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ELECTRONIC SUPPLEMENTARY INFORMATION for *Excited state characterization of carbonyl containing carotenoids: a comparison between single and multireference descriptions*

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	ν_1		ν_2	
	B3LYP	Exp	B3LYP	Exp
Astaxanthin (Keto)	1510 (1546)	1524[a]	1161 (1189)	1157 [a]
Astaxanthin (Eno)	1513 (1549)		1156 (1183)	
Fucoxanthin	1532 (1568)	1532[b]	1173 (1201)	1156[b]
Capsanthin	1521 (1557)		1164 (1192)	
Capsorubin	1523 (1559)		1164 (1192)	

Table S1. Vibrational frequencies of Astaxanthin and Fucoxanthin as obtained from B3LYP/6-311G(d,p) calculations. Values were scaled with the scaling factor of 0.9769. In parenthesis we report the unscaled frequencies. [a]Experiments from Ref. 1. [b]Experiments from Ref. 2.

	S1	S2	S3	S4
B3LYP	2.2714 (4.1763)	2.6408 (1.1660)	3.0590 (0.0038)	3.1800 (0.0081)
TPSS	1.8850 (1.3080)	2.1484 (0.7572)	2.2553 (2.7927)	2.4631 (0.1663)
Rev-TPSS	1.9020 (1.3388)	2.1583 (0.6852)	2.2718 (2.8813)	2.4865 (0.1488)
VSXC	1.9084 (1.4307)	2.2143 (1.7055)	2.2914 (1.9724)	2.5000 (0.1095)
VSXC/6-31+G(d)	1.9137 (1.4321)	2.2294 (1.9850)	2.3063 (1.7180)	2.5085 (0.0990)
HCTH	1.8304 (1.1764)	2.0524 (0.3569)	2.1963 (3.0843)	2.3893 (0.2135)
TPSSh	2.1315 (2.8506)	2.4400 (2.4712)	2.7738 (0.0469)	2.8037 (0.0157)
M06L	1.9627 (1.4958)	2.2852 (2.9377)	2.3911 (0.5880)	2.5628 (0.1133)
M11L	1.9176 (1.6170)	2.2057 (3.4969)	2.4936 (0.1928)	2.5157 (0.0105)
M11L/6-31+G(d)	1.9328 (1.6817)	2.2191 (3.5070)	2.5221 (0.1602)	2.5750 (0.0056)
MN12L	2.0571 (2.0991)	2.3599 (3.3675)	2.6944 (0.1059)	2.8019 (0.0107)
PBE	1.8211 (1.1476)	1.9804 (0.2394)	2.1837 (3.2356)	2.3764 (0.2686)
BLYP	1.8172 (1.1549)	2.0483 (0.4330)	2.1847 (3.0659)	2.3739 (0.1932)
PW91	1.8185 (1.1535)	1.9974 (0.2696)	2.1822 (3.2078)	2.3733 (0.2542)
M06	2.3365 (4.6220)	2.8127 (0.5035)	3.2370 (0.0099)	3.3428 (0.0042)
BHandH	2.6666 (5.0738)	3.6060 (0.0865)	3.8060 (0.0949)	3.9257 (0.0017)
HSEH1PBE	2.2367 (3.5231)	2.5719 (1.8584)	2.9908 (0.0117)	3.1769 (0.0120)
PBE0	2.3581 (4.6265)	2.7951 (0.7402)	3.2275 (0.0039)	3.3102 (0.0061)
CAM-B3LYP	2.6966 (4.8525)	3.7178 (0.0104)	3.7490 (0.0308)	3.8432 (0.1135)
LC-wPBE	3.0539 (4.6116)	3.8836 (0.0041)	4.1309 (0.0793)	4.8083 (0.1199)

Table S2. S_0-S_n (n=1-4) energies (in eV) and oscillator strengths (in parenthesis) for CC-echinenone as obtained from TDA/6-311+G(d,p) calculations (when specified 6-31+G(d) basis set was also used).

	S1	S2	S3	S4
B3LYP	2.2065 (4.3614)	2.5571 (1.5817)	3.0136 (0.0167)	3.0896 (0.0001)
TPSS	1.8302 (1.2087)	2.1287 (0.0012)	2.1944 (4.1764)	2.4369 (0.4336)
VSXC	1.8568 (1.3175)	2.1895 (0.0537)	2.2158 (4.3096)	2.4738 (0.3321)
RevTPSS	1.8468 (1.2417)	2.1316 (0.0004)	2.2113 (4.2057)	2.4606 (0.4043)
TPSSh	2.0688 (2.7624)	2.3791 (3.2352)	2.7063 (0.0013)	2.7622 (0.0875)
HCTC	1.7778 (1.0890)	2.0296 (0.0000)	2.1460 (3.9949)	2.3667 (0.5372)
M06L	1.9007 (1.3872)	2.2574 (4.2207)	2.3295 (0.0047)	2.5258 (0.2978)
M11L	1.8623 (1.4407)	2.1679 (4.3296)	2.4647 (0.3088)	2.4708 (0.0029)
MN12L	1.9956 (1.9322)	2.3094 (4.2282)	2.6557 (0.2101)	2.7460 (0.0013)
PBE	1.7702 (1.0719)	1.9564 (0.0000)	2.1380 (3.9966)	2.3534 (0.6191)
BLYP	1.7661 (1.0655)	2.0222 (0.0003)	2.1338 (4.0496)	2.3529 (0.5174)
PW91	1.7678 (1.0729)	1.9739 (0.0001)	2.1355 (4.0060)	2.3509 (0.6013)
M06	2.2682 (4.9567)	2.7165 (0.6954)	3.1870 (0.0013)	3.2508 (0.0001)
BHandH	2.5841 (5.4852)	3.4937 (0.1454)	3.7550 (0.0089)	3.8667 (0.0000)
HSEH1PBE	2.1664 (3.5229)	2.4928 (2.4847)	2.9399 (0.0426)	3.0855 (0.0006)
PBE0	No convergence			
CAM-B3LYP	2.6144 (5.2444)	3.6422 (0.0849)	3.6852 (0.0001)	3.7633 (0.0170)
LC-wPBE	2.9661 (4.9647)	3.8647 (0.0002)	4.0628 (0.0038)	4.6948 (0.0205)

Table S3. S_0-S_n (n=1-4) energies (in eV) and oscillator strengths (in parenthesis) for TC-echinenone as obtained from TDA/6-311+G(d,p) calculations.

	S1	S2	S3	S4
B3LYP	2.2722 (5.4210)	2.5276 (0.0000)	3.1008 (0.0755)	3.1909 (0.0000)
TPSS	1.9488 (0.0000)	2.0389 (3.9720)	2.0943 (0.0000)	2.0963 (0.8061)
RevTPSS	1.9651 (0.0000)	2.0507 (3.8361)	2.1027 (0.0000)	2.1054 (0.9647)
VSXC	1.9770 (0.0000)	2.0588 (4.8103)	2.1673 (0.1045)	2.1693 (0.0000)
HCTC	1.8900 (0.0000)	1.9702 (1.2553)	1.9939 (0.0000)	2.0197 (3.3279)
TPSSh	2.1915 (5.3523)	2.2687 (0.0000)	2.7305 (0.0002)	2.7343 (0.0000)
M06L	2.0366 (0.0000)	2.1073 (4.8805)	2.2927 (0.0427)	2.2959 (0.0000)
M11L	1.9891 (0.0000)	2.0471 (5.1852)	2.4279 (0.0009)	2.4313 (0.0000)
MN12L	2.1492 (0.0000)	2.1621 (5.4555)	2.7068 (0.0469)	2.7218 (0.0000)
PBE	1.8664 (0.0000)	1.9021 (0.2750)	1.9321 (0.0000)	2.0083 (4.3651)
BLYP	1.7548 (0.0000)	1.8756 (0.0042)	1.8756 (0.0000)	1.9282 (5.1527)
PW91	1.8701 (0.0000)	1.9191 (0.3938)	1.9440 (0.0000)	2.0059 (4.2335)
M06	2.3096 (5.2337)	2.7291 (0.0000)	3.3045 (0.0511)	3.3349 (0.0000)
BHandH	no convergence			
HSEH1PBE	2.2680 (5.4143)	2.4287 (0.0000)	3.0345 (0.1013)	3.1695 (0.0000)
PBE0	2.3420 (5.4765)	2.7002 (0.0000)	3.2903 (0.0489)	3.3324 (0.0000)
CAM-B3LYP	2.6392 (5.0468)	3.6905 (0.0000)	3.7304 (0.0000)	3.7750 (0.0017)
LC-wPBE	2.9872 (4.7272)	3.9164 (0.0000)	3.9207 (0.0012)	4.0624 (0.0000)

Table S4. S_0-S_n (n=1-4) energies (in eV) and oscillator strengths (in parenthesis) for CC-canthaxanthin as obtained from TDA/6-311+G(d,p) calculations.

	S1	S2	S3	S4
B3LYP	2.2234 (5.6707)	2.4542 (0.0908)	3.0422 (0.0478)	3.0544 (0.0129)
TPSS	1.8813 (0.1596)	2.0142 (3.8527)	2.0253 (0.0178)	2.0448 (1.0792)
RevTPSS	1.8975 (0.1729)	2.0259 (3.2946)	2.0284 (0.2474)	2.0539 (1.4257)
VSXC	1.9094 (0.1595)	2.0327 (5.0200)	2.0834 (0.0084)	2.1165 (0.0785)
HCTC	1.8264 (0.1283)	1.9253 (0.0000)	1.9335 (0.2740)	1.9830 (4.5024)
TPSSh	2.1383 (4.6897)	2.2076 (1.0177)	2.6362 (0.0001)	2.6922 (0.0002)
M06L	1.9611 (0.2742)	2.0767 (4.9476)	2.2276 (0.0007)	2.2407 (0.0247)
M11L	1.9170 (0.2538)	2.0184 (5.2500)	2.3729 (0.0005)	2.3802 (0.0011)
MN12L	2.0648 (0.8391)	2.1327 (4.9724)	2.6473 (0.0016)	2.6597 (0.0213)
PBE	1.8094 (0.1348)	1.8524 (0.0000)	1.8679 (0.0169)	1.9775 (4.8076)
BLYP	1.8113 (0.1136)	1.9186 (0.0023)	1.9305 (0.4813)	1.9713 (4.3039)
PW91	1.8106 (0.1288)	1.8698 (0.0002)	1.8823 (0.0501)	1.9744 (4.7702)
M06	2.2603 (5.5106)	2.6528 (0.0326)	3.2255 (0.0026)	3.2433 (0.0399)
BHandH	2.5603 (5.6003)	3.4607 (0.0063)	3.7034 (0.0275)	3.8571 (0.0001)
HSEH1PBE	2.2141 (5.4649)	2.3532 (0.2788)	2.9742 (0.0711)	3.0387 (0.0021)
PBE0	2.2915 (5.7583)	2.6234 (0.0476)	3.1929 (0.0005)	3.2293 (0.0395)
CAM-B3LYP	2.5890 (5.3257)	3.6141 (0.0037)	3.6778 (0.0004)	3.6907 (0.0272)
LC-wPBE	2.9411 (4.9977)	3.8620 (0.0002)	3.9160 (0.0032)	3.9908 (0.0235)

Table S5. S_0-S_n (n=1-4) energies (in eV) and oscillator strengths (in parenthesis) for TC-canthaxanthin as obtained from TDA/6-311+G(d,p) calculations.

	S1	S2	S3	S4
Ech-CC	2.1201 (0.16920)	2.3193 (3.57768)	2.5871 (0.04025)	2.9128 (0.00428)
Ech-TC	1.9646 (0.11007)	2.2380 (3.92380)	2.4357 (0.03813)	2.7410 (0.00001)
Ech-CT	1.9889 (0.12447)	2.2452 (3.83820)	2.4576 (0.06318)	2.9684 (0.00396)
Ech-TT	1.8614 (0.11348)	2.1724 (3.99291)	2.3149 (0.10270)	2.8074 (0.00016)
Canth-CC	2.0735 (0.00000)	2.2623 (3.97160)	2.5121 (0.00194)	2.9696 (0.00000)
Canth-TC	1.9586 (0.00920)	2.2065 (4.18587)	2.3779 (0.00043)	2.7882 (0.00002)
Canth-TT	1.8590 (0.00000)	2.1512 (4.40137)	2.2506 (0.01843)	2.7573 (0.00025)

Table S6. Electronic transition energies to the first 4 excited states (in eV) and oscillator strengths (in parenthesis) as obtained by DFT/MRCI calculations.

	Echinenone				*Cantaxanthin*			
	S_1	S_2	S_3	S_4	S_1	S_2	S_3	S_4
	CC							
B3LYP	2.27	2.64	3.06	3.18	2.27	2.53	3.10	3.19
TPSS	1.89	2.15	2.26	2.46	1.95	2.04	2.09	2.10
M06L	1.96	2.29	2.39	2.56	2.04	2.11	2.29	2.30
M11L	1.92	2.21	2.49	2.52	1.99	2.05	2.43	2.43
MN12L	2.06	2.36	2.69	2.80	2.15	2.16	2.71	2.72
MRCI	**2.12**	**2.40**	**2.54**	**2.71**	**2.01**	**2.34**	**2.60**	**2.64**
	TC							
B3LYP	2.21	2.56	3.01	3.09	2.22	2.45	3.04	3.05
TPSS	1.83	2.13	2.19	2.44	1.88	2.01	2.03	2.04
M06L	1.90	2.26	2.33	2.53	1.96	2.08	2.23	2.24
M11L	1.86	2.17	2.46	2.47	1.92	2.02	2.37	2.38
MN12L	2.00	2.31	2.66	2.75	2.06	2.13	2.65	2.66
MRCI	**1.96**	**2.32**	**2.50**	**2.55**	**1.92**	**2.29**	**2.42**	**2.49**
	CT							
B3LYP	2.21	2.56	3.01	3.24				
TPSS	1.84	2.17	2.22	2.44				
M06L	1.91	2.25	2.41	2.54				
M11L	1.87	2.16	2.48	2.55				
MN12L	2.00	2.30	2.67	2.84				
MRCI	**1.99**	**2.25**	**2.46**	**2.97**				
	TT							
B3LYP	2.13	2.50	2.96	3.09	2.18	2.38	2.98	3.04
TPSS	1.76	2.13	2.15	2.41	1.82	1.98	1.98	1.98
M06L	1.83	2.21	2.33	2.50	1.90	2.03	2.18	2.18
M11L	1.80	2.12	2.44	2.47	1.86	1.97	2.33	2.33
MN12L	1.92	2.26	2.63	2.74	2.00	2.08	2.60	2.61
MRCI	**1.86**	**2.17**	**2.31**	**2.81**	**1.86**	**2.15**	**2.25**	**2.76**
EXP	2.56-2.44				2.50-2.31			

Table S7. DFT/MRCI and TDA-DFT transition energies (in eV) for the first four excited states of Echinenone (CC, TC, CT and TT) and Canthaxanthin (CC, TC and TT). Experimental data are taken from Ref. 5: for Echinenone we report the values corresponding to OCP-o and OCP-r, and the range obtained for different isomers, while for Canthaxanthin we report the energy value range from experiments in different solvents.

