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A New Communic Acid Derivative from *Chromolaena collina* (DC) K. et R†.

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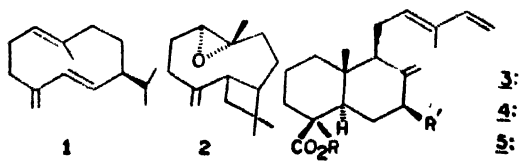
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The aerial parts of *Chromolaena collina* contain besides known compounds a new diterpenic acid, 7β-acetoxy-trans-communic acid (4), the unsubstituted acid also being present. The chemotaxonomical situation in this genus therefore still remaining complicated.

FROM the genus *Chromolaena* up to now 5 species have been investigated chemically. Besides flavones[1,2] some triterpenes[2] and several sesquiterpenes of different types[3,4] have been isolated so far. Therefore the chemotaxonomical situation still is not very clear. To learn more about the importance of the constituents in this genus a further species, *Chr. collina* (DC) K. et R. has been investigated.

The aerial parts of this species from Guatemala contain germacrene D (1) β-caryophyllenepoxide (2), trans-(+)-communic acid (3)[5] and a further acid showing the molecular formula $C_{22}H_{32}O_4$, elucidated by high resolution mass spectroscopy. All spectral data clearly show that we are dealing with an acid, which has a further acetoxy group. The ^{1}H-NMR-data are very similar to those of 3[6]. Therefore it was very probable that the new acid is an acetoxy derivative of 3. Using decoupling experiments and taking in mind the variation in chemical shifts of the 17-H signals in the spectrum of 3 and those of the new acid (see table) only the 7β-position for the acetoxy-group is possible, therefore the structure should be 4. Though the absolute configuration has not been proved with certainty the isolation of trans-(+) communic acid with known absolute stereochemistry makes it very probable that 4 has the same one.

The roots of *Chr. collina* also contain 1 and 3. 3 and related acids up to now in Compositae only have been found in *Mikania* species[7]. The constituents isolated now still do not clarify the chemotaxonomical situation in the genus *Chromolaena*. Surely much more species have to be investigated to see which compounds are really important in this connection.



	R	R'
3:	H	H
4:	H	OAc
5:	CH_3	OAc

^{1}H-NMR-DATA OF 4 AND 5
(270 MHz, TMS AS INTERNAL STANDARD, δ-VALUES)

	4 ($CDCl_3$)		5 (C_6D_6)	
3α-H			d(br)	1.94
3β-H			ddd	0.87
6α-H	dd	2.54	dd	2.60
6β-H	d(br)	2.23	d(br)	2.01
7α-H	s(br)	5.51	s(br)	5.63
11-H	dd(br)	2.45	m	2.3-2.4
11'-H				
12-H	t(br)	5.39	t(br)	5.53
14-H	dd	6.32	dd	6.53
15_o-H	d	4.89	d	4.97
$15'_t$-H	d	5.05	d	5.13
16-H	s(br)	1.76	s(br)	1.73
17-H	s(br)	4.86	s(br)	4.88
17'-H	s(br)	4.66	s(br)	4.73
18-H	s	0.99	s	1.16
19-H	s	1.31	s	1.08
OCH_3	—		s	3.26
OAc	s	1.91	s	1.77

J (Hz): 2α, 3β=3α, 3β=14; 2β, 3β=4; 6α, 6β=14; 6α, 7α=3; 11, 12=7; 14, 15_o=11; 14, 15_t=17. Irradiation at 7α-H sharpens the signal of 17-H and that of 6α-H forms a doublet (*J*=14); irradiation of the 12-H signal decouples the signals of 11-H and sharpens that of 16-H.

† Part 131. in the series "Naturally occurring Terpene-Derivatives"; for part 130. see: Bohlmann, F. and Mahanta, P. K. *Phytochemistry*, 1978, 17, 565.

Experimental

IR : Beckman IR 9, CCl_4 ; ^{1}H-NMR : Bruker WH 270, δ-values, TMS as internal standard ; MS : Varian MAT 711, 70 eV ; optical rotation : Perkin-Elmer-polarimeter, $CHCl_3$.

The air-dried plant-material (voucher RMK 7318) was extracted with ether-petrol (1:2) and the resulting extracts have been separated first by SC (sigel, act. grade II) and further by TLC (sigel, GF 254) using ether-petrol-mixtures as solvents. 50 g of roots afforded **1** (14 mg) and **3** (18 mg). 75 g of aerial parts yielded **1** (48 mg), **2** (11 mg), **3** (112 mg) and **4** (19 mg) (ether-petrol 1:1). **4** was esterified by CH_2N_2 in ether to give **5**, which also was purified by TLC (ether-petrol 1:3).

7β-Acetoxy-trans-communic acid (**4**) : Colorless oil, IR : CO_2H 3500-2400, 1695 ; OAc 1740 ; $C{=}CH_2$ 900 cm^{-1}. *MS* : M^+ m/e 360. 230 (2%) (calc. for $C_{22}H_{32}O_4$ 360.230) ; M^+-AcOH 300 (23) ; $300-{\cdot}CH_3$ 285 (8) ; $300-{\cdot}CO_2H$ 255 (8) ; $H_2C{=}CHC(CH_3){=}CHCH_2^+$ 81 (100) ; H_3CCO^+ 43 (85).

$$[\alpha]_{24°}^{\lambda} = \frac{489 \quad 578 \quad 546 \quad 436 \quad 365\ nm}{-0.4 \quad -0.4 \quad -1.2 \quad -7.2 \quad -15.9°} \qquad (c=1.75)$$

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