

Certificate of Analysis

Print Date: Jan 15th 2016

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Product Name: WZ 4003 Catalog No.: 5177 Batch No.: 1

CAS Number: 1214265-58-3

IUPAC Name: N-3-[[5-Chloro-2-[[2-methoxy-4-(4-methyl-1-piperazinyl)phenyl]amino]-4-pyrimidinyl]oxy]phenyl]propanamide

1. PHYSICAL AND CHEMICAL PROPERTIES

C₂₅H₂₉CIN₆O₃ **Batch Molecular Formula:**

496.99 **Batch Molecular Weight:**

Physical Appearance: Off White solid Solubility: 1eq. HCl to 50 mM

DMSO to 20 mM with gentle warming

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

R_f = 0.25 (Dichloromethane:Methanol [9:1]) TLC:

HPLC: Shows 98.4% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 60.42 5.88 16.91 Found 60.53 5.91 16.89



Product Information

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Description:

Potent and selective NUAK1/2 inhibitor (IC_{50} values are 20 and 100 nM respectively). Exhibits no significant inhibition against a panel of 139 kinases, including ten AMPK family members. Inhibits NUAK1-mediated MYPT1 phosphorylation. Also inhibits cell proliferation in U2OS cells.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₅H₂₉ClN₆O₃ Batch Molecular Weight: 496.99 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 50 mM

DMSO to 20 mM with gentle warming

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:

Zhou et al (2009) Novel mutant-selective EGFR kinase inhibitors against EGFR T790M. Nature 462 1070. PMID: 20033049.

Banerjee *et al* (2014) Interplay between Polo kinase, LKB1-activated NUAK1 kinase, PP1βMYPT1 phosphatase complex and the SCFβTrCP E3 ubiquitin ligase. Biochem.J. *461* 233. PMID: 24785407.

Banerjee *et al* (2014) Characterization of WZ4003 and HTH-01-015 as selective inhibitors of the LKB1-tumour-suppressor-activated NUAK kinases. Biochem.J. *457* 215. PMID: 24171924.