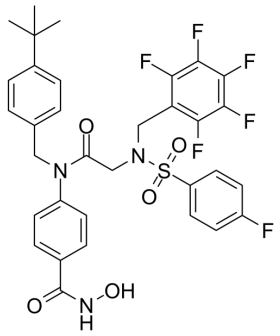
AES-135

Cat. No.:	HY-114483
CAS No.:	2361659-61-0
Molecular Formula:	$C_{33}H_{29}F_6N_3O_5S$
Molecular Weight:	693.66
Target:	HDAC
Pathway:	Cell Cycle/DNA Damage; 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 : 100 mg/mL (144.16 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	1.4416 mL	7.2081 mL	14.4163 mL
5 mM	0.2883 mL	1.4416 mL	2.8833 mL
10 mM	0.1442 mL	0.7208 mL	1.4416 mL

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.60 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

AES-135, a hydroxamic acid-based pan-HDAC inhibitor, prolongs survival in an orthotopic mouse model of pancreatic cancer. AES-135 inhibits HDAC3, HDAC6, HDAC8, and HDAC11 with IC_{50}s ranging from 190-1100 nM[1].

IC_{50} & Target

HDAC6	HDAC11	HDAC3	HDAC8
190 nM (IC_{50})	636 nM (IC_{50})	654 nM (IC_{50})	1100 nM (IC_{50})

In Vitro

AES-135 inhibits cancer cells growth with IC_{50} values of 2.3 μM, 1.4 μM, 0.27 μM, 0.94 μM, 1.9 μM, 2.72 μM, 2.1 μM, 15.0 μM, 1.6 μM and 19.2 μM for BT143, BT189, D425, D458, MV4-11, MOLM-13, MDA-MB-231, K562, PC-3 and MRC-9 cells, respectively[1].

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

In Vivo

AES-135 (50 mg/kg; intraperitoneal injection; 5 days a week; for 1 month) treatment significantly increases survival of C57Bl/6 mice implanted with KPC2 cells[1].

NSG mice are dosed with a single 20 mg/kg intraperitoneal (IP) injection, and blood is taken at 0.5 h, 1 h, 2 h, 4 h, 8 h, and 24 h. AES-135 achieved μM concentrations in the blood, reaching C_{max} 7452 ng/mL (10.74 μM) within 30 min, which is sustained for 8 h. The blood concentration of AES-135 is dose dependent, achieving an average of 323 ng/mL (0.47 μM) with 10 mg/kg dosing and 1829 ng/mL (2.64 μM) with 40 mg/kg. AES-135 shows an impressive pharmacokinetic profile in mice with an in vivo half-life of 5.0 h[1].

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

Animal Model:	C57Bl/6 mice injected with KPC2 cells[1]
Dosage:	50 mg/kg
Administration:	Intraperitoneal injection; 5 days a week; for 1 month
Result:	Significantly increased survival of mice.

CUSTOMER VALIDATION

- Cell Death Dis. 2021 May 18;12(6):501.

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REFERENCES

[1]. Shouksmith AE, et al. Identification and Characterization of AES-135, a Hydroxamic Acid-Based HDAC Inhibitor That Prolongs Survival in an Orthotopic Mouse Model of Pancreatic Cancer. J Med Chem. 2019 Mar 14;62(5):2651-2665.

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