N3PT

Cat. No.: HY-16339

CAS No.: 13860-66-7

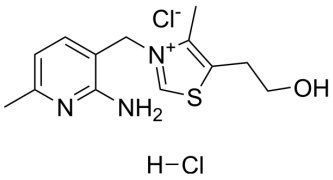
Molecular Formula: $C_{13}H_{19}Cl_2N_3OS$

Molecular Weight: 336.28

Target: Transketolase

Pathway: Metabolic Enzyme/Protease

Storage: 4°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 : 2.86 mg/mL (8.50 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.9737 mL	14.8686 mL	29.7371 mL
	5 mM	0.5947 mL	2.9737 mL	5.9474 mL
	10 mM	---	---	---

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 45% PEG300 >> 5% Tween-80 >> 50% saline
Solubility: 8 mg/mL (23.79 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

N3PT (N3-pyridyl thiamine) is a potent and selective transketolase inhibitor. N3PT is pyrophosphorylated and then binds to transketolase with an K_d value of 22 nM (Apo-TK, transketolase lacking bound thiamine)[1].

IC_{50} & Target

transketolase[1]

In Vitro

Arginase inhibitor 1inhibits human arginases I and II with IC_{50}s of 223±22.3 and 509±85.1 nM, respectively, and is active in a recombinant cellular assay overexpressing human arginase I (CHO cells). Arginase inhibitor 1 is a novel second generation arginase inhibitor with significant activity in a rat model of myocardial ischemia/reperfusion injury (MI/RI). Arginase inhibitor 1 is potent against hARG I in both in vitro enzyme and cellular assays. The IC_{50} for Arginase inhibitor 1 is 8 μM in CHO Cells Over-Expressing hArgI[1].

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

In Vivo

N3PT (compound 1) (100 mg/kg; i.v.; twice a day; 2 weeks) shows inhibitory effect on transketolase activity without significantly anti-tumor activity in HCT-116 tumor-bearing nude mice[1].

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Animal Model:	HCT-116 tumor-bearing nude mice[1]
Dosage:	100 mg/kg
Administration:	Intravenous injection; twice a day; 2 weeks
Result:	Decreased the activity of transketolase with no apparent effect on tumor size. Indicated that there were alternative pathways to generate ribose for DNA synthesis that were operating in these tumor cell lines.

REFERENCES

[1]. Thomas AA, et al. Synthesis, in vitro and in vivo activity of thiamine antagonist transketolase inhibitors. Bioorg Med Chem Lett. 2008 Mar 15;18(6):2206-10.

[2]. Allen A. Thomas, Josh Ballard, Bryan Bernat. Potent and Selective Thiamine Antagonists That Inhibit Transketolase.

[3]. Jeno Gyuris, May Han, Ronan C, N3-pyridyl-thiamine and its use in cancer treatments. Patent Numeber: WO2005094803 A2

[4]. Thomas AA, De Meese J, Le Huerou Y, Non-charged thiamine analogs as inhibitors of enzyme transketolase. Bioorg Med Chem Lett. 2008 Jan 15;18(2):509-12.

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