Certificate of Analysis

Product Name: **SB 612111 hydrochloride** **Catalog No.: 3573** **Batch No.: 3**

IUPAC Name: (5*S*,7*S*)-7-[[4-(2,6-Dichlorophenyl)-1-piperidinyl]methyl]-6,7,8,9-tetrahydro-1-methyl-5*H*-benzocyclohepten-5-ol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{29}Cl_2NO.HCl.¼H_2O$

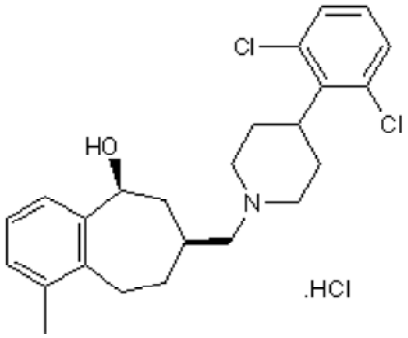
Batch Molecular Weight: 459.36

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.5 (DCM / MeOH / NH4OH (95:5:0.5))

HPLC: Shows 97.9% purity

Chiral HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -42.2 (Concentration = 1, Solvent = Ethanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.75	6.69	3.05
Found	62.67	6.67	3.22

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Product Information

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IUPAC Name: (5*S*,7*S*)-7-[[4-(2,6-Dichlorophenyl)-1-piperidinyl]methyl]-6,7,8,9-tetrahydro-1-methyl-5*H*-benzocyclohepten-5-ol hydrochloride

Description:

Selective NOP receptor antagonist (K_i values are 0.33, 57.6, 160.5 and 2109 nM for NOP, μ-, κ- and δ-receptors respectively). Antagonizes the pronociceptive action of nociceptin (Cat. No. 0910) in an acute pain model. Potentiates the action of morphine in morphine-tolerant animals and blocks hyperalgesia in an inflammatory pain model.

Physical and Chemical Properties:

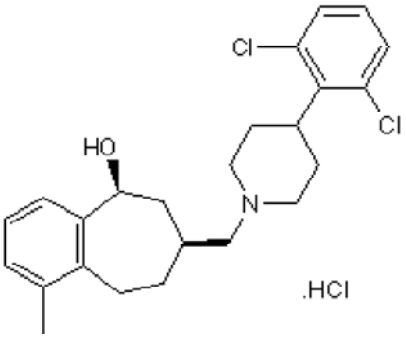
Batch Molecular Formula: $C_{24}H_{29}Cl_2NO.HCl.¼H_2O$

Batch Molecular Weight: 459.36

Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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.

Licensing Information:

Sold with the permission of GlaxoSmithKline

References:

Rizzi *et al* (2007) Pharmacological characterization of the nociceptin/orphanin FQ receptor antagonist SB-612111 [(-)-*cis*-1-methyl-7-[[4-(2,6-dichlorophenyl)piperidin-1-yl]methyl]-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-ol]: in vivo studies. J.Pharmacol.Exp.Ther. ***321*** 968. PMID: 17329551.

Spagnolo *et al* (2007) Pharmacological characterization of the nociceptin/orphanin FQ receptor antagonist SB-612111 [(-)-*cis*-1-Methyl-7-[[4-(2,6-dichlorophenyl)piperidin-1-yl]methyl]-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-ol]: in vitro studies. J.Pharm.Exp.Ther. ***106*** 961.

Zaratin *et al* (2004) Modification of nociception and mor. tolerance by the selective opiate receptor-like orphan receptor antagonist (-)-*cis*-1-methyl-7-[[4-(2,6-dichlorophenyl)piperidin-1-yl]methyl]-6,7,8,9-tetrahydro-5*H*-benzocyclohepten-5-ol (SB-612111) J.Pharmacol.Exp.Ther. ***308*** 454. PMID: 14593080.