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FUROCOUMARINS FROM *Prangos ferulacea*

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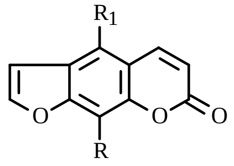
Plants of the genus *Prangos* (Apiaceae) are widely distributed around the world and number more than 30 species [1]. Coumarins were isolated in previous invetigations of plants from this genus [2, 3].

The raw material for our studies was collected in Turkey and until now had not been investigated chemically.

Ground air-dried roots (0.9 kg) were extracted with ethanol three times. The combined alcohol extracts were condensed, diluted with water in a 1:2 ratio, and worked up with ethylacetate to afford a thick brown extract (65 g), a portion of which (20 g) was placed on an Al_2O_3 column and eluted by a benzene:ethylacetate mixture (9:1) followed by an increased ethylacetate concentration. Fractions (200 mL) were collected.

Four coumarin-like compounds were isolated: **1**, $C_{16}H_4O_4$, mp 108-109°C; **2**, $C_{16}H_{14}O_4$, mp 102-103°C; **3**, $C_{19}H_{20}O_5$, mp 132-140°C; **4**, $C_{16}H_{16}O_6$, mp 132-133°C. The IR and PMR spectra and physical constants of **1**, **2**, and **4** identified them as isoimperatorin, imperatorin, and hydroxypeucedanin hydrate [4]. According to the literature, imperatorin exhibits anti-HIV activity [5].



1, 2

1: R = OCH_2-CH=$C(CH_3)_2$, R_1 = H
2: R = H, R_1 = OCH_2-CH=$C(CH_3)_2$

The structure of **3** was studied using PMR and ^{13}C NMR spectroscopy with computer analysis of the spectra.

The PMR spectrum of **3** exhibited the following signals: 6.01 (1H, d, J = 10 Hz, H-3), 7.52 (1H, d, J = 10 Hz, H-4), 6.55 (1H, s, H-5), 7.16 (1H, s, H-8), 3.13 (2H, d, J = 9 Hz, H-1′), 5.05 (1H, t, J = 9 Hz, H-2′), 1.42 (3H, s, H-4′), 1.51 (3H, s, H-5′) and signals for senecionic acid at 1.80* (3H, d, J = 1.5 Hz, H-4″), 2.03* (3H, d, J = 1.5 Hz, H-5″), and 5.44 (1H, m, H-2″). A double-resonance experiment showed spin—spin coupling between H-1′ and H-2′. An Overhauser effect on H-5′ was not observed with additional irradiation of methyl protons H-4′ and H-5′.

Base hydrolysis of **3** produced the hydroxycoumarin marmesin, the PMR spectrum of which exhibited the following signals: 6.14 (1H, d, J = 9 Hz, H-3), 7.86 (1H, d, J = 9 Hz, H-4), 6.71 (1H, s, H-5), 7.42 (1H, br. s, H-8), 3.12 (2H, d, J = 9 Hz, H-1′), 4.65 (1H, t, J = 9 Hz, H-2′), 1.09 (6H, s, H-4′, H-5′). The PMR spectra of **3** and its hydrolysis product showed no direct acylation effect, which was consistent with the ester in **3** on a quaternary C atom.

The ^{13}C NMR spectrum of **3** contained 18 signals (the two signals for C-4′ and C-5′ had the same chemical shifts). Signals were assigned based on calculations using the program ACD CNMR. First the molecular geometry was optimized. Then the chemical shifts were calculated. Table 1 gives the calculations, the assignments, and the absolute values of the differences between the calculated and observed signals. The maximum deviations between the calculated and experimental values in the corresponding pairs were observed for the quaternary C atoms.

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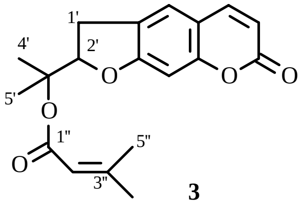
TABLE 1. ^{13}C Chemical Shifts of **3** and Calculated Using the Program ACD CNMR

C atom	CS		Absolute value of the difference of calculated and observed CS
	calculated	observed	
2	162.00	160.42 s	1.58
3	111.80	111.49 s	0.31
4	143.60	143.66 d	0.06
5	123.47	124.11 d	0.64
6	126.87	125.16 s	1.71
7	163.38	163.00	0.38
8	97.57	97.00	0.57
9	155.55	156.23	0.68
10	111.84	112.53	0.69
1′	28.51	29.03 t	0.52
2′	88.18	88.86 d	0.68
3′	82.32	81.16 s	1.16
4′	21.75	21.33 q	0.42
5′	21.75	21.33 q	0.42
1″	163.91	165.12 s	1.21
2″	116.25	116.72 d	0.47
3″	154.75	155.19 s	0.44
4″	26.14	26.78	0.64
5″	19.14	19.77	0.63

The chemical and spectral data for **3** identified it as pranchimgin [6].



3

These compounds were isolated for the first time from plants of the genus *Prangos* in Turkey.

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