1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: \( \text{C}_{18}\text{H}_{13}\text{N}_{3}\text{O}_{3}\text{S}_{2}\cdot\text{H}_{2}\text{O} \)

Batch Molecular Weight: 369.47

Physical Appearance: Beige solid

Solubility: DMSO to 20 mM with gentle warming

Storage: Store at +4°C

Batch Molecular Structure:

![Chemical Structure Image]

2. ANALYTICAL DATA

HPLC: Shows 98.0% purity

\(^1\text{H} \text{ NMR:}\) Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 58.52 4.09 11.37

Found 58.16 3.7 11.46
Product Name: Ro 3306
CAS Number: 872573-93-8
IUPAC Name: 5-(6-Quinolinyl)methylene)-2-[(2-thienylmethyl)amino]-4(5H)-thiazolone

Description:
ATP-competitive cyclin-dependent kinase 1 (cdk1) inhibitor (Ki values range from 35 to 240 nM depending on cdk1 binding partner). Also reported to inhibit other cdks (Ki values are 0.89-1.32, 0.03 and >2 μM 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).

Physical and Chemical Properties:
Batch Molecular Formula: C_{18}H_{13}N_{3}O_{2}S_{2}·H_{2}O
Batch Molecular Weight: 369.47
Physical Appearance: Beige solid

Minimum Purity: >98%

Batch Molecular Structure:

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.

References: