Certificate of Analysis

Product Name: **BAG 956** **Catalog No.: 3606** **Batch No.: 1**

CAS Number: 853910-02-8

IUPAC Name: α,α,-Dimethyl-4-[2-methyl-8-[2-(3-pyridinyl)ethynyl]-1*H*-imidazo[4,5-*c*]quinolin-1-yl]-benzeneacetonitrile

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{28}H_{21}N_5.½H_2O$

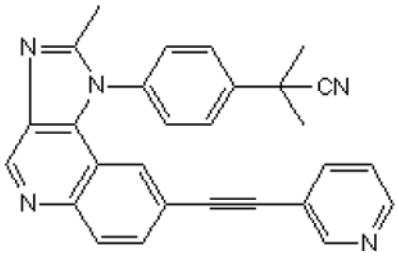
Batch Molecular Weight: 436.51

Physical Appearance: Red solid

Solubility: DMSO to 40 mM
ethanol to 20 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.3 (Dichloromethane:Methanol [95:5])

HPLC: Shows 99.1% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	77.04	5.08	16.04
Found	77.27	4.94	16.18

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Description:

BAG 956 is a dual PDPK1 (PDK1) and class I PI 3-K inhibitor (IC_{50} values are 245, 56, 446, 35 and 117 nM for PDPK1 and PI 3-K p110 -α, -β, -δ, and -γ respectively). Inhibits cellular AKT phosphorylation at Thr308. Blocks cell proliferation, causing arrest in G_1 phase of the cell cycle. Slows tumor progression in mouse xenograft models.

Physical and Chemical Properties:

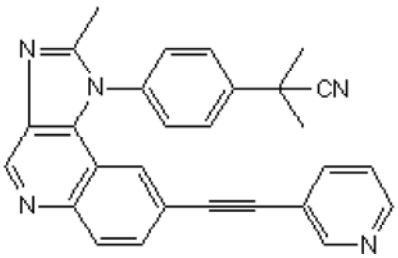
Batch Molecular Formula: $C_{28}H_{21}N_5.½H_2O$

Batch Molecular Weight: 436.51

Physical Appearance: Red solid

Minimum Purity: ≥98%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 40 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:

Marone *et al* (2009) Targeting melanoma with dual phosphoinositide 3-kinase/mammalian target of rapamycin inhibitors. Mol.Cancer Res. ***7*** 601. PMID: 19372588.

Stauffer *et al* (2008) Imidazo[4,5-*c*]quinolines as inhibitors of the PI3K/PKB-pathway. Bioorg.Med.Chem.Lett. ***18*** 1027. PMID: 18248814.

Weisberg *et al* (2008) Potentiation of antileukemic therapies by the dual PI3K/PDK-1 inhibitor, BAG956: effects on BCR-ABL- and mutant FLT3-expressing cells. Blood ***111*** 3723. PMID: 18184863.