1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{32}\text{H}_{40}\text{N}_{8}\text{O}_{2}\text{S}\cdot\text{H}_{2}\text{O} \)

Batch Molecular Weight: 618.8

Physical Appearance: Off White solid

Solubility: 1eq. HCl to 100 mM
            DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: \( R_f = 0.26 \) (Dichloromethane:Methanol [85:15])

HPLC: Shows >97.7% purity

Chiral HPLC: Shows >98.3% purity

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

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = -18.1\) (Concentration = 1, Solvent = Methanol)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>62.11</td>
<td>61.95</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>6.84</td>
<td>6.58</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>18.11</td>
<td>18.02</td>
</tr>
</tbody>
</table>
Product Information

Product Name: TC OT 39  Catalog No.: 4625  Batch No.: 1

CAS Number: 479232-57-0
IUPAC Name: \((2\text{S})_N-[(4,10-\text{Dihydro}-1-\text{methylpyrazolo}[3,4-b][1,5]\text{benzodiazepin}-5(1\text{H})-\text{yl})\text{carbonyl}]-2-\text{methyl}[\text{phenyl}][\text{methyl}]-2-\text{[(hexahydro}-4\text{-methyl}-1\text{H}-1,4-\text{diacepin}-1\text{-yl})\text{thioxomethyl}]-1\text{-pyrrolidinecarboxamide}

Description:
Potent non-peptide oxytocin receptor partial agonist (EC\(_{50}\) values are 33 nM and 850 nM for the oxytocin receptor and V\(_2\) vasopressin receptor respectively). Also a V\(_1\alpha\) vasopressin receptor antagonist (K\(_i\) = 330 nM). Active in vivo in a rat model of uterine response.

Physical and Chemical Properties:
Batch Molecular Formula: C\(_{32}\)H\(_{40}\)N\(_8\)O\(_5\)S\(_2\)H\(_2\)O
Batch Molecular Weight: 618.8
Physical Appearance: Off White solid
Minimum Purity: >97%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:
1eq. HCl to 100 mM
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: