Electronic Supporting Information to:

The limited extend of the electronic modulation of chlorins and bacteriochlorins through chromene-annulation

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meso-Tetrakis(pentafluorophenyl)porphyrin (4) (included for comparison)

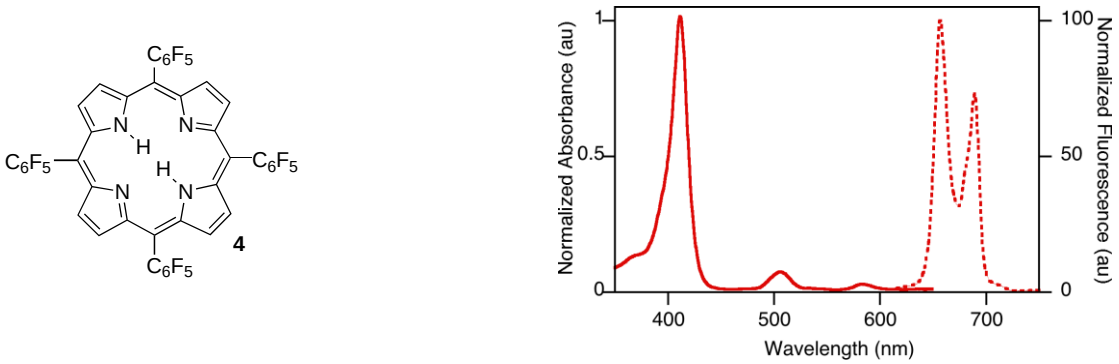


Figure S3. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **4**; $\lambda_{excitation} = \lambda_{Soret}$.

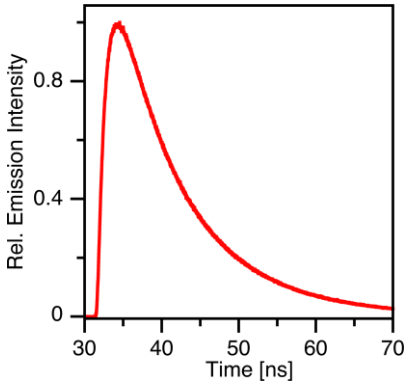


Figure S4. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **4**.

meso-Tetrakis(pentafluorophenyl)dihydroxychlorin (5)

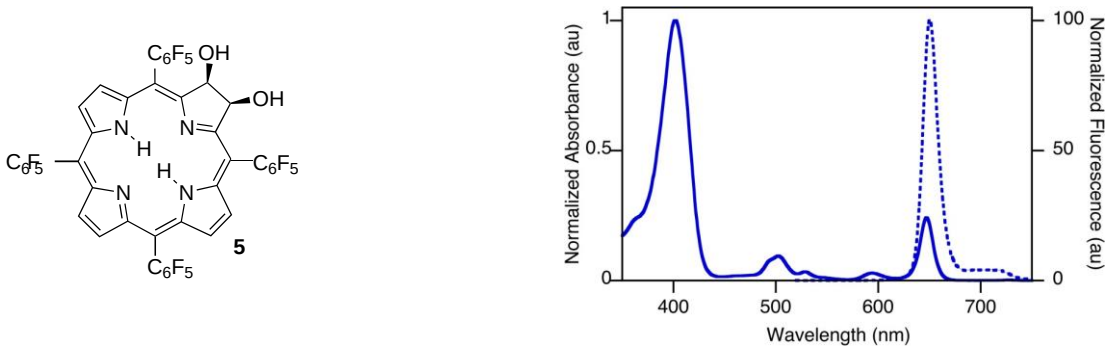


Figure S5. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **5**; $\lambda_{excitation} = \lambda_{Soret}$.

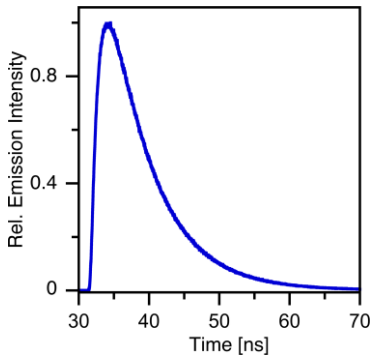


Figure S6. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **5**.

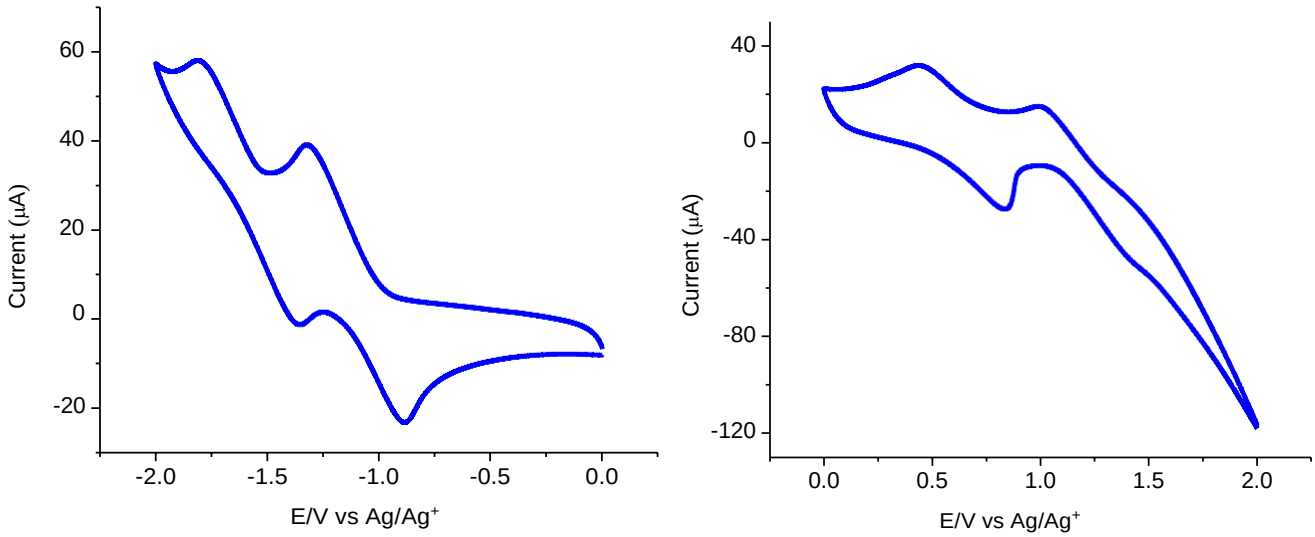
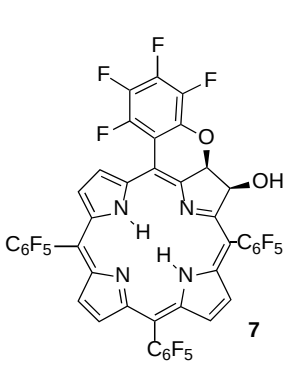


Figure S7. Cyclic voltammograms of **5** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**5**] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)dihydroxychlorin Mono-chromene-annulated (7)



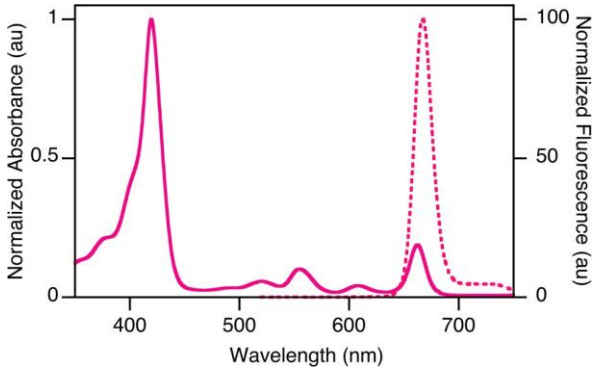


Figure S8. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **7**; $\lambda_{excitation} = \lambda_{Soret}$.

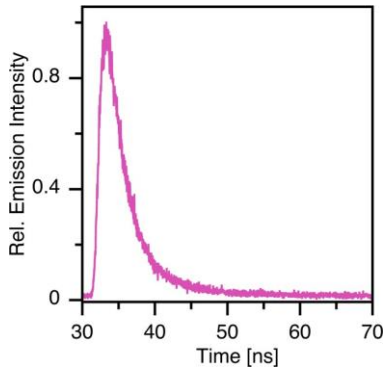


Figure S9. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **7**.

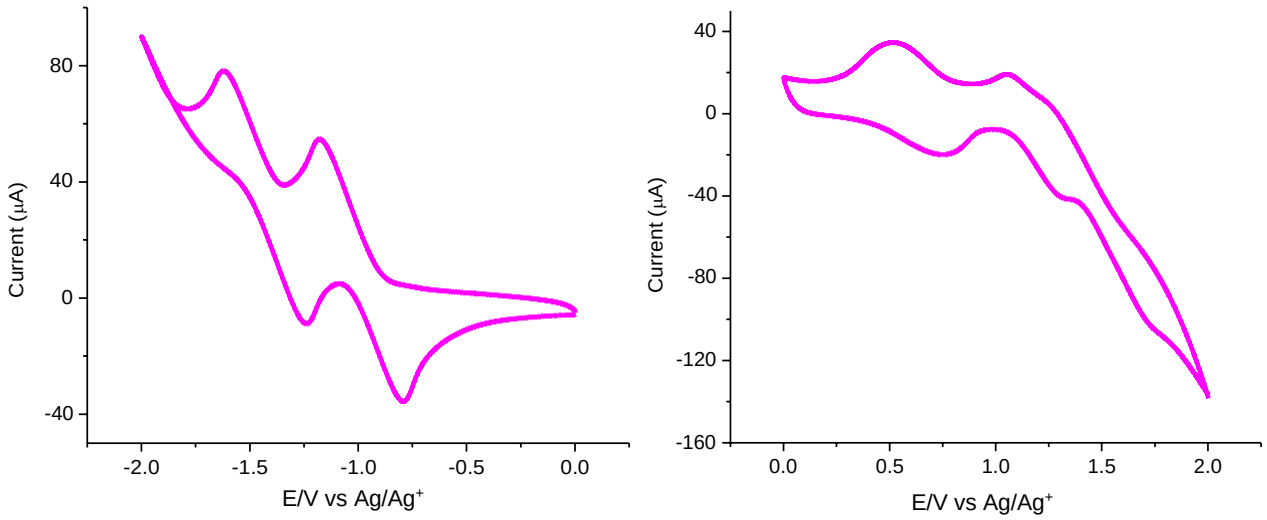
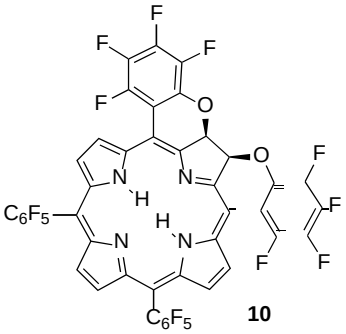


Figure S10. Cyclic voltammograms of **7** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**7**] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)dihydroxychlorin Bis-chromene-annulated (10)



10

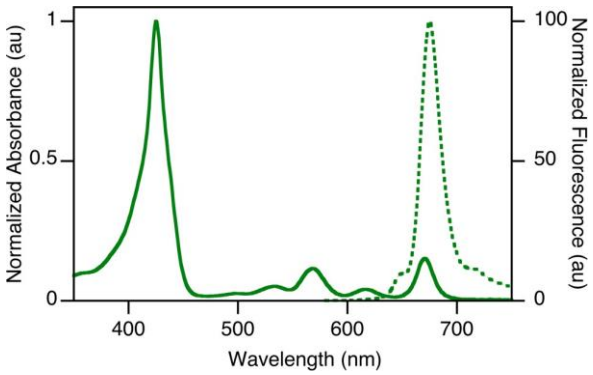


Figure S11. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **10**; $\lambda_{excitation} = \lambda_{Soret}$.

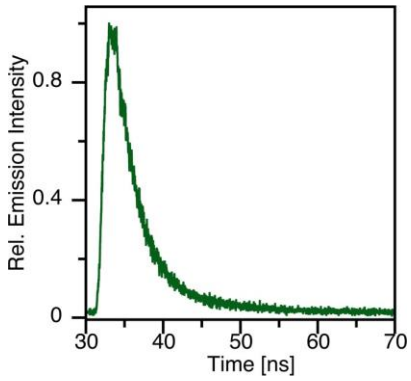


Figure S12. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **10**.

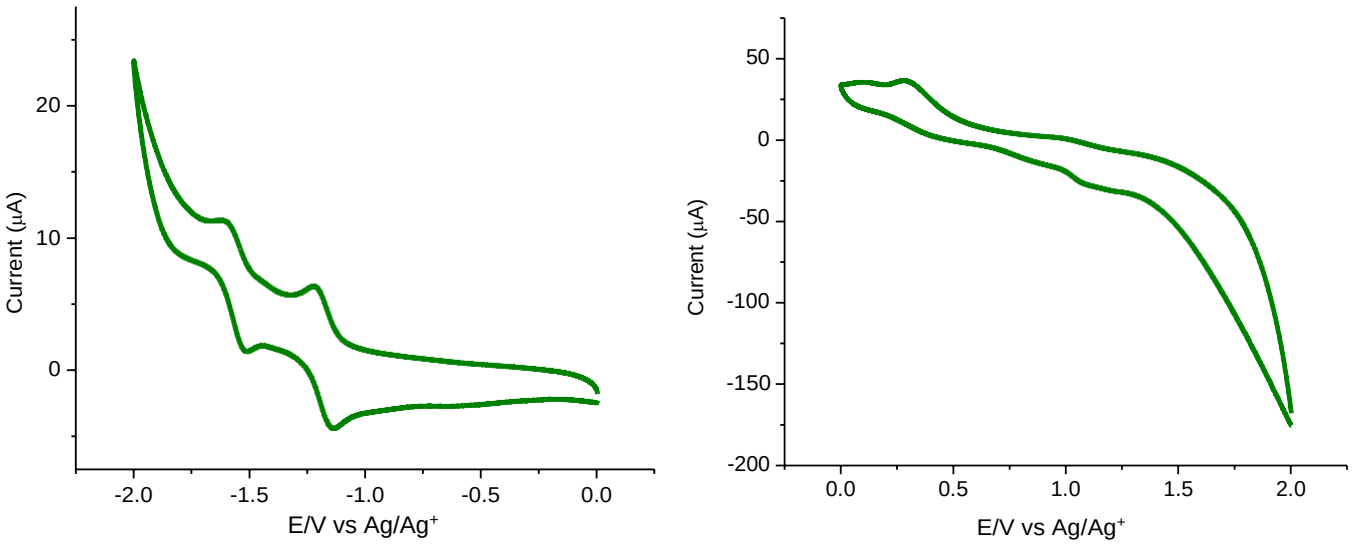


Figure S13. Cyclic voltammograms of **10** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**10**] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-Z (6-Z)

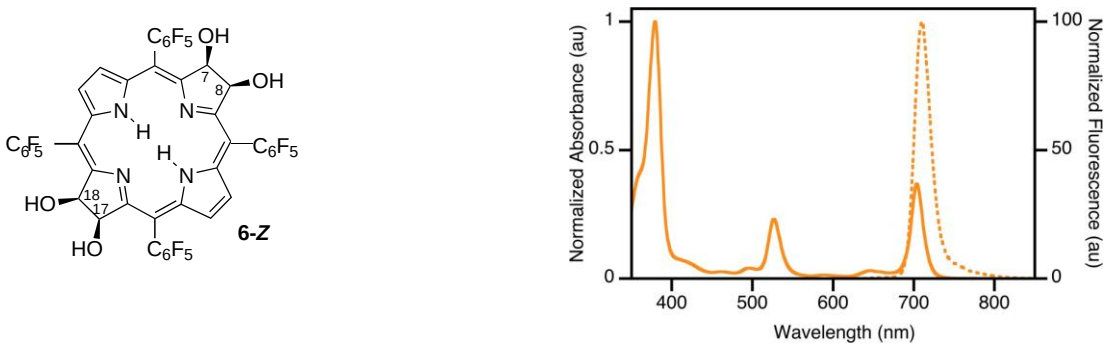


Figure S14. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **6-*Z***; $\lambda_{excitation} = \lambda_{Soret}$.

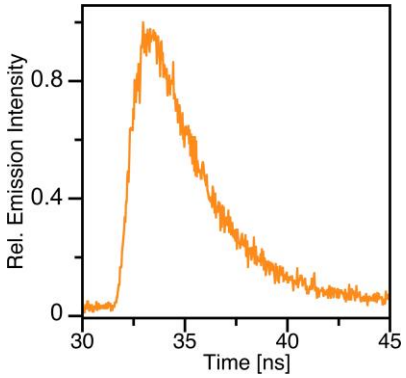


Figure S15. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **6-*Z***.

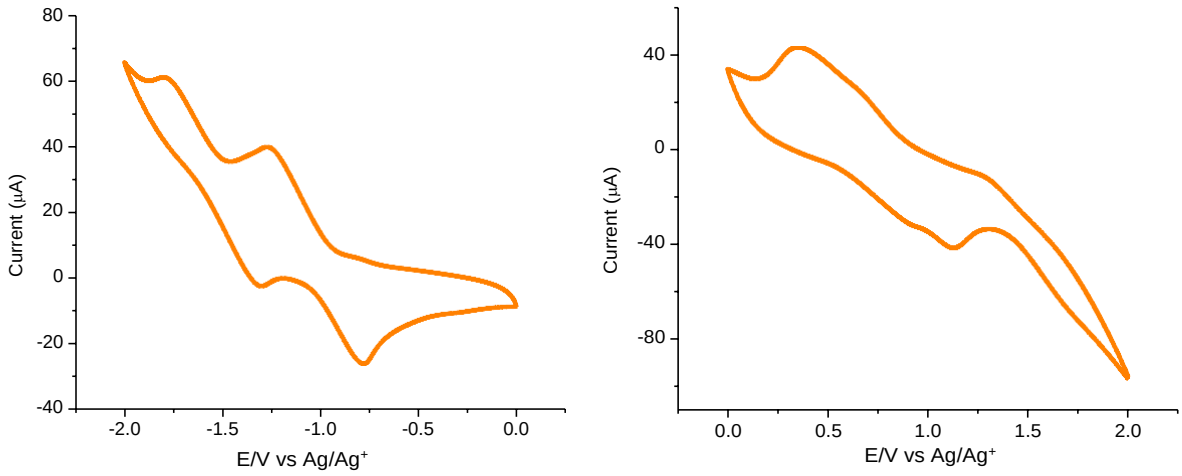
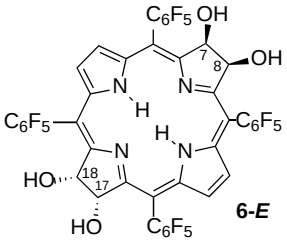


Figure S16. Cyclic voltammograms of **6-*Z*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**6-*Z***] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-E (6-E)



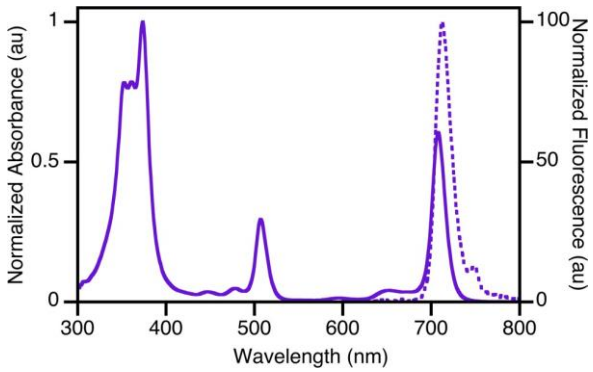


Figure S17. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **6-*E***; $\lambda_{excitation} = \lambda_{Soret}$.

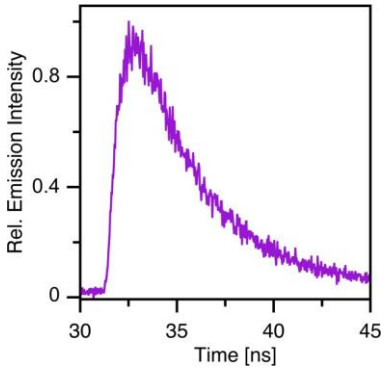


Figure S18. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **6-*E***.

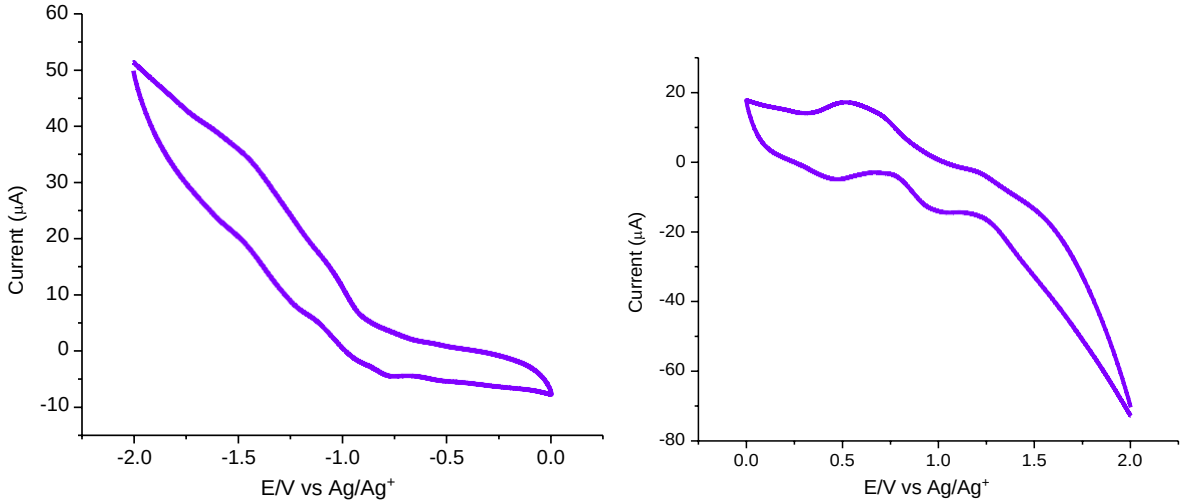
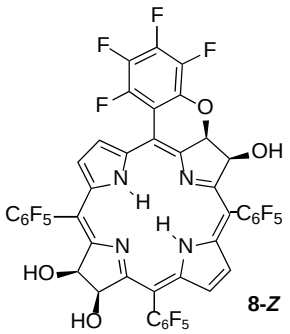


Figure S19. Cyclic voltammograms of **6-*E*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**6-*E***] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-Z Mono-chromene-annulated (8-Z)



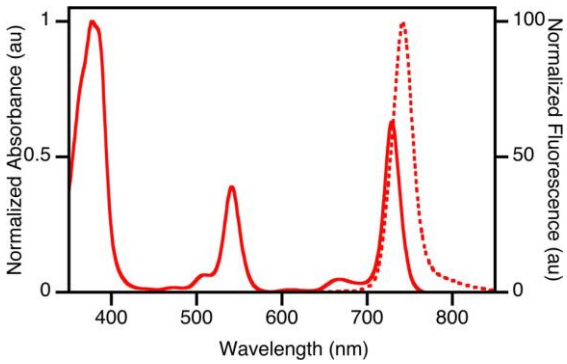


Figure S20. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **8-*Z***; $\lambda_{excitation} = \lambda_{Soret}$.

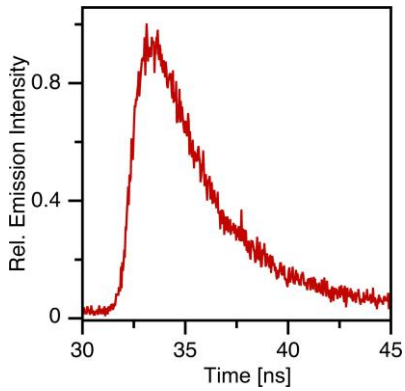


Figure S21. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **8-*Z***.

