

Certificate of Analysis

Print Date: Oct 18th 2017

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Product Name: AZ 10397767 Catalog No.: 5872 Batch No.: 1

CAS Number: 333742-63-5

 $IUPAC \ Name: \ 5-[[(3-Chloro-2-fluorophenyl)methyl]thio]-7-[[(1R)-2-hydroxy-1-methylethyl]amino]thiazolo[4,5-\emph{a}]pyrimidin-2(3H)-one$

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₁₅H₁₄CIFN₄O₂S₂

Batch Molecular Weight: 400.88

Physical Appearance:Pale orange solidSolubility:DMSO to 100 mMStorage:Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

TLC: $R_f = 0.48$ (Dichloromethane:Methanol [85:15])

HPLC: Shows >99.5% purity
Chiral HPLC: Shows 100% purity

1H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -14.4$ (Concentration = 1, Solvent = DMF)

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 44.94 3.52 13.97 Found 11.68 3.49 13.76

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



Product Information

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Description:

Potent CXCR2 antagonist ($IC_{50} = 1$ nM); attenuates oxaliplatin-induced NF- κ B activation, increases oxaliplatin cytotoxicity, and potentiates oxaliplatin-induced apoptosis in AIPC cells. Reduces the numbers of neutrophils infiltrating into tumors in both in vitro and in vivo models and delayed tumor growth. Orally bioavailable.

Physical and Chemical Properties:

Batch Molecular Formula: C₁₅H₁₄ClFN₄O₂S₂

Batch Molecular Weight: 400.88

Physical Appearance: Pale orange solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at -20°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:

Tazzyman *et al* (2011) Inhibition of neutrophil infiltration into A549 lung tumors *in vitro* and *in vivo* using a CXCR2-specific antagonist is associated with reduced tumor growth. Int.J.Cancer **129** 847. PMID: 21328342.

Walters et al (2008) Evaluation of a series of bicyclic CXCR2 antagonists. Bioorg.Med.Chem.Lett. 18 798. PMID: 18240390.

Wilson *et al* (2008) Chemotherapy-induced CXC-chemokine/CXC-chemokine receptor signaling in metastatic prostate cancer cells confers resistance to oxaliplatin through potentiation of nuclear factor-kappaB transcription and evasion of apoptosis. J.Pharmacol.Exp.Ther. **327** 746. PMID: 18780829.