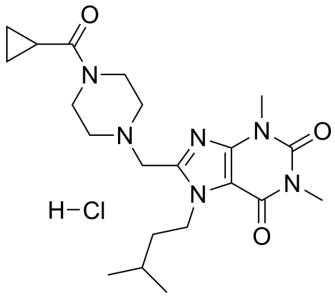
NCT-501 hydrochloride

Cat. No.:	HY-18768A
CAS No.:	2080306-22-3
Molecular Formula:	$C_{21}H_{33}ClN_6O_3$
Molecular Weight:	452.98
Target:	Aldehyde Dehydrogenase (ALDH)
Pathway:	Metabolic Enzyme/Protease
Storage:	Please store the product under the recommended conditions in the Certificate of Analysis.



BIOLOGICAL ACTIVITY

Description	NCT-501 hydrochloride 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)[1][2].
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.

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.

[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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