TOCRIS
a bio-techne brand

Print Date: Mar 10th 2022

Certificate of Analysis

www.tocris.com

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

Batch Molecular Formula: $C_{24}H_{37}N_3O_2$

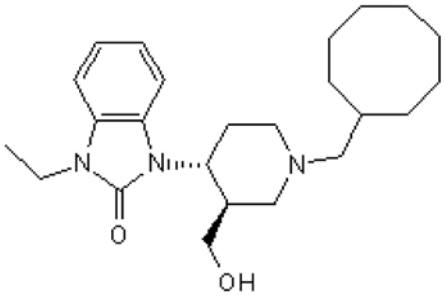
Batch Molecular Weight: 399.57

Physical Appearance: White solid

Solubility: DMSO to 50 mM
ethanol to 50 mM

Storage: Desiccate at RT

Batch Molecular Structure:



(and enantiomer)

2. ANALYTICAL DATA

HPLC: Shows 100% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.14	9.33	10.52
Found	72.32	9.41	10.53

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Product Information

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Description:

(±)-J 113397 is a potent and selective NOP receptor antagonist (IC_{50} 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:

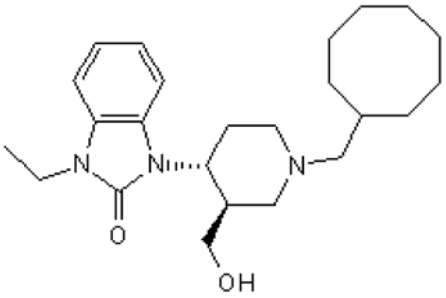
Batch Molecular Formula: $C_{24}H_{37}N_3O_2$

Batch Molecular Weight: 399.57

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



(and enantiomer)

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-piperidyl]-3-ethyl-1,3-dihydro-2*H*-benzimidazol-2-one (J-113397). J.Med.Chem. ***42*** 5061. PMID: 10602690.