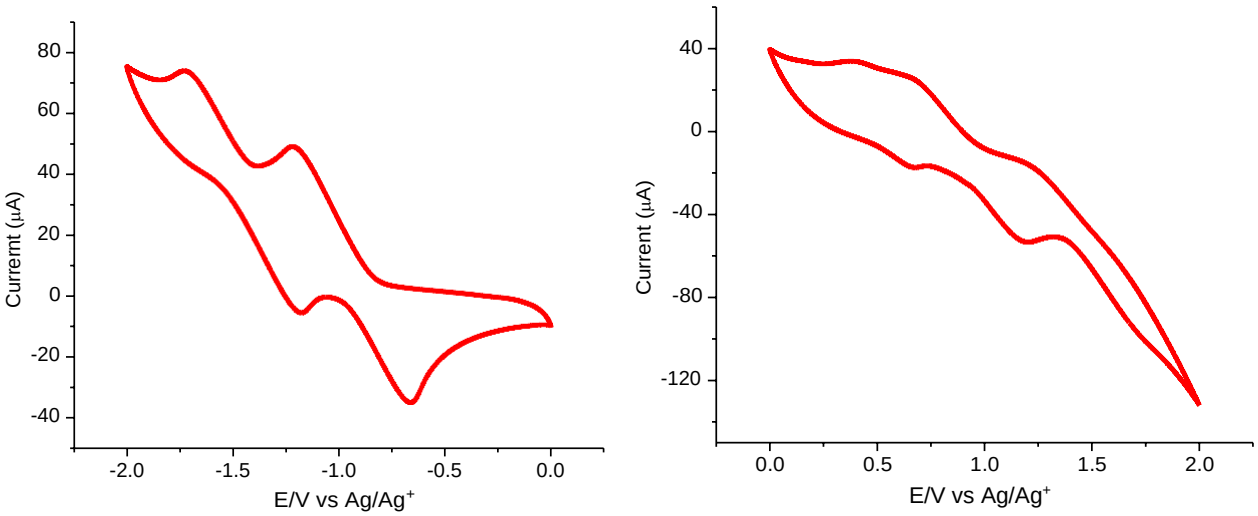
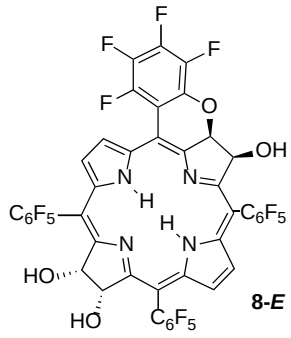


Figure S22. Cyclic voltammograms of **8-*Z*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**8-*Z***] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-E Mono-chromene-annulated (8-E)



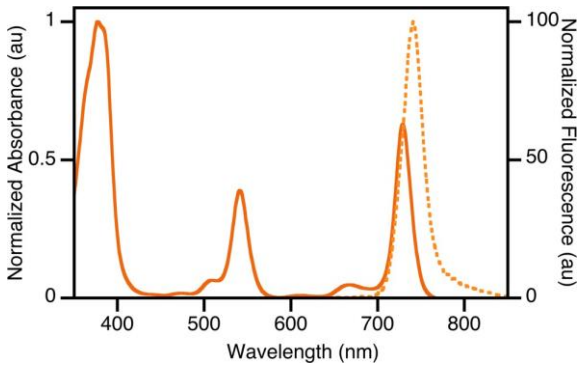


Figure S23. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **8-*E***; $\lambda_{excitation} = \lambda_{Soret}$.

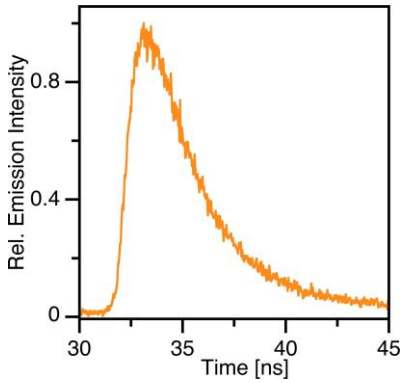


Figure S24. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **8-*E***.

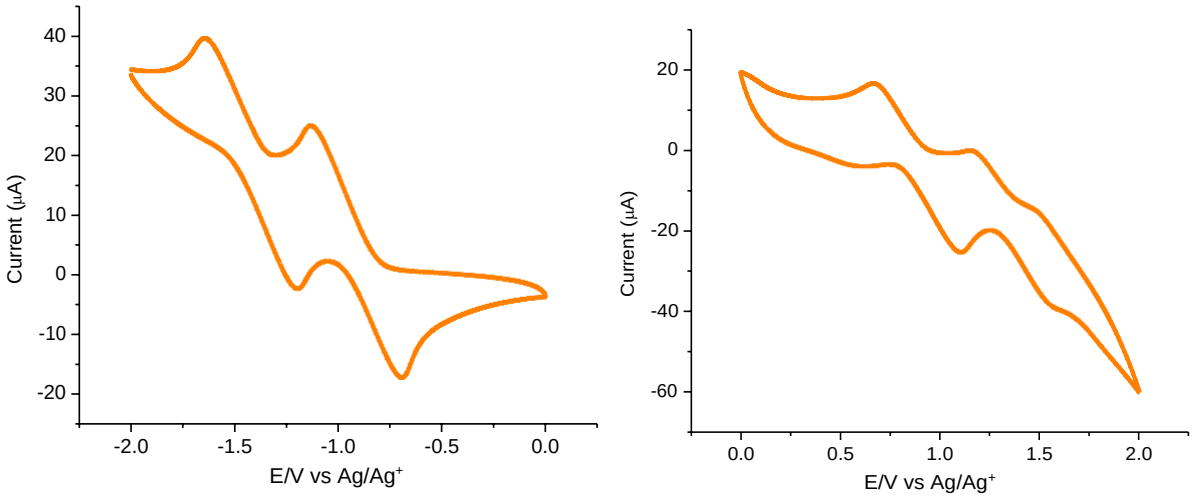


Figure S25. Cyclic voltammograms of **8-*E*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**8-*E***] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-Z Bis-chromene-annulated-s (9-Z-s)

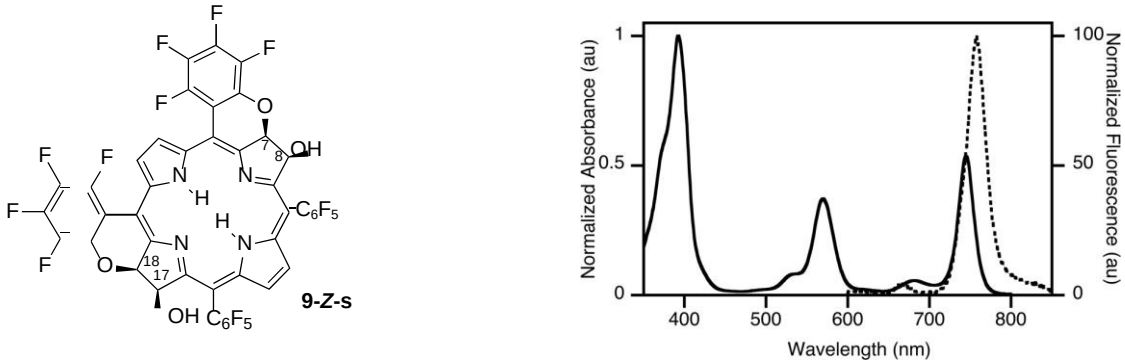


Figure S26. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **9-*Z*-*s***; $\lambda_{excitation} = \lambda_{Soret}$.

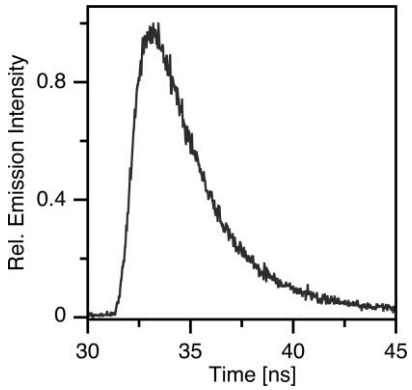


Figure S27. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **9-*Z*-*s*.**

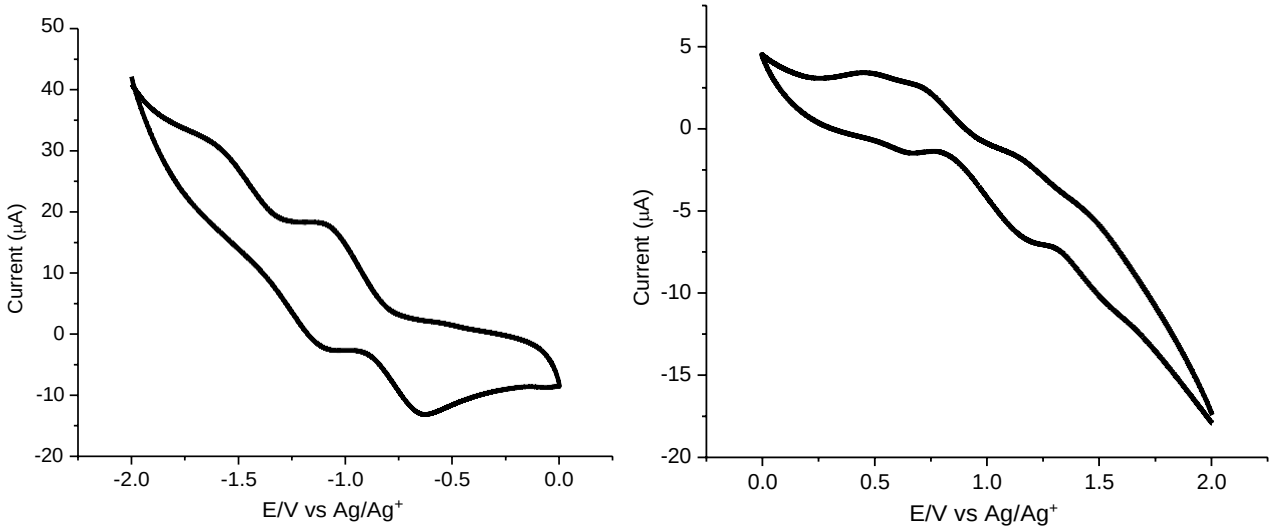


Figure S28. Cyclic voltammograms of **9-*Z*-*s*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**9-*Z*-*s***] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-E Bis-chromene-annulated-s (9-E-s)

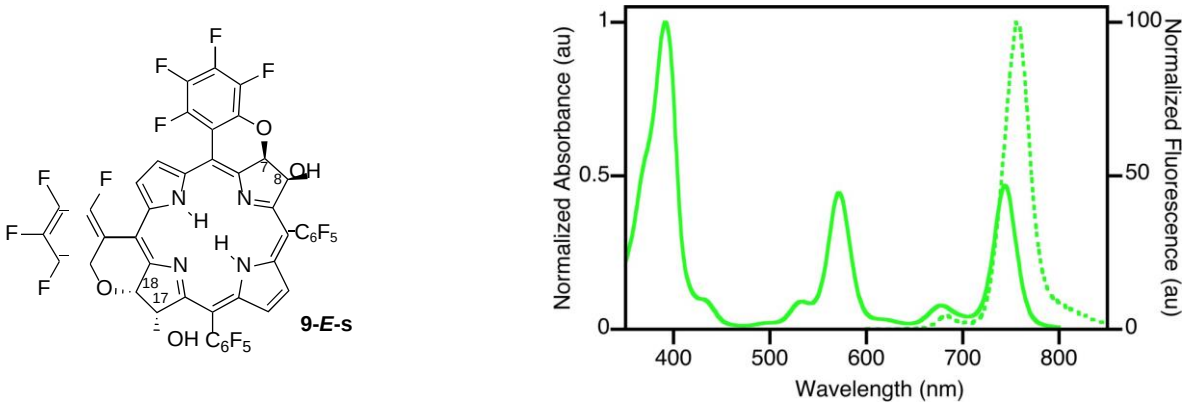


Figure S29. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **9-*E*-*s***; $\lambda_{excitation} = \lambda_{Soret}$.

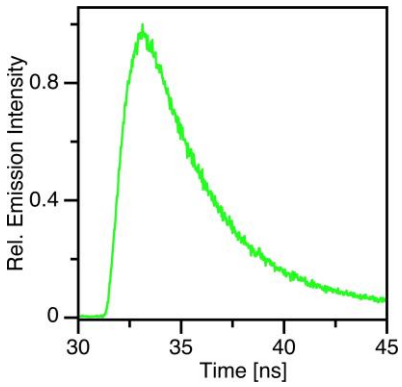


Figure S30. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **9-*E*-*s***

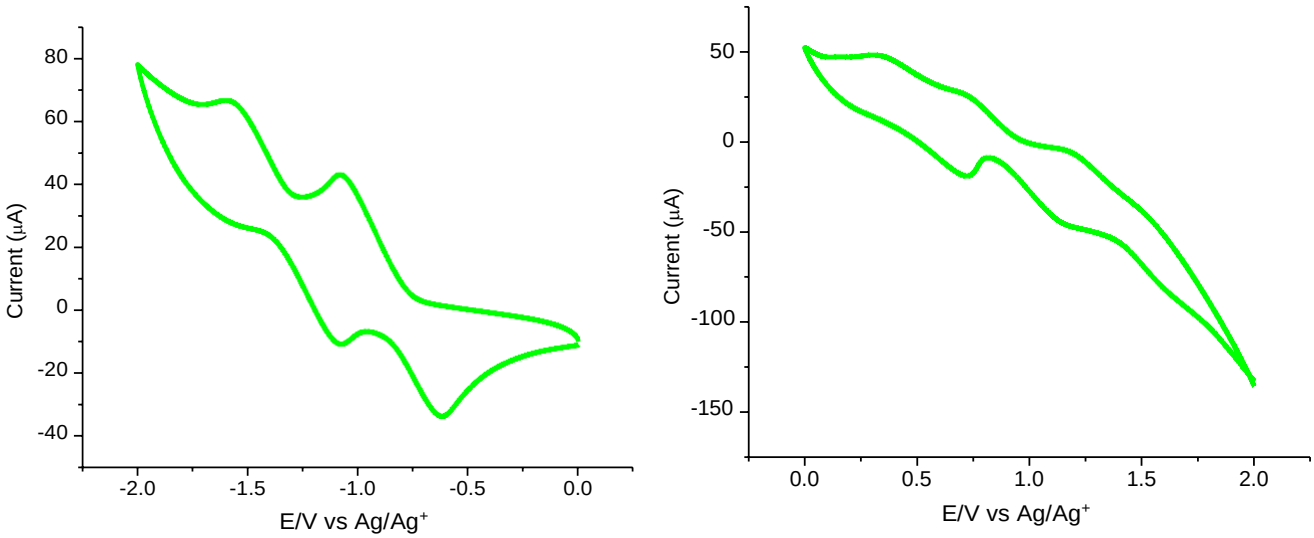
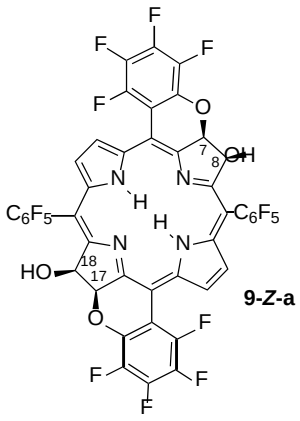