	S_1	S_2	S_3	S_4
	Astaxanthin-keto			
B3LYP	2.14	2.33	2.94	3.14
TPSS	1.78	1.93	2.23	2.24
M06L	1.85	1.98	2.40	2.42
M11L	1.82	1.94	2.39	2.52
MN12L	1.96	2.04	2.57	2.71
DFT/MRCI	**1.80**	**2.10**	**2.20**	**2.71**
	Astaxanthin-enol			
B3LYP	1.97	2.32	2.74	2.88
TPSS	1.51	1.95	2.15	2.28
M06L	1.59	2.01	2.25	2.36
M11L	1.57	1.95	2.22	2.32
MN12L	1.68	2.08	2.38	2.48
DFT/MRCI	**1.64**	**2.03**	**2.11**	**2.48**
EXP	2.33[a]			
	Fucoxanthin			
B3LYP	2.56	2.97	3.19	3.66
TPSS	2.25	2.31	2.60	2.86
M06L	2.33	2.52	2.66	3.06
M11L	2.29	2.56	2.66	3.01
MN12L	2.43	2.73	2.94	3.16
DFT/MRCI	**2.38**	**2.56**	**2.90**	**3.01**
EXP	2.40[b]; 2.74[b]			
	Capsanthin			
B3LYP	2.31	2.72	3.05	3.18
TPSS	1.95	2.10	2.37	2.59
M06L	2.02	2.28	2.43	2.68
M11L	1.94	2.33	2.43	2.62
MN12L	2.13	2.48	2.71	2.82
DFT/MRCI	**2.09**	**2.34**	**2.63**	**2.76**
EXP	2.64[c]			
	Capsorubin			
B3LYP	2.43	2.64	2.99	2.99
TPSS	1.95	1.95	2.10	2.27
M06L	2.13	2.14	2.19	2.32
M11L	2.13	2.25	2.30	2.30
MN12L	2.30	2.37	2.59	2.59
DFT/MRCI	**2.11**	**2.36**	**2.62**	**2.71**
EXP	2.64[c]			

Table S8. TDA-DFT and DFT/MRCI transition energies (in eV) for the first four excited states of Astaxanthin, Fucoxanthin, Capsanthin and Capsorubin. [a]Experiments in $CHCl_3$ from Ref. 6; [b]Experiments in THF from Ref. 7: a dark and a bright state were reported and assigned here to S_1 and S_2 based on our DFT/MRCI results. [c] Experiments in hexane from Ref. 8.

Molecule	Method	S_1	S_2	S_3	S_4
Astaxanthin (Keto)	old	1.7710 (0.00000)	2.1834 (4.48865)	2.3107 (0.12669)	2.7969 (0.00160)
	new	1.8029 (0.00000)	2.0977 (4.26632)	2.1972 (0.17686)	2.7086 (0.00034)
Astaxanthin (Enol)	old	1.7551 (0.09056)	2.1441 (3.92358)	2.2741 (0.60499)	2.6668 (0.03125)
	new	1.6411 (0.07569)	2.0276 (2.72719)	2.1096 (1.43195)	2.4789 (0.04582)
Fucoxanthin	old	2.3217 (0.13490)	2.4417 (0.00811)	2.5922 (3.52460)	3.0741 (0.00152)
	new	2.3832 (0.41177)	2.5633 (3.22006)	2.8966 (0.00109)	3.0107 (0.00341)
Capsanthin	old	2.0945 (0.08364)	2.2967 (0.01753)	2.4199 (3.82424)	2.7459 (0.01869)
	new	2.0916 (0.20117)	2.3417 (3.59539)	2.6270 (0.03250)	2.7569 (0.00033)
Capsorubin	old	2.0500 (0.00000)	2.3468 (0.03834)	2.3480 (0.00002)	2.4566 (4.00938)
	new	2.1109 (0.00000)	2.3567 (3.91292)	2.6179 (0.00473)	2.7140 (0.00001)

Table S9. Electronic transition energies (in eV) and oscillator strength (in parenthesis) for the first four excited states of Astaxanthin (keto and enol forms) Fucoxanthin, Capsanthin and Capsorubin as obtained by DFT/MRCI/def2-SV(P) calculations. The identifier ”old” refers to data obtained with the original parametrization of the DFT/MRCI Hamiltonian[3] while “new” refers to excited-state data calculated on the basis of the recently re-parametrized DFT/MRCI Hamiltonian[4].

XYZ coordinates of the optimized geometries (B3LYP/6-311G(d,p) level) of the new carotenoid structures. Echinenone and Canthaxanthin are available in Ref. 5.

Astaxanthin (keto)

C	11.686152	-1.348245	0.277605
C	13.140420	-1.836331	0.483822
C	14.109754	-1.284287	-0.544347
C	14.087523	0.231018	-0.458875
C	12.785208	0.894671	-0.273159
C	11.647040	0.176110	0.016383
C	10.395764	0.920755	0.073576
C	9.111785	0.474005	0.094822
C	7.934917	1.314712	0.107378
C	6.711397	0.699157	0.103906
C	5.416327	1.305142	0.111343
C	4.261813	0.580021	0.108597
C	2.920174	1.101585	0.112322
C	1.878959	0.207925	0.110293
C	0.480893	0.485381	0.111218
C	10.940664	-1.714795	1.584686
C	11.065703	-2.116047	-0.917985
C	12.816757	2.396880	-0.451860
C	8.105616	2.812385	0.123519
C	2.725411	2.597192	0.117906
O	15.412284	-1.778619	-0.334062
O	15.143686	0.841773	-0.574137
C	-11.686182	1.348267	0.277295
C	-13.140461	1.836363	0.483408
C	-14.109772	1.284132	-0.544683
C	-14.087518	-0.231159	-0.458953
C	-12.785196	-0.894761	-0.273094
C	-11.647041	-0.176130	0.016321
C	-10.395750	-0.920742	0.073623
C	-9.111777	-0.473971	0.094834
C	-7.934900	-1.314663	0.107496
C	-6.711386	-0.699096	0.103973
C	-5.416311	-1.305068	0.111479
C	-4.261802	-0.579940	0.108666
C	-2.920161	-1.101496	0.112440
C	-1.878949	-0.207832	0.110322
C	-0.480883	-0.485285	0.111268
C	-10.940725	1.715039	1.584332
C	-11.065726	2.115887	-0.918408
C	-12.816724	-2.397003	-0.451519
C	-8.105583	-2.812337	0.123798
C	-2.725392	-2.597102	0.118167
O	-15.143681	-0.841946	-0.574043
O	-15.412313	1.778478	-0.334504
H	13.498998	-1.530646	1.472896
H	13.163354	-2.929625	0.462623
H	13.771426	-1.545412	-1.560981
H	10.520109	1.995020	0.050575
H	8.904237	-0.587844	0.082577
H	6.713997	-0.389452	0.093133
H	5.354400	2.387245	0.118048

H	4.348051	-0.504955	0.102391
H	2.145209	-0.847524	0.107305
H	0.153115	1.520915	0.111540
H	9.860844	-1.594719	1.523761
H	11.298794	-1.103465	2.416888
H	11.143624	-2.761832	1.828473
H	11.614452	-1.930508	-1.843770
H	10.027994	-1.835427	-1.097973
H	11.093260	-3.191526	-0.720379
H	12.420738	2.922646	0.421688
H	12.237016	2.716399	-1.323519
H	13.848171	2.714041	-0.595260
H	7.154317	3.340170	0.149675
H	8.649719	3.152378	-0.763627
H	8.685041	3.128947	0.996577
H	1.675568	2.883633	0.119826
H	3.192129	3.052623	-0.761355
H	3.193313	3.046088	0.999910
H	15.994389	-1.014125	-0.469436
H	-13.499048	1.530835	1.472528
H	-13.163414	2.929653	0.462030
H	-13.771433	1.545090	-1.561355
H	-10.520075	-1.995011	0.050743
H	-8.904241	0.587879	0.082473
H	-6.713997	0.389512	0.093089
H	-5.354375	-2.387170	0.118290
H	-4.348046	0.505035	0.102356
H	-2.145203	0.847615	0.107234
H	-0.153103	-1.520819	0.111688
H	-9.860903	1.594969	1.523448
H	-11.298864	1.103839	2.416624
H	-11.143706	2.762113	1.827945
H	-11.614471	1.930210	-1.844167
H	-10.028017	1.835239	-1.098350
H	-11.093283	3.191396	-0.720963
H	-12.420661	-2.922604	0.422108
H	-12.237012	-2.716669	-1.323143
H	-13.848138	-2.714208	-0.594824
H	-7.154279	-3.340109	0.149998
H	-8.649694	-3.152431	-0.763304
H	-8.684994	-3.128812	0.996897
H	-1.675548	-2.883539	0.120099
H	-3.192119	-3.052620	-0.761044
H	-3.193279	-3.045914	1.000221
H	-15.994402	1.013947	-0.469737

Astaxanthin (enol)

C	11.539893	0.155735	0.044840
C	11.556700	-1.357385	0.373329
C	12.992114	-1.837230	0.706871
C	14.041380	-1.369574	-0.279516
C	13.953137	0.125458	-0.430748
C	12.810827	0.831140	-0.248494
C	10.727034	-1.692009	1.636803
C	11.032883	-2.166122	-0.838356
O	15.377904	-1.743911	0.109699
O	15.114820	0.721736	-0.809521
C	12.857918	2.328852	-0.451547
C	10.389089	0.897256	-0.042968
C	9.015460	0.494075	0.033670
C	7.913303	1.310386	-0.008397
C	7.990809	2.815955	-0.079213
C	6.610387	0.694930	0.019244
C	5.404326	1.329900	-0.011219
C	4.156690	0.632054	0.015720
C	2.890026	1.154349	-0.007191
C	2.609853	2.635870	-0.066734
C	1.773747	0.244070	0.027369
C	0.452077	0.571768	0.016709
C	-0.608286	-0.389586	0.049848
C	-1.931443	-0.068457	0.041731
C	-3.040758	-0.987856	0.067822
C	-2.748329	-2.467749	0.106068
C	-4.312713	-0.476926	0.055039
C	-5.550509	-1.190947	0.067014
C	-6.767445	-0.575742	0.057540
C	-8.056929	-1.218179	0.057943
C	-8.103515	-2.726675	0.069518
C	-9.176855	-0.422526	0.051973
C	-10.534984	-0.866382	-0.022446
C	-11.717287	-0.168403	0.028249
C	-11.834806	1.348934	0.307614
C	-13.223714	1.681464	0.910039
C	-14.387387	1.041259	0.218507
C	-14.159781	-0.295300	-0.326991
C	-12.934282	-0.898149	-0.335624
C	-10.817647	1.894246	1.339022
C	-11.668776	2.113130	-1.028387
O	-15.511741	1.530141	0.163999
O	-15.279975	-0.903218	-0.789089
C	-12.872349	-2.329399	-0.815683
H	-13.255515	1.331941	1.950825
H	-13.380984	2.762394	0.933856
H	-10.639934	-1.927955	-0.197837
H	-8.985689	0.641202	0.057505
H	-6.780739	0.512627	0.044990
H	-5.515696	-2.274484	0.081141
H	-4.400165	0.607934	0.030607
H	-2.193255	0.987657	0.010400
H	-0.312444	-1.435207	0.081869
H	-9.831730	2.076401	0.916078

