

NCT-505

Chemical Properties

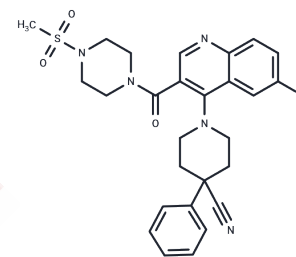
CAS No. : 2231079-74-4

Formula: C27H28FN5O3S

Molecular Weight: 521.61

Storage: Powder: -20°C for 3 years | In solvent: -80°C for 1 year

Actual storage temperature shall be subject to the COA.



Biological Description

Description	NCT-505 is a potent and selective inhibitor of aldehyde dehydrogenase (ALDH1A1, IC50 = 7 nM) and a weak inhibitor of hALDH1A2, hALDH1A3, hALDH2, hALDH3A1 with IC50 values of >57 μM, 22.8 μM, 20.1 μM, and >57 μM, respectively.
Targets(IC50)	Dehydrogenase
In vitro	NCT-505 (compound 86) is a potent and selective aldehyde dehydrogenase (ALDH1A1) inhibitor with IC50 of 7 nM, weakly inhibits hALDH1A2, hALDH1A3, hALDH2, hALDH3A1 (IC50s, >57, 22.8, 20.1, >57 μM). NCT-505 has no significant inhibitory effect on 5-hydroxyprostaglandin dehydrogenase (HPGD) and type 4 hydroxysteroid dehydrogenase (HSD17β4) (IC50, >57 μM). In addition, NCT-505 showed potent cellular viability, reducing the viability of OV-90 cells with EC50 of 2.10-3.92 μM. NCT-505 is also cytotoxic to SKOV-3-TR cells with IC50 of 1, 3, 10, 20, 30 μM in titration analysis[1].

Solubility Information

Solubility	DMSO: 55 mg/mL (105.44 mM), Sonication is recommended. (< 1 mg/ml refers to the product slightly soluble or insoluble)
In vivo Formulation	10% DMSO+40% PEG300+5% Tween 80+45% Saline: 2 mg/mL (3.83 mM), Sonication is recommended. <i>Please add the solvents sequentially, clarifying the solution as much as possible before adding the next one. Dissolve by heating and/or sonication if necessary. Working solution is recommended to be prepared and used immediately. The formulation provided above is for reference purposes only. In vivo formulations may vary and should be modified based on specific experimental conditions.</i>

Preparing Stock Solutions

	1mg	5mg	10mg
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
50 mM	0.0383 mL	0.1917 mL	0.3834 mL

Please select the appropriate solvent to prepare the stock solution, according to the solubility of the product in different solvents. Please use it as soon as possible.

Note: The dilution table applies only to solid products. For liquid products, please calculate the stock solution based on the stated concentration and/or density.

Reference

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.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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