

Product Name: Argatroban

Catalog No.: 1637

Batch No.: 1

CAS Number: 74863-84-6

IUPAC Name: (2*R*,4*R*)-1-[(2*S*)-5-[(aminoiminomethyl)amino]-1-oxo-2-[[[(1,2,3,4-tetrahydro-3-methyl-8-quinoliny)sulfonyl]amino]pentyl]-4-methyl-2-piperidinecarboxylic acid

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: C₂₃H₃₆N₆O₅S·1½H₂O

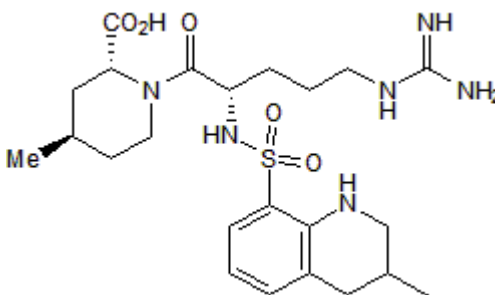
Batch Molecular Weight: 531.15

Physical Appearance: White solid

Solubility: DMSO to 100 mM
1eq. HCl to 10 mM
ethanol to 5 mM

Storage: Store at +4°C

Batch Molecular Structure:



2. ANALYTICAL DATA

HPLC: Shows 100% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Optical Rotation: [α]_D = +78 (Concentration = 1, Solvent = 0.2N HCl)

Microanalysis:

	Carbon	Hydrogen	Nitrogen
Theoretical	52.01	7.31	15.82
Found	51.86	7.24	15.7

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Description:

Potent inhibitor of thrombin mediated fibrinogen cleavage ($K_i = 19$ nM). Competitive inhibitor of thrombin-induced platelet activation and clotting. Shown to exhibit antithrombotic activity in animal models.

Physical and Chemical Properties:

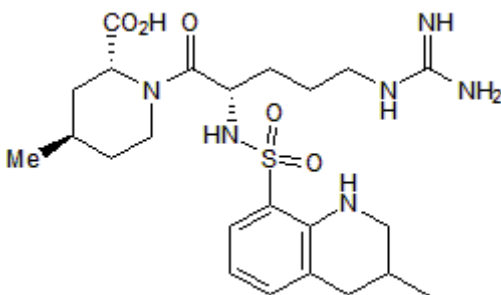
Batch Molecular Formula: $C_{23}H_{36}N_6O_5S \cdot 1\frac{1}{4}H_2O$

Batch Molecular Weight: 531.15

Physical Appearance: White solid

Minimum Purity: >99%

Batch Molecular Structure:



Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM
1eq. HCl to 10 mM
ethanol to 5 mM

This compound is a mixture of 2 diastereomers (approximate ratio 65/35)

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:

Kikumoto et al (1984) Selective inhibition of thrombin by (2R,4R)-4-methyl-1-[N2-[(3-methyl-1,2,3,4-tetrahydro-8-quinolinyl)++ +) sulfonyl]-1-arginyl]-2-piperidinecarboxylic acid. *Biochemistry* **23** 85. PMID: 6691968.

Fitzgerald and Fitzgerald (1989) Role of thrombin and thromboxane A_2 in reocclusion following coronary thrombolysis with tissue-type plasminogen activator. *Proc.Natl.Acad.Sci.USA* **86** 7585.

Jang et al (1990) Prevention of platelet-rich arterial thrombosis by selective thrombin inhibition. *Circulation* **81** 219. PMID: 2297828.

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