Figure S31. Cyclic voltammograms of **9-*Z*-*s*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**9-*E*-*s***] ~1 mM, scan rate of 200 mV/s)

meso-Tetrakis(pentafluorophenyl)tetrahydroxybacteriochlorin-Z Bis-chromene-annulated-a (9-Z-a)



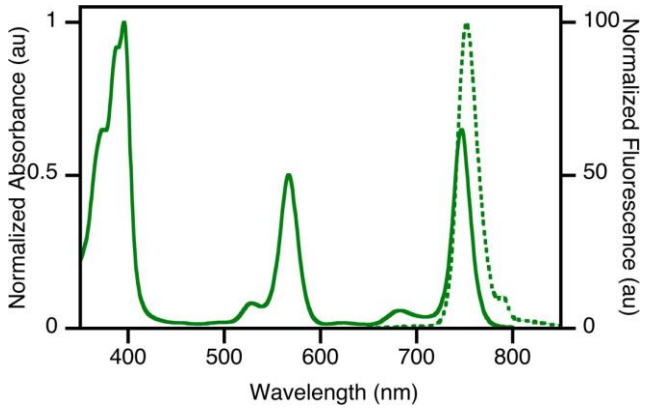


Figure S32. UV-vis absorption and normalized fluorescence emission spectra (CH_2Cl_2, 25°C) of **9-*Z*-*a***; $\lambda_{excitation} = \lambda_{Soret}$.

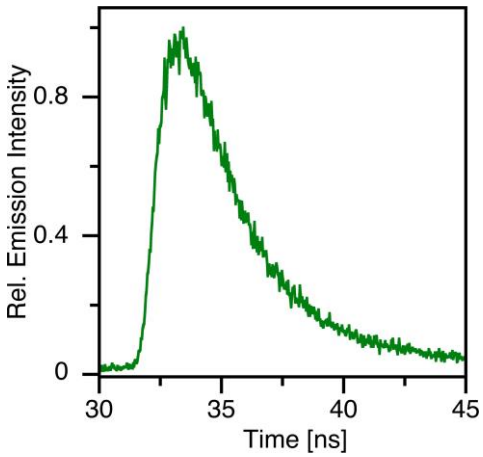


Figure S33. Time-dependent fluorescence emission traces (CH_2Cl_2, 25°C) of **9-*Z*-*a***

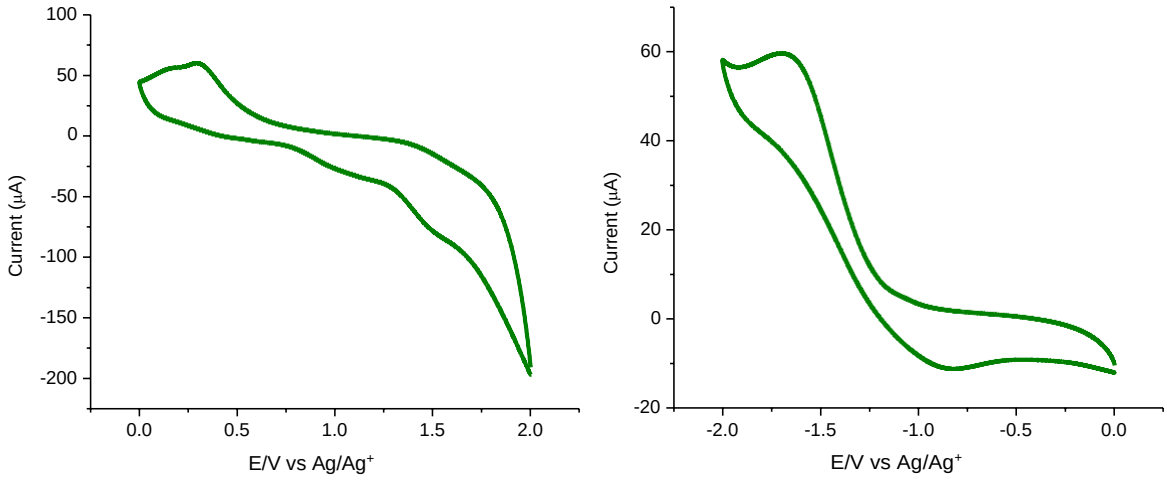


Figure S34. Cyclic voltammograms of **9-*Z*-*a*** (dry CH_2Cl_2, 0.1 M $TBAPF_6$, [**9-*Z*-*a***] ~1 mM, scan rate of 200 mV/s)

Table S1. Electrochemical half-wave potentials of the compounds investigated (in V vs NHE)

Compound[a]	**Reduction (V vs NHE)**[b]		**Oxidation (V vs NHE)**[b]		**HOMO-LUMO gap (V vs NHE)**
	$E_{red2}^{1/2}$	$E_{red1}^{1/2}$	$E_{ox1}^{1/2}$	$E_{ox2}^{1/2}$	
C diol **5**	-0.96	-0.50	1.23	1.82	1.73
Mono-fused C diol **7**	-0.81	-0.37	1.25	1.80	1.62
Bis-fused C diol **10**	-0.94	-0.56	(1.16)[c]	(1.66)[c]	(1.72)[c]
BC tetraol **6-*Z***	-0.93	-0.38	1.24	1.53	1.62
BC tetraol **6-*E***	(-0.70)[c]	(-0.29)[c]	(1.40)[c]	(1.48)[c]	(1.69)[c]
Mono-fused BC **8-*Z***	-0.83	-0.32	1.15	1.56	1.47
Mono-fused BC **8-*E***	-0.80	-0.29	1.24	1.76	1.53
Bis-fused BC **9-*Z*-*s***	-0.72	-0.24	1.20	1.58	1.44
Bis-fused BC **9-*E*-*s***	-0.71	-0.23	1.22	1.56	1.45
Bis-fused BC **9-*Z*-*a***	-	-0.61	0.96	-	1.57

[a] C = chlorin, BC = bacteriochlorin

[b] Potentials were referenced to Fc/Fc+ (0.02 V vs Ag/Ag^{+})

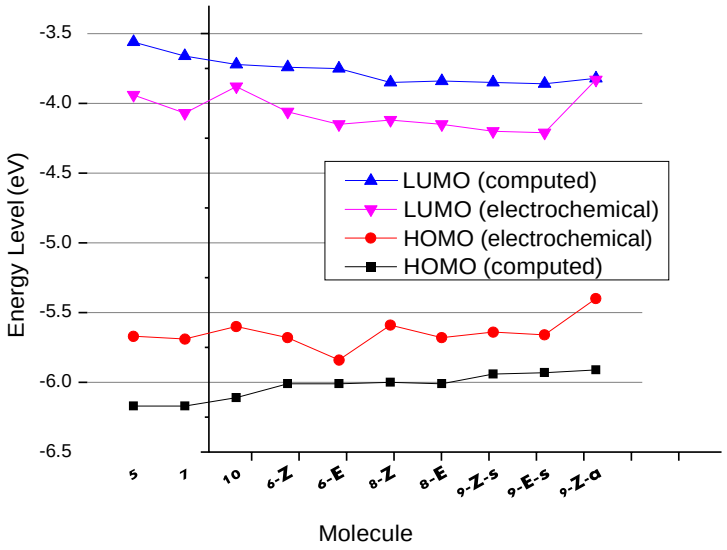


Figure S35. Comparison of HOMO and LUMO levels by computation or electrochemistry (based on oxidation and reduction potentials, respectively)

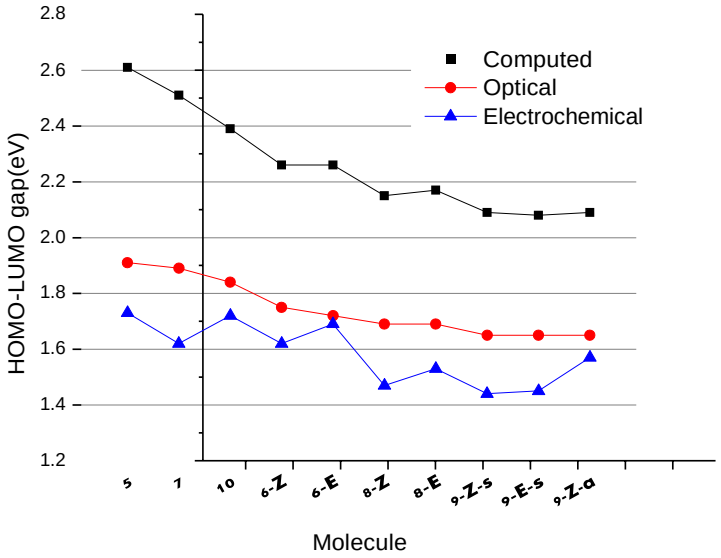


Figure S36. Comparison of the HOMO–LUMO energy gap based on the differences in HOMO and LUMO levels from **Figure S35** for computed and electrochemical results, and on the Q-state energy from optical results

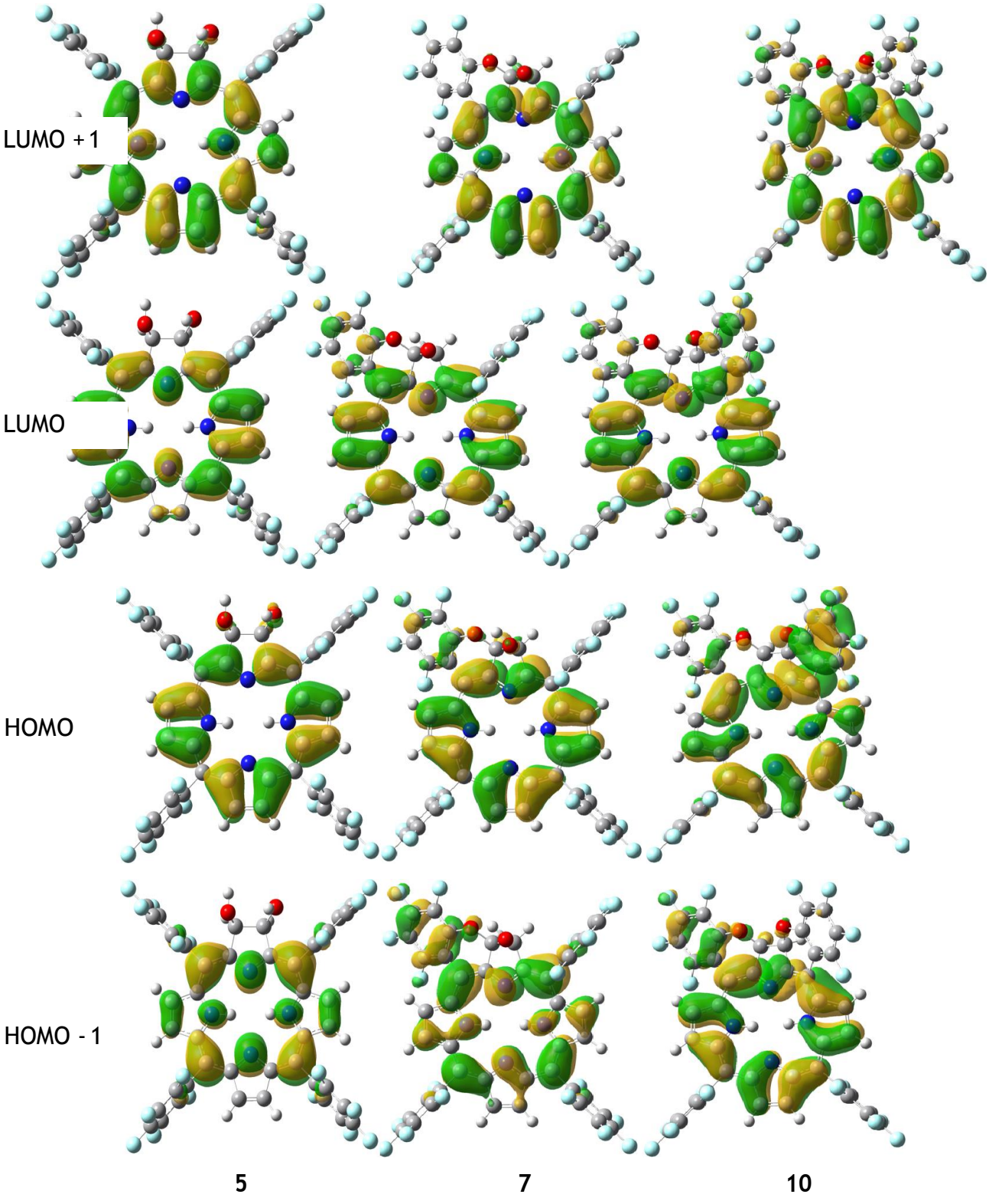


Figure S37. Representation of the frontier orbitals of the chlorin series **5**, **7** and **10** displayed at an isosurface value of 0.02 a.u.

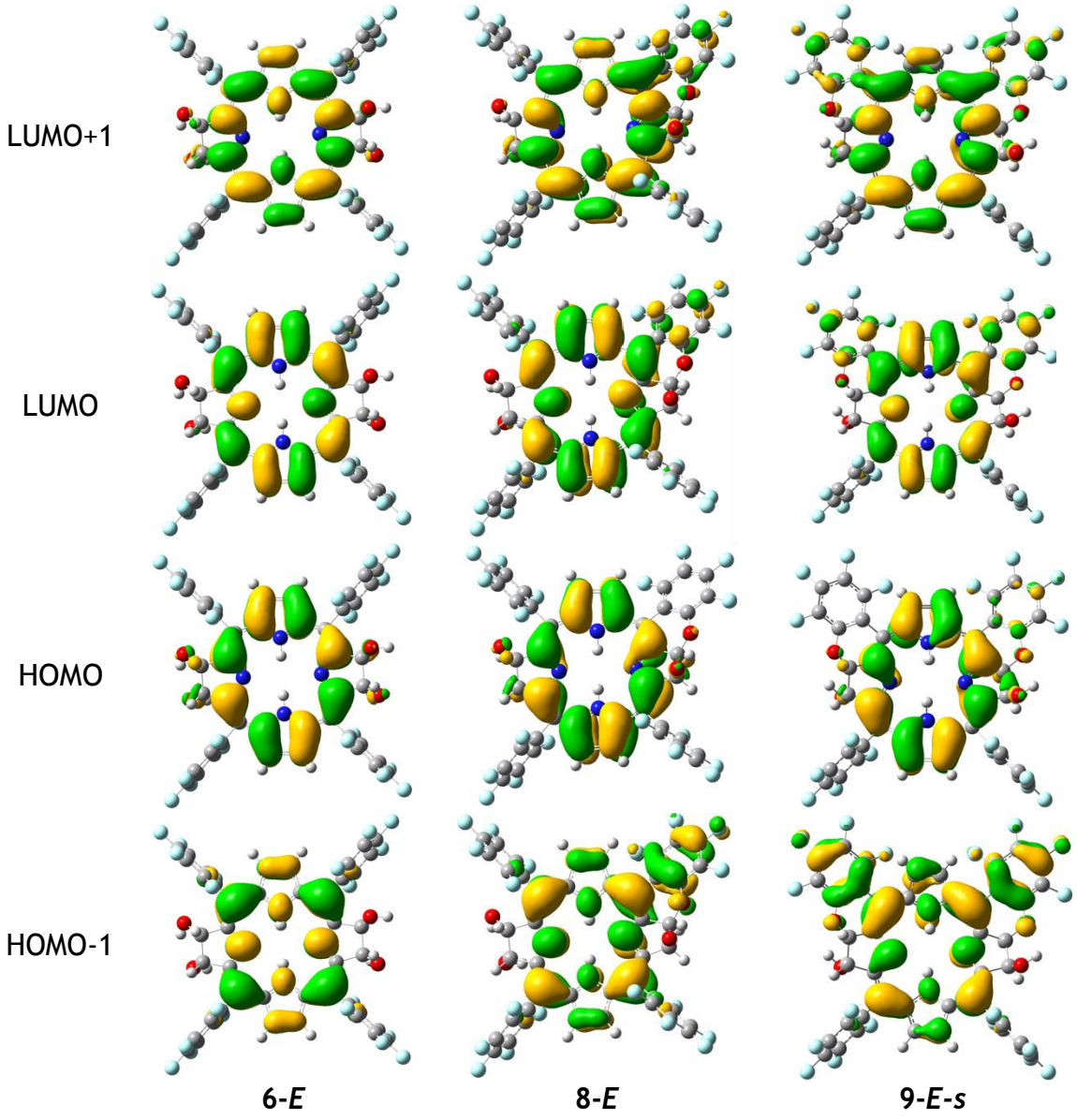


Figure S38. Representation of the frontier orbitals of the bacteriochlorin series 6-*E*, 8-*E*, 9-*E*-*s* displayed at an isosurface value of 0.02 a.u.

Table S2. Cartesian Coordinates of Computed Structures

All Structures were optimized at the B3LYP/6-31+g(d,p) level of theory with ultrafine integration grids, and confirmed to be local minima by a vibrational analysis.

C diol **5**
Total Energy = -4050.16020377 Hartrees
Lowest Vibrational Mode = 6.29 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-3.91490000	3.33695300	2.40409100
F	-6.00340500	5.05720500	2.40408300
F	3.59234800	3.75897100	-2.09063600
F	-4.03190300	3.21003600	-2.33591300
F	-7.11663600	5.86068000	0.04238300
F	-6.12091000	4.92965700	-2.32491200
F	5.26024300	5.88074600	-1.92190000
F	5.65741600	7.12544000	0.48036600
F	4.36594800	6.22714100	2.71288600
C	-1.14561000	4.21926200	0.04375000
H	-1.86445600	5.02488700	0.02567800
C	-4.40534000	0.34596800	0.03497100
H	-5.31776900	0.92450200	0.06255900
N	-0.27600700	2.13934900	0.06114500
H	-0.20986400	1.12888100	0.05811500
N	-2.12773300	-0.13121000	-0.01007000
C	-2.75063100	2.25554500	0.03049500
C	0.77882400	3.01211100	0.09049700
C	0.22056900	4.33304500	0.07365900
H	0.79492700	5.24683800	0.08259900
C	-5.57515000	4.53377300	-1.16672400
C	3.76196700	4.35086100	-0.89242700
C	-6.08448900	5.01018900	0.03970100
C	-1.47464100	2.82639500	0.03976000
C	3.31204800	4.52300100	1.43843900
C	2.15321700	2.68615000	0.13719600
C	-3.90388500	3.21470100	0.03392700
C	-3.04962100	0.87641700	0.02078300
C	-5.51479500	4.59937200	1.24324200
C	-4.49905800	3.64836300	-1.15524900
C	-4.28400700	-1.00622900	0.00837200
H	-5.07883400	-1.73849300	0.00964700
C	3.08466900	3.85908400	0.22752100
C	-4.43915700	3.71344600	1.22606400
C	4.62814700	5.44038500	-0.82414500
C	2.71657100	1.40812300	0.10693200

C	4.16949500	5.61652400	1.53567500
C	4.83121500	6.07631100	0.39841800
F	3.94858500	-2.69062100	-2.59477400
F	5.97375500	-4.46788600	-2.83086200
F	-3.20624000	-3.98498600	2.24050300
F	3.63125400	-3.68072500	2.03261800
F	6.83584600	-5.86395400	-0.64287500
F	5.65174900	-5.46097900	1.78622400
F	-4.95881100	-6.04551200	2.17977700
F	-3.47453200	-3.63019200	-2.48174400
F	-5.97821700	-6.90734200	-0.20364000
F	-5.22754000	-5.69071000	-2.53143400
C	0.97147100	-4.10464800	-0.27002400
H	1.69719500	-4.89929900	-0.35169300
N	0.09889700	-2.03869000	-0.08886700
H	-0.01218500	-1.03415300	-0.02703900
N	2.04206600	0.23738700	0.01177900
C	2.58704200	-2.14884900	-0.14737100
C	-0.96100000	-2.92433100	-0.13116800
C	-0.39254000	-4.23415100	-0.24184900
H	-0.95940500	-5.15159100	-0.29745100
C	5.22355900	-4.78235200	0.71178700
C	-3.68837200	-4.38558200	1.05245400
C	5.83283200	-4.98607600	-0.52506900
C	1.29070700	-2.70912700	-0.16771700
C	-3.82456100	-4.20617000	-1.31978900
C	-2.31668100	-2.59003000	-0.08614200
C	3.71138300	-3.13543800	-0.27431600
C	2.91643600	-0.79367700	-0.04411100
C	5.39275500	-4.27385500	-1.63767500
C	4.18157900	-3.86654900	0.82042800
C	-3.28224100	-3.73749100	-0.11866200
C	4.34454800	-3.36639100	-1.49810200
C	-4.59056400	-5.44767100	1.03835800
C	-2.85554500	-1.28599600	-0.02513300
C	-4.72807400	-5.26629000	-1.36250000
C	-5.11219100	-5.88857200	-0.17626100
C	4.37600100	-0.32039700	-0.02850200
O	5.20714500	-0.94499800	0.93259900
C	4.22559600	1.20638600	0.20072400
O	4.65417200	1.59288600	1.50856300
H	4.94001200	-0.61760000	1.80601700
H	4.84107000	-0.51886900	-0.99906200
H	4.76448800	1.78036400	-0.55964500
F	2.69348300	4.11099000	2.55434200
H	5.62027000	1.64835500	1.51332600

Mono-fused C diol **7**
Total Energy = -3949.71365202 Hartrees
Lowest Vibrational Mode = 7.49 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-4.01095400	2.32602200	2.89958500
F	-6.09193900	3.95166900	3.48375900
F	1.74303200	5.32362600	-1.71414000
F	-3.94011900	4.02636200	-1.52913500
F	-7.10415000	5.62240400	1.57434700
F	-6.01637400	5.65231500	-0.93144300
F	3.68476500	7.15486600	-1.78593200
F	6.17219000	6.59392400	-0.79645700
F	6.69878700	4.11528700	0.21677500
C	-1.14731600	4.16276000	0.59953100
H	-1.84012200	4.91713300	0.94180800
C	-4.40726400	0.33193200	-0.03464500
H	-5.32158100	0.89806900	0.07288300
N	-0.31524900	2.17499000	-0.05373800
H	-0.25760600	1.18835800	-0.27918400
N	-2.12957600	-0.12909100	-0.12827500
C	-2.75648000	2.21254300	0.33964100
C	0.72844900	3.06194700	-0.05268300
C	0.19626900	4.32140900	0.37480200
H	0.76857400	5.22434900	0.51474300
C	-5.51863100	4.83340100	0.00530500
C	2.92259100	5.00404100	-1.14452500
C	-6.07636700	4.81831400	1.28218800
C	-1.49026700	2.80239400	0.31198300
C	4.44662700	3.45797700	-0.13728100
C	2.07371700	2.71573600	-0.34653800
C	-3.90380600	3.12018800	0.66523700
C	-3.05342400	0.85536800	0.07093300
C	-5.55942500	3.96394200	2.25419400
C	-4.44694500	3.99147700	-0.28545600
C	-4.28230800	-0.99329100	-0.30754400
H	-5.07574700	-1.71238300	-0.45379100
C	3.11993900	3.75033600	-0.54321200
C	-4.48834800	3.13105300	1.93665500
C	3.92832000	5.96471100	-1.21619900
C	2.56178200	1.40453300	-0.31007600
C	5.45771200	4.41463700	-0.20066400
C	5.19845100	5.67850800	-0.72378500
F	4.46752100	-2.90600600	-1.87586000
F	6.49592500	-4.62575700	-1.38148400
F	-3.45686200	-4.16256400	1.57792100
F	3.01969900	-3.34057600	2.62137500

