

Supplemental Table 1 ¹H and ¹³C NMR data of oxidation products formed from xanthophylls

no	3'-hydroxy- ϵ,ϵ -caroten-3-one			3'-hydroxy- β,ϵ -coroten-3-one		
	$\delta^{13}\text{C}$	$\delta^1\text{H}$	mult (J in Hz)	$\delta^{13}\text{C}$	$\delta^1\text{H}$	mult (J in Hz)
1	36.6			39.4		
2	47.4	2.11 2.39	d (17) d (17)	54.7	2.43	s
3	199.7			210.5		
4	125.5	5.92	br. s	46.2	2.91	br. s
5	162.7			125.4		
6	56.3	2.61	d (10)	138.9		
7	125.5	5.54	dd (15, 9)	124.4	6.10	d (16)
8	138.4	6.24	d (15)	138.9	6.17	d (16)
9	134.4			135.2		
10	132.0	6.17	d (11)	131.9	6.20	d (11)
11	124.4	6.60	dd (16, 12)	124.7	~6.65	overlapped
12	138.3	6.39	d (15)	138.0	6.39	d (15)
13	136.3			136.4		
14	133.0	6.28	d (11)	132.9	6.28	d (9)
15	129.9	~6.65	overlapped	129.9	~6.65	overlapped
16	27.5/27.9	0.97/1.05	s	28.4	1.09	s
17	27.5/27.9	0.97/1.05	s	28.4	1.09	s
18	23.8	1.92	s	20.8	1.78	s
19	13.0	1.92	s	12.8	2.00	s
20	12.8	1.97	s	12.8	1.98	s
1'	34.0			34.0		
2'	44.6	1.37 1.85	dd (13, 7) dd (13, 6)	44.6	1.37 1.85	dd (13, 7) dd (13, 6)
3'	65.9	4.26	m	65.9	4.26	m
4'	124.4	5.55	br. s	124.4	5.55	br. s
5'	138.0			138.0		
6'	54.8	2.41	d (11)	54.8	2.41	d (9)
7'	128.8	5.43	d (15, 10)	128.8	5.43	d (16, 10)
8'	137.7	6.14	d (15)	137.6	6.15	d (16)
9'	135.2			135.2		
10'	130.7	6.15	d (11)	130.7	6.15	d (12)
11'	124.9	6.62	dd (15, 12)	124.8	6.62	dd (15, 11)
12'	137.5	6.37	d (15)	137.5	6.37	d (15)
13'	136.6			136.6		
14'	132.5	6.26	d (11)	132.5	6.26	d (10)
15'	130.3	~6.65	overlapped	130.2	~6.65	overlapped
16'	24.1/29.5	0.85/1.00	s	24.1/29.5	0.85/1.00	s
17'	24.1/29.5	0.85/1.00	s	24.1/29.5	0.85/1.00	s
18'	22.9	1.63	s	22.9	1.63	s
19'	13.1	1.92	s	13.1	1.92	s
20'	12.8	1.97	s	12.8	1.97	s

