114854.

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