

Certificate of Analysis

Print Date: Aug 26th 2022

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Product Name: ETP 45658 Catalog No.: 4702 Batch No.: 1

CAS Number: 1198357-79-7

IUPAC Name: 3-[1-Methyl-4-(4-morpholinyl)-1*H*-pyrazolo[3,4-*d*]pyrimidin-6-ylphenol

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{16}H_{17}N_5O_2$ Batch Molecular Weight:311.34Physical Appearance:White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.2$ (Ethyl acetate:Petroleum ether [1:1])

HPLC: Shows 99.3% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 61.72 5.5 22.49 Found 61.8 5.52 22.26

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Product Information

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Description:

ETP 45658 is a PI 3-kinase inhibitor (IC $_{50}$ values are 22, 30, 129 and 710 nM for PI 3-K α , PI 3-K δ , PI 3-K β and PI 3-K γ respectively). Also inhibits DNA-PK and mTOR (IC $_{50}$ values are 70.6 and 152 nM respectively). Inhibits proliferation of multiple cancer cell lines in vitro and reduces Akt phosphorylation levels in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₆H₁₇N₅O₂ Batch Molecular Weight: 311.34 Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 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:

Hill *et al* (2014) A novel phosphatidylinositol 3-kinase (PI3K) inhibitor directs a potent FOXO-dependent, p53-independent cell cycle arrest phenotype characterized by the differential induction of a subset of FOXO-regulated genes. Breast Cancer Res. *16* 482. PMID: 25488803.

Link et al (2009) Chemical interrogation of FOXO3a nuclear translocation identifies potent and selective inhibitors of phosphoinositide 3-kinases, J.Biol.Chem. **284** 28392, PMID: 19690175.

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