Electronic Supplementary Material (ESI) for Photochemical & Photobiological Sciences.

Conical Intersections and the Weak Fluorescence of Betalains

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Table S1. Calculated ADC (2) excitation energies, ΔE (eV, nm), oscillator strengths (*f*) and charge transfer character (*q*(CT), in units of *e*) of betanin, indicaxanthin and cBeet120 in the gas phase with two different basis sets for 10 excited states.

		ADC (2)					
		def2-TZVP			TZVP		
Compound	State	ΔE (eV, nm)	*f*	*q*(CT)	ΔE (eV, nm)	*f*	*q*(CT)
Betanin	S_1	2.25, 551	0.806	0.270	2.28(1.34), 543	0.829	0.250
	S_2	2.97, 417	0.092	0.461	2.99, 414	0.072	0.481
	S_3	3.68, 336	0.021	0.543	3.73, 332	0.027	0.540
	S_4	4.19, 295	0.001	0.014	4.24, 292	0.000	0.015
	S_5	4.53, 273	0.119	0.605	4.58, 270	0.215	0.378
	S_6	4.55, 272	0.133	0.543	4.62, 268	0.046	0.667
	S_7	4.61, 268	0.037	0.396	4.67, 265	0.023	0.498
	S_8	4.90, 253	0.007	0.696	4.94, 251	0.008	0.664
	S_9	4.94, 251	0.009	0.314	4.99, 248	0.010	0.341
	S_{10}	4.96, 250	0.010	0.200	5.01, 247	0.005	0.191
Indicaxanthin	S_1	2.69, 460	0.716	0.346	2.69(1.97), 460	0.729	0.355
	S_2	4.31, 287	0.003	0.093	4.36, 284	0.002	0.092
	S_3	4.61, 268	0.181	0.407	4.67, 265	0.186	0.407
	S_4	5.08, 244	0.009	0.522	5.12, 242	0.009	0.556
	S_5	5.12, 242	0.006	0.403	5.17, 239	0.007	0.381
	S_6	5.24, 236	0.092	0.349	5.29, 234	0.087	0.329
	S_7	5.71, 217	0.000	0.060	5.70, 217	0.000	0.055
	S_8	5.77, 214	0.002	0.074	5.76, 215	0.002	0.055
	S_9	6.14, 201	0.056	0.201	6.19, 200	0.048	0.224
	S_{10}	6.23, 199	0.001	0.255	6.22, 199	0.007	0.246
cBeet120	S_1	2.38, 521	0.876	0.322	2.39(1.77), 518	0.890	0.309
	S_2	3.18, 389	0.030	0.465	3.21, 386	0.024	0.478
	S_3	3.68, 336	0.014	0.589	3.74, 331	0.015	0.576
	S_4	3.93, 315	0.025	0.073	3.95, 313	0.023	0.082
	S_5	3.97, 312	0.000	0.251	3.98, 311	0.000	0.237
	S_6	4.43, 279	0.241	0.346	4.46, 278	0.220	0.295
	S_7	4.49, 276	0.069	0.287	4.53, 273	0.083	0.336
	S_8	4.71, 263	0.000	0.153	4.72, 262	0.000	0.150
	S_9	4.84, 256	0.031	0.240	4.88, 254	0.040	0.242
	S_{10}	4.98, 248	0.136	0.424	5.05, 245	0.146	0.417

Table S2. Calculated ADC (2)/TZVP excitation energies, ΔE (eV, nm), oscillator strengths *f* and charge transfer character (*q*(CT), in units of *e*) of betanin, indicaxanthin and cBeet120 in different polar environments (water and acetonitrile).

		water			acetonitrile		
Compound	State	ΔE(eV, nm)	*f*	*q*(CT)	ΔE(eV, nm)	*f*	q(CT)
Betanin	S_1	2.30, 539	0.890	0.152	2.29, 541	0.891	0.154
	S_2	3.42, 362	0.017	0.426	3.39, 365	0.014	0.431
	S_3	4.07, 304	0.074	0.509	4.04, 306	0.072	0.513
	S_4	4.53, 273	0.000	0.016	4.51, 274	0.000	0.015
	S_5	4.67, 265	0.183	0.359	4.66, 266	0.186	0.367
	S_6	4.81, 257	0.066	0.279	4.80, 258	0.066	0.281
	S_7	5.01, 247	0.015	0.345	5.01, 247	0.014	0.330
	S_8	5.30, 233	0.024	0.141	5.29, 234	0.023	0.136
	S_9	5.51, 225	0.033	0.093	5.49, 225	0.007	0.703
	S_{10}	5.54, 223	0.001	0.890	5.49, 225	0.027	0.273
Indicaxanthin	S_1	2.59, 478	0.729	0.358	2.58, 480	0.729	0.359
	S_2	4.65, 266	0.202	0.402	4.64, 267	0.202	0.402
	S_3	4.74, 261	0.000	0.078	4.72, 262	0.000	0.079
	S_4	5.10, 243	0.070	0.314	5.11, 242	0.069	0.317
	S_5	5.67, 218	0.013	0.339	5.65, 219	0.013	0.367
	S_6	5.70, 217	0.004	0.539	5.68, 218	0.005	0.522
	S_7	5.84, 212	0.002	0.113	5.83, 212	0.001	0.101
	S_8	5.90, 210	0.004	0.116	5.89, 210	0.003	0.110
	S_9	6.12, 202	0.000	0.145	6.12, 202	0.001	0.155
	S_{10}	6.42, 193	0.083	0.373	6.42, 193	0.090	0.325
cBeet120	S_1	2.37, 523	0.925	0.173	2.36, 525	0.924	0.174

