

**Product Name:** BIO 5192

**Catalog No.:** 5051

**Batch No.:** 2

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<sub>38</sub>H<sub>46</sub>Cl<sub>2</sub>N<sub>6</sub>O<sub>8</sub>S.½H<sub>2</sub>O

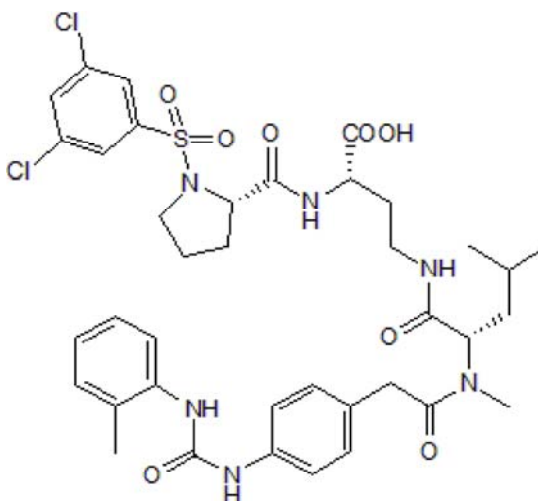
**Batch Molecular Weight:** 826.79

**Physical Appearance:** White solid

**Solubility:** DMSO to 100 mM

**Storage:** Store at -20°C

**Batch Molecular Structure:**



## 2. ANALYTICAL DATA

**HPLC:** Shows 98.5% purity

**<sup>1</sup>H NMR:** Consistent with structure

**Mass Spectrum:** Consistent with structure

**Microanalysis:**

	Carbon	Hydrogen	Nitrogen
Theoretical	55.2	5.73	10.16
Found	54.97	5.6	10.11

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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). Decreases oxidative damage and improves neurological function following spinal cord injury in rats. Please see product datasheet on www.tocris.com for full description.

**Physical and Chemical Properties:**

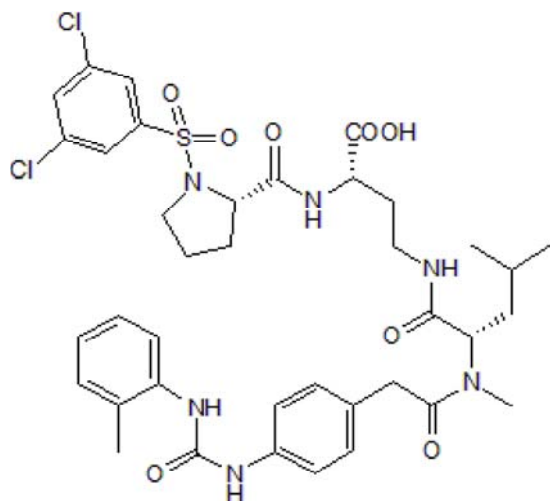
Batch Molecular Formula:  $C_{38}H_{46}Cl_2N_6O_8S \cdot \frac{1}{2}H_2O$

Batch Molecular Weight: 826.79

Physical Appearance: White solid

**Minimum Purity:**  $\geq 98\%$

**Batch Molecular Structure:**



**References:**

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

Bao *et al* (2008) An integrin inhibiting molecule decreases oxidative damage and improves neurological function after spinal cord injury. *Exp.Neurol* **214** 160. PMID: 18926823.

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

**Storage:** Store at  $-20^{\circ}C$

**Solubility & Usage Info:**

DMSO 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  $45-60^{\circ}C$  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  $-20^{\circ}C$  or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

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**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