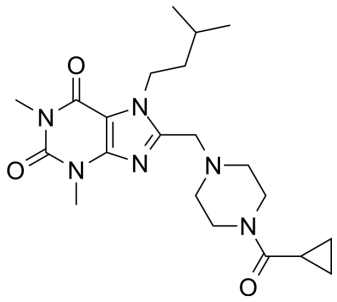
NCT-501

Cat. No.:	HY-18768
CAS No.:	1802088-50-1
Molecular Formula:	$C_{21}H_{32}N_6O_3$
Molecular Weight:	416.52
Target:	Aldehyde Dehydrogenase (ALDH)
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 : 3.57 mg/mL (8.57 mM; ultrasonic and warming and heat to 60°C)

Preparing Stock Solutions	Solvent / Mass / Concentration	1 mg	5 mg	10 mg
	1 mM	2.4008 mL	12.0042 mL	24.0085 mL
	5 mM	0.4802 mL	2.4008 mL	4.8017 mL
	10 mM	---	---	---

Please refer to the solubility information to select the appropriate solvent.

In Vivo

1. Add each solvent one by one: 10% DMSO >> 90% (20% SBE-β-CD in saline)
   Solubility: ≥ 1.25 mg/mL (3.00 mM); Clear solution
2. Add each solvent one by one: 10% DMSO >> 90% corn oil
   Solubility: ≥ 1.25 mg/mL (3.00 mM); Clear solution

BIOLOGICAL ACTIVITY

Description

NCT-501 is a potent and selective theophylline-based inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1), inhibits hALDH1A1 with IC_{50} of 40 nM, typically shows better selectivity over other ALDH isozymes and other dehydrogenases (hALDH1B1, hALDH3A1, and hALDH2, IC_{50} >57 μM).

IC_{50} & Target

ALDH1

In Vitro

NCT-501 shows a 16% decrease in the Cal-27 CisR cell line at 20 nM concentration, though the difference was not statistically significant[1].

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

In Vivo

NCT-501 (100 μg/animal; i.t.; every alternate day for 20 days) shows a 78% inhibition in tumor growth in Cal-27 CisR derived xenografts[1].

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

Animal Model:	5-6 weeks old male Hsd: Athymic Nude-Foxn1nu (immuno-deficient-mice bearing Cal-27 CisR cells)[1]
Dosage:	100μg/animal
Administration:	Intra-tumorally (i.t); every alternate day for 20 days
Result:	Showed a 78% inhibition in tumor growth in Cal-27 CisR derived xenografts.

CUSTOMER VALIDATION

- Free Radical Bio Med. 2020 May 20;152:8-17.
- Mol Cancer Ther. 2020 Jan;19(1):199-210.
- Mol Carcinog. 2017 Feb;56(2):694-711.
- Research Square Preprint. 2023 Jul 21.

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REFERENCES

[1]. Kulsum S et al. Cancer stem cell mediated acquired chemoresistance in head and neck cancer can be abrogated by Aldehydedehydrogenase 1 A1 inhibition.Mol Carcinog. 2016 Jul 6.

[2]. 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.

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