

Certificate of Analysis

Print Date: Jun 24th 2016

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Product Name: AZ 6102 Catalog No.: 5775 Batch No.: 1

CAS Number: 1645286-75-4

IUPAC Name: rel-2-[4-[6-[(3R,5S)-3,5-Dimethyl-1-piperazinyl]-4-methyl-3-pyridinyl]phenyl]-3,7-dihydro-7-methyl-4H-pyrrolo[2,3-d]

pyrimidin-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{28}N_6O$ Batch Molecular Weight: 428.53

Physical Appearance: Off White solid
Solubility: DMSO to 50 mM
Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99% purity

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

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 70.07 6.59 19.61 Found 70.19 6.58 19.4



Product Information

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Description:

Potent TNKS2 and TNKS1 inhibitor (IC₅₀ values are 1 and 3 nM, respectively). Exhibits >100-fold selectivity for TNKS1/2 over PARP-1, PARP-2 and PARP-6. Inhibits Wnt signaling in DLD-1 cells ($IC_{50} = 5$ nM). Exhibits moderate oral bioavailability.

Physical and Chemical Properties:

Batch Molecular Formula: C25H28N6O Batch Molecular Weight: 428.53 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO 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:

Johannes et al (2015) Pyrimidinone nicotinamide mimetics as selective tankyrase and wnt pathway inhibitors suitable for in vivo pharmacology. ACS Med.Chem.Lett. 13 254. PMID: 25815142.

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