Product Name: (S)-WAY 100135 dihydrochloride
Catalog No.: 1253
Batch No.: 6
CAS Number: 149007-54-5
IUPAC Name: (S)-N-tert-Butyl-3-(4-(2-methoxyphenyl)-piperazin-1-yl)-2-phenylpropanamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{24}H_{33}N_{3}O_{2}.2HCl.\frac{1}{2}H_{2}O
Batch Molecular Weight: 477.48
Physical Appearance: White solid
Solubility: DMSO to 100 mM
water to 5 mM with gentle warming
water to 10 mM with sonication
Storage: Desiccate at +4°C

2. ANALYTICAL DATA

TLC: R_{f} = 0.3 (Dichloromethane)
HPLC: Shows 99.5% purity
Chiral HPLC: Shows 99.2% purity
^1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [\alpha]_D = -50 (Concentration = 1, Solvent = Methanol)
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>60.37</td>
<td>60.41</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.6</td>
<td>7.43</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>8.8</td>
<td>8.76</td>
</tr>
</tbody>
</table>

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

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Description:
Potent, selective 5-HT_{1A} receptor antagonist (IC_{50} = 15 nM). Selective over 5-HT_{1B}, 1C, 2, α_1, α_2 and D_2 receptors (IC_{50} > 1000 nM). Centrally active on systemic administration.

Physical and Chemical Properties:
Batch Molecular Formula: C_{24}H_{33}N_3O_2·2HCl·½H_2O
Batch Molecular Weight: 477.48
Physical Appearance: White solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at +4°C

Solubility & Usage Info:
DMSO to 100 mM
ewater to 5 mM with gentle warming
water to 10 mM with sonication

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 Wyeth-Ayerst Research, US Patent 4,988,814

References: