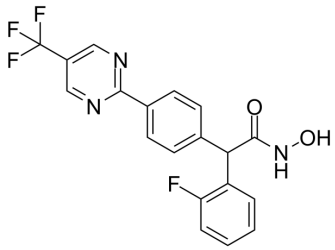
CHDI-390576

Cat. No.:	HY-119939
CAS No.:	1629729-98-1
Molecular Formula:	$C_{19}H_{13}F_4N_3O_2$
Molecular Weight:	391.32
Target:	HDAC
Pathway:	Cell Cycle/DNA Damage; Epigenetics
Storage:	Powder -20°C 3 years In solvent -80°C 6 months -20°C 1 month



SOLVENT & SOLUBILITY

In Vitro

DMSO : 250 mg/mL (638.86 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	2.5555 mL	12.7773 mL	25.5545 mL
	5 mM	0.5111 mL	2.5555 mL	5.1109 mL
	10 mM	0.2555 mL	1.2777 mL	2.5555 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 (5.32 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.08 mg/mL (5.32 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.08 mg/mL (5.32 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

CHDI-390576, a potent, cell permeable and CNS penetrant class IIa histone deacetylase (HDAC) inhibitor with IC_{50}s of 54 nM, 60 nM, 31 nM, 50 nM for class IIa HDAC4, HDAC5, HDAC7, HDAC9, respectively, shows >500-fold selectivity over class I HDACs (1, 2, 3) and ~150-fold selectivity over HDAC8 and the class IIb HDAC6 isoform[1].

IC_{50} & Target

HDAC4 54 nM (IC_{50})	HDAC5 60 nM (IC_{50})	HDAC7 31 nM (IC_{50})	hHDAC9 50 nM (IC_{50})
HDAC1 39.7 μM (IC_{50})	HDAC3 25.8 μM (IC_{50})	HDAC8 9.1 μM (IC_{50})	hHDAC6 6.2 μM (IC_{50})

In Vitro	The affinity (K_d) of CHDI-390576 to the catalytic domain of immobilized HDAC4 is 80 nM[1]. CHDI-390576 inhibits class I HDACs (1, 3, 8) and class IIb HDAC6 isoforms with IC_{50}s of 39.7μM, 25.8 μM, 9.1 μM, 6.2 μM, respectively[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

REFERENCES

[1]. Luckhurst CA, et al. Development and characterization of a CNS-penetrant benzhydryl hydroxamic acid class IIa histone deacetylase inhibitor. Bioorg Med Chem Lett. 2019 Jan 1;29(1):83-88.

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