Vorasidenib

Cat. No.: HY-104042

CAS No.: 1644545-52-7

Molecular Formula: $C_{14}H_{13}ClF_6N_6$

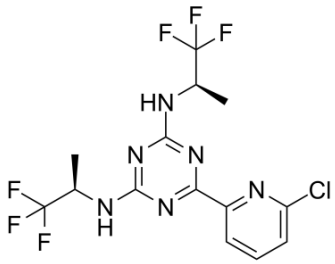
Molecular Weight: 414.74

Target: Isocitrate Dehydrogenase (IDH)

Pathway: Metabolic Enzyme/Protease

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 : 100 mg/mL (241.11 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4111 mL	12.0557 mL	24.1115 mL
	5 mM	0.4822 mL	2.4111 mL	4.8223 mL
	10 mM	0.2411 mL	1.2056 mL	2.4111 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 (5.02 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: 2.08 mg/mL (5.02 mM); Suspended solution; Need ultrasonic
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: 2.08 mg/mL (5.02 mM); Clear solution; Need warming
4. Add each solvent one by one: 5% DMSO >> 40% PEG300 >> 5% Tween-80 >> 50% saline
   Solubility: 2.5 mg/mL (6.03 mM); Suspended solution; Need ultrasonic
5. Add each solvent one by one: 5% DMSO >> 95% (20% SBE-β-CD in saline)
   Solubility: 2.4 mg/mL (5.79 mM); Suspended solution; Need ultrasonic

BIOLOGICAL ACTIVITY

Description

Vorasidenib (AG-881) is an orally available, brain penetrant second-generation dual mutant isocitrate dehydrogenases 1 and 2 (mIDH1/2) inhibitor. Vorasidenib (AG-881) exhibits nanomolar inhibition of (D)-2-hydroxyglutarate (D-2-HG), and the IC_{50} ranges of 0.04~22 nM against IDH1 R132C, IDH1 R132G, IDH1 R132H and IDH1 R132S and 7~14 nM against IDH2 R140Q and

	130 nM against IDH2 R172K[1][2].
IC_{50} & Target	IC50: 0.04~22 nM (IDH1 R132C, IDH1 R132G, IDH1 R132H, IDH1 R132S), 7~14 nM (IDH2 R140Q), 130 nM (IDH2 R172K)[2]
In Vitro	Vorasidenib has strong antiproliferative activity against human glioblastoma U-87 MG pLVX-IDH2 R140Q-neo, fibrosarcoma HT-1080 and neurosphere TS603 cells, all with IC_{50}s of less than 50 nM[2]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Theranostics. 2020 Jul 9;10(19):8757-8770.
- Metabolites. 2021, 11(2), 109.

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REFERENCES

[1]. Fujii T, et al. Targeting isocitrate dehydrogenase (IDH) in cancer. Discov Med. 2016 May;21(117):373-80.

[2]. Ma T, et al. Inhibitors of Mutant Isocitrate Dehydrogenases 1 and 2 (mIDH1/2): An Update and Perspective. J Med Chem. 2018 Oct 25;61(20):8981-9003.

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