

**Product Name:** (±)-J 113397

**Catalog No.:** 2598

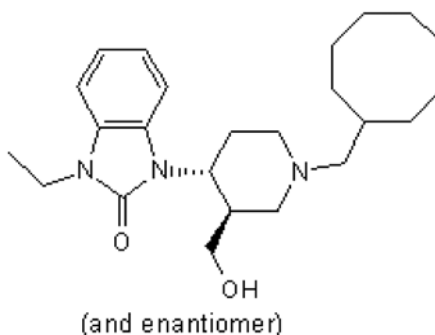
**Batch No.:** 6

**CAS Number:** 217461-40-0

**IUPAC Name:** (±)-1-[(3*R*\*,4*R*\*)-1-(Cyclooctylmethyl)-3-(hydroxymethyl)-4-piperidinyl]-3-ethyl-1,3-dihydro-2*H*-benzimidazol-2-one

## 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>24</sub> H <sub>37</sub> N <sub>3</sub> O <sub>2</sub>
<b>Batch Molecular Weight:</b>	399.57
<b>Physical Appearance:</b>	White solid
<b>Solubility:</b>	DMSO to 50 mM ethanol to 50 mM
<b>Storage:</b>	Desiccate at RT
<b>Batch Molecular Structure:</b>	



## 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 100% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	

	Carbon	Hydrogen	Nitrogen
Theoretical	72.14	9.33	10.52
Found	72.32	9.41	10.53

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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**Description:**

Potent and selective NOP receptor antagonist (IC<sub>50</sub> 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:**

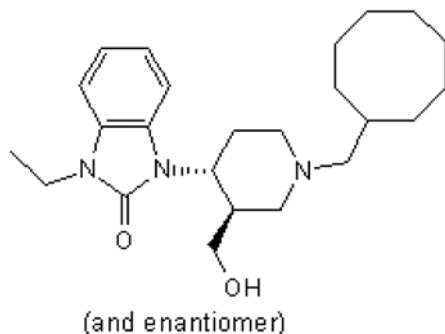
Batch Molecular Formula: C<sub>24</sub>H<sub>37</sub>N<sub>3</sub>O<sub>2</sub>

Batch Molecular Weight: 399.57

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**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:**

**Marti et al** (2007) The nociceptin/orphanin FQ receptor antagonist J-113397 and L-DOPA additively attenuate experimental Parkinsonism through overinhibition of nigrothalamic pathway. *J.Neurosci.* **27** 1297. PMID: 17287504.

**Ozaki et al** (2000) In vitro and in vivo pharmacological characterization of J-113397, a potent and selective non-peptidyl ORL1 receptor antagonist. *Eur.J.Pharmacol.* **402** 45. PMID: 10940356.

**Kawamoto et al** (1999) Discovery of the first potent and selective small molecule opioid receptor-like (ORL1) antagonist: 1-[(3*R*,4*R*)-1-cyclooctylmethyl-3-hydroxymethyl-4-piperidinyl]-3-ethyl-1,3-dihydro-2*H*-benzimidazol-2-one (J-113397). *J.Med.Chem.* **42** 5061. PMID: 10602690.

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