

**Product Name:** SB 224289 hydrochloride

**Catalog No.:** 1221

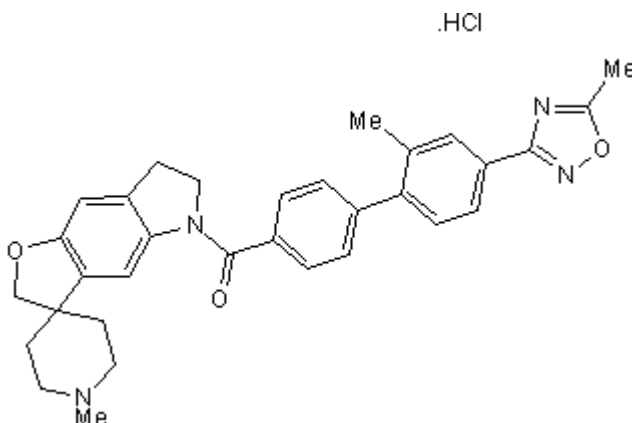
**Batch No.:** 3

CAS Number: 180084-26-8

IUPAC Name: 1'-Methyl-5-[[[2'-methyl-4'-(5-methyl-1,2,4-oxadiazol-3-yl)biphenyl-4-yl]carbonyl]-2,3,6,7-tetrahydrospiro[furo[2,3-f]indole-3,4'-piperidine hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	$C_{32}H_{32}N_4O_3 \cdot HCl \cdot \frac{1}{2}H_2O$
<b>Batch Molecular Weight:</b>	566.1
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 10 mM with gentle warming
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>TLC:</b>	$R_f = 0.51$ (Dichloromethane:Methanol [4:1])
<b>HPLC:</b>	Shows >98.1% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	67.89	6.05	9.9
Found	67.8	6.12	9.93

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**Description:**

Selective 5-HT<sub>1B</sub> receptor antagonist (pK<sub>i</sub> = 8.2). Displays > 60-fold selectivity over 5-HT<sub>1D</sub>, 5-HT<sub>1A</sub>, 5-HT<sub>1E</sub>, 5-HT<sub>1F</sub>, 5-HT<sub>2A</sub> and 5-HT<sub>2C</sub> receptors in radioligand binding and functional assays. Centrally active following oral administration in vivo.

**Physical and Chemical Properties:**

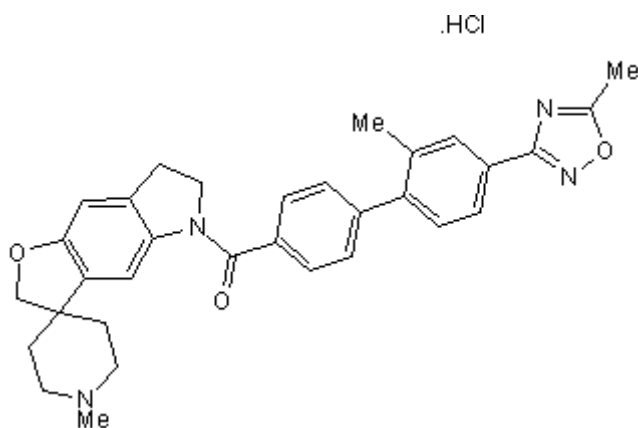
Batch Molecular Formula: C<sub>32</sub>H<sub>32</sub>N<sub>4</sub>O<sub>3</sub>.HCl.½H<sub>2</sub>O

Batch Molecular Weight: 566.1

Physical Appearance: White solid

**Minimum Purity:** >95%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 10 mM with gentle warming

**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:**

**Gaster et al (1998)** The selective 5-HT<sub>1B</sub> receptor inverse agonist 1'-methyl-5-[[[2'-methyl-4'-(5-methyl-1,2,4-oxadiazol-3-yl)biphenyl-4-yl]carbonyl]-2,3,6,7-tetrahydrospiro[furo[2,3-f]indole-3,4'-piperidine (SB-224289) potently blocks terminal 5-HT autoreceptor function both *in vitro* and *in vivo*. *J.Med.Chem.* **41** 1218. PMID: 9548813.

**Roberts et al (1998)** Differential effects of 5-HT<sub>1B/1D</sub> receptor antagonists in dorsal and median raphe innervated brain regions. *Eur.J.Pharmacol.* **346** 175. PMID: 9652357.

**Selkirk et al (1998)** SB-224289 - a novel selective (human) 5-HT<sub>1B</sub> receptor antagonist with negative intrinsic activity. *Br.J.Pharmacol.* **125** 202. PMID: 9776361.

**Hagan et al (1997)** Stimulation of 5-HT<sub>1B</sub> receptors causes hypothermia in the guinea-pig. *Eur.J.Pharmacol.* **331** 169. PMID: 9274976.

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