F	6.80039300	-5.70685200	1.11055900
F	5.05328800	-5.05408100	3.10540000
F	-5.18947800	-6.19114700	1.12579100
F	-3.19322100	-3.36033900	-3.08933900
F	-5.93411600	-6.81361900	-1.42763200
F	-4.92789200	-5.38956500	-3.53069200
C	0.97369500	-4.08878300	-0.25079900
H	1.70544500	-4.88234200	-0.22367300
N	0.08255800	-2.02497600	-0.20136000
H	-0.03937900	-1.02303500	-0.10506700
N	1.90956000	0.24031600	-0.15501000
C	2.54516100	-2.11095900	0.09774200
C	-0.95851400	-2.90794500	-0.40826600
C	-0.37854700	-4.21612000	-0.45458800
H	-0.92788000	-5.13209400	-0.61439700
C	4.90268100	-4.52331200	1.88447900
C	-3.80201400	-4.44452500	0.31087600
C	5.79596800	-4.85748000	0.86867800
C	1.26924100	-2.69570000	-0.09657400
C	-3.67106700	-4.04049400	-2.03404600
C	-2.31094100	-2.56336400	-0.49917300
C	3.67348800	-3.06160100	0.35751500
C	2.82337500	-0.74869600	0.05044100
C	5.63896000	-4.30549100	-0.40102200
C	3.86076200	-3.63659200	1.62018300
C	-3.26754200	-3.69288300	-0.74070300
C	4.58693700	-3.42402500	-0.63766900
C	-4.69597400	-5.49159200	0.09485900
C	-2.85374900	-1.26877700	-0.34198600
C	-4.56334200	-5.08272700	-2.27820000
C	-5.07755200	-5.81059300	-1.20695000
C	4.23059800	-0.18098800	0.26953200
O	4.45714600	-0.10818200	1.67096800
C	4.05721000	1.19600300	-0.38273400
O	4.77698400	2.21233400	0.32156400
H	5.07428000	0.61837800	1.84591000
H	5.01944300	-0.76321300	-0.21640800
H	4.40454600	1.17315200	-1.42682900

Bis-fused C diol **10**
Total Energy = -3849.24826294 Hartrees
Lowest Vibrational Model = 9.23 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-3.08534400	3.01312900	3.00484600
F	-4.59243700	5.11567900	3.78973700
F	3.12746200	4.55194200	-1.98293900
F	-2.71762900	4.91013100	-1.32956800
F	-5.16406500	7.12576400	2.03059500
F	-4.21659500	7.01208900	-0.52919200
F	5.53986800	5.71434400	-1.95970900
F	7.73346600	4.35097500	-1.06724700
F	7.49080300	1.76045000	-0.26255300
C	0.09271600	4.13661400	0.50975700
H	-0.32176500	5.04028100	0.93166200
C	-4.13393900	1.36111600	0.06486600
H	-4.85782600	2.14725600	0.22707000
N	0.26050800	2.03265700	-0.26836900
H	0.01235700	1.07594600	-0.49858600
N	-2.07119600	0.30682100	-0.14040000
C	-2.02063800	2.71879300	0.37544300
C	1.51084300	2.58468000	-0.34727400
C	1.40307100	3.91861200	0.15608400
H	2.21739900	4.61816300	0.25331000
C	-3.93384300	6.02710900	0.33425400
C	4.15978200	3.84754600	-1.47578800
C	-4.42055000	6.08584700	1.63861400
C	-0.64614100	2.94503000	0.23131900
C	5.14563400	1.83126400	-0.62613800
C	2.66459800	1.87285800	-0.78632800
C	-2.84826400	3.88820300	0.81041000
C	-2.68744000	1.50002900	0.11984300
C	-4.12957700	5.05814600	2.53361100
C	-3.15889000	4.93859800	-0.06101800
C	-4.37978600	0.06262400	-0.25495600
H	-5.34230600	-0.41162200	-0.38492100
C	3.97296900	2.54813000	-0.98267000
C	-3.35418700	3.97982900	2.11240700
C	5.40826200	4.46367400	-1.49080900
C	2.73266500	0.48323100	-0.84043700
C	6.39682900	2.44603700	-0.62602300
C	6.52864600	3.76855800	-1.04324200
F	6.51109900	-3.68171000	1.36204500
F	-4.08671600	-2.09210200	-3.16262000
F	1.35287200	-5.38146100	1.60206400
F	5.87845800	-6.03277000	2.58801600

F	3.25869800	-6.83807300	2.68163500
F	-6.30211000	-3.52970800	-3.74571800
F	-4.32860400	-3.56639200	1.34052800
F	-7.53770900	-4.99420300	-1.79851700
F	-6.53814600	-5.00627700	0.74386500
C	-0.18343700	-4.35727700	-0.31783500
H	0.29590000	-5.32043900	-0.36082300
N	-0.48367200	-2.13885800	-0.12441900
H	-0.33820200	-1.14500300	0.02080700
N	1.79431500	-0.42505900	-0.46650400
C	1.85960400	-2.83263400	0.15038200
C	-1.70843200	-2.68010200	-0.46496300
C	-1.49566900	-4.08803200	-0.61258000
H	-2.24881400	-4.80191000	-0.91185200
C	3.59730100	-5.71043800	2.03688600
C	-4.67342200	-2.79690500	-2.18089600
C	4.92350100	-5.29690500	2.00855100
C	0.46940900	-3.11728800	-0.00765300
C	-4.78935700	-3.54404100	0.07894400
C	-2.90903300	-1.97406300	-0.57118100
C	2.88442100	-3.75636300	0.70588400
C	2.38861300	-1.61560800	-0.31333600
C	5.23782300	-4.10507400	1.36862800
C	2.61551000	-4.94407400	1.41850300
C	-4.13073600	-2.78045200	-0.89116100
C	4.25059600	-3.33969800	0.74496900
C	-5.81279400	-3.53348000	-2.49815800
C	-3.08048100	-0.58445000	-0.35670300
C	-5.93089700	-4.28888400	-0.21122300
C	-6.44378500	-4.28253300	-1.50686600
C	3.84244600	-1.61525200	-0.74997400
O	4.68907300	-2.14309900	0.25339100
C	4.09237800	-0.14037500	-1.09755200
O	5.08176000	0.50702300	-0.28976700
H	4.39781900	-0.04211600	-2.14757700
H	3.95695800	-2.23044600	-1.65488200

BC tetraol **6-*Z***
Total Energy = -4201.81072453 Hartrees
Lowest Vibrational Mode = 6.12 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	1.36217800	4.33456600	-0.47186500
F	1.96708700	6.77652800	-1.46946200
F	6.71973200	-2.29910600	1.54813500
F	3.80262100	2.30040900	-3.99344600
F	3.49358800	6.99514300	-3.72531900
F	4.40768800	4.74686300	-4.97978600
F	8.86140200	-1.98712500	3.16948300
F	8.72872400	-0.28317900	5.30427000
F	6.43142700	1.10862000	5.79875900
C	4.32961500	2.03967300	-0.20682900
H	4.70962300	2.97771800	-0.58241200
C	0.16152500	1.92773300	-3.10961700
N	3.01928900	0.23378000	0.06472500
H	2.27055600	-0.43667000	-0.04017600
N	0.63623000	0.01883100	-1.75188000
C	2.23749400	1.88288000	-1.63394500
C	4.05697000	0.11341300	0.96213500
C	4.89033300	1.25549300	0.77594200
H	5.79835700	1.45645600	1.32385500
C	3.66080600	4.63979300	-3.87227600
C	6.62170500	-1.44860200	2.58805000
C	3.19581800	5.78796800	-3.23379600
C	3.13856800	1.39976000	-0.65822400
C	5.39812600	0.10796200	3.90957100
C	4.24040200	-0.92177700	1.90650700
C	2.56753000	3.23619500	-2.19534200
C	1.09118100	1.24972200	-2.11510100
C	2.41856800	5.67447800	-2.08271300
C	3.34323400	3.38806200	-3.34893400
C	-0.72669400	0.75424600	-3.57594700
C	5.42774800	-0.75578200	2.80899000
C	2.11830300	4.40998000	-1.58314100
C	7.73404200	-1.30368400	3.41493400
C	3.44370300	-2.05298000	2.08556000
C	6.49554800	0.27452800	4.75116000
C	7.66882000	-0.43548600	4.50224600
F	2.09620000	-6.64728400	0.48344100
F	1.48813200	-9.08157900	1.49552300
F	-0.79314300	-2.34499900	-5.09564400
F	-1.28657200	-4.69422400	3.17283000
F	-0.50934800	-9.33747300	3.34586700
F	-1.89192300	-7.13183400	4.17528600

F	-2.81203500	-2.70147300	-6.86183000
F	-3.93170700	-1.05963100	-1.78072800
F	-5.39807700	-2.24295700	-6.09895700
F	-5.94446800	-1.42402100	-3.55056900
C	-1.16217700	-4.53213500	-0.40958500
H	-1.48649800	-5.51240500	-0.09518500
N	0.00839200	-2.61196500	-0.51345100
H	0.70253000	-1.89698600	-0.34666500
N	2.35116300	-2.38409100	1.35095500
C	0.75345300	-4.23947100	1.22264400
C	-0.95854800	-2.54684800	-1.49283600
C	-1.69658800	-3.77185900	-1.41738100
H	-2.52628700	-4.03215400	-2.05674500
C	-0.91797900	-7.00731800	3.26227400
C	-2.05735700	-2.11789400	-4.68647700
C	-0.21094300	-8.13339600	2.84456900
C	-0.07311500	-3.80489100	0.17085100
C	-3.63080200	-1.47873000	-3.02190100
C	-1.17509400	-1.49470100	-2.40092500
C	0.41463200	-5.59019600	1.78424800
C	1.85928300	-3.56891500	1.76672600
C	0.80628500	-8.00091100	1.90280700
C	-0.59777500	-5.76089200	2.73270300
C	-2.29738700	-1.70425200	-3.37443100
C	1.10179000	-6.74018700	1.38841000
C	-3.08317200	-2.30026300	-5.61107800
C	-0.43840300	-0.30559000	-2.50096000
C	-4.67677800	-1.65518900	-3.92224400
C	-4.40037600	-2.06778100	-5.22445100
C	2.68873400	-4.17978900	2.90327300
O	1.95196000	-4.56185200	4.05097200
C	3.72756200	-3.06280200	3.19159500
O	3.49430800	-2.43230500	4.45392700
H	1.68130200	-3.74946800	4.50731500
H	3.18873300	-5.08839100	2.55424200
H	4.75111200	-3.44804100	3.14545100
O	-0.64310900	2.95368600	-2.49916600
H	-0.62486300	2.85732700	-1.53584300
O	-2.07871400	1.12019900	-3.74408500
H	-2.19836400	1.95198400	-3.25235600
H	0.67598600	2.40851400	-3.94264500
H	-0.35843000	0.37653300	-4.53899700
F	4.28776200	0.80839600	4.18207900
H	3.85186800	-2.99790400	5.15303500

BC tetraol **6-*E***
Total Energy = -4201.81044596 Hartrees
Lowest Vibrational Model = 6.25 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-3.85009800	2.91766100	2.59046900
F	-5.87020200	4.70236000	2.83164000
F	3.69625600	3.66498300	-2.29277300
F	-3.68902900	3.74276700	-2.07654800
F	-6.80756700	6.01839700	0.62495600
F	-5.70388400	5.53055600	-1.82627300
F	5.38510300	5.77724500	-2.26526200
F	5.88898900	7.09950800	0.07494000
F	4.68352700	6.28852500	2.38749200
C	-0.94562400	4.22261200	0.08317200
H	-1.66007500	5.03083900	0.11676900
C	-4.37077300	0.43163100	0.21084200
N	-0.09175800	2.14117400	0.02510400
H	-0.01418600	1.13381400	0.02259400
N	-2.04796300	-0.10205300	0.00680300
C	-2.57958800	2.28474100	0.12088400
C	0.97506600	3.01279700	0.01867200
C	0.42120300	4.33203400	0.04038000
H	0.99707900	5.24486000	0.03207500
C	-5.23913500	4.89034300	-0.74307800
C	3.91882100	4.29674500	-1.12398600
C	-5.80754800	5.13707100	0.50532000
C	-1.28275500	2.83215400	0.07306300
C	3.56548900	4.55195900	1.21611700
C	2.34336200	2.68057800	0.02200400
C	-3.69240400	3.28316300	0.25050300
C	-2.92106400	0.92699100	0.08508700
C	-5.32914300	4.46598000	1.62744300
C	-4.19894600	3.97319700	-0.85382500
C	-4.23083700	-1.05481200	-0.18087900
C	3.28391200	3.85031700	0.03865600
C	-4.28414100	3.55578500	1.48549200
C	4.79510600	5.38029000	-1.12835400
C	2.90618100	1.39746300	0.01997600
C	4.43437300	5.64040000	1.24073000
C	5.05245300	6.05557200	0.06244400
F	3.78896300	-3.56814400	2.20833800
F	5.79352500	-5.37790000	2.06502700
F	-3.04134100	-3.71889800	-2.56207200
F	4.09835100	-2.86450100	-2.47140100
F	6.96556700	-5.93855400	-0.33853100
F	6.10765400	-4.67115100	-2.60509500

