

Product Name: RS 102221 hydrochloride

Catalog No.: 1050

Batch No.: 14

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: $C_{27}H_{31}F_3N_4O_7S \cdot HCl \cdot \frac{1}{2}H_2O$

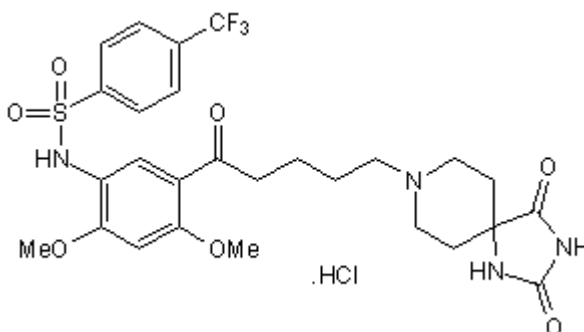
Batch Molecular Weight: 658.09

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.4$ (Dichloromethane:Methanol:Ammonia soln. [90:9:1])

HPLC: Shows 99.1% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	49.28	5.05	8.51
Found	49.15	4.85	8.45

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Description:

Potent and selective 5-HT_{2C} antagonist (pK_i = 8.7). Displays ~ 100-fold selectivity over the 5-HT_{2A} and 5-HT_{2B} subtypes and is > 100-fold selective over other 5-HT receptors, α- and β-adrenergic and muscarinic ACh receptors.

Physical and Chemical Properties:

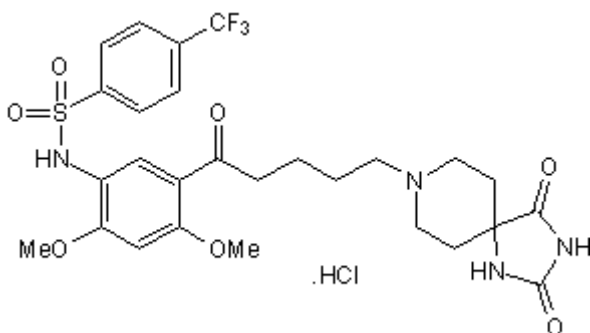
Batch Molecular Formula: C₂₇H₃₁F₃N₄O₇S.HCl.½H₂O

Batch Molecular Weight: 658.09

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_{2C} receptor. *Bioorg.Med.Chem.Lett.* **6** 2687.

Bonhaus et al (1997) RS-102221: a novel high affinity and selective 5-HT_{2C} receptor antagonist. *Neuropharmacology* **36** 621. PMID: 9225287.

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

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