

## Certificate of Analysis

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**Product Name:** Ro 3306

**Catalog No.:** 4181

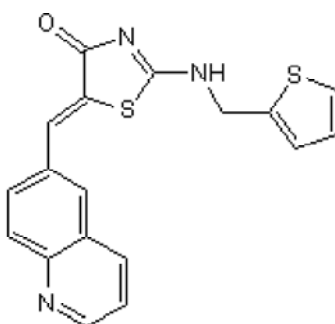
**Batch No.:** 2

CAS Number: 872573-93-8

IUPAC Name: 5-(6-Quinolinylmethylene)-2-[(2-thienylmethyl)amino]-4(5H)-thiazolone

### 1. PHYSICAL AND CHEMICAL PROPERTIES

<b>Batch Molecular Formula:</b>	C <sub>18</sub> H <sub>13</sub> N <sub>3</sub> OS <sub>2</sub> .H <sub>2</sub> O
<b>Batch Molecular Weight:</b>	369.47
<b>Physical Appearance:</b>	Beige solid
<b>Solubility:</b>	DMSO to 20 mM with gentle warming
<b>Storage:</b>	Store at +4°C
<b>Batch Molecular Structure:</b>	



### 2. ANALYTICAL DATA

<b>HPLC:</b>	Shows 98.0% 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	58.52	4.09	11.37
Found	58.16	3.7	11.46

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

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**Description:**

Ro 3306 is an ATP-competitive cyclin-dependent kinase 1 (cdk1) inhibitor ( $K_i$  values range from 35 to 240 nM depending on cdk1 binding partner). Also reported to inhibit other cdk's ( $K_i$  values are 0.89-1.32, 0.03 and  $>2$   $\mu$ M for cdk2, cdk3 and cdk4, respectively). Induces G2/M phase cell cycle arrest and apoptosis. Downregulates the expression of antiapoptotic proteins such as Bcl-2 and survivin and enhances downstream p53 signaling in acute myeloid leukemia (AML). RO 3306 also improves homology-directed repair (HDR) -mediated gene editing in hematopoietic stem and progenitor cells.

**Physical and Chemical Properties:**

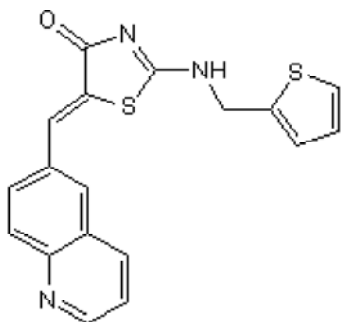
Batch Molecular Formula:  $C_{18}H_{13}N_3OS_2 \cdot H_2O$

Batch Molecular Weight: 369.47

Physical Appearance: Beige solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

**Azhagiri *et al*** (2021) Homology-directed gene-editing approaches for hematopoietic stem and progenitor cell gene therapy. *Stem Cell Res. Ther.* **12** 500. PMID: 34503562.

**Jorda *et al*** (2018) How selective are pharmacological inhibitors of cell-cycle-regulating cyclin-dependent kinases? *J. Med. Chem.* **61** 9105. PMID: 30234987.

**Yu *et al*** (2012) CDK1 regulates mediator of DNA damage checkpoint 1 during mitotic DNA damage. *Cancer Res.* **72** 5448. PMID: 22962268.

**Storage:** Store at +4°C

**Solubility & Usage Info:**

DMSO to 20 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.

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