



CAS Number:

IUPAC Name:

Storage:

Certificate of Analysis

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Batch No.: 4

Product Name: NNC 55-0396 dihydrochloride

Catalog No.: 2268

(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-(1S,2S)-2-[2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyl]-6-fluoro-1,2,3,4-tetrahydro-1-(1-methylethyl)-2-(1S,2S)-2-[[3-(1H-Benzimidazol-2-yl)propyl] methylamino] ethyllogolar ethylamino] ethyllogolar ethyllogolanaphthalenyl cyclopropanecarboxylate dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

357400-13-6

Batch Molecular Formula: C₃₀H₃₈FN₃O₂.2HCl.H₂O

Batch Molecular Weight: 582.59 **Physical Appearance:** White solid water to 25 mM Solubility:

Batch Molecular Structure:

2. ANALYTICAL DATA

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

Desiccate at RT

HPLC: Shows 99.0% 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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Product Information

Print Date: Feb 25th 2025

www.tocris.com

Batch No.: 4

Product Name: NNC 55-0396 dihydrochloride

CAS Number: 357400-13-6

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

naphthalenyl cyclopropanecarboxylate dihydrochloride

Description:

NNC 55-0396 dihydrochloride is a highly selective T-type calcium channel blocker. Displays IC $_{50}$ values of 6.8 and > 100 μ M for inhibition of Ca $_{v}$ 3.1 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:

J.2 HCI

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).

Catalog No.: 2268

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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-naphtyl cyclopropanecarboxylate dihydrochloride]: A new selective inhibitor of T-type calcium cha J.Pharmacol.Exp.Ther. *309* 193. PMID: 14718587.

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