

Certificate of Analysis

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Product Name: Quetiapine hemifumarate

Catalog No.: 4735

Batch No.: 1

CAS Number: 111974-72-2

IUPAC Name: 2-[2-(4-Dibenzo[*b,f*][1,4]thiazepin-11-yl-1-piperazinyl)ethoxy]ethanol hemifumarate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{25}N_3O_2S \cdot 0.5C_4H_4O_4$

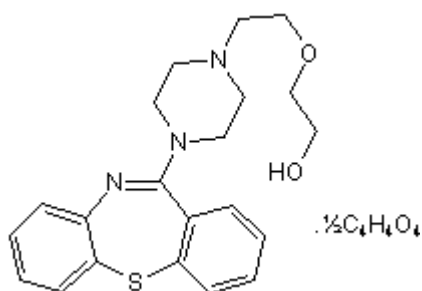
Batch Molecular Weight: 441.54

Physical Appearance: White solid

Solubility: DMSO to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

Melting Point: Between 173 - 175°C

HPLC: Shows 99.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.57	6.16	9.52
Found	62.81	6.19	9.61

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

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Description:

Atypical antipsychotic. Displays antagonist activity at serotonin (5-HT₂) and dopamine (D₂) receptors (IC₅₀ values are 148 and 329 nM respectively). Lacks affinity at either D₁ or muscarinic receptors.

Physical and Chemical Properties:

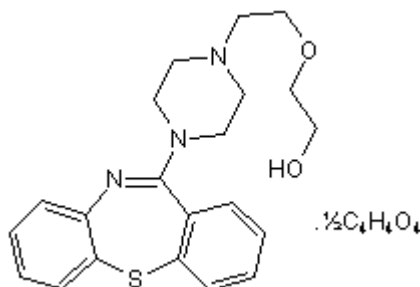
Batch Molecular Formula: C₂₁H₂₅N₃O₂S.0.5C₄H₄O₄

Batch Molecular Weight: 441.54

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 50 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:

Saller and Salama (1993) Seroquel: biochemical profile of a potential atypical antipsychotic. *Psychopharmacology (Berl.)* **112** 285. PMID: 7871032.

Ellenbroek et al (1996) Activity of "seroquel" (ICI 204,636) in animal models for atypical properties of antipsychotics: a comparison with clozapine. *Neuropsychopharmacology* **15** 406. PMID: 8887995.

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