



Certificate of Analysis

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Product Name: rac-CCT 250863 Catalog No.: 4546 Batch No.: 1

CAS Number: 1364269-06-6

IUPAC Name: 4-[2-Amino-5-[4-[(dimethylamino)methyl]-2-thienyl]-2-pyridinyl]-2-[[(2Z)-4,4,4-trifluoro-1-methyl-2-buten-1-yl]oxy]

benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{24}H_{25}F_3N_4O_2S.1\frac{1}{2}H_2O$

Batch Molecular Weight: 517.56 **Physical Appearance:** White solid

Solubility: 1eq. HCl to 100 mM

DMSO to 100 mM ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.32$ (Chloroform:Methanol [4:1])

HPLC: Shows 99.5% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 55.7 5.45 10.83 Found 55.57 5.11 10.89



Product Information

Print Date: Sep 16th 2016 **WWW.tocris.com**

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Description:

Potent Nek2 inhibitor (IC $_{50}$ = 73 nM). Exhibits selectivity for Nek2 over PLK1, MPS1, Cdk2 and Aurora A.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{24}H_{25}F_3N_4O_2S.11/2H_2O$

Batch Molecular Weight: 517.56 Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

1eq. HCl to 100 mM 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:

Innocenti et al (2012) Design of potent and selective hybrid inhibitors of the mitotic kinase Nek2: structure-activity relationship, structural biology, and cellular activity. J.Med.Chem. **55** 3228. PMID: 22404346.