

Isolation and Phytotoxicity of Apocarotenoids from *Chenopodium album*

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List of Supporting Information

Figure 1A. Effect of compounds **1-12**, **14-16** and **18** on germination of *Lactuca sativa* L.

Value presented as percentage differences from control; $P > 0.05$ for t-Student's test.

a, $P < 0.01$; b, $0.01 < P < 0.05$.

Figure 1B. Effect of compounds **1-12**, **14-16** and **18** on root length of *Lactuca sativa* L.

Value presented as percentage differences from control; $P > 0.05$ for t-Student's test.

a, $P < 0.01$; b, $0.01 < P < 0.05$.

Figure 1C. Effect of compounds **1-12**, **14-16** and **18** on shoot length of *Lactuca sativa* L.

Value presented as percentage differences from control; $P > 0.05$ for t-Student's test.

a, $P < 0.01$; b, $0.01 < P < 0.05$.

Table 1. NMR spectral data of compound **1** in CDCl_3

Table 2. NMR spectral data of compound **2** in CDCl_3

Figure 1A

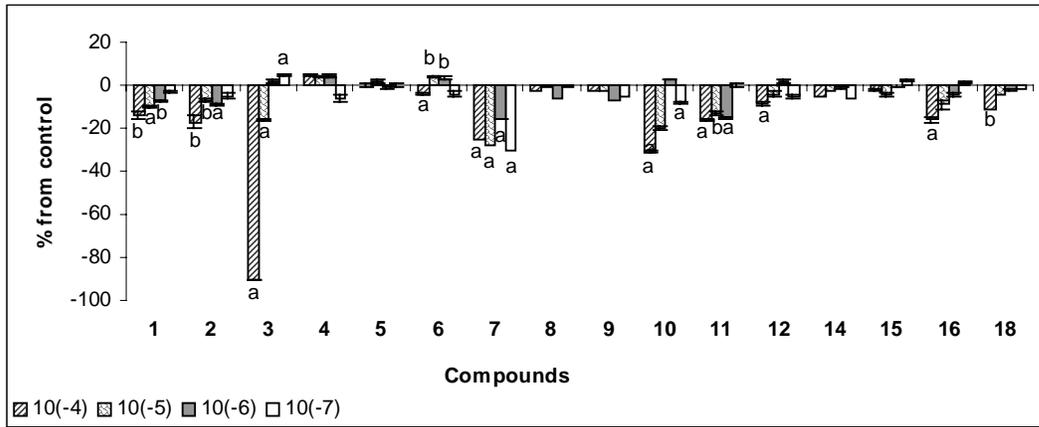


Figure 1B

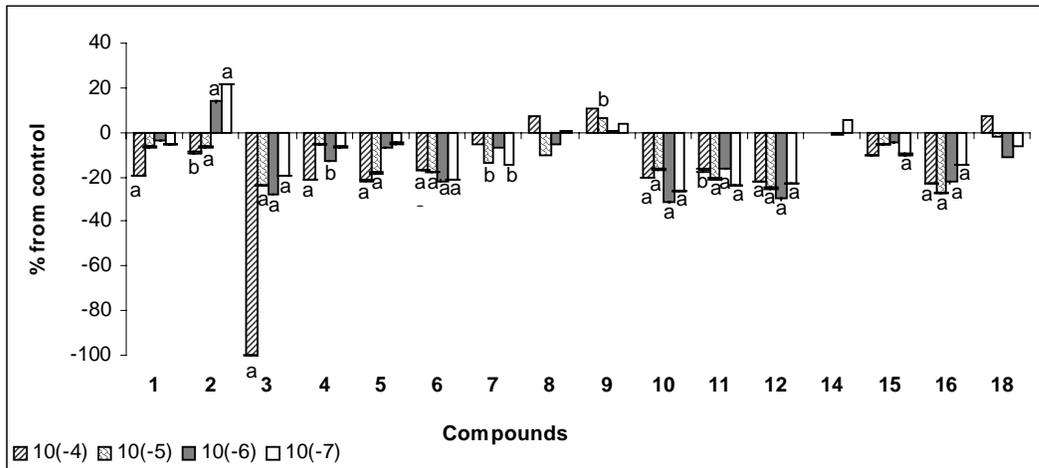


Figure 1C

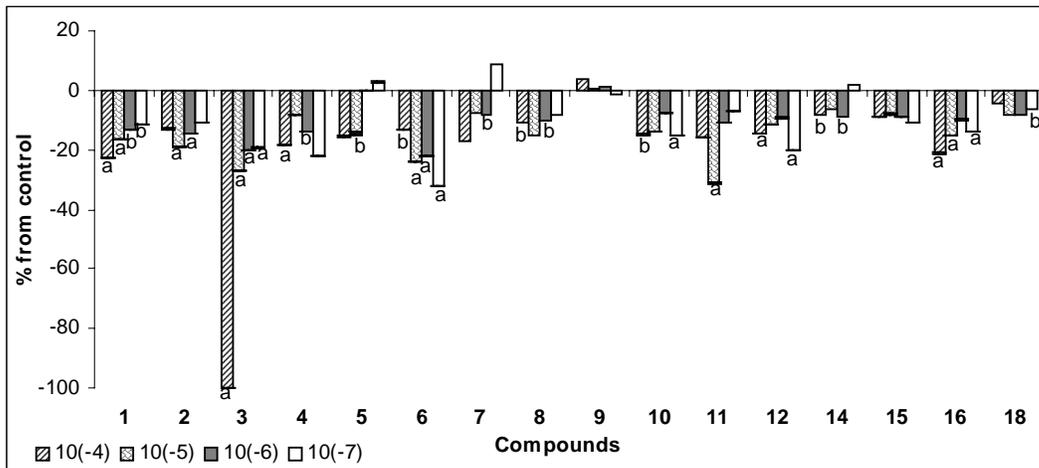


Table 1

Position	$\delta_{\text{H}}^{\text{a}}$	J (Hz)	^1H - ^1H COSY	ROESY	δ_{C}	HMBC ^b
1					34.0 (q) ^c	
2 <i>eq</i>	1.84 dd	17.5, 6.4	2 <i>ax</i> , 3	15, 16	44.5 (s)	1, 3, 15
2 <i>ax</i>	1.40 dd	17.5, 5.8	2 <i>eq</i> , 3	6, 15	44.5 (s)	1, 3, 15
3	4.26 brs		2	16	65.8 (q)	
4	5.58 brs		3	17	125.0(t)	2, 17
5					137.2 (q)	
6	2.44 d	9.5	7	2 <i>ax</i> , 8, 15	54.9 (q)	
7	5.69 dd	9.5, 15.0	8	16	133.6 (t)	5, 6, 9
8	6.20 d	15.0	7	6, 17	136.9 (t)	6, 9, 10, 18
9					144.5 (q)	
10	6.18 d	11.5	11		127.8 (t)	8, 18
