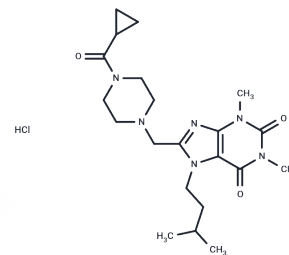


NCT-501 hydrochloride

Chemical Properties

CAS No. :	2080306-22-3
Formula:	C ₂₁ H ₃₃ ClN ₆ O ₃
Molecular Weight:	452.98
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-501 hydrochloride is a highly potent and selective inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1), which is based on theophylline. It effectively inhibits hALDH1A1 with an IC ₅₀ value of 40 nM, exhibiting superior selectivity towards hALDH1A1 compared to other ALDH isozymes and dehydrogenases such as hALDH1B1, hALDH3A1, and hALDH2 (with IC ₅₀ values exceeding 57 μM).
Targets(IC ₅₀)	Others, Dehydrogenase
In vitro	NCT-501 exhibited a 16% reduction in activity against the Cal-27 CisR cell line at a concentration of 20 nM; however, this difference was not statistically significant[1].
In vivo	NCT-501, administered intratracheally at a dose of 100 μg/animal on an alternate-day schedule for 20 days, demonstrates a 78% reduction in tumor growth in Cal-27 CisR-derived xenografts[1].

Preparing Stock Solutions

	1mg	5mg	10mg
1 mM	2.2076 mL	11.038 mL	22.076 mL
5 mM	0.4415 mL	2.2076 mL	4.4152 mL
10 mM	0.2208 mL	1.1038 mL	2.2076 mL
50 mM	0.0442 mL	0.2208 mL	0.4415 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

Kulsum S et al. Cancer stem cell mediated acquired chemoresistance in head and neck cancer can be abrogated by Aldehydedehydrogenase 1 A1 inhibition.

Yang SM, et al. Discovery of NCT-501, a Potent and Selective Theophylline-Based Inhibitor of Aldehyde Dehydrogenase 1A1(ALDH1A1). J Med Chem. 2015 Aug 13;58(15):5967-5978.

Inhibitor · Natural Compounds · Compound Libraries · Recombinant Proteins

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