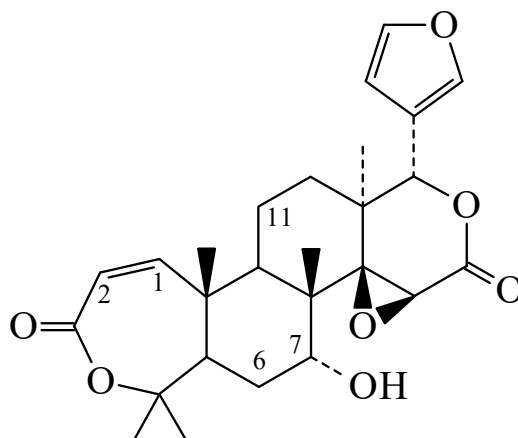




>>Entry Name: Obacunol

Synonym(s): Tricoccin S₂₃



CAS Registry Number: 17182-59-1

Molecular Formula: C₂₆H₃₂O₇

Molecular Weight: 456.535

Accurate Mass: 456.214805

Percentage Composition: C 68.40%; H 7.06%; O 24.53%

Biological Source: Constit. of *Lovoa trichiliodes* and *Cneorum tricoccon*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 256-260°

Optical Rotation: [α]_D +73.6

>>Derivative: 7-Ketone

Synonym(s): Obacunone. Casimirolide. Tricoccin S₃

CAS Registry Number: 751-03-1

Molecular Formula: C₂₆H₃₀O₇

Molecular Weight: 454.519

Accurate Mass: 454.199155

Percentage Composition: C 68.71%; H 6.65%; O 24.64%

Biological Source: Constit. of *Citrus* spp., *Poncirus trifoliata*, *Fortunella margarita*, *Casimiroa edulis*, *Phellodendron* spp. and others in the Rutaceae

Physical Description: Cryst. (MeOH)

Melting Point: Mp 229-230°

Optical Rotation: [α]_D -50 (CHCl₃)

UV: [neutral] $\lambda_{\max}$ 288 (ϵ 1360) (MeOH) (Derep)

>>Derivative: 6 β -Acetoxy

Synonym(s): 6 β -Acetoxyobacunol

Molecular Formula: C₂₈H₃₄O₉

Molecular Weight: 514.571

Accurate Mass: 514.220285

Percentage Composition: C 65.36%; H 6.66%; O 27.98%

Biological Source: Constit. of *Trichilia trifolia*

>>Derivative: 6 α -Acetoxy, 7-Ac

Synonym(s): 6 α -Acetoxyobacunol acetate

CAS Registry Number: 121959-09-9

Molecular Formula: C₃₀H₃₆O₁₀

Molecular Weight: 556.608

Accurate Mass: 556.23085

Percentage Composition: C 64.74%; H 6.52%; O 28.74%

Biological Source: Constit. of *Dysoxylum richii*

Physical Description: Amorph. solid

Melting Point: Mp 236-238°

>>Derivative: 7-Ac

Synonym(s): Cneorin I. Tricoccin S₄₁