

Product Name: (R)-PFI 2 hydrochloride

Catalog No.: 4892

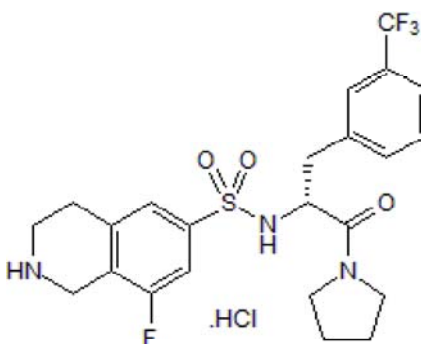
Batch No.: 2

CAS Number: 1627607-87-7

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₃ H ₂₅ F ₄ N ₃ O ₃ S.HCl.¾H ₂ O
Batch Molecular Weight:	549.49
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 20 mM with sonication
Storage:	Store at -20°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

TLC:	R _f = 0.33 (Chloroform:Methanol [9:1])
HPLC:	Shows 99.7% purity
Chiral HPLC:	Shows 100% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	50.27	5.04	7.65
Found	50.16	4.86	7.54

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

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Description:

Potent and selective SETD7 histone lysine methyltransferase inhibitor (IC₅₀ = 2 nM). Exhibits >1000-fold selectivity over DNMT1 and a panel of 18 other methyltransferases. Inhibits YAP nuclear translocation and function following activation of the Hippo signaling pathway in MCF7 cells. Negative Control also available.

Physical and Chemical Properties:

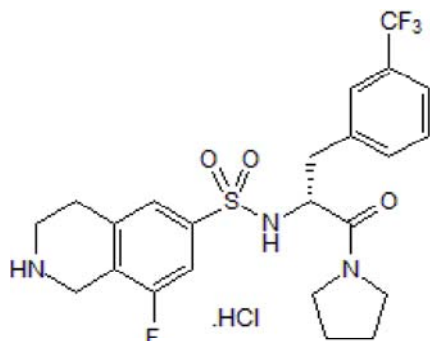
Batch Molecular Formula: C₂₃H₂₅F₄N₃O₃S.HCl.¾H₂O

Batch Molecular Weight: 549.49

Physical Appearance: White solid

Minimum Purity: ≥97%

Batch Molecular Structure:



Storage: Store at -20°C. This product is packaged under an inert atmosphere.

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 20 mM with sonication

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°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.

Licensing Information:

This probe 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:

Scheer et al (2019) A chemical biology toolbox to study protein methyltransferases and epigenetic signaling. *Nat.Commun.* **10** 19. PMID: 30604761.

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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