

Product Name: NNC 55-0396 dihydrochloride

Catalog No.: 2268

Batch No.: 4

CAS Number: 357400-13-6

IUPAC Name: (1*S*,2*S*)-2-[2-[[3-(1*H*-Benzimidazol-2-yl)propyl]methylamino]ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-naphthalenyl cyclopropanecarboxylate dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₀H₃₈FN₃O₂.2HCl.H₂O

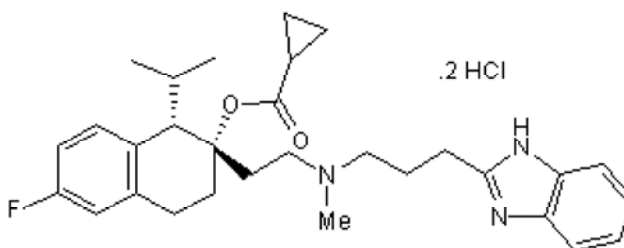
Batch Molecular Weight: 582.59

Physical Appearance: White solid

Solubility: water to 25 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.7 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99.1% purity

Chiral HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.85	7.27	7.21
Found	61.62	7.27	7.07

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Description:

Highly selective T-type calcium channel blocker. Displays IC₅₀ values of 6.8 and > 100 μM for inhibition of Ca_v3.1 T-type channels and HVA currents respectively in INS-1 cells.

Physical and Chemical Properties:

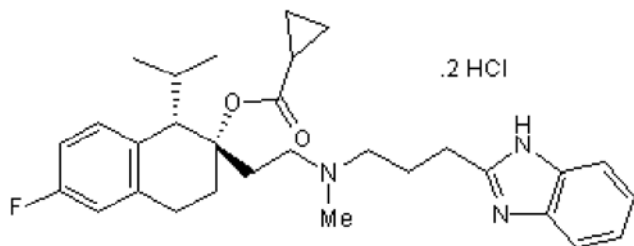
Batch Molecular Formula: C₃₀H₃₈FN₃O₂·2HCl·H₂O

Batch Molecular Weight: 582.59

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 25 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:

Chen et al (2010) Ca_v3.2 T-type Ca²⁺ channel-dependent activation of ERK in paraventricular thalamus modulates acid-induced chronic muscle pain. *J.Neurosci.* **30** 10360. PMID: 20685979.

Huang et al (2004) NNC 55-0396 [(1S,2S)-2-(2-(N-[(3-benzimidazol-2-yl)propyl]-N-methylamino)ethyl)-6-fluoro-1,2,3,4-tetrahydro-1-isopropyl-2-naphthyl cyclopropanecarboxylate dihydrochloride]: A new selective inhibitor of T-type calcium channels. *J.Pharmacol.Exp.Ther.* **309** 193. PMID: 14718587.

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