Certificate of Analysis

Product Name: **SU 9516** **Catalog No.: 2907** **Batch No.: 2**

CAS Number: 377090-84-1

IUPAC Name: (*Z*)-1,3-Dihydro-3-(1*H*-imidazol-4-ylmethylene)-5-methoxy-2*H*-indol-2-one

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{13}H_{11}N_3O_2.¼H_2O$

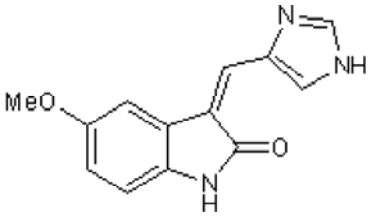
Batch Molecular Weight: 245.75

Physical Appearance: Orange solid

Solubility: DMSO to 100 mM
ethanol to 20 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.28 (Dichloromethane:Methanol:Ammonia soln. [98:1:1])

HPLC: Shows 99.9% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	63.54	4.72	17.1
Found	63.84	4.58	17.07

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Description:

Cyclin-dependent kinase (cdk) inhibitor (reported IC_{50} values are 0.02 - 0.03, 0.04 - 0.2, 0.2 - 1.7 and 0.9 µM for cdk2, cdk1, cdk4 and cdk9, respectively). Inhibits pRb phosphorylation causing enhanced pRB/E2F complex formation and induces G1 and G2-M cell cycle arrest. Transcriptionally downregulates Mcl-1 and has antiproliferative, cytostatic and pro-apoptotic effects in vitro.

Physical and Chemical Properties:

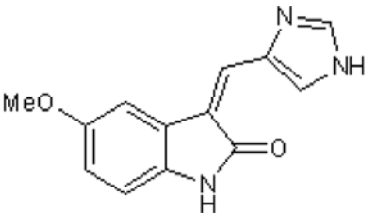
Batch Molecular Formula: $C_{13}H_{11}N_3O_2.¼H_2O$

Batch Molecular Weight: 245.75

Physical Appearance: Orange solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
ethanol to 20 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:

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

Gao *et al* (2006) The three-substituted indolinone cyclin-dependent kinase 2 inhibitor 3-[1-(3*H*-Imidazol-4-yl)-meth-(*Z*)-ylidene]-5-methoxy-1,3-dihydro-indol-2-one (SU9516) kills human leukemia cells via down-regulation of Mcl-1 through a transcriptional mechanism. Mol.Pharmacol. ***70*** 645. PMID: 16672643.

Yu *et al* (2002) SU9516, a cyclin-dependent kinase 2 inhibitor, promotes accumulation of high molecular weight E2F complexes in human colon carcinoma cells. Biochem.Pharmacol. ***64*** 1091. PMID: 12234612.

Lane *et al* (2001) A novel cdk2-selective inhibitor, SU9516, induces apoptosis in colon carcinoma cells. Cancer Res. ***61*** 6170. PMID: 11507069.