1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{26}\text{H}_{42}\text{N}_{4}\text{O}_{5}\text{S}_{2}\text{HCl} \cdot \frac{3}{4}\text{H}_{2}\text{O} \)

Batch Molecular Weight: 604.74

Physical Appearance: White solid

Solubility: water to 100 mM

DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

![Molecular Structure Image]

2. ANALYTICAL DATA

TLC: \( R_{f} = 0.5 \) (Dichloromethane:Methanol [9:1])

HPLC: Shows 98.4% purity

Chiral HPLC: Shows 100% purity

\(^1\text{H} \text{NMR}: \) Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_{D} = +22\) (Concentration = 1, Solvent = Methanol)

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>51.64</td>
<td>51.57</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>7.42</td>
<td>7.29</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>9.26</td>
<td>9.24</td>
</tr>
</tbody>
</table>
Product Information

Product Name: L-368,899 hydrochloride
Catalog No.: 2641
Batch No.: 3

CAS Number: 160312-62-9
IUPAC Name: (2S)-2-Amino-N-[(1S,2S,4R)-7,7-dimethyl-1-[[[4-(2-methylphenyl)-1-piperazinyl]sulfonyl]methyl]bicyclo[2.2.1]hept-2-yl]-4-(methylsulfonyl)butanamide

Description:
Potent, non-peptide and orally active oxytocin receptor antagonist (IC$_{50}$ = 8.9 nM) that displays > 40-fold selectivity over vasopressin V$_{1_a}$ and V$_{2}$ receptors (IC$_{50}$ values are 370 and 570 nM respectively). Antagonizes oxytocin-induced uterine contractions in vitro and in vivo.

Physical and Chemical Properties:
Batch Molecular Formula: C$_{26}$H$_{42}$N$_{4}$O$_{5}$S$_{2}$·HCl·½H$_{2}$O
Batch Molecular Weight: 604.74
Physical Appearance: White solid
Minimum Purity: >97%

Storage: Store at -20°C

Solubility & Usage Info:
- water to 100 mM
- DMSO to 100 mM
When purchased as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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: