Product Name: TASP 0390325

Catalog No.: 5729

Batch No.: 1

CAS Number: 1642187-96-9

IUPAC Name: 2-(3-Chloro-4-fluorophenyl)-N-(1-methylethyl)-6-[3-(4-morpholinyl)propoxy]-4-oxo-pyrido[2,3-d]pyrimidine-3(4H)-acetamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{25}\text{H}_{29}\text{ClF}_{2}\text{N}_{5}\text{O}_{4}\cdot\text{HCl} \cdot \frac{1}{3}\text{H}_{2}\text{O} \)

Batch Molecular Weight: 585.96

Physical Appearance: White solid

Solubility:
- Water to 100 mM
- DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows >99.7% purity

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

Mass Spectrum: Consistent with structure

Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
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<tbody>
<tr>
<td>Carbon</td>
<td>51.24</td>
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<tr>
<td>Hydrogen</td>
<td>5.76</td>
<td>5.63</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>11.95</td>
<td>12.09</td>
</tr>
</tbody>
</table>

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

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Product Name: TASP 0390325

CAS Number: 1642187-96-9
IUPAC Name: 2-(3-Chloro-4-fluorophenyl)-N-(1-methylethyl)-6-[3-(4-morpholinyl)propoxy]-4-oxo-pyrido[2,3-d]pyrimidine-3(4H)-acetamide hydrochloride

Description:
Potent and selective V₁B receptor antagonist (IC₅₀ = 2.22 nM for rat pituitary receptor). Exhibits no significant affinity for 85 other receptors, ion channels and transporters at 10 μM, including V₁A and V₂. Increases ACTH levels in rats. Orally bioavailable. Antidepressant and anxiolytic.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₅H₂₉ClFNN₂O₄.HCl.1½H₂O
Batch Molecular Weight: 585.96
Physical Appearance: White solid
Minimum Purity: >98%

Storage: Store at -20°C

Solubility & Usage Info:
- water 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: