Print Date: Jan 11th 2022

Certificate of Analysis

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Product Name: **ML 218 hydrochloride** **Catalog No.: 4507** **Batch No.: 1**

CAS Number: 2319922-08-0

IUPAC Name: 3,5-Dichloro-*N*-[[(1α,5α,6-exo,6α)-3-(3,3-dimethylbutyl)-3-azabicyclo[3.1.0]hex-6-yl]methyl]-benzamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{26}Cl_2N_2O.HCl$

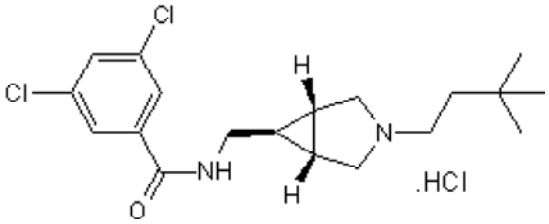
Batch Molecular Weight: 405.79

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.16 (Dichloromethane)

HPLC: Shows 99.5% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	56.24	6.71	6.9
Found	56.11	6.66	6.91

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Description:

ML 218 hydrochloride is a selective inhibitor of T-type calcium channels (IC_{50} values are 270 and 310 nM for $Ca_v3.3$ and $Ca_v3.2$ respectively in a patch EP assay). Decreases burst activity in STN neurons; reduces cataleptic behaviour in an in vivo rat model of Parkinson's disease. Displays no significant inhibition of L- or N-type calcium channels, $K_{ir}6$ (K_{ATP}) or $K_V11.1$ (hERG) potassium channels. ML 218 hydrochloride inhibits oral cancer cell proliferation. Orally active.

Physical and Chemical Properties:

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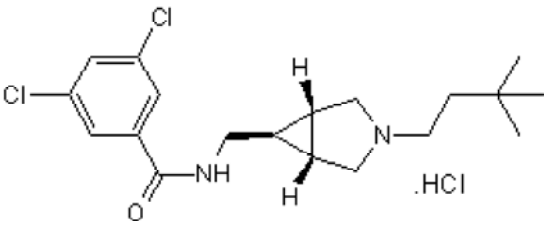
Batch Molecular Weight: 405.79

Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Chakraborty *et al* (2021) ML218 HCl is more efficient than capsaicin in inhibiting bacterial antigen-induced Cal 27 oral cancer cell proliferation. Int.J.Mol.Sci. ***22*** 12559. PMID: 34830441.

Galvan *et al* (2016) Lack of antiparkinsonian effects of systemic injections of the specific T-type calcium channel blocker ML218 in MPTP-treated monkeys. ACS Chem.Neurosci ***7*** 1543. PMID: 27596273 .

Xiang *et al* (2011) The discovery and characterization of ML218: A novel, centrally active T-type calcium channel inhibitor with robust effects in STN neurons and in a rodent model of Parkinson's disease. ACS Chem.Neurosci. ***2*** 730. PMID: 22368764.

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