

Product Name: SSR 146977 hydrochloride

Catalog No.: 3297

Batch No.: 1

CAS Number: 264618-38-4

IUPAC Name: *N*1-[1-3-[(3*R*)-1-Benzoyl-3-(3-(3,4-dichlorophenyl)-3-piperidinyl)propyl]-4-phenyl-piperidinyl]-*N,N*-dimethylurea hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₅H₄₂Cl₂N₄O₂.HCl.2H₂O

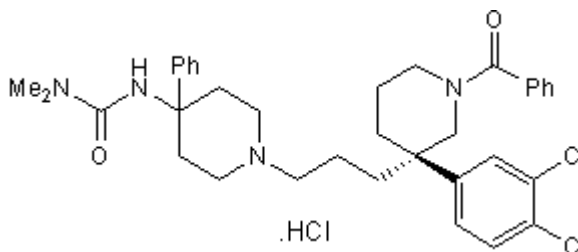
Batch Molecular Weight: 694.14

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (Dichloromethane:Ethanol:Ammonia soln. [90:9:1])

HPLC: Shows >98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +23.6 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	60.56	6.82	8.07
Found	60.52	6.31	7.94

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

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Description:

Potent and selective NK₃ receptor antagonist (K_i values are 0.26 and 19.3 nM in CHO cells expressing the human NK₃ and NK₂ receptor respectively). Also inhibits senktide-induced inositol monophosphate formation and intracellular calcium mobilization (IC₅₀ = 10 nM).

Physical and Chemical Properties:

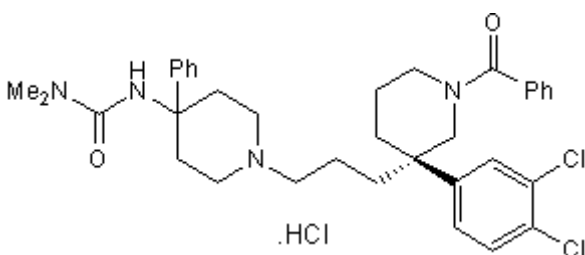
Batch Molecular Formula: C₃₅H₄₂Cl₂N₄O₂.HCl.2H₂O

Batch Molecular Weight: 694.14

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol 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:

Emonds-Alt et al (2002) Biochemical and pharmacological activities of SSR 146977, a new potent nonpeptide tachykinin NK3 receptor antagonist. *Can.J.Physiol.Pharmacol.* **80** 482. PMID: 12056557.

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