



Certificate of Analysis

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Product Name: Catalog No.: 2961 Batch No.: 4 **Batimastat**

CAS Number: 130370-60-4

IUPAC Name: (2R,3S)-N⁴-Hydroxy-N1-[(1S)-2-(methylamino)-2-oxo-1-(phenylmethyl)ethyl]-2-(2-methylpropyl)-3-[(2-thienylthio)

methyl]butanediamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{23}H_{31}N_3O_4S_2$

Batch Molecular Weight: 477.64 **Physical Appearance:** White solid

DMSO to 100 mM Solubility: Storage: Store at -20°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.8% purity

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

 $[\alpha]_D$ = -78.2 (Concentration = 0.5, Solvent = Methanol) **Optical Rotation:**

Microanalysis: Carbon Hydrogen Nitrogen

> Theoretical 57.84 6.54 8.8 Found 57.64 6.53 8.87

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

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Product Information

Print Date: Jan 27th 2020

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methyl]butanediamide

Description:

Potent, broad spectrum MMP inhibitor (IC $_{50}$ values are 3, 4, 4, 6 $\,$ and 20 nM for MMP -1, -2, -9, -7 and -3 respectively). Exhibits antiproliferative, anti-invasive and antimetastatic activity in human ovarian carcinoma xenografts in vivo.

Physical and Chemical Properties:

Batch Molecular Formula: C₂₃H₃₁N₃O₄S₂

Batch Molecular Weight: 477.64 Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

When purchsed as a 1mg unit, this product is supplied as a lyophilized solid and may be very hard to visualize. Solutions should be made by adding solvent directly to the vial. The vial should then be vortexed vigorously to ensure the product has completely dissolved.

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:

Kohn and Liotta (1995) Molecular insights into cancer invasion: strategies for prevention and intervention. Cancer Res. 55 1856. PMID:

Wang et al (1994) Matrix metalloproteinase inhibitor BB-94 (Batimastat) inhibits human colon tumor growth and spread in a patient-like orthotopic model in nude mice. Cancer Res. 54 4726. PMID: 8062271.

Davies et al (1993) A synthetic matrix metalloproteinase inhibitor decreases tumor burden and prolongs survival of mice bearing human ovarian carcinoma xenografts. Cancer Res. 53 2087. PMID: 8347186.