

Product Name: SB 223412

Catalog No.: 4672

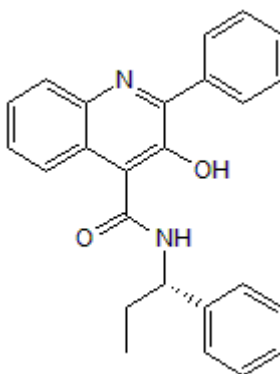
Batch No.: 1

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: C₂₅H₂₂N₂O₂·¼H₂O
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
¹H 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

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

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Description:

Potent and selective non-peptide NK₃ receptor antagonist (K_i values are 1, 144 and >100000 nM for human NK₃, NK₂ and NK₁ receptors respectively). Selective over a panel of >60 receptors, enzymes and ion channels at concentrations of 1 or 10 μM. Inhibits NKB-induced Ca²⁺ mobilization in vitro (IC₅₀ = 16.6 nM) and inhibits NK₃-agonist-induced behavioral responses in vivo. Orally active and brain penetrant.

Physical and Chemical Properties:

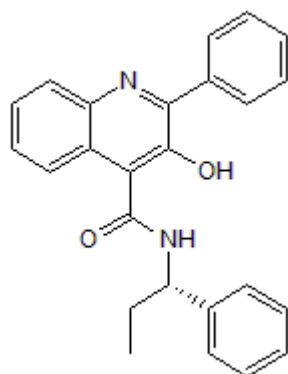
Batch Molecular Formula: C₂₅H₂₂N₂O₂ · ¼H₂O

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 NK₃ receptor. *Eur.J.Pharmacol.* **413** 143. PMID: 11226387.

de la Flor and Dawson (2009) Augmentation of antipsychotic-induced neurochemical changes by the NK₃ receptor antagonist taltetant (SB-223412). *Neuropharmacol.* **56** 342. PMID: 18822303.

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