1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_8\text{H}_9\text{NO}_4.\frac{1}{2}\text{H}_2\text{O} \)

Batch Molecular Weight: 196.67

Physical Appearance: Off White solid

Solubility:
- Water to 50 mM
- Phosphate buffered saline to 50 mM
- DMSO to 20 mM with gentle warming

Storage: Desiccate at -20°C

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

TLC: \( R_f = 0.36 \) (Pyridine:Acetic acid:Water:Butanol [3:8:11:33])

HPLC: Shows >99% purity

Chiral HPLC: Shows >99% purity

\(^1\)H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = +133.7 \) (Concentration = 1, Solvent = 6N HCl)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>48.86</td>
<td>5.38</td>
<td>7.12</td>
</tr>
<tr>
<td>Found</td>
<td>48.69</td>
<td>5.38</td>
<td>7.12</td>
</tr>
</tbody>
</table>
Description:
Selective group I mGlu receptor agonist. Available as part of the Group I mGlu Receptor Tocriset™ and Mixed mGlu Receptor Tocriset™. Racemate also available.

Physical and Chemical Properties:
Batch Molecular Formula: C6H6NO3.¾H2O
Batch Molecular Weight: 196.67
Physical Appearance: Off White solid

Minimum Purity: >98%

Response Image

Storage: Desiccate at -20°C
CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:
- water to 50 mM
- phosphate buffered saline to 50 mM
- DMSO to 20 mM with gentle warming

Whilst supplied of high purity, this product is very sensitive to air and light promoted oxidation, and may discolour slightly over time. Chemical and pharmacological analysis shows that this discoulouration has no noticeable effect on its properties and can be safely ignored. Further analysis has shown that this product rapidly decomposes when dissolved in alkaline solution. Therefore, as a precautionary measure we recommend that the solid material be stored at -20°C, away from light, under which conditions it should be stable for 6 months from the date of purchase. When made up, stock solutions should be aliquoted, stored at -20°C and used within one week.

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: