Product Name: BMY 14802 hydrochloride

CAS Number: 105565-55-7

IUPAC Name: α-(4-Fluorophenyl)-4-(5-fluoro-2-pyrimidinyl)-1-piperazinebutanol hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{18}\text{H}_{22}\text{F}_{2}\text{N}_{4}\text{O}.\text{HCl} \)

Batch Molecular Weight: 384.86

Physical Appearance: White solid

Solubility:
- Water to 25 mM
- DMSO to 100 mM
- Ethanol to 10 mM

Storage: Desiccate at RT

Batch Molecular Structure:

![Molecular Structure](image)

2. ANALYTICAL DATA

TLC: \( R_f = 0.73 \) (Chloroform:Methanol:Ammonia soln. [95:5:0.1])

Melting Point: Between 233 - 234°C

HPLC: Shows 98.2% purity

\(^1\text{H} \text{NMR}:\) Consistent with structure

Microanalysis:

<table>
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<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
<th>Carbon</th>
<th>Hydrogen</th>
<th>Nitrogen</th>
<th>Chlorine</th>
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Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: BMY 14802 hydrochloride

CAS Number: 105565-55-7
IUPAC Name: α-(4-Fluorophenyl)-4-(5-fluoro-2-pyrimidinyl)-1-piperazinebutanol hydrochloride

Description:
Potent sigma receptor antagonist (IC₅₀ = 112 nM) with modest to weak affinity for 5-HT₁A and α₁ receptors. Antipsychotic following oral administration and acts via indirect modulation of central dopaminergic systems.

Physical and Chemical Properties:
Batch Molecular Formula: C₁₉H₂₂F₂N₄O.HCl
Batch Molecular Weight: 384.86
Physical Appearance: White solid
Minimum Purity: >98%

Storage:
Desiccate at RT

Solubility & Usage Info:
- water to 25 mM
- DMSO to 100 mM
- ethanol to 10 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:
