Supplementary Information

for

Dyads with Tunable Near-Infrared Donor−Acceptor Excited-State Energy Gaps: Molecular Design and Förster Analysis for Ultrafast Energy Transfer

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Table S1. Excited-state energies from TDDFT calculations.[a]

Dyad	S_2 λ_D (nm)	S_1 λ_A (nm)	$\Delta\lambda$ $\lambda_A - \lambda_D$ (nm)	S_2 E_D (cm^{-1})	S_2 E_A (cm^{-1})	Observed $E_D - E_A$ (cm^{-1})
1	746.8	760.3	13.5	13,390	13,153	238
2	737.4	752.8	15.4	13,561	13,284	277
3	765.8	789.6	23.8	13,058	12,665	394
4	737.5	759.6	22.1	13,559	13,165	394
5	729.8	752.2	22.4	13,702	13,294	408
6	730.2	769.5	39.3	13,695	12,995	699
7	738.0	788.2	50.2	13,550	12,687	863
8	729.8	787.6	57.8	13,702	12,697	1,006
9	729.6	796.6	67	13,706	12,553	1,153

[a]For dyads in toluene.

Table S2. S_1 and S_2 NTO summary for dyads.

Dyad	S2-S1 energy gap (cm^{-1})	S1 Fraction donor NTOs	S1 Fraction acceptor NTOs	S2 Fraction donor NTOs	S2 Fraction acceptor NTOs
1	197	0.130	0.8696	0.868	0.132
2	235	0.071	0.9285	0.920	0.080
3	303	0.086	0.9138	0.905	0.095
4	335	0.039	0.9605	0.960	0.040
5	345	0.033	0.9671	0.967	0.033
6	628	0.000	1.0000	0.992	0.008
7	772	0.013	0.9870	0.986	0.014
8	876	0.009	0.9909	0.989	0.011
9	1089	0.000	1.0000	0.992	0.008

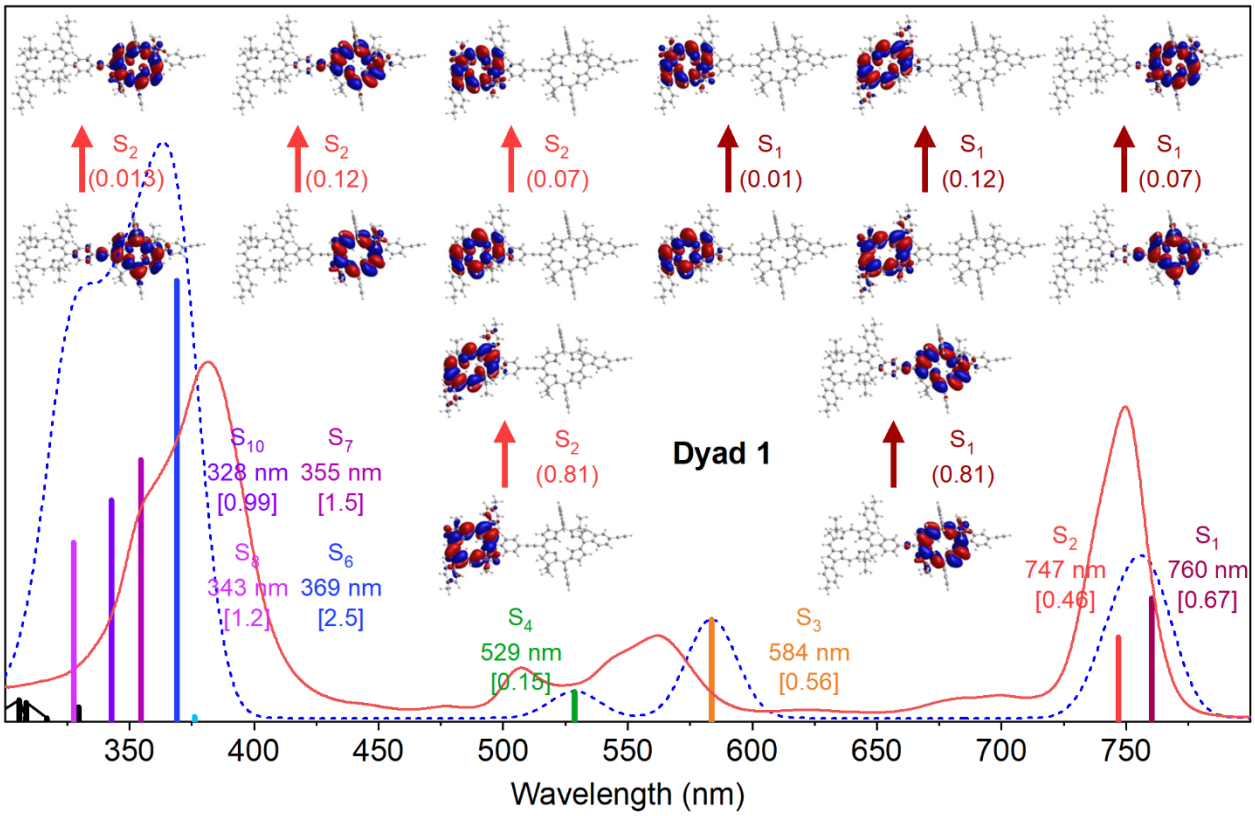


Figure S1. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-1** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

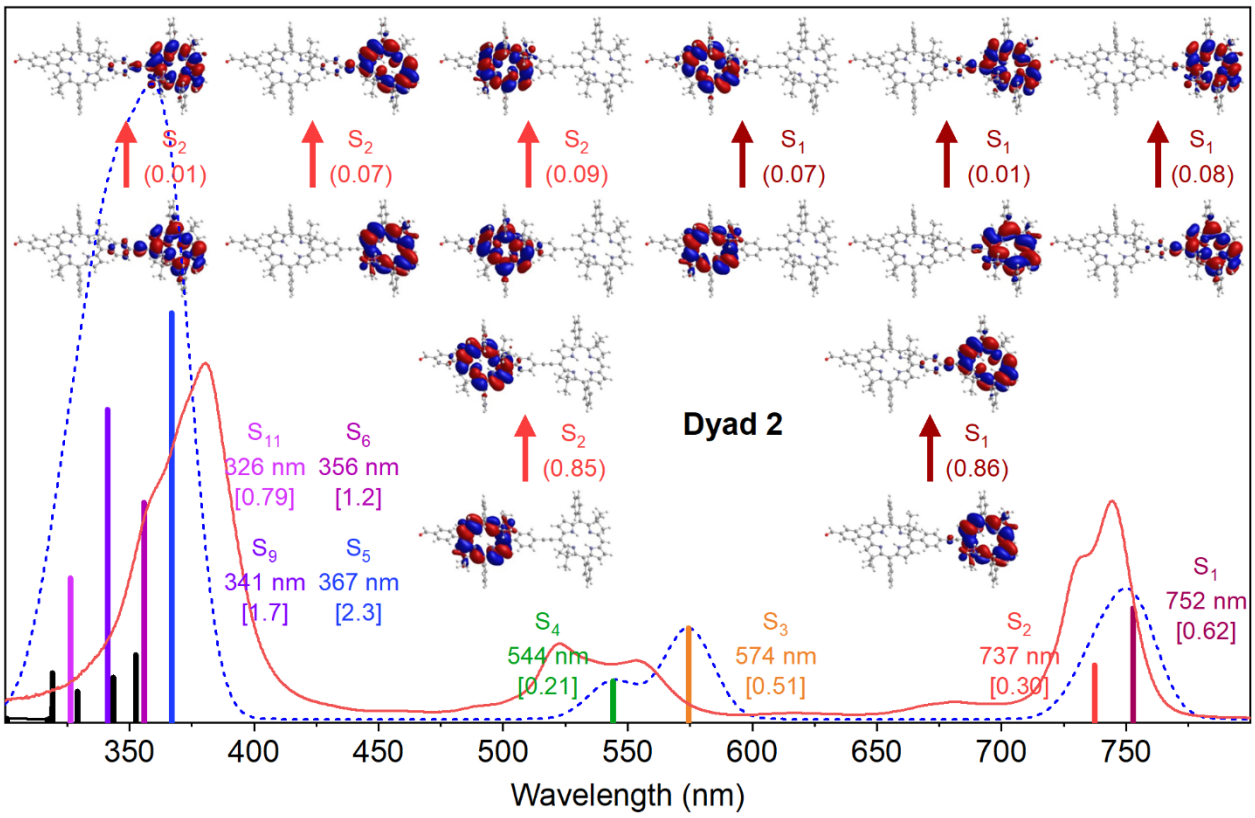


Figure S2. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-2** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

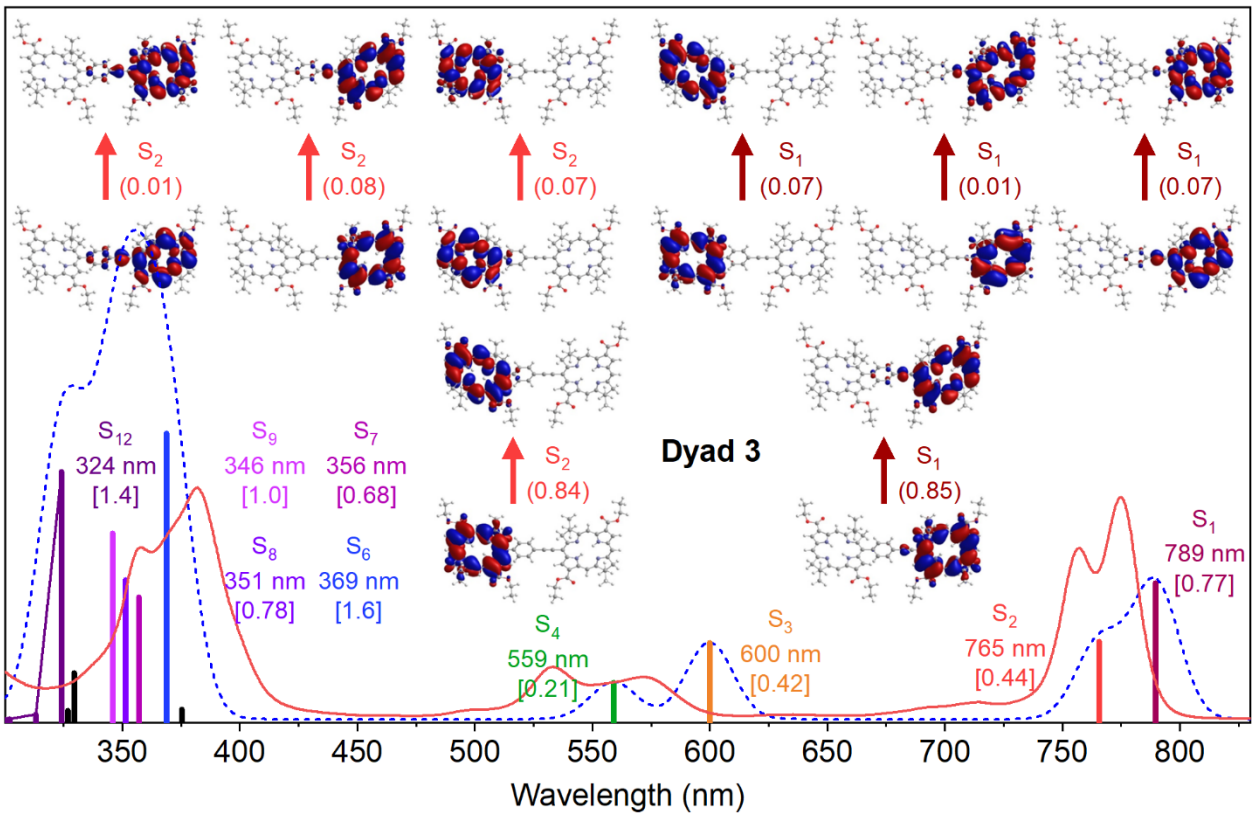


Figure S3. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-3** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

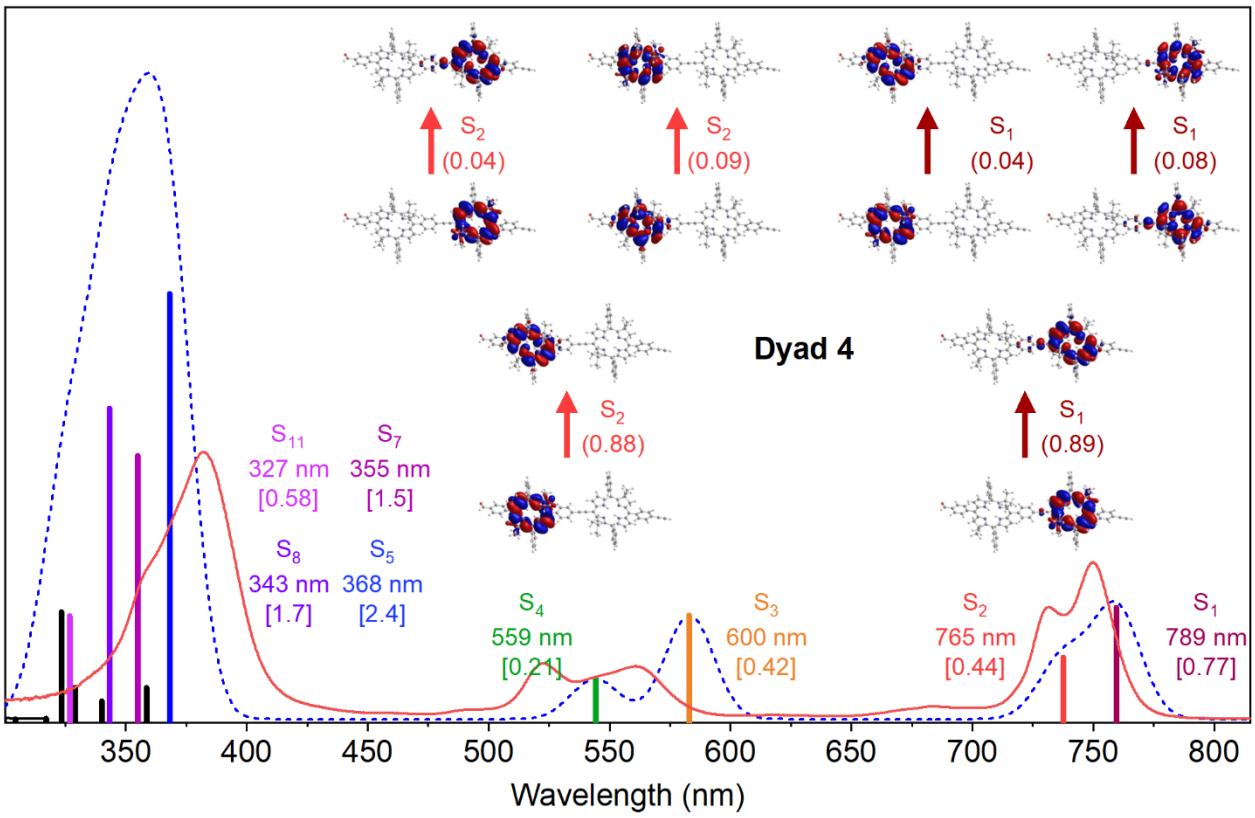


Figure S4. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-4** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

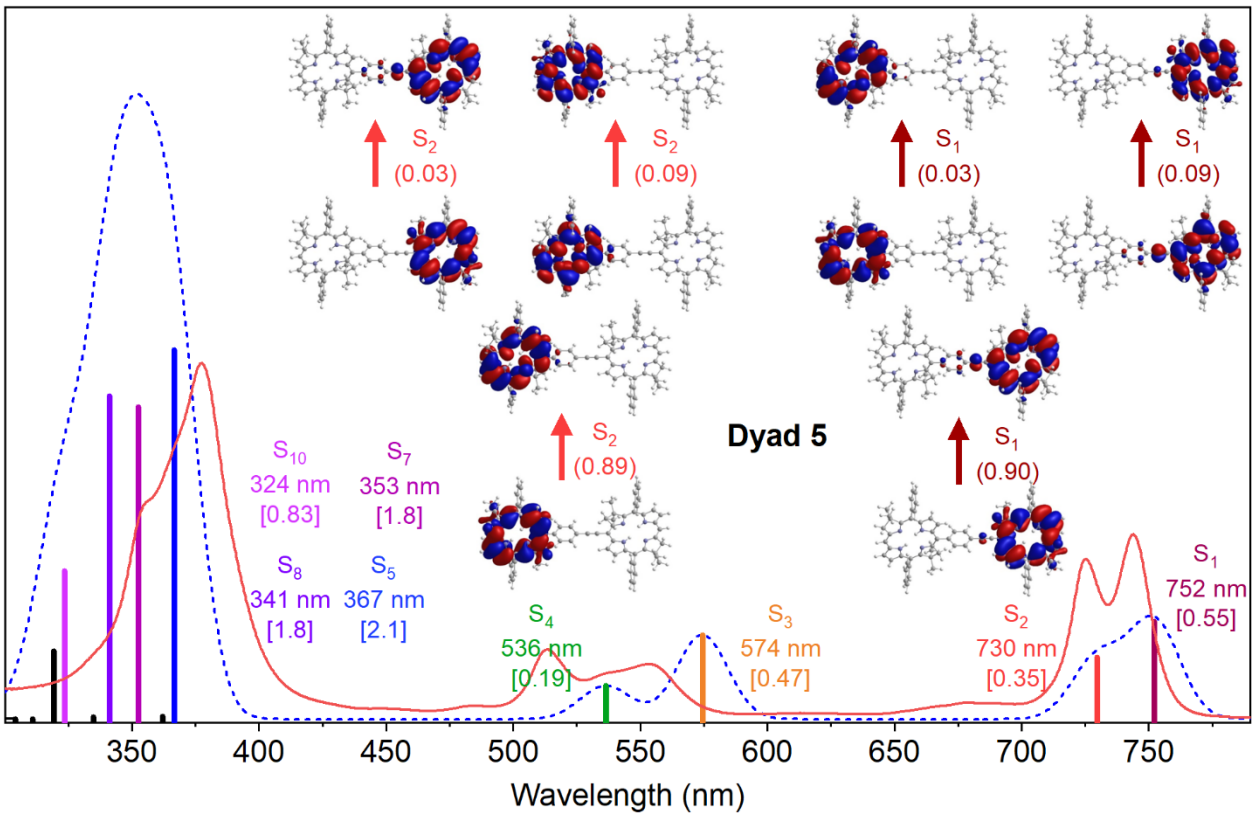


Figure S5. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-5** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

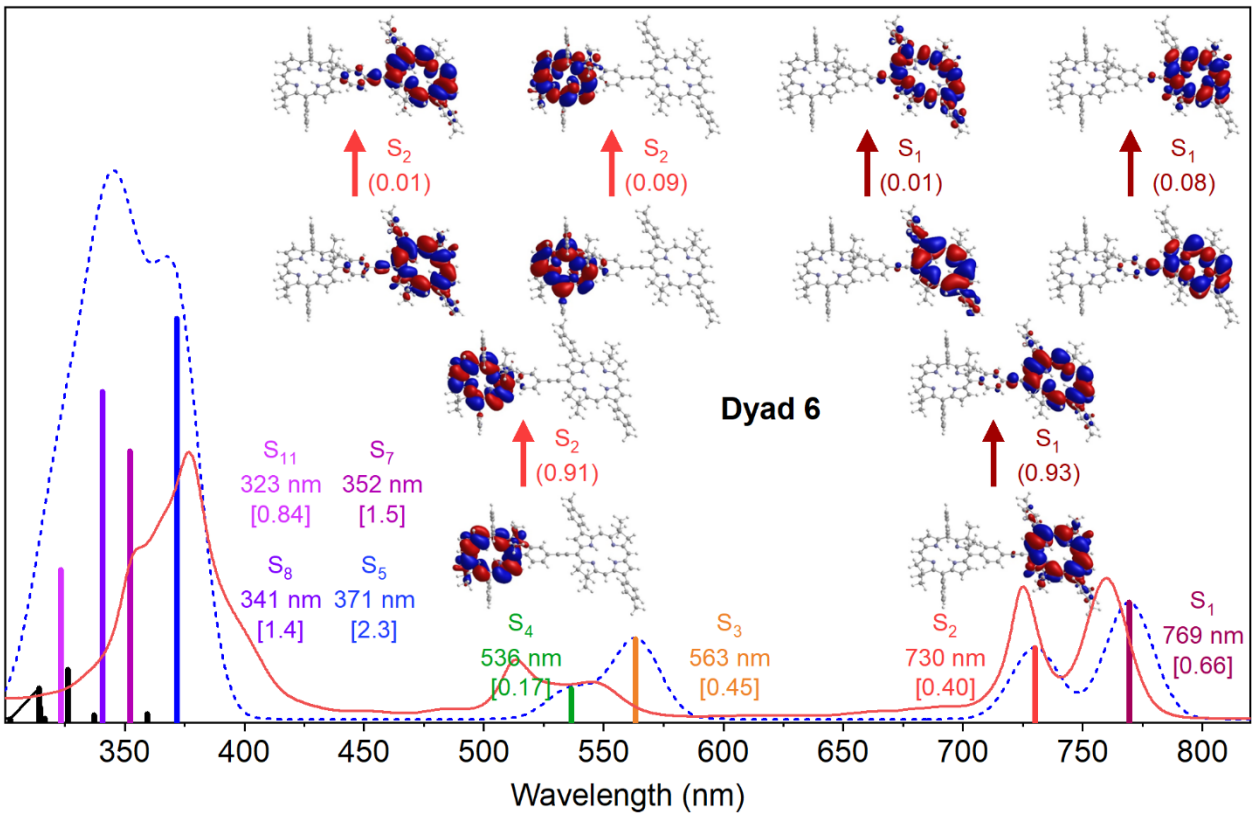


Figure S6. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-6** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

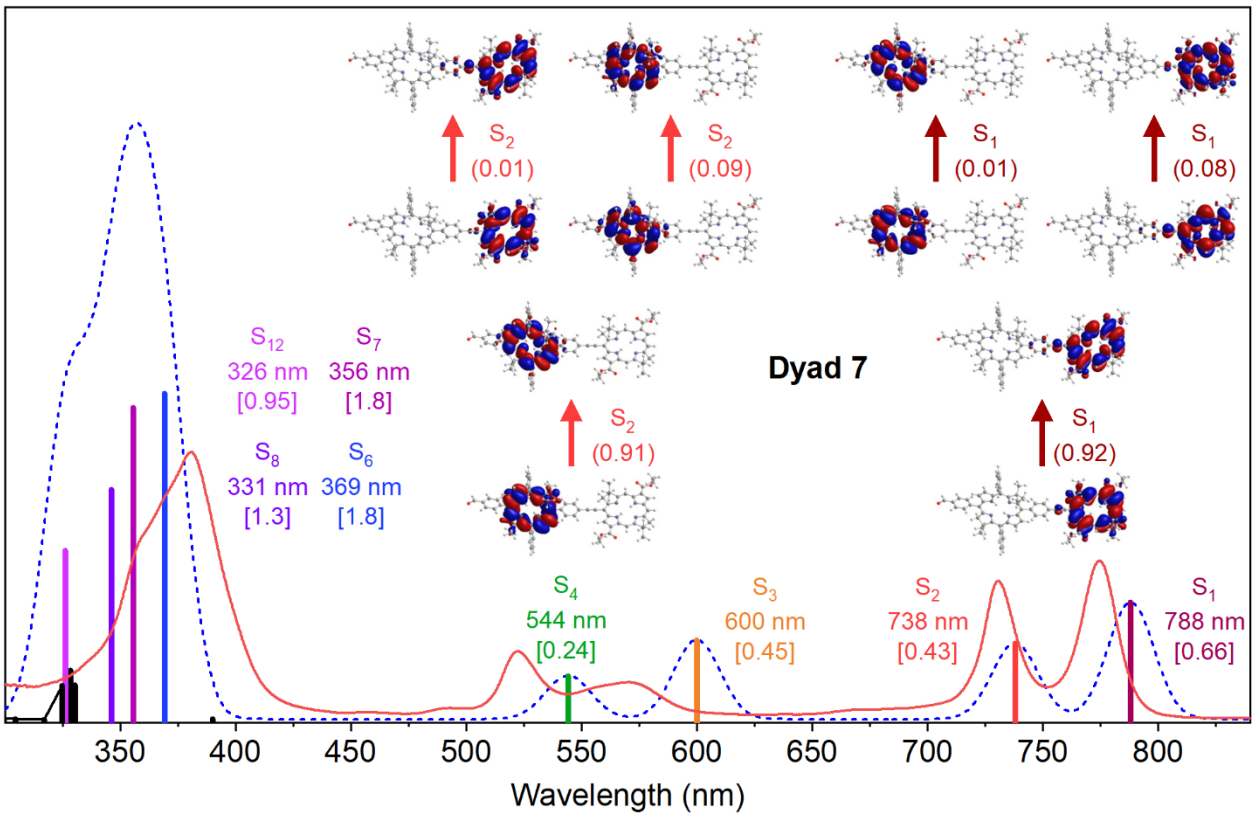


Figure S7. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-7** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

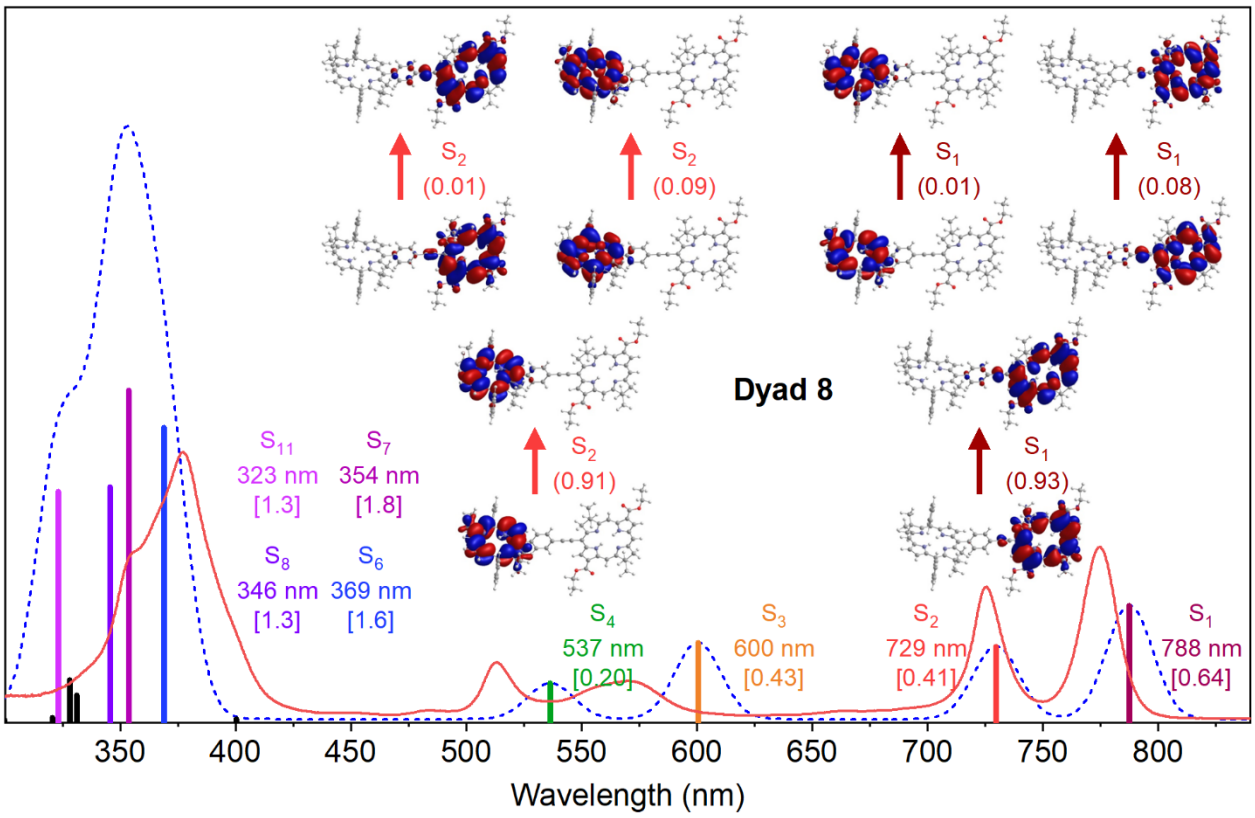


Figure S8. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-8** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

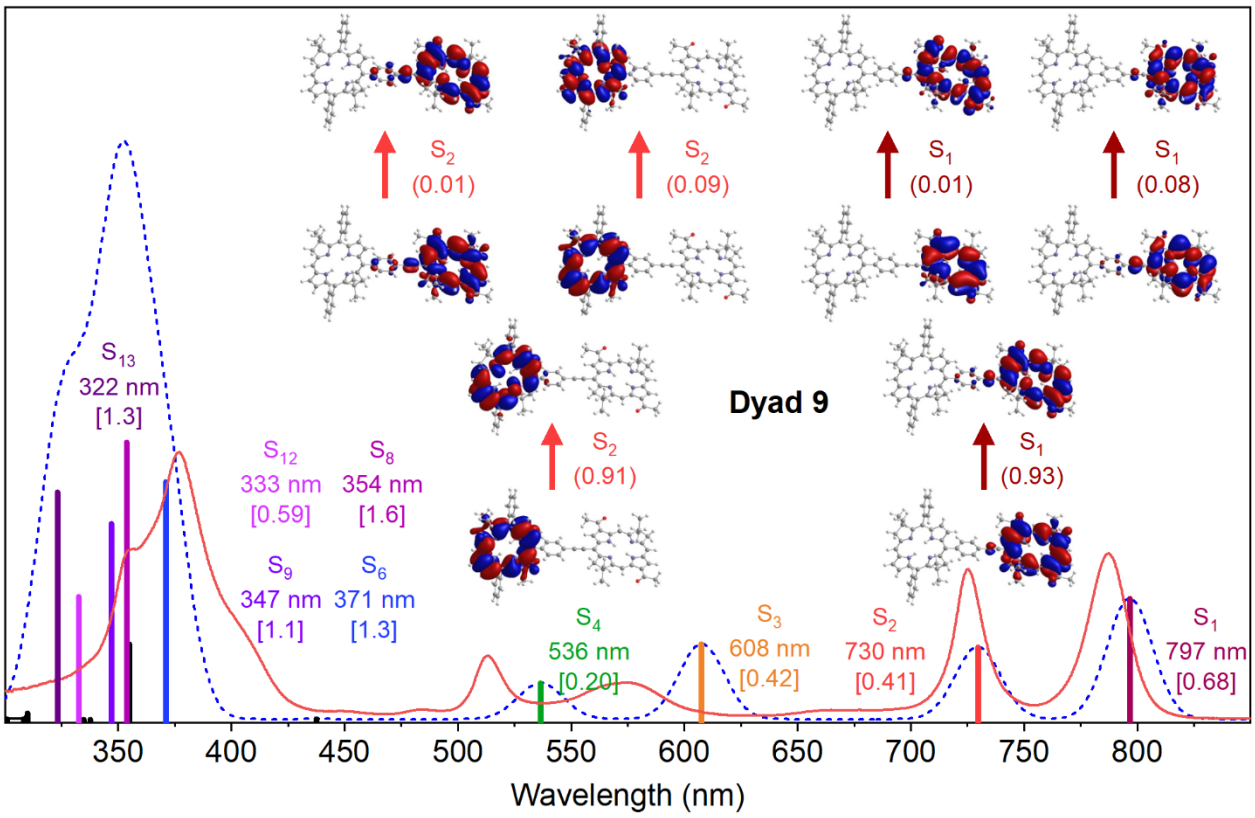
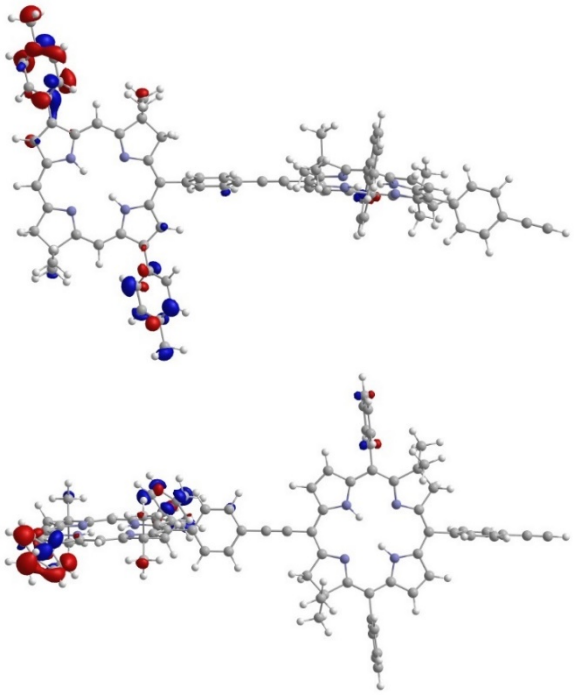
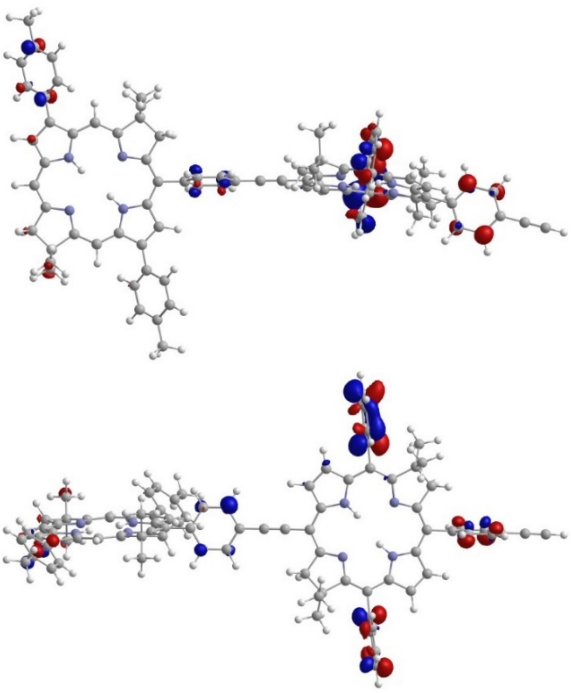
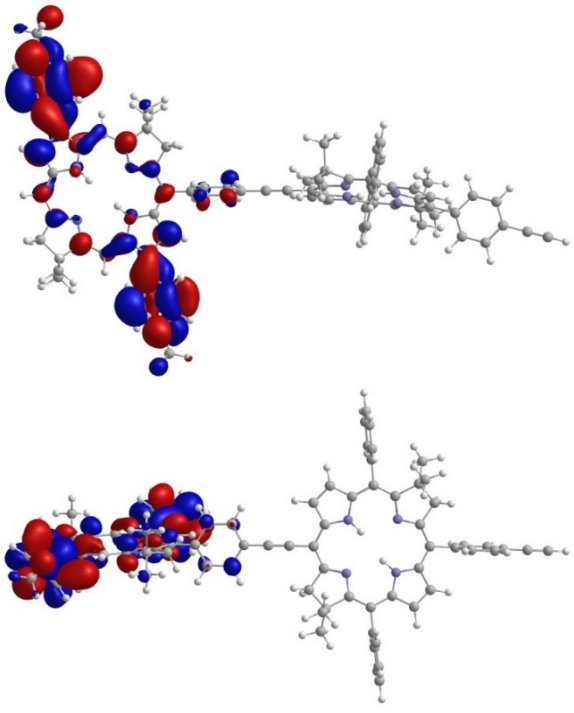
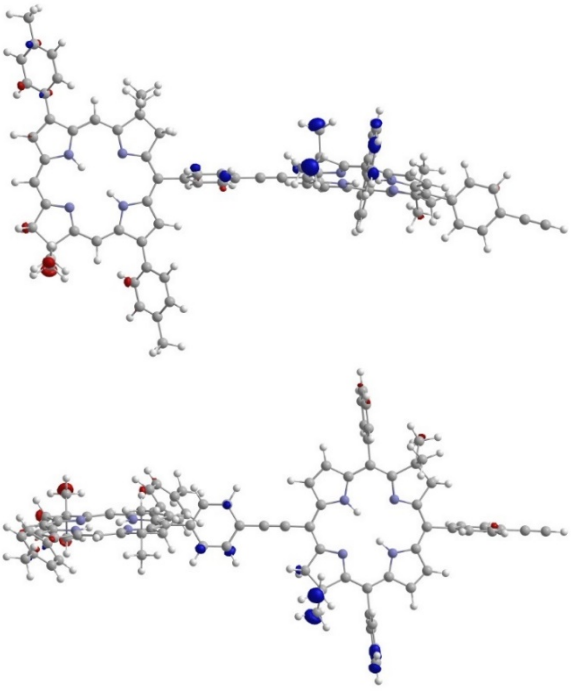
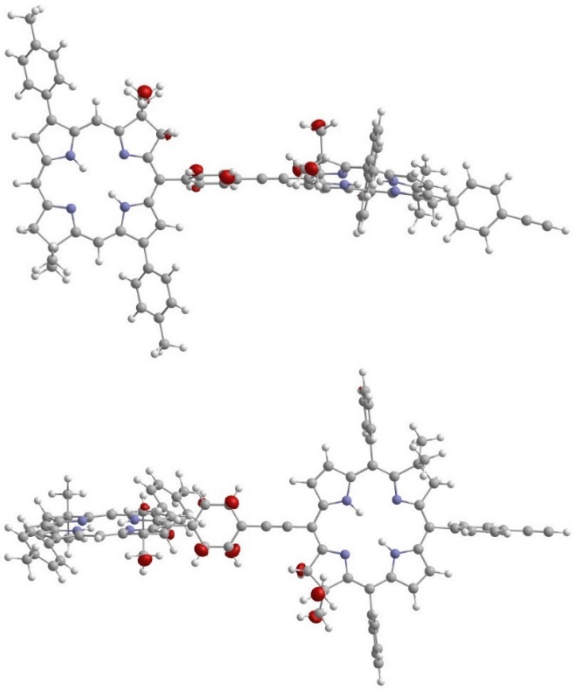
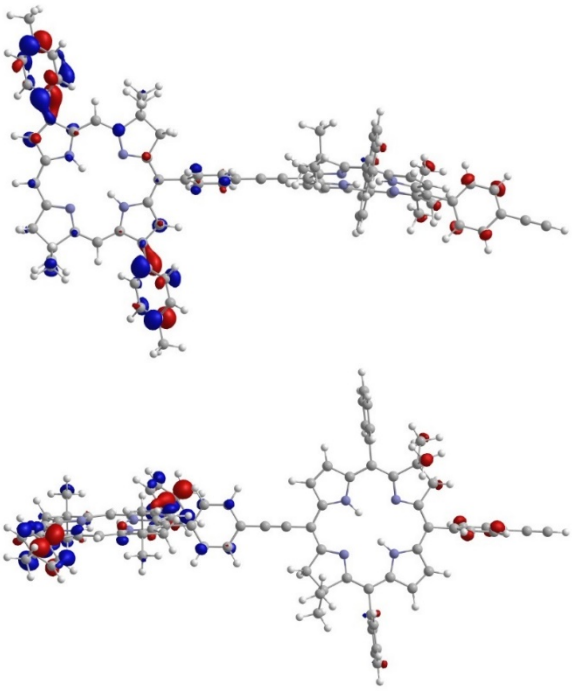
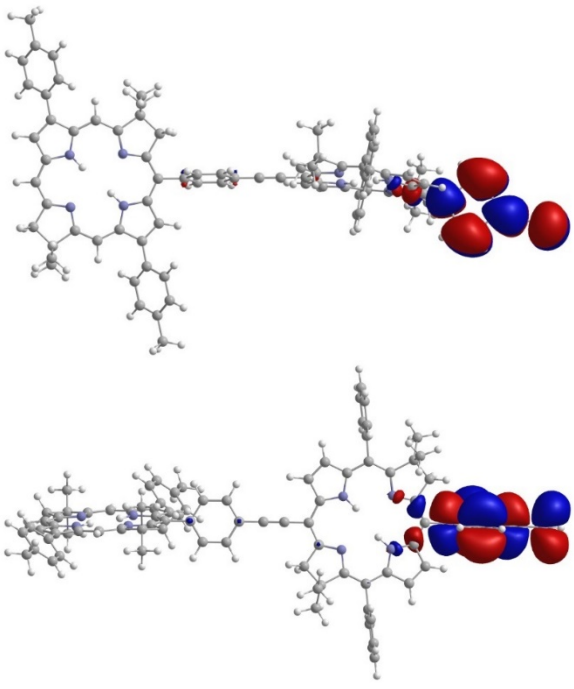
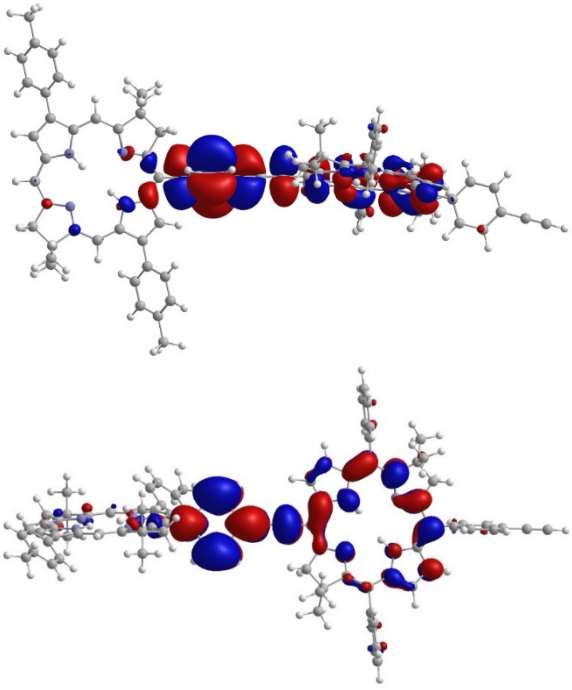
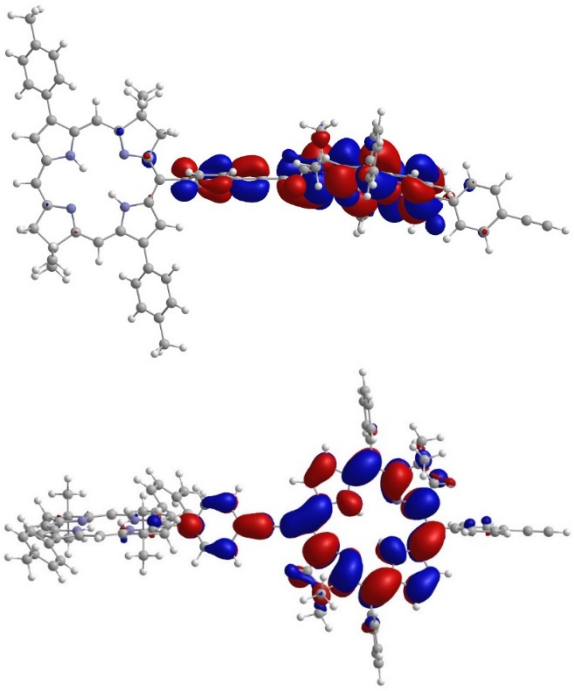
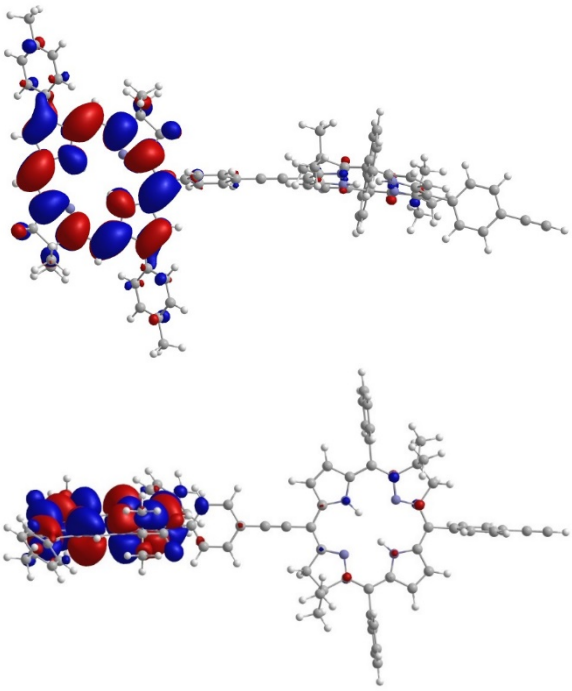
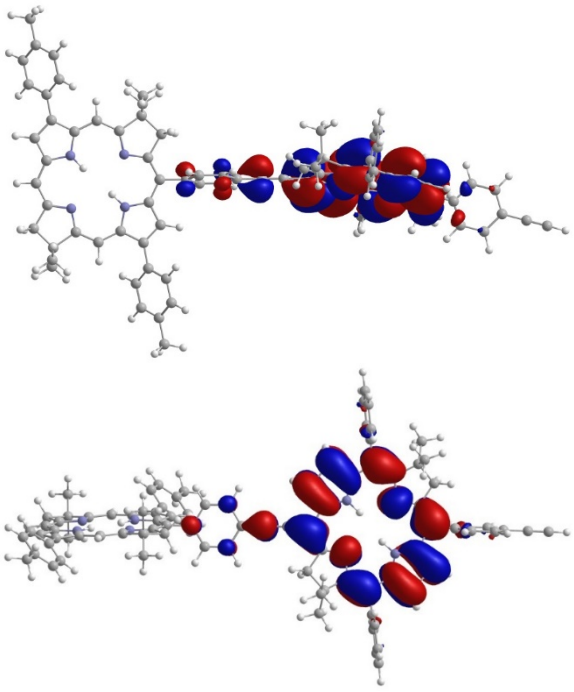
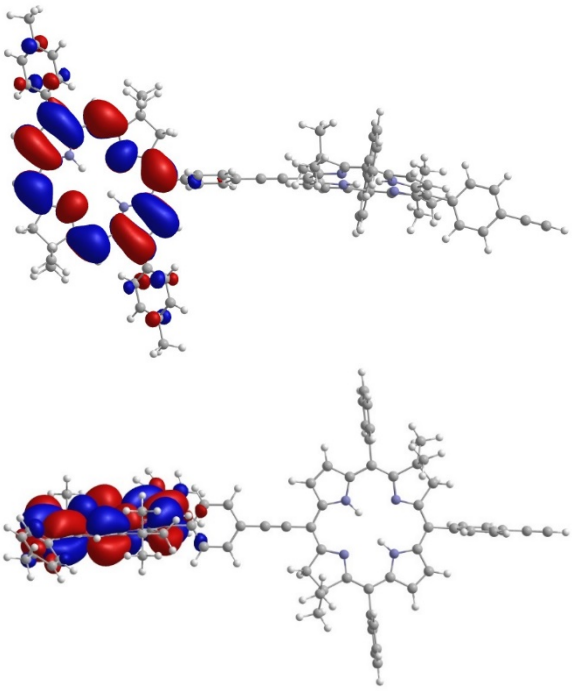


