Product Name: GR 55562 dihydrochloride
Catalog No.: 1054 Batch No.: 7
CAS Number: 159533-25-2
IUPAC Name: 3-[3-(Dimethylamino)propyl]-4-hydroxy-N-[4-(4-pyridinyl)phenyl]benzamide dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{23}H_{25}N_{3}O_{2}.2HCl.\frac{1}{2}H_{2}O
Batch Molecular Weight: 457.4
Physical Appearance: Pale yellow solid
Solubility: water to 100 mM
Storage: Desiccate at +4°C

2. ANALYTICAL DATA

TLC: R_f = 0.42 (Chloroform:Methanol:Ammonia soln. [85:13.5:1.5])
HPLC: Shows 99.8% purity
^1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>60.4</td>
<td>60.25</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.17</td>
<td>6.29</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>9.19</td>
<td>9.14</td>
</tr>
</tbody>
</table>

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

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CAS Number: 159533-25-2

IUPAC Name: 3-[3-(Dimethylamino)propyl]-4-hydroxy-N-[4-(4-pyridyl)phenyl]benzamide dihydrochloride

Description:
A selective competitive 5-HT_{1B} (5-HT_{1D} silent antagonist with pK_{a} values of 7.3 and 6.3 for human cloned 5-HT_{1B} and 5-HT_{1D} receptors respectively and only weak binding at a number of other 5-HT subtypes.

Physical and Chemical Properties:
Batch Molecular Formula: C_{23}H_{22}N_{3}O_{2}·2HCl·½H_{2}O

Batch Molecular Weight: 457.4

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Desiccate at +4°C

Solubility & Usage Info:
water 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:
