Ebselen

Cat. No.: HY-13750

CAS No.: 60940-34-3

Molecular Formula: $C_{13}H_9NOSe$

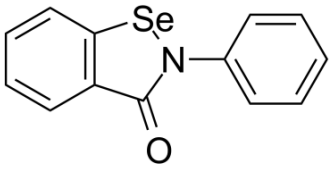
Molecular Weight: 274.18

Target: Calcium Channel; Virus Protease; HIV; Phosphatase

Pathway: Membrane Transporter/Ion Channel; Neuronal Signaling; Anti-infection; 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 : 50 mg/mL (182.36 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.6472 mL	18.2362 mL	36.4724 mL
5 mM	0.7294 mL	3.6472 mL	7.2945 mL
10 mM	0.3647 mL	1.8236 mL	3.6472 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 (9.12 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (9.12 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Ebselen (SPI-1005), a glutathione peroxidase mimetic, is a potent voltage-dependent calcium channel (VDCC) blocker[1][2]. Ebselen potently inhibits M^{pro} (IC_{50}=0.67 μM) and COVID-19 virus (EC_{50}=4.67 μM)[3].Ebselen is an inhibitor of HIV-1 capsid CTD dimerization. Ebselen, an organoselenium compound, can permeate the blood-brain barrier and has anti-inflammatory, antioxidant and anticancer activity[4][5].

IC_{50} & Target

IC50: 0.67 μM (M^{pro})[3]
EC50: 4.67 μM (COVID-19 virus)[3]

In Vitro

Ebselen (SPI-1005; 0.4-100 μM; 20-24 hours) shows strong antiviral effects at a concentration of 10 μM treatment in COVID-19

virus infected Vero cells. Ebsele covalently binds to C145 of the catalytic dyad in COVID-19 virus Mpro[3].
Ebselen inhibits early viral postentry events of the HIV-1 life cycle by impairing the incoming capsid uncoating process[4].
Ebselen permeates the blood-brain barrier and inhibits endogenous inositol monophosphatase in mouse brain. Ebselen inhibits inositol monophosphatase (IMPase)[5].
Ebselen inhibits QSOX1 enzymatic activity and suppresses invasion of pancreatic, renal cancer cell lines[6].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

RT-PCR[3]

Cell Line:	COVID-19 virus infected Vero cells
Concentration:	0.4, 1.2, 3.7, 11.1, 33.3, 100 μM
Incubation Time:	20-24 hours
Result:	Showed strong antiviral effects at a concentration of 10 μM treatment.

In Vivo

Ebselen (5, 10 mg/kg; IP) decreases 5-HT_2 agonist-induced head twitches in a dose-dependent manner[5].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	20-25 g 10-12 week old male C57Bl6 mice[5]
Dosage:	5, 10 mg/kg
Administration:	IP
Result:	Decreased 5-HT_2 agonist-induced head twitches in a dose-dependent manner.

CUSTOMER VALIDATION

- J Enzyme Inhib Med Chem. 2020 Dec;35(1):906-912.
- Int J Antimicrob Agents. 2019 Dec;54(6):814-819.
- Antiviral Res. 2019 Jun 27;169:104544.
- SLAS Discov. 2020 Jun 22;2472555220932552.
- Exp Ther Med. 2019 Feb;17(2):1412-1419.

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REFERENCES

[1]. Thenin-Houssier S, et al. Ebselen, a Small-Molecule Capsid Inhibitor of HIV-1 Replication. Antimicrob Agents Chemother. 2016 Mar 25;60(4):2195-208.

[2]. Singh N, et al. A safe lithium mimetic for bipolar disorder. Nat Commun. 2013;4:1332. doi: 10.1038/ncomms2320.

[3]. Hanavan PD, et al. Ebselen inhibits QSOX1 enzymatic activity and suppresses invasion of pancreatic and renal cancer cell lines. Oncotarget. 2015 Jul 30;6(21):18418-28.

[4]. Liang Q, et al. Electrical Stimulation Degenerated Cochlear Synapses Through Oxidative Stress in NeonatalCochlear Explants. Front Neurosci. 2019 Oct 14;13:1073.

[5]. H Sies, et al. Ebselen, a Selenoorganic Compound as Glutathione Peroxidase Mimic

[6]. Jin Z, et al. Structure of M^{pro} from COVID-19 virus and discovery of its inhibitors. Nature. 2020 Apr 9.

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

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