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Print Date: Jan 14th 2016

Certificate of Analysis

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Product Name: **SB 223412** **Catalog No.: 4672** **Batch No.: 1**

CAS Number: 174636-32-9

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{22}N_2O_2 \cdot ¼H_2O$

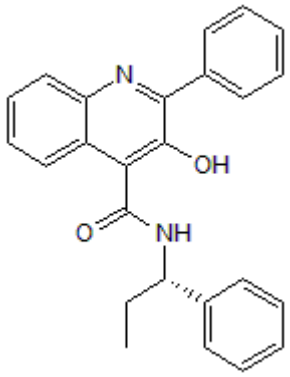
Batch Molecular Weight: 386.95

Physical Appearance: Off-white 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 (Chloroform:Methanol [95:5])

HPLC: Shows >99.8% purity

Chiral HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	77.6	5.86	7.24
Found	77.97	5.67	7.38

bio-techne.com
info@bio-techne.com
techsupport@bio-techne.com

North America
Tel: (800) 343 7475

China
info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa
Tel: +44 (0)1235 529449

Rest of World
www.tocris.com/distributors
Tel:+1 612 379 2956

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

Description:

Potent and selective non-peptide NK_3 receptor antagonist (K_i values are 1, 144 and >100000 nM for human NK_3, NK_2 and NK_1 receptors respectively). Selective over a panel of >60 receptors, enzymes and ion channels at concentrations of 1 or 10 µM. Inhibits NKB-induced Ca^{2+} mobilization in vitro (IC_{50} = 16.6 nM) and inhibits NK_3-agonist-induced behavioral responses in vivo. Orally active and brain penetrant.

Physical and Chemical Properties:

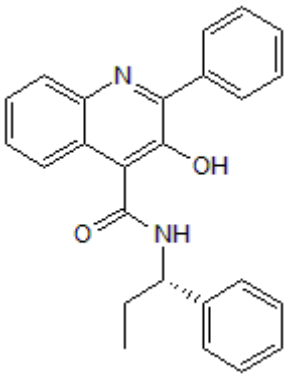
Batch Molecular Formula: $C_{25}H_{22}N_2O_2.¼H_2O$

Batch Molecular Weight: 386.95

Physical Appearance: Off-white 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:

Sarau *et al* (1997) Nonpeptide tachykinin receptor antagonists: I. Pharmacological and pharmacokinetic characterization of SB 223412, a novel, potent and selective neurokinin-3 receptor antagonist. J.Pharmacol.Ther.Exp. ***281*** 1303. PMID: 9190866.

Sarau *et al* (2001) Molecular and pharmacological characterization of the murine tachykinin NK_3 receptor. Eur.J.Pharmacol. ***413*** 143. PMID: 11226387.

de la Flor and Dawson (2009) Augmentation of antipsychotic-induced neurochemical changes by the NK_3 receptor antagonist talnetant (SB-223412). Neuropharmacol. ***56*** 342. PMID: 18822303.