BI-3231

Cat. No.: HY-148814

CAS No.: 2894848-07-6

Molecular Formula: $C_{16}H_{14}F_2N_4O_3S$

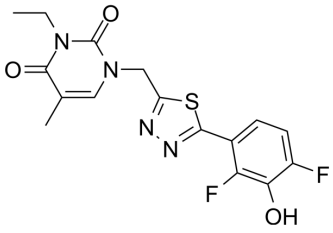
Molecular Weight: 380.37

Target: 17β-HSD

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
In solvent	-80°C	6 months
	-20°C	1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 125 mg/mL (328.63 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.6290 mL	13.1451 mL	26.2902 mL
	5 mM	0.5258 mL	2.6290 mL	5.2580 mL
	10 mM	0.2629 mL	1.3145 mL	2.6290 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: ≥ 2.08 mg/mL (5.47 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.47 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.47 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

BI 3231 is a potent and selective hydroxysteroid 17ß-dehydrogenase 13 (HSD17B13) inhibitor, with IC_{50}s of 1 and 13 nM for hHSD17B13 and mHSD17B13, respectively. BI 3231 has the potential for the research of nonalcoholic steatohepatitis (NASH) and other liver diseases[1].

IC_{50} & Target

hydroxysteroid 17ß-dehydrogenase 13 (HSD17B13)[1]

In Vitro

BI 3231 demonstrates high metabolic stability in liver microsomes and moderate metabolic stability in hepatocytes[1].

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

In Vivo	BI 3231 is rapidly cleared from plasma, considerable hepatic exposure was maintained over 48 h[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Thamm S, et, al. Discovery of a Novel Potent and Selective HSD17B13 Inhibitor, BI-3231, a Well-Characterized Chemical Probe Available for Open Science. J Med Chem. 2023 Feb 2.

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