Supporting Information

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Thermal Oxidation Of 9'-cis-Neoxanthin In A Model System Containing Peroxyacetic Acid Leads To The Potent Odorant β-Damascenone

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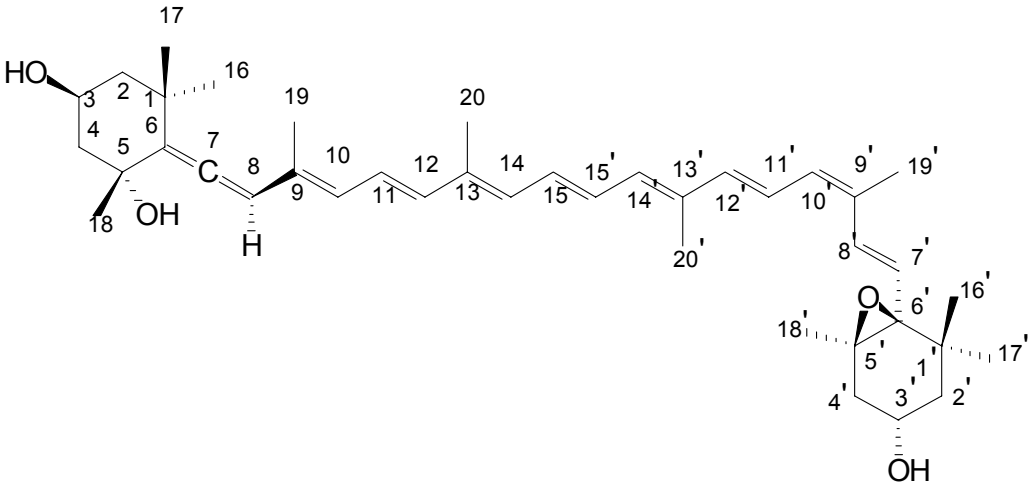

Figure S1. Structure of 9’-cis-neoxanthin

Table S1. NMR data for 9'-cis-neoxanthin**.**

Position	δ(^{13}C)	δ(^{13}C')	δ(^{1}H)	δ(^{1}H')
Polyene moiety				
7(7')	202.27(C)	125.80(CH)	-	6.03(d, $J_{7',8'}$=15.5Hz)
8(8')	102.41(CH)	129.09(CH)	6.06	6.84(d, $J_{7',8'}$=15.5Hz)
9(9')	131.69(C)	132.19(C)	-	-
10(10')	128.08(CH)	130.63(CH)	6.13(d,$J_{10,11}$=11.0Hz)	6.11(d,$J_{10',11'}$=11.0Hz)
11(11')	124.63(CH)	123.04(CH)	6.62(dd, $J_{10,11}$=11.0Hz; $J_{11,12}$=15.0Hz)	6.79(dd, $J_{10',11'}$=11.0Hz; $J_{11',12'}$=15.0Hz)
12(12')	136.89(CH)	137.28(CH)	6.37(d,$J_{11,12}$=15.0Hz)	6.34(d,$J_{11',12'}$=15.0Hz)
13(13')	136.10(C)	135.82(C)	-	-
14(14')	132.62(CH)	132.62(CH)	6.28(m)	6.28(m)
15(15')	129.77(CH)	129.99(CH)	6.66(m)	6.66(m)
Cyclohexane moieties				
1(1')	35.24(C)	34.78(C)		
2(2')	49.18(CH_2)	47.15(CH_2)	1.91(H_{eq},m)* 1.27(H_{ax},m)*	1.58(H_{eq},m)* 1.21(H_{ax},m)*
3(3')	63.31(CH)	63.10(CH)	4.21(m)*	3.78(m)*
4(4')	48.68(CH_2)	40.18(CH_2)	2.19(H_{eq},m)* 1.32(H_{ax},m)*	2.34(H_{eq},m)* 1.63(H_{ax},m)*
5(5')	67.39(C)	71.72(C)		
6(6')	117.01(C)	70.84(C)		
Methyl groups				
16(16')	29.93	23.75	1.36	1.00
17(17')	31.49	29.33	1.08	1.21
18(18')	29.33	18.84	1.21	1.17
19(19')	12.76	19.53	1.83	1.95
20(20')	11.42	11.38	1.98	1.98

*Only some of the ^{1}H-^{1}H hyperfine coupling constants, J(Hz), could be estimated from ^{1}H-NMR-spectrum: $J_{4'eq,3ax'}$~5Hz, $J_{4'eq,4'ax}$=14.5Hz, $J_{4'eq,2'eq}$~0.5Hz, $J_{4'ax,3'ax}$=9.5Hz, $J_{2eq,2ax}$~11Hz, $J_{2eq,3ax}$~5Hz, $J_{2eq,4eq}$~0.5Hz.

Table S2. The two bond and three bond ^{1}H-^{13}C long range hyperfine interactions in 9'-cis-neoxanthin (HMBC data).

Position of hydrogen	H	H'
4(4')	C_2, C_3, C_5, C_6, C_{18}	$C_{2'}$, $C_{3'}$, $C_{5'}$, $C_{6'}$, $C_{18'}$
(7')		$C_{5'}$, $C_{6'}$, $C_{9'}$, $C_{10'}$
8(8')	C_6, C_7, C_9,C_{10},C_{19}	$C_{6'}$, $C_{7'}$, $C_{9'}$,$C_{10'}$,$C_{19'}$
10(10')	C_8, C_{19}	$C_{8'}$, $C_{19'}$
11(11')	C_9, C_{10}, C_{12}, C_{13}	$C_{9'}$, $C_{10'}$, $C_{12'}$, $C_{13'}$
12(12')	C_{10}, C_{13},C_{14}	$C_{10'}$, $C_{13'}$,$C_{14'}$
14(14')	C_{12}, C_{13}, C_{15}, C_{20}	$C_{12'}$, $C_{13'}$, $C_{15'}$, $C_{20'}$
15(15')	C_{13}, C_{14}, $C_{15'}$	$C_{13'}$, $C_{14'}$, C_{15}
16(16')	C_1, C_2, C_6, C_{17}	$C_{1'}$, $C_{2'}$, $C_{6'}$, $C_{17'}$
17	C_1, C_2, C_6, C_{16}	
19(19')	C_8, C_9, C_{10}	$C_{8'}$, $C_{9'}$, $C_{10'}$