

Product Name: UK 370106

Catalog No.: 2900

Batch No.: 2

CAS Number: 230961-21-4

IUPAC Name: (βR)- β -[[[(1S)-1-[[[(1S)-2-Methoxy-1-phenylethyl]amino]carbonyl]-2,2-dimethylpropyl]amino]carbonyl]-2-methyl-[1,1'-biphenyl]-4-hexanoic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₃₅H₄₄N₂O₅·½H₂O

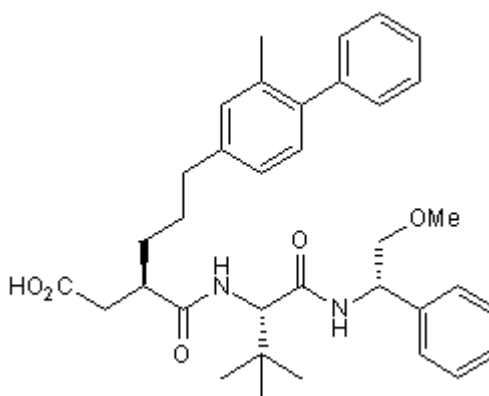
Batch Molecular Weight: 577.23

Physical Appearance: White solid

Solubility: DMSO to 100 mM
ethanol to 25 mM

Storage: Store at -20°C

Batch Molecular Structure:



2. ANALYTICAL DATA

TLC: R_f = 0.45 (Diethyl ether:Petroleum ether:Acetic acid [1:1:1])

HPLC: Shows 95.9% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	72.83	7.77	4.85
Found	72.64	7.83	4.93

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

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Description:

Highly selective MMP-3 and MMP-12 inhibitor (IC₅₀ values are 0.023, 0.042, 1.75, 2.3, 5.8, 30.4, 34.2 and 66.9 μ M at MMP 3, 12, 8, 13, 7, 9, 2 and 14 respectively.) Inhibits fibronectin cleavage (IC₅₀ = 320 nM) and has little effect on keratinocyte migration in vitro. Substantially inhibits MMP-3 in an ex vivo model of chronic dermal ulcers.

Physical and Chemical Properties:

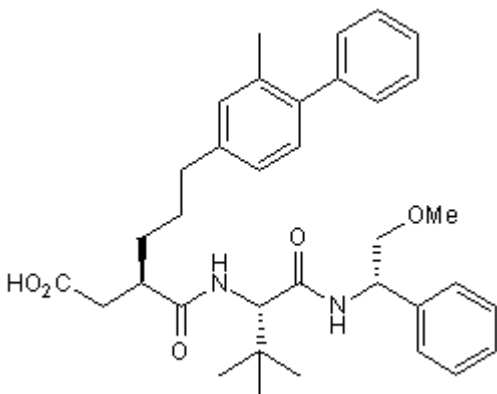
Batch Molecular Formula: C₃₅H₄₄N₂O₅. $\frac{1}{4}$ H₂O

Batch Molecular Weight: 577.23

Physical Appearance: White solid

Minimum Purity: >95%

Batch Molecular Structure:



References:

Fray et al (2003) A potent, selective inhibitor of matrix metalloproteinase-3 for the topical treatment of chronic duodenal ulcers. *J.Med.Chem.* **46** 3514. PMID: 12877590.

Whitlock et al (2007) A novel series of highly selective inhibitors of MMP-3. *Bioorg.Med.Chem.Letts.* **17** 6750.

Matthews et al (2008) Formulation, stability and thermal analysis of lyophilised wound healing wafers containing an insoluble MMP-3 inhibitor and a non-ionic surfactant. *Int.J.Pharmaceutics* **356** 110.

Storage: Store at -20°C

Solubility & Usage Info:

DMSO to 100 mM

ethanol to 25 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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