Product Name: L-733,060 hydrochloride
Catalog No.: 1145
Batch No.: 5
CAS Number: 148687-76-7
IUPAC Name: (2S,3S)-3-[[3,5-bis(Trifluoromethyl)phenyl]methoxy]-2-phenylpiperidine hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{20}\text{H}_{19}\text{F}_{6}\text{NO.HCl} \)
Batch Molecular Weight: 439.83
Physical Appearance: White solid
Solubility: water to 50 mM with gentle warming
Storage: Store at RT

2. ANALYTICAL DATA

TLC: \( R_f = 0.44 \) (Chloroform:Methanol [9:1])
HPLC: Shows 100% purity
Chiral HPLC: Shows >99.3% purity
\(^1\)H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: \( [\alpha]_D = +83 \) (Concentration = 1, Solvent = Methanol)
Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>54.62</td>
<td>4.58</td>
<td>3.18</td>
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<tr>
<td>Found</td>
<td>54.74</td>
<td>4.7</td>
<td>3.1</td>
</tr>
</tbody>
</table>
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Description:
Potent NK₁ antagonist (Kᵢ values are 0.08, 0.2 and 93.13 nM for gerbil, human and rat receptors, respectively). Produces anxiolytic-like effects in the gerbil elevated plus-maze. Exhibits antitumor activity in vitro. Also decreases HER2 activity and tumor growth in mice bearing HER2⁺ or EGFR⁺ breast tumors. Orally bioavailable and brain penetrant.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₀H₁₆F₆NO.HCl
Batch Molecular Weight: 439.83
Physical Appearance: White solid
Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at RT

Solubility & Usage Info:
Water to 50 mM with gentle warming.

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: