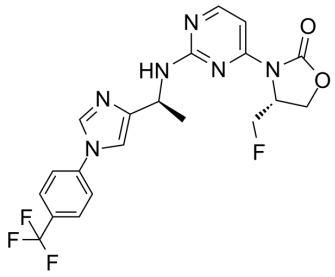
IDH1 Inhibitor 1

Cat. No.:	HY-112601
CAS No.:	2234285-81-3
Molecular Formula:	$C_{20}H_{18}F_4N_6O_2$
Molecular Weight:	450.39
Target:	Isocitrate Dehydrogenase (IDH)
Pathway:	Metabolic Enzyme/Protease
Storage:	4°C, sealed storage, away from moisture and light * In solvent : -80°C, 6 months; -20°C, 1 month (sealed storage, away from moisture and light)



SOLVENT & SOLUBILITY

In Vitro

DMSO : ≥ 100 mg/mL (222.03 mM)

* "≥" means soluble, but saturation unknown.

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.2203 mL	11.1015 mL	22.2030 mL
5 mM	0.4441 mL	2.2203 mL	4.4406 mL
10 mM	0.2220 mL	1.1101 mL	2.2203 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: ≥ 2.5 mg/mL (5.55 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (5.55 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.55 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

IDH1 Inhibitor 1 is a potent, orally bioavailable, brain-penetrant and selective mutant IDH1 inhibitor with IC_{50}s of 0.021 μM, 0.045 μM, and 2.52 μM for $IDH1^{R132H}$, $IDH1^{R132C}$, and $IDH1^{WT}$, respectively[1]. Anticancer activity[1].

IC_{50} & Target

IC50: 0.021 μM ($IDH1^{R132H}$), 0.045 μM ($IDH1^{R132C}$), and 2.52 μM ($IDH1^{WT}$)[1]

In Vitro

IDH1 Inhibitor 1 (Compound 19) inhibits cellular HCT116-$IDH1^{R132H/+}$ with an IC_{50} of 0.039 μM[1].

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

In Vivo	IDH1 Inhibitor 1 (Compound 19) inhibits 2-hydroxyglutarate (2-HG) production in a preclinical xenograft tumor model. IDH1 Inhibitor 1 is also profiled in a patient-derived IDH1 mutant HCT116-IDH1$^{R132H/+}$ mechanistic xenograft tumor model in mice to evaluate in vivo inhibition of 2-HG production. IDH1 Inhibitor 1, dosed orally at 150 mg/kg, inhibits new 2-HG production [1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Zhao Q, et al. Optimization of 3-Pyrimidin-4-yl-oxazolidin-2-ones as Orally Bioavailable and Brain Penetrant Mutant IDH1 Inhibitors. ACS Med Chem Lett. 2018 Jun 11;9(7):746-751.

Tel: 609-228-6898 Fax: 609-228-5909 E-mail: tech@MedChemExpress.com
Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA