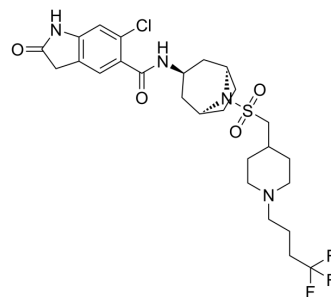


## EPZ031686

<b>Cat. No.:</b>	HY-19324		
<b>CAS No.:</b>	2095161-11-6		
<b>Molecular Formula:</b>	C <sub>26</sub> H <sub>34</sub> ClF <sub>3</sub> N <sub>4</sub> O <sub>4</sub> S		
<b>Molecular Weight:</b>	591.09		
<b>Target:</b>	Histone Methyltransferase		
<b>Pathway:</b>	Epigenetics		
<b>Storage:</b>	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	2 years
		-20°C	1 year



### SOLVENT & SOLUBILITY

#### In Vitro

DMSO : 35 mg/mL (59.21 mM); ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	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

Please refer to the solubility information to select the appropriate solvent.

#### In Vivo

- Add each solvent one by one: 30% PEG300 >> 70% (20% SBE-β-CD in saline)  
Solubility: 10 mg/mL (16.92 mM); Suspended solution; Need ultrasonic and warming
- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
Solubility: ≥ 1.75 mg/mL (2.96 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)  
Solubility: ≥ 1.75 mg/mL (2.96 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
Solubility: ≥ 1.75 mg/mL (2.96 mM); Clear solution

### BIOLOGICAL ACTIVITY

#### Description

EPZ031686 is an potent and orally active SMYD3 inhibitor and with an IC<sub>50</sub> value of 3 nM. EPZ031686 can be used for cancer research<sup>[1]</sup>.

#### IC<sub>50</sub> & Target

SMYD3  
3 nM (IC<sub>50</sub>)

## In Vivo

EPZ031686 (1-50 mg/mL; p.o. and i.v.; Male CD-1 mice) has good bioavailability following oral dosing in mice<sup>[1]</sup>.

Pharmacokinetic Analysis in Male CD-1 mice<sup>[1]</sup>

Route	Dose (mg/kg)	CL (mL/min/kg)	CL <sub>r</sub> (mL/min/kg)	V <sub>ss</sub> (L/kg)	t <sub>max</sub> (h)	t <sub>max</sub> (h)	C <sub>max</sub> (ng/mL)	AUC <sub>last</sub> (ng·h/mL)	AUC <sub>INF_obs</sub> (ng·h/mL)
i.v.	1	27	5.3	2.3	1.7	/	/	603	616
p.o.	5	/	/	/	2.7/td>	0.89	345	1281	1479
p.o.	50	/	/	/	2.2	1.3	4693	21158	21170

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

## CUSTOMER VALIDATION

- Acta Pharm Sin B. 2020 Dec 15.
- Sci Adv. 2023 Nov 15;9(46):eadi5921.
- Eur J Med Chem. 2022 Sep 8;243:114683.
- Aging. 2020 Nov 3;12(21):21423-21445.

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## REFERENCES

[1]. 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.

**Caution: Product has not been fully validated for medical applications. For research use only.**

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