Imidazole ketone erastin

Cat. No.: HY-114481

CAS No.: 1801530-11-9

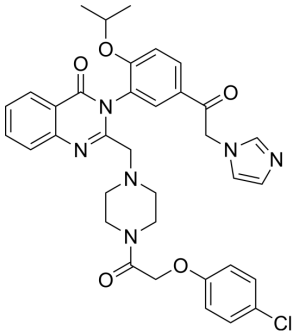
Molecular Formula: $C_{35}H_{35}ClN_6O_5$

Molecular Weight: 655.14

Target: Ferroptosis

Pathway: Apoptosis

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 (152.64 mM; Need ultrasonic)

Preparing Stock Solutions	Mass / Solvent / Concentration	1 mg	5 mg	10 mg
	1 mM	1.5264 mL	7.6320 mL	15.2639 mL
	5 mM	0.3053 mL	1.5264 mL	3.0528 mL
	10 mM	0.1526 mL	0.7632 mL	1.5264 mL

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

In Vivo

1. Add each solvent one by one: 50% PEG300 >> 50% saline
   Solubility: 16.67 mg/mL (25.44 mM); Suspended solution; Need ultrasonic
2. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 2.5 mg/mL (3.82 mM); Clear solution
3. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (3.82 mM); Clear solution
4. Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline
   Solubility: ≥ 2.08 mg/mL (3.17 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

Imidazole ketone erastin is a potent, selective, and metabolically stable inhibitor of the cystine-glutamate antiporter, system x_c^- and an activator of ferroptosis. Imidazole ketone erastin has anti-tumor activity[1].

IC_{50} & Target

System X_c^-, ferroptosis[1]

In Vitro

Imidazole ketone erastin (IKE) (0.1 nM-100 μM; 24 h) potently reduces diffuse large B cell lymphoma (DLBCL) cell number by

lipid peroxidation and ferroptosis[1].
?IKE (1-250 nM; 24 h) depletes reduced glutathione (GSH) in a dose-dependent manner with an IC_{50} of 34 nM in SUDHL6 cells [1].
?IKE (125-500 nM) increases lipid ROS in a dose-dependent manner in SUDHL-6 cells[1].
?IKE (500 nM; 5-360 min) increases the system x_c^- component SLC7A11, prostaglandin-endoperoxide synthase 2 (PTGS2), and ChaC glutathione-specific gamma-glutamylcyclotransferase 1 (CHAC1) expression in SUDHL-6 cells[1].
?IKE (500 nM and 1 μM) changes the relative abundance of 62 lipid species including lysophosphatidylcholines (LPC), phosphatidylcholines (PC), phosphatidylethanolamines (PE), and triglycerides (TAGs) in SUDHL6 cells[1].
?IKE (500 nM) activates de novo lipid biosynthesis pathways, phospholipid remodeling pathways, and arachidonic acid oxidation pathways in SUDHL6 cells[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

In Vivo

IKE (23-40 mg/kg; i.p. once daily for 13 d) inhibits tumor growth in mice[1].
?IKE (50 mg/kg; a single i.p) depletes GSH significantly starting from 4 h, and increases in the relative abundance of free fatty acids, phospholipids, and diacylglycerols (DAG) in mice[1].
?IKE (50 mg/kg) exhibits half-life (1.82, 1.31, and 0.96 h) and C_{max} (19515, 11384, and 5203 ng/mL) following different administration (i.p., i.v., and p.o. respectively) in mice[1].
MCE has not independently confirmed the accuracy of these methods. They are for reference only.

Animal Model:	Male NCG mice bearing SUDHL6 subcutaneous xenografts[1]
Dosage:	23, 40 mg/kg
Administration:	I.p. injection once daily for 13 days
Result:	Caused a significant decrease in tumor growth starting from day 9. Had a weight loss starting from day 9.

Animal Model:	NOD/SCID mice (12 weeks old; ~28 g weight)[1]
Dosage:	50 mg/kg (Pharmacokinetic Analysis)
Administration:	A single i.p., i.v., and p.o. administration
Result:	I.p.: $T_{1/2}$=1.82 h, C_{max}=19515 ng/mL. I.v.: $T_{1/2}$=1.31 h, C_{max}=11384 ng/mL. P.o.: $T_{1/2}$=0.96 h, C_{max}=5203 ng/mL.

CUSTOMER VALIDATION

- Nature. 2022 Jun;606(7915):776-784.
- Cell. 2023 Jun 22;186(13):2748-2764.e22.
- Nat Cancer. 2022 Apr;3(4):471-485.
- Nat Commun. 2021 Mar 11;12(1):1589.
- Redox Biol. 2023 Mar 8;62:102661.

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REFERENCES

[1]. Zhang Y, et al. Imidazole Ketone Erastin Induces Ferroptosis and Slows Tumor Growth in a Mouse Lymphoma Model. Cell Chem Biol. 2019 Jan 31. pii: S2451-9456(19)30030-3.

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