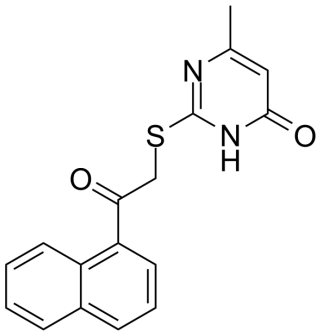
I3MT-3

Cat. No.:	HY-128206
CAS No.:	459420-09-8
Molecular Formula:	$C_{17}H_{14}N_2O_2S$
Molecular Weight:	310.37
Target:	Hippo (MST)
Pathway:	Stem Cell/Wnt
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (402.75 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	3.2220 mL	16.1098 mL	32.2196 mL
	5 mM	0.6444 mL	3.2220 mL	6.4439 mL
	10 mM	0.3222 mL	1.6110 mL	3.2220 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 (6.70 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (6.70 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

I3MT-3 (HMPSNE) is a potent, selective, and cell-membrane permeable inhibitor of 3-Mercaptopyruvate sulfurtransferase (3MST) (IC_{50}=2.7 μM). I3MT-3 is inactive for other H2S/sulfane sulfur-producing enzymes. I3MT-3 targets a persulfurated cysteine residue located in the active site of 3MST[1].

IC_{50} & Target

IC50: 2.7 μM (3-Mercaptopyruvate sulfurtransferase (3MST))[1]

In Vitro

I3MT-3 (1 μM) is selective for 3MST and shows a high inhibitory activity (80–90%) even at 10 μM in cell lysate of 3MST-overexpressing HEK293 cells. Besides, it is almost inactive towards the other two H2S-producing enzymes even at 100 μM[1]. I3MT-3 (1 μM) shows a high selectivity for 3MST, it completely suppresses the 3MST activity in COS7 cells living cells[1]. I3MT-3 produces a concentration-dependent inhibition of the AzMC (the fluorescent H2S probe) signal when incubated with purified human recombinant enzyme, the inhibition of the catalytic activity of 3-MST produces a concentration-dependent

inhibition of H2S production with an IC_{50} of 13.6 μM[1].
I3MT-3 shows a dose-dependent inhibition of 3-MST activity from CT26 homogenates, which contain the murine form of the enzyme. The IC_{50} of HMPSNE for murine 3-MST is calculated as 2.3 μM with a cozncentration-dependent decrease of AzMC fluorescence[1].
I3MT-3 (10 μM-100 μM; after 3 h probe AzMC) causes a partial inhibition of the signal, while at 100 μM, HMPSNE causes a complete inhibition of the AzMC-guided H2S fluorescence at 100 μM, Additionally, HMPSNE is capable of inhibiting its target in situ in CT26 cells (with an IC_{50} of approximately 30 μM)[2].
I3MT-3 (0-300 μM; 5-50 hours) does not enhance MTT conversion at 10 μM, while at 100 and 300 μM it produces an inhibitory response, without increasing the LDH signal, i.e., without inducing any detectable degree of cell necrosis. It also produces a decreased oxygen consumption rate (OCR) profiles in CT26 cells[2].
I3MT-3 (0-300 μM; 48 hours) inhibits CT26 cells proliferate with increasing concentrations of I3MT-3. Confluence of cells treated with HMPSNE is recorded each hour for 48 h by the IncuCyte method[2].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Cell Proliferation Assay[2]

Cell Line:	CT26 cells
Concentration:	0 μM; 10 μM; 30 μM; 100 μM; 300 μM
Incubation Time:	48 hours
Result:	Slowed down proliferation of CT26 cells.

CUSTOMER VALIDATION

- Cell Death Dis. 2022 Oct 30;13(10):913.
- J Biol Chem. 2023 Apr 13;104710.

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REFERENCES

[1]. Kenjiro Hanaoka, et al. Discovery and Mechanistic Characterization of Selective Inhibitors of H 2 S-producing Enzyme: 3-Mercaptopyruvate Sulfurtransferase (3MST) Targeting Active-site Cysteine Persulfide. Sci Rep. 2017 Jan 12;7:40227

[2]. Fiona Augsburger, et al. Role of 3-Mercaptopyruvate Sulfurtransferase in the Regulation of Proliferation, Migration, and Bioenergetics in Murine Colon Cancer Cells. Biomolecules. 2020 Mar 13;10(3):447.

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