

DS18561882

Chemical Properties

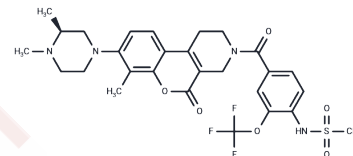
CAS No. : 2227149-22-4

Formula: C₂₈H₃₁F₃N₄O₆S

Molecular Weight: 608.63

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

Description	DS18561882 is an orally available, selective and potent inhibitor of methylenetetrahydrofolate dehydrogenase 2 (MTHFD2) with antitumor activity, inhibits MTHFD1 activity and can be used in the study of breast cancer.
Targets(IC50)	Dehydrogenase,DHFR
In vitro	DS18561882 (0-150 nM) achieves the lowest GI50 value (140 nM) against the MDA-MB-231 cell line.
In vivo	DS18561882 (oral; 10mg/kg, 30mg/kg, 100mg/kg or 300mg/kg) has good oral pharmacokinetics, including ACU (64.6, 264, 726ug.H/ml); Cmax (11.4, 56.5, 90.1° g) /ml). T1/2 (2.21, 2.16, 2.32 hours) are 30 mg/kg; 100 mg/kg; 200 mg/kg respectively. DS18561882 was suspended in 0.5% (W/V) methylcellulose 400 solution. DS18561882 (oral; 30, 100 or 300 mg/kg); tumor growth inhibition was inhibited in a dose-dependent manner and was completely inhibited at 300 mg/kg in mice (TGI: 67%).[1]

Solubility Information

Solubility	DMSO: 245 mg/mL (402.54 mM),Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 5 mg/mL (8.22 mM),Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.643 mL	8.2152 mL	16.4303 mL
5 mM	0.3286 mL	1.643 mL	3.2861 mL
10 mM	0.1643 mL	0.8215 mL	1.643 mL
50 mM	0.0329 mL	0.1643 mL	0.3286 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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