1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( C_{24}H_{29}Cl_2NO.HCl.\frac{1}{4}H_2O \)

Batch Molecular Weight: 459.36

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Store at -20°C

2. ANALYTICAL DATA

TLC: \( R_f = 0.5 \) (DCM / MeOH / NH4OH (95:5:0.5))

HPLC: Shows 97.9% purity

Chiral HPLC: Shows 99.9% purity

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

Mass Spectrum: Consistent with structure

Optical Rotation: \([\alpha]_D = -42.2\) (Concentration = 1, Solvent = Ethanol)

Microanalysis:

<table>
<thead>
<tr>
<th></th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theoretical</td>
<td>62.75</td>
<td>6.69</td>
<td>3.05</td>
</tr>
<tr>
<td>Found</td>
<td>62.67</td>
<td>6.67</td>
<td>3.22</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: SB 612111 hydrochloride

CAS Number: 371980-94-8

IUPAC Name: 7-[[4-(2,6-Dichlorophenyl)-1-piperidinyl][methyl]-6,7,8,9-tetrahydro-1-methyl-5H-benzocyclohepten-5-ol hydrochloride

Description:
Selective NOP receptor antagonist (Kᵢ values are 0.33, 57.6, 160.5 and 2109 nM for NOP, μ-, κ- and δ-receptors respectively). Antagonizes the pronociceptive action of nociceptin (Cat. No. 0910) in an acute pain model. Potentiates the action of morphine in morphine-tolerant animals and blocks hyperalgesia in an inflammatory pain model.

Physical and Chemical Properties:
Batch Molecular Formula: C₂₃H₂₉Cl₂NO.HCl.½H₂O
Batch Molecular Weight: 459.36
Physical Appearance: White solid
Minimum Purity: >97%

Storage: Store at -20°C

Solubility & Usage Info:
DMSO to 100 mM
Ethanol to 50 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.

Licensing Information:
Sold with the permission of GlaxoSmithKline

References:
