

Product Name: TL4-12

Catalog No.: 5910

Batch No.: 1

CAS Number: 1620820-12-3

IUPAC Name: 4-Methyl-3-[[6-(methylamino)-4-pyrimidinyl]oxy]-N-[3-(4-methyl-1-piperazinyl)-5-(trifluoromethyl)phenyl]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₅H₂₇F₃N₆O₂·½H₂O

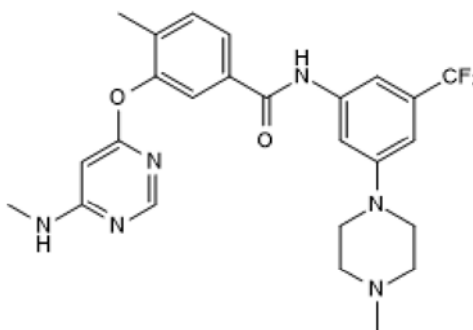
Batch Molecular Weight: 509.54

Physical Appearance: White solid

Solubility: DMSO to 20 mM
1eq. HCl to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Methanol [4:1])

HPLC: Shows 99% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	58.93	5.54	16.49
Found	59.06	5.42	16.47

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

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Description:

Potent MAP4K2 (GCK) inhibitor ($IC_{50} = 37$ nM). Exhibits >70-fold selectivity for MAP4K2 over TAK1 ($IC_{50} = 2.7$ μ M for TAK1). Inhibits IL-1 and TGF β -induced p38 MAPK phosphorylation, in vitro.

Physical and Chemical Properties:

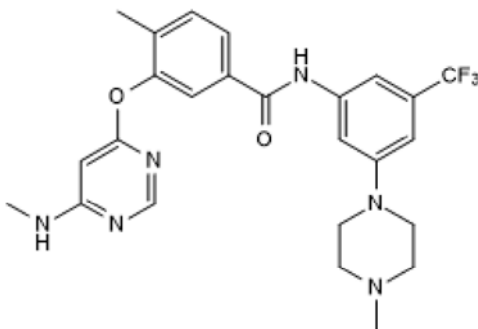
Batch Molecular Formula: C₂₅H₂₇F₃N₆O₂·½H₂O

Batch Molecular Weight: 509.54

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 20 mM

1eq. HCl to 20 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 under license from Dana-Farber Cancer Institute.

References:

Tan *et al* (2015) Discovery of type II inhibitors of TGF β -activated kinase 1 (TAK1) and mitogen-activated protein kinase kinase kinase 2 (MAP4K2). *J.Med.Chem.* **58** 183. PMID: 25075558.

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