

**Product Name:** PFI 3

**Catalog No.:** 5072

**Batch No.:** 2

**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<sub>19</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub>·¼H<sub>2</sub>O

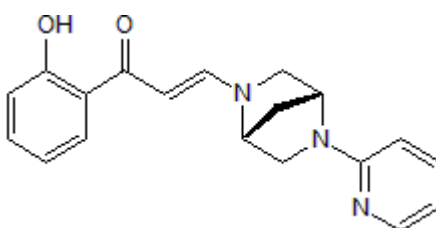
**Batch Molecular Weight:** 325.87

**Physical Appearance:** Yellow solid

**Solubility:** DMSO to 100 mM  
ethanol to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.25 (Ethyl acetate:Petroleum ether [1:1])

**HPLC:** Shows >99.9% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Optical Rotation:** [α]<sub>D</sub> = +258.9 (Concentration = 0.22, Solvent = Methanol)

**Microanalysis:**

	Carbon Hydrogen Nitrogen		
Theoretical	70.03	6.03	12.89
Found	70.05	5.8	12.82

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

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**Description:**

Potent and selective polybromo 1 and SMARCA4 inhibitor ( $K_d$  values are 48 and 89 nM respectively). Also inhibits SMARCA2. Displays 30-fold selectivity over other sub-family branches. Accelerates FRAP recovery in cells at a concentration of 1  $\mu$ M.

**Physical and Chemical Properties:**

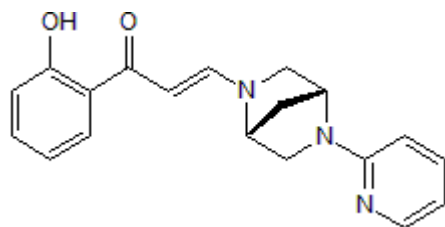
Batch Molecular Formula:  $C_{19}H_{19}N_3O_2 \cdot \frac{1}{4}H_2O$

Batch Molecular Weight: 325.87

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at -20°C

**Solubility & Usage Info:**

DMSO to 100 mM

ethanol to 100 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.

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