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Print Date: Jan 13th 2016

Certificate of Analysis

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Product Name: **SB 222200** **Catalog No.: 1393** **Batch No.: 2**

CAS Number: 174635-69-9

IUPAC Name: 3-Methyl-2-phenyl-*N*-[(1*S*)-1-phenylpropyl]-4-quinolinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{24}N_2O$

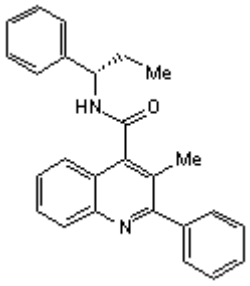
Batch Molecular Weight: 380.48

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.64 (Ethyl acetate:Petroleum ether [1:2])

Melting Point: Between 154 - 157°C

HPLC: Shows >98.5% purity

^{1}H NMR: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -37 (Concentration = 10, Solvent = methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	82.08	6.36	7.36
Found	82.13	6.32	7.4

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CAS Number: 174635-69-9

IUPAC Name: 3-Methyl-2-phenyl-*N*-[(1*S*)-1-phenylpropyl]-4-quinolinecarboxamide

Description:

Potent and selective non-peptide NK_3 receptor antagonist (K_i values are 4.4, > 100,000 and 250 nM for human NK_3, NK_1 and NK_2 receptors respectively). Antihypertensive in vivo. Brain penetrant.

Physical and Chemical Properties:

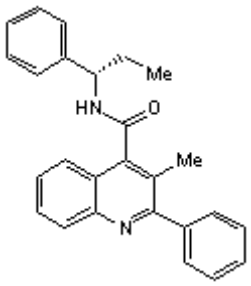
Batch Molecular Formula: $C_{26}H_{24}N_2O$

Batch Molecular Weight: 380.48

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at RT

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:

Medhurst *et al* (1997) *In vitro* and *in vivo* characterization of NK_3 receptors in the rabbit eye by use of selective non-peptide NK_3 receptor antagonists. Br.J.Pharmacol. ***122*** 469. PMID: 9351503.

Sarau *et al* (2000) Nonpeptide tachykinin receptor antagonists. II. Pharmacological and pharmacokinetic profile of SB-222200, a central nervous system penetrant, potent and selective NK-3 receptor antagonist. J.Pharmacol.Exp.Ther. ***295*** 373. PMID: 10992004.

De Brito Gariepy and Couture (2010) Blockade of tachykinin NK3 receptor reverses hypertension through a dopaminergic mechanism in the ventral tegmental area of spontaneously hypertensive rats. Br.J.Pharmacol. ***161*** 1868. PMID: 20804497.