TH588

Cat. No.: HY-12814

CAS No.: 1609960-31-7

Molecular Formula: $C_{13}H_{12}Cl_2N_4$

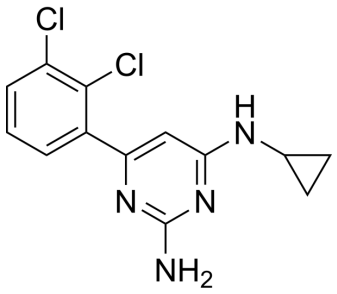
Molecular Weight: 295.17

Target: DNA/RNA Synthesis

Pathway: Cell Cycle/DNA Damage

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 16 mg/mL (54.21 mM; Need ultrasonic and warming)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.3879 mL	16.9394 mL	33.8788 mL
	5 mM	0.6776 mL	3.3879 mL	6.7758 mL
	10 mM	0.3388 mL	1.6939 mL	3.3879 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: ≥ 2.5 mg/mL (8.47 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (8.47 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (8.47 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

TH588 is first-in-class nudix hydrolase family inhibitor that potently and selectively engage and inhibit the MTH1 (IC_{50}= 5 nM).

IC_{50} & Target

IC50: 5 nM (MTH1)[1]

In Vitro

TH588 (2-10μM; 7-10 days) selectively and effectively kills U2OS, HeLa, MDA-MB-231, MCF-7, SW480, and SW620 cells with IC_{50}s of 1.38, 0.83, 1.03, 1.08, 1.72, 0.8 μM[1].

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

Cell Viability Assay[1]

Cell Line:	U2OS, HeLa, MDA-MB-231, MCF-7, SW480, SW620, VH10, HDFn cells
Concentration:	2, 4, 6, 8, 10 μM
Incubation Time:	7-10 days
Result:	Selectively and effectively killed U2OS, HeLa, MDA-MB-231, MCF-7, SW480, and SW620 cells with IC_{50}s of 1.38, 0.83, 1.03, 1.08, 1.72, 0.8 μM, but was less toxic to several primary or immortalized cells.

In Vivo

TH588 (30 mg/kg; s.c.; once daily for 35 days) reduces tumour growth in SW480 xenograft cancer model[1].

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

Animal Model:	5-6 weeks female SCID mice (SW480 xenograft cancer model)[1]
Dosage:	30 mg/kg
Administration:	Subcutaneous injection; once daily for 35 days
Result:	Reduced tumour growth in SW480 xenograft cancer model.

CUSTOMER VALIDATION

- J Mol Med (Berl). 2019 Aug;97(8):1183-1193.

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REFERENCES

[1]. Gad H, et al. MTH1 inhibition eradicates cancer by preventing sanitation of the dNTP pool. Nature. 2014 Apr 10;508(7495):215-21.

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