

Product Name: NCT 501 hydrochloride

Catalog No.: 5934

Batch No.: 1

CAS Number: 2080306-22-3

IUPAC Name: 8-[[4-(Cyclopropylcarbonyl)-1-piperazinyl]methyl]-3,7-dihydro-1,3-dimethyl-7-(3-methylbutyl)-1*H*-purine-2,6-dione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₃₂N₆O₃.HCl.¼H₂O

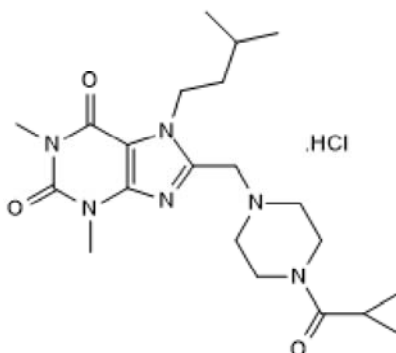
Batch Molecular Weight: 457.48

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.15 (Ethyl acetate)

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.13	7.38	18.37
Found	55.23	7.4	18.46

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Description:

NCT 501 hydrochloride is a potent and selective ALDH1A1 inhibitor (IC₅₀ = 40 nM). Exhibits >1000-fold selectivity for ALDH1A1 over ALDH3A1, ALDH1B1, ALDH2, HPGD and HSD17β4. Also selective over a panel of 168 GPCRs. Blood-brain barrier permeable.

Physical and Chemical Properties:

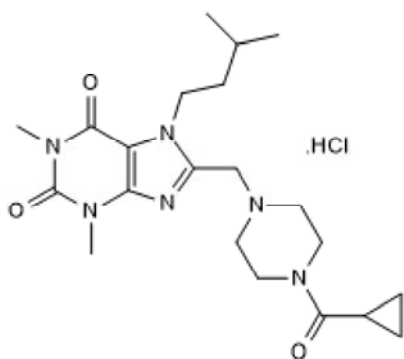
Batch Molecular Formula: C₂₁H₃₂N₆O₃.HCl.¼H₂O

Batch Molecular Weight: 457.48

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Yang *et al* (2015) Discovery of NCT-501, a potent and selective theophylline-based inhibitor of aldehyde dehydrogenase 1A1 (ALDH1A1). *J.Med.Chem.* **58** 5967. PMID: 26207746.

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