

Certificate of Analysis

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Product Name: SKI 178

Catalog No.: 5452

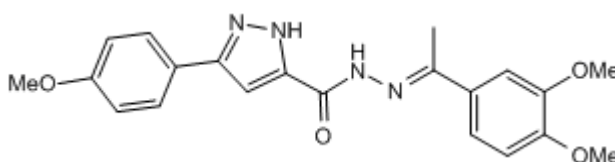
Batch No.: 1

CAS Number: 1259484-97-3

IUPAC Name: *N*-(1-(3,4-Dimethoxyphenyl)ethylidene)-3-(4-methoxyphenyl)-1*H*-pyrazole-5-carbohydrazide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₁H₂₂N₄O₄·H₂O
Batch Molecular Weight: 412.44
Physical Appearance: White solid
Solubility: DMSO to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.43 (Dichloromethane:Methanol [9:1])
HPLC: Shows >98.3% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	61.16	5.86	13.58
Found	61.11	5.83	13.55

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

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IUPAC Name: *N*-(1-(3,4-Dimethoxyphenyl)ethylidene)-3-(4-methoxyphenyl)-1*H*-pyrazole-5-carbohydrazide

Description:

Non-lipid sphingosine kinase 1 (SphK1) inhibitor (IC₅₀ = 0.1-1.8 μM). Induces CDK1-dependent apoptosis in human acute myeloid leukemia cell lines. Active in vivo.

Physical and Chemical Properties:

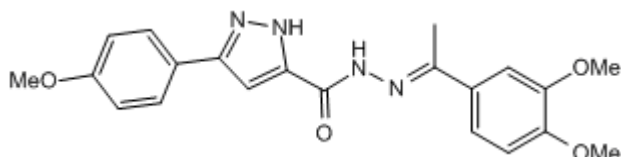
Batch Molecular Formula: C₂₁H₂₂N₄O₄.H₂O

Batch Molecular Weight: 412.44

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Store at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

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:

Dick et al (2015) The apoptotic mechanism of action of the sphingosine kinase 1 selective inhibitor SKI-178 in human acute myeloid leukemia cell lines. *J.Pharmacol.Exp.Ther.* **352** 494. PMID: 25563902.

Hengst et al (2010) Development of a sphingosine kinase 1 specific small-molecule inhibitor. *Bioorg.Med.Chem.Lett.* **20** 7498. PMID: 21050755.

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