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New Coumarins From *Peacedanum Decursivum*

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Abstract: Four new Coumarins named Decursitin B, C, D, F have been isolated from traditional Chinese medicine - the root of *Peacedanum decursivum*. Their structures were elucidated by chemical evidences and spectral analysis.

Keywords: *Peacedanum decursivum*; decursitin B; decursitin C; decursitin D; decursitin F.

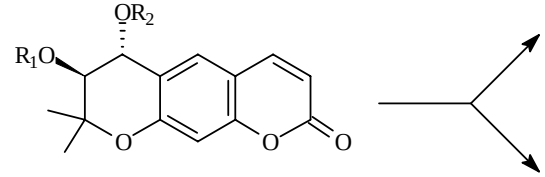
The root of *Peucedanum decursivum* (Miq.) Maxim (umbelliferae) is known as a famous traditional chinese medicine. Its chemical constituents were studied. Compound **1**, **2**, **3**, **4** were isolated from the extract of the root by combination of silica gel column Chromatography and preparative HPLC.

1, colorless, glassy substance, $[\alpha]_{23}^{D}$ -53.43 [$CHCl_3$], $C_{24}H_{26}O_7$ (HREIMS mol. wt. calcd. 426.1631, obs. 426.1654), UVspectra (λ max 322.8 nm and 221.0 nm), ^{1}HNMR indicates **1** is a xanthyletin-type coumarin. $J_{3',4'}$=6.0 Hz indicates a *trans* configuration at the 3' -and 4'-position [1]. δ 6.18 (1H, m), 6.12 (1H, m), 2.03 (3H, d), 1.93 (3H, d) and 1.88 (6H, s) show the existence of two angeloyloxys. **1** formed (-)-*cis*-decursidinol and (+)-*trans*-decursidinol after basic hydrolysis[1], indicating the absolute configurations are of 3'S, 4'R. The oxygen functionality at 4' had suffered randomization during basic hydrolysis. Therefore the structure of **1** is 3'(S), 4'(R) –biangeloyloxy-3',4'-dihydroxanthyletin, named decursitin B.

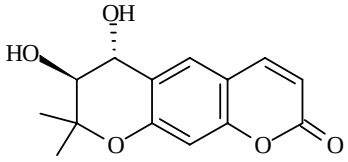
2, colorless glassy substance, $[\alpha]_{23}^{D}$ -58.41 [$CHCl_3$], $C_{24}H_{26}O_7$ (HREIMS mol. wt. calcd. 426.1675, obs. 426.1676), UVspectra (λ max 324.8 nm and 257.2 nm), ^{1}HNMR indicates **2** is a xanthyletin-type coumarin. $J_{3',4'}$=5.7 Hz indicates a *trans* configuration at the 3'- and 4'-position[1]. δ 2.08 (3H, d), 1.87 (3H, s) and 6.17 (1H, q) show the existence of angeloyloxy. δ 1.89 (3H, s), 2.16 (3H, s) and 5.69 (1H, brs) show the existence of senecioyloxy. HMBC indicates senecioyloy is attached to C-3' and angeloyloxy to C-4'. **2** formed (-)-*cis*-decursidinol and (+)-*trans*-decursidinol after basic hydrolysis[1], indicating the absolute configurations are of 3'S, 4'R. Therefore the structure of **2** is 3'(S)-senecioyloxy-4'(R)-angeloyloxy-3',4'-dihydroxanthyletin, named decursitin C**.**

3, white powder, m.p.: 100-102℃, $[\alpha]_{23}^{D}$ -14.60 [$CHCl_3$], $C_{19}H_{20}O_6$ (HREIMS mol. wt. calcd. 344.1172, obs. 344.1215), UVspectra (λ max 324.8 nm and 257.2 nm), ^{1}HNMR indicates **3** is a xanthyletin-type coumarin, $J_{3',4'}$=7.0 Hz indicates a *trans* configuration at the 3'- and 4'- position[1]. δ 6.22 (1H, m), 2.05 (3H, d) and 1.93 (3H, s) show the existence of angeloyloxy. H-3' and H-4' are 3.91 ppm and 6.00 ppm, which indicate the angeloyloxy group is linked to the C-4'[2]. **3** formed (-)-*cis*-decursidinol and (+)-*trans*-decursidinol after basic hydrolysis[1], indicating the absolute configurations are of 3'S, 4'R. Therefore the structure of **3** is 3'(S)-hydroxy-4'(R)-angeloyloxy-3',4'-dihydroxanthyletin, named decursitin D.

