Product Name: JNJ 10181457 dihydrochloride
Catalog No.: 4019 Batch No.: 1
CAS Number: 544707-20-2
IUPAC Name: 4-[3-[4-[Piperidinyl]but-1-ynyl]benzyl]morpholine dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{20}H_{28}N_{2}O.2HCl.\frac{1}{2}H_{2}O
Batch Molecular Weight: 394.38
Physical Appearance: Tan solid
Solubility: water to 100 mM, ethanol to 25 mM
Storage: Desiccate at RT

2. ANALYTICAL DATA

TLC: R_f = 0.38 (Chloroform:Methanol [9:1])
HPLC: Shows 98.9% purity
^1H 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>60.91</td>
<td>61.01</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.92</td>
<td>7.76</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7.10</td>
<td>7.15</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
Histamine H3 receptor antagonist (pK values are 8.15 and 8.93 for rat and human H3 receptors respectively). Increases extracellular norepinephrine and acetylcholine levels in rat frontal cortex but does not stimulate dopamine release. Brain penetrant.

Physical and Chemical Properties:
Batch Molecular Formula: C20H26N2O.2HCl.½H2O
Batch Molecular Weight: 394.38
Physical Appearance: Tan solid
Minimum Purity: >98%

Storage: Desiccate at RT

Solubility & Usage Info:
- Water to 100 mM
- Ethanol to 25 mM

USE WITH CARE; NOT FULLY TESTED - YOUR SUBLICENSE UNDER CERTAIN PATENT RIGHTS OF ORTHO-MCNEIL-JANSSEN PHARMACEUTICAL, INC. RESTRICTS USE TO INTERNAL RESEARCH ONLY - MAY NOT BE USED IN HUMANS - MAY NOT BE SOLD, TRANSFERRED, OR USED IN COMMERCIAL SERVICES

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:

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