H	-10.705803	1.215715	2.187640
H	-11.175898	2.855137	1.719569
H	-12.428596	1.819183	-1.756653
H	-10.689444	1.912998	-1.468636
H	-11.756014	3.191861	-0.864047
H	-12.484058	-2.992371	-0.035898
H	-12.221203	-2.431306	-1.688492
H	-13.866012	-2.678377	-1.086998
H	-7.571746	-3.120673	0.941263
H	-7.614034	-3.138590	-0.818927
H	-9.118034	-3.117751	0.104333
H	-2.171230	-2.772906	-0.772796
H	-3.652657	-3.072559	0.135030
H	-2.150220	-2.722115	0.986936
H	13.271060	-1.447294	1.694487
H	13.002489	-2.928967	0.772607
H	13.914795	-1.850288	-1.255419
H	10.531513	1.947719	-0.255298
H	8.797149	-0.564395	0.091304
H	6.602863	-0.392903	0.066941
H	5.385920	2.412828	-0.058754
H	4.232396	-0.453317	0.059670
H	2.028442	-0.813750	0.065647
H	0.159511	1.617995	-0.019451
H	9.656486	-1.558715	1.502316
H	11.035648	-1.062898	2.475569
H	10.895182	-2.736739	1.917170
H	11.633142	-1.981588	-1.732611
H	10.004400	-1.899245	-1.082892
H	11.063279	-3.239275	-0.623234
H	12.406570	2.856671	0.393782
H	12.318921	2.633373	-1.355091
H	13.888298	2.663999	-0.552092
H	7.454161	3.269780	0.760131
H	7.524468	3.188472	-0.997384
H	9.013481	3.186207	-0.050003
H	2.033069	2.958628	0.806252
H	2.016756	2.884418	-0.952829
H	3.520128	3.231641	-0.100248
H	15.467555	-1.566542	1.054152
H	-15.986487	-0.244549	-0.652909
H	15.802683	0.042572	-0.718096

Fucoxanthin

C	-9.647839	2.124663	-1.079848
C	-9.659851	3.556116	-0.570877
C	-10.114118	3.668316	0.880714
C	-11.460531	2.987549	1.026050
C	-11.472356	1.463226	0.734439
C	-10.515789	1.083877	-0.438294
C	-10.870771	-0.174250	-1.246175
C	-10.988359	-1.529594	-0.516231
C	-9.796288	-2.359213	-0.210022
C	-8.537614	-1.870189	-0.374098
C	-7.297922	-2.542145	-0.099978
C	-6.095663	-1.923495	-0.252399
C	-4.793685	-2.493546	-0.008027
C	-3.696584	-1.696706	-0.204172
C	-2.319079	-2.028967	-0.029869
C	-1.302124	-1.143775	-0.242159
C	0.078223	-1.463914	-0.069335
C	1.163297	-0.645733	-0.244803
C	2.477825	-1.191422	-0.007476
C	3.661598	-0.530635	-0.116566
C	4.931380	-1.149631	0.137438
C	-9.121623	2.020513	-2.498473
C	-12.936703	1.101449	0.401565
C	-11.030058	0.694645	1.999028
C	-4.706516	-3.926930	0.452071
O	-9.102013	1.192593	-0.124147
O	-10.296119	5.036243	1.261782
H	-3.680172	-4.257052	0.601119
H	-5.170068	-4.598299	-0.277867
H	-5.240481	-4.063544	1.398010
H	-8.648980	3.968282	-0.688908
H	-10.327682	4.165916	-1.189895
H	-9.372681	3.194070	1.533747
H	-11.842366	3.158810	2.036325
H	-12.149470	3.496894	0.342048
H	-11.844522	-0.022310	-1.714099
H	4.890169	-2.201760	0.413753
H	2.508120	-2.237799	0.290656
H	0.285014	-2.485986	0.242808
H	-1.568014	-0.139096	-0.558456
H	-2.059259	-3.034110	0.289304
H	-3.890880	-0.677008	-0.532130
H	-6.104022	-0.887463	-0.585351
H	-8.435305	-0.843585	-0.707808
H	-8.954627	0.995148	-2.821578
H	-8.165417	2.547648	-2.569192
H	-9.814883	2.496300	-3.198521
H	-9.435825	5.466965	1.242826
H	-13.093705	0.028240	0.302486
H	-13.260550	1.587058	-0.524784
H	-13.584221	1.469193	1.202944
H	-11.086096	-0.386112	1.858423
H	-11.688181	0.951355	2.833884
H	-10.004811	0.945720	2.276207

