

Product Name: PNU 142633

Catalog No.: 1985

Batch No.: 2

CAS Number: 187665-65-2

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₃₀N₄O₃·½H₂O

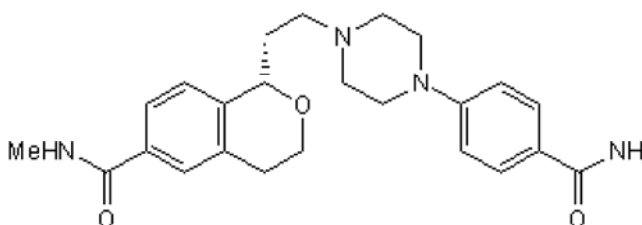
Batch Molecular Weight: 431.54

Physical Appearance: Off White solid

Solubility: DMSO to 100 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.54 (Chloroform:Methanol [8:2])

HPLC: Shows 98.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.8	7.24	12.98
Found	67.1	7.1	12.92

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Description:

Very selective, high affinity 5-HT_{1D} receptor agonist (K_i values are 6 and > 18000 nM at human 5-HT_{1D} and 5-HT_{1B} receptors respectively). Inhibits sympathetically-induced tachycardic responses and blocks neurogenic plasma protein extravasation in vivo.

Physical and Chemical Properties:

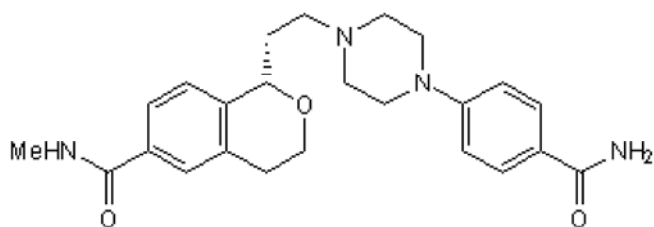
Batch Molecular Formula: C₂₄H₃₀N₄O₃·½H₂O

Batch Molecular Weight: 431.54

Physical Appearance: Off White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

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.

References:

Sanchez-Lopez et al (2003) Pharmacological profile of the 5-HT-induced inhibition of cardioaccelerator sympathetic outflow in pithed rats: correlation with 5-HT₁ and putative 5-HT_{5A/5B} receptors. *Br.J.Pharmacol.* **140** 725. PMID: 14504136.

McCall et al (2002) Preclinical studies characterizing the anti-migraine and cardiovascular effects of the selective 5-HT_{1D} receptor agonist PNU-142633. *Cephalalgia* **22** 799. PMID: 12485205.

Roon et al (1999) Bovine isolated middle cerebral artery contractions to antimigraine drugs. *Naunyn-Schmied.Arch.Pharmacol.* **360** 591.

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