Supplemental Table 1 continued

no	β,ϵ -caroten-3'-one			β,β -caroten-3-one		
	$\delta^{13}\text{C}$	$\delta^1\text{H}$	mult (J in Hz)	$\delta^{13}\text{C}$	$\delta^1\text{H}$	mult (J in Hz)
1	34.2			39.4		
2	39.5	1.47	m	54.7	2.43	s
3	19.2	1.61	m	210.5		
4	33.1	2.02	t (6)	46.2	2.91	br. s
5	129.5			125.4		
6	137.8			138.9		
7	126.7	6.16	d (16)	124.4	6.10	d (16)
8	137.7	6.14	d (16)	138.9	5.17	d (16)
9	136.2			135.1		
10	130.8	6.16	d (12)	132.0	6.20	d (11)
11	125.2	~6.65	overlapped	124.6	~6.65	overlapped
12	137.1	6.36	d (15)	138.0	6.40	d (15)
13	136.8			136.3		
14	132.3	6.26	d (10)	132.9	6.28	d (9)
15	130.4	~6.65	overlapped	129.8	~6.65	overlapped
16	28.9	1.03	s	28.4	1.09	s
17	28.9	1.03	s	28.4	1.09	s
18	21.8	1.72	s	20.8	1.78	s
19	12.9	1.98	s	12.8	2.00	s
20	12.8	1.98	s	12.8	1.98	s
1'	36.6			34.2		
2'	47.4	2.11	d (17)	39.5	1.47	m
		2.39	d (17)			
3'	199.6			19.2	1.61	m
4'	125.5	5.91	br. s	33.1	2.02	t (6)
5'	162.7			129.5		
6'	56.3	2.61	d (9)	137.8		
7'	125.4	5.53	dd (15, 9)	126.7	6.18	br.d (16)
8'	138.4	6.24	d (15)	137.7	6.14	d (16)
9'	134.4			136.2		
10'	132.1	6.18	br.d (11)	130.8	6.16	br.d (12)
11'	124.3	6.59	dd(15, 11)	125.1	~6.65	overlapped
12'	138.3	6.39	d (15)	137.1	6.37	d (15)
13'	136.1			136.7		
14'	133.1	6.28	d (10)	132.3	6.26	d (9)
15'	129.7	~6.65	overlapped	130.3	~6.65	overlapped
16'	27.5/27.9	0.97/1.05	s	28.9	1.03	s
17'	27.5/27.9	0.97/1.05	s	28.9	1.03	s
18'	23.8	1.92	s	21.8	1.72	s
19'	13.1	1.92	s	12.8	1.98	s
20'	12.8	1.97	s	12.9	1.98	s

Supplemental Table 1 continued

3-hydroxy- β,ϵ -caroten-3'-one				ϵ,ϵ -carotene-3,3'-dione			
no	$\delta^{13}\text{C}$	$\delta^1\text{H}$	mult (J in Hz)	no	$\delta^{13}\text{C}$	$\delta^1\text{H}$	mult (J in Hz)
1	37.1			1, 1'	36.6		
2	48.2	1.48	dd (12, 12)	2, 2'	47.4	2.11	d (17)
		1.78	m			2.39	d (17)
3	65.0	4.01	br. s	3, 3'	199.6		
4	42.4	2.05	dd (17, 10)	4, 4'	125.5	5.92	br. s
		2.39	dd (17, 7)				
5	126.2			5, 5'	162.7		
6	137.6			6, 6'	56.3	2.61	d (9)
7	125.6	6.10	d (16)	7, 7'	125.6	5.54	dd (15, 9)
8	138.5	6.13	d (16)	8, 8'	138.4	6.24	d (15)
9	135.8			9, 9'	134.5		
10	131.2	6.16	d (10)	10, 10'	132.0	6.18	d (11)
11	125.0	~6.65	overlapped	11, 11'	124.5	6.68	dd(15, 11)
12	137.5	6.37	d (14)	12, 12'	138.2	6.39	d (15)
13	136.7			13, 13'	136.5		
14	132.5	6.26	d (11)	14, 14'	133.0	6.28	br.d (10)
15	130.3	~6.65	overlapped	15, 15'	130.2	6.66	multiplet
16	28.7/30.2	1.07	s	16, 16'	27.5/27.9	0.97/1.05	s
17	28.7/30.2	1.07	s	17, 17'	27.5/27.9	0.97/1.05	s
18	21.7	1.74	s	18, 18'	23.8	1.92	s
19	12.8	1.97	s	19, 19'	13.1	1.92	s
20	12.8	1.98	s	20, 20'	12.8	1.98	s
1'	36.6						
2'	47.4	2.10	d (17)				
		2.39	d (17)				
3'	199.6						
4'	125.5	5.92	br. s				
5'	162.7						
6'	56.3	2.61	d (9)				
7'	125.5	5.54	dd (15, 9)				
8'	138.4	6.24	d (15)				
9'	134.4						
10'	132.0	6.18	d (10)				
11'	124.4	6.60	dd (15, 11)				
12'	138.3	6.39	d (14)				
13'	136.2						
14'	133.0	6.28	d (11)				
15'	129.9	~6.65	overlapped				
16'	27.4/27.9	0.97/1.05	s				
17'	27.4/27.9	0.97/1.05	s				
18'	23.8	1.92	s				
19'	13.1	1.92	s				
20'	12.8	1.97	s				