

## Certificate of Analysis

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**Product Name:** RS 102221 hydrochloride

**Catalog No.:** 1050

**Batch No.:** 10

**CAS Number:** 187397-18-8

**IUPAC Name:** 8-[5-(2,4-Dimethoxy-5-(4-trifluoromethylphenylsulphonamido)phenyl-5-oxopentyl]-1,3,8-triazaspiro[4.5]decane-2,4-dione hydrochloride

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:**  $C_{27}H_{31}F_3N_4O_7S \cdot HCl \cdot H_2O$

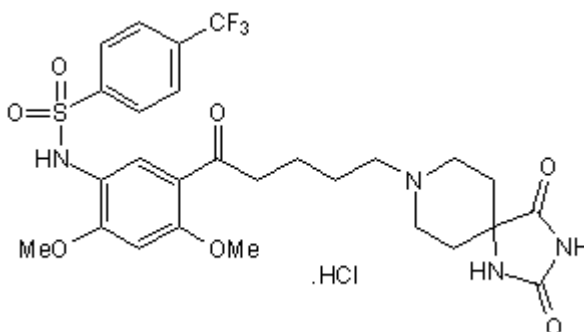
**Batch Molecular Weight:** 667.1

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at RT

**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.32$  (Dichloromethane:Methanol [9:1])

**HPLC:** Shows >98.4% purity

**$^1H$  NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

Carbon Hydrogen Nitrogen

|             |       |      |      |
|-------------|-------|------|------|
| Theoretical | 48.61 | 5.14 | 8.4  |
| Found       | 48.32 | 5    | 8.19 |

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

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**Description:**

Potent and selective 5-HT<sub>2C</sub> antagonist ( $pK_i = 8.7$ ). Displays ~ 100-fold selectivity over the 5-HT<sub>2A</sub> and 5-HT<sub>2B</sub> subtypes and is > 100-fold selective over other 5-HT receptors,  $\alpha$ - and  $\beta$ -adrenergic and muscarinic ACh receptors.

**Physical and Chemical Properties:**

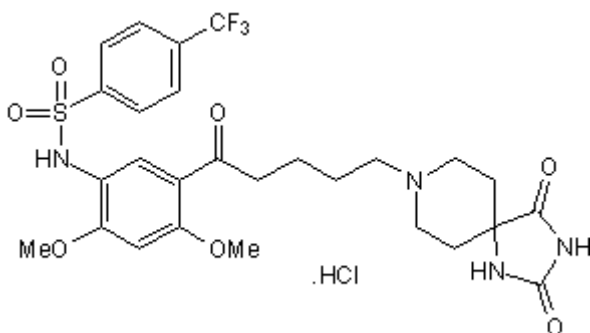
Batch Molecular Formula: C<sub>27</sub>H<sub>31</sub>F<sub>3</sub>N<sub>4</sub>O<sub>7</sub>S.HCl.H<sub>2</sub>O

Batch Molecular Weight: 667.1

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store 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.

**References:**

**Weinhardt et al** (1996) Some benzenesulphonamido-substituted valerophenones that are selective antagonists for the 5-HT<sub>2C</sub> receptor. *Bioorg.Med.Chem.Lett.* **6** 2687.

**Bonhaus et al** (1997) RS-102221: a novel high affinity and selective 5-HT<sub>2C</sub> receptor antagonist. *Neuropharmacology* **36** 621. PMID: 9225287.

**Bonhaus et al** (1998) Absorption and brain penetration of a high affinity, highly selective 5-HT<sub>2C</sub> receptor antagonist, RS-102221. *Ann.N.Y.Acad.Sci.* **861** 269. PMID: 9928284.

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