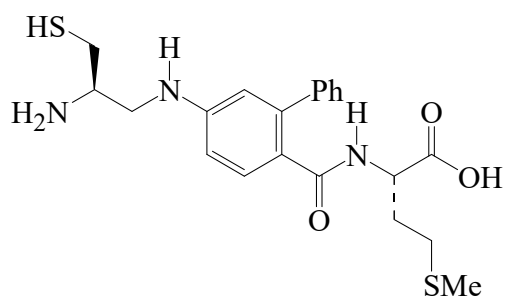




>>Entry Name: *N*-[[5-[(2-Amino-3-mercaptopropyl)amino][1,1']-biphenyl]-2-yl]carbonylmethionine, 9Cl

Synonym(s): FTI 276



Molecular Formula: C₂₁H₂₇N₃O₃S₂

Molecular Weight: 433.595

Accurate Mass: 433.149382

Percentage Composition: C 58.17%; H 6.28%; N 9.69%; O 11.07%; S 14.79%

Biological Use/Importance: Peptidomimetic inhibitor of protein farnesyl transferase. Antineoplastic agent

>>Variant: (L)-(R)-form

CAS Registry Number: 170006-72-1

Molecular Formula: C₂₁H₂₇N₃O₃S₂

Molecular Weight: 433.595

Accurate Mass: 433.149382

Percentage Composition: C 58.17%; H 6.28%; N 9.69%; O 11.07%; S 14.79%

Optical Rotation: $[\alpha]_{\text{D}}^{25} -13.6$ (c, 0.005 in MeOH)

>>Derivative: Me ester

Synonym(s): FTI 277

CAS Registry Number: 170006-73-2

Molecular Formula: C₂₂H₂₉N₃O₃S₂

Molecular Weight: 447.621

Accurate Mass: 447.165032

Percentage Composition: C 59.03%; H 6.53%; N 9.39%; O 10.72%; S 14.33%

>>Derivative: Me ester; hydrochloride

CAS Registry Number: 180977-34-8

Optical Rotation: $[\alpha]_{\text{D}}^{25} -12.1$ (c, 0.008 in MeOH)

Other Data: Not clear whether reported optical rotation refers to hydrochloride salt or base

References:

Sun, J. *et al.*, *Cancer Res.*, 1995, **55**, 4243-4247, (*pharmacol*)

Lerner, E.C. *et al.*, *J. Biol. Chem.*, 1995, **270**, 26802-26806, (*synth, Me ester, activity*)

Bernhard, E.J. *et al.*, *Cancer Res.*, 1996, **56**, 1727-1730, (*FTI 277 pharmacol*)

Pat. Coop. Treaty (WIPO), 1996, *Univ. of Pittsburgh*, 96 21 456; *CA*, **125**, 212665v, (*R-form, synth, Me ester, pharmacol*)