

Product Name: TMI 1

Catalog No.: 5960

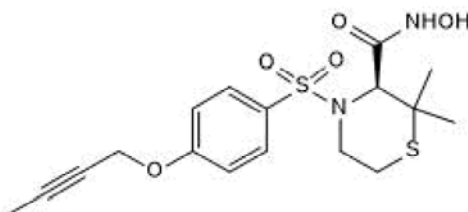
Batch No.: 1

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: C₁₇H₂₂N₂O₅S₂
Batch Molecular Weight: 398.49
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 ethanol to 20 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 99.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	51.24	5.56	7.03
Found	51.15	5.6	6.95

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

bio-techne.com

info@bio-techne.com
techsupport@bio-techne.com

North America

Tel: (800) 343 7475

China

info.cn@bio-techne.com
Tel: +86 (21) 52380373

Europe Middle East Africa

Tel: +44 (0)1235 529449

Rest of World

www.tocris.com/distributors
Tel: +1 612 379 2956

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Description:

ADAM17 (TACE) and MMP inhibitor (IC₅₀ 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:

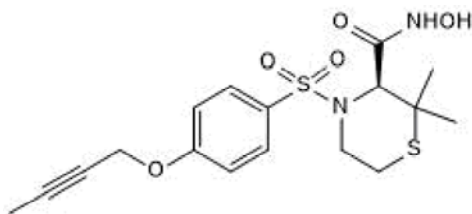
Batch Molecular Formula: C₁₇H₂₂N₂O₅S₂

Batch Molecular Weight: 398.49

Physical Appearance: White solid

Minimum Purity: \geq 98%

Batch Molecular Structure:



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

References:

Mezil *et al* (2012) Tumor selective cytotoxic action of a thiomorpholin hydroxamate inhibitor (TMI-1) in breast cancer PLoS One **7** e43409. PMID: 23028451.

Levin (2006) Heterocyclic inhibitors of tumor necrosis factor- α converting enzyme (TACE) Heterocycles **70** 691.

Zhang *et al* (2004) Identification and characterization of 4-[[4-(2-butyn-1-yloxy)phenyl]sulfonyl]-N-hydroxy-2,2-dimethyl-(3S) thiomorpholinecarboxamide (TMI-1), a novel dual tumor necrosis factor- α -converting enzyme/matrix meta J.Pharmacol.Exp.Ther. **309** 348. PMID: 14718605.

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