上海源叶生物科技有限公司
Shanghai yuanye Bio-Technology Co., Ltd
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产品名称：Ebselen
CAS 号：60940-34-3
产品货号：S85955

生物活性：

Description

Ebselen (SPI-1005) 是一种谷胱甘肽过氧化物酶模拟物，有效的电压依赖性钙通道 (VDCC) 阻断剂。Ebselen 有效抑制 Mpro (IC50=0.67 μM) 和 COVID-19 病毒 (EC50=4.67 μM)。Ebselen 是 HIV-1 衣壳 CTD 二聚化的抑制剂。Ebselen 是一种有机硒化合物，可透过血脑屏障，具有抗炎，抗氧化和抗癌活性。

IC50 & Target

HIV-1

Cellular Effect

Cell Line	Type	Value	Description
184B5	GI_{50}	30.1 μM	Antiproliferative activity against human 184B5 cells after 72 hrs by MTT assay
A549	IC_{50}	> 100 μM	Antiproliferative activity against human A549 cells assessed as cell viability after 48 hrs by MTT assay
A549	IC_{50}	16.8 μM	Cytotoxicity in human A549 cells assessed as reduction in cell viability incubated for 48 hrs by resazurin dye based assay
A549	IC_{50}	3.75 μM	Antiproliferative activity against human A549 cells after 48 hrs by CCK-8 assay
BEAS-2B	GI_{50}	49.5 μM	Antiproliferative activity against human BEAS2B cells after 72 hrs by MTT assay
Bel-7402	IC_{50}	68.2 μM	Antiproliferative activity against human Bel7402 cells assessed as cell viability after 48 hrs by MTT assay
Calu-1	GI_{50}	68.6 μM	Antiproliferative activity against human HTB-54 cells after 72 hrs by MTT assay
CCRF-CEM	GI_{50}	57.1 μM	Antiproliferative activity against human CCRF-CEM cells after 72 hrs by MTT assay
CHO-K1	EC_{50}	6.1 μM	Cytotoxicity against CHO-K1 cells by Alamar blue assay
HCT-116	IC_{50}	50 μM	Cytotoxicity in human HCT-116 cells assessed as reduction in cell viability incubated for 48 hrs by resazurin dye based assay
HeLa	IC_{50}	78.5 μM	Antiproliferative activity against human HeLa cells assessed as cell viability after 48 hrs by MTT assay
HT-29	GI_{50}	> 100 μM	Antiproliferative activity against human HT-29 cells after 72 hrs by MTT assay
HT-29	IC_{50}	50.4 μM	Cytotoxicity in human HT-29 cells assessed as reduction in cell viability incubated for 48 hrs by resazurin dye based assay
MCF7	IC_{50}	> 100 μM	Antiproliferative activity against human MCF7 cells assessed as cell viability after 48 hrs by MTT assay
MCF7	IC_{50}	15.02 μM	Antiproliferative activity against human MCF7 cells after 48 hrs by CCK-8 assay

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	MCF7	GI_{50}	58.8 μM	Antiproliferative activity against human MCF7 cells after 72 hrs by MTT assay
	MDA-MB-231	IC_{50}	42.3 μM	Antiproliferative activity against human MDA231 cells after 72 hrs by MTT assay
	NCI-H1299	IC_{50}	27.7 μM	Cytotoxicity in human NCI-H1299 cells assessed as reduction in cell viability incubated for 48 hrs by resazurin dye based assay
	PC-3	GI_{50}	> 100 μM	Antiproliferative activity against human PC3 cells after 72 hrs by MTT assay
	U-266	IC_{50}	40 μM	Anticancer activity against human U-266 cells assessed as cell growth inhibition incubated for 24 hrs by MTS assay

In Vitro

Ebselen (SPI-1005；0.4-100 μM；20-24 小时) 在 10 μM 浓度下对 COVID-19 病毒感染的 Vero 细胞表现出强大的抗病毒作用。Ebsele 与 COVID-19 病毒 Mpro 中催化二元体的 C145 共价结合[3]。

Ebselen 通过削弱进入的衣壳脱壳过程来抑制 HIV-1 生命周期的早期病毒进入后事件[4]。

Ebselen 可渗透血脑屏障并抑制小鼠脑中的内源性肌醇单磷酸酶。Ebselen 抑制肌醇单磷酸酶 (IMPase)[5]。

Ebselen 可抑制 QSOX1 酶活性并抑制胰腺癌细胞系和肾癌细胞系的侵袭[6]。

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）以剂量依赖性方式减少 5-HT2 激动剂引起的头部抽搐[5]。

Animal Model:	20-25 g 10-12 week old male C57Bl6 mice[5]
Dosage:	5, 10 mg/kg
Administration:	IP
Result:	Decreased 5-HT2 agonist-induced head twitches in a dose-dependent manner.

