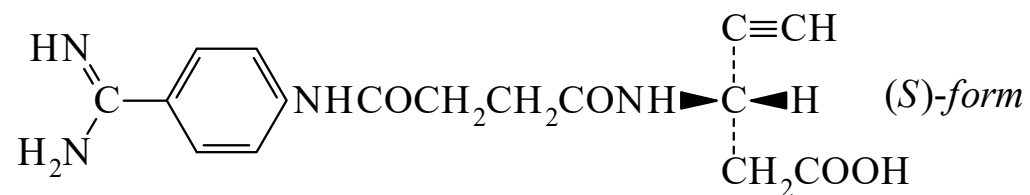




>>Entry Name: 3-[[4-[[4-(Aminoiminomethyl)phenyl]amino]-1,4-dioxobutyl]amino]-4-pentynoic acid, 9Cl



Related CAS Registry Numbers(s): 149727-64-0 149727-65-1 169237-79-0 169237-81-4 169275-97-2 169275-98-3

Molecular Formula: C₁₆H₁₈N₄O₄

Molecular Weight: 330.343

Accurate Mass: 330.132806

Percentage Composition: C 58.17%; H 5.49%; N 16.96%; O 19.37%

Use/Importance: Fibrinogen binding antagonist

>>Variant: (S)-form

Synonym(s): SC 54701A

CAS Registry Number: 149193-61-3

Molecular Formula: C₁₆H₁₈N₄O₄

Molecular Weight: 330.343

Accurate Mass: 330.132806

Percentage Composition: C 58.17%; H 5.49%; N 16.96%; O 19.37%

Other Data: Pharmacol. active isomer

>>Derivative: Hydrochloride

CAS Registry Number: 149177-89-9

Optical Rotation: [α]_D -33.7 (c, 1.45 in MeOH)

>>Derivative: Et ester

Synonym(s): Xemilofiban, INN. SC 54684A

CAS Registry Number: 149820-74-6

Molecular Formula: C₁₈H₂₂N₄O₄

Molecular Weight: 358.396

Accurate Mass: 358.164106

Percentage Composition: C 60.32%; H 6.19%; N 15.63%; O 17.86%

Use/Importance: Platelet aggregation inhibitor, glycoprotein receptor GP IIb/IIIa antagonist. Antithrombotic agent

Development Status: In clinical trials (1996)

Other Data: Prodrug of parent acid

>>Derivative: Et ester, hydrochloride

Synonym(s): Xemilofiban hydrochloride, USAN

CAS Registry Number: 156586-91-3

>>Variant: (±)-form

CAS Registry Number: 149251-13-8

Molecular Formula: C₁₆H₁₈N₄O₄

Molecular Weight: 330.343

Accurate Mass: 330.132806

Percentage Composition: C 58.17%; H 5.49%; N 16.96%; O 19.37%

Physical Description: Solid (as trifluoroacetate)

>>Derivative: Et ester

CAS Registry Number: 149193-59-9

Physical Description: Solid (as trifluoroacetate)

References: