Certificate of Analysis

Product Name: **CCT 241533 dihydrochloride** **Catalog No.: 4968** **Batch No.: 1**

CAS Number: 1962925-28-5

IUPAC Name: (3*R*,4*S*)-4-[[2-(5-Fluoro-2-hydroxyphenyl)-6,7-dimethoxy-4-quinazolinyl]amino]-α,α-dimethyl-3-pyrrolidinemethanol dihydrochloride

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{27}FN_4O_4.2HCl.½H_2O$

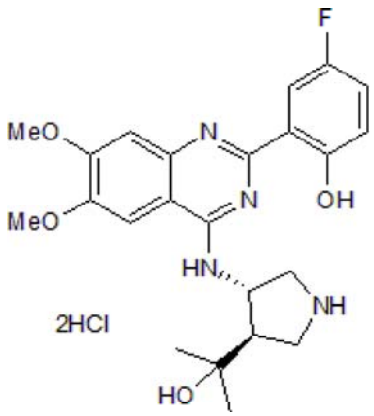
Batch Molecular Weight: 524.42

Physical Appearance: Pale yellow solid

Solubility: water to 10 mM with gentle warming
DMSO to 100 mM

Storage: Desiccate at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.72 (Pyridine:Acetic acid:Water:Butanol [4:1:1:4])

HPLC: Shows 98.7% purity

Chiral HPLC: Shows 99.2% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -35.4 (Concentration = 0.5, Solvent = Water)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.68	5.77	10.68
Found	52.52	5.84	10.58

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Product Information

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Description:

Potent Chk2 inhibitor (IC_{50} = 3 nM). Shows >63-fold selectivity for Chk1 over Chk2 and a panel of 84 other kinases. Inhibits Chk2 activation in response to etoposide-induced DNA damage in HT29 cells. Blocks ionizing radiation-induced apoptosis of mouse thymocytes.

Physical and Chemical Properties:

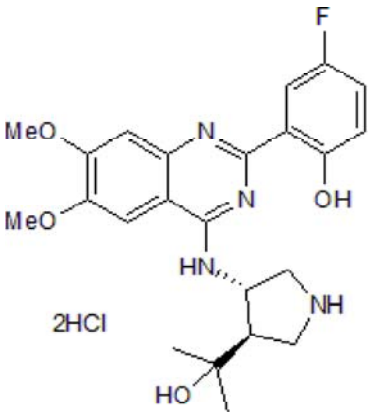
Batch Molecular Formula: $C_{23}H_{27}FN_4O_4.2HCl.½H_2O$

Batch Molecular Weight: 524.42

Physical Appearance: Pale yellow solid

Minimum Purity: >98%

Batch Molecular Structure:



Storage: Desiccate at RT

Solubility & Usage Info:

water to 10 mM with gentle warming
DMSO to 100 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:

Caldwell *et al* (2011) Structure-based design of potent and selective 2-(quinazolin-2-yl)phenol inhibitors of checkpoint kinase 2. J.Med.Chem. ***54*** 580. PMID: 21186793.

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