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

CAS Number: 130370-60-4
IUPAC Name: (2R,3S)-N\(^4\)-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: \(\text{C}_{23}\text{H}_{31}\text{N}_{3}\text{O}_{4}\text{S}_{2}\)
   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

   HPLC: Shows 99.8% purity
   \(^1\)H NMR: Consistent with structure
   Mass Spectrum: Consistent with structure
   Optical Rotation: \([\alpha]\) = -78.2 (Concentration = 0.5, Solvent = Methanol)
   Microanalysis:

<table>
<thead>
<tr>
<th>Element</th>
<th>Theoretical</th>
<th>Found</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>57.84</td>
<td>57.64</td>
</tr>
<tr>
<td>H</td>
<td>6.54</td>
<td>6.53</td>
</tr>
<tr>
<td>N</td>
<td>8.8</td>
<td>8.87</td>
</tr>
</tbody>
</table>

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use
Product Name: Batimastat
Catalog No.: 2961
Batch No.: 4

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

Description:
Potent, broad spectrum MMP inhibitor (IC₅₀ 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: C₂₃H₂₅N₇O₄S₂
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 purchased 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: