Product Name: SSR 146977 hydrochloride  
Catalog No.: 3297  
Batch No.: 1  
CAS Number: 264618-38-4  
IUPAC Name: N1-[1-3-[(3R)-1-Benzoyl-3-(3,4-dichlorophenyl)-3-piperidinyl]propyl]-4-phenyl-piperidinyl]-N,N-dimethylurea hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₅H₄₂Cl₂N₄O₂.HCl.2H₂O
Batch Molecular Weight: 694.14
Physical Appearance: Pale yellow solid
Solubility: DMSO to 100 mM, ethanol to 100 mM
Storage: Store at +4°C

2. ANALYTICAL DATA

TLC: Rₛ = 0.5 (Dichloromethane:Ethanol:Ammonia soln. [90:9:1])
HPLC: Shows >98.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]D = +23.6 (Concentration = 1, Solvent = Methanol)

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
<td>60.56</td>
<td>60.52</td>
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<tr>
<td>Hydrogen</td>
<td>6.82</td>
<td>6.31</td>
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<tr>
<td>Nitrogen</td>
<td>8.07</td>
<td>7.94</td>
</tr>
</tbody>
</table>
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**Description:**
Potent and selective NK₃ receptor antagonist (Kᵢ values are 0.26 and 19.3 nM in CHO cells expressing the human NK₃ and NK₂ receptor respectively). Also inhibits senktide-induced inositol monophosphate formation and intracellular calcium mobilization (IC₅₀ = 10 nM).

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C₉₅H₇₀Cl₄N₂O₁₂.HCl.2H₂O
- **Batch Molecular Weight:** 694.14
- **Physical Appearance:** Pale yellow solid
- **Minimum Purity:** >98%

**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:**