Product Name: SB 222200
Catalog No.: 1393
Batch No.: 2

CAS Number: 174635-69-9
IUPAC Name: 3-Methyl-2-phenyl-N-[(1S)-1-phenylpropyl]-4-quinolinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

- Batch Molecular Formula: C_{26}H_{24}N_{2}O
- Batch Molecular Weight: 380.48
- Physical Appearance: White solid
- Solubility: DMSO to 100 mM, ethanol to 100 mM
- Storage: Store at RT

2. ANALYTICAL DATA

- TLC: R_f = 0.64 (Ethyl acetate:Petroleum ether [1:2])
- Melting Point: Between 154 - 157°C
- HPLC: Shows >98.5% purity
- ^1H NMR: Consistent with structure
- Optical Rotation: [\alpha]_D = -37 (Concentration = 10, Solvent = methanol)
- Microanalysis:

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>82.08</td>
<td>6.36</td>
</tr>
<tr>
<td>Found</td>
<td>82.13</td>
<td>6.32</td>
</tr>
</tbody>
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<td><strong>Description:</strong></td>
<td>Potent and selective non-peptide NK₃ receptor antagonist (Kᵢ values are 4.4, &gt; 100,000 and 250 nM for human NK₃, NK₁ and NK₂ receptors respectively). Antihypertensive in vivo. Brain penetrant.</td>
</tr>
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**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₂₀H₂₂N₂O  
- **Batch Molecular Weight:** 380.48  
- **Physical Appearance:** White solid  
- **Minimum Purity:** >98%  

**Storage:** Store at RT

**Solubility & Usage Info:**
- DMSO to 100 mM  
- Ethanol to 100 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:**