O	-12.101937	-1.965840	-0.254583
C	-10.119465	-3.733253	0.315675
H	-9.230462	-4.347040	0.454844
H	-10.644233	-3.663179	1.273046
H	-10.800481	-4.253157	-0.362776
H	-7.327111	-3.569656	0.243289
C	1.048644	0.796476	-0.671600
H	1.483270	1.459828	0.083117
H	1.595066	0.969087	-1.604345
H	0.017681	1.106639	-0.829861
C	6.166526	-0.579484	0.075656
H	3.652685	0.513597	-0.408287
C	6.416518	0.861221	-0.280499
H	7.067109	0.933021	-1.157791
H	5.500079	1.408226	-0.494948
H	6.933892	1.373943	0.536377
C	7.330396	-1.411493	0.376303
H	7.123965	-2.453534	0.619774
C	8.590353	-1.026218	0.379781
C	9.847682	-0.676342	0.399607
C	10.528426	-0.170177	1.696139
C	10.701424	-0.770583	-0.881766
C	11.383792	1.081441	1.370106
C	11.478539	0.547061	-1.079587
C	12.287428	0.905970	0.160264
H	11.988242	1.341720	2.244692
H	10.719802	1.931476	1.175869
H	12.144944	0.442657	-1.941567
H	10.776880	1.359107	-1.298770
H	13.049767	0.146667	0.331628
C	11.405558	-1.289544	2.306624
H	11.878341	-0.927137	3.225324
H	10.785349	-2.152611	2.561366
H	12.175445	-1.632847	1.619476
C	9.482344	0.237051	2.748263
H	8.822238	1.024258	2.375130
H	8.862229	-0.612287	3.041955
H	9.986083	0.612040	3.644003
C	9.877417	-1.091679	-2.130618
H	9.359313	-2.043120	-2.008136
H	9.139670	-0.314915	-2.342751
H	10.544710	-1.170412	-2.994755
O	11.636896	-1.846361	-0.652571
H	12.246502	-1.866939	-1.399738
O	12.969100	2.178708	-0.035426
C	14.141678	2.153215	-0.707684
O	14.634194	1.153056	-1.168362
C	14.734284	3.537936	-0.798766
H	14.874606	3.950483	0.202566
H	15.686853	3.491075	-1.322093
H	14.047791	4.200308	-1.331128
H	-10.144661	-0.292827	-2.047426

Capsanthin

C	9.246090	-0.357664	0.164925
C	10.493408	-0.874745	0.167171
H	9.130957	0.717501	0.055397
H	10.594757	-1.955940	0.203542
C	8.005790	-1.109316	0.261119
C	6.826502	-0.423028	0.200021
H	6.895763	0.658064	0.092305
C	5.494945	-0.950339	0.249998
C	4.379892	-0.172935	0.172722
H	5.374723	-2.023548	0.346270
H	4.517878	0.902398	0.076246
C	3.012986	-0.630242	0.197073
C	2.011676	0.301764	0.100449
H	2.321637	1.341971	0.018019
C	0.602950	0.079196	0.087449
C	-0.324088	1.077010	-0.015642
H	0.236331	-0.940909	0.158710
H	0.036392	2.099154	-0.086521
C	-1.730345	0.839709	-0.038392
C	-2.746171	1.755438	-0.138831
H	-2.026072	-0.205797	0.030542
C	-4.100654	1.266392	-0.150066
C	-5.236702	2.012208	-0.247263
H	-4.213164	0.186238	-0.075058
H	-5.153042	3.090190	-0.323860
C	-6.544232	1.429195	-0.254161
C	-7.753091	2.060617	-0.351621
H	-6.567329	0.343726	-0.173070
C	-8.945058	1.234955	-0.337854
H	-8.759137	0.173628	-0.240647
C	11.757732	-0.128512	0.032571
C	12.049507	0.967860	0.768035
C	12.750979	-0.743562	-0.979960
C	13.335679	1.748885	0.594116
C	13.899767	0.238850	-1.310485
C	14.461223	1.005996	-0.124077
H	13.693519	2.081447	1.577581
H	13.113273	2.675916	0.044727
H	14.708706	-0.305917	-1.806857
H	13.531463	0.983228	-2.025790
H	15.192552	1.739443	-0.493745
C	11.156125	1.545077	1.839849
H	10.716417	2.499226	1.521889
H	10.342294	0.879175	2.119146
H	11.746599	1.763646	2.736828
C	13.322466	-2.066320	-0.411108
H	12.532221	-2.801025	-0.234880
H	14.021835	-2.507665	-1.128446
H	13.859021	-1.889736	0.519148
C	12.030130	-1.052837	-2.312372
H	11.261841	-1.819599	-2.192334
H	11.547576	-0.158775	-2.717380
H	12.751361	-1.415348	-3.051805
O	15.131202	0.078844	0.738553

H	15.472246	0.569004	1.492975
C	-7.906134	3.554442	-0.474274
H	-8.427491	3.816924	-1.400329
H	-8.504348	3.953289	0.351153
H	-6.949294	4.073381	-0.472831
C	-2.513000	3.242039	-0.239818
H	-2.932279	3.639360	-1.169917
H	-3.003494	3.768963	0.585081
H	-1.456517	3.502463	-0.215624
C	2.750702	-2.110660	0.321121
H	3.200838	-2.655617	-0.514869
H	3.194638	-2.506830	1.239933
H	1.689138	-2.349191	0.338290
C	8.084328	-2.606785	0.416135
H	7.104224	-3.071918	0.503484
H	8.592874	-3.061283	-0.440668
H	8.660636	-2.874015	1.307611
C	-10.215653	1.690785	-0.424245
H	-10.389065	2.759144	-0.505178
C	-11.512431	0.974991	-0.384881
O	-12.511657	1.682898	-0.366934
C	-11.678132	-0.569083	-0.370333
C	-11.531867	-1.194340	1.091384
C	-13.148113	-0.925793	-0.714564
C	-12.328273	-2.521398	0.956777
C	-13.422967	-2.311116	-0.116564
H	-13.328517	-0.935297	-1.791237
H	-13.814452	-0.179381	-0.286795
H	-11.666002	-3.321633	0.613304
H	-12.734601	-2.831761	1.924300
H	-14.426987	-2.347045	0.322659
C	-10.774831	-1.255711	-1.422497
H	-10.892226	-0.755271	-2.387768
H	-9.714636	-1.248048	-1.177980
H	-11.085755	-2.292190	-1.561191
C	-10.100439	-1.482310	1.564914
H	-9.550409	-2.110040	0.860099
H	-9.533604	-0.564219	1.734235
H	-10.133346	-2.019702	2.518208
C	-12.208420	-0.292556	2.146805
H	-11.673711	0.652684	2.268958
H	-13.242441	-0.051945	1.893927
H	-12.208632	-0.801197	3.115592
O	-13.347732	-3.286509	-1.170221
H	-13.543305	-4.148121	-0.788309

