TOCRIS
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Print Date: Feb 15th 2022

Certificate of Analysis

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Product Name: **KU 55933** **Catalog No.: 3544** **Batch No.: 5**

CAS Number: 587871-26-9

IUPAC Name: 2-(4-Morpholinyl)-6-(1-thianthrenyl)-4*H*-pyran-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{21}H_{17}NO_3S_2.¼H_2O$

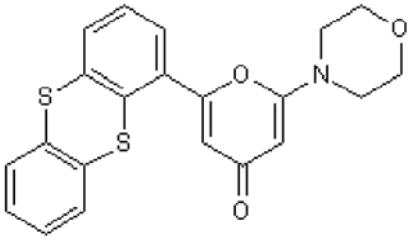
Batch Molecular Weight: 399.99

Physical Appearance: Tan solid

Solubility: DMSO to 100 mM
ethanol to 50 mM

Storage: Desiccate at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.29 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.0% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.06	4.41	3.5
Found	63.25	4.32	3.53

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Description:

KU 55933 is a potent, selective and competitive ATM kinase inhibitor (K_i = 2.2 nM, IC_{50} values are 13, 2500, 9300, 16600, > 100000 and > 100000 nM at ATM, DNA-PK, mTOR, PI 3-kinase, PI 4-K and ATR respectively). Decreases viability of MCF-7, A549 and HCT116 cells and decreases $p21^{CIP1}$ levels in vitro. Acts as a radio- and chemosensitizer for the treatment of cancer.

Physical and Chemical Properties:

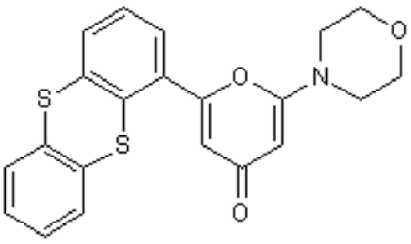
Batch Molecular Formula: $C_{21}H_{17}NO_3S_2.¼H_2O$

Batch Molecular Weight: 399.99

Physical Appearance: Tan solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Desiccate at -20°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 50 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:

Crescenzi *et al* (2008) Ataxia telangiectasia mutated and p21CIP1 modulate cell survival of drug-induced senescent tumor cells: implications for chemotherapy. Clin.Cancer Res. ***14*** 1877. PMID: 18347191.

Eaton *et al* (2007) Ataxia-telangiectasia mutated kinase regulates ribonucleotide reductase and mitochondrial homeostasis. J.Clin.Invest. ***117*** 2723. PMID: 17786248.

Hickson *et al* (2004) Identification and characterization of a novel and specific inhibitor of the ataxia-telangiectasia mutated kinase ATM. Cancer Res. ***64*** 9152. PMID: 15604286.

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