Product Name: **Batimastat** **Catalog No.: 2961** **Batch No.: 3**

CAS Number: 130370-60-4

IUPAC Name: (2*R*,3*S*)-*N*^{4}-Hydroxy-*N*^{1}-[(1*S*)-2-(methylamino)-2-oxo-1-(phenylmethyl)ethyl]-2-(2-methylpropyl)-3-[(2-thienylthio)methyl]butanediamide

1. PHYSICAL AND CHEMICAL PROPERTIES

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

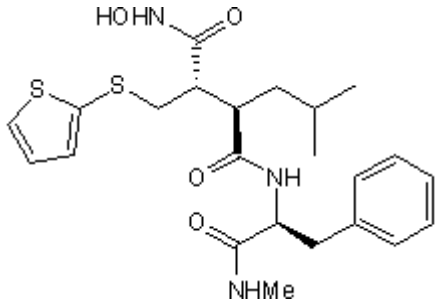
Batch Molecular Weight: 477.64

Physical Appearance: White solid

Solubility: DMSO to 100 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.6 (Dichloromethane:Methanol [85:15])

HPLC: Shows 99.8% purity

^{1}H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D$ = -84 (Concentration = 0.5, Solvent = Methanol)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	57.84	6.54	8.8
Found	57.97	6.62	8.89

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Description:

Potent, broad spectrum matrix metalloprotease (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:

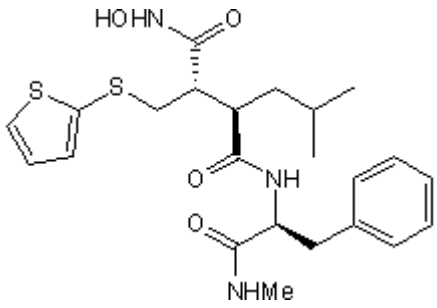
Batch Molecular Formula: $C_{23}H_{31}N_3O_4S_2$

Batch Molecular Weight: 477.64

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at -20°C

Solubility & Useage 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:

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.

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.

Kohn and Liotta (1995) Molecular insights into cancer invasion: strategies for prevention and intervention. Cancer Res. ***55*** 1856. PMID: 7728753.