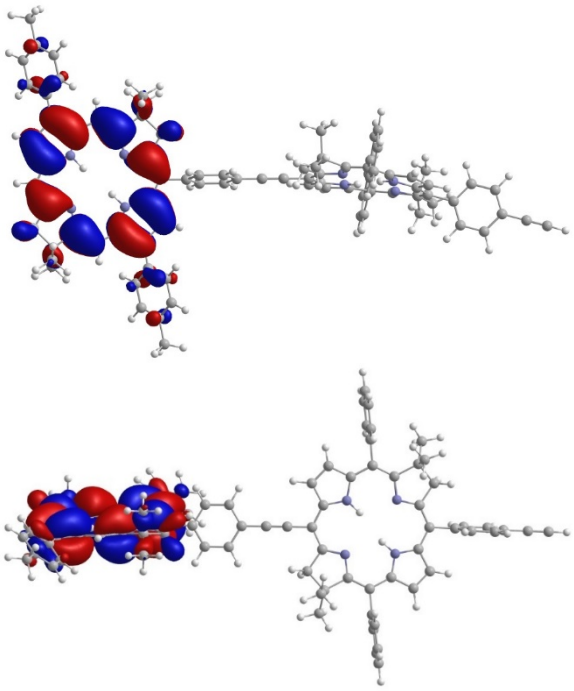
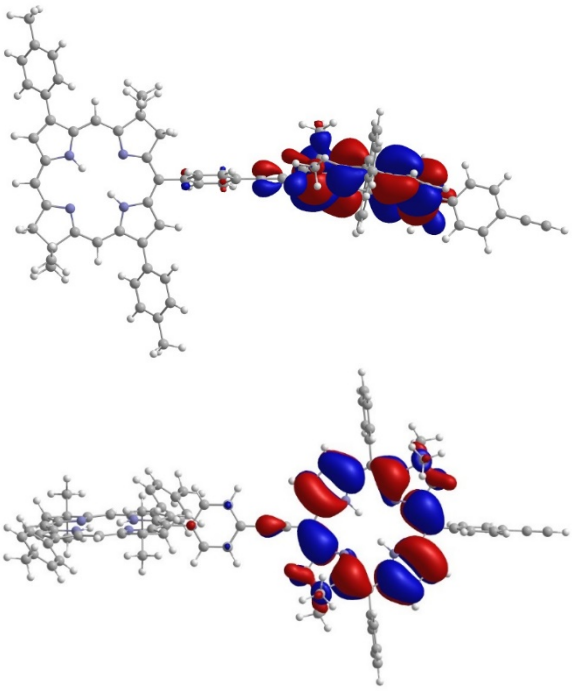
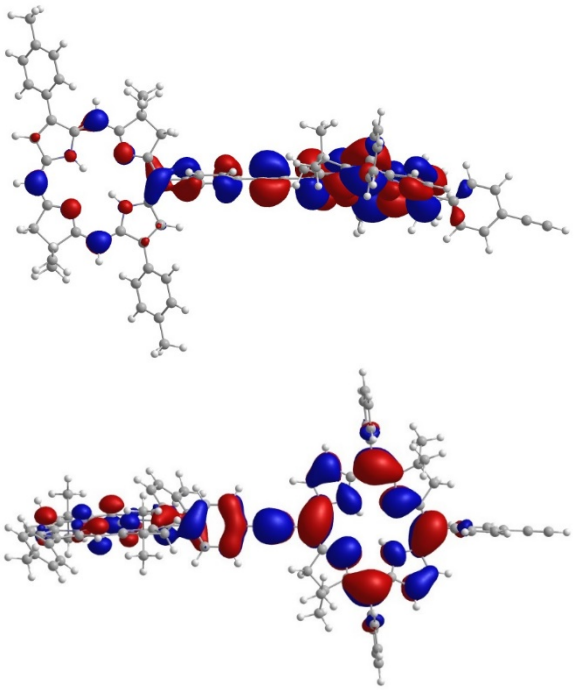
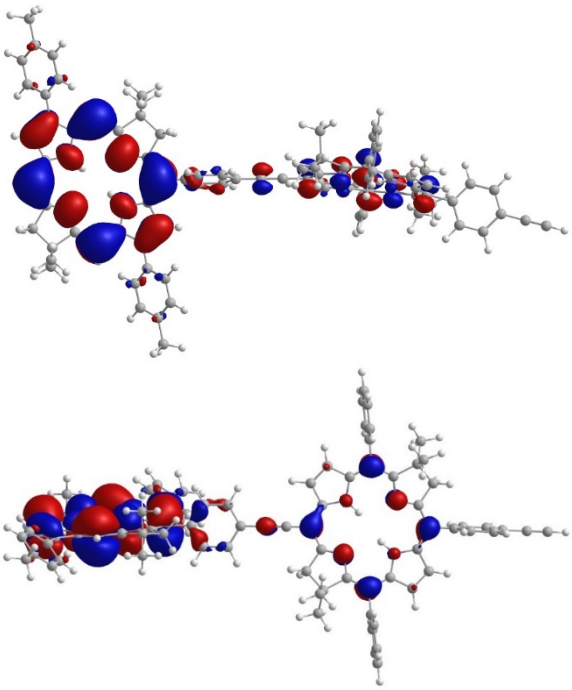
Figure S9. Absorption spectra measured (red) and calculated by TDDFT (colored sticks and blue dashed lines using 10-nm Gaussian skirts) for **Dyad-9** in toluene. The $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transitions both have multiple pairs of occupied and virtual NTOs with relative weights indicated in parenthesis. The calculated wavelength and oscillator strength (in square brackets) for each transition are given at the bottom of each panel.

Table S3. MOs for **Dyad-1** in toluene.

	
LUMO+10 +1.15 eV	LUMO+11 +1.16 eV
	
LUMO+8 +1.07 eV	LUMO+9 +1.13 eV

	
LUMO+6 +1.00 eV	LUMO+7 +1.06 eV
	
LUMO+4 +0.47 eV	LUMO+5 +0.74 eV

	
LUMO+2 -0.09 eV	LUMO+3 +0.12 eV
	
LUMO -1.70 eV	LUMO+1 -1.46 eV

	
HOMO -6.07 eV	HOMO-1 -6.26 eV
	
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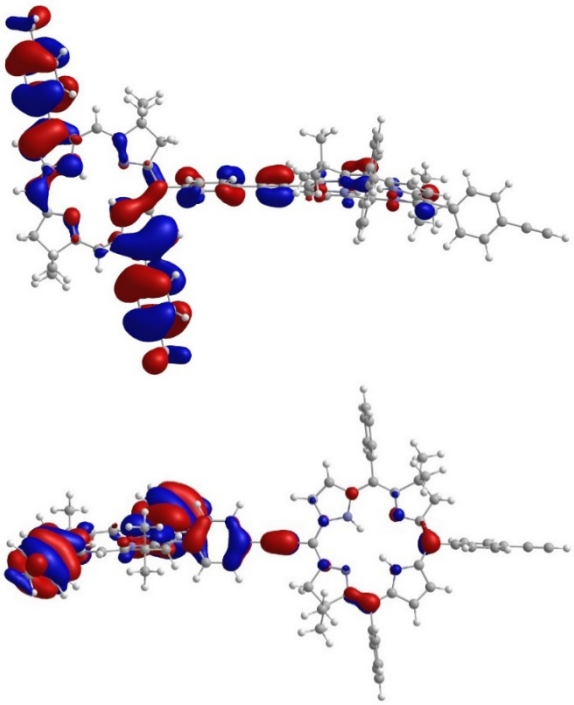
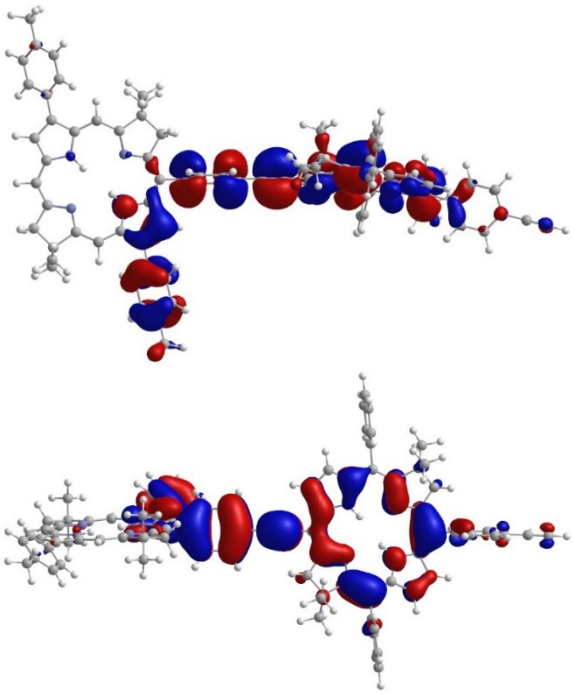
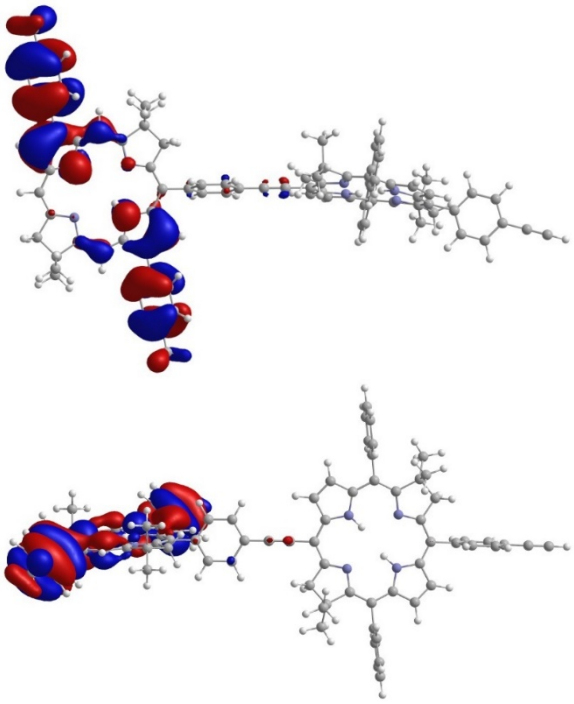
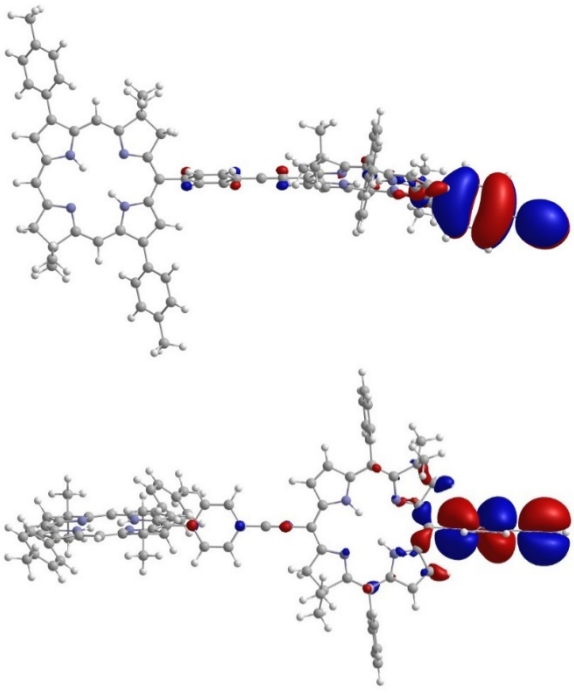
	
