

Certificate of Analysis

Print Date: Feb 9th 2017

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Product Name: NU 7441 Catalog No.: 3712 Batch No.: 6

CAS Number: 503468-95-9

IUPAC Name: 8-(4-Dibenzothienyl)-2-(4-morpholinyl)-4*H*-1-benzopyran-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{25}H_{19}NO_3S.1/4H_2O$

Batch Molecular Weight: 417.99

Physical Appearance: Light Beige solid

Solubility: DMSO to 5 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.36$ (Dichloromethane:Methanol [9:1])

HPLC: Shows >99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 71.84 4.7 3.35 Found 72.05 4.74 3.54



Product Information

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Description:

Potent and selective DNA-PK inhibitor (IC $_{50}$ = 14 nM). Selective for DNA-PK over a range of kinases including mTOR, PI 3-K, ATM and ATR. Potentiates the effects of doxorubicin (Cat. No. 2252) and etoposide (Cat. No. 1226) in vitro and etoposide in vivo. Also enhances CRISPR-Cas9-mediated homology-directed repair (HDR) efficiency 2 to 3-fold, and decreases nonhomologous end-joining (NHEJ) frequency ~40%.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₅H₁₉NO₃S.1/4H₂O

Batch Molecular Weight: 417.99

Physical Appearance: Light Beige solid

Minimum Purity: >99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 5 mM with gentle warming

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:

Robert et al (2015) Pharmacological inhibition of DNA-PK stimulates Cas9-mediated genome editing. Genome Med. 7 93. PMID: 26307031.

Willmore et al (2008) DNA-dependent protein kinase is a therapeutic target and an indicator of poor prognosis in B-cell chronic lymphocytic leukemia. Clin.Cancer Res. 14 3984. PMID: 18559621.

Zhao et al (2006) Preclinical evaluation of a potent novel DNA-dependent protein kinase inhibitor NU7441. Cancer Res. **66** 5354. PMID: 16707462.

Leahy et al (2004) Identification of a highly potent and selective DNA-dependent protein kinase (DNA-PK) inhibitor (NU7441) by screening of chromenone libraries. Bioorg.Med.Chem.Lett. 14 6083. PMID: 15546735.

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