



# **Certificate of Analysis**

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Product Name: NSC 109555 ditosylate Catalog No.: 3034 Batch No.: 1

CAS Number: 66748-43-4

IUPAC Name: 4,4'-diacetyldiphenylurea bis(guanylhydrazone) ditosylate

### 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{19}H_{24}N_{10}O.2C_7H_8O_3S.1\frac{1}{4}H_2O$ 

Batch Molecular Weight: 775.38

Physical Appearance: off-white solid

Solubility: DMSO to 10 mM

Storage: Store at -20°C

**Batch Molecular Structure:** 

.2C7H8O3S

#### 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.4$  (Methanol:Ammonia soln. [9:1])

HPLC: Shows >98.4% purity
 1H NMR: Consistent with structure
 Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 51.12 5.52 18.06 Found 50.89 5.33 18.41



## **Product Information**

Print Date: Mar 9th 2013

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**IUPAC Name:** 4,4'-diacetyldiphenylurea bis(guanylhydrazone) ditosylate

#### **Description:**

Selective, reversible, ATP-competitive Chk2 inhibitor ( $IC_{50} = 0.2 \mu M$ ) that Solubility & Usage Info: displays no effect on a range of other kinases including Chk1 (IC<sub>50</sub> > 10  $\mu$ M). Inhibits histone H1 phosphorylation (IC<sub>50</sub> = 0.24  $\mu$ M) and attenuates DMSO to 10 mM mitochondrial ATP synthesis. Exhibits antiproliferative activity in a number Stability and Solubility Advice: of leukemias in vivo.

#### **Physical and Chemical Properties:**

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Batch Molecular Weight: 775.38 Physical Appearance: off-white solid

Minimum Purity: >98%

#### **Batch Molecular Structure:**

 $.2C_7H_8O_3S$ 

Storage: Store at -20°C

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).

Catalog No.: 3034

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:

Byczkowski et al (1981) Actions of bis(guanylhydrazones) on isolated rat liver mitochondria. Biochem. Pharmacol. 30 2851. PMID: 6895596.

Byczkowski et al (1982) Potentiation of the antimitochondrial and antiproliferative effects of bis(guanylhydrazones) by phenethylbiquanide. Cancer Res. 42 3592. PMID: 6896674.

Jobson et al (2007) Identification of a bis-guanylhydrazone [4,4'-diacetyldiphenylurea-bis(guanylhydrazone); NSC 109555] as a novel chemotype for inhibition of Chk2 kinase. Mol. Pharmacol. 72 876. PMID: 17616632.

