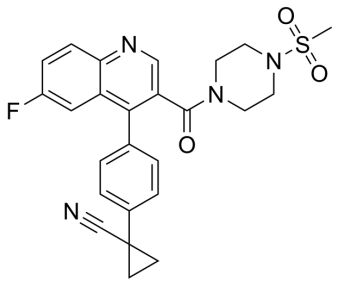
NCT-506

Cat. No.:	HY-112278
CAS No.:	2231098-99-8
Molecular Formula:	$C_{25}H_{23}FN_4O_3S$
Molecular Weight:	478.54
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 : 33.33 mg/mL (69.65 mM; Need ultrasonic)

Preparing Stock Solutions

Solvent / Mass / Concentration	1 mg	5 mg	10 mg
1 mM	2.0897 mL	10.4484 mL	20.8969 mL
5 mM	0.4179 mL	2.0897 mL	4.1794 mL
10 mM	0.2090 mL	1.0448 mL	2.0897 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 (5.22 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 2.5 mg/mL (5.22 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NCT-506 is an orally bioavailable aldehyde dehydrogenase 1A1 (ALDH1A1) inhibitors with an IC_{50} of 7 nM[1].

IC_{50} & Target

ALDH1

In Vitro

NCT-506 inhibits ALDH1A1, hALDH1A3, hALDH2 with IC_{50}s of 0.007±0.001, 16.4±3.99, and 21.5 μM, respectively[1].
NCT-506 (100, 10, 1, 0.1 μM, 6 days) decreases significantly cell viability with an EC_{50} of 45.6 μM in OV-90 cells. NCT-506 inhibits MIA PaCa-2, OV-90, and HT-29 cells with IC_{50}s of 0.077±0.040, 0.161±0.038, and 0.048±0.022 μM in aldefluor cell-based assays, respectively[1].
NCT-506 is treated in combined with Paclitaxel, IC_{50}s of 1202, 924, 870, 411, 102, and 31.8 nM with concentrations of NCT-506 at 0 (DMSO), 1, 3, 10, 20, 30 μM in SKOV-3-TR cells, respectively[1].

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

Cell Viability Assay[1]

Cell Line:	OV-90 and SKOV-3-TR cells
Concentration:	100, 10, 1, 0.1 μM
Incubation Time:	6 days for OV-90 cells; 4 days for SKOV-3-TR cells
Result:	Decreased significantly cell viability with an EC_{50} of 45.6 μM in OV-90 cells. Decreased cell viability in combined treatments (Paclitaxel concentration of 100 nM) with an EC_{50} of 11.2 μM in SKOV-3-TR cells.

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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