

Product Name: PF 3644022

Catalog No.: 4279

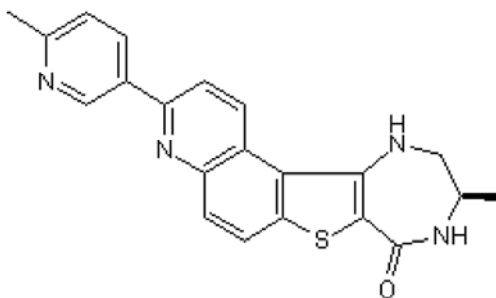
Batch No.: 2

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: C₂₁H₁₈N₄OS.¼H₂O
Batch Molecular Weight: 378.96
Physical Appearance: Yellow solid
Solubility: DMSO to 40 mM
Storage: Store at +4°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.41 (5% 7M methanolic ammonia/DCM)
HPLC: Shows 99.7% purity
Chiral HPLC: Shows 99.7% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	66.56	4.92	14.78
Found	66.7	4.95	14.68

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

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Description:

Potent, ATP-competitive inhibitor of mitogen-activated protein kinase (MAPK)-activated protein kinase-2 (MK2) (IC₅₀ = 5.2 nM; K_i = 3 nM). Inhibits tumor necrosis factor α (TNFα) production in U937 monocytic cells and peripheral blood mononuclear cells (PBMCs) (IC₅₀ = 160 nM); exhibits oral efficacy in acute and chronic inflammatory models.

Physical and Chemical Properties:

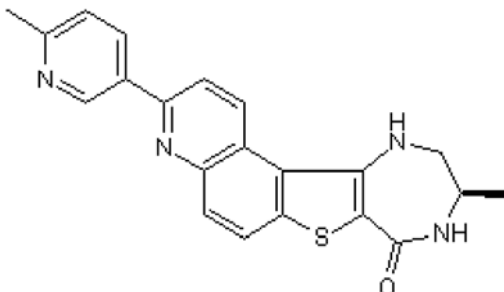
Batch Molecular Formula: C₂₁H₁₈N₄OS.¼H₂O

Batch Molecular Weight: 378.96

Physical Appearance: Yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

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

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 40 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.

Licensing Information:

Sold for research purposes under agreement from Pfizer Inc.

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