1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{24}\text{H}_{37}\text{N}_{3}\text{O}_{2} \)

Batch Molecular Weight: 399.57

Physical Appearance: White solid

Solubility: DMSO to 50 mM, ethanol to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 100% purity

\(^1\text{H NMR:}\) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>72.14</td>
<td>9.33</td>
<td>10.52</td>
</tr>
<tr>
<td>Found</td>
<td>72.32</td>
<td>9.41</td>
<td>10.53</td>
</tr>
</tbody>
</table>
**Product Information**

**Product Name:** (±)-J 113397  
**Catalog No.:** 2598  
**Batch No.:** 6

**CAS Number:** 217461-40-0  
**IUPAC Name:** (±)-1-{(3R*, 4R*)-1-(Cyclooctylmethyl)-3-(hydroxymethyl)-4-piperidinyl}-3-ethyl-1,3-dihydro-2H-benzimidazol-2-one

**Description:** Potent and selective NOP receptor antagonist (IC₅₀ values are 2.3, 1400, 2200 and > 10000 nM for NOP, κ, μ and δ-opioid receptors respectively). Inhibits nociceptin/orphanin FQ-induced hyperalgesia in the mouse tail-flick test.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₂₄H₃₁N₅O₂  
- **Batch Molecular Weight:** 399.57  
- **Physical Appearance:** White solid  
- **Minimum Purity:** >98%

**Storage:** Desiccate at RT

**Solubility & Usage Info:**
- DMSO to 50 mM  
- ethanol 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:**