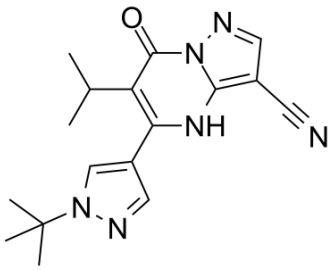
KDM5-IN-1

Cat. No.:	HY-100422
CAS No.:	1628210-26-3
Molecular Formula:	$C_{17}H_{20}N_6O$
Molecular Weight:	324.38
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 : ≥ 30 mg/mL (92.48 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	3.0828 mL	15.4140 mL	30.8280 mL
5 mM	0.6166 mL	3.0828 mL	6.1656 mL
10 mM	0.3083 mL	1.5414 mL	3.0828 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 (6.41 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (6.41 mM); Clear solution
3. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline
   Solubility: ≥ 2.5 mg/mL (7.71 mM); Clear solution

BIOLOGICAL ACTIVITY

Description	KDM5-IN-1 is a potent, selective and orally bioavailable KDM5 inhibitor with an IC_{50} of 15.1 nM.
IC_{50} & Target	IC50: 15.1 nM (KDM5); EC50: 0.34 μM (PC9 H3K4Me3)[1]
In Vitro	KDM5-IN-1 is found to potently inhibit KDM5B and KDM5C isoforms (IC_{50} of 4.7 and 65.5 nM, respectively). It is significantly less potent against other KDM enzymes (1A, 2B, 3B, 4C, 5A, 6A, 7B), inhibiting KDM4C the strongest with an IC_{50} of 1.9 μM.

	KDM5-IN-1 still displays more than 100-fold selectivity for KDM4C vs. KDM5A[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	When dosed orally in mice at 50 mg/kg twice a day, KDM5-IN-1 shows an unbound maximal plasma concentration C_{max}>15-fold over its cell EC_{50}, thereby providing a robust chemical probe for studying KDM5 biological functions in vivo[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Liang J, et al. Lead optimization of a pyrazolo[1,5-a]pyrimidin-7(4H)-one scaffold to identify potent, selective and orally bioavailable KDM5 inhibitors suitable for in vivo biological studies. Bioorg Med Chem Lett. 2016 Aug 15;26(16):4036-41.

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