Print Date: Aug 30th 2012

Certificate of Analysis

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Product Name: Astemizole **Catalog No.: 3489** **Batch No.: 2**

CAS Number: 68844-77-9 EC Number: 272-441-9

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{31}FN_4O$

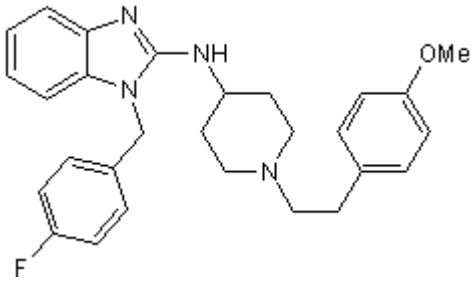
Batch Molecular Weight: 458.57

Physical Appearance: white solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	73.33	6.81	12.22
Found	73.28	6.73	12.26

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Description:

Orally active, potent histamine H_1 antagonist (IC_{50} = 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_{50} = 227 - 734 nM). Also potent K_V11.1 (hERG) channel blocker (IC_{50} = 0.9 nM) that displays cardiotoxicity in vivo.

Physical and Chemical Properties:

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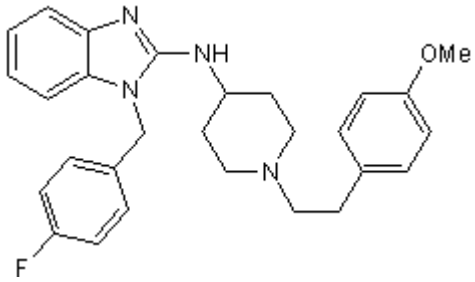
Batch Molecular Weight: 458.57

Physical Appearance: white solid

Minimum Purity: >99%

Batch Molecular Structure:



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.

References:

Laduron *et al* (1981) *In vitro* and *in vivo* binding characteristics of a new long-acting histamine H_1 antagonist, astemizole. Mol.Pharmacol. ***21*** 294.

Cavalli *et al* (2002) Towards a pharmacophore for drugs inducing the long QT syndrome: Insights from a CoMFA study of hERG K^+ channel blockers. J.Med.Chem. ***45*** 3844. PMID: 12190308.

Chong *et al* (2006) A clinical drug library screen identifies astemizole as an antimalarial agent. Nat.Chem.Biol. ***2*** 415. PMID: 16816845.