HOMO-4 -8.21 eV	HOMO-5 -8.25 eV
	
HOMO-6 -8.35 eV	HOMO-7 -8.57 eV

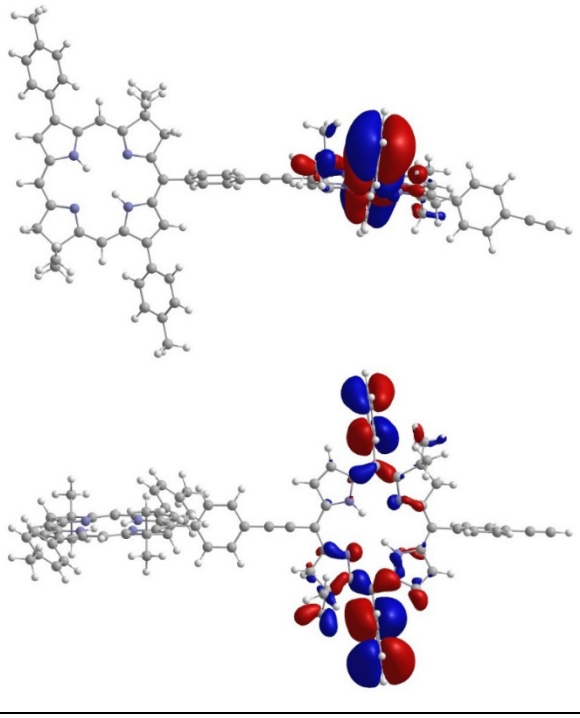
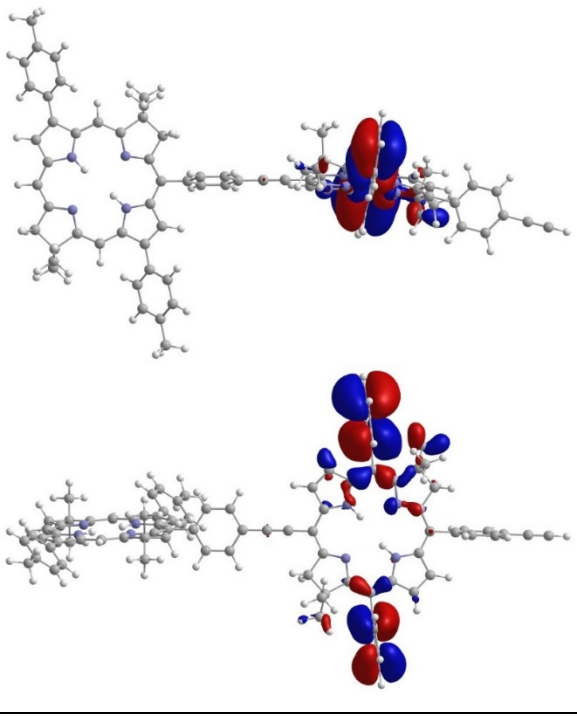
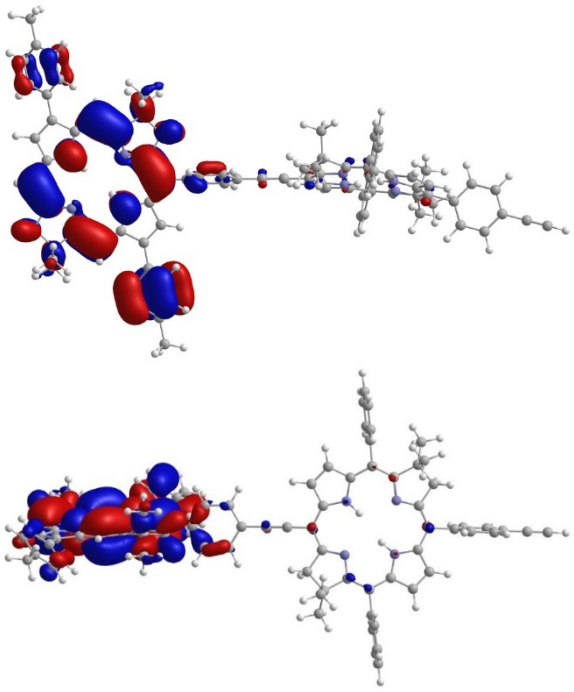
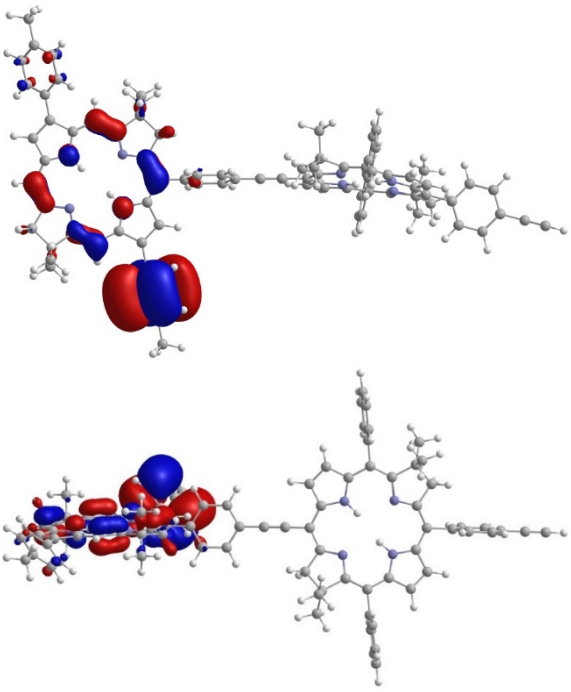
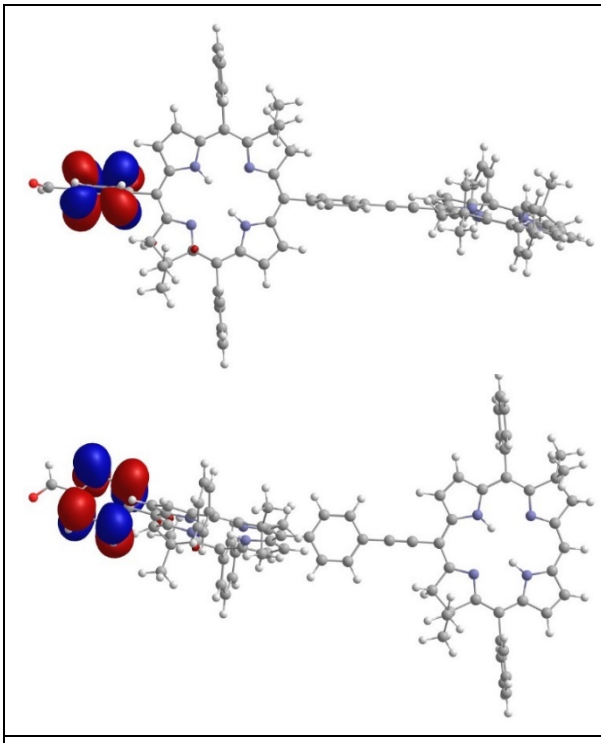
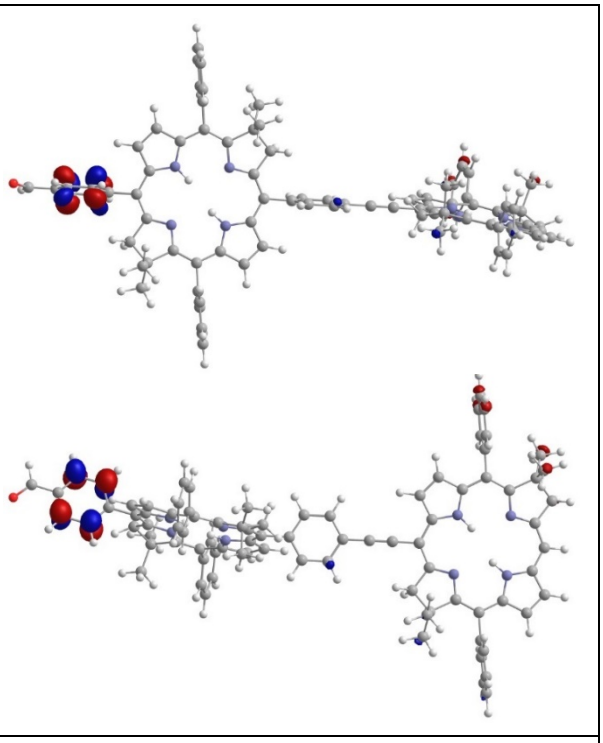
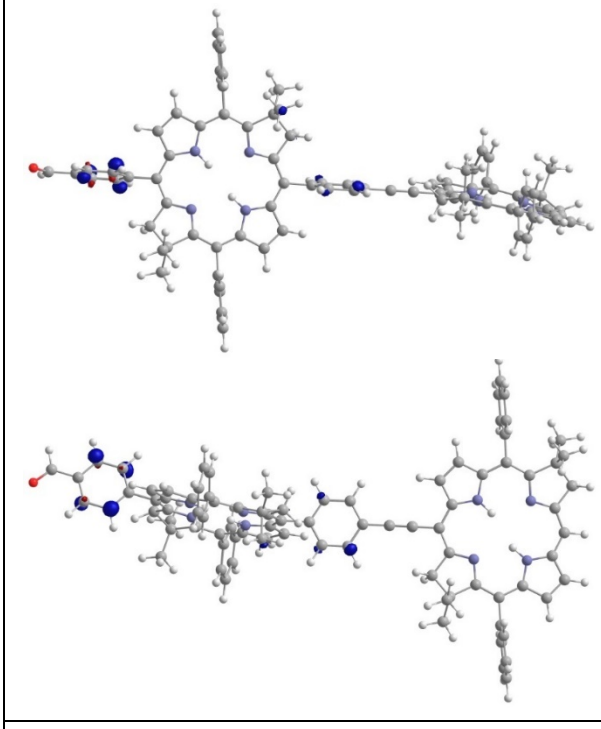
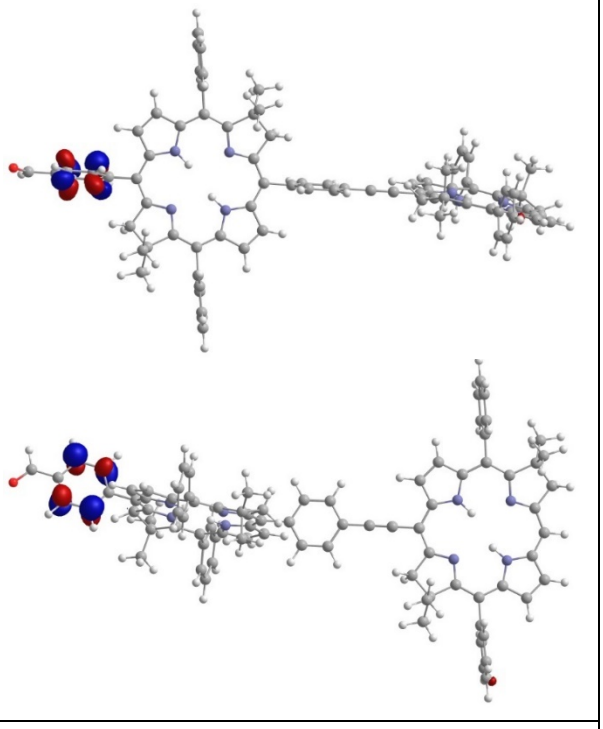
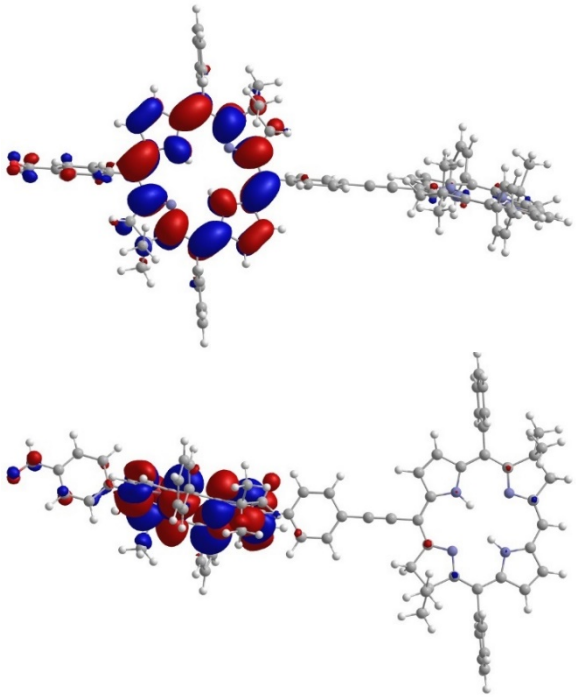
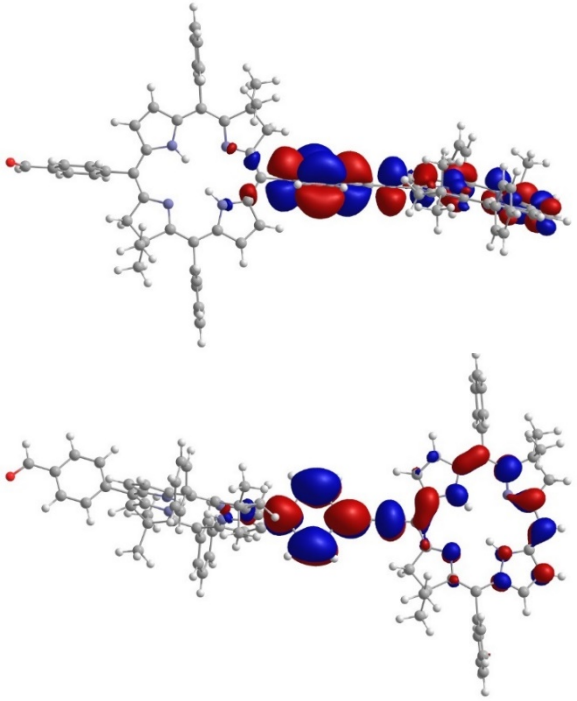
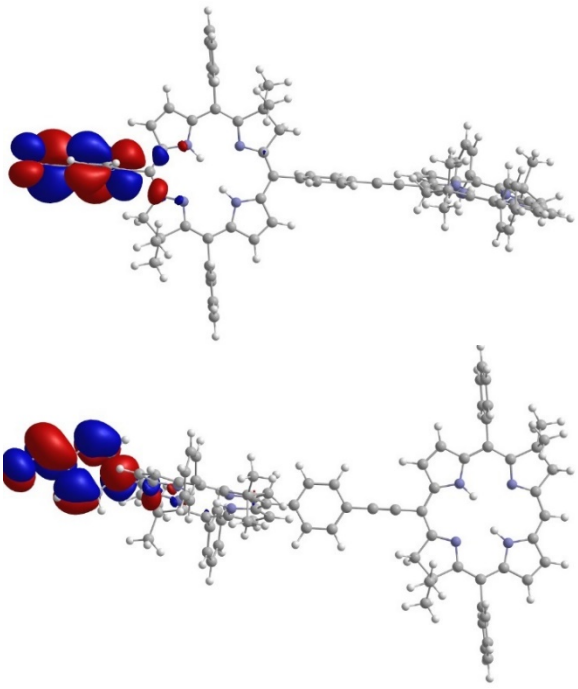
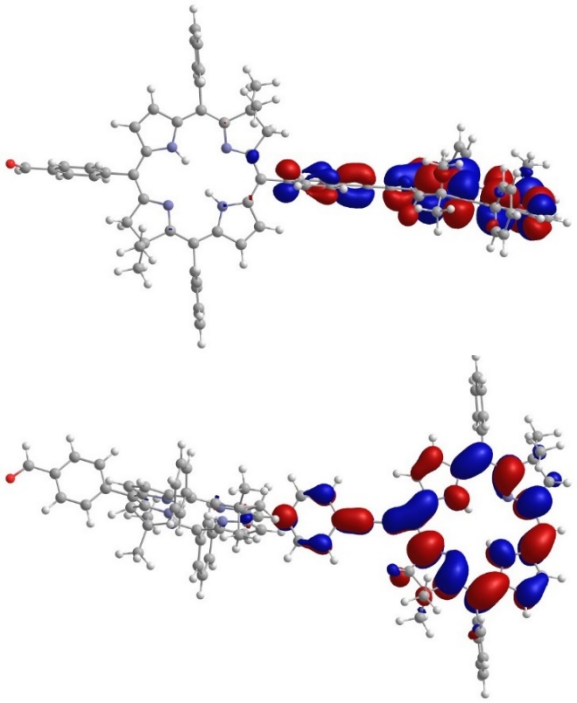
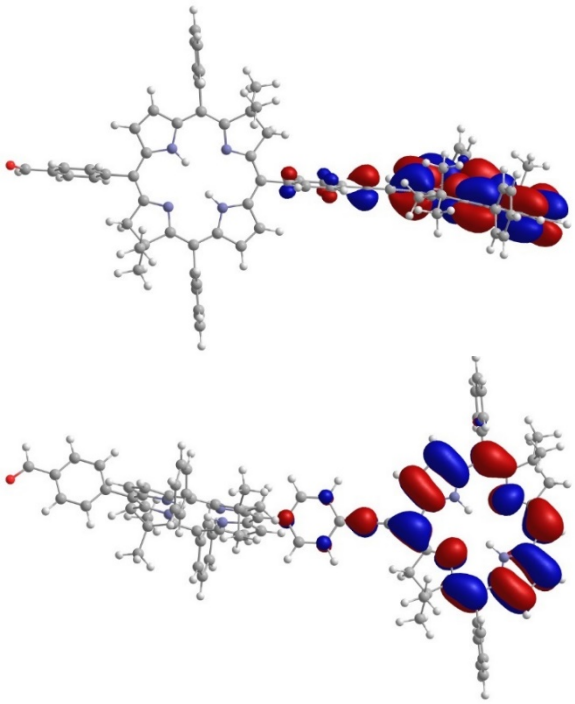
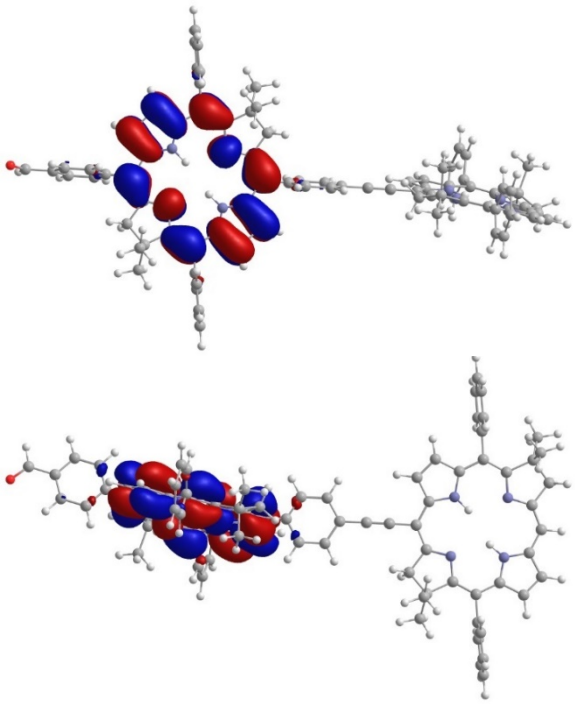
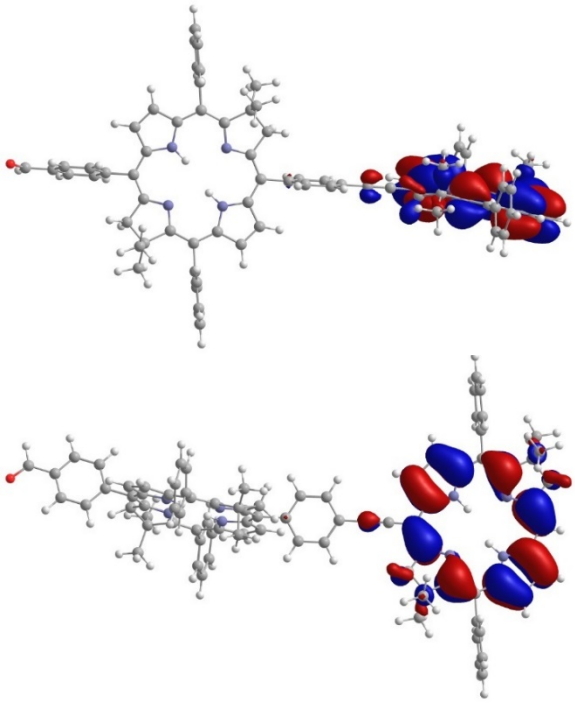
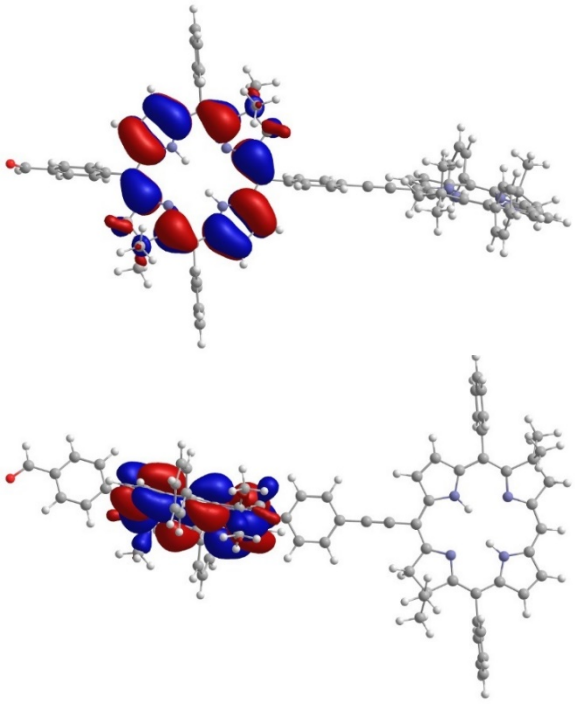
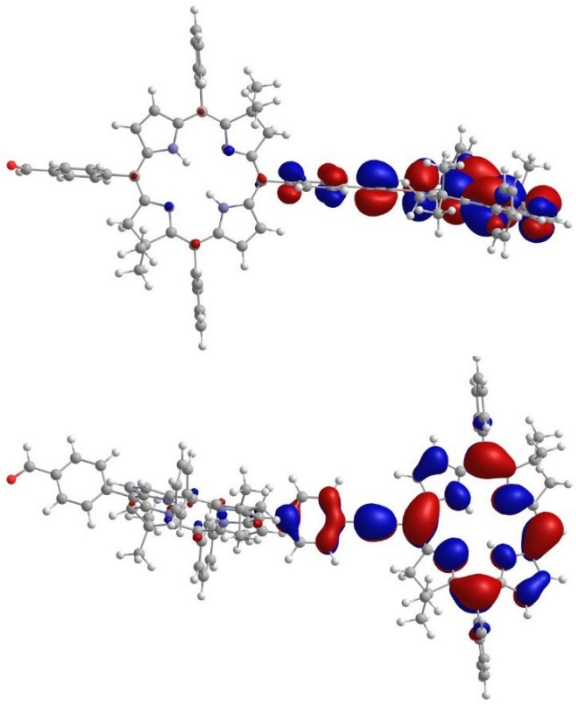
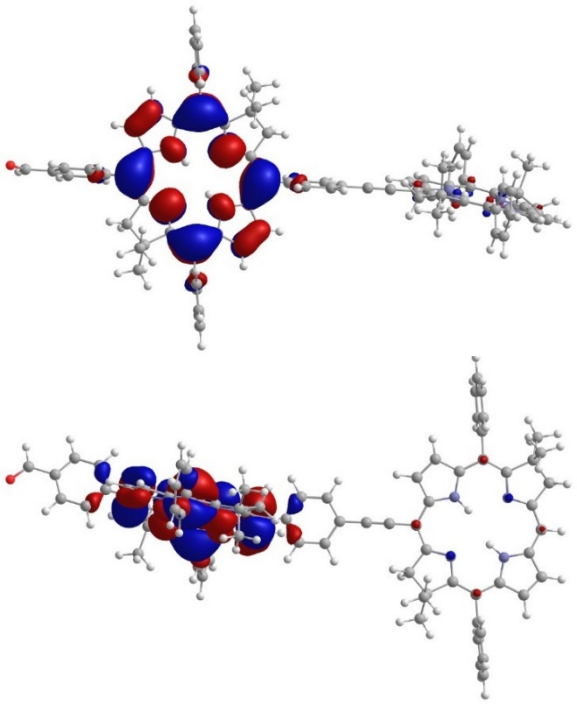
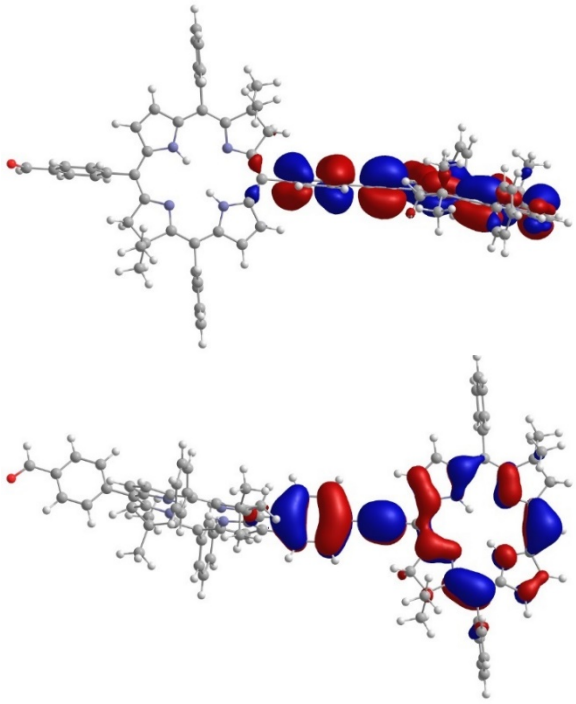
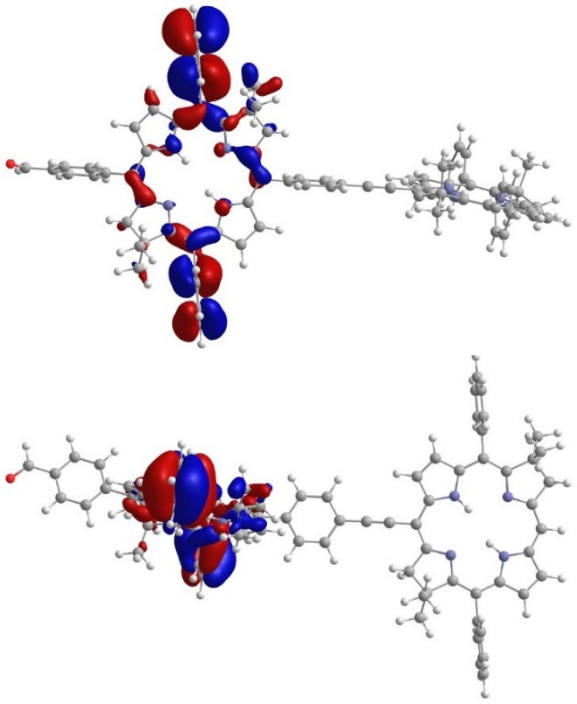
	
HOMO-8 -8.96 eV	HOMO-9 -8.99 eV
	
HOMO-10 -9.01 eV	HOMO-11 -9.04 eV

Table S4. MOs for **Dyad-2** in toluene.

