

## Certificate of Analysis

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**Product Name:** BIIB 021

**Catalog No.:** 4608

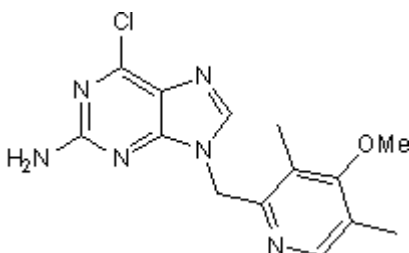
**Batch No.:** 1

CAS Number: 848695-25-0

IUPAC Name: 6-Chloro-9-[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]-9H-purin-2-amine

### 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>14</sub> H <sub>15</sub> ClN <sub>6</sub> O.½H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	327.77
<b>Physical Appearance:</b>	White crystalline solid
<b>Solubility:</b>	DMSO to 100 mM
<b>Storage:</b>	Store at -20°C
<b>Batch Molecular Structure:</b>	



### 2. ANALYTICAL DATA

<b>TLC:</b>	R <sub>f</sub> = 0.3 (Ethyl acetate (100%))
<b>HPLC:</b>	Shows 98.7% purity
<b><sup>1</sup>H NMR:</b>	Consistent with structure
<b>Mass Spectrum:</b>	Consistent with structure
<b>Microanalysis:</b>	
	Carbon Hydrogen Nitrogen
	Theoretical 51.3 4.92 25.64
	Found 51.35 4.93 25.48

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

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**Description:**

Selective, Hsp90 competitive inhibitor ( $K_i = 1.7$  nM). Displays no significant activity at a range of ATP-binding kinases or Na<sup>+</sup>K<sup>+</sup> ATPase. Induces degradation of HER-2 in vitro ( $EC_{50} = 38$  nM in MCF-7 cells). Inhibits growth and promotes cell death in a variety of human tumor cells. Orally bioavailable.

**Physical and Chemical Properties:**

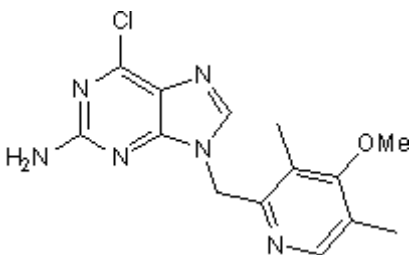
Batch Molecular Formula: C<sub>14</sub>H<sub>15</sub>ClN<sub>6</sub>O.½H<sub>2</sub>O

Batch Molecular Weight: 327.77

Physical Appearance: White crystalline solid

**Minimum Purity:** >98%

**Batch Molecular Structure:**



**References:**

**Lundgren et al** (2009) BIIB021, an orally available, fully synthetic small-molecule inhibitor of the heat shock protein Hsp90. *Mol.Cancer Ther.* **8** 921. PMID: 19372565.

**Yin et al** (2010) BIIB021, a novel Hsp90 inhibitor, sensitizes head and neck squamous cell carcinoma to radiotherapy. *Int.J.Cancer* **126** 1216. PMID: 19662650.

**Storage:** Store at -20°C

**Solubility & Usage Info:**

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.

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