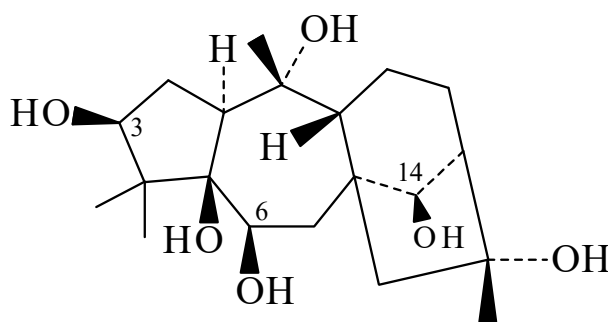




>>Entry Name: 3,5,6,10,14,16-Grayanotoxanehexol



Molecular Formula: C₂₀H₃₄O₆

Molecular Weight: 370.485

Accurate Mass: 370.23554

Percentage Composition: C 64.84%; H 9.25%; O 25.91%

>>Variant: (1 α ,3 β ,5 β ,6 β ,10 α ,14 β ,16 α)-form

Synonym(s): Grayanotoxin III. Andromedol

CAS Registry Number: 4678-45-9

Molecular Formula: C₂₀H₃₄O₆

Molecular Weight: 370.485

Accurate Mass: 370.23554

Percentage Composition: C 64.84%; H 9.25%; O 25.91%

Biological Source: Toxic constit. of *Leucothoe grayana*

Physical Description: Cryst. + 1/2EtOAc

Melting Point: Mp 218 dec.°

Optical Rotation: [α]_D¹⁵ -12

Hazard & Toxicity: Toxic

Sigma: G2786

>>Derivative: 14-Ac

Synonym(s): Grayanotoxin I. Andromedotoxin

CAS Registry Number: 4720-09-6

Molecular Formula: C₂₂H₃₆O₇

Molecular Weight: 412.522

Accurate Mass: 412.246105

Percentage Composition: C 64.06%; H 8.80%; O 27.15%

Biological Source: Toxic agent from *Rhododendron*, *Kalmia*, *Leucothoe* and *Lyonia* spp.

Physical Description: Cryst. (EtOAc/pentane)

Melting Point: Mp 267-270°

Optical Rotation: [α]_D²⁵ -8.8 (c, 2.3 in EtOH)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 1.3 mg/kg

>>Derivative: 6,14-Di-Ac

Synonym(s): Rhodojaponin IV

CAS Registry Number: 30460-34-5

Molecular Formula: C₂₄H₃₈O₈

Molecular Weight: 454.559

Accurate Mass: 454.25667

Percentage Composition: C 63.42%; H 8.43%; O 28.16%

Biological Source: Constit. of *Rhododendron* spp.

Physical Description: Cryst.

Melting Point: Mp 245-247°