



Certificate of Analysis

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Product Name: Zoledronic Acid Catalog No.: 6111 Batch No.: 1

CAS Number: 118072-93-8

IUPAC Name: [1-Hydroxy-2-(1*H*-imidazol-1-yl)ethylidene]bisphosphonic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_5H_{10}N_2O_7P_2.2H_2O$

Batch Molecular Weight: 308.12

Physical Appearance: Off White solid

Solubility: 1.1eq. NaOH to 50 mM

water to 3 mM

Storage: Store at +4°C

Batch Molecular Structure:

N OH OH

2. ANALYTICAL DATA

Microanalysis:

HPLC: Shows 99.4% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Carbon Hydrogen Nitrogen

Theoretical 19.49 4.58 9.09 Found 19.5 4.2 8.89



Product Information

Print Date: Feb 16th 2017

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CAS Number: 118072-93-8

IUPAC Name: [1-Hydroxy-2-(1*H*-imidazol-1-yl)ethylidene]bisphosphonic acid

Description:

Potent bisphophonate farnesyl diphosphate (FPP) synthase inhibitor (IC_{50} = 20 nM). Inhibits osteoclast-mediated bone resorption. Also inhibits Ras signaling and tumor growth, and induces apoptosis in pancreatic cancer cells. Reverses epithelial-mesenchymal transition and inhibits breast cancer cell renewal via inactivation of NF- κ B.

Physical and Chemical Properties:

Batch Molecular Formula: $C_5H_{10}N_2O_7P_2.2H_2O$

Batch Molecular Weight: 308.12 Physical Appearance: Off White solid

Minimum Purity: >98%

Batch Molecular Structure:

Storage: Store at +4°C

CAUTION - This product is light sensitive and we recommend that the solid material and any solutions obtained are protected from exposure to light.

Solubility & Usage Info:

1.1eq. NaOH to 50 mM water to 3 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:

Schech *et al* (2013) Zoledronic acid reverses the epithelial-mesenchymal transition and inhibits self-renewal of breast cancer cells through inactivation of NF-κB. Mol.Cancer Ther. *12* 1356. PMID: 23619300.

Tassone *et al* (2003) Zoledronic acid induces antiproliferative and apoptotic effects in human pancreatic cancer cells *in vitro*. Br.J.Cancer *88* 1971. PMID: 12799645.

Dunford *et al* (2001) Structure-activity relationships for inhibition of farnesyl diphosphate synthase *in vitro* and inhibition of bone resorption *in vivo* by nitrogen-containing bisphosphonates. J.Pharmacol.Exp.Ther. **296** 235. PMID: 11160603.