	S_2	3.81, 325	0.169	0.504	3.79, 327	0.154	0.508
	S_3	4.15, 298	0.025	0.558	4.14, 299	0.025	0.568
	S_4	4.48, 276	0.307	0.537	4.49, 276	0.317	0.543
	S_5	4.65, 266	0.027	0.064	4.61, 268	0.026	0.067
	S_6	4.83, 256	0.062	0.215	4.81, 257	0.066	0.206
	S_7	4.95, 250	0.028	0.485	4.95, 250	0.026	0.490
	S_8	5.07, 244	0.000	0.222	5.03, 246	0.001	0.227
	S_9	5.12, 242	0.008	0.400	5.12, 242	0.011	0.376
	S_{10}	5.23, 237	0.031	0.157	5.21, 238	0.034	0.166

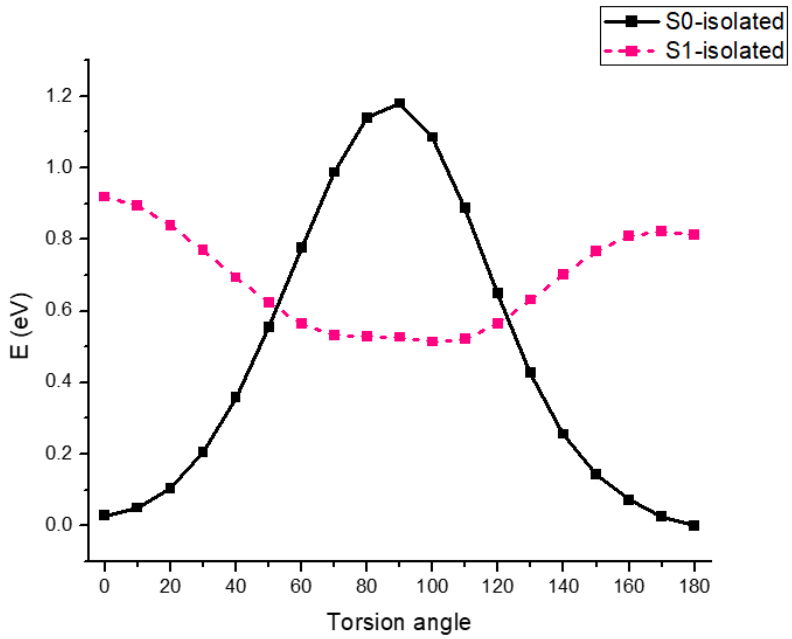

Figure S1. PES curve along the torsional angle ω (see Scheme 3) of betanin-H for the S_1 and S_0 states by ADC (2)/def2-TZVP single point calculation based on geometry optimized at ADC (2)/TZVP level.

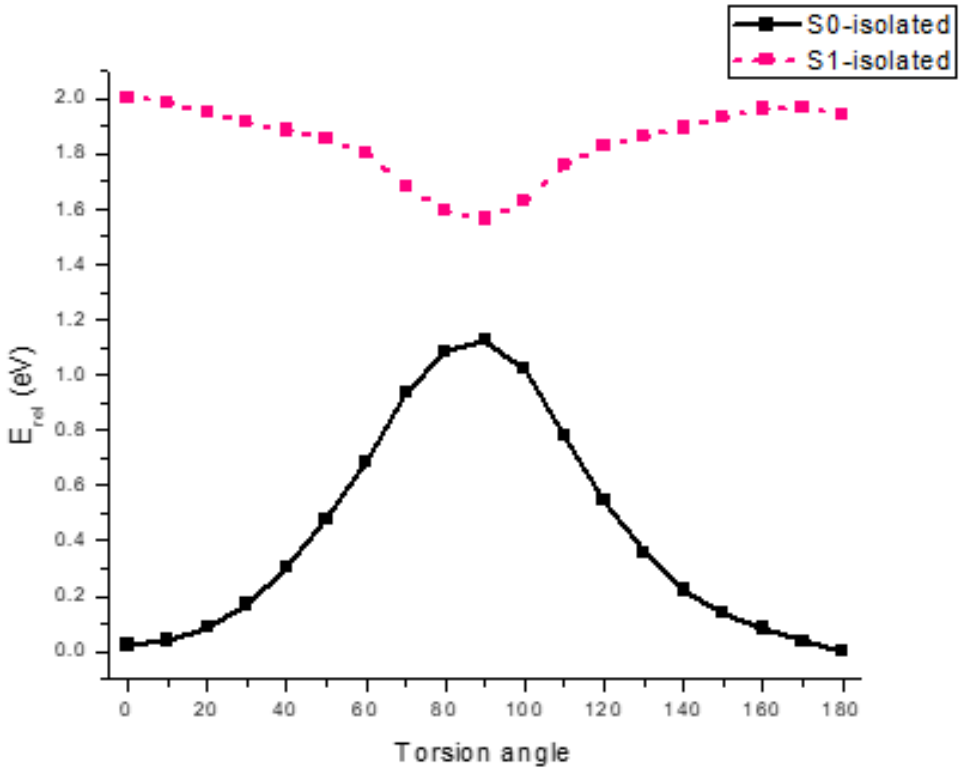

Figure S2. PES curve along the torsional angle ω (see Scheme 3) of betanin-H for the S_1 and S_0 states by CASSCF (8,8)/6-31G* based on geometry optimized at ADC (2)/TZVP level.

