

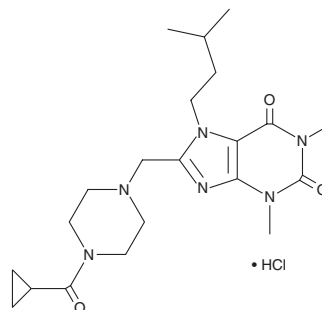
PRODUCT INFORMATION



NCT-501 (hydrochloride)

Item No. 18319

CAS Registry No.: 2080306-22-3
Formal Name: 8-[[4-(cyclopropylcarbonyl)-1-piperazinyl]methyl]-3,7-dihydro-1,3-dimethyl-7-(3-methylbutyl)-1H-purine-2,6-dione, monohydrochloride
MF: C₂₁H₃₂N₆O₃ • HCl
FW: 453.0
Purity: ≥98%
Stability: ≥2 years at -20°C
Supplied as: A crystalline solid
UV/Vis.: λ_{max}: 277 nm



Laboratory Procedures

For long term storage, we suggest that NCT-501 (hydrochloride) be stored as supplied at -20°C. It should be stable for at least two years.

NCT-501 (hydrochloride) is supplied as a crystalline solid. A stock solution may be made by dissolving the NCT-501 (hydrochloride) in the solvent of choice. NCT-501 (hydrochloride) is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide (DMF), which should be purged with an inert gas. The solubility of NCT-501 (hydrochloride) in ethanol is approximately 20 mg/ml and approximately 30 mg/ml in DMSO and DMF.

Further dilutions of the stock solution into aqueous buffers or isotonic saline should be made prior to performing biological experiments. Ensure that the residual amount of organic solvent is insignificant, since organic solvents may have physiological effects at low concentrations. Organic solvent-free aqueous solutions of NCT-501 (hydrochloride) can be prepared by directly dissolving the crystalline solid in aqueous buffers. The solubility of NCT-501 (hydrochloride) in PBS, pH 7.2, is approximately 10 mg/ml. We do not recommend storing the aqueous solution for more than one day.

Description

Aldehyde dehydrogenases (ALDHs) catalyze the NAD(P)⁺-dependent oxidation of aldehyde-containing substrates to the corresponding carboxylic acids.¹ ALDH1A1 activity is elevated in certain stem cells and cancers.¹ NCT-501 is a potent, reversible, theophylline-based inhibitor of ALDH1A1 (IC₅₀ = 40 nM for the human form).² It is selective for ALDH1A1 over other ALDH isozymes as well as other dehydrogenases. Pharmacokinetic studies indicate that NCT-501 has high bioavailability when delivered intraperitoneally, with rapid phase I modification in the liver.²

References

1. Tomita, H., Tanaka, K., Tanaka, T., *et al.* Aldehyde dehydrogenase 1A1 in stem cells and cancer. *Oncotarget* (2016).
2. Yang, S.-M., Yasgar, A., Miller, B., *et al.* Discovery of NCT-501, a potent and selective theophylline-based inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1). *J. Med. Chem.* **58**, 5967-5978 (2015).

WARNING

THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

SAFETY DATA

This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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