

Product Name: Terfenadine

Catalog No.: 3948

Batch No.: 1

CAS Number: 50679-08-8

EC Number: 256-710-8

IUPAC Name: α -[4-(1,1-Dimethylethyl)phenyl]-4-(hydroxydiphenylmethyl)-1-piperidinebutanol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{32}H_{41}NO_2 \cdot \frac{1}{4}H_2O$

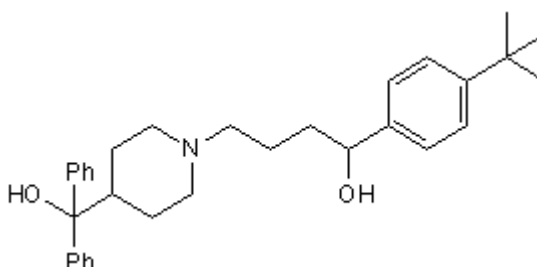
Batch Molecular Weight: 476.17

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 98.7% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	80.72	8.78	2.94
Found	80.99	8.79	3.06

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

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 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

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Product Name: Terfenadine

Catalog No.: 3948 **Batch No.:** 1

CAS Number: 50679-08-8

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IUPAC Name: α -[4-(1,1-Dimethylethyl)phenyl]-4-(hydroxydiphenylmethyl)-1-piperidinebutanol

Description:

Histamine H₁ receptor antagonist. Also blocks K_v11.1 (hERG) and K_{ir}6 (K_{ATP}) channels (IC₅₀ values are 204 nM and 1.2 μ M respectively). Inhibits the delayed rectifier K⁺ current (I_{Kr}) in guinea pig ventricular myocytes (IC₅₀ = 50 nM). Activity prolongs QT and induces Torsades de pointes (TdP); cardiotoxic in vivo.

Physical and Chemical Properties:

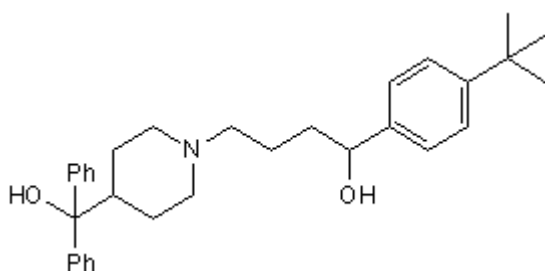
Batch Molecular Formula: C₃₂H₄₁NO₂ · ¼H₂O

Batch Molecular Weight: 476.17

Physical Appearance: white solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Crumb (2000) Loratadine blockade of K⁺ channels in human heart: comparison with terfenadine under physiological conditions. *J.Pharmacol.Exp.Ther.* **292** 261. PMID: 10604956.

Zunkler et al (2000) Mechanism of terfenadine block of ATP-sensitive K⁺ channels. *Br.J.Pharmacol.* **130** 1571. PMID: 10928959.

Stork et al (2007) State dependent dissociation of HERG channel inhibitors. *Br.J.Pharmacol.* **151** 136.

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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