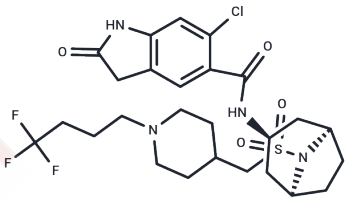
Data Sheet (Cat.No.TQ0263)

EPZ031686

Chemical Properties



CAS No. : 1808011-22-4

Formula: C26H34ClF3N4O4S

Molecular Weight: 591.09

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	EPZ031686 is an effective inhibitor of SMYD3 inhibitor with an IC50 of 3 nM and can be used in studies about cancer.
Targets(IC50)	Histone Methyltransferase
In vivo	In male CD-1 mice, EPZ031686 (1 mg/kg; i.v.) shows a moderate clearance (CL) of 27 ± 3.9 mL/min/kg, in very good agreement with the mouse microsomal data, with a volume of distribution at steady state (Vss) of 2.3 ± 0.29 L/kg, translating to a mean terminal half-life (t1/2) of 1.7 ± 0.13 h. After the treatment of EPZ031686 (5 and 50 mg/kg; p.o.), both Cmax and AUC0-last increased in a slightly higher than dose-proportional manner, while t1/2 remained unchanged. Bioavailability (F) of 48 ± 5.4% and 69 ± 8.2%, respectively, leading to EPZ031686 unbound blood concentration remaining above the SMYD3 ICW IC50 value for more than 12 h after a 50 mg/kg p.o.[1].

Solubility Information

Solubility	DMSO: 30 mg/mL (50.75 mM),Sonication and heating to 60°C are recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 1 mg/mL (1.69 mM),Sonication is recommended. *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.*

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	1.6918 mL	8.4589 mL	16.9179 mL
5 mM	0.3384 mL	1.6918 mL	3.3836 mL
10 mM	0.1692 mL	0.8459 mL	1.6918 mL
50 mM	0.0338 mL	0.1692 mL	0.3384 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

Mitchell LH et al. Novel Oxindole Sulfonamides and Sulfamides: EPZ031686, the First Orally Bioavailable Small Molecule SMYD3 Inhibitor. ACS Med Chem Lett. 2015 Aug 27;7(2):134-8.