SHMT-IN-2

Cat. No.: HY-129226

CAS No.: 2102681-49-0

Molecular Formula: $C_{22}H_{24}F_3N_5O$

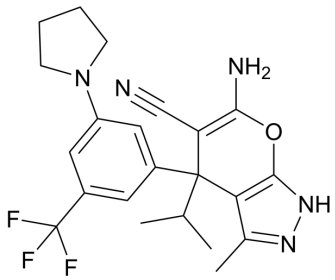
Molecular Weight: 431.45

Target: SHMT

Pathway: Metabolic Enzyme/Protease

Storage: 4°C, protect from light

* In solvent : -80°C, 6 months; -20°C, 1 month (protect from light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (231.78 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.3178 mL	11.5888 mL	23.1777 mL
	5 mM	0.4636 mL	2.3178 mL	4.6355 mL
	10 mM	0.2318 mL	1.1589 mL	2.3178 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 (5.79 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

SHMT-IN-2 is a stereo specific inhibitor of human SHMT1/2 with IC_{50} values of 13 nM and 66 nM for SHMT1 and SHMT2, respectively. SHMT-IN-2 can block the growth of many human cancer cells, and has sensitivity for B-cell lymphomas[1].

IC_{50} & Target

IC50: 2800 nM (SHMT1); IC50: 36 nM (SHMT2) [1]

In Vitro

SHMT-IN-2 (compound 2) can inhibit cell growth with cellular IC_{50} values of 2800 nM and 36 nM for SHMT1 and SHMT2, respectively[1].

SHMT-IN-2 (30 μM) shows the growth sensitivity with the median IC_{50} was 4 μM to a panel of nearly 300 human cancer cell lines (with IC_{50} values of 1.72 μM and 1.73 μM for CCRF-CEM and HT,respectively), cell lines of B-cell lymphoma origin were enriched in the more sensitive half of cells[1].

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

REFERENCES

[1]. regory S Ducker, et al. Human SHMT inhibitors reveal defective glycine import as a targetable metabolic vulnerability of diffuse large B-cell lymphoma. Proc Natl Acad Sci U S A. 2017 Oct 24;114(43):11404-11409.

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