

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]-3-pyridinyl]-2-[[[(2Z)-4,4,4-trifluoro-1-methyl-2-buten-1-yl]oxy]benzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₄H₂₅F₃N₄O₂S.1½H₂O

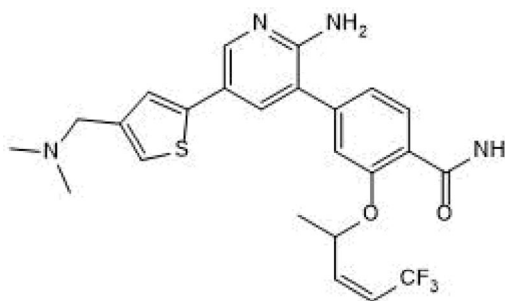
Batch Molecular Weight: 517.56

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 99.0% 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

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use

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Description:

rac-CCT 250863 is a potent Nek2 inhibitor (IC_{50} = 73 nM). Exhibits selectivity for Nek2 over PLK1, MPS1, Cdk2 and Aurora A.

Physical and Chemical Properties:

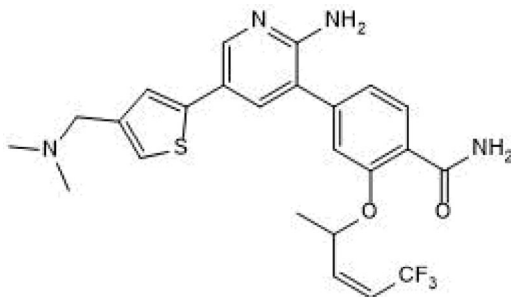
Batch Molecular Formula: $C_{24}H_{25}F_3N_4O_2S \cdot 1\frac{1}{2}H_2O$

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. *Unless contradicted by product-specific protocols or instructions, our standard recommendations apply:

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 .

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