F	-4.73653300	-5.82234500	-2.71887700
F	-3.32704200	-3.85192900	2.17031500
F	-5.73083800	-6.95379600	-0.43883500
F	-5.01732300	-5.95885700	2.00355300
C	1.11668300	-4.10312200	-0.12252700
H	1.83125300	-4.91133200	-0.15618000
N	0.26009000	-2.02605300	-0.03512400
H	0.18072500	-1.01921700	-0.00295400
N	2.22666500	0.23007000	-0.00887200
C	2.75054500	-2.16416900	-0.05703200
C	-0.80520800	-2.89778600	-0.08161400
C	-0.25422600	-4.21306800	-0.12979300
H	-0.83066500	-5.12493400	-0.16959900
C	5.53265000	-4.39967800	-1.42423000
C	-3.51252700	-4.25609900	-1.42086100
C	5.97047200	-5.04655100	-0.27144400
C	1.45154600	-2.71663200	-0.06435300
C	-3.65378100	-4.32271900	0.95346500
C	-2.17483300	-2.55694000	-0.10442000
C	3.86646100	-3.16627400	-0.12776100
C	3.09449300	-0.81048400	-0.02372100
C	5.36752000	-4.76238100	0.95254400
C	4.49288000	-3.47624100	-1.33714100
C	-3.12259000	-3.71895400	-0.19063500
C	4.33349700	-3.83281100	1.00835800
C	-4.38427500	-5.33709200	-1.52091300
C	-2.73036900	-1.27578600	-0.06636500
C	-4.52819600	-5.40547200	0.88543600
C	-4.89326800	-5.91473400	-0.35935000
C	4.55575600	-0.34641400	-0.05084400
O	5.39363300	-0.91693300	0.93856900
C	4.41602500	1.19364300	0.08803000
O	4.88073100	1.65725300	1.35802000
H	5.13749500	-0.53603600	1.79333500
H	5.01229800	-0.60585700	-1.01093000
H	4.93777700	1.71700500	-0.71982800
H	-4.66625800	0.50622200	1.26602100
H	-4.82640800	-1.70642100	0.45975700
O	-5.33869500	1.11176900	-0.55722900
O	-4.71915400	-1.26886400	-1.51811800
H	-3.98266800	-1.24127000	-2.14633000
H	-5.49078000	0.56543500	-1.34869000
F	2.99096200	4.18268100	2.36985100
H	5.84756600	1.69467100	1.33840600

Mono-fused BC **8-*Z***
Total Energy = -4101.36439102 Hartrees
Lowest Vibrational Mode = 8.50 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-3.27176200	2.91110500	3.00667800
F	-5.15863100	4.73396400	3.66902200
F	2.27446700	5.12194700	-1.98022800
F	-3.82644400	4.01331800	-1.57301800
F	-6.38276300	6.20877200	1.72130000
F	-5.70648700	5.84017500	-0.89991500
F	4.33900100	6.80742500	-2.13236200
F	6.77710000	6.12707100	-1.09801100
F	7.12797000	3.67392300	0.04341700
C	-0.69790100	4.25534400	0.41807400
H	-1.33953500	5.06634500	0.72822800
C	-4.30964400	0.67490100	0.21512000
N	0.00341800	2.19668400	-0.14051900
H	0.01990800	1.20008900	-0.31339200
N	-2.04618500	0.00881400	-0.12871100
C	-2.43032400	2.39689900	0.33274200
C	1.10268400	3.02444300	-0.20664800
C	0.65075800	4.32766800	0.15358900
H	1.27105400	5.20634700	0.22772300
C	-5.10429700	5.11890100	0.05548900
C	3.42683000	4.75028700	-1.38806900
C	-5.45143900	5.30789400	1.39196200
C	-1.11915500	2.90616000	0.22017300
C	4.83774800	3.15418100	-0.29452700
C	2.41880600	2.57069900	-0.47932000
C	-3.48270700	3.40462000	0.69521300
C	-2.84662500	1.07788300	0.12463600
C	-4.82565500	4.55534700	2.38384100
C	-4.13149000	4.17725000	-0.27338900
C	-4.29641500	-0.71539900	-0.45573600
C	3.53574100	3.51726800	-0.72422800
C	-3.85758900	3.62134300	2.02435200
C	4.49695300	5.63388700	-1.50159000
C	2.81675200	1.23320300	-0.37264400
C	5.91222500	4.03572400	-0.39791500
C	5.74249000	5.28592700	-0.98607800
F	4.43537300	-3.24553700	-1.71547500
F	6.33186600	-5.08337200	-1.12871000
F	-3.37545300	-2.78747200	-3.13268000
F	2.89952900	-3.41687600	2.77016700
F	6.52585100	-6.09261500	1.40402100
F	4.80136900	-5.24905000	3.34640800

F	-5.16549400	-4.71453200	-3.76586400
F	-3.40211300	-4.25629100	1.37693400
F	-6.07883300	-6.42536900	-1.83713900
F	-5.18367100	-6.18644000	0.73332400
C	0.85529100	-4.12200600	-0.15337400
H	1.52915100	-4.96421300	-0.10138500
N	0.09663600	-2.00557400	-0.13801400
H	0.05705300	-0.99709100	-0.07156700
N	2.08396300	0.12580300	-0.16309100
C	2.54522800	-2.25088000	0.19871000
C	-0.98996700	-2.81574100	-0.37653300
C	-0.49629200	-4.15803100	-0.40479900
H	-1.09902800	-5.03556300	-0.58298800
C	4.70499400	-4.75365700	2.10544300
C	-3.79943300	-3.61958800	-2.16084500
C	5.58663000	-5.18510200	1.11650100
C	1.24064200	-2.75505100	0.00034100
C	-3.80553400	-4.36104200	0.09822400
C	-2.32796300	-2.39300500	-0.51998700
C	3.60225300	-3.26654400	0.50867500
C	2.92249100	-0.91224100	0.09936900
C	5.48614200	-4.66944700	-0.17413500
C	3.73099100	-3.80723600	1.79345100
C	-3.31420800	-3.47028300	-0.85984600
C	4.50193300	-3.72600600	-0.45836300
C	-4.72622200	-4.60139600	-2.50375300
C	-2.80763700	-1.08668100	-0.36011800
C	-4.72890700	-5.35345000	-0.21450900
C	-5.19206500	-5.47340600	-1.52354900
C	4.36312100	-0.43288800	0.30841300
O	4.57670400	-0.29754600	1.70775700
C	4.29272100	0.91455700	-0.42121200
O	5.08165100	1.91535600	0.22985900
H	5.25679200	0.37768500	1.85176600
H	5.11647300	-1.09299100	-0.13195700
H	4.64316500	0.80671800	-1.45913700
O	-4.77655800	0.56748800	1.57258800
H	-4.02328500	0.47507700	2.17426100
O	-5.21863700	-1.60928300	0.12344400
H	-5.40701700	-1.26725600	1.01524700
H	-4.99397400	1.36567000	-0.27884400
H	-4.55457800	-0.61000900	-1.51828700

Mono-fused BC **8-*E***
Total Energy = -4101.36482695 Hartrees
Lowest Vibrational Mode = 8.33 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-3.75256200	2.24656900	3.00267600
F	-5.76085500	3.90315600	3.73683300
F	1.89168400	5.25916700	-1.87531400
F	-3.78624400	4.14752300	-1.34303700
F	-6.78960300	5.69138600	1.94142600
F	-5.78817400	5.80478000	-0.59791200
F	3.83612800	7.08237500	-2.03634900
F	6.33454100	6.54933600	-1.06140200
F	6.87127700	4.10667000	0.02872900
C	-0.95162800	4.16575800	0.56350600
H	-1.63218600	4.92543200	0.91705900
C	-4.36462700	0.36399400	0.19672000
N	-0.14816200	2.16857000	-0.08447100
H	-0.08159900	1.17914000	-0.28342100
N	-2.04251700	-0.11157800	-0.09474000
C	-2.58497500	2.22445800	0.40429000
C	0.90316300	3.05708400	-0.13120200
C	0.38266200	4.32248700	0.28440400
H	0.95693900	5.22941800	0.38648400
C	-5.27792400	4.93368600	0.28485300
C	3.07877400	4.95592000	-1.31354600
C	-5.79503600	4.87349700	1.57765400
C	-1.30554100	2.80106000	0.31175500
C	4.61462400	3.43988300	-0.27542900
C	2.23705500	2.69743000	-0.43341100
C	-3.68920800	3.15383300	0.80942800
C	-2.91892300	0.88345800	0.15038700
C	-5.27037000	3.96200000	2.49006900
C	-4.24206200	4.07969400	-0.08034100
C	-4.21636900	-1.02650300	-0.45762500
C	3.28365300	3.72147400	-0.67521500
C	-4.23205600	3.12116200	2.09613500
C	4.08479600	5.91131000	-1.43099400
C	2.72644500	1.38323000	-0.35760400
C	5.62560300	4.39312900	-0.38348000
C	5.36097400	5.63879700	-0.94566100
F	3.17379800	-3.22907900	2.77229800
F	5.19717100	-4.93338500	3.32693600
F	-2.88611300	-3.36095700	-3.08634800
F	4.61554800	-3.00011200	-1.74210800
F	6.93621300	-5.68361100	1.35953900
F	6.63381200	-4.70990800	-1.17675600

F	-4.55556300	-5.42264000	-3.62163300
F	-3.43226800	-4.13616000	1.56089500
F	-5.66453900	-6.85440800	-1.57549000
F	-5.09350700	-6.20216300	1.01528400
C	1.11488300	-4.08617600	-0.07784200
H	1.83430100	-4.88870000	-0.01117500
N	0.23893600	-2.01831000	-0.11556900
H	0.14814200	-1.01208400	-0.06374000
N	2.07494300	0.23109000	-0.15287400
C	2.70108200	-2.10987300	0.19801400
C	-0.80303000	-2.89469300	-0.31083700
C	-0.24152500	-4.20465400	-0.30002900
H	-0.79828100	-5.11988700	-0.43496900
C	5.78086700	-4.34189100	-0.20970900
C	-3.41649200	-4.04754200	-2.05704300
C	5.93670000	-4.83923200	1.08251200
C	1.42399600	-2.69990700	0.02759300
C	-3.68674600	-4.43811600	0.27522100
C	-2.16552200	-2.54366900	-0.45776300
C	3.82503900	-3.05428500	0.49729200
C	2.98845100	-0.75474900	0.09008200
C	5.04747300	-4.45549100	2.08427700
C	4.73418100	-3.46458900	-0.48278400
C	-3.09837400	-3.68403800	-0.74510900
C	4.01049200	-3.57468900	1.78346800
C	-4.27332400	-5.10504700	-2.35121800
C	-2.72155700	-1.27064200	-0.33372300
C	-4.54732000	-5.50181600	0.01185400
C	-4.84053100	-5.83580500	-1.30907900
C	4.39518900	-0.17961100	0.28109300
O	4.62533100	-0.04564900	1.67796600
C	4.22105400	1.16896000	-0.42940800
O	4.95047500	2.21236400	0.22380300
H	5.26386300	0.66974400	1.81833500
H	5.18348100	-0.78159700	-0.18124700
H	4.56141600	1.09916600	-1.47391300
H	-4.65572700	0.24148100	1.24844100
H	-4.83468900	-1.77959400	0.03189800
O	-5.33971000	1.16647800	-0.42978800
O	-4.65956800	-0.98300000	-1.82716000
H	-3.89919000	-0.86655100	-2.41511200
H	-5.45895600	0.80224200	-1.32462700

