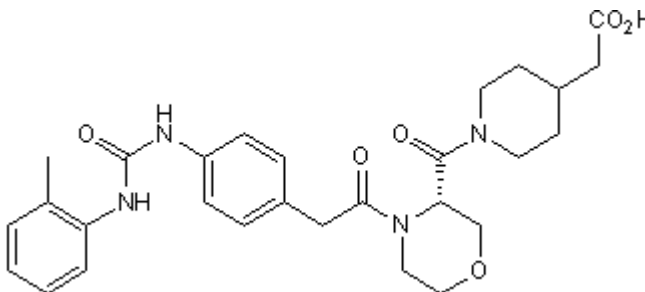


Product Name: TCS 2314 **Catalog No.:** 3900 **Batch No.:** 1
CAS Number: 317353-73-4
IUPAC Name: 1-[[[(3S)-4-[2-[4-[[[(2-Methylphenyl)amino]carbonyl]amino]phenyl]acetyl]-3-morpholinyl]carbonyl]-4-piperidinediacetic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₄N₄O₆·H₂O
Batch Molecular Weight: 540.61
Physical Appearance: Off-white solid
Solubility: DMSO to 100 mM
 ethanol to 50 mM
Storage: Store at RT
Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.11 (Dichloromethane:Methanol [9:1])
HPLC: Shows 99.2% purity
Chiral HPLC: Shows 98.4% purity
¹H NMR: Consistent with structure
Mass Spectrum: Consistent with structure
Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	62.21	6.71	10.36
Found	62.02	6.67	10.28

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

Product Name: TCS 2314

Catalog No.: 3900

Batch No.: 1

CAS Number: 317353-73-4

IUPAC Name: 1-[[[(3S)-4-[2-[4-[[[(2-Methylphenyl)amino]carbonyl]amino]phenyl]acetyl]-3-morpholinyl]carbonyl]-4-piperidinediacetic acid

Description:

Integrin very late antigen-4 (VLA-4; $\alpha_4\beta_1$) antagonist ($IC_{50} = 4.4$ nM). Blocks the activation of inflammatory cells.

Physical and Chemical Properties:

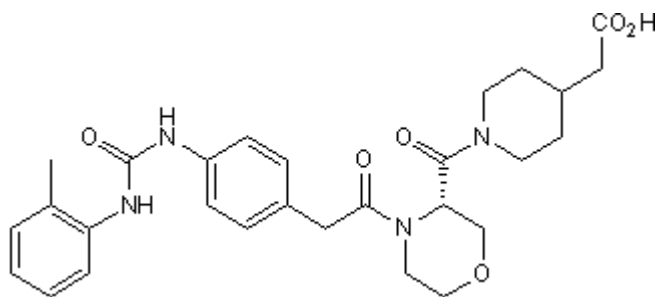
Batch Molecular Formula: $C_{28}H_{34}N_4O_6 \cdot H_2O$

Batch Molecular Weight: 540.61

Physical Appearance: Off-white solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at RT

Solubility & Usage Info:

DMSO to 100 mM

ethanol 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.

References:

Muro et al (2009) Discovery of *trans*-4-[1-[[[2,5-Dichloro-4-(1-methyl-3-indolyl)carboxamido]phenyl]acetyl]]-(4S)-methoxy-(2S)-pyrrolidinylmethoxy]cyclohexanecarboxylic acid: an orally active, selective very late antigen-4 antagonist. *J.Med.Chem.* **52** 7974. PMID: 19891440.

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