KDM5A-IN-1

Cat. No.: HY-100014

CAS No.: 1905481-36-8

Molecular Formula: $C_{15}H_{22}N_4O_2$

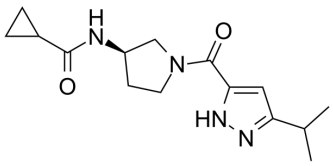
Molecular Weight: 290.36

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



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 50 mg/mL (172.20 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.4440 mL	17.2200 mL	34.4400 mL
5 mM	0.6888 mL	3.4440 mL	6.8880 mL
10 mM	0.3444 mL	1.7220 mL	3.4440 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: ≥ 2.75 mg/mL (9.47 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.75 mg/mL (9.47 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.75 mg/mL (9.47 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

KDM5A-IN-1 is a potent, orally bioavailable pan-histone lysine demethylases 5 (KDM5) inhibitor with IC_{50}s of 45 nM, 56 nM and 55 nM for KDM5A, KDM5B and KDM5C, respectively, and with an EC_{50} value of 960 nM for PC9 H3K4Me3. KDM5A-IN-1 is significantly less potent against other KDM5B enzymes (1A, 2B, 3B, 4C, 6A, 7B)[1].

IC_{50} & Target

IC50: 45 nM (KDM5A), 56 nM (KDM5B) and 55 nM (KDM5C)[1]

In Vivo

KDM5A-IN-1 (Compound 50, 5 mg/kg; oral administration; female CD-1 mice) treatment shows moderate clearance (28 mL/min/kg) in mice with good oral bioavailability (F% 34) and remarkably low plasma protein binding in mice (40%), with $t_{1/2}$ of 0.4 hours[1].

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

Animal Model:	Female CD-1 mice[1]
Dosage:	5 mg/kg
Administration:	Oral administration (Pharmacokinetic study)
Result:	Moderate clearance (28 mL/min/kg) in mice with good oral bioavailability (F% 34), and showed remarkably low plasma protein binding in mice (40%).

CUSTOMER VALIDATION

- Life Sci. 2019 Dec 15;239:116868.
- Hum Cell. 2022 Jul 27.

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REFERENCES

[1]. Liang J, et al. From a novel HTS hit to potent, selective, and orally bioavailable KDM5 inhibitors. Bioorg Med Chem Lett. 2017 Jul 1;27(13):2974-2981.

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