4, white powder, m.p.: 158-160℃, $[\alpha]_{23}^{D}$ +61.53 [$CHCl_3$], $C_{16}H_{16}O_6$ (HREIMS mol. wt. calcd. 304.0915, obs. 304.0930), UVspectra (λ max 324.4 nm and 219.8 nm), ^{1}HNMR indicates **4** is a xanthyletin-type coumarin, $J_{3',4'}$=7.0 Hz indicates a *trans* configuration at the 3'-and 4'-position[1]. ^{1}HNMR δ 2.13 (3H, s) and ^{13}CNMR δ 170.86, 21.63 show the existence of acetyl. H-3' and H-4' are 5.08 ppm and 4.75 ppm, which indicate C-3'-OH is acylated[2]. **4** formed (-)-*cis*-decursidinol and (+)-*trans*-decursidinol after basic hydrolysis[1], indicating the absolute configurations are of 3'S, 4'R. Therefore the structure of **4** is 3'(S)-acetoxy-4'(R)-hydroxy-3',4'-dihydroxanthyletin, named decursitin F.

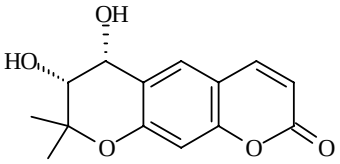


	R_1	R_2
1	angeloyloxy	angeloyloxy
2	senecioyloxy	angeloyloxy
3	H	angeloyloxy
4	Ac	H



(+) - *trans* - Decursidinol

+



(-) - *cis* - Decursidinol

Table 1. the ^{1}HNMR data of compounds **1, 2, 3, 4**

	H-3	H-4	H-5	H-8	H-3'	H-4'	gem-$(Me)_2$
1	6.25	7.59	7.39	6.81	7.37	6.16	1.41
		J=9.5			J=6.0		1.48
2	6.25	7.60	7.42	6.82	5.30	6.11	1.40
		J=9.5			J=5.7		1.47
3	6.24	7.60	7.35	6.78	3.91	6.0	1.35
		J=9.3			J=7.0		1.53
4	6.25	7.94	7.76	6.71	5.08	4.75	1.29
		J=9.5			J=7.5		1.41
(+)-*trans*-	6.40	8.05	7.88	6.86	3.72	4.73	1.43
decursidinol		J=9.5			J=8.5		1.67
(-)-*cis*-	6.23	8.01	7.73	6.67	3.63	4.73	1.25
decursidinol		J=9.5			J=3.5		1.40

Table 2. the ^{13}CNMR data of compounds **1, 2, 3, 4**

NO	**1**	**2**	**3**	**4**	(+)-*trans*-decursidinol	(-)-*cis*-decursidinol
C-2	160.8	160.8	160.9	161.1	163.5	161.4
C-3	113.8	113.8	113.6	113.9	113.7	113.1
C-4	143.1	143.2	143.2	144.7	146.0	144.4
C-5	129.0	129.0	128.4	129.9	129.7	129.0
C-6	117.1	117.0	117.6	122.5	124.5	123.8
C-7	156.2	156.2	156.2	156.4	157.9	156.5
C-8	104.9	104.9	104.8	104.3	104.8	103.6
C-9	155.4	155.4	155.2	155.8	156.4	154.9
C-10	113.3	113.3	113.2	114.0	114.5	112.7
C-2'	77.9	77.8	79.8	79.1	81.7	81.0
C-3'	72.0	71.2	73.5	76.1	76.6	75.4
C-4'	66.7	66.7	70.9	66.5	69.6	68.5
C-2'-CH_3	22.5	22.7	20.2	20.9	20.0	20.0
	25.2	25.0	25.7	26.0	27.3	27.0

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References

1. K. Sano, I. T. Yosioka, and I. Kitagawa, *Chem. Pharm. Bull.*, **1975,** *23*(1), 20.
2. I. Sakakibara, T. Okayama and S. Shibata, *Planta Medica*, **1982**, *44*, 199.
3. Y. Matano, T. Okuyama, and S. Shibata, *Planta Medica*, **1986**, 135.
4. T. Kozawa, K. Sakai, and M. Uchida, *J. Pharm. Pharmacol.*, **1983,** *33*, 317.

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