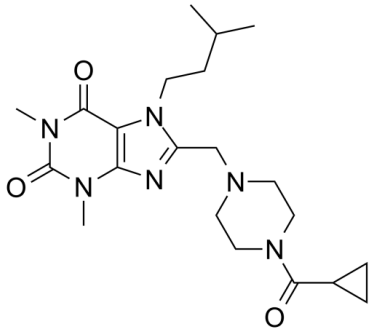
Data Sheet

Product Name:	NCT-501
Cat. No.:	CS-5116
CAS No.:	1802088-50-1
Molecular Formula:	C21H32N6O3
Molecular Weight:	416.52
Target:	Aldehyde Dehydrogenase (ALDH)
Pathway:	Metabolic Enzyme/Protease
Solubility:	DMSO : ≥ 28 mg/mL (67.22 mM)



BIOLOGICAL ACTIVITY:

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).

PROTOCOL (Extracted from published papers and Only for reference)

Enzymatic assay [1] An amount of 3 μL of enzyme (final concentration 20, 50, 20, and 5 nM for ALDH1A1, ALDH1B1, ALDH2, and ALDH3A1, respectively) or assay buffer (100 mM HEPES, pH 7.5, with 0.01% Tween 20) is dispensed into a 1536-well solid-bottom black plate followed by pin-tool transfer (23 nL) of NCT-501 (final concentration range 968 pM to 57.2 μM) and control (Bay 11-7085, final concentration range from 1.31 nM to 2.86 μM). Samples are incubated (rt, protected from light) for 15 min followed by a 1 μL substrate addition of NAD+ and propionaldehyde (final concentrations of 1 mM and 80 μM, respectively, for ALDH1A1, ALDH1B1, and ALDH2; or NAD+ and benzaldehyde at 1 mM and 200 μM, respectively, for ALDH3A1). Plates are centrifuged at 1000 rpm for 15 s, then read in kinetic mode on a ViewLux high-throughput CCD imager equipped with standard UV fluorescence optics (340 nm excitation, 450 nm emission) for 10 min (ALDH1A1, ALDH1B1, ALDH2) or 4 min (ALDH3A1). The change in fluorescence intensity over the 4 or 10 min reaction period is normalized against no-inhibitor and no-enzyme controls, and the resulting percent inhibition data were fitted for biological activity.

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.

CAIndexNames:

1H-Purine-2,6-dione, 8-[[4-(cyclopropylcarbonyl)-1-piperazinyl]methyl]-3,7-dihydro-1,3-dimethyl-7-(3-methylbutyl)-

SMILES:

O=C(N1C)N(C)C2=C(N(CCC(C)C)C(CN3CCN(C(C4CC4)=O)CC3)=N2)C1=O

Caution: Product has not been fully validated for medical applications. For research use only.

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