

**Product Name:** Trap 101

**Catalog No.:** 2508

**Batch No.:** 1

CAS Number: 1216621-00-9

IUPAC Name: 1-[1-(Cyclooctylmethyl)-1,2,3,6-tetrahydro-5-(hydroxymethyl)-4-pyridinyl]-3-ethyl-1,3-dihydro-2H-benzimidazol-2-one hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>24</sub>H<sub>35</sub>N<sub>3</sub>O<sub>2</sub>·HCl·½H<sub>2</sub>O

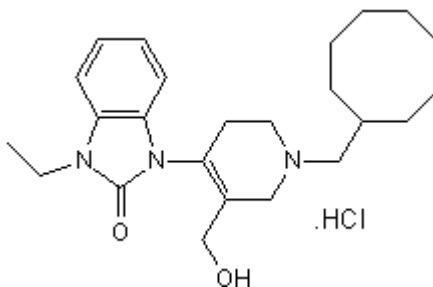
**Batch Molecular Weight:** 443.03

**Physical Appearance:** White solid

**Solubility:** DMSO to 50 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.25 (Ethyl acetate:Petroleum ether [3:7])

**HPLC:** Shows >98.8% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	65.07	8.42	9.48
Found	65.21	8.74	9.1

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**Description:**

Potent and selective nociceptin/orphanin FQ (NOP) receptor antagonist ( $pA_2 = 7.75$ ). Displays selectivity for NOP receptors over classical opioid receptors ( $pK_i$  values are 8.65, 6.60, 6.14 and  $< 5$  for NOP,  $\mu$ -,  $\kappa$ -, and  $\delta$ -opioid receptors respectively). Attenuates motor deficits in a rat model of Parkinson's Disease. Active in vivo.

**Physical and Chemical Properties:**

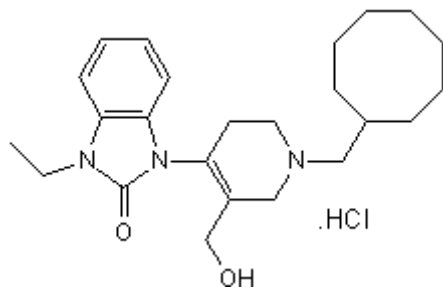
Batch Molecular Formula:  $C_{24}H_{35}N_3O_2 \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 443.03

Physical Appearance: White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO 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:**

**Trapella et al** (2006) Identification of an achiral analogue of J-113397 as potent nociceptin/orphanin FQ receptor antagonist. *Bioorg.Med.Chem.* **14** 692. PMID: 16202610.

**Marti et al** (2008) The novel nociceptin/orphanin FQ receptor antagonist Trap-101 alleviates experimental parkinsonism through inhibition of the nigro-thalamic pathway: positive interaction with  $L$ -DOPA. *J.Neurochem.* **107** 1683. PMID: 19014386.

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