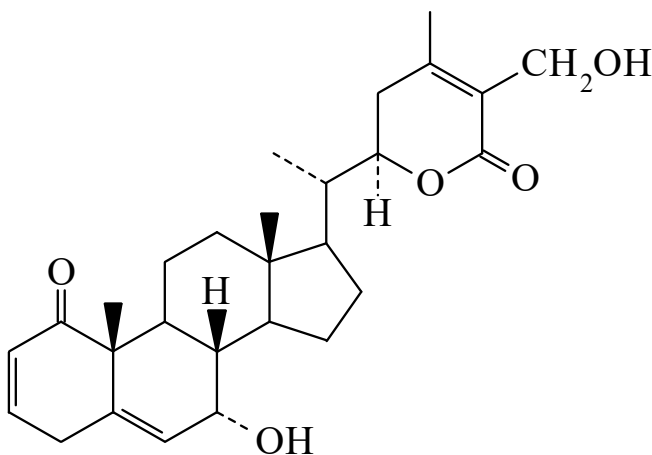




>>Entry Name: 7,27-Dihydroxy-1-oxowitha-2,5,24-trienolide



Molecular Formula: C₂₈H₃₈O₅

Molecular Weight: 454.605

Accurate Mass: 454.271925

Percentage Composition: C 73.98%; H 8.42%; O 17.60%

>>Variant: (7 α ,22*R*)-form

Type of Compound Code(s): AJ1400 VT1400

Molecular Formula: C₂₈H₃₈O₅

Molecular Weight: 454.605

Accurate Mass: 454.271925

Percentage Composition: C 73.98%; H 8.42%; O 17.60%

Biological Source: Constit. of *Withania somnifera*

>>Derivative: Di-Ac

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 208-209°

Optical Rotation: [α]_D -119 (c, 0.26 in CHCl₃)

>>Derivative: 27-*O*- β -D-Glucopyranoside

Synonym(s): Daturataturin A

CAS Registry Number: 133360-51-7

Type of Compound Code(s): VT1400

Molecular Formula: C₃₄H₄₈O₁₀

Molecular Weight: 616.747

Accurate Mass: 616.32475

Percentage Composition: C 66.21%; H 7.84%; O 25.94%

Biological Source: Constit. of *Datura tatura*

Physical Description: Amorph. powder

Optical Rotation: [α]_D²¹ -38.1 (c, 0.72 in Py)

References:

Lavie, D. *et al.*, *J.C.S.(C)*, 1971, 2032

Shinga, K. *et al.*, *Chem. Pharm. Bull.*, 1990, **38**, 3485, (*Daturataturin A*)