Terpenoids from Conyza Linifolia

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From the terpenoid extract of *Conyza linifolia* a rare daucane, an eudesmanolide and a triterpene were isolated.

Conyza (Family Asteraceae, tribe Astereae) is a genus with about 50 species and is distributed in the tropical regions¹. It has been placed in the subtribe Conyziinae and close to Microglossa and Nidorella. The genus is known to produce acetylenes and diterpenes²⁻⁴. While triterpenes, flavones and coumarins were reported from some species⁵. Previously, we reported a new glucoside form Conyza linifolia⁶, and reinvestigation of the species afforded a sesquiterpene with a rare skeleton, an eudesmanolide and a triterpene.

The present paper reports the isolation and structural elucidation of three terpenoid compounds from the leaves of *C. linifolia*. The structures were established by spectroscopic techniques as 10-oxo-isodauc-3-ene-15-al (1), taurin (2) and 23-hydroxyerthrodiol (3).

The aerial parts of *C. linifolia* (Willd.) Tackh. (= *Erigeron bonariensis* L.) were collected from El-Minia University campus in April 1987. A voucher specimen was deposited in the Herbarium of the University of Egypt. The ground aerial parts (600 g) were extracted with MeOH: $Et_2O:PE\ (1:1:1)$ and the extract was separated by CC (Silica gel), TLC and HPLC to give 10 mg 1, 15 mg 2 and 6 mg 3.

Compound (1)

The structure of 1 was deduced from the 1 H-NMR spectrum. The aldehydic proton appeared as a sharp singlet at δ 9.34. Spin decoupling allowed the assignment of all signals. The olefinic double doublet at δ 6.63 which is assigned to H-4 showed a coupling with a signal at δ 2.53, H-5, and a small coupling with H-2 at δ 2.45. In addition the multiplet at δ 2.71 was typical for a methylene group adjacent to a keto group. The other signals agreed with a compound previously isolated from *Chromolaena laevigata*⁷. The structure of 1 was further supported by 13 C-NMR which is reported for the first time.

10-Oxo-isodauc-3-ene-15-al 1: IR $v_{max}^{CHCl_3}$ cm⁻¹: 2750, 1670, 1700. MS m/z (rel. int.) 243 [M]⁺ (50), 219 [M—CH₃]⁺ (22), 191 [M—C₃H₇]⁺ (100), 163

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[191—CO]⁺ (83), 151 (95). ¹H-NMR (400 MHz, CDCl₃, δ -values: 9.34 (S, H-15), 6.63 (1H, dd, J = 6 and 1.5 Hz, H-4), 2.8–2.71 (2H, m, H-1), 2.53 (1H, dd, J = 9 and 5 Hz, H-5). 2.45 (2H, m, H-2), 2.20 (1H, ddd, J = 6, 10 and 14 Hz, H-8), 1.86 (1H, m, H-7), 1.82 (1H, ddd, J = 7, 7 and 9 Hz, H-6), 1.65 (1H, m, H-11), 1.43 (1H, m, H-7), 1.42 (1H, m, H-8), 1.31 (3H, S, H-14), 0.93 (6H, d, J = 7 Hz, H-12 and H-13). ¹³C-NMR (100.6 MHz, CDCl₃, δ -value): 38.9 (C-1, t), 35.1 (C-2, t), 143.7 (C-3, s), 158.5 (C-4, d), 55.4 (C-5, d), 53.2 (C-6, d), 19.7 (C-7, t) 26.7 (C-8, t), 59.6 (C-9, s), 212.1 (C-10, s), 32.3 (C-11, d), 21.9 (C-12, q), 19.4 (C-13, q), 25.0 (C-14, q), 192.7 (C-15, d), some signals may be

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interchangeable.

Compound (2)

The ¹H-NMR of 2 suggested that we were dealing with eudesmanolide skeleton. The IR, MS and ¹H-NMR spectral data were consistent with taurin⁸. Taurin 2: IR $v_{\text{max}}^{\text{CHCl}_3}$ cm⁻¹: 1770, 1700, 1200, 1480, MS m/z (rel. int.) 248

 $[M]^+$ (35), 233 $[M—CH₃]^+$ (10), 220 $[M—CO]^+$ (16), 1H -NMR (400 MHz, CDCl₃, δ -value): 4.59 (1H, brd, J = 12 Hz, H-6), 2.63 (1H ddd, J = 6, 7 and 13 Hz, H-2), 2.49 (1H, ddd, J = 0.7, 7 and 13 Hz, H-2'), 2.40–2.35 (2H, m, H-3), 2.30 (1H, m, H-11) 2.00 (1H, m, H-8), 1.96 (3H, br.s, H-15), 1.86 (1H, ddd, J = 4, 4 and 13 Hz, H-9), 1.73 (1H, dddd, J = 3.5, 12, 12 and 13 Hz, H-7), 1.61 (1H, m, H-8), 1.53 (1H, ddd, J = 4.5, 4.5 and 13 Hz), 1.32 (3H, s, H-14), 1.24 (3H, d, J = 7 Hz, H-13).

Compound (3)

Compound 3 showed a molecular ion at m/z 458 (C₃₀H₅₀O₃), indicating an oleanane triterpene with two hydroxylated methyl groups. The fragmentation pattern of MS and ¹H-NMR spectrum suggested that 3 is 23-hydroxyerthridiol⁹.

23-Hydroxyerthridiol 3: $IRv_{max}^{CHCl_3}$ cm⁻¹ 3510, 3460, 3430, 1725, 1340, MS m/z (rel. int.): 458 [M]⁺ (5), 440 [M—H₂O]⁺ (5) 427 [M—CH₂—CH₂—OH]⁺ (3), 409 [440—CH₂—OH]⁺ (6), 205 (15), 203 (30) 149 (70). ¹H-NMR (400 MHz, CDCl₃, δ -value): 5.26 (1H, t, J = 3.5 and 3.5 Hz, H-11) 3.74 (1H d, J = 10 Hz, H-23), 3.65 (1H, dd, J = 7 and 9 Hz, H-3), 3.55 (1H, d, J = 11, Hz, H-28), 3.44 (1H, d, J = 10 Hz, H-23), 3.21 (1H, d, J = 11 Hz, H-28), 1.15 (3H, s), 0.98 (3H, s),0.94 (3H, s), 0.91 (3H, s), 0.88 (3H, s), 0.87 (3H, s).

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