TOCRIS
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Print Date: Jan 16th 2016

# Certificate of Analysis

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**Product Name:** **CGP 74514 dihydrochloride** **Catalog No.: 5472** **Batch No.: 1**

IUPAC Name: *rel*-$N^2$-[(1*R*,2*S*)-2-Aminocyclohexyl]-$N^6$-(3-chlorophenyl)-9-ethyl-9*H*-purine-2,6-diamine dihydrochloride

## 1. PHYSICAL AND CHEMICAL PROPERTIES

**Batch Molecular Formula:** $C_{19}H_{24}ClN_7.2HCl.1½H_2O$

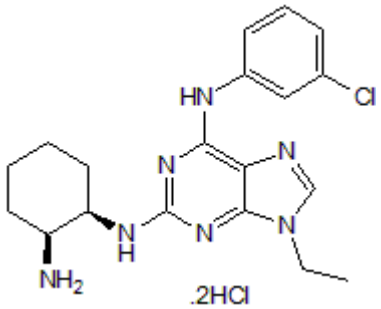
**Batch Molecular Weight:** 485.84

**Physical Appearance:** Off White solid

**Solubility:** water to 50 mM
DMSO to 100 mM

**Storage:** Desiccate at RT

**Batch Molecular Structure:**




## 2. ANALYTICAL DATA

**TLC:** $R_f$ = 0.37 (Dichloromethane:Methanol:Ammonia soln. [89:10:0.1])

**HPLC:** Shows 98.8% purity

**$^1$H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

| | Carbon | Hydrogen | Nitrogen |
|---|---|---|---|
| Theoretical | 46.97 | 6.02 | 20.18 |
| Found | 46.78 | 5.71 | 19.93 |



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**Description:**

Potent cdk1 inhibitor ($IC_{50}$ = 25 nM). Reduces Akt phosphorylation and increases mitochondrial damage in leukemia cells in vitro in combination with LY 294002.

**Physical and Chemical Properties:**

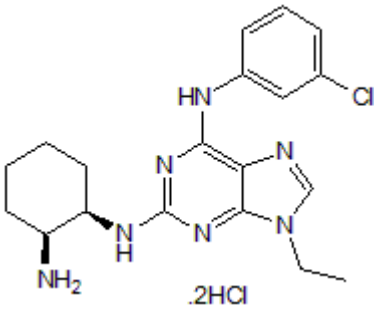
Batch Molecular Formula: $C_{19}H_{24}ClN_7.2HCl.1½H_2O$

Batch Molecular Weight: 485.84

Physical Appearance: Off White solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**




**Storage:** Desiccate at RT

**Solubility & Usage Info:**

water to 50 mM
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:**

**Furet** *et al* (2000) Structure-based design of potent CDK1 inhibitors derived from olomoucine. J.Comput.Aided Mol.Des. ***14*** 403. PMID: 10896313.

**Yu** *et al* (2013) The lethal effects of pharmacological cyclin-dependent kinase inhibitors in human leukemia cells proceed through a phosphatidylinositol 3-kinase/Akt-dependent process. Cancer Res. ***63*** 1822. PMID: 12702569.



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