Product Name: TCS OX2 29  
Catalog No.: 3371  
Batch No.: 2  
CAS Number: 372523-75-6  
IUPAC Name: (2S)-1-(3,4-Dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)-3,3-dimethyl-2-[(4-pyridinylmethyl)amino]-1-butanone hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

   Batch Molecular Formula: $C_{23}H_{31}N_3O_3\cdot HCl\cdot 3H_2O$
   Batch Molecular Weight: 488.02
   Physical Appearance: Pale yellow solid
   Solubility:
   - water to 100 mM
   - DMSO to 25 mM
   - ethanol to 5 mM
   Storage: Desiccate at +4°C
   Batch Molecular Structure:

   ![Molecular Structure](image)

2. ANALYTICAL DATA

   HPLC:
   - Shows 98.3% purity
   \(^1\)H NMR:
   - Consistent with structure
   Mass Spectrum:
   - Consistent with structure
   Optical Rotation: $[\alpha]_D = +48$ (Concentration = 1, Solvent = Water)
   Microanalysis:
   
<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon</td>
<td>56.61</td>
<td>56.61</td>
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<tr>
<td>Hydrogen</td>
<td>7.85</td>
<td>7.36</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>8.61</td>
<td>8.65</td>
</tr>
</tbody>
</table>

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

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**Description:**
Potent and selective OX₂ receptor antagonist (IC₅₀ = 40 nM). Displays >250-fold selectivity for OX₂ over OX₁ and a range of receptors, ion channels and transporters. Inhibits orexin A induced IP₃ accumulation and ERK1/2 phosphorylation in CHO cells transfected with the OX₂ receptor.

**Physical and Chemical Properties:**
- Batch Molecular Formula: C₂₃H₂₁N₂O₅.HCl.3H₂O  
- Batch Molecular Weight: 488.02  
- Physical Appearance: Pale yellow solid  
- Minimum Purity: >98%

**Solubility & Usage Info:**
- Water to 100 mM  
- DMSO to 25 mM  
- Ethanol to 5 mM

**Storage:** Desiccate at +4°C

**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:**