

# **Certificate of Analysis**

Print Date: Apr 9th 2020

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Product Name: (-)-Pentazocine Catalog No.: 5519 Batch No.: 2

CAS Number: 7488-49-5

IUPAC Name: (2R,6R,11R)-1,2,3,4,5,6-Hexahydro-6,11-dimethyl-3-(3-methyl-2-buten-1-yl)-2,6-methano-3-benzazocin-8-ol

#### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C<sub>19</sub>H<sub>27</sub>NO Batch Molecular Weight: 285.42

Physical Appearance: White crystalline solid

Solubility: 1eq. HCl to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.22 (Dichloromethane:Methanol [4:1])

HPLC: Shows >99.4% purity

<sup>1</sup>H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

**Optical Rotation:**  $[\alpha]_D = -118.9$  (Concentration = 0.19, Solvent = Chloroform)



## **Product Information**

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#### **Description:**

κ-opioid agonist. Displays antinociceptive in vivo.

## **Physical and Chemical Properties:**

Batch Molecular Formula: C<sub>19</sub>H<sub>27</sub>NO Batch Molecular Weight: 285.42

Physical Appearance: White crystalline solid

**Minimum Purity**: ≥98%

#### **Batch Molecular Structure:**

Storage: Store at -20°C

#### Solubility & Usage Info:

1eq. HCl to 100 mM DMSO to 100 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.

#### Other Information:

#### INFORMATION FOR CUSTOMERS IN THE UK ONLY

This product is a Schedule 3 Home Office controlled substance and customers in the UK are required to hold the relevant licence or be exempt from restrictions in order to purchase and possess this material.

#### References:

Mori et al (2015) Effects of (+)-pentazocine on the antinociceptive effects of (-)-pentazocine in mice. Synapse 69 166. PMID: 25559075.

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