Product Name: R-96544 hydrochloride  
Catalog No.: 1742  
Batch No.: 3

CAS Number: 167144-80-1  
IUPAC Name: (2R,4R)-5-[2-[2-[2-(3-Methoxyphenyl)ethyl]phenoxy]ethyl]-1-methyl-3-pyrrolidinol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{22}\text{H}_{29}\text{NO}_{3}\cdot\text{HCl} \)

Batch Molecular Weight: 391.94

Physical Appearance: White solid

Solubility: water to 100 mM  
DMSO to 100 mM

Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.02 \) (Chloroform:Methanol [9:1])

HPLC: Shows >99.5% purity

\(^1\text{H} \) NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = -14.7 \) (Concentration = 1.5, Solvent = Methanol)

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>67.42</td>
<td>67.37</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.71</td>
<td>7.75</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>3.57</td>
<td>3.6</td>
</tr>
</tbody>
</table>

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

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Product Name: R-96544 hydrochloride

CAS Number: 167144-80-1

IUPAC Name: (2R,4R)-5-[2-[2-(3-Methoxyphenyl)ethyl]phenoxy]ethyl]-1-methyl-3-pyrrolidinol hydrochloride

Description:
Potent, selective 5-HT<sub>2</sub> receptor antagonist; displays some selectivity for 5-HT<sub>2A</sub> receptors (K<sub>i</sub> = 1.6 nM). IC<sub>50</sub> values are 2.2, 310, 2400, 3700, > 5000 and > 5000 nM for 5-HT<sub>2A</sub>, α<sub>1</sub>-adrenergic, D<sub>2</sub> dopamine, 5-HT<sub>1</sub>, 5-HT<sub>3</sub> and β-adrenergic receptors respectively. Inhibits 5-HT-induced platelet aggregation and pressor responses in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C<sub>22</sub>H<sub>29</sub>NO<sub>5</sub>.HCl
Batch Molecular Weight: 391.94
Physical Appearance: White solid
Minimum Purity: >99%

Storage: Store at RT

Solubility & Usage Info:
water to 100 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.

References: