

Certificate of Analysis

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Product Name: ML 3403

Catalog No.: 4586

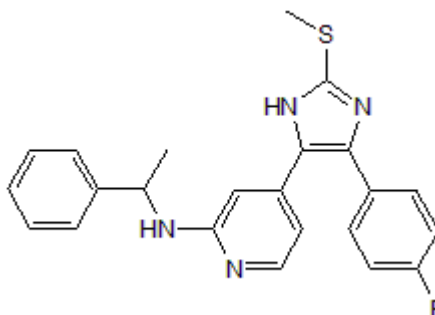
Batch No.: 1

CAS Number: 549505-65-9

IUPAC Name: [5-[4-(4-Fluorophenyl)-2-methylthio-1*H*-imidazol-4-yl]-*N*-(1-phenylethyl)-2-pyridinamine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:	C ₂₃ H ₂₁ FN ₄ S
Batch Molecular Weight:	404.5
Physical Appearance:	White solid
Solubility:	DMSO to 100 mM ethanol to 50 mM
Storage:	Store at +4°C
Batch Molecular Structure:	



2. ANALYTICAL DATA

HPLC:	Shows 98.4% purity
¹H NMR:	Consistent with structure
Mass Spectrum:	Consistent with structure
Microanalysis:	

	Carbon	Hydrogen	Nitrogen
Theoretical	68.29	5.23	13.85
Found	67.92	5.29	13.53

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

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Description:

p38 MAPK inhibitor ($IC_{50} = 0.38 \mu\text{M}$). Inhibits the release of IL-1 β and TNF- α in a peripheral blood mononuclear cell (PBMC) assay (IC_{50} values are 0.039 and 0.16 μM respectively).

Physical and Chemical Properties:

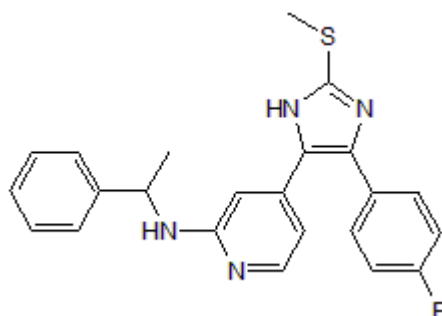
Batch Molecular Formula: $C_{23}H_{21}FN_4S$

Batch Molecular Weight: 404.5

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 50 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:

Laufer et al (2003) Novel substituted pyridinyl imidazoles as potent anticytokine agents with low activity against hepatic cytochrome P450 enzymes. *J. Med. Chem.* **46** 3230. PMID: 12852754.

Kammerer et al (2007) Pharmacokinetics of ML3403 ({4-[5-(4-fluorophenyl)-2-methylsulfanyl-3H-imidazol-4-yl]-pyridin-2-yl)-(1-phenylethyl)-amine), a 4-pyridinylimidazole-type p38 mitogen-activated protein kinase inhibitor. *Drug Metab. Dispos.* **35** 875. PMID: 17344341.

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