

Product Name: TCN 237 dihydrochloride

Catalog No.: 4072

Batch No.: 1

CAS Number: 700878-19-9

IUPAC Name: 2-[[4-[(2-Fluorophenyl)methyl]-1-piperidiny]methyl]-1*H*-benzimidazol-6-ol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₂FN₃O.2HCl

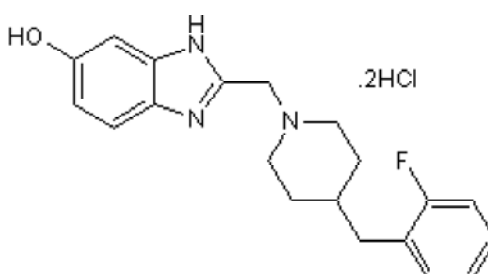
Batch Molecular Weight: 412.33

Physical Appearance: White solid

Solubility: water to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.31 (Chloroform:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows >99.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.26	5.87	10.19
Found	58.27	5.9	10.2

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

Highly potent GluN2B (formally NR2B) selective NMDA receptor antagonist ($K_i = 0.8$ nM); blocks GluN2B-mediated calcium influx in Ltk cells ($K_i = 9.7$ nM). Selective for GluN2B subunit over α_1 -adrenergic receptors and hERG channels (IC_{50} values are 730 nM and 2900 nM respectively). Displays efficacy in the rat carrageenan-induced mechanical hyperalgesia assay. Please refer to IUPHAR Guide to Pharmacology for the most recent naming conventions.

Physical and Chemical Properties:

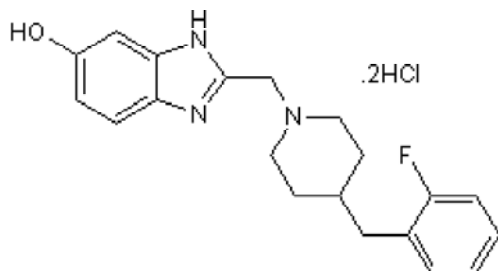
Batch Molecular Formula: $C_{20}H_{22}FN_3O \cdot 2HCl$

Batch Molecular Weight: 412.33

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

McCauley et al (2004) NR2B-selective N-methyl-D-aspartate antagonists: synthesis and evaluation of 5-substituted benzimidazoles. *J. Med. Chem.* **47** 2089. PMID: 15056006.

Storage: Store at -20°C

Solubility & Usage Info:

water 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.

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