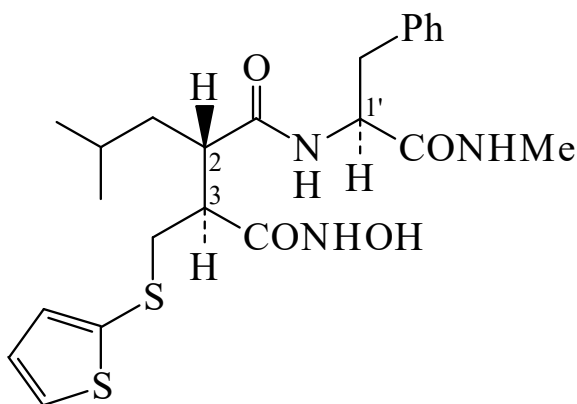




>>Entry Name: Batimastat, BAN, INN, USAN

Synonym(s): *N*⁴-Hydroxy-*N*¹-[2-(methylamino)-2-oxo-1-(phenylmethyl)ethyl]-2-(2-methylpropyl)-3-[(2-thienylthio)methyl]butanediamide, 9Cl. [4-(*N*-Hydroxyamino)-2-isobutyl-3-(thiophen-2-ylthiomethyl)succinyl]phenylalanine *N*-methanamide. Barinatrix. BB-94



CAS Registry Number: 130370-60-4

Molecular Formula: C₂₃H₃₁N₃O₄S₂

Molecular Weight: 477.648

Accurate Mass: 477.175597

Percentage Composition: C 57.84%; H 6.54%; N 8.80%; O 13.40%; S 13.43%

Use/Importance: Matrix metalloproteinase inhibitor. Restricts tumour growth

Physical Description: Cryst. (MeOH aq.)

Melting Point: Mp 236-238°

Calculated Log P Data: Log P 3.09 (calc)

Other Data: Stereochem. is (2*R*,3*S*,1'*S*)

>>Derivative: Na salt

CAS Registry Number: 130464-84-5

Physical Description: Solid

Melting Point: Mp 170°

Optical Rotation: [α]_D -67 (c, 1 in MeOH)

References:

Pat. Coop. Treaty (WIPO), 1990, *British Biotech*, 90 05 719; *CA*, **113**, 212677c, (*synth, pharmacol*)

Davies, B. *et al.*, *Cancer Res.*, 1993, **53**, 2087, (*pharmacol*)

Wang, X. *et al.*, *Cancer Res.*, 1994, **54**, 4726, (*pharmacol*)

Chirivi, R.G.S. *et al.*, *Int. J. Cancer*, 1994, **58**, 460, (*pharmacol*)

Taraboletti, G. *et al.*, *J. Natl. Cancer Inst.*, 1995, **87**, 293, (*pharmacol*)