

Product Name: CP 122721 hydrochloride

Catalog No.: 3649

Batch No.: 1

CAS Number: 145877-52-7

IUPAC Name: (2S,3S)-N-[[2-Methoxy-5-(trifluoromethoxy)phenyl]methyl]-2-phenyl-3-piperidinamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₃F₃N₂O₂.2HCl

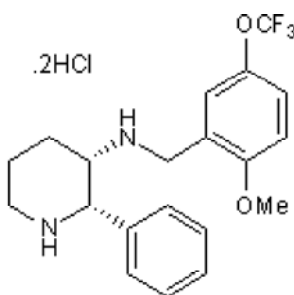
Batch Molecular Weight: 453.33

Physical Appearance: White solid

Solubility: water to 100 mM
DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.35 (DCM / MeOH / NH₄OH (90:9:1))

HPLC: Shows 99.8% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +65.8 (Concentration = 1.09, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.99	5.56	6.18
Found	52.77	5.54	6.18

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Description:

High affinity NK₁ antagonist (pIC₅₀ = 9.8). Suppresses recruitment of immunocytes in respiratory syncytial virus (RSV)-infected rats after capsaicin stimulation. Also blocks substance P-induced excitation of locus ceruleus cells in guinea pig brain slices (IC₅₀ = 7 nM). Exhibits anxiolytic and antidepressant-like effects. Active in vivo.

Physical and Chemical Properties:

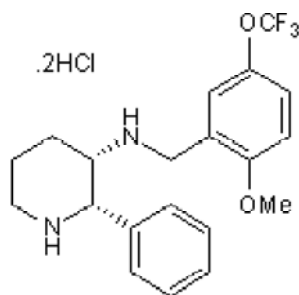
Batch Molecular Formula: C₂₀H₂₃F₃N₂O₂.2HCl

Batch Molecular Weight: 453.33

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

water to 100 mM

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.

References:

Auais *et al* (2003) Immunomodulatory effects of sensory nerves during respiratory syncytial virus infection in rats. *Am.J.Physiol. Lung Cell Mol.Physiol.* **285** L105. PMID: 12639840.

Gonsalves *et al* (1996) Broad spectrum antiemetic effects of CP-122,721, a tachykinin NK1 receptor antagonist, in ferrets. *Eur.J.Pharmacol.* **305** 181. PMID: 8813551.

McLean *et al* (1996) Characterization of CP-122,721; a nonpeptide antagonist of the neurokinin NK1 receptor. *J.Pharmacol.Exp.Ther.* **277** 900. PMID: 8627572.

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