

Certificate of Analysis

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Product Name: SB 269970 hydrochloride

Catalog No.: 1612

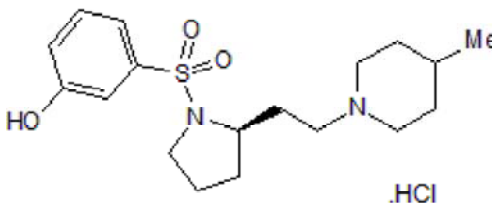
Batch No.: 10

CAS Number: 261901-57-9

IUPAC Name: (2*R*)-1-[(3-Hydroxyphenyl)sulfonyl]-2-[2-(4-methyl-1-piperidinyl)ethyl]pyrrolidine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₈H₂₈N₂O₃S.HCl
Batch Molecular Weight: 388.95
Physical Appearance: White solid
Solubility: water to 20 mM
 phosphate buffered saline to 5 mM
 DMSO to 100 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.21 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +86.2 (Concentration = 0.47, Solvent = DMSO)
Microanalysis:

| | Carbon Hydrogen Nitrogen | | |
|-------------|--------------------------|------|------|
| Theoretical | 55.58 | 7.52 | 7.2 |
| Found | 55.26 | 7.48 | 7.16 |

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

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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Description:

Potent and selective 5-HT₇ receptor antagonist (pK_i values are 8.9, 7.2 and 6.0 for 5-HT_{7A}, 5-HT_{5A} and 5-HT_{1B} and < 6.0 for 5-HT_{1A}, 5-HT_{1D}, 5-HT_{1E}, 5-HT_{1F}, 5-HT_{2A}, 5-HT_{2B}, 5-HT_{2C}, 5-HT₄ and 5-HT₆ receptors respectively). Brain penetrant in vivo.

Physical and Chemical Properties:

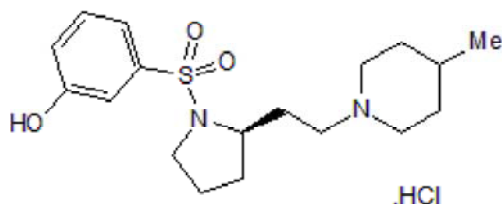
Batch Molecular Formula: C₁₈H₂₈N₂O₃S.HCl

Batch Molecular Weight: 388.95

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

water to 20 mM
phosphate buffered saline to 5 mM
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.

Licensing Information:

Sold for research purposes under agreement from GlaxoSmithKline.

References:

Kogan et al (2002) DR4004, a putative 5-HT₇ receptor antagonist, also has functional activity at the dopamine receptor. *Eur.J.Pharmacol.* **449** 105. PMID: 12163113.

Hagan et al (2000) Characterization of SB-269970-A, a selective 5-HT₇ receptor antagonist. *Br.J.Pharmacol.* **130** 539. PMID: 10821781.

Lovell et al (2000) A novel, potent, and selective 5-HT₇ antagonist: (*R*)-3-(2-(2-(4-methylpiperidin-1-yl)-ethyl)pyrrolidine-1-sulfonyl) phenol (SB-269970) *J.Med.Chem.* **43** 342. PMID: 10669560.

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