



Certificate of Analysis

www.tocris.com

Product Name: LIMKi 3 Catalog No.: 4745 Batch No.: 3

CAS Number: 1338247-35-0

IUPAC Name: N-[5-[1-(2,6-Dichlorophenyl)-3-(difluoromethyl)-1*H*-pyrazol-5-yl]-2-thiazolyl]-2-methylpropanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{17}H_{14}Cl_2F_2N_4OS$

Batch Molecular Weight: 431.29 **Physical Appearance:** White solid

Solubility: DMSO to 100 mM

ethanol to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.55$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.1% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 47.34 3.27 12.99
Found 47.35 3.27 12.88



Product Information

Print Date: Jan 13th 2016

www.tocris.com

Product Name: LIMKi 3 Catalog No.: 4745 Batch No.: 3

CAS Number: 1338247-35-0

IUPAC Name: N-[5-[1-(2,6-Dichlorophenyl)-3-(difluoromethyl)-1H-pyrazol-5-yl]-2-thiazolyl]-2-methylpropanamide

Description:

Potent LIM kinase inhibitor (IC_{50} values are 7 and 8 nM for LIMK1 and LIMK2 respectively). Inhibits cofilin phosphorylation in MDA-MB-231 breast cancer cells. Reduces MDA-MB-231 tumor cell invasion in a 3D matrigel invasion assay.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{17}H_{14}Cl_2F_2N_4OS$

Batch Molecular Weight: 431.29 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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.

References:

Ross-Macdonald *et al* (2008) Identification of a nonkinase target mediating cytotoxicity of novel kinase inhibitors. Mol.Cancer Ther. **7** 3490. PMID: 19001433.

Scott et al (2010) LIM kinases are required for invasive path generation by tumor and tumor-associated stromal cells. J.Cell Biol. 191 169. PMID: 20876278.

Sparrow *et al* (2012) The actin-severing protein cofilin is downstream of neuregulin signaling and is essential for Schwann cell myelination. J.Neurosci. **32** 5284. PMID: 22496574.