

**Product Name:** UK 370106

**Catalog No.:** 2900

**Batch No.:** 2

**CAS Number:** 230961-21-4

**IUPAC Name:** ( $\beta R$ )- $\beta$ -[[[(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:** C<sub>35</sub>H<sub>44</sub>N<sub>2</sub>O<sub>5</sub>·½H<sub>2</sub>O

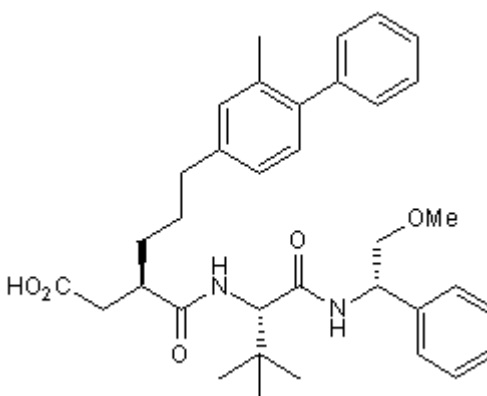
**Batch Molecular Weight:** 577.23

**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<sub>f</sub> = 0.45 (Diethyl ether:Petroleum ether:Acetic acid [1:1:1])

**HPLC:** Shows 95.9% purity

**<sup>1</sup>H 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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SYSTEMS®

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**Description:**

Highly selective MMP-3 and MMP-12 inhibitor (IC<sub>50</sub> values are 0.023, 0.042, 1.75, 2.3, 5.8, 30.4, 34.2 and 66.9  $\mu$ M at MMP 3, 12, 8, 13, 7, 9, 2 and 14 respectively.) Inhibits fibronectin cleavage (IC<sub>50</sub> = 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:**

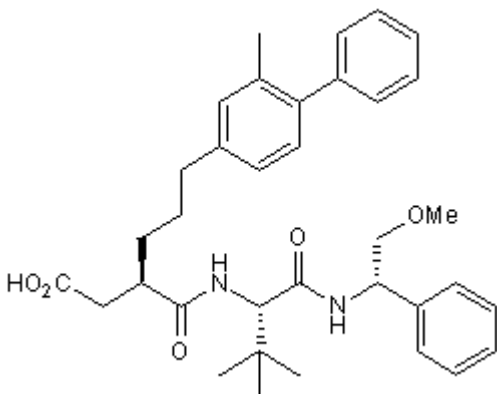
Batch Molecular Formula: C<sub>35</sub>H<sub>44</sub>N<sub>2</sub>O<sub>5</sub>.<sup>1</sup>/<sub>4</sub>H<sub>2</sub>O

Batch Molecular Weight: 577.23

Physical Appearance: White solid

**Minimum Purity:** >95%

**Batch Molecular Structure:**



**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.

**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.

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