Product Data Sheet

Oxythiamine

Cat. No.: HY-107430 CAS No.: 136-16-3 Molecular Formula: $C_{12}H_{16}N_3O_2S$ Molecular Weight: 266.34

Target: Apoptosis; Endogenous Metabolite Pathway: Apoptosis; Metabolic Enzyme/Protease Storage: -20°C, sealed storage, away from moisture

* In solvent: -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture)

SOLVENT & SOLUBILITY

In Vitro

DMSO: 51.67 mg/mL (194.00 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	3.7546 mL	18.7730 mL	37.5460 mL
	5 mM	0.7509 mL	3.7546 mL	7.5092 mL
	10 mM	0.3755 mL	1.8773 mL	3.7546 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: ≥ 2.58 mg/mL (9.69 mM); Clear solution
- 2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline) Solubility: ≥ 2.58 mg/mL (9.69 mM); Clear solution
- 3. Add each solvent one by one: 10% DMSO >> 90% corn oil Solubility: ≥ 2.58 mg/mL (9.69 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Oxythiamine (Hydroxythiamin), an analogue of anti-metabolite, can suppress the non-oxidative synthesis of ribose and induce cell apoptosis. Oxythiamine is a thiamine antagonist and inhibits transketolase (TK). Oxythiamine inhibits cancer cell apoptosis and inhibits cell proliferation ^{[1][2][3]} .
IC ₅₀ & Target	Vitamin B1, Thiamine, Transketolase ^[1] .
In Vitro	Oxythiamine (0-40 μ M, 2 days) inhibits cell viability of MIA PaCa-2 cells (IC ₅₀ : 14.95 μ M) ^[1] . Oxythiamine chloride hydrochloride (0-500 μ M, 48 h) suppresses expression of 14-3-3 protein beta/alpha in MIA PaCa-2 cells ^[1] .

Oxythiamine (0.1-100 μM, 6-48 h) inhibits A549 cell proliferation^[3].

Oxythiamine (0.1-100 μ M, 24 h) induces A549 cell apoptosis^[3].

Oxythiamine (0-20 µM) inhibits the invasion and migration (IC₅₀: 8.75 µM) of Lewis lung carcinoma (LLC) cells^[4].

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

Cell Viability Assay^[1]

Cell Line:	MIA PaCa-2 cells
Concentration:	0-40 μΜ
Incubation Time:	2 days
Result:	Inhibited cell viability with an IC $_{50}$ of 14.95 $\mu\text{M}.$

Western Blot Analysis^[1]

Cell Line:	MIA PaCa-2 cells	
Concentration:	0, 5, 50, 500 μΜ	
Incubation Time:	48 h	
Result:	Inhibited 14-3-3 protein beta/alpha expression, and increased alpha-enolase.	

In Vivo

Oxythiamine (100-500 mg/kg, i.p. 4 days) inhibits tumor growth in Ehrlich's ascites tumor hosting mice^[2]. Oxythiamine (250 or 500 mg/kg, daily for 5 week) inhibits tumor cell metastasis via inhibition of MMPs in mice implanted (s.c.) with LLC cells^[4].

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

Animal Model:	Ehrlich's ascites tumor hosting mice ^[2]
Dosage:	100-500 mg/kg
Administration:	i.p., 4 days
Result:	Inhibited tumor growth by 43% at 300 mg/kg and 84% at 500 mg/kg.

CUSTOMER VALIDATION

• Nat Commun. 2022 Oct 17;13(1):6121.

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REFERENCES

- [1]. Wang J, et al. Inhibition of transketolase by oxythiamine altered dynamics of protein signals in pancreatic cancer cells. Exp Hematol Oncol. 2013 Jul 27;2:18.
- [2]. Rais B, et al. Oxythiamine and dehydroepiandrosterone induce a G1 phase cycle arrest in Ehrlich's tumor cells through inhibition of the pentose cycle. FEBS Lett. 1999 Jul 30;456(1):113-8.
- [3]. Bai L, et al. A dose- and time-dependent effect of oxythiamine on cell growth inhibition in non-small cell lung cancer. Cogn Neurodyn. 2022 Jun;16(3):633-641.
- [4]. Yang CM, et al. The in vitro and in vivo anti-metastatic efficacy of oxythiamine and the possible mechanisms of action. Clin Exp Metastasis. 2010 May;27(5):341-9.

 $\label{lem:caution:Product} \textbf{Caution: Product has not been fully validated for medical applications. For research use only.}$

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