11	7.58 dd	15.0, 11.5	10, 12	14, 18	139.0 (t)	9, 13
12	6.20 d	15.0	11		129.8 (t)	10, 13, 14
13					198.6 (s)	
14	2.30 s			11	27.7 (p)	12, 13
15	1.01 s			6, 2 <i>ax</i> , 2 <i>eq</i>	29.5 (p)	1, 2, 6, 16
16	0.86 s			2 <i>eq</i> , 3, 7	24.9 (p)	1, 2, 6, 15
17	1.62 s			4	22.8 (p)	4, 5, 6
18	2.01 s			11	13.5 (p)	8, 9, 10

^a ^1H chemical shift values (δ ppm from SiMe_4) followed by multiplicity and then the coupling constants (J in Hz).

^b HMBC correlations from H to C.

^c Letters, p, s, t and q, in parentheses indicate, respectively, the primary, secondary, tertiary and quaternary carbons, assigned by DEPT.

Table 2

Position	$\delta_{\text{H}}^{\text{a}}$	J (Hz)	^1H - ^1H COSY	ROESY	δ_{C}	HMBC(C) ^b
1					41.6 (q) ^c	
2 <i>eq</i>	2.50 d	17.5	2	16	49.7 (s)	1, 3, 15
2 <i>ax</i>	2.30 d	17.5	2		49.7 (s)	1, 3, 15
3					198.4 (q)	
4	5.94 s			17	127.1(t)	2, 17
5					161.0 (q)	
6					80.1 (q)	
7	5.96 d	15.9	8	15, 16, 18	132.0 (t)	5, 6, 9
8	6.47 d	15.9	7	10, 17	134.6 (t)	6, 9, 10, 18
9					143.2 (q)	
10	6.26 d	11.5	11	8	130.3 (t)	8, 18
11	7.55 dd	15.5, 11.5	10, 12	14, 18	138.4 (t)	9, 13
12	6.24 d	15.5	11		130.3 (t)	10, 13, 14
13					198.4 (s)	
14	2.30 s			11	28.5 (p)	12, 13
15	1.11 s			7	23.1 (p)	1, 2, 6, 16
16	1.03 s			2 <i>eq</i> , 8	24.3 (p)	1, 2, 6, 15
17	1.91 s			4, 8	18.9 (p)	4, 5, 6
18	2.02 s			7, 11	14.0 (p)	8, 9, 10

^a ^1H chemical shift values (δ ppm from SiMe_4) followed by multiplicity and then the coupling constants (J in Hz).

^b HMBC correlations from H to C.

^c Letters, p, s, t and q, in parentheses indicate, respectively, the primary, secondary, tertiary and quaternary carbons, assigned by DEPT.