

Product Name: TC-I 15

Catalog No.: 4527

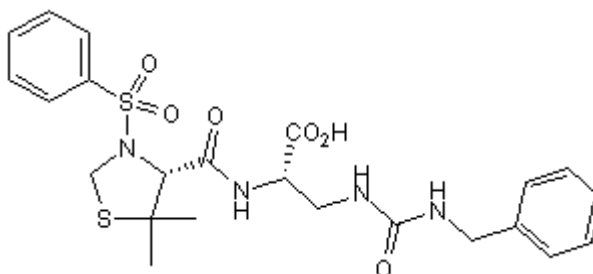
Batch No.: 1

CAS Number: 916734-43-5

IUPAC Name: *N*-[[[(4*R*)-5,5-Dimethyl-3-(phenylsulfonyl)-4-thiazolidinyl]carbonyl]-3-[[[(phenylmethyl)amino]carbonyl]amino]-L-alanine

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₈N₄O₆S₂·½H₂O
Batch Molecular Weight: 529.63
Physical Appearance: White solid
Solubility: DMSO to 100 mM
 1.1eq. NaOH to 25 mM
 ethanol to 100 mM
Storage: Store at -20°C
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.43 (Chloroform:Methanol [9:1] + 1% AcOH)
HPLC: Shows 98.5% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Optical Rotation: [α]_D = +1.6 (Concentration = 2.225, Solvent = Chloroform)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.16	5.52	10.58
Found	52.5	5.53	10.3

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

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Description:

Potent $\alpha_2\beta_1$ integrin inhibitor (IC₅₀ values for the inhibition of human platelet adhesion to type I collagen are 12 and 715 nM for platelets under static conditions and under flow, respectively). Displays selectivity for $\alpha_2\beta_1$ over $\alpha_v\beta_3$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_{IIb}\beta_3$ at concentrations exceeding 1000 nM. Reduces collagen IV production in mesangial cells. Active in vivo; prevents ferric chloride-induced clot formation in mice.

Physical and Chemical Properties:

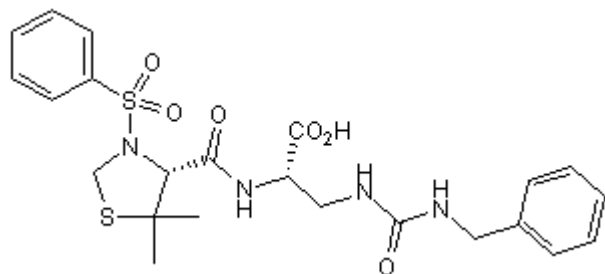
Batch Molecular Formula: C₂₃H₂₈N₄O₆S₂·½H₂O

Batch Molecular Weight: 529.63

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Miller et al (2009) Small-molecule inhibitors of integrin $\alpha_2\beta_1$ that prevent pathological thrombus formation via an allosteric mechanism. *Proc.Natl.Acad.Sci.U.S.A.* **106** 719. PMID: 19141632.

Borza et al (2012) Inhibition of integrin $\alpha_2\beta_1$ ameliorates glomerular injury. *J.Am.Soc.Nephrol.* **23** 1027. PMID: 22440900.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

1.1eq. NaOH to 25 mM

ethanol 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.

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