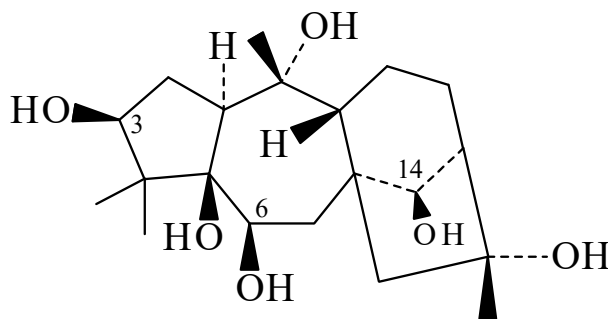




>>Entry Name: 3,5,6,10,14,16-Grayanotoxanehexol



**Molecular Formula:** C<sub>20</sub>H<sub>34</sub>O<sub>6</sub>

**Molecular Weight:** 370.485

**Accurate Mass:** 370.23554

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

>>Variant: (1 $\alpha$ ,3 $\beta$ ,5 $\beta$ ,6 $\beta$ ,10 $\alpha$ ,14 $\beta$ ,16 $\alpha$ )-form

**Synonym(s):** Grayanotoxin III. Andromedol

**CAS Registry Number:** 4678-45-9

**Molecular Formula:** C<sub>20</sub>H<sub>34</sub>O<sub>6</sub>

**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. + ½EtOAc

**Melting Point:** Mp 218 dec.°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>15</sup> -12

**Hazard & Toxicity:** Toxic

**Sigma:** G2786

>>Derivative: 14-Ac

**Synonym(s):** Grayanotoxin I. Andromedotoxin

**CAS Registry Number:** 4720-09-6

**Molecular Formula:** C<sub>22</sub>H<sub>36</sub>O<sub>7</sub>

**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:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> -8.8 (c, 2.3 in EtOH)

**Hazard & Toxicity:** BERDY HAZD : LD<sub>50</sub> (mus, ipr) 1.3 mg/kg

>>Derivative: 6,14-Di-Ac

**Synonym(s):** Rhodojaponin IV

**CAS Registry Number:** 30460-34-5

**Molecular Formula:** C<sub>24</sub>H<sub>38</sub>O<sub>8</sub>

**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°