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Print Date: Jan 15th 2016

Certificate of Analysis

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Product Name: **BMY 14802 hydrochloride** **Catalog No.: 1440** **Batch No.: 1**

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: $C_{18}H_{22}F_2N_4O.HCl$

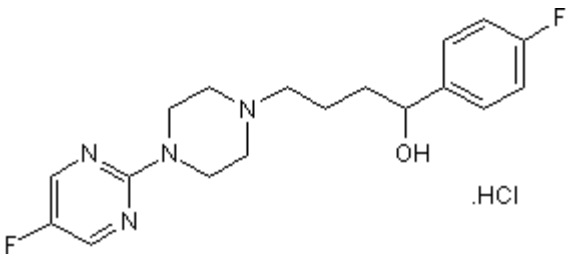
Batch Molecular Weight: 384.86

Physical Appearance: White solid

Solubility: water to 25 mM
DMSO to 100 mM
ethanol to 10 mM

Storage: Desiccate at RT

Batch Molecular Structure:



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}H NMR: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen	Chlorine
Theoretical	56.18	6.02	14.56	9.21
Found	56.05	6.06	14.44	9.31

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Description:

Potent sigma receptor antagonist (IC_{50} = 112 nM) with modest to weak affinity for 5-HT_{1A} and α_1 receptors. Antipsychotic following oral administration and acts via indirect modulation of central dopaminergic systems.

Physical and Chemical Properties:

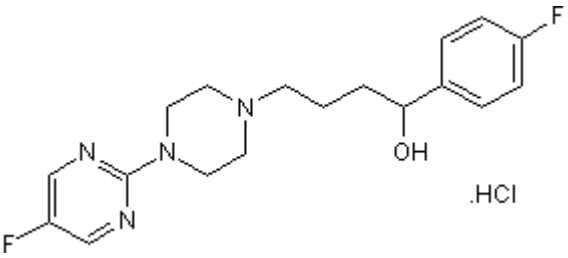
Batch Molecular Formula: $C_{18}H_{22}F_2N_4O.HCl$

Batch Molecular Weight: 384.86

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



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:

Yevich *et al* (1992) Synthesis and biological characterization of α-(4-fluorophenyl)-4-(5-fluoro-2-pyrimidinyl)-1-piperazinebutanol and analogues as potential atypical antipsychotic agents. J.Med.Chem. ***35*** 4516. PMID: 1361578.

Zhang *et al* (1993) Further characterization of the effects of BMY 14802 on dopamine neuronal activity. Synapse ***15*** 276. PMID: 7908761.

Taylor *et al* (1993) A role for sigma binding in the antipsychotic profile of BMY 14802? NIDA Res.Monogr. ***133*** 125. PMID: 8232511.