Product Name: TMI 1
Catalog No.: 5960
Batch No.: 1
CAS Number: 287403-39-8
IUPAC Name: (3S)-4-[(4-(2-Butyn-1-yloxy)phenyl)sulfonyl]-N-hydroxy-2,2-dimethyl-3-thiomorpholinecarboxamide

1. PHYSICAL AND CHEMICAL PROPERTIES

- Batch Molecular Formula: C_{17}H_{22}N_{2}O_{5}S_{2}
- Batch Molecular Weight: 398.49
- Physical Appearance: White solid
- Solubility: DMSO to 100 mM, ethanol to 20 mM
- Storage: Store at -20°C

2. ANALYTICAL DATA

- HPLC: Shows 99.4% purity
- $^1$H NMR: Consistent with structure
- Mass Spectrum: Consistent with structure
- Microanalysis:
  
<table>
<thead>
<tr>
<th></th>
<th>Theoretical</th>
<th>Found</th>
</tr>
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<tbody>
<tr>
<td>Carbon</td>
<td>51.24</td>
<td>51.15</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.56</td>
<td>5.6</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>7.03</td>
<td>6.95</td>
</tr>
</tbody>
</table>

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

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**Catalog No.:** 5960

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**IUPAC Name:** (3S)-4-[[4-(2-Butyn-1-yloxy)phenyl]sulfonyl]-N-hydroxy-2,2-dimethyl-3-thiomorpholinecarboxamide

**Description:**
Adam 17 (TACE) and MMP inhibitor (IC_{50} values are 3, 4.7, 6.6, 8.4, 12, 26 and 26 nM for MMP-13, MMP-2, MMP-1, ADAM 17, MMP-9, MMP-7 and MMP-14, respectively). Suppresses TNF-α production in an acute LPS-mouse model. Reduces severity score in an in vivo model of rheumatoid arthritis. Displays selective cytotoxicity to tumor cells and cancer stem cells in vitro. Induces tumor apoptosis in a breast cancer in vivo model. Orally bioavailable.

**Physical and Chemical Properties:**
- **Batch Molecular Formula:** C_{17}H_{22}N_{2}O_{3}S_{2}
- **Batch Molecular Weight:** 398.49
- **Physical Appearance:** White solid
- **Minimum Purity:** >98%

**Storage:** Store at -20°C

**Solubility & Usage Info:**
- DMSO to 100 mM
- Ethanol to 20 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.

**Licensing Information:**
Sold for research purposes under agreement from Pfizer Inc

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**References:**