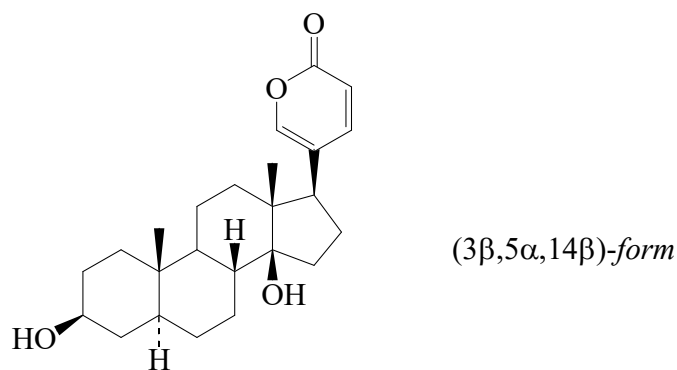




>>Entry Name: 3,14-Dihydroxybufa-20,22-dienolide



Molecular Formula: C₂₄H₃₄O₄

Molecular Weight: 386.53

Accurate Mass: 386.24571

Percentage Composition: C 74.58%; H 8.87%; O 16.56%

Other Data: All refs. before 1997 refer principally to Bufalin and its derivs.

>>Variant: (3β,5α,14β)-form

Molecular Formula: C₂₄H₃₄O₄

Molecular Weight: 386.53

Accurate Mass: 386.24571

Percentage Composition: C 74.58%; H 8.87%; O 16.56%

>>Derivative: 3-*O*-[β-D-Glucopyranosyl-(1→4)-α-L-rhamnopyranoside]

Synonym(s): 4,5-Dihydroscillaren A

CAS Registry Number: 131221-53-9

Molecular Formula: C₃₆H₅₄O₁₃

Molecular Weight: 694.815

Accurate Mass: 694.356445

Percentage Composition: C 62.23%; H 7.83%; O 29.93%

Biological Source: Constit. of *Urginea sanguinea*

Physical Description: Needles (MeOH)

Melting Point: Mp 192-194°

Optical Rotation: [α]_D -44.4 (c, 0.12 in MeOH)

UV: [neutral] λ_{max} 298 () (MeOH)

>>Variant: (3β,5β,14β)-form

Synonym(s): Bufalin

CAS Registry Number: 465-21-4

Molecular Formula: C₂₄H₃₄O₄

Molecular Weight: 386.53

Accurate Mass: 386.24571

Percentage Composition: C 74.58%; H 8.87%; O 16.56%

Biological Source: Constit. of toad venom

Use/Importance: Cardiotonic agent

Physical Description: Cryst. (EtOAc)

Melting Point: Mp 240-243°

Optical Rotation: [α]_D -9 (CHCl₃)

Hazard & Toxicity: Highly toxic, LD₅₀ (cat, ivn) 0.14 mg/kg, LD₅₀ (mus, ivn) 0.74 mg/kg

Sigma: B0261

>>Derivative: 3-Ac

Melting Point: Mp 230°. Mp 247° (double Mp)

Optical Rotation: [α]_D -6 (CHCl₃)