

Certificate of Analysis

Print Date: Jan 15th 2016 **WWW.tocris.com**

Product Name: TC-A 2317 hydrochloride Catalog No.: 4066 Batch No.: 1

CAS Number: 1245907-03-2

IUPAC Name: 2-[(5-Hydroxy-1,5-dimethylhexyl)amino]-4-methyl-6-[(5-methyl-1/H-pyrazol-3-yl)amino]-3-pyridinecarbonitrile

hydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{19}H_{28}N_6O.HCl.$ ¹/₄H₂O

Batch Molecular Weight: 397.43

Physical Appearance: Pale yellow solid

Solubility: DMSO to 100 mM ethanol to 50 mM

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.33$ (Ethyl acetate/1% NH3)

HPLC: Shows 98.6% purity

1H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 57.42 7.48 21.15 Found 57.32 7.34 21.34



Product Information

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Description:

Product Name:

Potent Aurora kinase A inhibitor ($K_i = 1.2$ nM compared to 101 nM for inhibition of Aurora kinase B). Selective over 60 other kinases (IC_{50} values > 1000 nM). Exhibits good cell permeability and antitumor activity.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{19}H_{28}N_6O.HCl.$ 1/4 H_2O

Batch Molecular Weight: 397.43 Physical Appearance: Pale yellow 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:

Ando et al (2010) 3-Cyano-6-(-5-methyl-3-pyrazoloamino)pyridines: Selective Aurora A kinase inhibitors. Bioorg.Med.Chem.Lett. 20 4709. PMID: 20573509.