<table>
<thead>
<tr>
<th><strong>Product Name:</strong> Astemizole</th>
<th><strong>Catalog No.:</strong> 3489</th>
<th><strong>Batch No.:</strong> 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>CAS Number: 68844-77-9</td>
<td>EC Number: 272-441-9</td>
<td></td>
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<tr>
<td>IUPAC Name: 1-[(4-Fluorophenyl)methyl]-N-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinyl]-1H-benzimidazol-2-amine</td>
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</tbody>
</table>

### 1. PHYSICAL AND CHEMICAL PROPERTIES

- **Batch Molecular Formula:** $\text{C}_{28}\text{H}_{31}\text{FN}_{4}\text{O}$
- **Batch Molecular Weight:** 458.57
- **Physical Appearance:** White solid
- **Solubility:** DMSO to 100 mM, ethanol to 25 mM
- **Storage:** Store at +4°C
- **Batch Molecular Structure:**

![Molecular Structure Image](image)

### 2. ANALYTICAL DATA

- **TLC:** $R_f = 0.6$ (Chloroform:Methanol [9:1])
- **HPLC:** Shows >99.6% purity
- **$^1$H NMR:** Consistent with structure
- **Mass Spectrum:** Consistent with structure
- **Microanalysis:**
  
<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
<td>73.34</td>
<td>73.42</td>
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<tr>
<td>Hydrogen</td>
<td>6.81</td>
<td>6.75</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.22</td>
<td>12.23</td>
</tr>
</tbody>
</table>

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

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### Description:
Orally active, potent histamine H₁ antagonist (IC₅₀ = 4 nM) that displays 20-fold, > 250-fold and > 250-fold selectivity over 5-HT, dopamine and muscarinic acetylcholine receptors respectively. Exhibits antimalarial activity in multidrug resistant strains in vitro (IC₅₀ = 227 - 734 nM). Also potent Kᵢ11.1 (hERG) channel blocker (IC₅₀ = 0.9 nM) that displays cardiotoxicity in vivo.

### Physical and Chemical Properties:
- **Batch Molecular Formula:** C₂₁H₂₀FN₂O
- **Batch Molecular Weight:** 458.57
- **Physical Appearance:** White solid
- **Minimum Purity:** >99%
- **Storage:** Store at +4°C
- **Solubility & Usage Info:**
  - DMSO to 100 mM
  - Ethanol to 25 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.

### Batch Molecular Structure:
![Molecular Structure](image)

### References: