Certificate of Analysis

Product Name: **CP 99994 dihydrochloride** **Catalog No.: 3417** **Batch No.: 1**

CAS Number: 145148-39-6

IUPAC Name: (2*S*,3*S*)-*N*-[(2-Methoxyphenyl)methyl]-2-phenyl-3-piperidinamine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{24}N_2O.2HCl.¼H_2O$

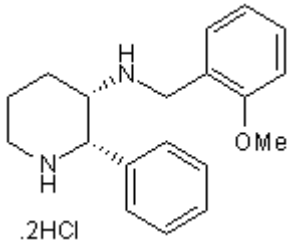
Batch Molecular Weight: 373.83

Physical Appearance: White solid

Solubility: water to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.05	7.14	7.49
Found	61.03	7.14	7.56

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Description:

High affinity NK_1 antagonist (K_i = 0.145 nM in vitro). Also displays high ex vivo binding potency in gerbil striatum (IC_{50} = 36.8 nM). Attenuates endothelium-dependent contraction induced by substance P.

Physical and Chemical Properties:

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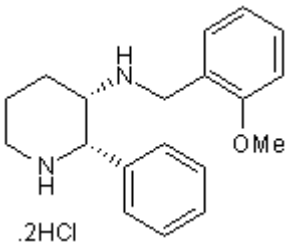
Batch Molecular Weight: 373.83

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Desiccate at RT

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.

References:

Shirahase *et al* (1995) Endothelium-dependent contraction in intrapulmonary arteries: mediation by endothelial NK_1 receptors and TXA_2. Br.J.Pharmacol. ***115*** 1215. PMID: 7582548.

Duffy *et al* (2002) Correlation of neurokinin (NK) 1 receptor occupancy in gerbil striatum with behavioral effects of NK1 antagonists. J.Pharmacol.Exp.Ther. ***301*** 536. PMID: 11961054.

Lindstrom *et al* (2007) Neurokinin 1 receptor antagonists: correlation between in vitro receptor interaction and in vivo efficacy. J.Pharmacol.Exp.Ther. ***322*** 1286. PMID: 17575073.