

Certificate of Analysis

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Product Name: SB 271046 hydrochloride

Catalog No.: 3368

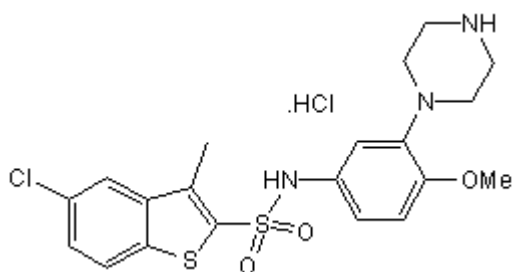
Batch No.: 2

CAS Number: 209481-24-3

IUPAC Name: 5-Chloro-N-[4-methoxy-3-(1-piperazinyl)phenyl]-3-methyl-benzo[b]thiophen-2-sulfonamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₀H₂₂ClN₃O₃S₂.HCl.H₂O
Batch Molecular Weight: 506.47
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Desiccate at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.29 (Dichloromethane:Methanol [95:5])
HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	47.43	4.98	8.3	14
Found	47.38	4.6	8.2	14.36

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

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Description:

Selective, orally active 5-HT₆ antagonist (pK_i values are 9.02-8.92, 6.55, 6.35, 6.27, 6.05, 5.95, 5.76, 5.73, 5.62, 5.55, 5.41, 5.39, 5.27 and < 4.99 at 5-HT₆, 5-HT_{1D}, 5-HT_{1A}, D₃, 5-HT_{1B}, 5-HT_{1F}, α_{1B}, 5-HT_{2C}, 5-HT_{2A}, D₂, 5-HT_{2B}, 5-HT₇, 5-HT₄ and 5-HT_{1E} respectively) and is > 200-fold selective over 55 other receptors, enzymes and ion channels. Increases extracellular glutamate and aspartate in the frontal cortex, and exhibits anticonvulsant activity (EC₅₀ = 0.16 μM).

Physical and Chemical Properties:

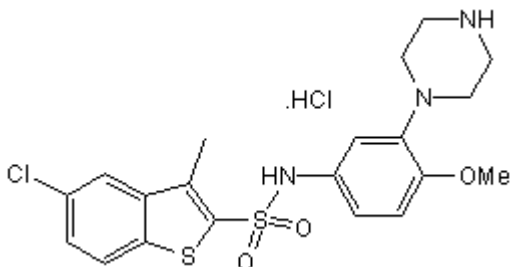
Batch Molecular Formula: C₂₀H₂₂ClN₃O₃S₂.HCl.H₂O

Batch Molecular Weight: 506.47

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Bromidge et al (1999) 5-Chloro-N-(4-methoxy-3-piperazin-1-yl-phenyl)-3-methyl-2-benzothiophenesulfonamide (SB-271046): a potent, selective, and orally bioavailable 5-HT₆ receptor antagonist. *J.Med.Chem.* **42** 202. PMID: 9925723.

Dawson et al (2000) *In vivo* effects of the 5-HT₆ antagonist SB-271046 on striatal and frontal cortex extracellular concentrations of noradrenaline, dopamine, 5-HT, glutamate and aspartate. *Br.J.Pharmacol.* **130** 23. PMID: 10780993.

Routledge et al (2000) Characterization of SB-271046: a potent, selective and orally active 5-HT₆ receptor antagonist. *Br.J.Pharmacol.* **130** 1606. PMID: 10928964.

Marcos et al (2008) Effects of 5-HT₆ receptor antagonism and cholinesterase inhibition in models of cognitive impairment in the rat. *Br.J.Pharmacol.* **155** 434. PMID: 18622410.

Storage: Desiccate at RT

Solubility & Usage Info:

DMSO 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.

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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