Product Name: Zatebradine hydrochloride
Catalog No.: 2202
Batch No.: 1
CAS Number: 91940-87-3
IUPAC Name: 3-[[2-(3,4-Dimethoxyphenyl)ethyl]methylamino]propyl]-1,3,4,5-tetrahydro-7,8-dimethoxy-2H-3-benzazepin-2-one hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{26}H_{36}N_2O_5\cdot HCl\cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 502.05

Physical Appearance: White solid

Solubility: water to 100 mM

Storage: Desiccate at +4°C

2. ANALYTICAL DATA

TLC: $R_f = 0.28$ (Dichloromethane:Methanol [4:1])

Melting Point: Between 186 - 188°C

HPLC: Shows 98.5% purity

$^1$H NMR: Consistent with structure

$^{13}$C 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>62.2</td>
<td>61.9</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.63</td>
<td>7.52</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>5.58</td>
<td>5.54</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Description:
Bradycardic agent that produces use-dependent inhibition of hyperpolarization-activated current $I_h$ (HCN channel) in sinoatrial node cells ($EC_{50} = 480$ nM) and Purkinje fibres. Displays negative chronotropic activity in isolated guinea pig atria ($EC_{50}$ of 13.4 μM).

Physical and Chemical Properties:
Batch Molecular Formula: $C_{26}H_{32}N_2O_6 \cdot HCl$.½$H_2O$
Batch Molecular Weight: 502.05
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Desiccate at +4°C. This product is packaged under an inert atmosphere.

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:
