Certificate of Analysis

Product Name: **PFI 3** **Catalog No.: 5072** **Batch No.: 3**

CAS Number: 1819363-80-8

IUPAC Name: (2*E*)-1-(2-Hydroxyphenyl)-3-[(1*R*,4*R*)-5-(pyridin-2-yl)-2,5-diazabicyclo[2.2.1]heptan-2-yl]prop-2-en-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{19}N_3O_2$

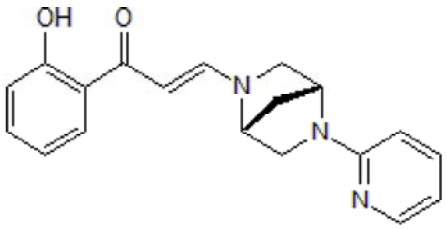
Batch Molecular Weight: 321.37

Physical Appearance: Yellow solid

Solubility: DMSO to 100 mM
ethanol to 5 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = +250 (Concentration = 0.22, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	71.01	5.96	13.08
Found	70.83	6.01	13.18

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Product Information

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Description:

PFI 3 is a potent and selective polybromo 1 (PBRM1) and SMARCA4 inhibitor (K_d values are 48 and 89 nM respectively) that also inhibits SMARCA2. This compoud displays 30-fold selectivity over other sub-family branches. PFI 3 accelerates FRAP recovery in cells at a concentration of 1 µM.

Physical and Chemical Properties:

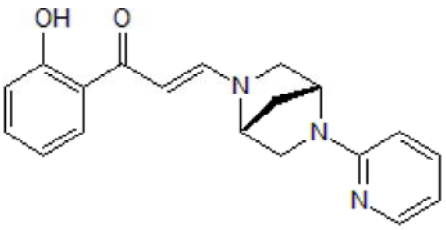
Batch Molecular Formula: $C_{19}H_{19}N_3O_2$

Batch Molecular Weight: 321.37

Physical Appearance: Yellow solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 5 mM with gentle warming

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 PFI 3 probe summary on the SGC website.

References:

Gerstenberger *et al* (2016) Identification of a chemical probe for family VIII bromodomains through optimization of a fragment hit. J.Med.Chem. ***59*** 4800. PMID: 27115555.

Vangamudi *et al* (2015) The SMARCA2/4 ATPase domain surpasses the bromodomain as a drug target in SWI/SNF mutant cancers: Insights from cDNA rescue and PFI-3 inhibitor studies Cancer Res. ***75*** 3865. PMID: 26139243.

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