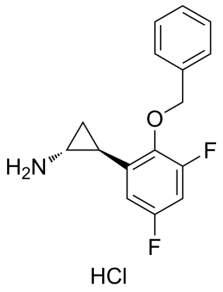
S2101

Cat. No.:	HY-110277
CAS No.:	1239262-36-2
Molecular Formula:	$C_{16}H_{16}ClF_2NO$
Molecular Weight:	311.75
Target:	Histone Demethylase
Pathway:	Epigenetics
Storage:	Powder -20°C 3 years 4°C 2 years In solvent -80°C 6 months -20°C 1 month



Relative stereochemistry

SOLVENT & SOLUBILITY

In Vitro

DMSO : 100 mg/mL (320.77 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	3.2077 mL	16.0385 mL	32.0770 mL
	5 mM	0.6415 mL	3.2077 mL	6.4154 mL
	10 mM	0.3208 mL	1.6038 mL	3.2077 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: 5 mg/mL (16.04 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 5 mg/mL (16.04 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 5 mg/mL (16.04 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

S2101 is a lysine-specific demethylase 1 (LSD1) inhibitor with an IC_{50} of 0.99 μM, K_i of 0.61 μM and K_{inact}/K_i of 4560 M/s[1].

IC_{50} & Target

KDM1/LSD1

In Vitro

S2101 is a lysine-specific demethylase 1 (LSD1) inhibitor with an IC_{50} of 0.99 μM, K_i of 0.61 μM and K_{inact}/K_i of 4560 M/s. S2101 also displays much lower inhibition activity toward MAO-B (K_i=17 μM, K_{inact}/K_i=18 M/s) and MAO-A (K_i=110 μM, K_{inact}/K_i=60 M/s). The treatment of HEK293T cells with S2101 results in a dose-dependent increase in the level of H3K4me2, which

must have accumulated by the inactivation of LSD1. During the course of S2101 treatment, the amounts of histone H3 and LSD1 in the nuclear extracts remain essentially unaffected. Because the treatment with 1 μM S2101 generates a level of H3K4me2 similar to that elicited by 50 μM 2-PCPA, S2101 is assumed to have approximately 50-fold stronger LSD1 inhibition activity than 2-PCPA in human cells[1].

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

REFERENCES

[1]. Mimasu S, et al. Structurally designed trans-2-phenylcyclopropylamine derivatives potently inhibit histone demethylase LSD1/KDM1 . Biochemistry. 2010 Aug 3;49(30):6494-503.

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