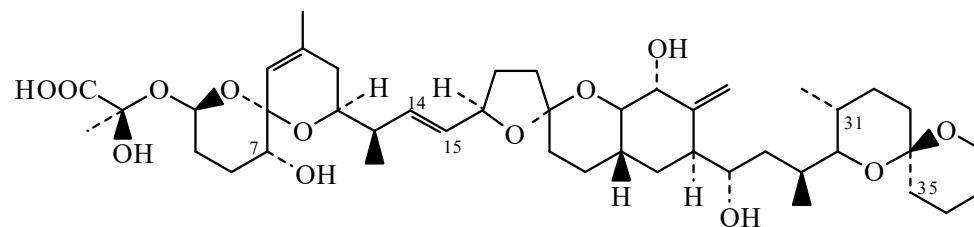




>>Entry Name: Okadaic acid

Synonym(s): 9,10-Deepithio-9,10-didehydroacanthifolicin. PL toxin II



CAS Registry Number: 78111-17-8

Molecular Formula: C₄₄H₆₈O₁₃

Molecular Weight: 805.013

Accurate Mass: 804.465995

Percentage Composition: C 65.65%; H 8.51%; O 25.84%

Biological Source: Found in *Halichondria okadai* and *Halichondria melanodocia*. Metab. of *Prorocentrum lima*

Use/Importance: Mammalian toxin. Shows cytotoxic properties against human epidermoid carcinoma

Physical Description: Cryst. (C₆H₆/CHCl₃)

Melting Point: Mp 164-166°

Optical Rotation: $[\alpha]_D^{20} +53.3$ (c, 0.182 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, hexane; poorly sol. H₂O, hexane

UV: [neutral] $\lambda_{\max}$ 0 (end) (ϵ) (MeOH) (Derep) [neutral] $\lambda_{\max}$ (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ 192 µg/kg (i.p. mice) ; BERDY HAZD : LD₅₀ (mus, ivn) .192 mg/kg

Sigma: O4511

>>Derivative: Me ester

Molecular Formula: C₄₅H₇₀O₁₃

Molecular Weight: 819.04

Accurate Mass: 818.481645

Percentage Composition: C 65.99%; H 8.61%; O 25.39%

Physical Description: Cryst. (hexane/C₆H₆)

Melting Point: Mp 127-133°

Optical Rotation: $[\alpha]_D^{25} +28$ (c, 0.38 in CHCl₃)

>>Derivative: *p*-Bromophenacyl ester

Melting Point: Mp 134-135°

>>Derivative: 6-Hydroxy-2-methyl-2*E*,4*E*-hexadienoyl ester

CAS Registry Number: 145781-81-3

Molecular Formula: C₅₁H₇₈O₁₄

Molecular Weight: 915.169

Accurate Mass: 914.53916

Percentage Composition: C 66.93%; H 8.59%; O 24.48%

Biological Source: Isol. from *Prorocentrum concavum*

>>Derivative: 7-Hydroxy-2-methyl-2*E*,4*E*-heptadienoyl ester

CAS Registry Number: 145814-30-8

Molecular Formula: C₅₂H₈₀O₁₄

Molecular Weight: 929.196

Accurate Mass: 928.55481

Percentage Composition: C 67.22%; H 8.68%; O 24.11%

Biological Source: Isol. from *Prorocentrum concavum* and *Prorocentrum lima*

>>Derivative: 7-Hydroxy-2,4-dimethyl-2*E*,4*E*-heptadienoyl ester

CAS Registry Number: 157376-74-4