

Certificate of Analysis

Product Name: EMD 281014 hydrochloride

Catalog No.: 4470

Batch No.: 1

CAS Number: 443144-27-2

IUPAC Name: 7-[[4-[2-(4-Fluorophenyl)ethyl]-1-piperazinyl]carbonyl]-1*H*-indole-3-carbonitrile hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₂H₂₁FN₄O.HCl

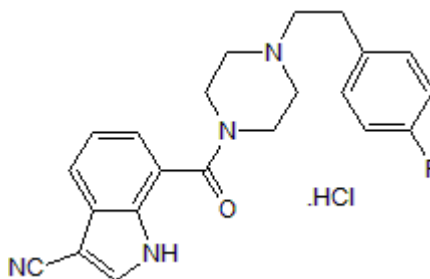
Batch Molecular Weight: 412.89

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Chloroform:Methanol [95:5])

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	64	5.37	13.57
Found	63.67	5.34	13.51

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

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Description:

Selective 5-HT_{2A} antagonist; displays high affinity for human 5-HT_{2A} over 5-HT_{2C} receptors (K_i values are 0.87 and 557 nM respectively). Exhibits low off-target activity (K_i values are >1000 and 1268 nM for human D₂ receptors and IKr channels, respectively).

Physical and Chemical Properties:

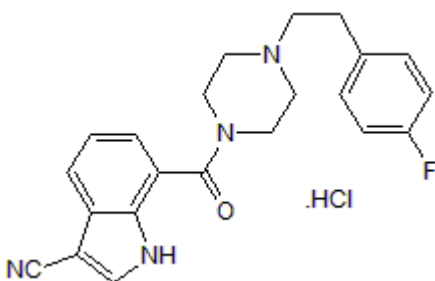
Batch Molecular Formula: C₂₂H₂₁FN₄O.HCl

Batch Molecular Weight: 412.89

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 25 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:

Bartoszyk et al (2003) EMD 281014, a new selective serotonin 5-HT_{2A} receptor antagonist. *Eur.J.Pharmacol.* **473** 229.

Patel et al (2004) The highly selective 5-hydroxytryptamine (5-HT)_{2A} receptor antagonist, EMD 281014, significantly increases swimming and decreases immobility in male congenital learned helpless rats in the forced swim test. *Synapse* **52** 73. PMID: 14755634.

Ladduwahetty et al (2006) A new class of selective, non-basic 5-HT_{2A} receptor antagonists. *Bioorg.Med.Chem.Lett.* **16** 3201. PMID: 16632354.

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