Product Name: PNU 142633  
Catalog No.: 1985  
Batch No.: 2  
CAS Number: 187665-65-2  
IUPAC Name: (1S)-1-[2-[4-[(Aminocarbonyl)phenyl]-1-piperazinyl]ethyl]-3,4-dihydro-N-methyl-1H-2-benzopyran-6-carboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C_{24}H_{30}N_{4}O_{3}\cdot\frac{1}{2}H_{2}O  
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 98.6% purity  
^1H NMR: Consistent with structure  
Mass Spectrum: Consistent with structure  
Microanalysis:  
<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>66.8</td>
<td>67.1</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.24</td>
<td>7.1</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>12.98</td>
<td>12.92</td>
</tr>
</tbody>
</table>

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

**Product Name:** PNU 142633  
**Catalog No.:** 1985  
**Batch No.:** 2

---

**Description:**
Very selective, high affinity 5-HT₁D receptor agonist (Kᵢ values are 6 and > 18000 nM at human 5-HT₁D and 5-HT₁B receptors respectively). Inhibits sympathetically-induced tachycardic responses and blocks neurogenic plasma protein extravasation in vivo.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₂₈H₃₉N₅O₅·½H₂O
- **Batch Molecular Weight:** 431.54
- **Physical Appearance:** Off White solid

**Minimum Purity:** >98%

**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:**