

## Certificate of Analysis

**Product Name:** PNU 109291

**Catalog No.:** 2556

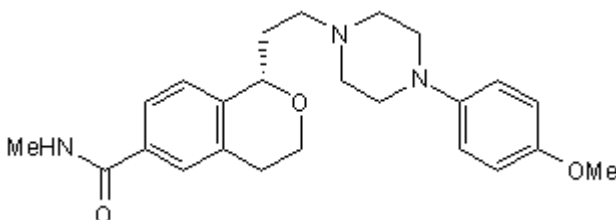
**Batch No.:** 3

CAS Number: 187665-60-7

IUPAC Name: (S)-3,4-Dihydro-1-[2-[4-(4-methoxyphenyl)-1-piperazinyl]ethyl]-N-methyl-1H-2-benzopyran-6-carboxamide

### 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>24</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>  
**Batch Molecular Weight:** 409.52  
**Physical Appearance:** Off-white solid  
**Solubility:** DMSO to 100 mM  
 ethanol to 100 mM  
**Storage:** Store at +4°C  
**Batch Molecular Structure:**



### 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.42 (Chloroform:Methanol [9:1])  
**HPLC:** Shows 98.0% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Optical Rotation:** [α]<sub>D</sub> = -66 (Concentration = 0.49, Solvent = Methanol:Dichloromethane (1:1))  
**Microanalysis:**

|             | Carbon | Hydrogen | Nitrogen |
|-------------|--------|----------|----------|
| Theoretical | 70.39  | 7.63     | 10.26    |
| Found       | 70.06  | 7.59     | 9.9      |

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**Description:**

Potent and selective 5-HT<sub>1D</sub> receptor agonist that displays > 600-fold selectivity over 5-HT<sub>1A</sub> and 5-HT<sub>2A</sub> receptors and no activity at 5-HT<sub>1B</sub>, 5-HT<sub>1E</sub>, 5-HT<sub>2B</sub>, 5-HT<sub>2C</sub>, 5-HT<sub>6</sub> and 5-HT<sub>7</sub> receptors. Reduces dural plasma extravasation evoked by trigeminal ganglion stimulation.

**Physical and Chemical Properties:**

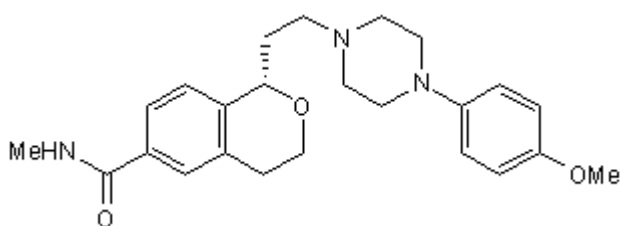
Batch Molecular Formula: C<sub>24</sub>H<sub>31</sub>N<sub>3</sub>O<sub>3</sub>

Batch Molecular Weight: 409.52

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 100 mM  
ethanol 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.

**References:**

**Ennis et al (1998)** Isochroman-6-carboxamides as highly selective 5-HT<sub>1D</sub> agonists: potential new treatment for migraine without cardiovascular side effects. *J.Med.Chem.* **41** 2180. PMID: 9632349.

**Cutrer et al (1999)** Effects of PNU-109,291, a selective 5-HT<sub>1D</sub> receptor agonist, on electrically induced dural plasma extravasation and capsaicin-evoked c-fos immunoreactivity within trigeminal nucleus caudalis. *Neuropharmacology* **38** 1043. PMID: 10428423.

**Bhattacharya et al (2004)** 5-Hydroxytryptamine<sub>1B</sub> receptor-mediated contraction of rabbit saphenous vein and basilar artery: role of vascular endothelium. *J.Pharmacol.Exp.Ther.* **309** 825. PMID: 14724223.

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**bio-techne.com**

info@bio-techne.com

techsupport@bio-techne.com

**North America**

Tel: (800) 343 7475

**China**

info.cn@bio-techne.com

Tel: +86 (21) 52380373

**Europe Middle East Africa**

Tel: +44 (0)1235 529449

**Rest of World**

www.tocris.com/distributors

Tel: +1 612 379 2956