

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]-1-3-morpholinyl]carbonyl]-4-piperidinediacetic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₈H₃₄N₄O₆·H₂O

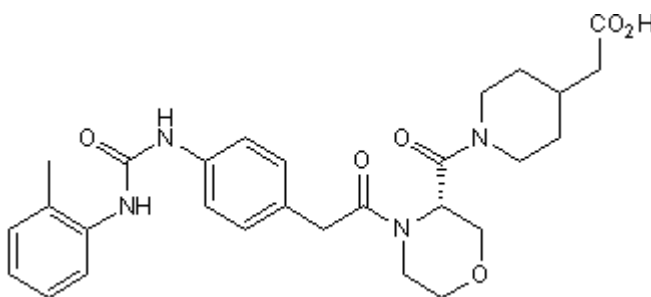
Batch Molecular Weight: 540.61

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

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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:

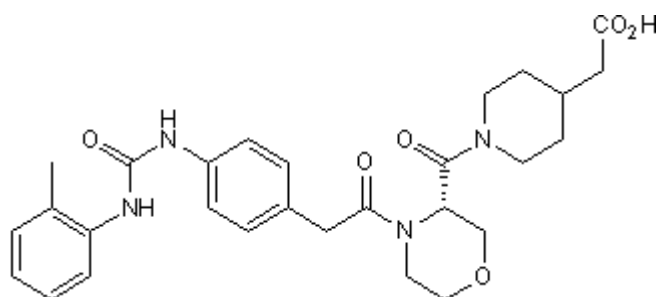
Batch Molecular Formula: $C_{28}H_{34}N_4O_6 \cdot H_2O$

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-indolylcarboxamido)phenyl]acetyl]-(4S)-methoxy-(2S)-pyrrolidinylmethoxy]cyclohexanecarboxylic acid: an orally active, selective very late antigen-4 antagonist. *J.Med.Chem.* **52** 7974. PMID: 19891440.

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