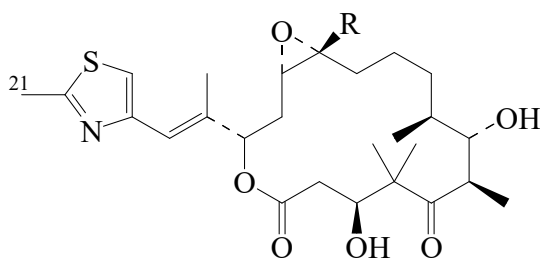




>>Entry Name: Epothilone A



R = H

CAS Registry Number: 152044-53-6

Type of Compound Code(s): VC0100 VX6935

Molecular Formula: C₂₆H₃₉NO₆S

Molecular Weight: 493.663

Accurate Mass: 493.249809

Percentage Composition: C 63.26%; H 7.96%; N 2.84%; O 19.45%; S 6.50%

Biological Source: Prod. by *Sorangium cellulosum*

Biological Use/Importance: Induces cellular microtubuli assembly and stabilisation by a Taxol™-like mechanism. Competes for same binding site on microtubules as Taxol™. Antiproliferative and potential anticancer agent. Antifungal and cytotoxic agent

Physical Description: Cryst. (EtOAc/toluene)

Melting Point: Mp 95°

Optical Rotation: $[\alpha]_D^{21}$ -47.1 (c, 1 in MeOH)

UV: [neutral] $\lambda_{\max}$ 211 (ϵ 17800); 249 (ϵ 12500) (MeOH) [neutral] $\lambda_{\max}$ 211 (ϵ 17800); 249 (ϵ 12500) (MeOH) (Berdy)

>>Derivative: 21-Hydroxy

Synonym(s): Epothilone E

CAS Registry Number: 201049-37-8

Type of Compound Code(s): VX6935 VC0100

Molecular Formula: C₂₆H₃₉NO₇S

Molecular Weight: 509.663

Accurate Mass: 509.244724

Percentage Composition: C 61.27%; H 7.71%; N 2.75%; O 21.97%; S 6.29%

Biological Source: Prod. by *Sorangium cellulosum*

Biological Use/Importance: Antitumour agent

Optical Rotation: $[\alpha]_D^{22}$ -27.5 (c, 0.2 in CHCl₃)

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