

**Product Name:** PNU 96415E

**Catalog No.:** 2735

**Batch No.:** 2

CAS Number: 170856-41-4

IUPAC Name: 1-[2-(3,4-Dihydro-1*H*-2-benzopyran-1-yl)ethyl]-4-(4-fluorophenyl)piperazine dihydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>21</sub>H<sub>25</sub>FN<sub>2</sub>O.2HCl

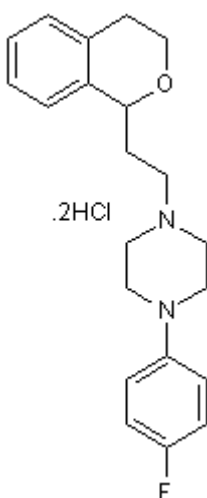
**Batch Molecular Weight:** 413.36

**Physical Appearance:** Off-white solid

**Solubility:** water to 10 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**TLC:** R<sub>f</sub> = 0.5 (Chloroform:Methanol:Ammonia soln. [9:1:3])

**HPLC:** Shows >99.3% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	61.02	6.58	6.78
Found	61.21	6.53	6.72

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**Description:**

Antipsychotic agent. Displays high affinity for dopamine D<sub>4</sub> and serotonergic 5-HT<sub>2A</sub> receptors and relatively weak affinity at D<sub>2</sub> receptors (K<sub>i</sub> values are 3.0, 5.8, 134, 181, 199, 240, 411 and > 678 nM for D<sub>4</sub>, 5-HT<sub>2A</sub>, 5-HT<sub>1A</sub>, α<sub>1</sub>, D<sub>2</sub>, D<sub>3</sub>, D<sub>1</sub>, α<sub>2</sub> and muscarinic receptors respectively). Inhibits exploratory locomotor activity and antagonizes d-amphetamine-induced locomotor stimulation in rats.

**Physical and Chemical Properties:**

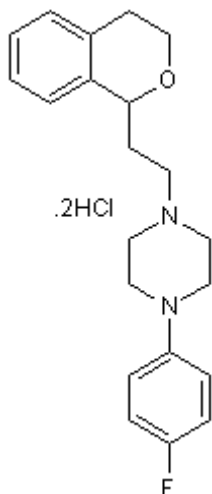
Batch Molecular Formula: C<sub>21</sub>H<sub>25</sub>N<sub>2</sub>O<sub>2</sub>.2HCl

Batch Molecular Weight: 413.36

Physical Appearance: Off-white solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Tang et al** (1997) PNU-96415E, a potential antipsychotic agent with clozapine-like pharmacological properties. *J.Pharmacol.Exp.Ther.* **281** 440. PMID: 9103528.

**Goudie et al** (1998) Discriminative stimulus properties of the atypical neuroleptic clozapine in rats: tests with subtype selective receptor ligands. *Behav.Pharmacol.* **9** 699. PMID: 9890260.

**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water 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.

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