Product Name: Zatebradine hydrochloride
Catalog No.: 2202
Batch No.: 1

CAS Number: 91940-87-3
IUPAC Name: 3-[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: \( \text{C}_{26}\text{H}_{36}\text{N}_{2}\text{O}_{5}\cdot \text{HCl}\cdot \frac{1}{2}\text{H}_{2}\text{O} \)
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 98.2% purity
\(^1\text{H NMR}: \) Consistent with structure
\(^{13}\text{C NMR}: \) Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
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<td>Theoretical</td>
<td>62.2</td>
<td>7.63</td>
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<tr>
<td>Found</td>
<td>61.9</td>
<td>7.52</td>
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</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
Zatebradine hydrochloride is a bradycardic agent that produces use-dependent inhibition of hyperpolarization-activated current I\(_{\text{HCN}}\) (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\(_{36}\)N\(_2\)O\(_5\).HCl.½H\(_2\)O
Batch Molecular Weight: 502.05
Physical Appearance: White solid
Minimum Purity: ≥98%

Batch Molecular Structure:

![Molecular Structure](image)

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: