

# **Certificate of Analysis**

Print Date: Jan 26th 2017

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Product Name: L189 Catalog No.: 3561 Batch No.: 1

CAS Number: 64232-83-3

IUPAC Name: 6-Amino-2,3-dihydro-5-[(phenylmethylene)amino]-2-4(1*H*)-pyrimidineone

## 1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula:  $C_{11}H_{10}N_4OS.1/4H_2O$ 

Batch Molecular Weight: 250.79
Physical Appearance: Yellow solid

**Solubility:** DMSO to 100 mM **Storage:** Store at -20°C

**Batch Molecular Structure:** 

## 2. ANALYTICAL DATA

**TLC:**  $R_f = 0.45$  (Ethyl acetate:Petroleum ether [1:1])

<sup>1</sup>H NMR: Consistent with structure Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 52.68 4.22 22.34 Found 52.28 4.44 22.31



# **Product Information**

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#### **Description:**

DNA ligase I, III and IV inhibitor (IC $_{50}$  values are 5, 9 and 5  $\mu$ M respectively) that blocks DNA binding ( $K_i$  = 5  $\mu$ M for DNA ligase I). Preferentially inhibits step 2 of the ligation reaction, and inhibits base excision repair (BER) and non-homologous end joining (NHEJ). Specifically sensitizes cancer cells to DNA damage and increases the cytotoxicity of DNA-damaging agents.

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

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

**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.

#### References:

**Chen** *et al* (2008) Rational design of human DNA ligase inhibitors that target cellular DNA replication and repair. Cancer Res. *68* 3169. PMID: 18451142.