

## Certificate of Analysis

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**Product Name:** Astemizole

**Catalog No.:** 3489

**Batch No.:** 4

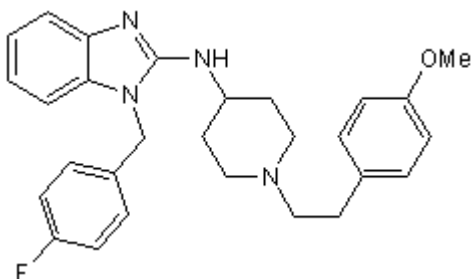
CAS Number: 68844-77-9

EC Number: 272-441-9

IUPAC Name: 1-[(4-Fluorophenyl)methyl]-N-[1-[2-(4-methoxyphenyl)ethyl]-4-piperidiny]-1H-benzimidazol-2-amine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>28</sub>H<sub>31</sub>FN<sub>4</sub>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:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.6 (Chloroform:Methanol [9:1])  
**HPLC:** Shows >99.6% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	73.34	6.81	12.22
Found	73.42	6.75	12.23

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

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**Description:**

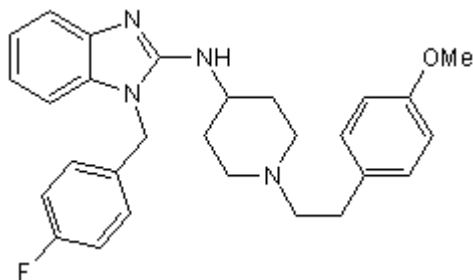
Orally active, potent histamine H<sub>1</sub> antagonist (IC<sub>50</sub> = 4 nM) that displays 20-fold, > 250-fold and > 250-fold selectivity over 5-HT, dopamine and muscarinic acetylcholine receptors respectively. Exhibits antimalarial activity in multidrug resistant strains in vitro (IC<sub>50</sub> = 227 - 734 nM). Also potent K<sub>v</sub>11.1 (hERG) channel blocker (IC<sub>50</sub> = 0.9 nM) that displays cardiotoxicity in vivo.

**Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>28</sub>H<sub>31</sub>FN<sub>4</sub>O  
 Batch Molecular Weight: 458.57  
 Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**References:**

**Chong et al** (2006) A clinical drug library screen identifies astemizole as an antimalarial agent. *Nat.Chem.Biol.* **2** 415. PMID: 16816845.  
**Cavalli et al** (2002) Towards a pharmacophore for drugs inducing the long QT syndrome: Insights from a CoMFA study of hERG K<sup>+</sup> channel blockers. *J.Med.Chem.* **45** 3844. PMID: 12190308.  
**Laduron et al** (1981) *In vitro* and *in vivo* binding characteristics of a new long-acting histamine H<sub>1</sub> antagonist, astemizole. *Mol.Pharmacol.* **21** 294.

**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.

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