NCT-505

Cat. No.: HY-112277

CAS No.: 2231079-74-4

Molecular Formula: $C_{27}H_{28}FN_5O_3S$

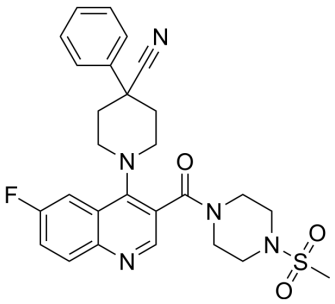
Molecular Weight: 521.61

Target: Aldehyde Dehydrogenase (ALDH)

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 (191.71 mM; Need ultrasonic)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	1.9171 mL	9.5857 mL	19.1714 mL
	5 mM	0.3834 mL	1.9171 mL	3.8343 mL
	10 mM	0.1917 mL	0.9586 mL	1.9171 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: ≥ 2.5 mg/mL (4.79 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (4.79 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NCT-505 is a potent and selective aldehyde dehydrogenase (ALDH1A1) inhibitor, with an IC_{50} of 7 nM, and weakly inhibits hALDH1A2, hALDH1A3, hALDH2, hALDH3A1 (IC_{50}s, >57, 22.8, 20.1, >57 μM).

IC_{50} & Target

ALDH1

In Vitro

NCT-505 (Compound 86) is a potent and selective aldehyde dehydrogenase (ALDH1A1) inhibitor, with an IC_{50} of 7 nM, and weakly inhibits hALDH1A2, hALDH1A3, hALDH2, hALDH3A1 (IC_{50}s, >57, 22.8, 20.1, >57 μM). NCT-505 has no obvious inhibitory effec on 5-hydroxyprostaglandin dehydrogenase (HPGD) and type-4 hydroxysteroid dehydrogenase (HSD17β4) (IC_{50}, >57 μM). Moreover, NCT-505 shows potent cellular activities, reducing the viability of OV-90 cells with an EC_{50} of 2.10-3.92 μM. NCT-505 is also cytotoxic to SKOV-3-TR cells, with IC_{50}s of 1, 3, 10, 20, 30 μM, respectively, in the titration assay[1].

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

PROTOCOL

Cell Assay [1]

Cells are harvested, and an equal volume of first compound (NCT-505 or paclitaxel (Taxol)) at the indicated concentration or vehicle DMSO (final DMSO concentration is the same in all conditions) is added to the cell suspension before dispensing. Cells are dispensed into 384-well, white, TC-treated plates at a density of 3000 cells/well in a volume of 30 µL of growth media/well using a Multidrop Combi dispenser. Immediately after dispensing, the second compound (ALDH1A1 inhibitor or paclitaxel) and control solutions (92 nL) are transferred using a pintool. Plates are covered with a breathable seal and incubated for 4 days at 37°C, 5% CO_2, 85% RH followed by addition of 20 µL of CellTiter-Glo. After a -30 min incubation at rt, samples are analyzed for luminescence intensity using a ViewLux high-throughput CCD imager equipped with clear filters. Pinned compounds are tested as 16-point dilution series, with concentrations ranging from 30.7 µM to 70.1 nM for ALDH1A1 inhibitors (NCT-505, etc.) or 31.7 µM to 0.034 nM for paclitaxel, in triplicate. Data are normalized to positive control bortezomib (1 µM final) and neutral control DMSO[1].

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

REFERENCES

[1]. Yang SM, et al. Discovery of Orally Bioavailable, Quinoline-Based Aldehyde Dehydrogenase 1A1 (ALDH1A1) Inhibitors with Potent Cellular Activity. J Med Chem. 2018 Jun 14;61(11):4883-4903.

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