

Certificate of Analysis

Print Date: Apr 9th 2020

Batch No.: 5

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Product Name: Clocinnamox mesylate Catalog No.: 0898

CAS Number: 117332-69-1

IUPAC Name: 14β-(p-Chlorocinnamoylamino)-7,8-dihydro-*N*-cyclopropylmethylmorphinone mesylate

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₉H₂₉ClN₂O₄.CH₃SO₃H.H₂O

Batch Molecular Weight: 619.13 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 25 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.5$ (Chloroform:Methanol [9:1])

HPLC: Shows 98.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -1.58$ (Concentration = 1, Solvent = DMSO)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.2 5.7 4.52 Found 58.28 5.72 4.5

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



Product Information

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IUPAC Name: 14β-(p-Chlorocinnamoylamino)-7,8-dihydro-*N*-cyclopropylmethylmorphinone mesylate

Description:

Systemically active, irreversible μ -opioid receptor antagonist (apparent K_i values are 0.7, 1.9 and 5.7 nM for mouse μ , δ and κ receptors respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C₂₉H₂₉CIN₂O₄.CH₃SO₃H.H₂O

Batch Molecular Weight: 619.13 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

HO CH₃SO₃H

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Broadbear *et al* (2000) Methocinnamox is a potent, long-lasting, and selective antagonist of morphine-mediated antinociception in the mouse: comparison with clocinnamox, β -funaltrexamine, and β -chlornaltrexamine. J.Pharmacol.Exp.Ther. **294** 933. PMID: 10945843.

Zernig *et al* (1996) Mechanism of clocinnamox blockade of opioid receptors: evidence from *in vitro* and *ex vivo* binding and behavioural assays. J.Pharmacol.Exp.Ther. **279** 23. PMID: 8858971.

Burke *et al* (1994) Irreversible opioid antagonist effects of clocinnamox on opioid analgesia and mu receptor binding in mice. J.Pharmacol.Exp.Ther. **271** 715. PMID: 7965787.

Aceto *et al* (1989) Very long-acting narcotic antagonists. The 14β-p-substituted cinnamoylaminomorphinones and their partial mu agonist codeinone relatives. Arzneimittelforschung **39** 570. PMID: 2547389.

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