

Product Name: TC-I 15

Catalog No.: 4527

Batch No.: 3

CAS Number: 916734-43-5

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

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₂₈N₄O₆S₂ · ¼H₂O

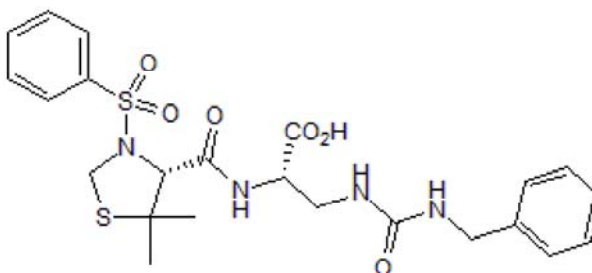
Batch Molecular Weight: 525.12

Physical Appearance: White solid

Solubility: DMSO to 100 mM
1eq. NaOH to 50 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 98.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.61	5.47	10.67
Found	52.22	5.43	10.71

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

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:

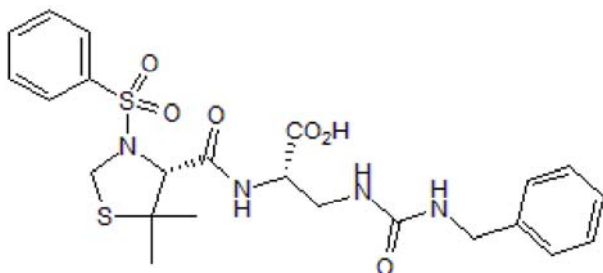
Batch Molecular Formula: C₂₃H₂₈N₄O₆S₂·¼H₂O

Batch Molecular Weight: 525.12

Physical Appearance: White solid

Minimum Purity: ≥98%

Batch Molecular Structure:



References:

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

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.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

1eq. NaOH to 50 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 under license from the University of Pennsylvania.

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