

Product Name: SR 140333

Catalog No.: 4012

Batch No.: 2

CAS Number: 153050-21-6

IUPAC Name: 1-[2-[(3S)-3-(3,4-Dichlorophenyl)-1-[2-[3-(1-methylethoxy)phenyl]acetyl]-3-piperidiny]ethyl]-4-phenyl-1-azoniabicyclo[2.2.2]octane chloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₇H₄₅Cl₃N₂O₂ · 1³/₄H₂O

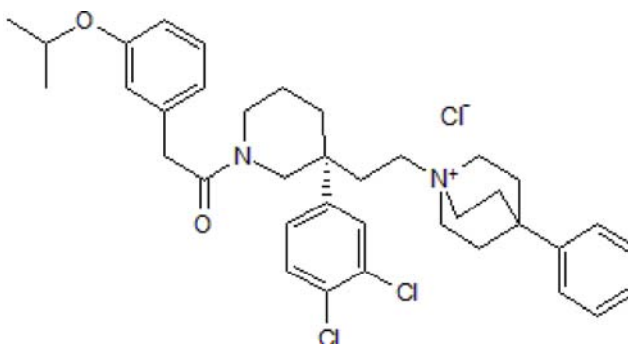
Batch Molecular Weight: 687.64

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 97.0% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +13.8 (Concentration = 1, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64.63	7.11	4.07
Found	63.79	6.93	4.14

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Description:

SR 140333 is a potent NK₁ receptor antagonist (K_i = 0.74 nM. IC₅₀ = 1.6 nM). Inhibits substance P-invoked calcium mobilization and outward current (IC₅₀ = 1.3 nM); blocks NK₁-mediated nitric oxide-dependent vasodilation *in vivo*.

Physical and Chemical Properties:

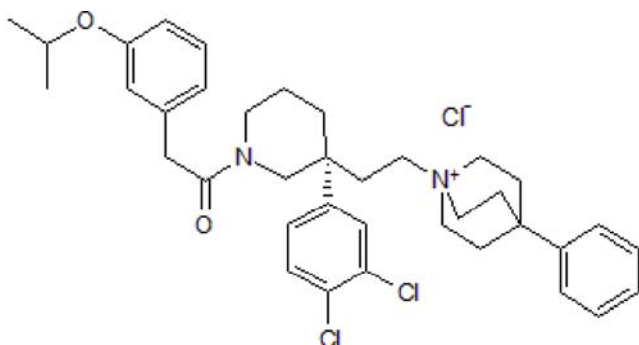
Batch Molecular Formula: C₃₇H₄₅Cl₃N₂O₂·1¾H₂O

Batch Molecular Weight: 687.64

Physical Appearance: Off White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°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:

Nieuwmeier *et al* (2006) Ava[L-Pro9,N-MeLeu10] substance P(7-11) (GR 73632) and Sar9, Met(O2)11 increase distention-induced peristalsis through activation of neurokinin-1 receptors on smooth muscle and interstitial cells of Caj J.Pharmacol.Exp.Ther. **317** 439. PMID: 16330493.

Hall and Brain (1994) Inhibition by SR140333 of NK₁ tachykinin receptor-evoked, nitric oxide-dependent vasodilation in the hamster cheek pouch microvasculature *in vivo*. Br.J.Pharmacol. **113** 522. PMID: 7530573.

Oury-Donat *et al* (1994) SR 140333, a novel, selective, and potent nonpeptide antagonist of the NK1 tachykinin receptor: characterization on the U373MG cell line. J.Neurochem. **62** 1399. PMID: 7510780.

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