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Product Data Sheet

Oxythiamine chloride hydrochloride

Cat. No.: HY-107430A CAS No.: 614-05-1 Molecular Formula: $C_{12}H_{17}Cl_2N_3O_2S$

Molecular Weight: 338.25

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)

HO S-		D N N	
Н	CI (CI ⁻	

SOLVENT & SOLUBILITY

In Vitro

DMSO: 50 mg/mL (147.82 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent Mass Concentration	1 mg	5 mg	10 mg
	1 mM	2.9564 mL	14.7820 mL	29.5639 mL
	5 mM	0.5913 mL	2.9564 mL	5.9128 mL
	10 mM	0.2956 mL	1.4782 mL	2.9564 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: ≥ 2.08 mg/mL (6.15 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	Oxythiamine (Hydroxythiamine) chloride hydrochloride, an analogue of anti-metabolite, can suppress the non-oxidative synthesis of ribose and induce cell apoptosis. Oxythiamine chloride hydrochloride is a thiamine antagonist and inhibits transketolase (TK). Oxythiamine chloride hydrochloride inhibits cancer cell apoptosis and inhibits cell proliferation ^{[1][2][3]} .
IC ₅₀ & Target	Vitamin B1, Thiamine, Transketolase ^[1] .
In Vitro	Oxythiamine chloride hydrochloride (0-40 µM, 2 days) inhibits cell viability of MIA PaCa-2 cells (IC ₅₀ : 14.95 µM) ^[1] . Oxythiamine chloride hydrochloride (0-500 µM, 48 h) suppresses expression of 14-3-3 protein beta/alpha in MIA PaCa-2 cells ^[1] . Oxythiamine chloride hydrochloride (0.1-100 µM, 6-48 h) inhibits A549 cell proliferation ^[3] . Oxythiamine chloride hydrochloride (0.1-100 µM, 24 h) induces A549 cell apoptosis ^[3] . Oxythiamine chloride hydrochloride (0-20 µM) inhibits the invasion and migration (IC ₅₀ : 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 μM.	
Western Blot Analysis ^[1]		
Cell Line:	MIA PaCa-2 cells	
Concentration:	0, 5, 50, 500 μM	
Incubation Time:	48 h	
Result:	Inhibited 14-3-3 protein beta/alpha expression, and increased alpha-enolase.	

In Vivo

Oxythiamine chloride hydrochloride (100-500 mg/kg, i.p. 4 days) inhibits tumor growth in Ehrlich's ascites tumor hosting $mice^{[2]}$.

Oxythiamine chloride hydrochloride (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]. Raïs 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.

Page 2 of 3 www.MedChemExpress.com

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

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Page 3 of 3 www.MedChemExpress.com