Capsorubin

C	-9.034185	-1.267610	-0.345733
H	-8.921376	-0.191703	-0.341064
C	-7.785749	-2.006656	-0.382985
C	-6.624476	-1.286011	-0.403905
H	-6.722119	-0.201820	-0.395160
C	-5.279280	-1.777075	-0.429983
C	-4.194814	-0.953467	-0.441144
H	-5.124449	-2.849777	-0.436467
H	-4.375705	0.119773	-0.433719
C	-2.810867	-1.354663	-0.457019
C	-1.854000	-0.372654	-0.460124
H	-2.211970	0.655306	-0.455043
C	-0.435562	-0.525744	-0.464804
C	0.435672	0.525723	-0.464875
H	-0.018415	-1.528480	-0.464993
H	0.018523	1.528458	-0.465156
C	1.854111	0.372638	-0.460226
C	2.810974	1.354651	-0.457251
H	2.212085	-0.655320	-0.455046
C	4.194923	0.953461	-0.441364
C	5.279386	1.777075	-0.430289
H	4.375817	-0.119778	-0.433832
H	5.124549	2.849775	-0.436862
C	6.624585	1.286020	-0.404163
C	7.785853	2.006674	-0.383281
H	6.722234	0.201831	-0.395321
C	9.034291	1.267636	-0.345937
H	8.921488	0.191727	-0.341199
C	7.833807	3.512262	-0.392425
H	8.331004	3.891025	0.506219
H	8.407203	3.876611	-1.250514
H	6.843509	3.961295	-0.439622
C	2.485304	2.827149	-0.465988
H	2.897786	3.321417	0.419419
H	2.923877	3.316063	-1.341714
H	1.414317	3.018735	-0.482938
C	-2.485202	-2.827163	-0.465615
H	-2.897674	-3.321342	0.419845
H	-2.923789	-3.316162	-1.341287
H	-1.414216	-3.018754	-0.482560
C	-7.833711	-3.512244	-0.392025
H	-6.843414	-3.961286	-0.439168
H	-8.330931	-3.890941	0.506634
H	-8.407090	-3.876650	-1.250101
C	-10.268146	-1.817331	-0.301050
H	-10.363904	-2.898305	-0.285749
C	-11.614825	-1.198821	-0.216611
O	-12.544298	-1.978173	-0.060830
C	-11.904078	0.325180	-0.325052
C	-13.427613	0.537447	-0.555886
C	-11.655594	1.113138	1.041839
C	-13.829052	1.864259	0.113252
H	-13.995371	-0.265259	-0.090446
H	-13.667786	0.518592	-1.621378

C	-12.563023	2.351354	0.843859
H	-14.160035	2.606326	-0.624076
H	-12.044032	3.096147	0.231219
H	-12.803082	2.835184	1.796139
C	-11.156960	0.944327	-1.530203
H	-10.075125	0.977546	-1.421890
H	-11.377601	0.369922	-2.434195
H	-11.498753	1.966903	-1.708814
C	-12.158720	0.290724	2.247398
H	-12.074508	0.893096	3.157330
H	-13.202835	-0.000841	2.139880
H	-11.560676	-0.612771	2.391929
C	-10.212141	1.551856	1.324309
H	-9.563868	0.703214	1.551540
H	-9.776177	2.115156	0.495306
H	-10.200049	2.207075	2.201019
O	-14.917461	1.578911	1.003885
H	-15.194455	2.407428	1.407862
C	10.268249	1.817363	-0.301234
H	10.364019	2.898337	-0.285999
C	11.614911	1.198839	-0.216702
O	12.544409	1.978187	-0.061053
C	11.904096	-0.325181	-0.325052
C	13.427635	-0.537579	-0.555748
C	11.655422	-1.113059	1.041842
C	13.828897	-1.864399	0.113482
H	13.995419	0.265099	-0.090293
H	13.667896	-0.518789	-1.621221
C	12.562753	-2.351367	0.843979
H	14.159897	-2.606522	-0.623782
H	12.043752	-3.096123	0.231304
H	12.802676	-2.835199	1.796292
C	11.157017	-0.944317	-1.530232
H	10.075169	-0.977419	-1.421993
H	11.377782	-0.369988	-2.434242
H	11.498718	-1.966937	-1.708758
C	12.158517	-0.290650	2.247418
H	12.074200	-0.892991	3.157362
H	13.202656	0.000847	2.139968
H	11.560516	0.612885	2.391879
C	10.211897	-1.551613	1.324196
H	9.563692	-0.702891	1.551324
H	9.775948	-2.114904	0.495179
H	10.199653	-2.206787	2.200939
O	14.917234	-1.579104	1.004220
H	15.194137	-2.407631	1.408240

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