LDH-IN-1

Cat. No.: HY-111108

CAS No.: 1964515-43-2

Molecular Formula: $C_{30}H_{26}N_4O_4S_2$

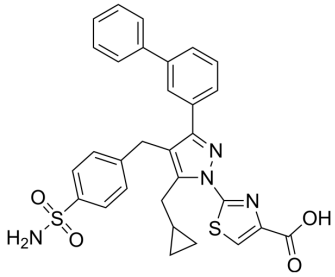
Molecular Weight: 570.68

Target: Lactate Dehydrogenase

Pathway: Metabolic Enzyme/Protease

Storage:

Powder	-20°C	3 years
	4°C	2 years
In solvent	-80°C	2 years
	-20°C	1 year



SOLVENT & SOLUBILITY

In Vitro

DMSO : 52 mg/mL (91.12 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.7523 mL	8.7615 mL	17.5230 mL
	5 mM	0.3505 mL	1.7523 mL	3.5046 mL
	10 mM	0.1752 mL	0.8761 mL	1.7523 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: ≥ 2.17 mg/mL (3.80 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.17 mg/mL (3.80 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

LDH-IN-1 is a novel pyrazole-based inhibitor of human lactate dehydrogenase (LDH) with IC_{50}s of 32 and 27 nM for LDHA and LDHB, respectively.

IC_{50} & Target

IC50: 32 nM (LDHA), 27 nM (LDHB)[1]

In Vitro

LDH-IN-1 exhibits low nM inhibition of both LDHA and LDHB (IC_{50}=32, 27 nM, respectively), submicromolar inhibition of lactate production, and inhibition of lactate in MiaPaCa2 pancreatic cancer and A673 sarcoma cells (IC_{50}=0.517, 0.854μM, respectively). LDH-IN-1 inhibits the growth of MiaPaCa2 pancreatic cancer and A673 sarcoma cells with IC_{50}s of 2.23 and 1.21 μM). Dose?response treatment of MiaPaCa-2 cells with LDH-IN-1 shows effects on cellular proliferation at concentrations as low as 250 nM and with nearly complete arrest of cell growth at 20 μM[1].

	MCE has not independently confirmed the accuracy of these methods. They are for reference only.
In Vivo	LDH-IN-1 shows clearance values that far exceed hepatic blood flow (HBF) in mouse species (90 mL/min/kg), with in vivo clearances of 227 mL/min/kg[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

PROTOCOL

Cell Assay [1]	A673 and MiaPaCa-2 cellsA673 and MiaPaCa-2 cells are cultured and plated in 1536-well white solid tissue culture plates. A 1536-well pintool dispenser outfitted with 20 nL pins is used to transfer 23 nL of LDH-IN-1 in DMSO to the 1536-well assay plates. After a 48 h incubation at 37°C, 2.5 µL of CellTiter-Glo is dispensed into each well using a BioRAPTR FRD dispenser. Plates are incubated at room temperature for 10 min, transferred to a ViewLux microplate imager, and the ATP-coupled luminescence is measured using a 1 s exposure[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.
Animal Administration [1]	Mice[1] Male CD1 mice approximately 6–8 weeks of age and a weight of approximately 20–30 g, are dosed with LDH-IN-1 at 2 mg/ kg (iv) and 50 mg/kg (po). Each cohort had three mice, and plasma is collected at 5 min, 15 min, 30 min, 1 h, 2 h, 4 h, 8 h, 12 h, and 24h postdose for iv and 15 min 30 min, 1 h, 2 h, 4 h, 8 h, 12 h, and 24 h for po. Approximately 0.025 mL of blood is collected via the dorsal metatarsal vein at each time point. Blood samples are then transferred into plastic microcentrifuge tubes containing heparin–Na as anticoagulant. Samples are then centrifuged at 4000g for 5 min at 4 °C to obtain plasma. Plasma samples are then stored in polypropylene tubes, quickly frozen, and kept at −75 °C until analyzed by LC/MS/MS[1]. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

CUSTOMER VALIDATION

- Cell Rep. 2022 Jun 21;39(12):110986.

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REFERENCES

[1]. Rai G, et al. Discovery and Optimization of Potent, Cell-Active Pyrazole-Based Inhibitors of Lactate Dehydrogenase (LDH). J Med Chem. 2017 Nov 22;60(22):9184-9204.

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