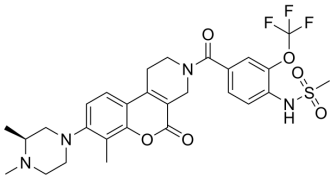
DS18561882

Cat. No.:	HY-130251
CAS No.:	2227149-22-4
Molecular Formula:	$C_{28}H_{31}F_3N_4O_6S$
Molecular Weight:	608.63
Target:	Methylenetetrahydrofolate Dehydrogenase (MTHFD)
Pathway:	Metabolic Enzyme/Protease
Storage:	4°C, stored under nitrogen * In solvent : -80°C, 2 years; -20°C, 1 year (stored under nitrogen)



SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (164.30 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.6430 mL	8.2152 mL	16.4303 mL
	5 mM	0.3286 mL	1.6430 mL	3.2861 mL
	10 mM	0.1643 mL	0.8215 mL	1.6430 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 (4.11 mM); Clear solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.5 mg/mL (4.11 mM); Clear solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.5 mg/mL (4.11 mM); Clear solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

DS18561882 is a highly potent, isozyme-selective methylenetetrahydrofolate dehydrogenase 2 (MTHFD2) inhibitor with an IC_{50} value of 0.0063 μM. DS18561882 also has inhibitory effect on MTHFD1 (IC_{50}=0.57 μM). DS18561882 exhibits a good oral pharmacokinetic profile[1].

IC_{50} & Target

IC50: 0.0063 μM (MTHFD2); 0.57 μM (MTHFD1)[1]

In Vitro

DS18561882 (0-150 nM) gives the lowest GI_{50} value (140 nM) against the MDA-MB-231 cell line[1].

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

In Vivo

DS18561882 (oral administration; 30, 100 or 300 mg/kg; twice daily) inhibits tumor growth inhibition with a dose-dependent manner, the tumor is completely inhibited (TGI: 67%) at the dose of 300 mg/kg in mice[1].

DS18561882 (oral administration; 10, 30, 100, or 300 mg/kg) has a good oral pharmacokinetic profile, including ACU (64.6, 264, 726 μg.h/ml); C_{max} (11.4, 56.5, 90.1 μg/ml); $t_{1/2}$ (2.21, 2.16, 2.32 hours) for 30 mg/kg; 100mg/kg; 200 mg/kg, respectively [1].

DS18561882 is suspended in a 0.5% (w/v) methyl cellulose 400 solution in this article[1].

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

Animal Model:	Five week old female BALB/cAJcl-nu/nu mice with MDA-MB-231 luc tumor cells (4×10^6 cells/mouse)[1]
Dosage:	30, 100 or 300 mg/kg
Administration:	Oral administration; 30, 100 or 300 mg/kg; twice daily; until day 11
Result:	Suppressed tumor growth in a dose-dependent manner.

CUSTOMER VALIDATION

- Nat Metab. 2022 Sep;4(9):1119-1137.
- Cell Stem Cell. 2024 Aug 21:S1934-5909(24)00285-6.
- J Exp Clin Cancer Res. 2022 Apr 5;41(1):125.
- Redox Biol. 2025 Jun 9:85:103715.
- Cancer Lett. 2022 Nov 28:549:215903.

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REFERENCES

[1]. Kawai J, et al. Discovery of a Potent, Selective, and Orally Available MTHFD2 Inhibitor (DS18561882) with In Vivo Anti-Tumor Activity. J Med Chem. 2019 Oct 22.

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