

# Certificate of Analysis

**Product Name:** PNU 177864 hydrochloride

**Catalog No.:** 3355

**Batch No.:** 1

CAS Number: 250266-51-4

IUPAC Name: *N*-[4-[2-(Propylamino)ethyl]phenyl]-4-(trifluoromethoxy)-benzenesulfonamide hydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>18</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>S.HCl

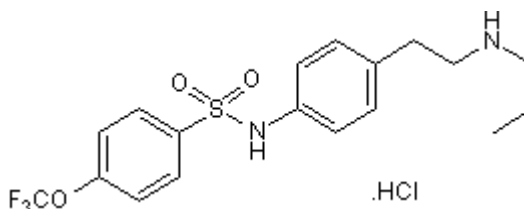
**Batch Molecular Weight:** 438.89

**Physical Appearance:** White solid

**Solubility:** water to 20 mM  
DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.2 (Dichloromethane:Methanol [9:1])

**HPLC:** Shows >99.7% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	49.26	5.05	6.38
Found	49.35	5.1	6.45

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**Description:**

Highly selective dopamine D<sub>3</sub> receptor antagonist. Induces phospholipidosis and exhibits antischizophrenic activity in vivo.

**Physical and Chemical Properties:**

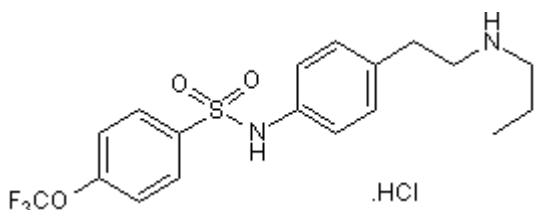
Batch Molecular Formula: C<sub>18</sub>H<sub>21</sub>F<sub>3</sub>N<sub>2</sub>O<sub>3</sub>S.HCl

Batch Molecular Weight: 438.89

Physical Appearance: White solid

**Minimum Purity:** >99%

**Batch Molecular Structure:**



**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 20 mM

DMSO to 100 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:**

**Vonderfecht et al (2004)** Myopathy related to administration of a cationic amphiphilic drug and the use of multidose drug distribution analysis to predict its occurrence. *Toxicol.Pathol.* **32** 318. PMID: 15204973.

**Rudmann et al (2004)** Epididymal and systemic phospholipidosis in rats and dogs treated with dopamine D<sub>3</sub> selective antagonist PNU-177864. *Toxicol.Pathol.* **32** 326. PMID: 15204974.

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