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_{3}N_{4}O_{7}S.HCl.\frac{1}{2}H_{2}O
Batch Molecular Weight: 658.09
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at RT

2. ANALYTICAL DATA

TLC: R_{f} = 0.4 (Dichloromethane:Methanol:Ammonia soln. [90:9:1])
HPLC: Shows 99.1% purity
{^1}H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>49.28</td>
<td>49.15</td>
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<tr>
<td>Hydrogen</td>
<td>5.05</td>
<td>4.85</td>
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<tr>
<td>Nitrogen</td>
<td>8.51</td>
<td>8.45</td>
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</tbody>
</table>
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Description:
Potent and selective 5-HT₂ subtype antagonist (pKᵢ = 8.7). Displays ~100-fold selectivity over the 5-HT₁ subtype 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: C₂₂H₂₃F₃N₂O₇S.HCl.H₂O
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: