

**Product Name:** PF 3644022

**Catalog No.:** 4279

**Batch No.:** 1

**CAS Number:** 1276121-88-0

**IUPAC Name:** (10*R*)-9,10,11,12-Tetrahydro-10-methyl-3-(6-methyl-3-pyridinyl)-8*H*-[1,4]diazepino[5',6':4,5]thieno[3,2-*f*]quinolin-8-one

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** C<sub>21</sub>H<sub>18</sub>N<sub>4</sub>OS.¾H<sub>2</sub>O

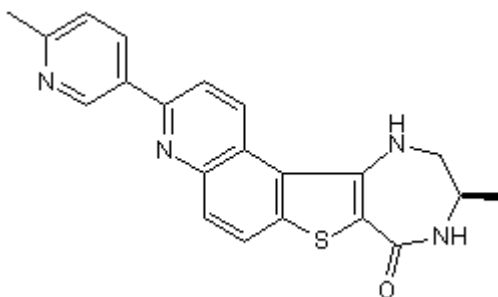
**Batch Molecular Weight:** 387.97

**Physical Appearance:** Yellow solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at +4°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**TLC:** R<sub>f</sub> = 0.36 (Chloroform:Methanol:Ammonia soln. [90:9:1])

**HPLC:** Shows 99.1% purity

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

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	65.01	5.07	14.44
Found	65.05	4.92	14.41

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**Description:**

Potent, ATP-competitive inhibitor of mitogen-activated protein kinase (MAPK)-activated protein kinase-2 (MK2) ( $IC_{50}$  = 5.2 nM;  $K_i$  = 3 nM). Inhibits tumor necrosis factor  $\alpha$  (TNF $\alpha$ ) production in U937 monocytic cells and peripheral blood mononuclear cells (PBMCs) ( $IC_{50}$  = 160 nM); exhibits oral efficacy in acute and chronic inflammatory models.

**Physical and Chemical Properties:**

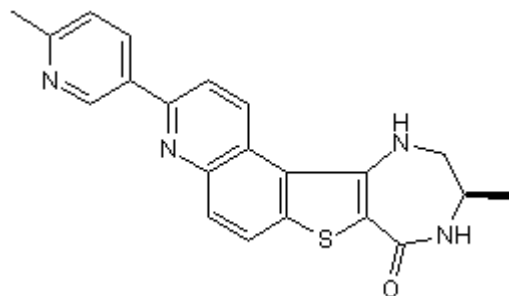
Batch Molecular Formula:  $C_{21}H_{18}N_4OS \cdot \frac{3}{4}H_2O$

Batch Molecular Weight: 387.97

Physical Appearance: Yellow solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO 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.

**References:**

**Mourey *et al*** (2010) A benzothienopyridine inhibitor of mitogen-activated protein kinase-activated protein kinase 2 inhibits tumor necrosis factor  $\alpha$  production and has oral anti-inflammatory efficacy in acute and chronic models of inflammation. *J.Pharmacol.Exp.Ther.* **333** 797. PMID: 20237073.

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