Solvent&Solubility

细胞实验:

DMSO 中的溶解度 ：50 mg/mL (182.36 mM; 超声助溶; 吸湿的 DMSO 对产品的溶解度有显著影响，请使用新开封的 DMSO)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.6472 mL	18.2361 mL	36.4723 mL
	5 mM	0.7294 mL	3.6472 mL	7.2945 mL
	10 mM	0.3647 mL	1.8236 mL	3.6472 mL

*请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液；一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。

储备液的保存方式和期限：-80°C, 1 year; -20°C, 6 months。-80°C 储存时，请在 1 年内使用， -20°C 储存时，请在 6 个月内使用。

动物实验：

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	请根据您的 实验动物和给药方式 选择适当的溶解方案。 以下溶解方案都请先按照 In Vitro 方式配制澄清的储备液，再依次添加助溶剂： ——为保证实验结果的可靠性，澄清的储备液可以根据储存条件，适当保存；体内实验的工作液，建议您现用现配，当天使用； 以下溶剂前显示的百分比是指该溶剂在您配制终溶液中的体积占比；如在配制过程中出现沉淀、析出现象，可以通过加热和/或超声的方式助溶 方案 一 请依序添加每种溶剂： 10% DMSO → 40% PEG300 → 5% Tween-80 → 45% Saline Solubility: ≥ 2.5 mg/mL (9.12 mM); 澄清溶液 此方案可获得 ≥ 2.5 mg/mL（饱和度未知）的澄清溶液。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 400 μL PEG300 中，混合均匀；再向上述体系中加入 50 μL Tween-80，混合均匀；然后再继续加入 450 μL 生理盐水 定容至 1 mL。 生理盐水的配制：将 0.9 g 氯化钠，溶解于 ddH₂O 并定容至 100 mL，可以得到澄清透明的生理盐水溶液。 方案 二 请依序添加每种溶剂： 10% DMSO → 90% Corn Oil Solubility: ≥ 2.5 mg/mL (9.12 mM); 澄清溶液 此方案可获得 ≥ 2.5 mg/mL（饱和度未知）的澄清溶液，此方案实验周期在半个月以上的动物实验酌情使用。 以 1 mL 工作液为例，取 100 μL 25.0 mg/mL 的澄清 DMSO 储备液加到 900 μL 玉米油中，混合均匀。
参考文献	[1]. Liang Q, et al. Electrical Stimulation Degenerated Cochlear Synapses Through Oxidative Stress in NeonatalCochlear Explants. Front Neurosci. 2019 Oct 14;13:1073. [2]. H Sies, et al. Ebselen, a Selenoorganic Compound as Glutathione Peroxidase Mimic [3]. Jin Z, et al. Structure of Mpro from COVID-19 virus and discovery of its inhibitors. Nature. 2020 Apr 9. [4]. 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. [5]. Singh N, et al. A safe lithium mimetic for bipolar disorder. Nat Commun. 2013;4:1332. doi: 10.1038/ncomms2320. [6]. 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

完整储备液配制表：

请根据产品在不同溶剂中的溶解度选择合适的溶剂配制储备液；一旦配成溶液，请分装保存，避免反复冻融造成的产品失效。

储备液的保存方式和期限：-80°C, 1 year; -20°C, 6 months。-80°C 储存时，请在 1 年内使用， -20°C 储存时，请在 6 个月内使用。

可选溶剂	质量 / 溶剂体积 / 浓度	1 mg	5 mg	10 mg	25 mg
DMSO	1 mM	3.6472 mL	18.2361 mL	36.4723 mL	91.1806 mL
	5 mM	0.7294 mL	3.6472 mL	7.2945 mL	18.2361 mL

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	10 mM	0.3647 mL	1.8236 mL	3.6472 mL	9.1181 mL
	15 mM	0.2431 mL	1.2157 mL	2.4315 mL	6.0787 mL
	20 mM	0.1824 mL	0.9118 mL	1.8236 mL	4.5590 mL
	25 mM	0.1459 mL	0.7294 mL	1.4589 mL	3.6472 mL
	30 mM	0.1216 mL	0.6079 mL	1.2157 mL	3.0394 mL
	40 mM	0.0912 mL	0.4559 mL	0.9118 mL	2.2795 mL
	50 mM	0.0729 mL	0.3647 mL	0.7294 mL	1.8236 mL
	60 mM	0.0608 mL	0.3039 mL	0.6079 mL	1.5197 mL
	80 mM	0.0456 mL	0.2280 mL	0.4559 mL	1.1398 mL
	100 mM	0.0365 mL	0.1824 mL	0.3647 mL	0.9118 mL