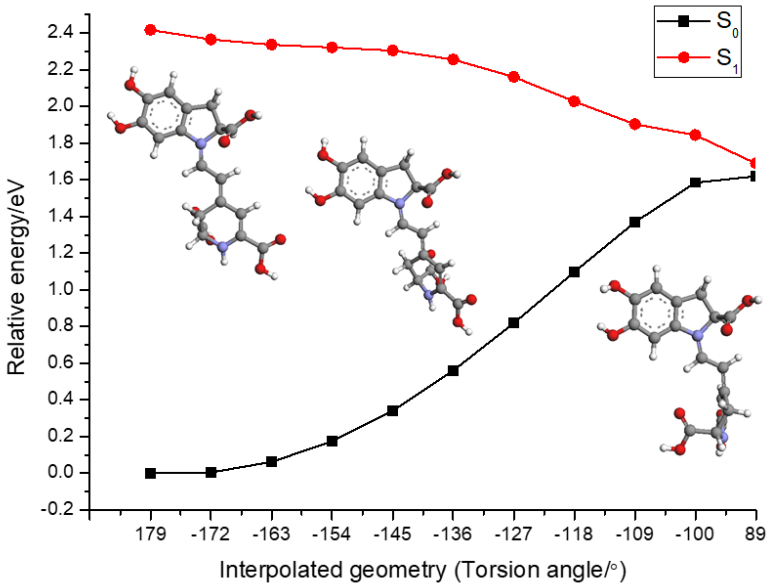

Figure S3. Potential energy curves of betanin-H (**5**) calculated by ADC (2)/TZVP based on linear interpolation geometries (see text). The first point is for the ground state geometry and the last one for the MXS structure, both optimized at SA-CASSCF (6,6)/6-31G* level.

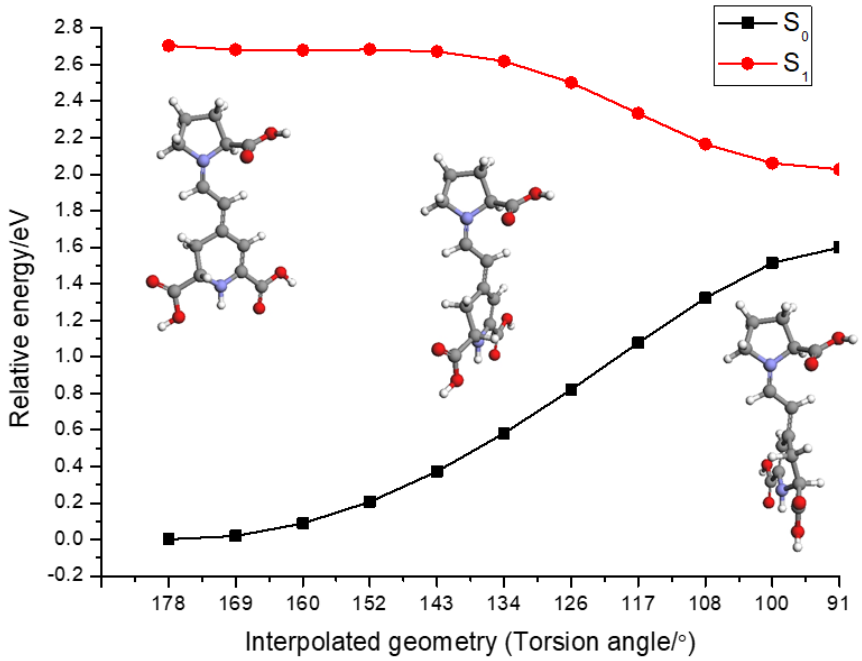

Figure S4. Potential energy curves of indicaxanthin (**3**) calculated by ADC (2)/TZVP based on linear interpolation geometries (see text). The first point is for the ground state geometry and the last one for the MXS structure, both optimized at SA-CASSCF (6,6)/6-31G* level.

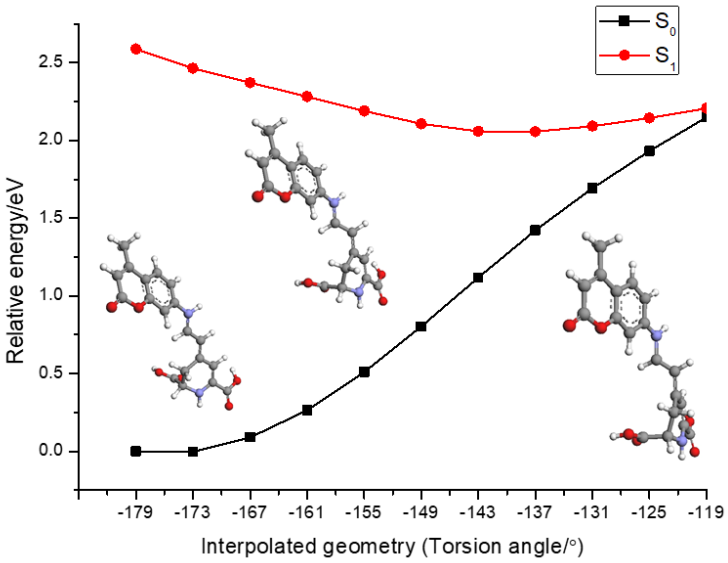

Figure S5. Potential energy curves of cBeet 120 (**4**) calculated by ADC (2)/TZVP based on linear interpolation geometries (see text). The first point is for the ground state geometry and the last one for the MXS structure, both optimized at SA-CASSCF (6,6)/6-31G* level.

Cartesian coordinates of the optimized structures calculated by the different methods and def2-TZVP basis set. of betanin, indicaxanthin and cBeet 120. If not informed, the calculations are in gas phase.

(1) Betanin

DFT/B3-LYP

C	-4.0306208	4.7957654	1.0105739
O	-3.1553693	4.3494464	-0.0393560
C	-3.4329188	3.0418005	-0.4709440
C	-4.8347445	2.9532538	-1.0517161
C	-5.8482427	3.4339870	-0.0293275
C	-5.4751502	4.8162403	0.4938818
O	-2.5183667	2.7186852	-1.4938317
O	-5.0510788	1.5892794	-1.3975436
O	-7.1136384	3.4118866	-0.6658736
O	-6.4051878	5.1090213	1.5311213
C	-3.5165238	6.1582978	1.4376725
O	-2.1942943	6.0913067	1.9371404
C	-0.2223462	2.4888531	-0.8573417
C	0.8498169	1.6601620	-0.5701812
C	0.6629633	0.2833623	-0.5838965
C	-0.5529221	-0.3099909	-0.8823901
C	-1.6332846	0.5199846	-1.1781211
C	-1.4540335	1.9233662	-1.1525842
C	2.2792574	2.0000201	-0.2574138
C	2.8678394	0.6347544	0.1866052
N	1.8765261	-0.3666524	-0.2484920
O	-2.8052226	-0.0560242	-1.4685408
C	2.0757918	-1.6724794	-0.2380804
C	3.2529554	-2.3205938	0.1228180
C	3.3941223	-3.6995504	0.1675248
C	4.6131523	-4.2816891	0.5636178
C	4.7651407	-5.6490175	0.6295833
N	3.8277924	-6.5057106	0.1948614
C	2.7309402	-6.0022366	-0.6091297
C	2.2468112	-4.6547846	-0.0734632
C	6.0358705	-6.2121969	1.2041743
O	6.9433889	-5.5372148	1.6001027
O	6.0189307	-7.5589188	1.2136724
C	3.0553412	0.5570979	1.7044534
O	4.0341440	1.3944920	2.0806354
O	2.4250401	-0.1436440	2.4437445

C	3.0901753	-5.8892231	-2.1064658
O	4.0321672	-6.7746786	-2.4629306
O	2.5436777	-5.1299754	-2.8564184
H	-3.9641600	4.1075491	1.8641034
H	-3.3266077	2.3322194	0.3638802
H	-4.8761868	3.5895182	-1.9423028
H	-5.8395720	2.7400034	0.8241045
H	-5.5574978	5.5385497	-0.3270861
H	-5.9699937	1.4777057	-1.6722733
H	-7.7765074	3.7009787	-0.0262388
H	-6.5159402	6.0614196	1.6180713
H	-4.1368380	6.5386543	2.2500589
H	-3.5903113	6.8507270	0.5875903
H	-1.6399881	5.7228943	1.2389397
H	-0.1311946	3.5668073	-0.8680386
H	-0.7143665	-1.3787368	-0.8880808
H	2.3868829	2.7502116	0.5249810
H	2.8069873	2.3726722	-1.1378016
H	3.8300357	0.4403657	-0.2872002
H	-3.5332863	0.5891254	-1.5987355
H	1.2220756	-2.2538126	-0.5556063
H	4.1144970	-1.7318533	0.4108788
H	5.4453330	-3.6715216	0.8832776
H	4.0590110	-7.4863948	0.1523873
H	1.9108144	-6.7226567	-0.5617164
H	1.7346192	-4.8110876	0.8807922
H	1.5190336	-4.2638650	-0.7798438
H	6.8541223	-7.8776527	1.5919437
H	4.1288157	1.3501122	3.0464501
H	4.1823229	-6.6984149	-3.4206758

DFT/B3-LYP/ /COSMO (water)

C	-4.0223685	4.8315468	0.9714009
O	-3.1694037	4.3531083	-0.0814886
C	-3.4603473	3.0283273	-0.4593131
C	-4.8732647	2.9230772	-1.0161895
C	-5.8758838	3.4679195	-0.0124428
C	-5.4720997	4.8559922	0.4747201
O	-2.5627608	2.6682738	-1.4839028
O	-5.0968658	1.5388333	-1.2820933
O	-7.1495637	3.4796113	-0.6448129
O	-6.3712032	5.2022056	1.5271391
C	-3.5000343	6.2000246	1.3573627

O	-2.1823028	6.1337444	1.8961952
C	-0.2665171	2.4546797	-0.8028435
C	0.8039357	1.6302657	-0.4994400
C	0.6259499	0.2524720	-0.5163645
C	-0.5840334	-0.3475712	-0.8299580
C	-1.6599898	0.4811277	-1.1387173
C	-1.4892112	1.8794440	-1.1183201
C	2.2268694	1.9804028	-0.1702512
C	2.8451381	0.6081437	0.2171567
N	1.8378839	-0.3914485	-0.1796447
O	-2.8412197	-0.0958996	-1.4499358
C	2.0481667	-1.6987699	-0.1914234
C	3.2417236	-2.3255427	0.1349592
C	3.3997298	-3.7077817	0.1496593
C	4.6261493	-4.2779495	0.5280542
C	4.7800340	-5.6499128	0.5975256
N	3.8579427	-6.5008766	0.1444556
C	2.7577361	-6.0031608	-0.6549317
C	2.2613356	-4.6660634	-0.1073629
C	6.0365341	-6.2198525	1.1976833
O	6.9380662	-5.5385637	1.6204136
O	6.0244695	-7.5529364	1.1987837
C	3.1086480	0.5411357	1.7182807
O	4.2247962	1.2077106	2.0148582
O	2.3963416	-0.0050328	2.5224798
C	3.1207073	-5.8855050	-2.1477129
O	4.2051099	-6.5836727	-2.4760134
O	2.4502441	-5.2543504	-2.9277263
H	-3.9488571	4.1597767	1.8365562
H	-3.3400841	2.3537301	0.3995549
H	-4.9200038	3.5062960	-1.9411562
H	-5.8930829	2.7963690	0.8566086
H	-5.5586973	5.5635072	-0.3560451
H	-5.8982074	1.4375364	-1.8112511
H	-7.7944625	3.8064960	-0.0029264
H	-6.5518579	6.1486385	1.4981268
H	-4.1360735	6.6232359	2.1345466
H	-3.5335170	6.8579884	0.4806593
H	-1.6122742	5.7238816	1.2320354
H	-0.1733441	3.5328173	-0.8111140
H	-0.7283463	-1.4187296	-0.8387855
H	2.3078069	2.7015457	0.6427334
H	2.7487067	2.3969405	-1.0321105
H	3.7771595	0.4270802	-0.3143688
H	-3.5622527	0.5630359	-1.5523766
H	1.1925961	-2.2882734	-0.4888961

H	4.1022132	-1.7284978	0.4083743
H	5.4490547	-3.6550581	0.8453102
H	4.0383297	-7.4928446	0.1706955
H	1.9464281	-6.7310409	-0.6141475
H	1.7474409	-4.8393457	0.8423907
H	1.5265522	-4.2713000	-0.8039179
H	6.8457733	-7.8934810	1.5933106
H	4.3618593	1.2095542	2.9785507
H	4.3666980	-6.5030145	-3.4325969

MP2

C	-3.9153694	4.6900771	1.0124153
O	-3.0813993	4.2756613	-0.0811247
C	-3.4431406	3.0018706	-0.5454168
C	-4.8481844	3.0079596	-1.1011255
C	-5.8050964	3.4828808	-0.0340706
C	-5.3552539	4.8181678	0.5242993
O	-2.5755738	2.6591941	-1.6007181
O	-5.1271518	1.6750069	-1.4984476
O	-7.0831788	3.5390570	-0.6336479
O	-6.2508654	5.1153975	1.5867907
C	-3.3244380	5.9915858	1.5043991
O	-1.9889015	5.8237089	1.9336161
C	-0.2694334	2.4434919	-0.9766770
C	0.7875469	1.6033627	-0.6523719
C	0.5668239	0.2312771	-0.5933368
C	-0.6648775	-0.3609122	-0.8409622
C	-1.7258620	0.4791107	-1.1737090
C	-1.5130591	1.8771310	-1.2289126
C	2.2322844	1.9176688	-0.3928849
C	2.7754720	0.5761851	0.1455682
N	1.7733560	-0.4215861	-0.2505185
O	-2.9212722	-0.0737363	-1.4186392
C	1.9669287	-1.7202370	-0.1948907
C	3.1629813	-2.3299466	0.1977051
C	3.3316540	-3.7006119	0.2511040
C	4.5719875	-4.2528874	0.6234243
C	4.7542439	-5.6217940	0.6621605
N	3.8329202	-6.4878258	0.2137694
C	2.7596707	-5.9575005	-0.5957107
C	2.2131574	-4.6877187	0.0391523
C	6.0350953	-6.1651672	1.2095297
O	6.9303211	-5.4774425	1.6343944

O	6.0506268	-7.5099111	1.1587759
C	2.8789945	0.5787878	1.6653471
O	3.8874627	1.3785879	2.0423966
O	2.1575464	-0.0379634	2.4061426
C	3.2125677	-5.6436907	-2.0280908
O	4.2136111	-6.4455135	-2.4196770
O	2.6886284	-4.8038725	-2.7175959
H	-3.8677241	3.9412279	1.8167519
H	-3.3569325	2.2604980	0.2668067
H	-4.8780891	3.6885744	-1.9607803
H	-5.8005728	2.7560539	0.7928800
H	-5.4084313	5.5757603	-0.2678537
H	-6.0710256	1.6236099	-1.7130398
H	-7.7007945	3.8469276	0.0461829
H	-6.3124453	6.0733181	1.6906052
H	-3.8877665	6.3454726	2.3681501
H	-3.3959289	6.7387110	0.7029490
H	-1.5113818	5.4540420	1.1786787
H	-0.1584332	3.5192443	-1.0539695
H	-0.8476182	-1.4271234	-0.7816755
H	2.3804989	2.7217570	0.3289548
H	2.7498927	2.1945867	-1.3146905
H	3.7474868	0.3257026	-0.2832816
H	-3.6018754	0.6054312	-1.6241283
H	1.1172157	-2.3200669	-0.4985853
H	4.0149361	-1.7143413	0.4666346
H	5.3991442	-3.6305164	0.9423508
H	4.1027768	-7.4590587	0.1219660
H	1.9707166	-6.7111198	-0.6695674
H	1.7773758	-4.9330337	1.0147115
H	1.4224448	-4.3023685	-0.6011265
H	6.9031880	-7.8032186	1.5284247
H	3.9088174	1.3819643	3.0173289
H	4.4137020	-6.2198870	-3.3471397

(2) Indicaxanthin

DFT/B3-LYP

C	2.9174661	-1.7647632	-1.6907187
C	4.3367314	-1.8392935	-1.1393745
C	4.6488753	-0.3768063	-0.8003371
C	3.2928332	0.1989572	-0.3167739
N	2.2904984	-0.7394406	-0.8345839
C	3.0764490	1.6069972	-0.8627459
O	2.3603713	1.8850900	-1.7832536

O	3.8346602	2.4788881	-0.1813438
C	1.0010776	-0.6905520	-0.5783829
C	0.3539569	0.2419906	0.2281794
C	-3.3647319	-0.3240580	-0.2017621
C	-1.9387795	-0.8454911	-0.0314081
C	-1.0115336	0.2325745	0.4847175
C	-1.5823246	1.1866930	1.3465987
C	-2.9339740	1.1631432	1.6349798
N	-3.7959275	0.3740847	0.9958500
C	-3.5754863	2.0283448	2.6904471
O	-4.7584797	1.9983612	2.9017594
O	-2.6942423	2.7987269	3.3328676
C	-4.3134518	-1.4488794	-0.6030458
O	-3.9648453	-2.4064066	-1.2326450
O	-5.5718388	-1.2014052	-0.2074283
H	2.3604680	-2.6979616	-1.6273459
H	4.3577011	-2.4586246	-0.2406525
H	4.9766327	0.1544330	-1.6955151
H	3.7356599	3.3595958	-0.5805887
H	3.2400485	0.2268258	0.7736586
H	5.4199211	-0.2582013	-0.0432636
H	5.0372405	-2.2593675	-1.8588495
H	2.9093019	-1.4145452	-2.7268679
H	0.9340167	1.0326602	0.6859094
H	-3.3812822	0.3914639	-1.0394259
H	-1.9365380	-1.6704431	0.6900086
H	-0.9617878	1.9097078	1.8533778
H	0.4270381	-1.4769968	-1.0525939
H	-3.1724725	3.3322931	3.9894118
H	-4.7807423	0.4545921	1.2200404
H	-1.6244209	-1.2609282	-0.9840547
H	-6.1480888	-1.9212588	-0.5148447

DFT/B3-LYP/ COSMO (water)

C	2.9268823	-1.7475067	-1.7282631
C	4.3189191	-1.8345146	-1.1149203
C	4.6321522	-0.3746272	-0.7694713
C	3.2644158	0.2030131	-0.3249850
N	2.2750447	-0.7144218	-0.9007919
C	3.0926693	1.6266114	-0.8303546
O	2.4483059	1.9473032	-1.7980307
O	3.7923068	2.4721455	-0.0703613
C	0.9877830	-0.6866649	-0.6475304
C	0.3412122	0.2461646	0.1649707
C	-3.3712824	-0.3571053	-0.1865381
C	-1.9404567	-0.8717956	-0.0407946

C	-1.0153268	0.2205448	0.4430986
C	-1.5747320	1.1830983	1.3090413
C	-2.9168963	1.1555136	1.6221836
N	-3.7856396	0.3424886	1.0172880
C	-3.5274960	2.0427635	2.6710592
O	-4.7120892	2.0290393	2.9168271
O	-2.6359361	2.8175026	3.2791081
C	-4.3366842	-1.4699788	-0.5650571
O	-4.0154358	-2.4354977	-1.2121949
O	-5.5788556	-1.2218206	-0.1462398
H	2.3538662	-2.6706840	-1.6873567
H	4.2910269	-2.4454853	-0.2110668
H	4.9870658	0.1523243	-1.6566789
H	3.7185271	3.3735401	-0.4301804
H	3.1716136	0.1987118	0.7617426
H	5.3759468	-0.2605155	0.0149585
H	5.0447010	-2.2626234	-1.8039781
H	2.9693839	-1.3968188	-2.7626166
H	0.9197079	1.0386077	0.6214778
H	-3.4058676	0.3522278	-1.0277917
H	-1.9134310	-1.6833335	0.6941604
H	-0.9408121	1.9134562	1.7874147
H	0.4212363	-1.4757642	-1.1248515
H	-3.0858036	3.3731087	3.9390200
H	-4.7692251	0.4454295	1.2274225
H	-1.6318860	-1.2899657	-0.9939504
H	-6.1749106	-1.9344710	-0.4357690

MP2

C	2.9160682	-1.7602434	-1.7101720
C	4.3065739	-1.8440288	-1.1029507
C	4.6151726	-0.3778584	-0.7979421
C	3.2634061	0.1884592	-0.3151711
N	2.2769691	-0.7422023	-0.8615552
C	3.0417665	1.5840673	-0.8660189
O	2.3905743	1.8369744	-1.8478680
O	3.7181455	2.4748121	-0.1265575
C	0.9901655	-0.6890201	-0.6101178
C	0.3657890	0.2659603	0.1954847
C	-3.3225182	-0.3185970	-0.1915494
C	-1.9127917	-0.8519804	0.0001692
C	-0.9939217	0.2475781	0.4706227
C	-1.5616128	1.2102699	1.3215592
C	-2.9110598	1.1562431	1.6358281
N	-3.7651965	0.3474326	1.0137470

C	-3.5532450	2.0024033	2.6932770
O	-4.7410249	1.9537587	2.9164180
O	-2.6729609	2.7803434	3.3266789
C	-4.2716518	-1.4262569	-0.6083068
O	-3.9270411	-2.4027228	-1.2224318
O	-5.5320336	-1.1459121	-0.2401759
H	2.3410729	-2.6848109	-1.6749290
H	4.2788535	-2.4343110	-0.1845993
H	4.9210939	0.1353845	-1.7128553
H	3.6199119	3.3459559	-0.5541482
H	3.1942058	0.1981929	0.7765471
H	5.3937578	-0.2351219	-0.0511415
H	5.0309090	-2.2916017	-1.7821568
H	2.9508371	-1.3882270	-2.7386336
H	0.9544868	1.0637210	0.6355493
H	-3.3134135	0.4203185	-1.0111112
H	-1.9256850	-1.6434383	0.7608070
H	-0.9477034	1.9527659	1.8138361
H	0.4060395	-1.4720874	-1.0823311
H	-3.1711025	3.3007380	3.9839776
H	-4.7527681	0.4211714	1.2447672
H	-1.5988717	-1.3078877	-0.9364727
H	-6.1011964	-1.8702427	-0.5600729

(3) cBeet 120

DFT/B3-LYP

C	-4.1506848	-1.8450947	0.2645807
C	-2.8047226	-2.1433978	0.3482783
C	-1.8596454	-1.1176400	0.2361420
C	-2.2663344	0.1974033	0.0519102
C	-3.6236058	0.4778890	-0.0384793
C	-4.5979707	-0.5321785	0.0673545
N	-0.4961892	-1.4721369	0.3245768
C	0.5630404	-0.7335882	0.0155249
C	1.8713423	-1.1502626	0.1951911
C	2.9966818	-0.4099044	-0.1613673
C	4.2851206	-0.9228885	0.0449529
C	5.4125203	-0.2110591	-0.3375862
N	5.3435834	1.0355489	-0.7883961
C	4.1298680	1.8038803	-0.6302804
C	2.9063441	0.9137436	-0.8903646
C	6.8285344	-0.7672503	-0.3314179
O	7.0658212	-1.8710448	0.3809490

O	7.6857709	-0.2184546	-0.9611737
C	4.0973730	2.4336616	0.7781218
O	3.0113103	3.2139000	0.9047688
O	4.9238420	2.2557941	1.6244567
H	-4.8699629	-2.6472880	0.3506213
H	-2.4846118	-3.1686243	0.4891659
H	-1.5782548	1.0287440	-0.0008701
H	0.3445887	0.2396849	-0.4004986
H	2.0362955	-2.1253127	0.6441458
H	4.3920676	-1.9276479	0.4292243
H	6.2217151	1.4897177	-1.0100708
H	4.1298814	2.6251031	-1.3479733
H	2.8495310	0.6955336	-1.9618413
H	2.0157902	1.4796697	-0.6289353
C	-5.9962103	-0.1489287	-0.0224331
C	-6.2917314	1.1563918	-0.2031302
C	-5.2867415	2.2004165	-0.3119286
O	-3.9497590	1.7735171	-0.2181119
O	-5.4794770	3.3684727	-0.4707522
C	-7.0684230	-1.1894446	0.0883040
H	-7.3125690	1.5048300	-0.2767951
H	-6.9607850	-1.9448285	-0.6945658
H	-8.0573148	-0.7442163	-0.0008513
H	-7.0109242	-1.7063138	1.0497578
H	-0.3223654	-2.4118370	0.6601373
H	6.3302704	-2.1163021	0.9573510
H	3.0269903	3.6317425	1.7823081

DFT/B3-LYP/ COSMO (water)

C	-4.1258766	-1.8408358	0.2923430
C	-2.7809319	-2.1276051	0.3841969
C	-1.8357600	-1.0990216	0.2608735
C	-2.2467842	0.2140815	0.0614211
C	-3.6042028	0.4773910	-0.0311892
C	-4.5765322	-0.5285254	0.0782025
N	-0.4811109	-1.4516302	0.3558434
C	0.5717733	-0.7097896	0.0401265
C	1.8756741	-1.1383169	0.2225516
C	2.9950495	-0.4011493	-0.1461510
C	4.2841995	-0.9188095	0.0636752
C	5.4058510	-0.2057921	-0.3203760
N	5.3426864	1.0533699	-0.7426636
C	4.1187210	1.8096723	-0.6120128
C	2.9094662	0.9088084	-0.8915888
C	6.8021099	-0.7860202	-0.3339519

O	7.0060621	-1.9634547	0.2467568
O	7.7111259	-0.1963078	-0.8656202
C	4.0413483	2.4610658	0.7789576
O	2.9424412	3.2118816	0.8753594
O	4.8584417	2.3246373	1.6537023
H	-4.8412013	-2.6457968	0.3840754
H	-2.4490721	-3.1459098	0.5417657
H	-1.5549656	1.0410060	-0.0044093
H	0.3583368	0.2619400	-0.3817715
H	2.0332051	-2.1109129	0.6769149
H	4.3811096	-1.9178520	0.4637494
H	6.2033049	1.5224443	-0.9887267
H	4.1293996	2.6225348	-1.3374327
H	2.8891653	0.6763454	-1.9601686
H	2.0037342	1.4662689	-0.6716185
C	-5.9693066	-0.1521561	-0.0287226
C	-6.2724128	1.1550663	-0.2229459
C	-5.2668142	2.1816683	-0.3253792
O	-3.9506397	1.7820372	-0.2243258
O	-5.4651575	3.3685764	-0.4934398
C	-7.0394080	-1.1925061	0.0739531
H	-7.2955513	1.4928678	-0.3101358
H	-6.9123379	-1.9507282	-0.7028636
H	-8.0279516	-0.7490141	-0.0293746
H	-6.9848060	-1.7063169	1.0369045
H	-0.3020165	-2.3916087	0.6914928
H	6.2203698	-2.3236824	0.6852803
H	2.8992644	3.6220788	1.7567225

MP2

C	-1.6325581	4.1417508	-0.4384383
C	-0.5370019	3.4371215	0.0317886
C	-0.6581352	2.0666336	0.2796792
C	-1.8645963	1.4063219	0.0827578
C	-2.9495425	2.1264294	-0.4059511
C	-2.8592440	3.5024694	-0.6740478
N	0.4831866	1.3720926	0.7455044
C	0.7174237	0.0774114	0.6212292
C	1.8506702	-0.5536318	1.1203362
C	2.0887035	-1.9169452	0.9950892
C	3.2487919	-2.4923353	1.5300344
C	3.4594186	-3.8649984	1.4571783
N	2.6773266	-4.6606790	0.7421390
C	1.7732505	-4.0754157	-0.2142763
C	1.0760362	-2.8737380	0.4161243
C	4.5498576	-4.6142197	2.1880029

O	5.5938333	-3.9104791	2.6311343
O	4.4508589	-5.8031722	2.3555989
C	2.5699200	-3.6581707	-1.4583714
O	1.7431730	-3.1008131	-2.3592108
O	3.7541078	-3.8139495	-1.6007840
H	-1.5370140	5.2031379	-0.6317901
H	0.4107649	3.9412894	0.1897062
H	-2.0131639	0.3606567	0.3249542
H	-0.0389436	-0.4760342	0.0777761
H	2.5931215	0.0496070	1.6374754
H	3.9307169	-1.8714504	2.0981505
H	2.9295577	-5.6455863	0.7175666
H	1.0319219	-4.8176879	-0.5174124
H	0.4345620	-3.2244206	1.2340160
H	0.4373288	-2.4150497	-0.3363170
C	-4.0391308	4.1844641	-1.1667936
C	-5.1666536	3.4561807	-1.3401193
C	-5.2579526	2.0310485	-1.0589559
O	-4.0903318	1.4216759	-0.5820831
O	-6.2292720	1.3393130	-1.1980128
C	-3.9892762	5.6479760	-1.4683995
H	-6.0815158	3.9068249	-1.7061601
H	-3.7282712	6.2211226	-0.5755187
H	-4.9545876	5.9988428	-1.8303877
H	-3.2372623	5.8631228	-2.2313439
H	1.1896858	1.9386916	1.2074178
H	5.5945406	-3.0159210	2.2592284
H	2.2756949	-2.8894870	-3.1485142