Certificate of Analysis

Product Name: **Compound 401** **Catalog No.: 3271** **Batch No.: 1**

CAS Number: 168425-64-7

IUPAC Name: 2-(4-Morpholinyl)-4*H*-pyrimido[2,1-*a*]isoquinolin-4-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{15}N_3O_2$

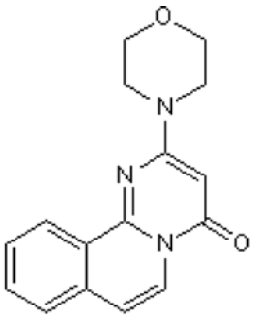
Batch Molecular Weight: 281.31

Physical Appearance: Beige solid

Solubility: DMSO to 10 mM
ethanol to 5 mM

Storage: Store at RT

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows >99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	68.31	5.37	14.94
Found	68.49	5.28	14.97

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Description:

Reversible and selective inhibitor of DNA-dependent protein kinase (DNA-PK) and mammalian target of rapamycin (mTOR) (IC_{50} values are 0.28 and 5.3 μM respectively). Displays little affinity for other commonly studied kinases including PI 3-K, ATM and ATR (IC_{50} values are all > 100 μM). Induces apoptosis in vitro.

Physical and Chemical Properties:

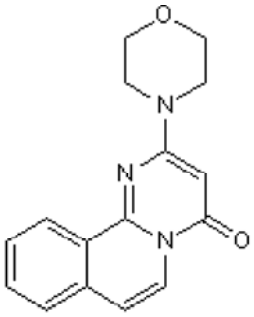
Batch Molecular Formula: $C_{16}H_{15}N_3O_2$

Batch Molecular Weight: 281.31

Physical Appearance: Beige solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 10 mM
ethanol to 5 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:

Ballo *et al* (2007) Inhibition of mammalian target of rapamycin signaling by 2-(morpholin-1-yl)oyrimido[2,1-α]isoquinolin-4-one. J.Biol.Chem. ***282*** 24463. PMID: 17562705.

Griffen *et al* (2005) Selective benzopyranone and pyrimido[2,1-α]isoquinolin-4-one inhibitors of DNA-dependent protein kinase: synthesis, structure-activity studies and radiosensitization of a human tumor cell line in vitro. J.Med.Chem. ***48*** 569. PMID: 15658870.