

**Product Name:** (S)-PFI 2 hydrochloride

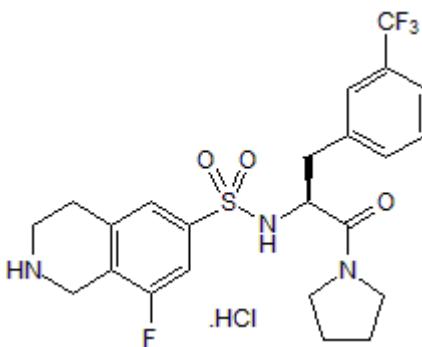
**Catalog No.:** 5400

**Batch No.:** 1

**IUPAC Name:** (1S)-1-[[3-(Trifluoromethyl)phenyl]methyl]-2-oxo-2-(1-pyrrolidinyl)ethyl]1,2,3,4-tetrahydro-6-isoquinolinesulfonamide hydrochloride

**1. PHYSICAL AND CHEMICAL PROPERTIES**

**Batch Molecular Formula:** C<sub>23</sub>H<sub>25</sub>F<sub>4</sub>N<sub>3</sub>O<sub>3</sub>S.HCl.2H<sub>2</sub>O  
**Batch Molecular Weight:** 572.01  
**Physical Appearance:** White solid  
**Solubility:** DMSO to 100 mM  
ethanol to 20 mM  
**Storage:** Store at -20°C  
**Batch Molecular Structure:**



**2. ANALYTICAL DATA**

**HPLC:** Shows 97.8% purity  
**Chiral HPLC:** Shows 99.4% purity  
**<sup>1</sup>H NMR:** Consistent with structure  
**Mass Spectrum:** Consistent with structure  
**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	48.29	5.29	7.35
Found	48.13	5.19	7.33

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

**Product Name:** (S)-PFI 2 hydrochloride

**Catalog No.:** 5400

**Batch No.:** 1

**IUPAC Name:** (1S)-1-[[3-(Trifluoromethyl)phenyl]methyl]-2-oxo-2-(1-pyrrolidinyl)ethyl]1,2,3,4-tetrahydro-6-isoquinolinesulfonamide hydrochloride

**Description:**

Negative control of (R)-PFI 2 hydrochloride (Cat. No. 4892). Exhibits 500-fold lower activity in a SETD7 enzymatic assay ( $IC_{50} = 1 \mu M$ ) compared to the active enantiomer.

**Physical and Chemical Properties:**

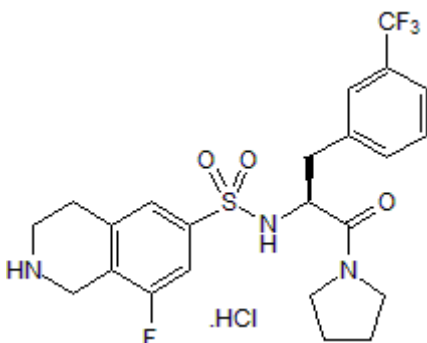
Batch Molecular Formula:  $C_{23}H_{25}F_4N_3O_3S \cdot HCl \cdot 2H_2O$

Batch Molecular Weight: 572.01

Physical Appearance: White solid

**Minimum Purity:** >97%

**Batch Molecular Structure:**



**Storage:** Store at  $-20^{\circ}C$ . This product is packaged under an inert atmosphere.

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 20 mM

This product has been packed under inert atmosphere, and should be stored under inert atmosphere after use.

**Stability and Solubility Advice:**

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

**References:**

**Baryte-Lovejoy et al (2014)** (R)-PFI-2 is a potent and selective inhibitor of SETD7 methyltransferase activity in cells. Proc.Natl.Acad.Sci.U S A **111** 12853. PMID: 25136132.

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

Tocris Bioscience is an R&D Systems company  
 USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373  
[www.RnDSystems.com](http://www.RnDSystems.com)