

Certificate of Analysis

Product Name: MCOPPB trihydrochloride

Catalog No.: 3763

Batch No.: 1

CAS Number: 1108147-88-1

IUPAC Name: 1-[1-(1-Methylcyclooctyl)-4-piperidiny]-2-(3*R*)-3-piperidiny-1*H*-benzimidazole trihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₆H₄₀N₄·3HCl·3H₂O

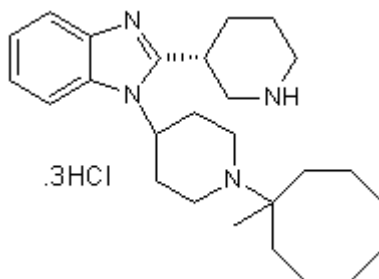
Batch Molecular Weight: 588.1

Physical Appearance: White solid

Solubility: water to 30 mM
DMSO to 60 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	55.14	9.08	9.53
Found	55.01	8.78	9.83

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

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Description:

High affinity NOP receptor agonist ($pK_i = 10.07$ for the human NOP receptor). Exhibits anxiolytic effects with no effect on memory or locomotion. Regarded as one of the most potent, non-peptide NOP full agonists in vitro.

Physical and Chemical Properties:

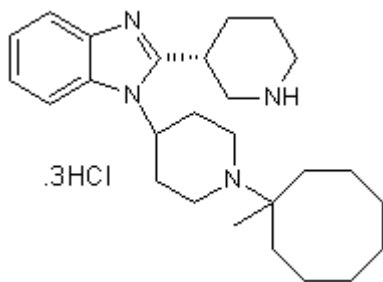
Batch Molecular Formula: $C_{26}H_{40}N_4 \cdot 3HCl \cdot 3H_2O$

Batch Molecular Weight: 588.1

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



References:

Hirao et al (2008) Pharmacological characterization of the newly synthesized nociceptin/orphanin FQ-receptor agonist 1-[1-(1-methylcyclooctyl)-4-piperidiny]-2-[(3*R*)-3-piperidiny]-1*H*-benzimidazole as an anxiolytic agent. *J.Pharmacol.Sci.* **106** 361. PMID: 18319566.

Hayashi et al (2009) Novel non-peptide nociceptin/orphanin FQ receptor agonist, 1-[1-(1-Methylcyclooctyl)-4-piperidiny]-2-[(3*R*)-3-piperidiny]-1*H*-benzimidazole: design, synthesis, and structure-activity relationship of oral receptor occupancy in the brain for orally potent antianxiety drug. *J.Med.Chem.* **52** 610. PMID: 19125610.

Storage: Store at -20°C

Solubility & Usage Info:

water to 30 mM
DMSO to 60 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.

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