

Certificate of Analysis

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Product Name: 3PO

Catalog No.: 5121

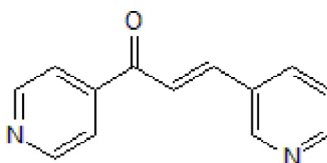
Batch No.: 1

CAS Number: 13309-08-5

IUPAC Name: 3-(3-Pyridinyl)-1-(4-pyridinyl)-2-propen-1-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₃H₁₀N₂O
Batch Molecular Weight: 210.23
Physical Appearance: Yellow solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.6% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon Hydrogen Nitrogen		
Theoretical	74.27	4.79	13.33
Found	74.19	4.73	13.3

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

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IUPAC Name: 3-(3-Pyridinyl)-1-(4-pyridinyl)-2-propen-1-one

Description:

3PO is originally reported to inhibit PFKFB3 (IC_{50} = 25 μ M). More recent reports failed to demonstrate activity in a PFKFB3 kinase assay. Reduces glycolytic flux and suppresses glucose uptake. Inhibits endothelial cell proliferation and causes G₂/M cell cycle arrest in vitro. Attenuates vessel sprouting and tumor growth in vivo. Amplifies the antiangiogenic effect of VEGFR blockade.

Physical and Chemical Properties:

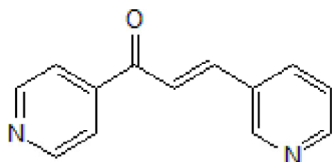
Batch Molecular Formula: C₁₃H₁₀N₂O

Batch Molecular Weight: 210.23

Physical Appearance: Yellow solid

Minimum Purity: ≥99%

Batch Molecular Structure:



Storage: Store at -20°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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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:

Boyd *et al* (2015) Structure-based design of potent and selective inhibitors of the metabolic kinase PFKFB3. *J.Med.Chem.* **58** 3611. PMID: 25849762.

Schoors *et al* (2014) Partial and transient reduction of glycolysis by PFKFB3 blockade reduces pathological angiogenesis. *Cell Metab.* **19** 37. PMID: 24332967.

Clem *et al* (2008) Small-molecule inhibition of 6-phosphofructo-2-kinase activity suppresses glycolytic flux and tumor growth. *Mol.Cancer Ther.* **7** 110. PMID: 18202014.

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