Bis-fused BC **9-*Z*-*s***
Total Energy = -4000.90519902 Hartrees
Lowest Vibrational mode = 10.14 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	-6.84733300	3.80427600	-0.46929800
F	2.91124300	4.60665600	2.47414900
F	-1.80016500	4.98642500	-2.10109700
F	-6.38050300	5.96535500	-2.06404300
F	-3.81795800	6.51289600	-2.87755500
F	5.18139600	5.97341800	2.80450800
F	7.50413600	5.12858100	1.63296200
F	7.52192300	2.82702700	0.16742700
C	-0.15084000	4.45383900	-0.03128200
H	-0.67876400	5.38120000	-0.17641900
C	-3.90682400	1.38610000	0.87578700
N	0.29405700	2.26073600	0.18294900
H	0.20731100	1.25191300	0.16713800
N	-1.91941500	0.31627900	0.25412200
C	-2.08188600	2.75662700	-0.20058600
C	1.47287400	2.92943000	0.42411900
C	1.17347500	4.32447400	0.29527900
H	1.87511200	5.13159200	0.42670600
C	-4.05721900	5.50142300	-2.02844600
C	4.00279000	4.17337400	1.81016500
C	-5.35975700	5.21540500	-1.63425700
C	-0.73109000	3.14303500	-0.09931300
C	5.18396700	2.57145100	0.48066900
C	2.71073100	2.28696800	0.64010400
C	-3.17831400	3.64689900	-0.66055600
C	-2.54426600	1.48688500	0.22865500
C	-5.58583600	4.12198700	-0.80904000
C	-3.00878500	4.71264400	-1.56919600
C	-4.24087500	-0.10448600	0.72765500
C	3.94337300	3.04021400	0.98349600
C	-4.52929500	3.33038500	-0.35135200
C	5.18052900	4.88635400	2.01787000
C	2.93343100	0.92051200	0.37553600
C	6.36657500	3.28189600	0.67900800
C	6.36670200	4.45250400	1.43242400
F	4.08205700	-3.82457800	1.24499100
F	5.70083400	-5.81905700	0.39709600
F	-3.97156400	-3.41913200	-1.48258000
F	2.33646400	-3.39172100	-3.14538500
F	5.65116600	-6.60661200	-2.21995400
F	3.96284900	-5.38216900	-3.98306800
F	-6.02744900	-5.10790800	-1.01075800
F	-3.55165200	-2.64150300	3.17908600

F	-6.85623900	-5.57888000	1.54843600
F	-5.60726700	-4.33836800	3.64018300
C	0.34909900	-4.12519600	-0.15289500
H	0.90003900	-5.03818000	-0.32363600
N	-0.12554300	-1.94592500	0.07463000
H	-0.03950500	-0.93819600	0.08019400
N	2.06873000	-0.05386900	0.08376700
C	2.24471300	-2.43777500	-0.46636600
C	-1.29432700	-2.63041400	0.30780200
C	-0.98900400	-4.01266100	0.18246200
H	-1.69264300	-4.82061300	0.31681100
C	3.98577800	-4.99504500	-2.70057700
C	-4.35370600	-3.62421800	-0.21463700
C	4.84837400	-5.62116100	-1.80320200
C	0.89689800	-2.81499600	-0.21186200
C	-4.14252100	-3.23980500	2.12671600
C	-2.55380300	-2.02909300	0.57501000
C	3.15420700	-3.53751900	-0.92290300
C	2.77380600	-1.16854600	-0.29909900
C	4.87222600	-5.21834900	-0.46958900
C	3.15489400	-3.96914400	-2.25443500
C	-3.69103400	-2.97172000	0.83095600
C	4.02963500	-4.19156000	-0.05052200
C	-5.41328800	-4.49971800	0.01360300
C	-2.82592200	-0.67062400	0.57147900
C	-5.20108200	-4.10820600	2.38279000
C	-5.83903500	-4.74089800	1.31819600
C	4.24808500	-0.82907900	-0.53584000
C	4.36005600	0.42259400	0.34306200
H	-3.78234200	1.62362500	1.94427100
H	-4.76407500	-0.49072000	1.60937900
O	-4.91931800	2.23510700	0.35857400
O	-4.97101600	-0.38900000	-0.45838100
H	-5.74171100	0.19783600	-0.48872300
O	4.41810700	-0.54893200	-1.91962300
H	4.93901100	-1.61437000	-0.21477300
H	5.18508600	0.03414200	-2.02410300
H	4.70628200	0.14942600	1.35180400
O	5.25815400	1.39145600	-0.20666800

Bis-fused BC **9-*E-s***
Total Energy = -4000.90354620 Hartrees
Lowest Vibrational Mode = 8.24 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	7.29627000	3.21199200	-0.76870600
F	-2.31984500	5.39288200	1.08411300
F	2.49107600	5.41105500	0.48376000
F	7.09896000	5.86538600	-0.16682100
F	4.64835900	6.91710800	0.47733400
F	-4.40281900	7.05046600	0.94566500
F	-6.84380200	6.16158900	0.09353000
F	-7.17557800	3.53193900	-0.55715100
C	0.62665500	4.28144200	-0.99030600
H	1.22668500	5.05379900	-1.44284400
C	4.11169500	0.76846100	-1.00157600
N	0.01979800	2.31606100	-0.08762600
H	0.06197500	1.38052500	0.29635000
N	2.03366500	0.13990300	-0.13326500
C	2.46104000	2.57843500	-0.40443400
C	-1.13571200	3.04564600	-0.27241000
C	-0.74178200	4.27327200	-0.88141300
H	-1.41661200	5.04158800	-1.22497800
C	4.75481500	5.63548400	0.09291400
C	-3.46934300	4.90280500	0.58092400
C	6.00145400	5.10242500	-0.21201700
C	1.12644800	3.05525900	-0.45515000
C	-4.87235900	3.11431100	-0.17014300
C	-2.43813800	2.60596000	0.06761600
C	3.64513300	3.47950200	-0.37884400
C	2.78250300	1.20731100	-0.43028100
C	6.08868700	3.75565700	-0.53633000
C	3.62247700	4.82966100	0.03824100
C	4.30173900	-0.61231000	-0.37306300
C	-3.56777100	3.56598200	0.15586500
C	4.94926600	2.94920300	-0.58693700
C	-4.55118000	5.77878200	0.54457200
C	-2.81530100	1.26142300	0.21041300
C	-5.95830700	3.98631600	-0.21641100
C	-5.79860800	5.32664300	0.12309300
F	-3.13397200	-3.77212800	-2.18487100
F	-5.05180400	-5.67256900	-2.28723400
F	3.50561100	-3.19804200	2.54357200
F	-4.14984100	-3.00596700	2.38645300
F	-6.52551600	-6.25564400	-0.06315900
F	-6.06315100	-4.91411300	2.27342500
F	5.41824300	-5.09959800	2.73293100

F	3.56694000	-3.61695800	-2.18080100
F	6.41085200	-6.27468500	0.47647700
F	5.47449100	-5.52656000	-1.98029000
C	-0.73776800	-4.07978100	0.37326900
H	-1.38644300	-4.93733800	0.47150700
N	-0.04881600	-1.95287800	0.14239900
H	-0.05645600	-0.94699300	0.02439800
N	-2.07644700	0.14473500	0.15667300
C	-2.51277600	-2.26625400	0.15695500
C	1.08142000	-2.73393600	0.20923700
C	0.64129400	-4.07960800	0.36793200
H	1.29032700	-4.93776400	0.45732500
C	-5.34031700	-4.62866200	1.18052000
C	3.97645300	-3.74880000	1.41580100
C	-5.57762400	-5.31335500	-0.00945100
C	-1.17818800	-2.73335300	0.22618000
C	4.00312700	-3.96806000	-0.95587500
C	2.41597100	-2.28099100	0.07697700
C	-3.57450100	-3.32234500	0.10365100
C	-2.91044800	-0.93447400	0.11833600
C	-4.82346500	-5.01463800	-1.14229900
C	-4.34886500	-3.65127400	1.22076000
C	3.47381900	-3.34043700	0.17562500
C	-3.83924500	-4.03070900	-1.07441100
C	4.95863900	-4.73068900	1.52931200
C	2.83067900	-0.97460800	-0.15013500
C	4.98738700	-4.95007600	-0.87171900
C	5.46671100	-5.33188100	0.37965200
C	-4.37257800	-0.51552000	-0.06249500
O	-4.70040000	-0.66747700	-1.43853000
C	-4.28573500	0.95060000	0.37694500
O	-5.10798600	1.79498400	-0.43602600
H	-5.38822100	-0.02348400	-1.66503500
H	-5.07184500	-1.08212700	0.56040600
H	-4.59812200	1.05995100	1.42647400
H	3.98335400	0.65052300	-2.09014800
H	4.81707400	-1.30055100	-1.05097400
O	5.21465900	1.62727900	-0.77592300
O	4.95427000	-0.56084900	0.88870200
H	5.78067000	-0.06585800	0.78279800

Bis-fused BC **9-*Z*-*a***
Total Energy = -4000.91770265 Hartrees
Lowest Vibrational Mode = 10.09 cm^{-1}

Atom	X (Å)	Y (Å)	Z (Å)
F	3.18205700	-2.69794100	3.10526100
F	5.25923300	-4.18111500	3.99687300
F	-1.46503500	-5.23152200	-2.26752800
F	4.79816200	-3.11760900	-1.33487000
F	7.11182000	-5.14351200	2.23638400
F	6.87015900	-4.60656200	-0.43281200
F	-3.30924700	-7.14005600	-2.56823000
F	-5.84499200	-6.79549100	-1.60445300
F	-6.52274300	-4.45476500	-0.37809200
C	1.29013800	-4.10715900	0.31967700
H	2.01415700	-4.84225800	0.63826200
C	4.36403600	-0.01191300	0.28606500
N	0.36528200	-2.13547900	-0.22418100
H	0.23595500	-1.13935800	-0.34814400
N	2.04156000	0.22965300	-0.24108600
C	2.76923200	-2.02836300	0.36805300
C	-0.61739600	-3.08737800	-0.37175700
C	-0.02262000	-4.33811100	-0.02683700
H	-0.52833000	-5.29037000	-0.01885800
C	5.96078000	-4.13446500	0.43235700
C	-2.67457400	-5.02346000	-1.71024700
C	6.08609500	-4.40847000	1.79276000
C	1.54571400	-2.70974800	0.18278900
C	-4.30129300	-3.65343600	-0.60919300
C	-1.96557600	-2.77986700	-0.68831100
C	3.91959500	-2.85587400	0.85574300
C	2.99250200	-0.67435400	0.11937200
C	5.13927200	-3.91659400	2.68878500
C	4.88622600	-3.36930200	-0.01428300
C	4.14075400	1.25705500	-0.54965100
C	-2.95307000	-3.84092000	-1.00587400
C	4.07569400	-3.15119100	2.21476400
C	-3.62724400	-6.02105600	-1.89969400
C	-2.52363300	-1.50220400	-0.54860000
C	-5.25906000	-4.64984200	-0.78902600
C	-4.92215200	-5.84412100	-1.41994200
F	-3.13496000	2.64740900	3.00989400
F	-5.22772900	4.14243400	3.84299800
F	-4.66977100	3.00576500	-1.46434700
F	-7.04787100	5.08032100	2.03592100
F	-6.75770800	4.50672500	-0.62070800
F	6.63251400	4.35728500	-0.31613300
F	1.61099400	5.10757600	-2.30993800

F	5.97810800	6.68087000	-1.58703200
F	3.46084500	7.01190800	-2.60251800
C	-1.19236400	4.01853300	0.24090400
H	-1.92220600	4.75776800	0.53570300
N	-0.25757100	2.03974900	-0.25827600
H	-0.12591400	1.04203900	-0.36600000
N	-1.93372500	-0.32559000	-0.27463200
C	-2.67228500	1.94037300	0.29018200
C	0.72769700	2.98972600	-0.40064400
C	0.12658000	4.24500600	-0.08448600
H	0.63197100	5.19746400	-0.08037200
C	-5.86426200	4.04666100	0.26723900
C	4.41553800	3.55275300	-0.57734900
C	-6.01432100	4.33937600	1.62123900
C	-1.44543000	2.61931800	0.11843600
C	2.80985600	4.90737000	-1.72727100
C	2.08155300	2.67804300	-0.68773600
C	-3.83132200	2.77431900	0.74533000
C	-2.89106600	0.58309000	0.05578400
C	-5.08408100	3.86000100	2.54107800
C	-4.78183900	3.27556600	-0.14917500
C	3.07494800	3.73469100	-1.00152000
C	-4.01212400	3.08825100	2.09708200
C	5.37669300	4.54663900	-0.75312200
C	2.63666000	1.40247500	-0.52015000
C	3.76608500	5.90228900	-1.91274300
C	5.05181300	5.73207200	-1.40657800
C	-4.26551500	-0.07729000	0.20619800
O	-4.48307100	-0.33157200	1.58804300
C	-4.02692300	-1.35746800	-0.60787900
O	-4.70636700	-2.47994800	-0.03708200
H	-5.07557300	-1.09395000	1.67178000
H	-5.08511700	0.51890900	-0.20759600
H	-4.37353000	-1.22290900	-1.64397400
O	4.55627200	0.26119300	1.66807200
H	5.19099200	-0.61367300	-0.10440900
H	5.14695700	1.02489000	1.75229400
H	4.50647300	1.10842400	-1.57724400
O	4.80964400	2.38728200	0.01826400