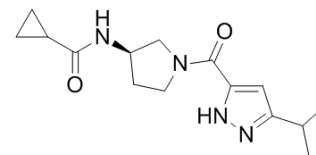


KDM5A-IN-1

Cat. No.:	HY-100014		
CAS No.:	1905481-36-8		
Molecular Formula:	C ₁₅ H ₂₂ N ₄ O 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 Concentration	Mass		
		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

- 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
- 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
- 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 IC₅₀s of 45 nM, 56 nM and 55 nM for KDM5A, KDM5B and KDM5C, respectively, and with an EC₅₀ 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].

IC₅₀ & 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].

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 Oct.

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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.

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

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