Product Name: JNJ 16259685
Catalog No.: 2333
Batch No.: 4
CAS Number: 409345-29-5
IUPAC Name: (3,4-Dihydro-2H-pyrano[2,3-b]quinolin-7-yl)-(cis-4-methoxycyclohexyl)-methanone

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{20}H_{23}NO_{3}
Batch Molecular Weight: 325.41
Physical Appearance: White solid
Solubility: ethanol to 100 mM
DMSO to 25 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.14 \) (Ethyl acetate:Petroleum ether [1:1])
HPLC: Shows 99.9% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>73.82</td>
<td>73.71</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.12</td>
<td>7.14</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>4.3</td>
<td>4.34</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Description:
Sub-nanomolar potent, non-competitive mGlu1 antagonist (Kᵢ = 0.34 nM). Inhibits glutamate-induced Ca²⁺ response at the human mGlu1 receptor with an IC₅₀ value of 0.55 nM. Selective over mGlu₂, mGlu₃, mGlu₄, mGlu₆, AMPA or NMDA receptors (IC₅₀ > 10 μM). Centrally active following systemic administration.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₀H₂₃NO₃
Batch Molecular Weight: 325.41
Physical Appearance: White solid
Minimum Purity: >98%

Storage:
Store at +4°C

Solubility & Usage Info:
ethanol to 100 mM
DMSO 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.

References: