

Product Name: BAG 956

Catalog No.: 3606

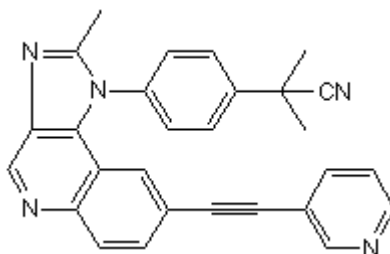
Batch No.: 1

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: $C_{28}H_{21}N_5 \cdot \frac{1}{2}H_2O$
Batch Molecular Weight: 436.51
Physical Appearance: red solid
Solubility: DMSO to 40 mM
ethanol to 20 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: $R_f = 0.3$ (Dichloromethane:Methanol [95:5])
HPLC: Shows 99.1% purity
¹H 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 |

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

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Description:

Dual PDK1 and class I PI 3-K inhibitor (IC_{50} values are 245, 56, 446, 35 and 117 nM for PDK1 and PI 3-K p110 $-\alpha$, $-\beta$, $-\delta$, and $-\gamma$ respectively). Inhibits cellular AKT phosphorylation at Thr308. Blocks cell proliferation, causing arrest in G₁ phase of the cell cycle. Slows tumor progression in mouse xenograft models.

Physical and Chemical Properties:

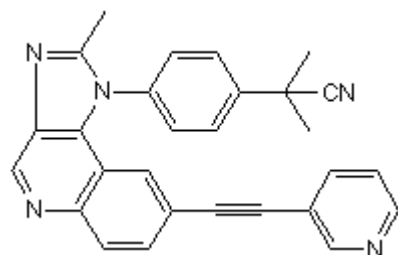
Batch Molecular Formula: C₂₈H₂₁N₅ · ½H₂O

Batch Molecular Weight: 436.51

Physical Appearance: red solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

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:

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.

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

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