

Product Name: BIO 5192

Catalog No.: 5051

Batch No.: 1

CAS Number: 327613-57-0

IUPAC Name: (2S)-2-[[[(2S)-1-[(3,5-Dichlorophenyl)sulfonyl]-2-pyrrolidinyl]carbonyl]amino]-4-[[[(2S)-4-methyl-2-[methyl[2-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]acetyl]amino]-1-oxopentyl]amino]butanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{38}H_{46}Cl_2N_6O_8S \cdot H_2O$

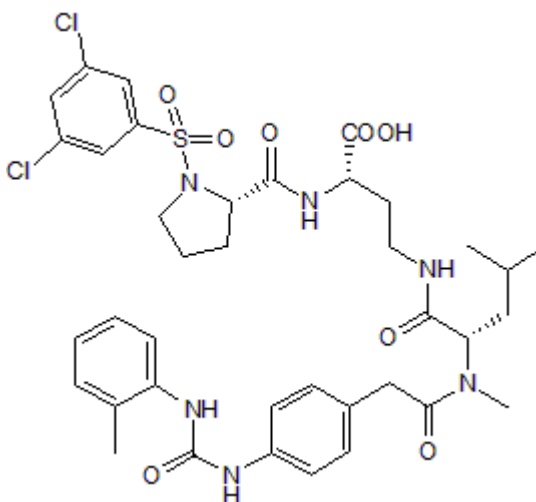
Batch Molecular Weight: 835.8

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

TLC: $R_f = 0.4$ (Dichloromethane:IPA [9:1])

HPLC: Shows >98.2% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: $[\alpha]_D = -102.7$ (Concentration = 1, Solvent = Ethanol)

Microanalysis:

Carbon Hydrogen Nitrogen

Theoretical 54.61 5.79 10.06

Found 54.63 5.7 9.9

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USA & CANADA Tel: (800) 343-7475 EUROPE Tel: +44 (0)1235 529449 CHINA Tel: +86 (21) 52380373
www.RnDSystems.com

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Description:

Highly selective and potent inhibitor of integrin $\alpha_4\beta_1$ (Very Late Antigen 4; VLA-4) ($K_d < 10$ pM). Selectively binds $\alpha_4\beta_1$ over a range of other integrins (IC_{50} values are 1.8, 138, 1053, > 500 and > 10,000 nM for $\alpha_4\beta_1$, $\alpha_9\beta_1$, $\alpha_2\beta_1$, $\alpha_4\beta_7$ and $\alpha_{11b}\beta_3$, respectively). Induces a 30-fold increase in mobilization of murine hematopoietic stem and progenitor cells; displays a 3-fold additive effect with AMD 3100 (Cat. No. 3299).

Physical and Chemical Properties:

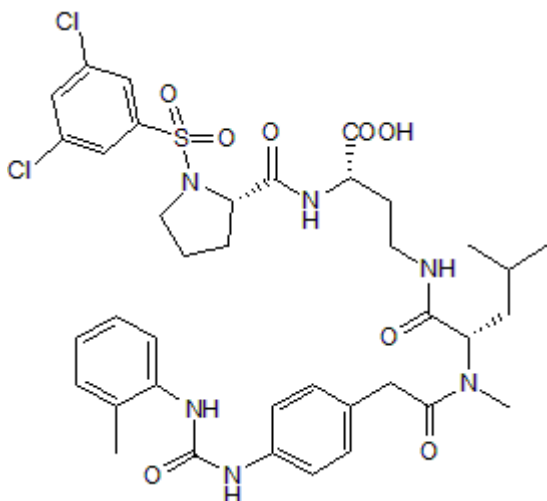
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Batch Molecular Weight: 835.8

Physical Appearance: White solid

Minimum Purity: >98%

Batch Molecular Structure:



References:

Leone *et al* (2003) An assessment of the mechanistic differences between two integrin alpha 4 beta 1 inhibitors, the monoclonal antibody TA-2 and the small molecule BIO5192, in rat experimental autoimmune encephalomyelitis. *J.Pharmacol.Exp.Ther.* **305** 1150. PMID: 12626659.

Xu *et al* (2008) A chemical approach to stem-cell biology and regenerative medicine. *Nature* **453** 338. PMID: 18480815.

Ramirez *et al* (2009) BIO5192, a small molecule inhibitor of VLA-4, mobilizes hematopoietic stem and progenitor cells. *Blood*. **1340** 1340. PMID: 19571319.

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.

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