

Product Name: (S)-PFI 2 hydrochloride

Catalog No.: 5400

Batch No.: 2

CAS Number: 1627607-88-8

IUPAC Name: 8-Fluoro-1,2,3,4-tetrahydro-*N*-[(1*S*)-2-oxo-2-(1-pyrrolidinyl)-1-[[3-(trifluoromethyl)phenyl]methyl]ethyl]-6-isoquinolinesulfonamide hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₅F₄N₃O₃S.HCl.½H₂O

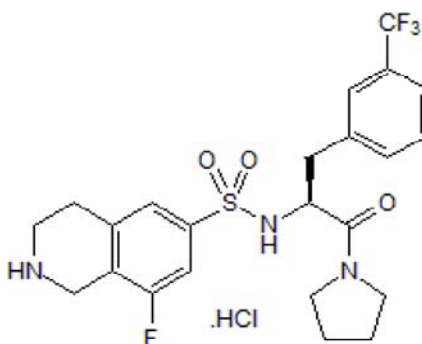
Batch Molecular Weight: 544.99

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Methanol [9:1])

HPLC: Shows 99% purity

Chiral HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	50.69	4.99	7.71
Found	50.88	5.01	7.71

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Description:

Negative control of (R)-PFI 2 hydrochloride. Exhibits 500-fold lower activity in a SETD7 enzymatic assay ($IC_{50} = 1 \mu M$) compared to the active enantiomer. Active Analog also available.

Physical and Chemical Properties:

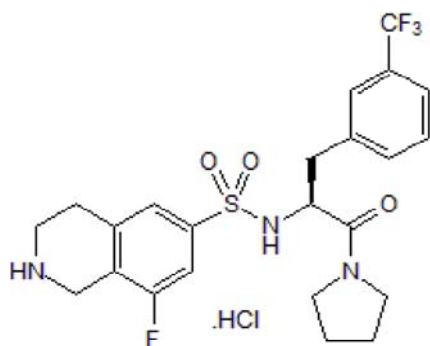
Batch Molecular Formula: $C_{23}H_{25}F_4N_3O_3S \cdot HCl \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 544.99

Physical Appearance: White solid

Minimum Purity: $\geq 97\%$

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.

Licensing Information:

This compound is supplied in conjunction with the Structural Genomics Consortium. For further characterization details, please visit the (R)-PFI 2 probe summary on the SGC website.

References:

Barsyte-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.

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