Product Name: PD 168368
Catalog No.: 2603 Batch No.: 1
CAS Number: 204066-82-0
IUPAC Name: \((S)-\alpha\text{-Methyl-}\alpha\text{-[[(4-nitrophenyl)amino]carbonyl]amino}]\text{-N-[[1-(2-pyridinyl)cyclohexyl]methyl]}\text{-1H-indole-3-propanamide}\)

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: \(C_{31}H_{34}N_{6}O_{4}\cdot H_{2}O\)
   Batch Molecular Weight: 572.67
   Physical Appearance: Pale yellow solid
   Solubility: DMSO to 100 mM
   Storage: Store at +4°C

2. ANALYTICAL DATA

   TLC: \(R_f = 0.69\) (Ethyl acetate)
   HPLC: Shows 96.7% purity
   \(^1\)H NMR: Consistent with structure
   Mass Spectrum: Consistent with structure
   Optical Rotation: \([\alpha]_D = +38.4\) (Concentration = 1, Solvent = DMSO)
   Microanalysis:

<table>
<thead>
<tr>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>65.02</td>
<td>6.34</td>
</tr>
<tr>
<td>Found</td>
<td>64.98</td>
<td>5.89</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
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Catalog No.: 2603
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CAS Number: 204066-82-0
IUPAC Name: (S)-α-Methyl-α-[[4-nitrophenyl]amino]carbonyl]amino]-N-[1-(2-pyridinyl)cyclohexyl][methyl]-1H-indole-3-propanamide

Description:
Potent neuromedin B receptor antagonist (NMB-R, BB₁) (IC₅₀ = 40 nM) that displays ~ 40-fold selectivity over the gastrin-releasing peptide receptor (GRP-R, BB₂) and > 300-fold selectivity over BRS-R (bb₂). Antagonizes neuromedin B-stimulated calcium release and inhibits proliferation of rat glioma cells (IC₅₀ = 2 μM).

Physical and Chemical Properties:
Batch Molecular Formula: C₄₇H₄₃N₁₂O₉.H₂O
Batch Molecular Weight: 572.67
Physical Appearance: Pale yellow solid
Minimum Purity: >96%

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: