

Certificate of Analysis

Product Name: Nepicastat hydrochloride

Catalog No.: 5037

Batch No.: 1

CAS Number: 170151-24-3

IUPAC Name: 5-(Aminomethyl)-1-[(2*S*)-5,7-difluoro-1,2,3,4-tetrahydro-2-naphthalenyl]-1,3-dihydro-2*H*-imidazole-2-thione hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₄H₁₅F₂N₃S.HCl.¼H₂O

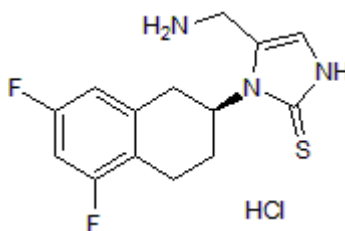
Batch Molecular Weight: 336.31

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50	4.95	12.49
Found	50.36	4.84	12.21

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

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Description:

Potent and selective dopamine β -hydroxylase (DBH) inhibitor (IC_{50} = 9 nM). Selective for DBH over 12 other enzymes. Decreases noradrenaline and increases dopamine levels in tissues and plasma in hypertensive rats. Prevents progressive left ventricular dysfunction in an in vivo heart failure model. Also potentiates the stimulus effects of cocaine without producing cocaine-like effects in rats. Orally bioavailable.

Physical and Chemical Properties:

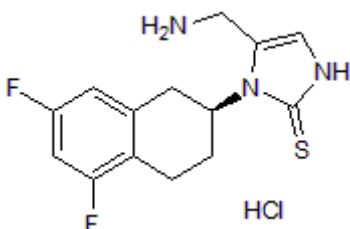
Batch Molecular Formula: $C_{14}H_{15}F_2N_3S \cdot HCl \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 336.31

Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Stanley et al (1997) Catecholamine modulatory effects of nepicastat (RS-25560-197), a novel, potent and selective inhibitor of dopamine-beta-hydroxylase. *Br.J.Pharmacol.* **121** 1803. PMID: 9283721.

Sabbah et al (2000) Effects of dopamine β -hydroxylase inhibition with nepicastat on the progression of left ventricular dysfunction and remodeling in dogs with chronic heart failure. *Circulation* **102** 1990. PMID: 11034950.

Manvich et al (2013) Dopamine β -hydroxylase inhibitors enhance the discriminative stimulus effects of cocaine in rats. *J.Pharmacol.Exp.Ther.* **347** 564. PMID: 24068832.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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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