New Triterpene from *Conyza aegyptiaca L.**

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Triterpene, *Conyza aegyptiaca L.*

A reinvestigation of *C. aegyptiaca L.* gave in addition to phytol a new triterpene. Its structure was determined by IR, ^{1}H NMR and mass spectral data.

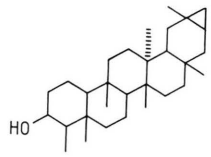
Introduction

From the large genus Conyza (tribe Astereae, family Compositae) about 10% of the approximately 2000 species in this tribe have been subjected to chemical scruting. However, work has been confined largely to root constituents. Among these, polyacetylenes, polyenes and related substances and, in certain groups, coumarins are very characteristic. Less widely distributed, perhaps because they are less intensively searched for, are diterpenoids, so far largely of the labdane and clerodane type.

Our previous investigation [1] of *C. aegyptiaca L.* resulted in isolation of α-curcumene, germacrene D, β-farnesene, caryophyllenepoxide, lachnophyllum ester, matricaria ester, stigmasterol, squalene and some acetylenic compounds from the plant material collected in August. In continuation of our study on the Egyptian Compositae [2] the present work deals with investigation of the same plant collected in April.

A reinvestigation of *C. aegyptiaca L.* afforded a phytol and a new triterpene. The molecular formula of the triterpene is $C_{30}H_{50}O$, was deduced from the chemical ionization mass spectrum, while the IR spectrum showed a well-defined absorption due to OH (3620 cm^{-1}). The ^{1}H NMR spectrum showed the presence of seven methyl groups, H-3 (3.73, dd, 1H, J = 5 Hz), with a (1H, dddd) centered at 0.35 (J = 7 Hz) suggesting the attachement of a cyclopropane ring to C-21 in epifriedelinol and the absence of the methyl group at C-30 (see Experimental). The triterpene gave molecular ion $[M]^+$ at m/z 426 corresponding to $C_{30}H_{50}O$. The fragment m/z 411, produced from $[M]^+$ after removal of a methyl group. The appearance of fragments m/z 394, 341, 275, 205 and 109 can be explained on the basis of elimination of OH, C_4H_5, C_5H_6, C_5H_{10} and C_7H_{12} from the fragment m/z 411. The m/z 109 ion is converted into the fragment ion m/z 55 (base peak) by loss of C_4H_6. Thus, the structure of the triterpene was settled to be 1.

The seasonal difference in the constituents of *C. aegyptiaca L.* is worthy of comment. The sample collected in August from the same locality did not contain this type of triterpene.



1

Experimental

The air dried plant material, collected in April, from the garden of Mansoura University, was extracted with $C_2H_5OC_2H_5$/petroleum ether/CH_3OH (1:3:1). The extract of the aerial parts of *C. aegyptiaca* (150 g) was first treated with CH_3OH to remove long chain hydrocarbons and then partially separated by CC (SiO_2) with petroleum ether and increasing amounts of $C_2H_5OC_2H_5$ and finally $C_2H_5OC_2H_5$/CH_3OH (10:1). The fraction obtained with petroleum ether/$C_2H_5OC_2H_5$ (9:1) afforded 10 mg phytol. The fraction obtained with petroleum ether/$C_2H_5OC_2H_5$ (3:1) afforded (1) 5 mg colourless oil; IR νCCl_4/max. cm^{-1}: 3620 (OH); MS m/z (rel. int.): 426.386 $[M]^+$ (2) (calcd for $C_{30}H_{50}O$: 426.386), 411 $[M-CH_3]^+$ (45), 394 $[411\text{-}OH]^+$ (8), 341 $[394\text{-}C_4H_5]^+$ (2), 275 $[341\text{-}C_5H_6]^+$ (35), 205 $[275\text{-}C_5H_{10}]^+$ (22), 109 $[205\text{-}C_7H_{12}]^+$ (61), 55 $[109\text{-}C_4H_6]^+$ (100); ^{1}H NMR (400 MHz) $CDCl_3$: δ 0.7, 0.83, 0.93, 0.94, 0.98, 0.99, 1.01 (7CH_3), 3.73 (dd, 1H, H-3, J = 5 Hz) and 0.35 (dddd, 1H, C-30 CH_2, J = 7 Hz).

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* Part 18 in the series of Egyptian Compositae, for part 17, see M. A. Metwally, Pharmazie 1989.

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[1] M. A. Metwally and A. M. Dawidar, Pharmazie **39,** H8, 575 (1984).

[2] M. A. Metwally, Pharmazie, communicated.