Batch No.: 1



Certificate of Analysis

www.tocris.com

Product Name: (R)-PFI 2 hydrochloride

Catalog No.: 4892

IUPAC Name: (1R)-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: $C_{23}H_{25}F_4N_3O_3S.HCl.$ ³/₄H₂O

Batch Molecular Weight: 549.49

Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM

ethanol to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.33$ (Chloroform:Methanol [9:1])

HPLC: Shows 99% purity
Chiral HPLC: Shows 99.33% purity

1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -220$ (Concentration = 0.01, Solvent = Methanol)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 50.27 5.04 7.65 Found 50.19 5.05 7.56

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





Batch No.: 1



Product Information

www.tocris.com

Product Name: (R)-PFI 2 hydrochloride

Catalog No.: 4892

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

isoquinolinesulfonamide hydrochloride

Description:

Potent and selective SETD7 histone lysine methyltransferase inhibitor ($IC_{50} = 2$ nM). Exhibits > 100-fold selectivity for SETD7 over other methyltransferases.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{23}H_{25}F_4N_3O_3S.HCl.^3/_4H_2O$

Batch Molecular Weight: 549.49 Physical Appearance: Off-white solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol to 20 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.