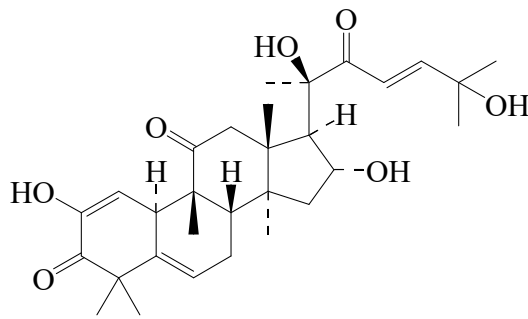




>>Entry Name: 2,16,20,25-Tetrahydroxycucurbita-1,5,23-triene-3,11,22-trione

Synonym(s): 16,20,25-Trihydroxycucurbita-5,23-diene-2,3,11,22-tetrone



Molecular Formula: C₃₀H₄₂O₇

Molecular Weight: 514.658

Accurate Mass: 514.293055

Percentage Composition: C 70.01%; H 8.23%; O 21.76%

Biological Use/Importance: Cucurbitacins possess antihepatotoxic, antineoplastic and cathartic activity

Solubility: BERDY SOL: Sol. bases, EtOAc, Et₂O; poorly sol. H₂O, hexane, C₆H₆

UV: [base] λ_{max} 234 (ε 11400); 314 (ε 6750) (NAOH) (Berdy) [neutral] λ_{max} 234 (ε 11000); 269 (ε 6850) (EtOH) (Berdy)

>>Variant: (16α,20R,23E)-form

Synonym(s): Cucurbitacin I. Elatericin B

CAS Registry Number: 2222-07-3

Molecular Formula: C₃₀H₄₂O₇

Molecular Weight: 514.658

Accurate Mass: 514.293055

Percentage Composition: C 70.01%; H 8.23%; O 21.76%

Physical Description: Cryst.

Melting Point: Mp 148-149 dec.°

Optical Rotation: [α]_D²⁰ -58.5 (MeOH)

>>Derivative: 2-O-β-D-Glucopyranoside

CAS Registry Number: 29803-94-9

Molecular Formula: C₃₆H₅₂O₁₂

Molecular Weight: 676.8

Accurate Mass: 676.34588

Percentage Composition: C 63.89%; H 7.74%; O 28.37%

Biological Source: Constit. of *Citrullus lanatus*

Melting Point: Mp 241-243°

Optical Rotation: [α]_D²⁰ -72.6 (EtOH)

>>Derivative: 20-Ac

Synonym(s): Datiscacin‡

CAS Registry Number: 38308-89-3

Molecular Formula: C₃₂H₄₄O₈

Molecular Weight: 556.695

Accurate Mass: 556.30362

Percentage Composition: C 69.04%; H 7.97%; O 22.99%

Biological Source: Constit. of *Datisca glomerata*

Biological Use/Importance: Antineoplastic agent

Melting Point: Mp 208-212°

Optical Rotation: [α]_D²³ -18 (c, 0.87 in CHCl₃)

Calculated Log P Data: Log P 0.32 (uncertain value) (calc)

UV: [neutral] λ_{max} 231 (ε 9600); 268 (ε 5400) (EtOH) (Berdy)