	
LUMO+8 +1.10 eV	LUMO+9 +1.13 eV
	
LUMO+6 +0.99 eV	LUMO+7 +1.05 eV

	
LUMO+4 +0.02 eV	LUMO+5 +0.72 eV
	
LUMO+2 -0.28 eV	LUMO+3 -0.08 eV

	
LUMO -1.66 eV	LUMO+1 -1.56 eV
	
HOMO -6.24 eV	HOMO-1 -6.25 eV

	
HOMO-2 -6.72 eV	HOMO-3 -6.89 eV
	
HOMO-4 -8.27 eV	HOMO-5 -8.95 eV

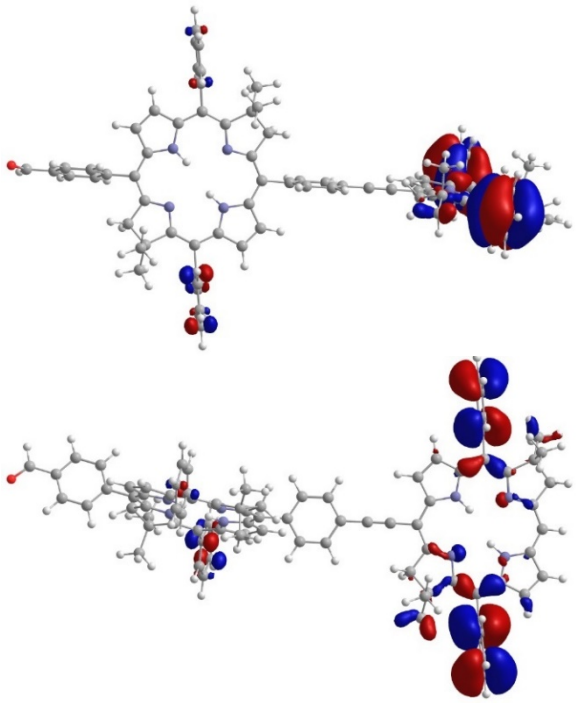
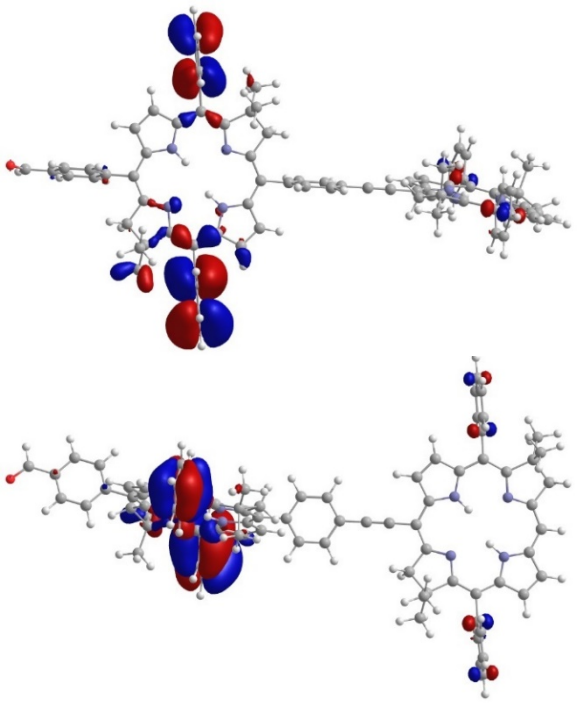
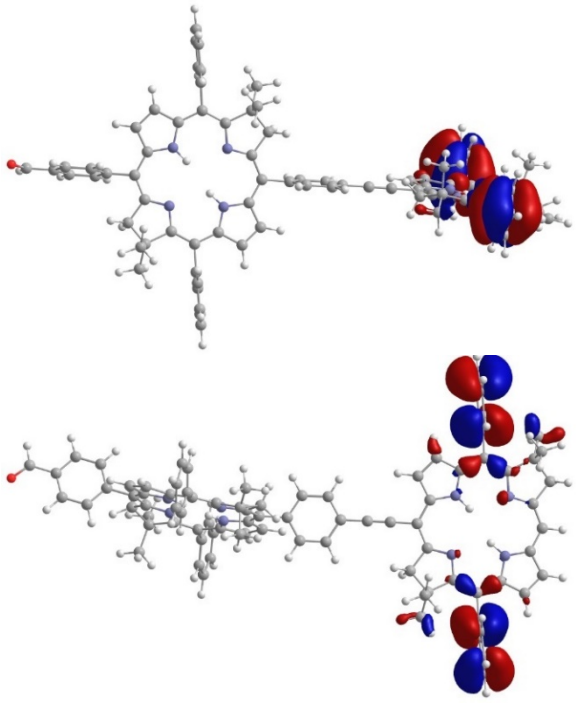
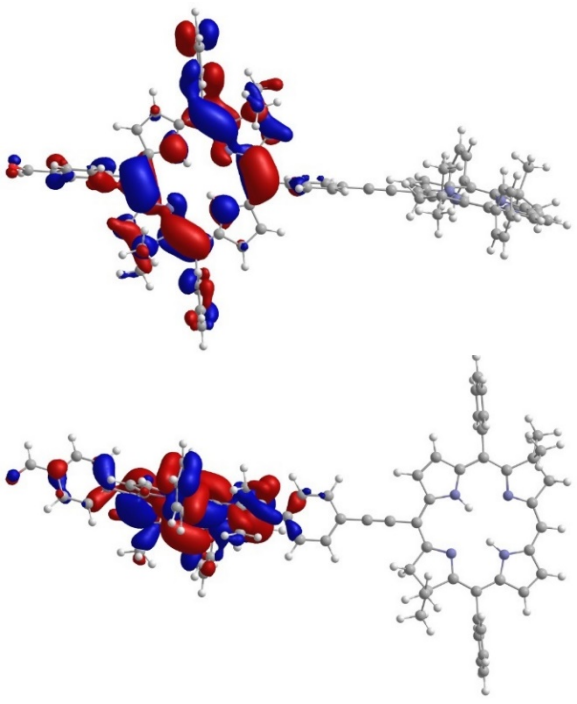
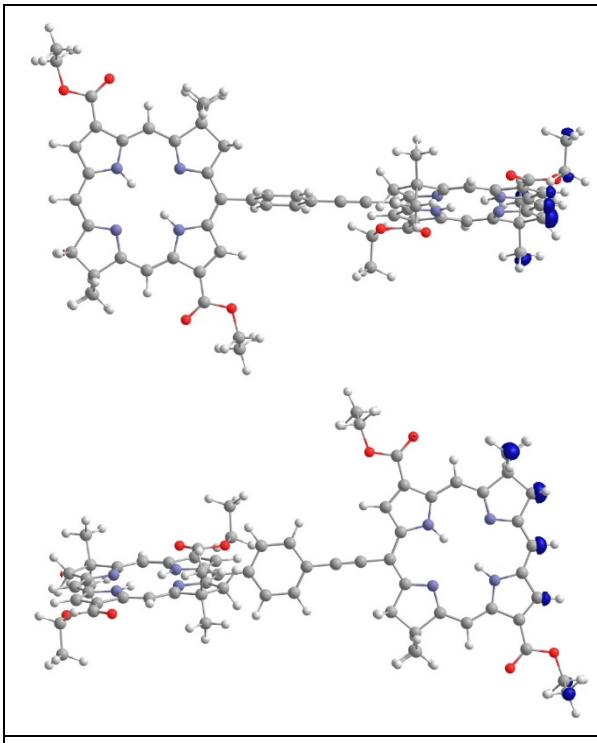
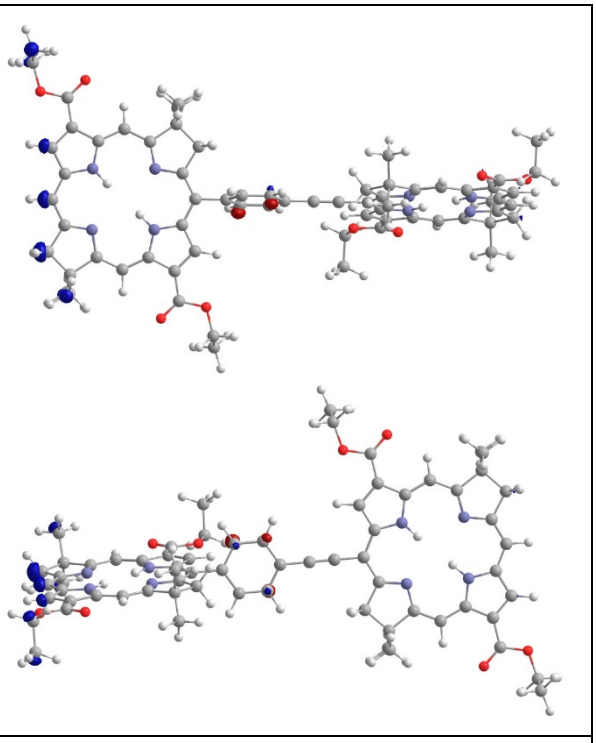
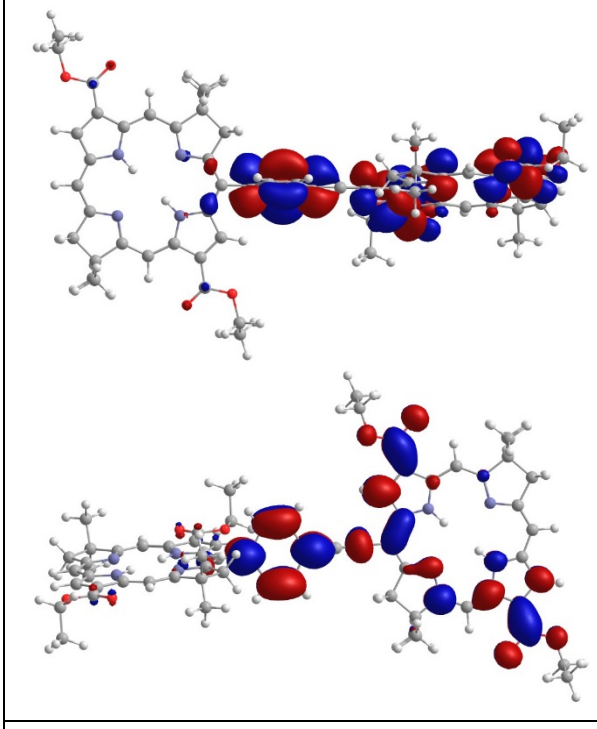
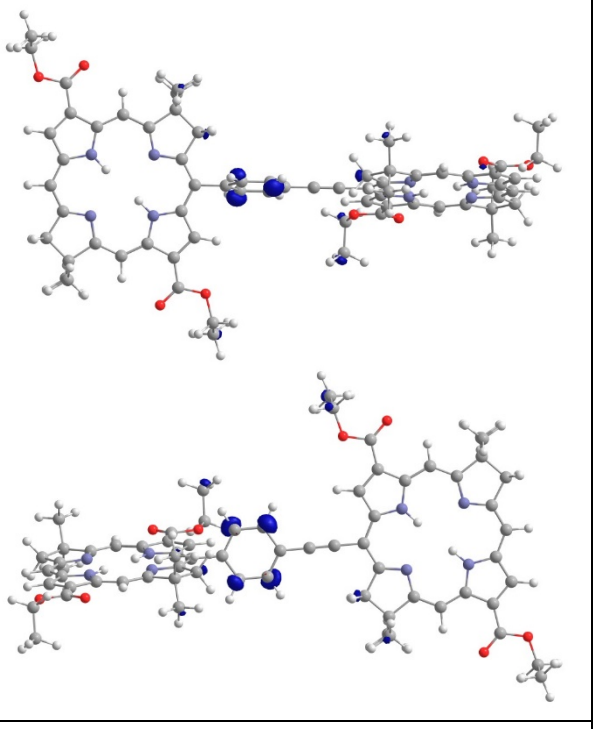
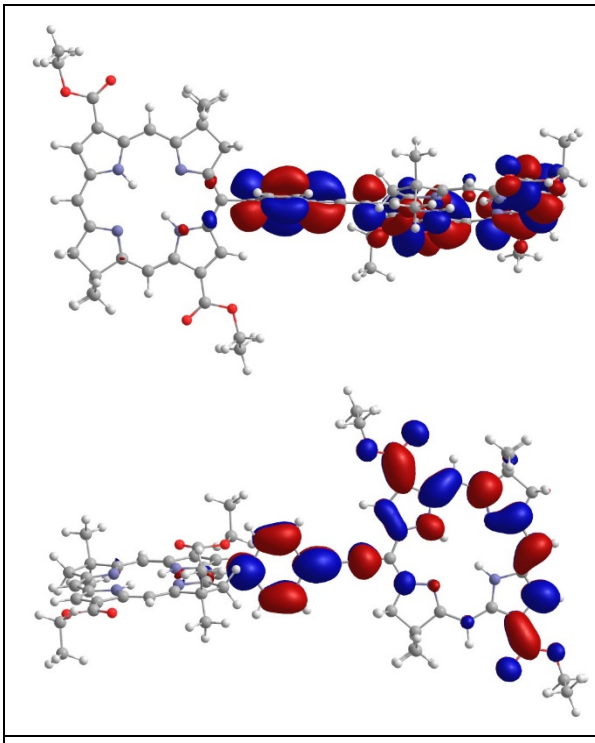
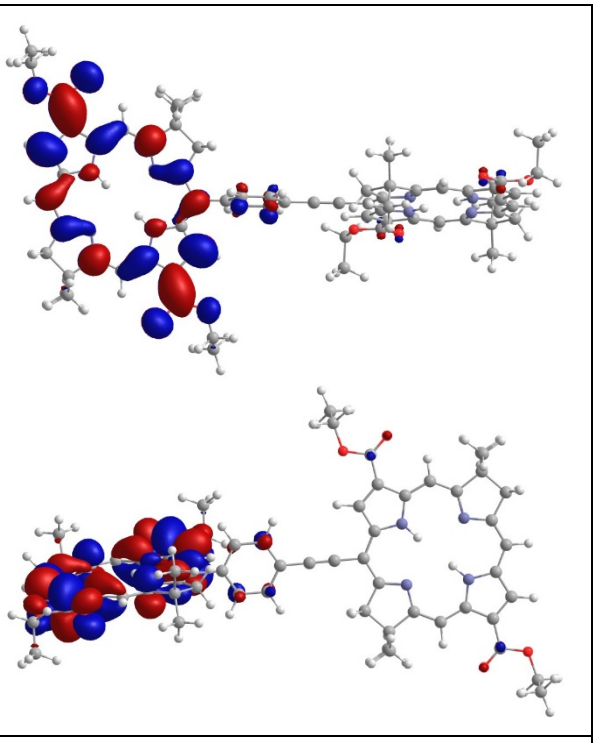
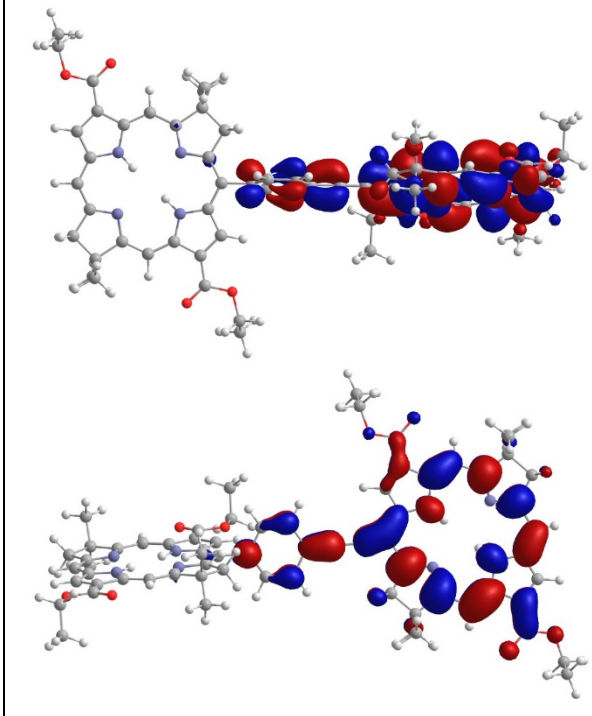
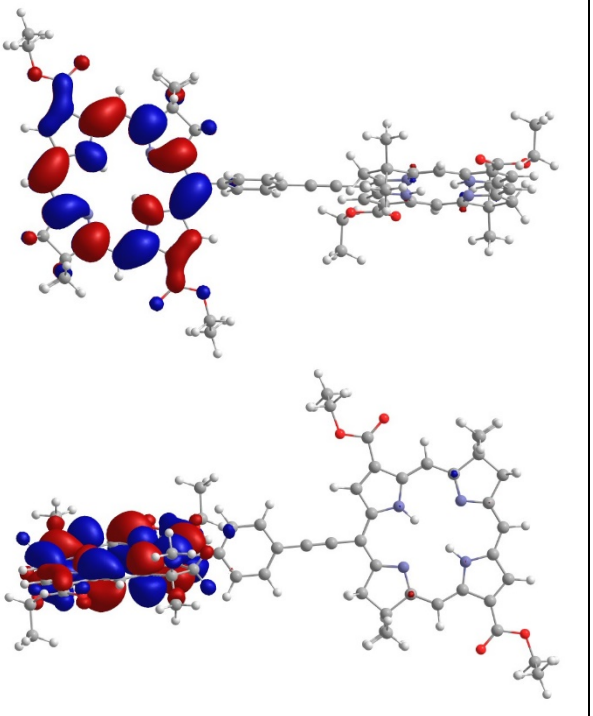
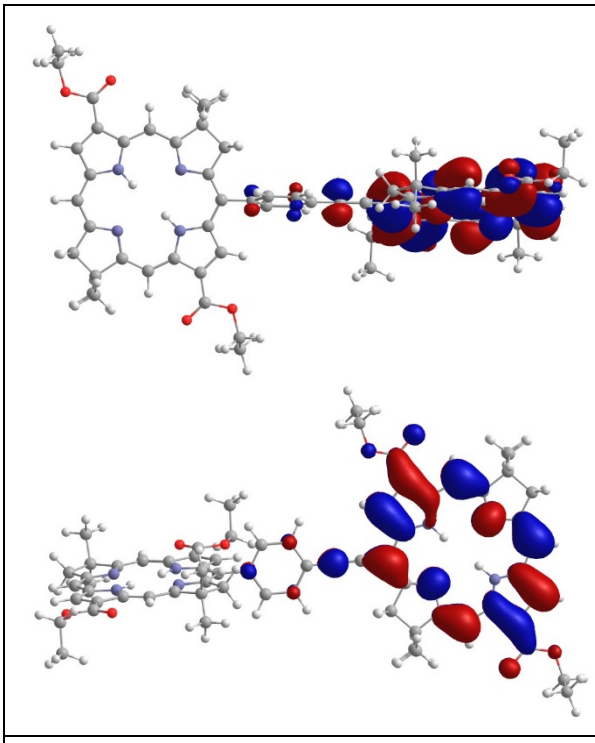
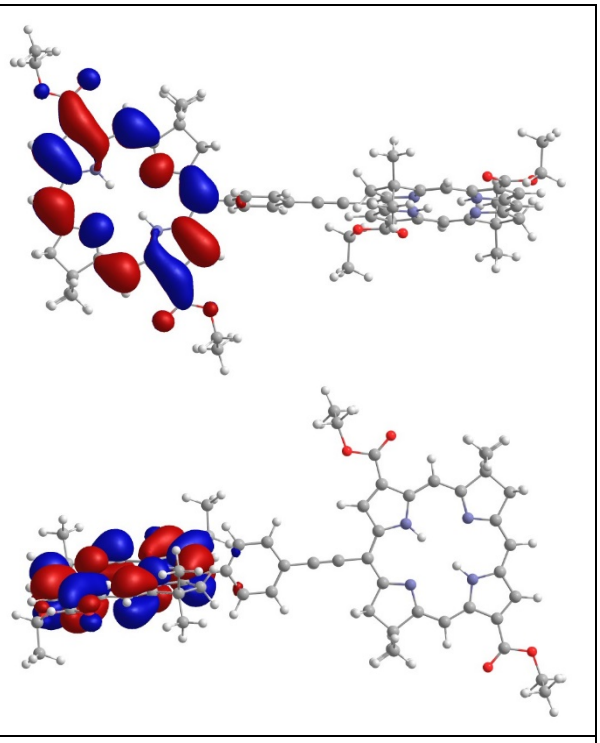
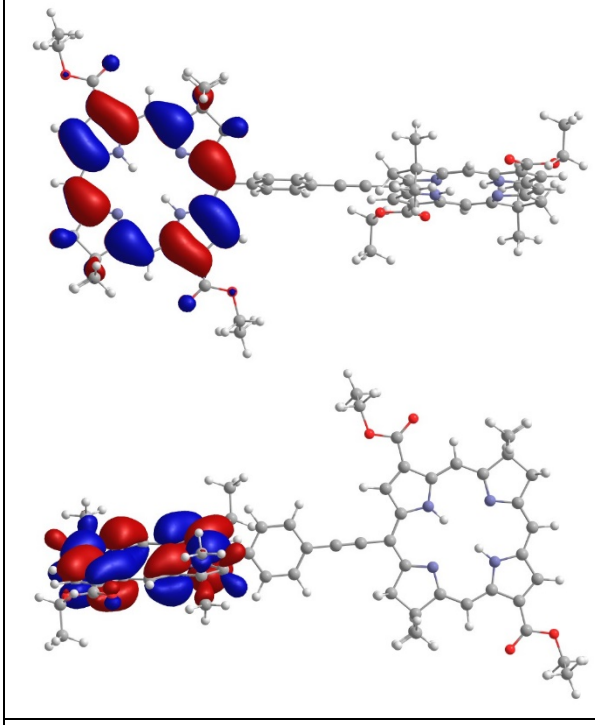
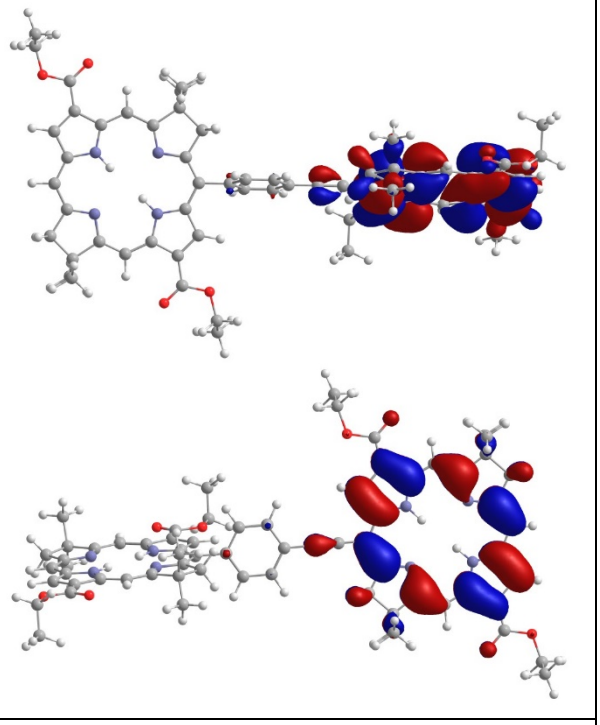
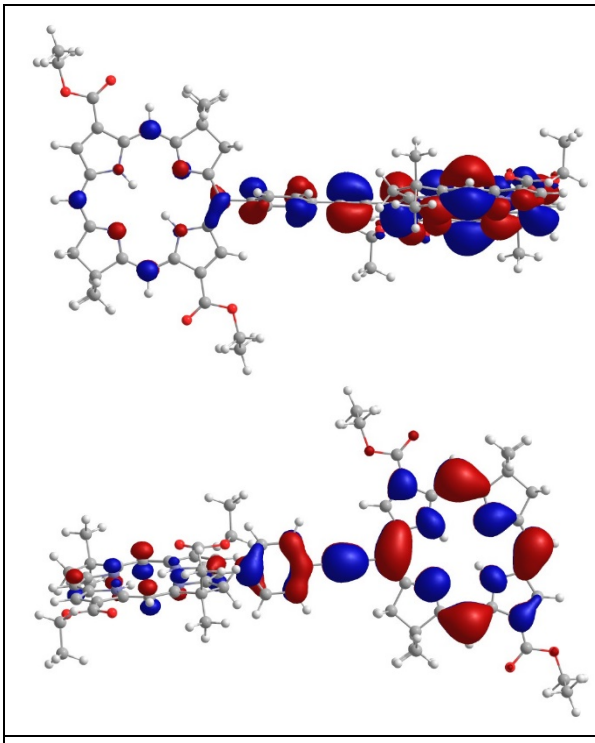
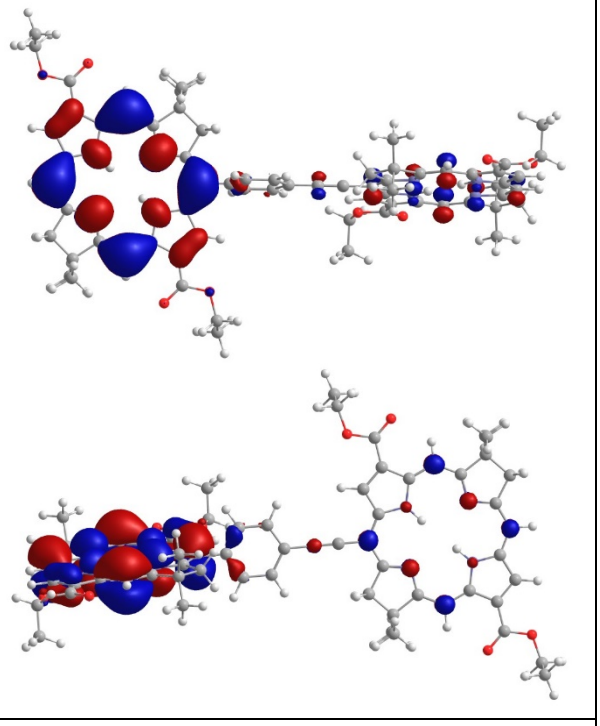
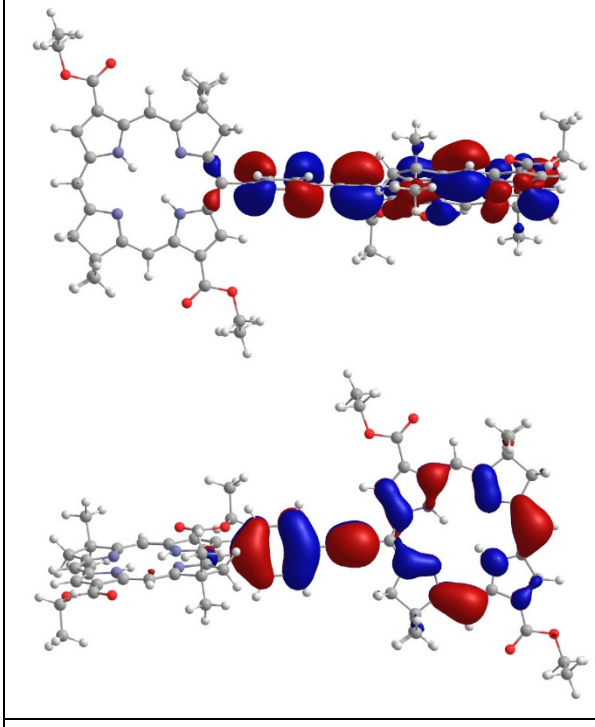
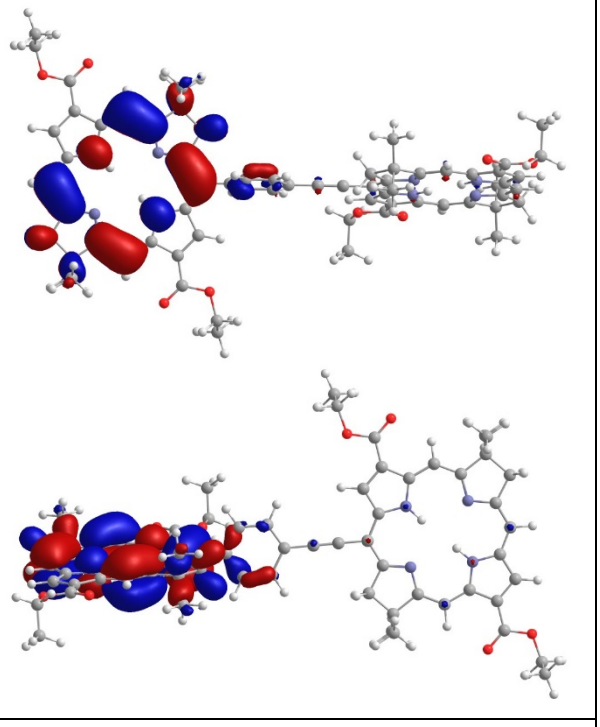
	
HOMO-6 -8.97 eV	HOMO-7 -8.98 eV
	
HOMO-8 -8.99 eV	HOMO-9 -9.01 eV

Table S5. MOs for **Dyad-3** in toluene.

	
LUMO+8 +1.10 eV	LUMO+9 +1.14 eV
	
LUMO+6 +0.83 eV	LUMO+7 +0.98 eV

	
LUMO+4 +0.52 eV	LUMO+5 +0.72 eV
	
LUMO+2 -0.30 eV	LUMO+3 -0.08 eV

	
LUMO -2.05 eV	LUMO+1 -1.89 eV
	
HOMO -6.40 eV	HOMO-1 -6.46 eV

	
HOMO-2 -6.91 eV	HOMO-3 -7.07 eV
	
HOMO-4 -8.43 eV	HOMO-5 -9.16 eV

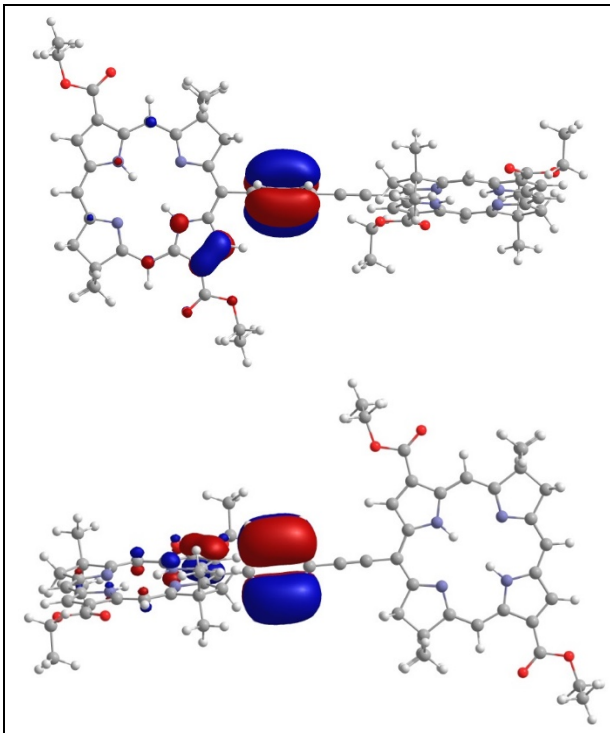
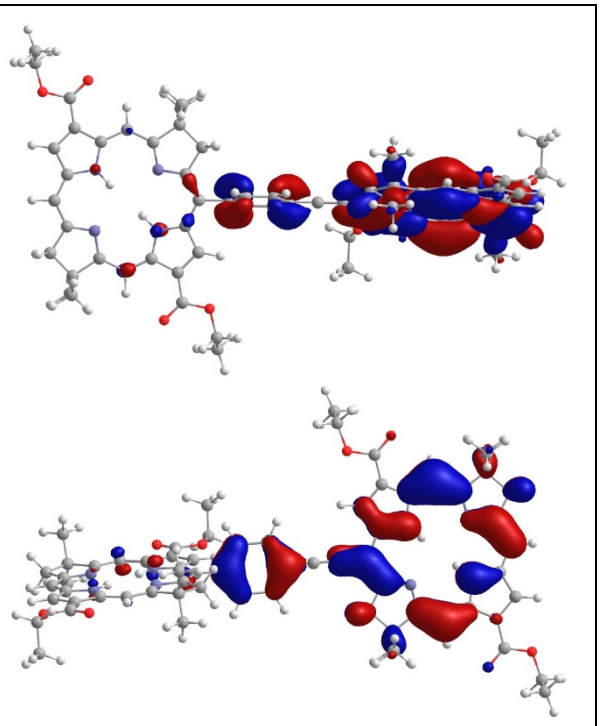
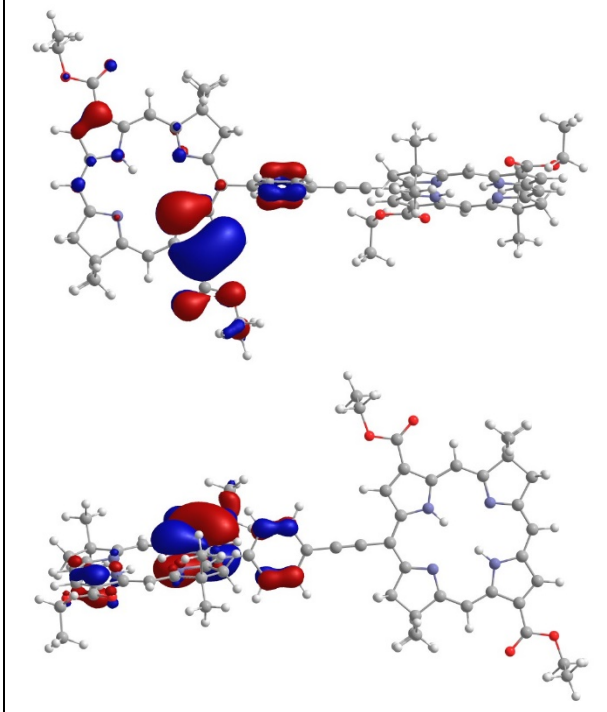
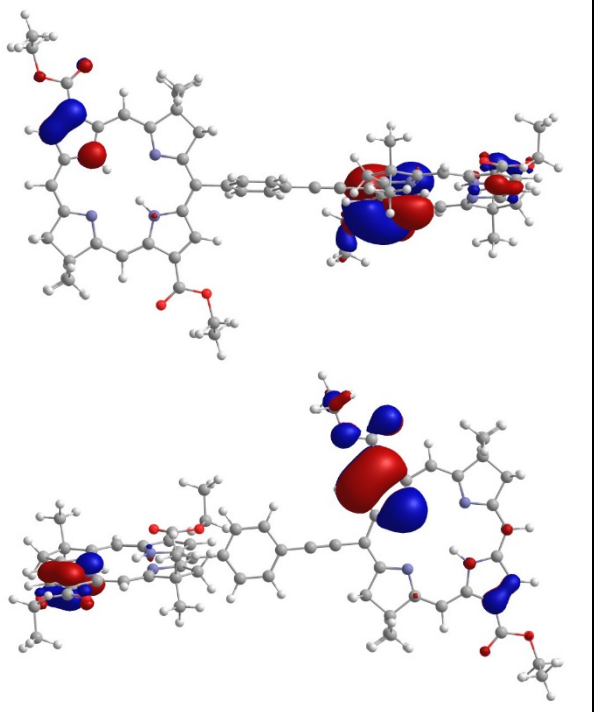
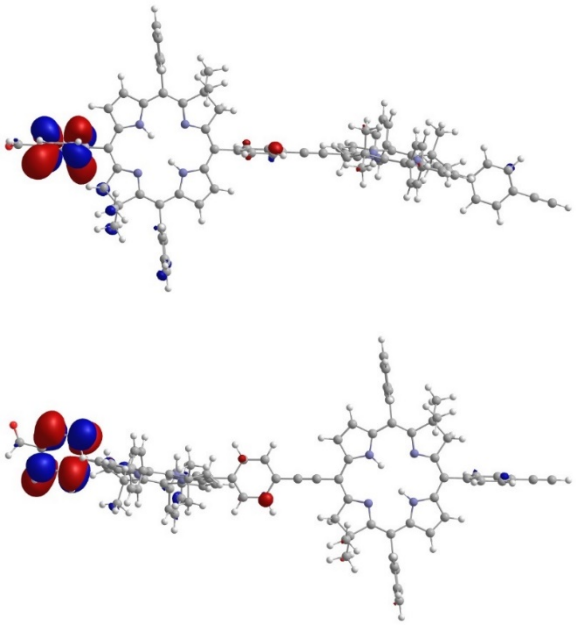
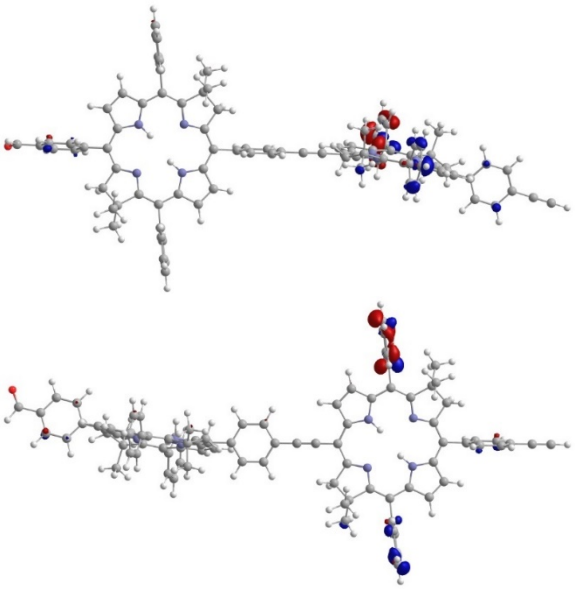
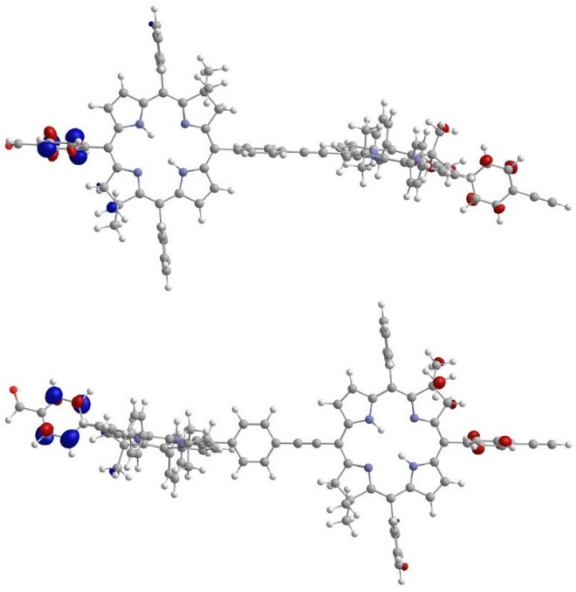
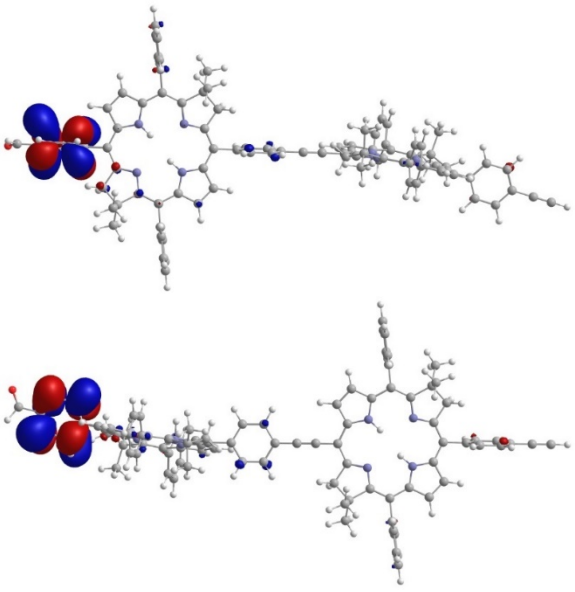
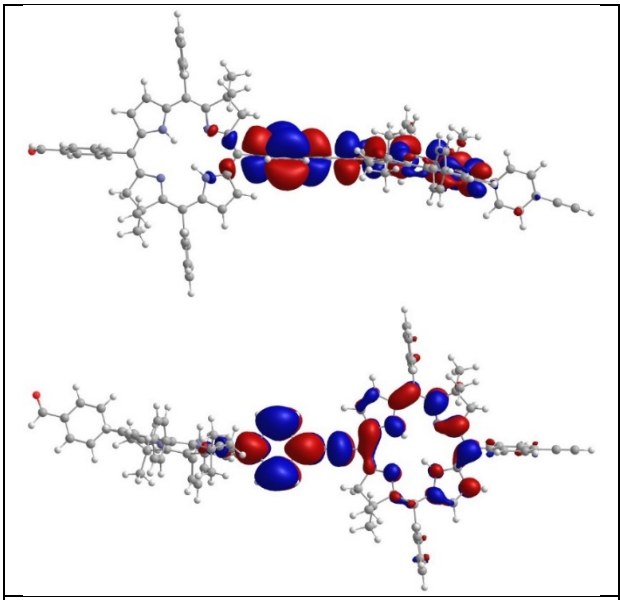
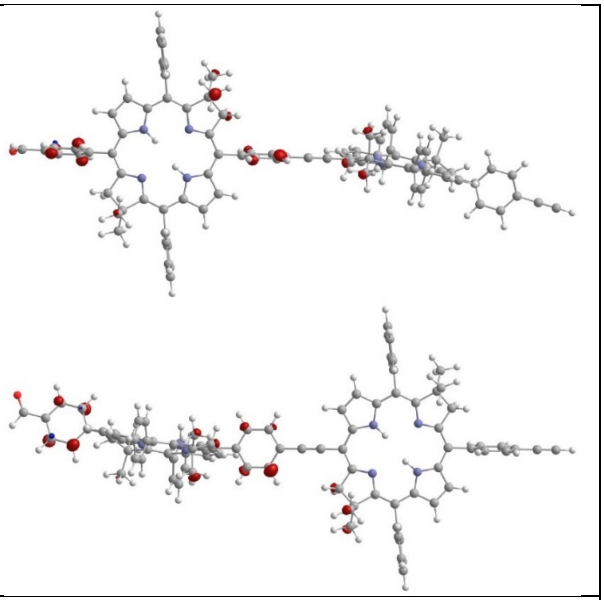
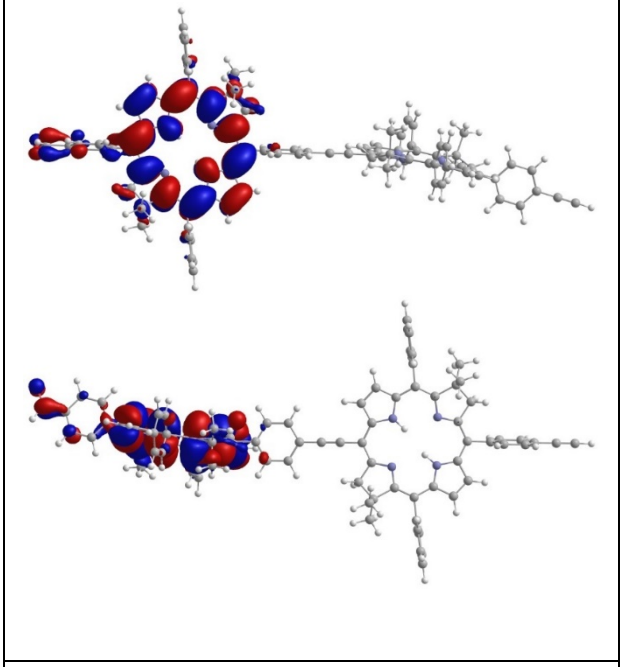
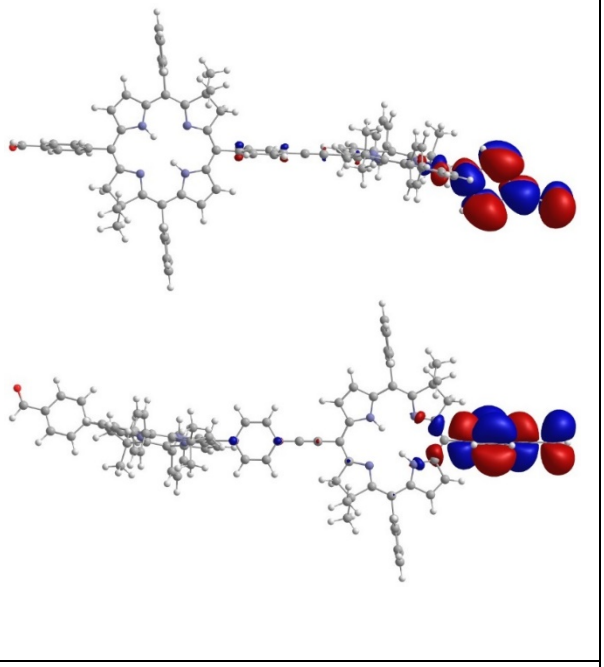
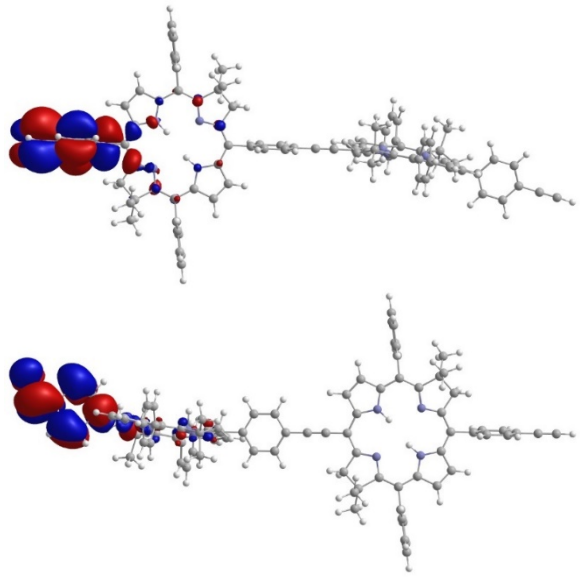
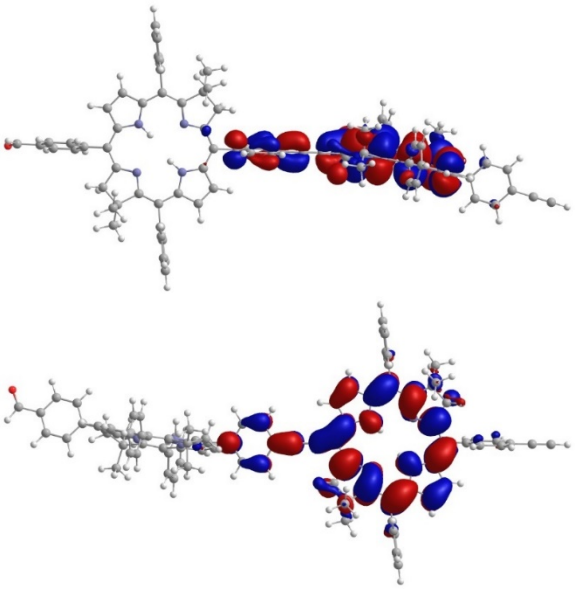
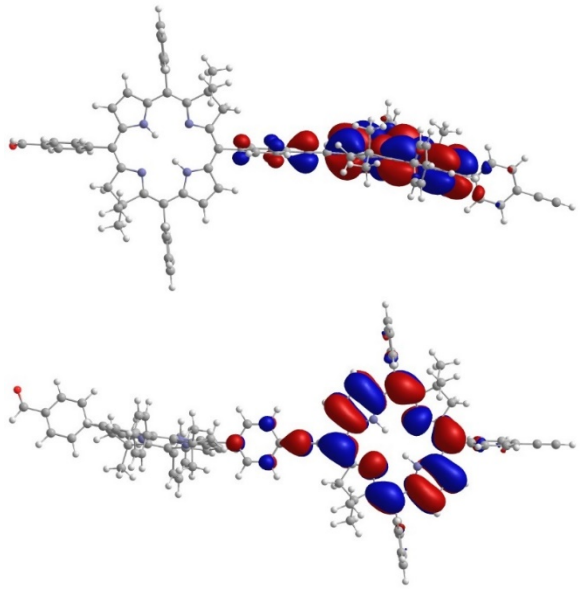
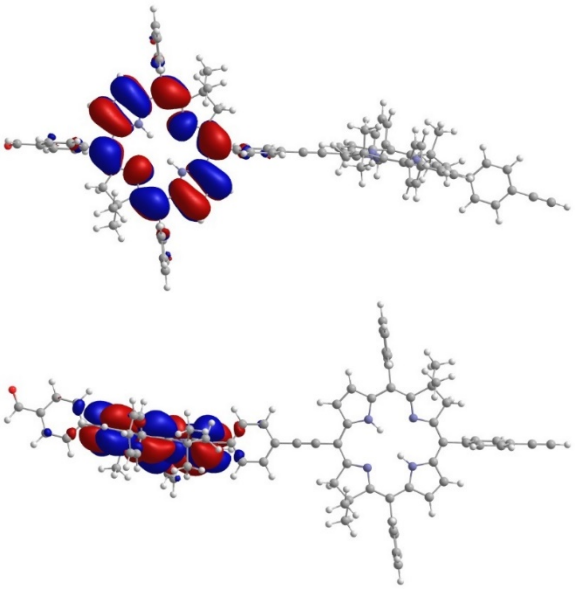
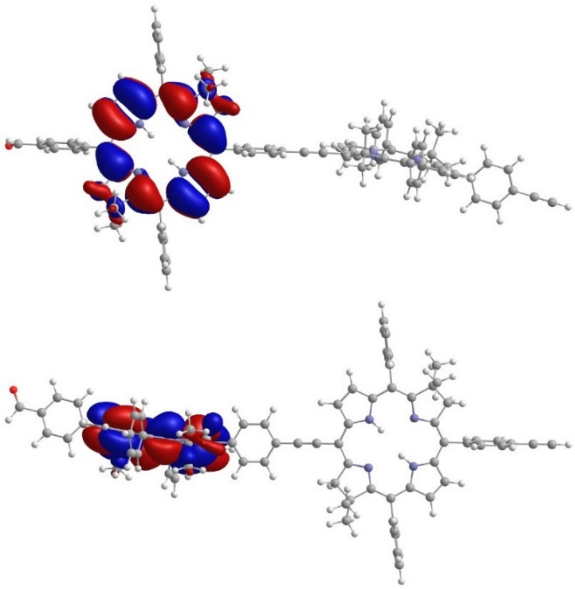
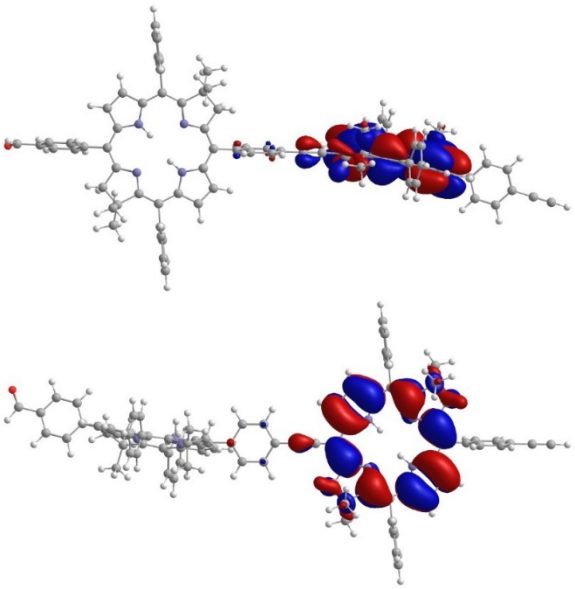
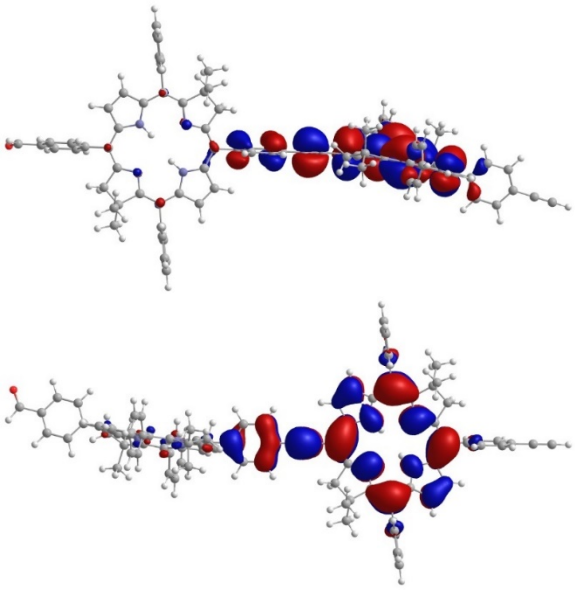
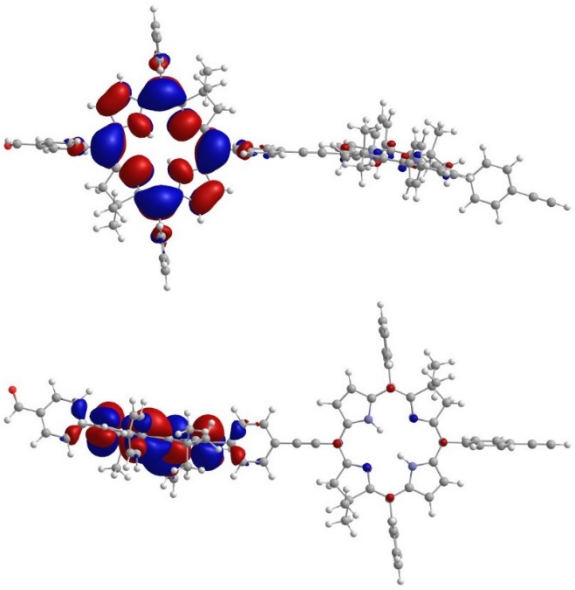
	
