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_{3}O_{2}S.0.5C_{4}H_{4}O_{4}
Batch Molecular Weight: 441.54
Physical Appearance: White solid
Solubility: DMSO to 50 mM
Storage: Store at +4°C
Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

Melting Point: Between 173 - 175°C
HPLC: Shows 99.9% purity
^{1}H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>62.57</td>
<td>62.81</td>
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<tr>
<td>Hydrogen</td>
<td>6.16</td>
<td>6.19</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>9.52</td>
<td>9.61</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
A typical 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: C₂₁H₂₂N₆O₇S.0.5C₄H₉O₄
Batch Molecular Weight: 441.54
Physical Appearance: White solid
Minimum Purity: >99%

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: