

Certificate of Analysis

Product Name: PNU 22394 hydrochloride

Catalog No.: 2201

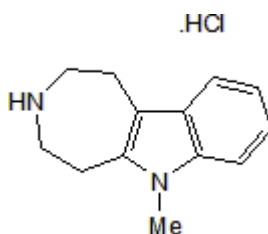
Batch No.: 1

CAS Number: 15923-42-9

IUPAC Name: 1,2,3,4,5,6-Hexahydro-6-methyl-azepino[4,5-*b*]indole hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₆N₂·HCl
Batch Molecular Weight: 236.74
Physical Appearance: Off-white solid
Solubility: water to 100 mM
Storage: Desiccate at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.55 (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])
Melting Point: Between 212 - 214°C
HPLC: Shows >99.8% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	65.96	7.24	11.83
Found	65.6	7.26	11.84

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

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Description:

Potent 5-HT_{2C} agonist and partial 5-HT_{2A}/5-HT_{2B} agonist. Non-selective between 5-HT₂ receptor subtypes (K_i values are 18, 18 and 66 nM for human recombinant 5-HT_{2C}, 5-HT_{2A} and 5-HT_{2B} receptors respectively). Reduces food intake in rats following subcutaneous administration and displays anorexigenic effects in humans.

Physical and Chemical Properties:

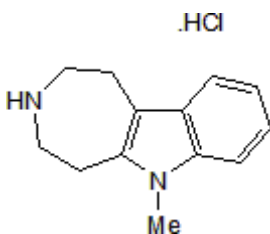
Batch Molecular Formula: C₁₃H₁₆N₂.HCl

Batch Molecular Weight: 236.74

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

McCall et al (2001) PNU-22394, a 5-HT_{2C} receptor agonist, reduces feeding in rodents and produces weight loss in humans. Soc.Neurosci.Abstr. **27** 309.

Jensen et al (2013) Design, synthesis and pharmacological characterization of *N*- and *O*-substituted 5,6,7,8-tetrahydro-4*H*-isoxazolo [4,5-*d*]azepin-3-ol analogues: novel 5-HT_{2A}/5-HT_{2C} receptor agonists with pro-cognitive properties. J.Med.Chem. **56** 1211.

Storage: Desiccate at +4°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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