HOMO-6 -9.34 eV	HOMO-7 -9.44 eV
	
HOMO-8 -9.59 eV	HOMO-9 -9.55 eV

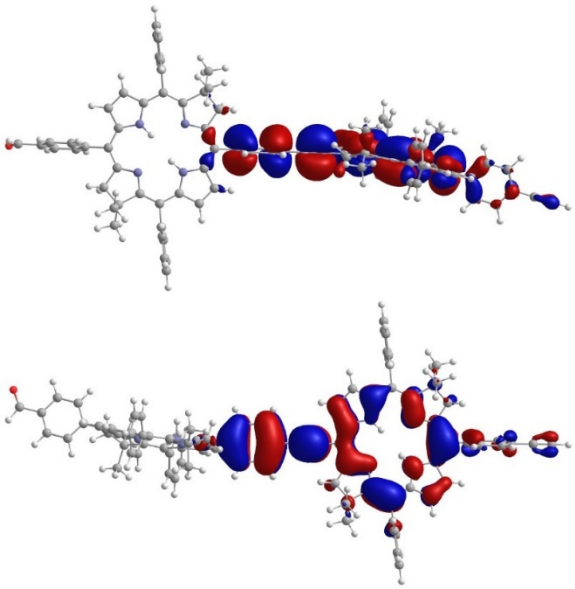
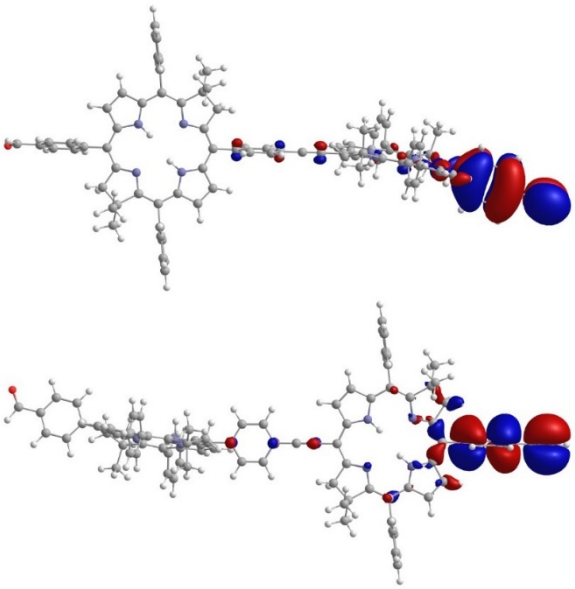
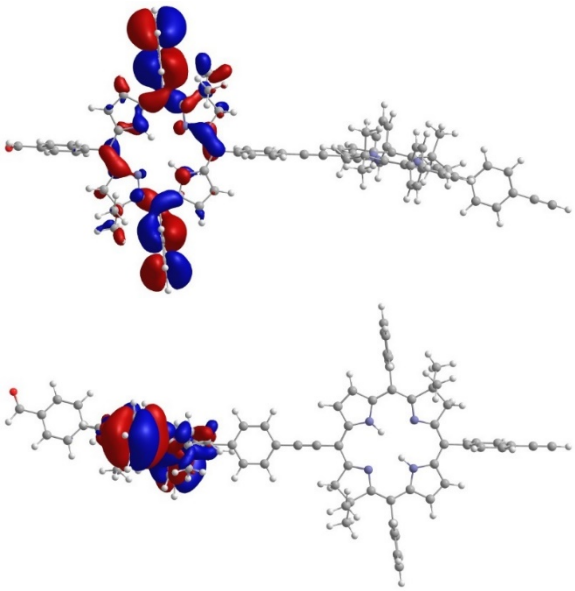
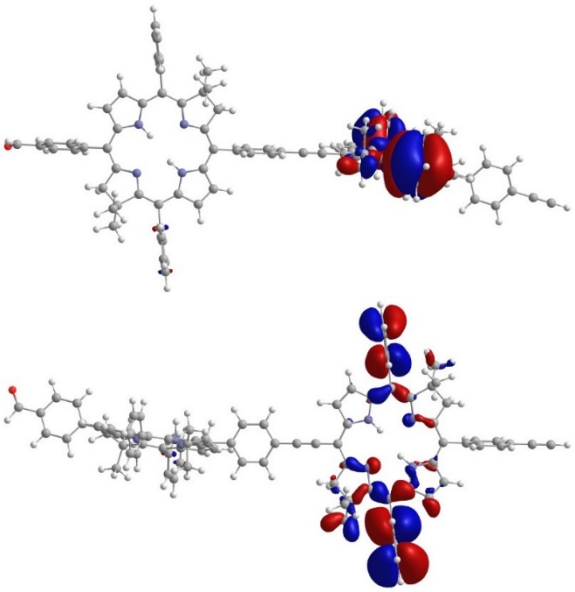
Table S6. MOs for **Dyad-4** in toluene.

	
LUMO+10 +1.11 eV	LUMO+11 +1.14 eV
	
LUMO+8 +1.03 eV	LUMO+9 +1.09 eV

	
LUMO+6 +0.70 eV	LUMO+7 +0.98 eV
	
LUMO+4 +0.02 eV	LUMO+5 +0.46 eV

	
LUMO+2 -0.29 eV	LUMO+3 -0.11 eV
	
LUMO -1.17 eV	LUMO+1 -1.57 eV

	
HOMO -6.26 eV	HOMO-1 -6.28 eV
	
HOMO-2 -6.73 eV	HOMO-3 -6.89 eV

	
HOMO-4 -8.27 eV	HOMO-5 -8.58 eV
	
HOMO-6 -8.96 eV	HOMO-7 -8.97 eV

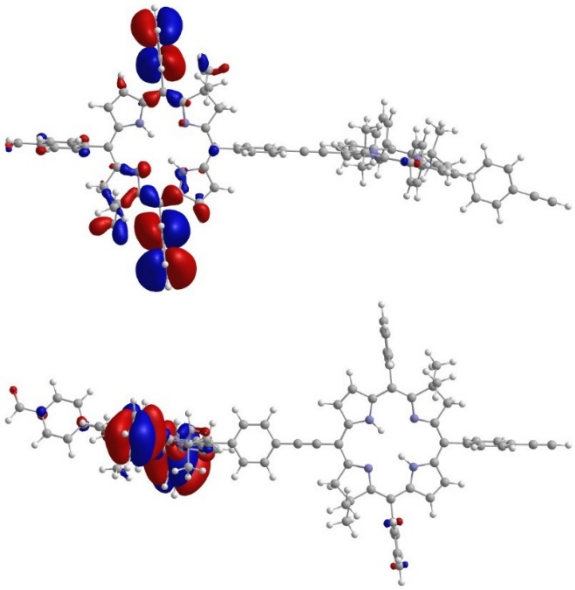
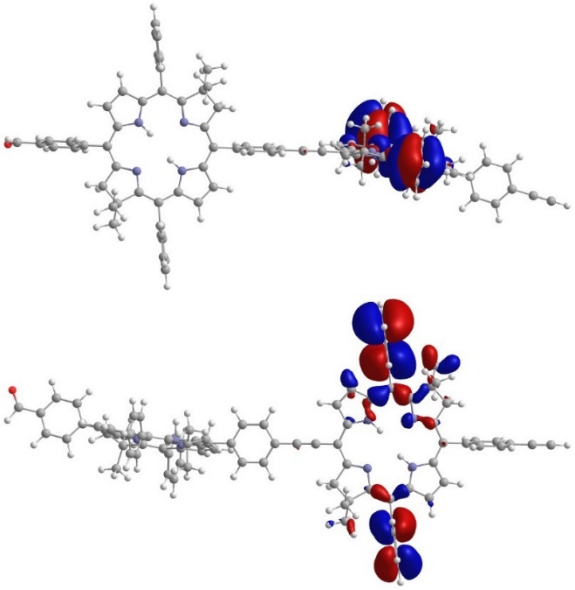
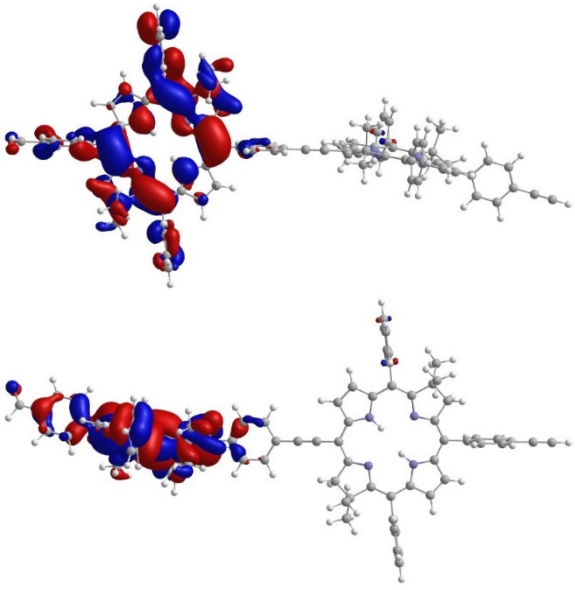
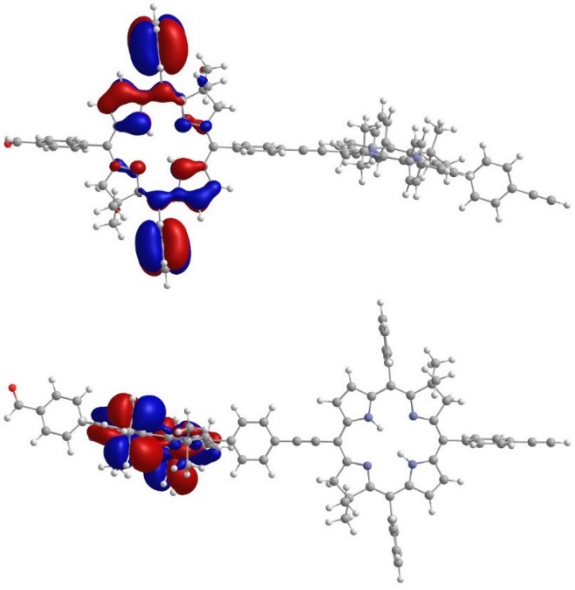
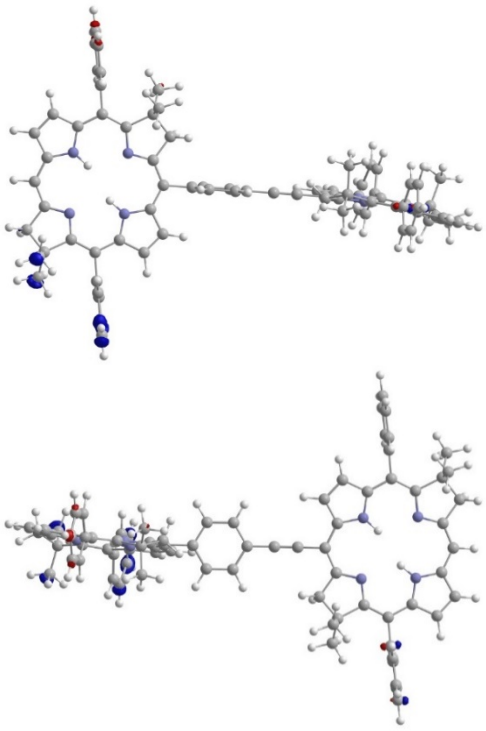
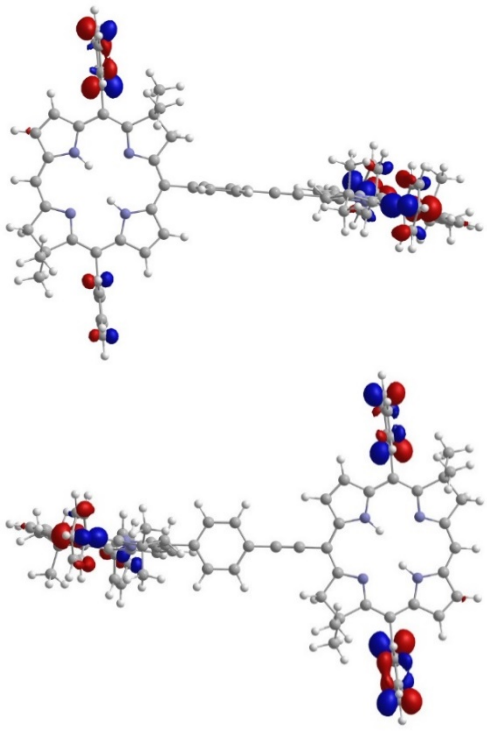
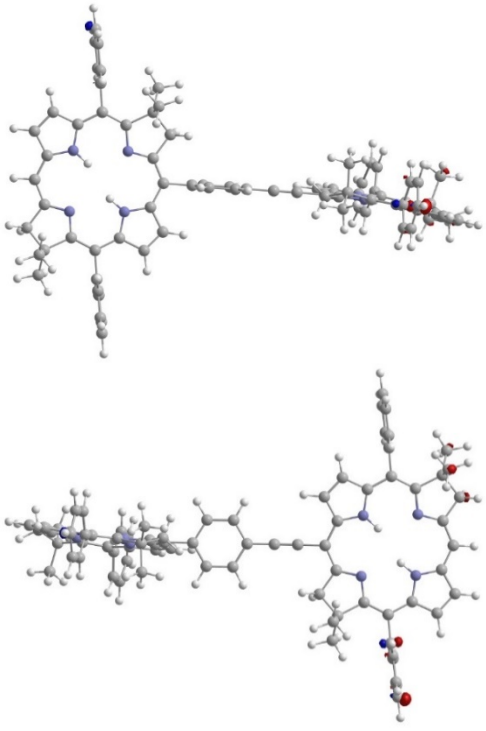
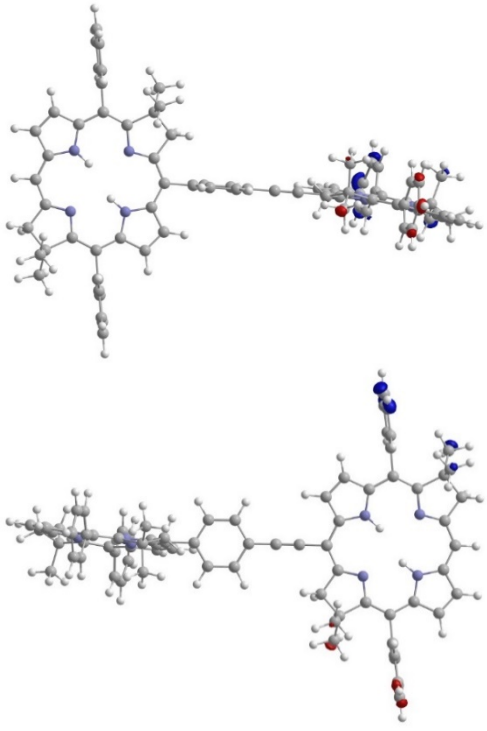
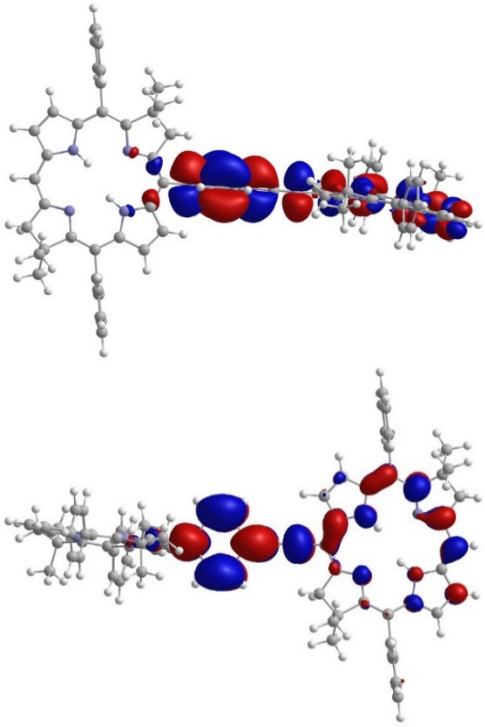
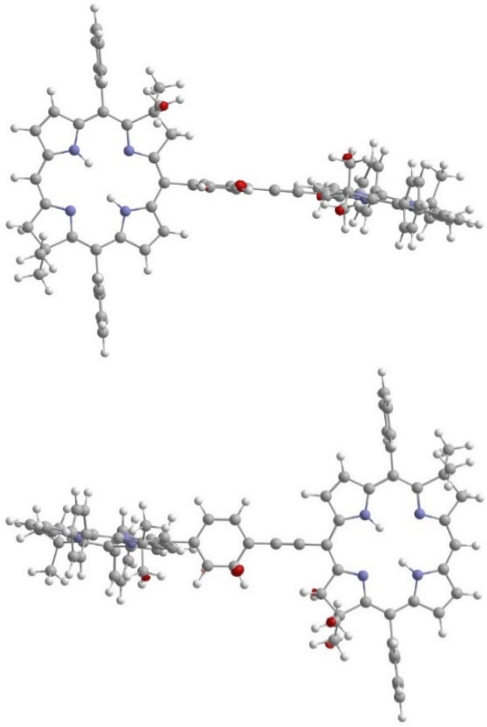
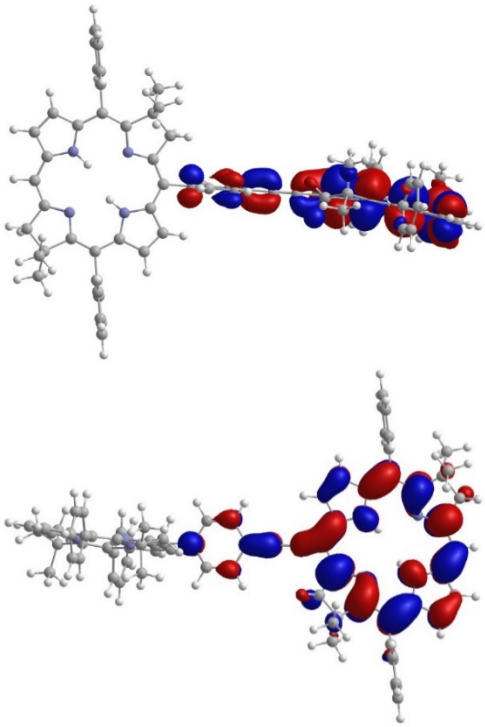
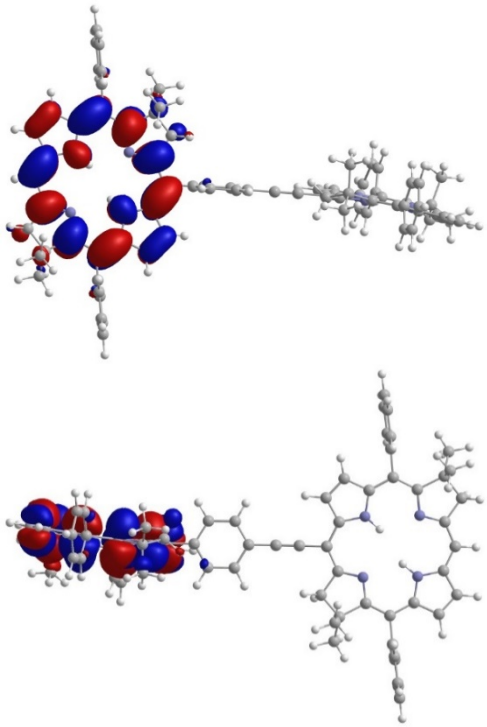
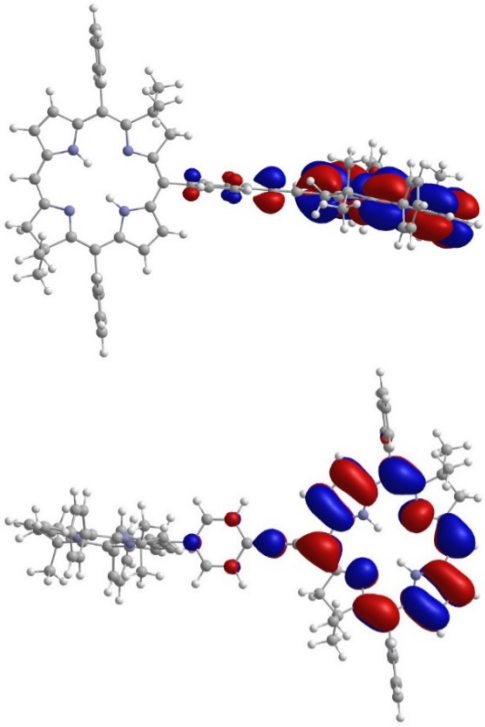
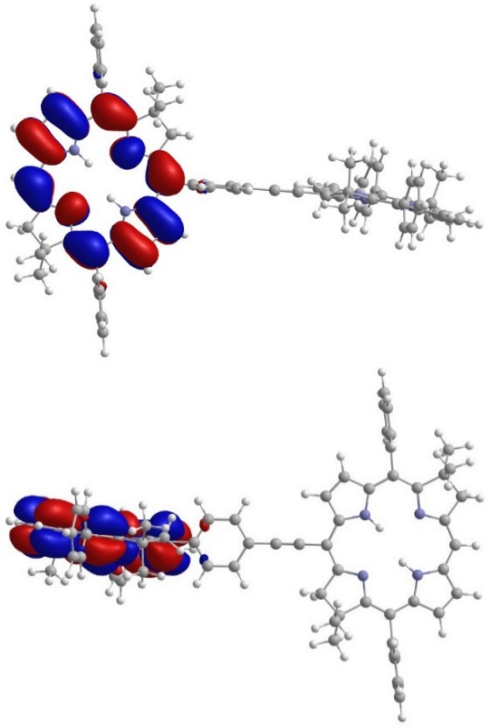
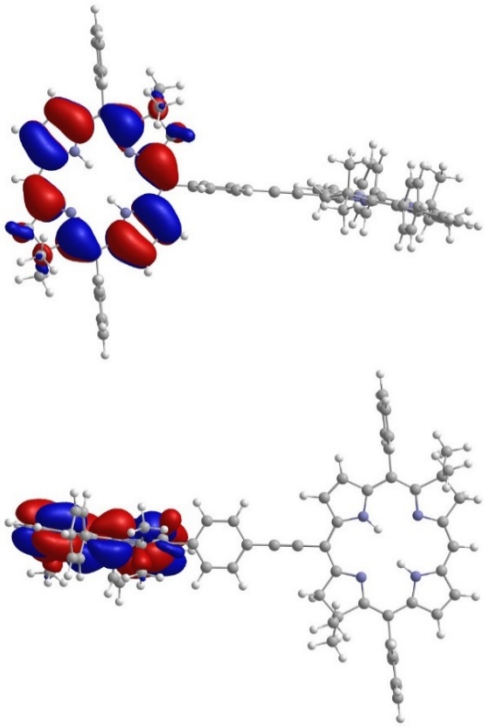
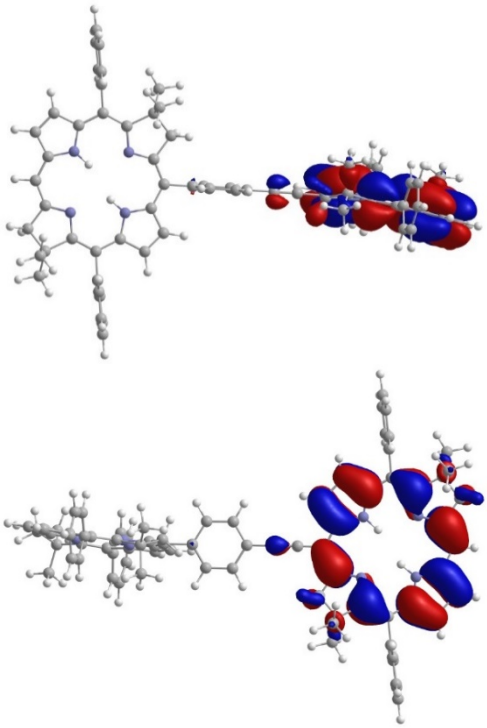
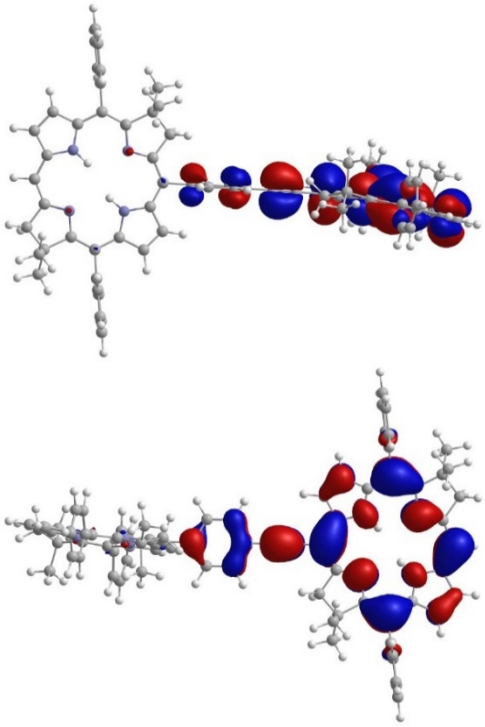
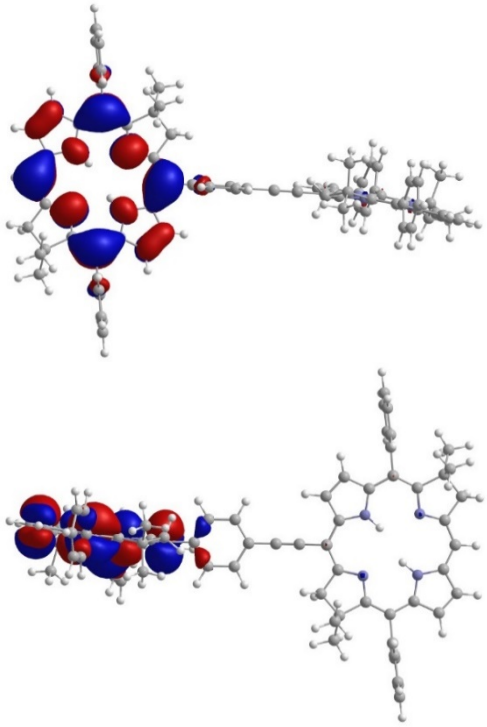
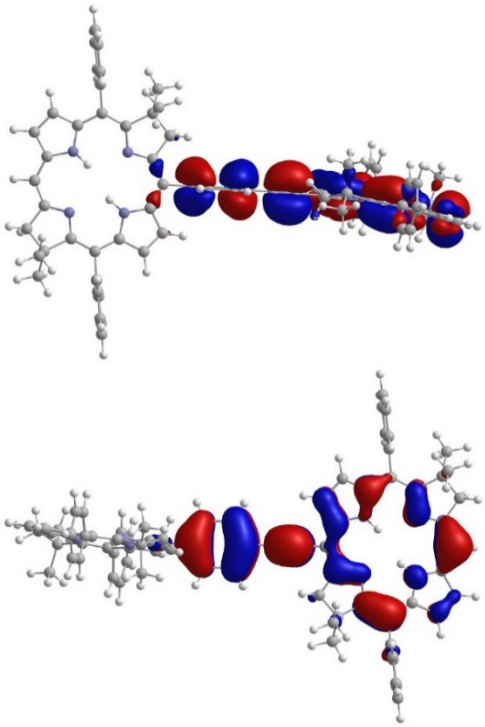
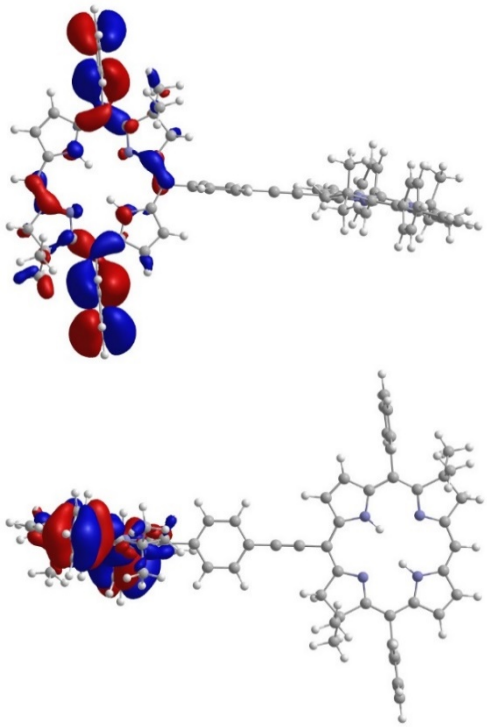
	
