

Print Date: Nov 21st 2018

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Product Name: NU 6140 Catalog No.: 3301 Batch No.: 1

Certificate of Analysis

CAS Number: 444723-13-1

IUPAC Name: 4-[[6-(Cyclohexylmethoxy)-1H-purin-2-yl]amino]-N,N-diethylbenzamide

1. PHYSICAL AND CHEMICAL PROPERTIES

 $C_{23}H_{30}N_6O_2.1/4H_2O$ **Batch Molecular Formula:**

Batch Molecular Weight: 427.02

Physical Appearance: Off-white solid

DMSO to 100 mM Solubility:

ethanol to 100 mM

Storage: Desiccate at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 64.69 7.2 19.68 Found 64.7 7.14 19.57

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



Product Information

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IUPAC Name: 4-[[6-(Cyclohexylmethoxy)-1*H*-purin-2-yl]amino]-*N*,*N*-diethylbenzamide

Description:

Cyclin-dependent kinase 2 (cdk2) inhibitor (IC $_{50}$ values are 0.42 - 1.1 μ M). Displays some selectivity for cdk2 (IC $_{50}$ value = 0.94 μ M for cdk4 and >2.3 μ M for other cdks). Induces cell-cycle arrest at the G2-M phase. Potentiates the apoptotic effect of taxol (Cat. No. 1097) in HeLa cells; down-regulates the antiapoptotic protein survivin. Also potently inhibits aurora kinases (IC $_{50}$ values are 0.035 and 0.067 μ M for aurora kinase B and A, respectively).

Physical and Chemical Properties:

Batch Molecular Formula: C23H30N6O2.14H2O

Batch Molecular Weight: 427.02 Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Desiccate at +4°C

Solubility & Usage Info:

DMSO to 100 mM ethanol 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:

Jorda et al (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? J.Med.Chem. 61 9105. PMID: 30234987.

Pennati *et al* (2005) Potentiation of paclitaxel-induced apoptosis by the novel cyclin-dependent kinase inhibitor NU6140: a possible role for survivin down-regulation. Mol.Cancer.Ther. *4* 1328. PMID: 16170024.