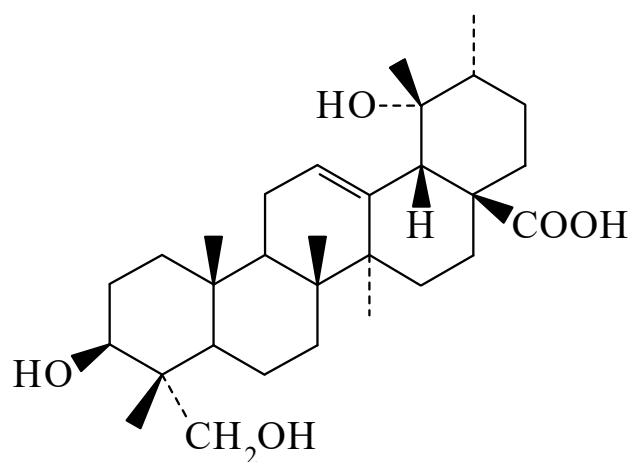




>>Entry Name: 3,19,23-Trihydroxy-12-ursen-28-oic acid



Molecular Formula: C₃₀H₄₈O₅

Molecular Weight: 488.706

Accurate Mass: 488.350175

Percentage Composition: C 73.73%; H 9.90%; O 16.37%

>>Variant: (3β,19α)-form

Synonym(s): Rotundic acid

CAS Registry Number: 20137-37-5

Molecular Formula: C₃₀H₄₈O₅

Molecular Weight: 488.706

Accurate Mass: 488.350175

Percentage Composition: C 73.73%; H 9.90%; O 16.37%

>>Derivative: Me ester

Molecular Formula: C₃₁H₅₀O₅

Molecular Weight: 502.733

Accurate Mass: 502.365825

Percentage Composition: C 74.06%; H 10.02%; O 15.91%

Physical Description: Cryst.

Melting Point: Mp 257°

Optical Rotation: [α]_D²⁴+38

>>Derivative: β-D-Glucopyranosyl ester

Synonym(s): Pedunculoside

CAS Registry Number: 42719-32-4

Molecular Formula: C₃₆H₅₈O₁₀

Molecular Weight: 650.848

Accurate Mass: 650.403

Percentage Composition: C 66.44%; H 8.98%; O 24.58%

Biological Source: Isol. from *Ilex oldhami*, *Ilex pedunculosa* and *Ilex rotunda*

Physical Description: Prisms (EtOAc)

Melting Point: Mp 213-214°

Optical Rotation: [α]_D²⁵+22 (c, 0.05 in MeOH)

>>Derivative: 3-O-α-L-Arabinopyranoside, 28-O-β-D-glucopyranosyl ester

Synonym(s): Ilekudinoside D

CAS Registry Number: 147235-21-0

Molecular Formula: C₄₁H₆₆O₁₄

Molecular Weight: 782.964

Accurate Mass: 782.44526

Percentage Composition: C 62.90%; H 8.50%; O 28.61%

Biological Source: Constit. of *Ilex kudincha*

Physical Description: Amorph. powder

Optical Rotation: [α]_D²³+11.5 (c, 2.16 in MeOH)