HOMO-8 -8.98 eV	HOMO-9 -9.00 eV
	
HOMO-10 -9.02 eV	HOMO-11 -9.09 eV

Table S7. MOs for **Dyad-5** in toluene.

	
LUMO+8 +1.17 eV	LUMO+9 +1.19eV
	
LUMO+6 +1.09 eV	LUMO+7 +1.15 eV

	
LUMO+4 +0.76 eV	LUMO+5 +1.03 eV
	
LUMO+2 -0.05 eV	LUMO+3 +0.11 eV

	
LUMO -1.64 eV	LUMO+1 -1.46 eV
	
HOMO -6.16 eV	HOMO-1 -6.22 eV

	
HOMO-2 -6.70 eV	HOMO-3 -6.83 eV
	
HOMO-4 -8.24 eV	HOMO-5 -8.91 eV

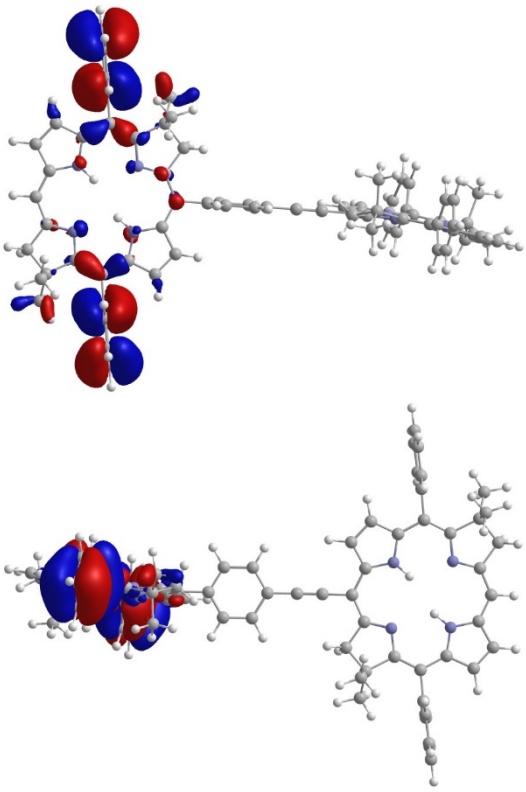
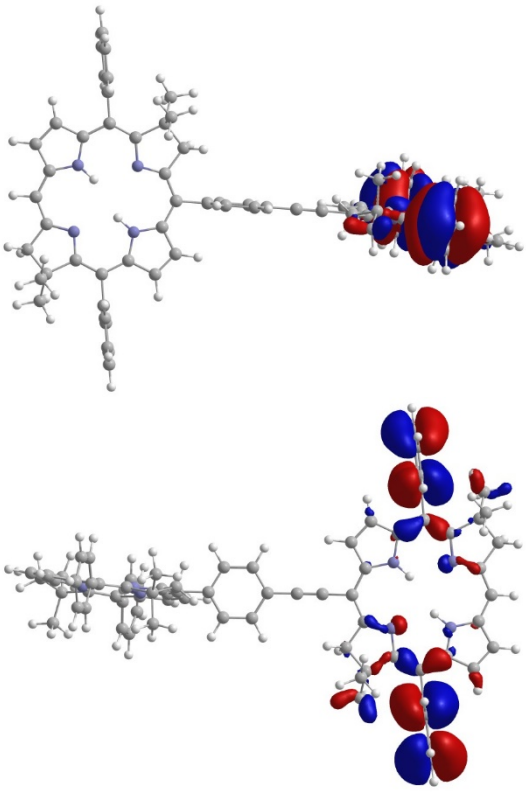
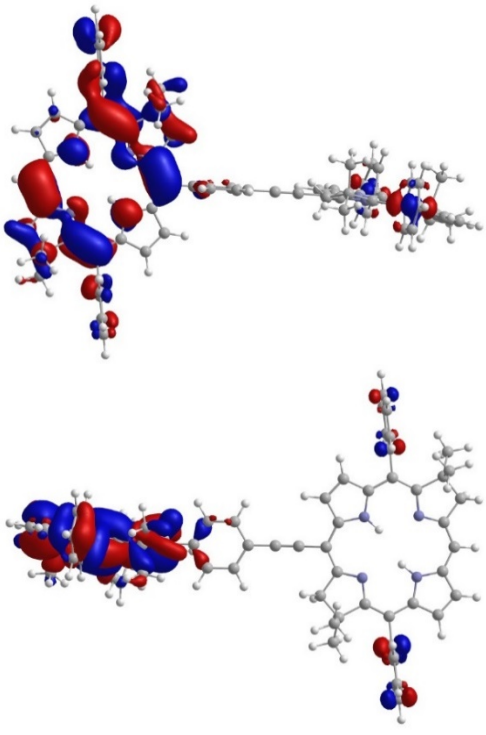
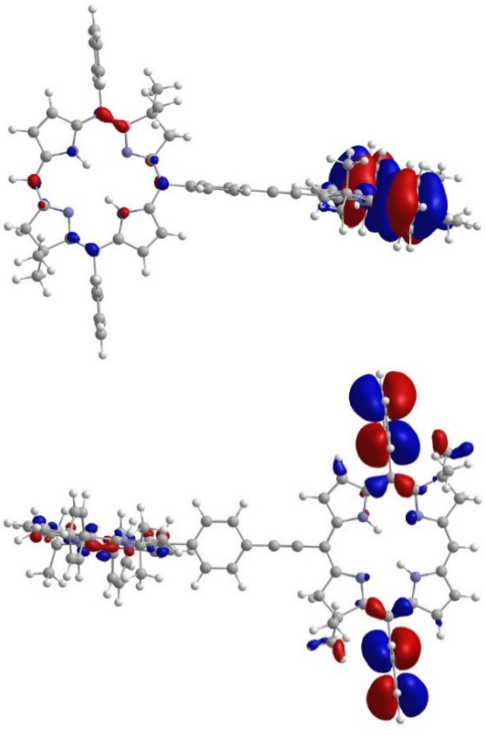
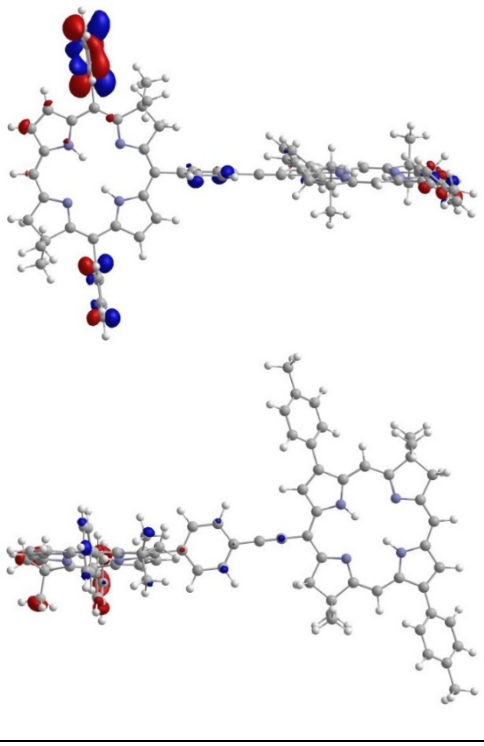
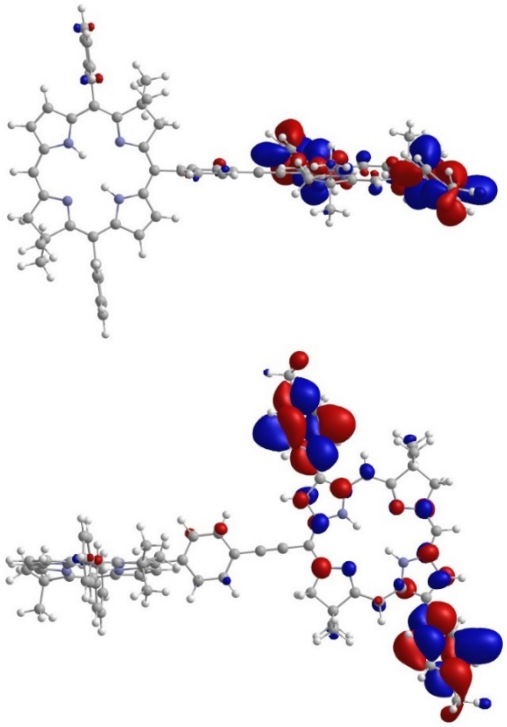
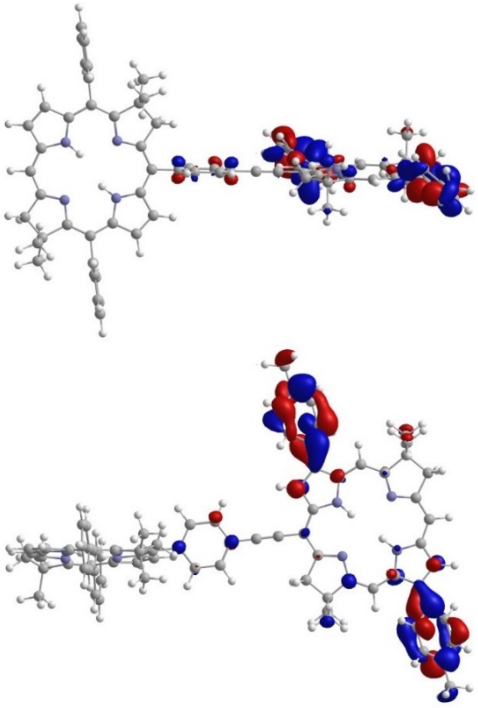
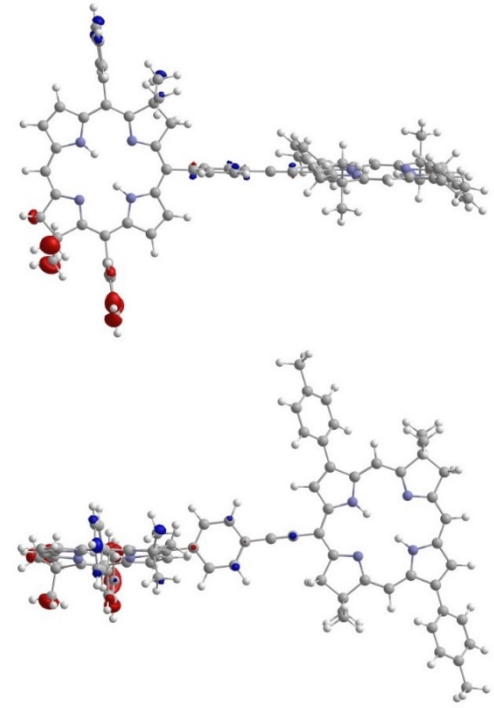
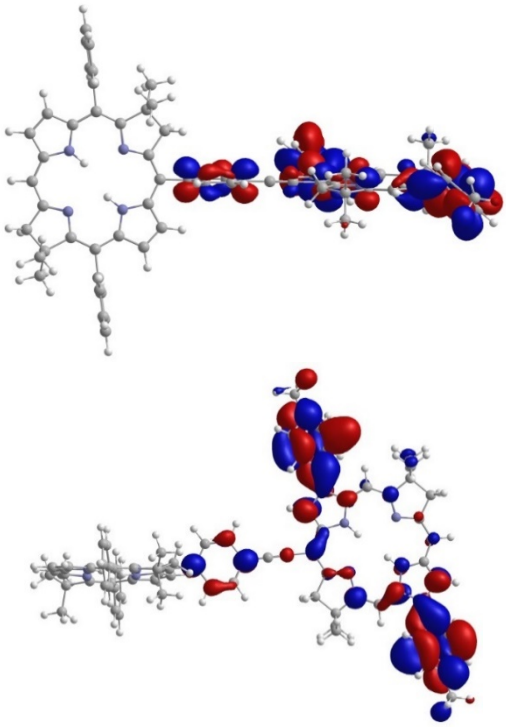
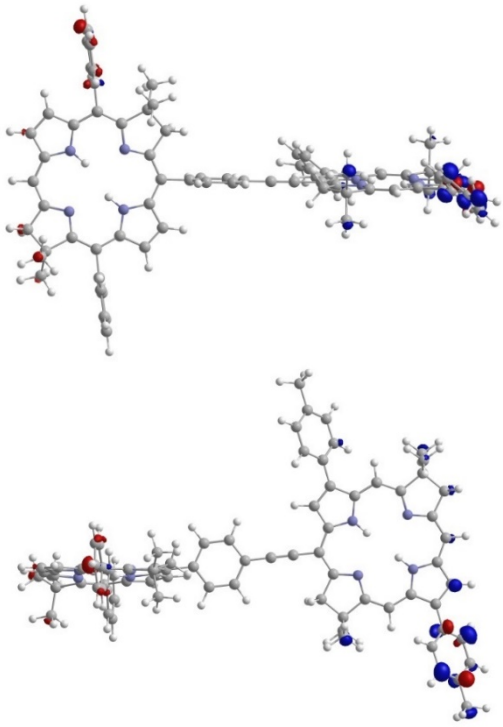
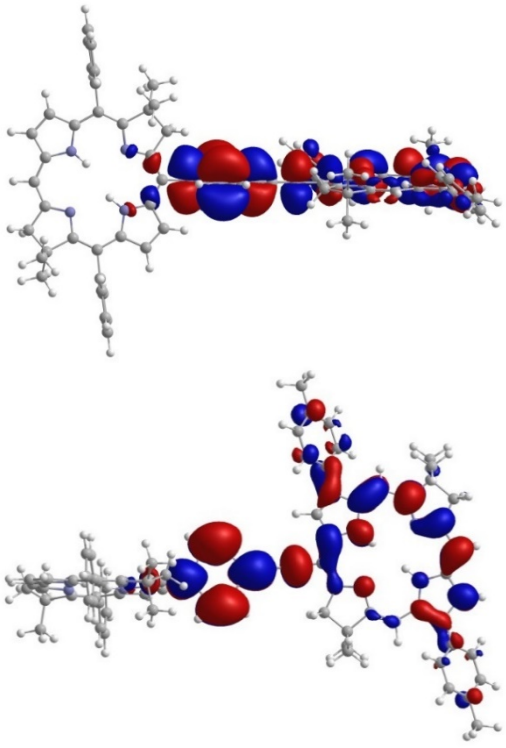
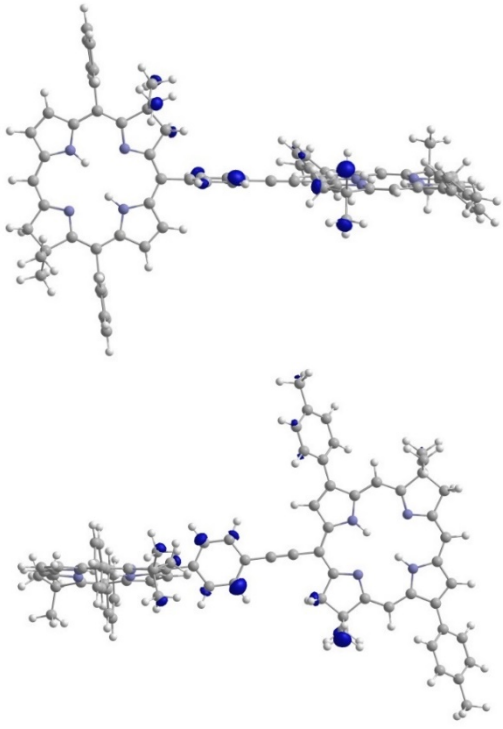
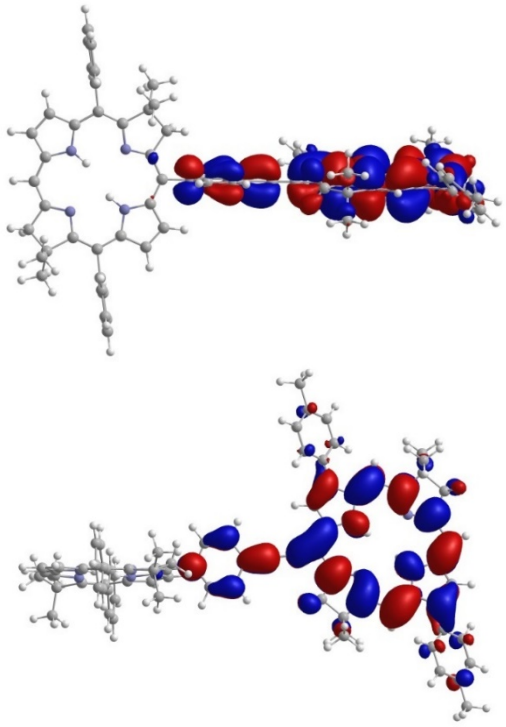
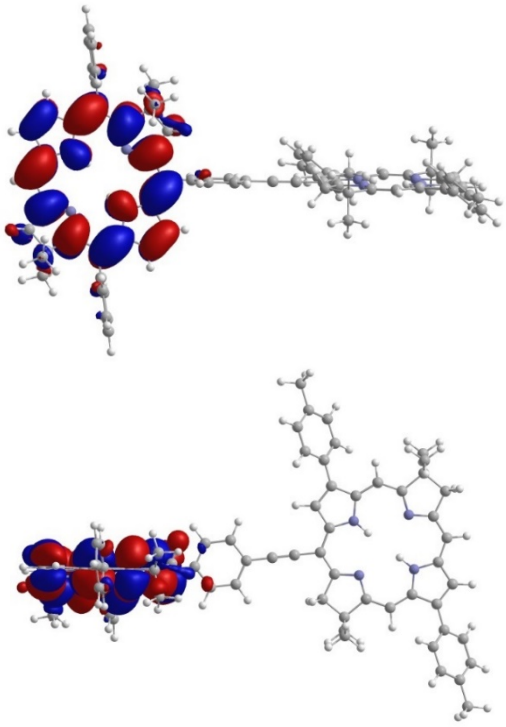
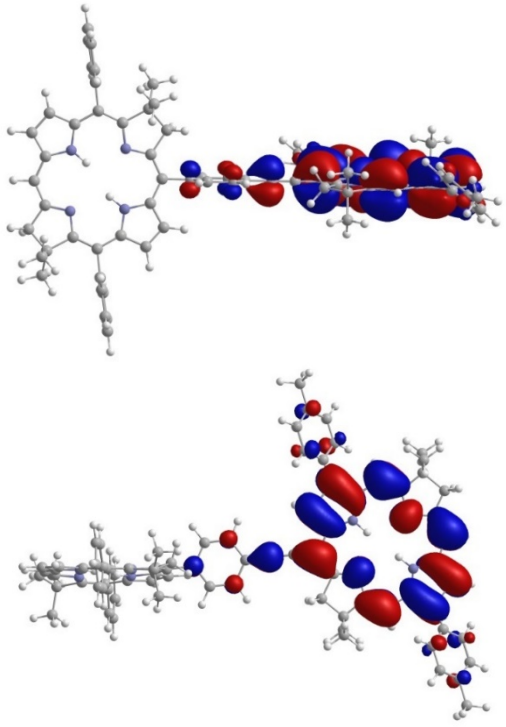
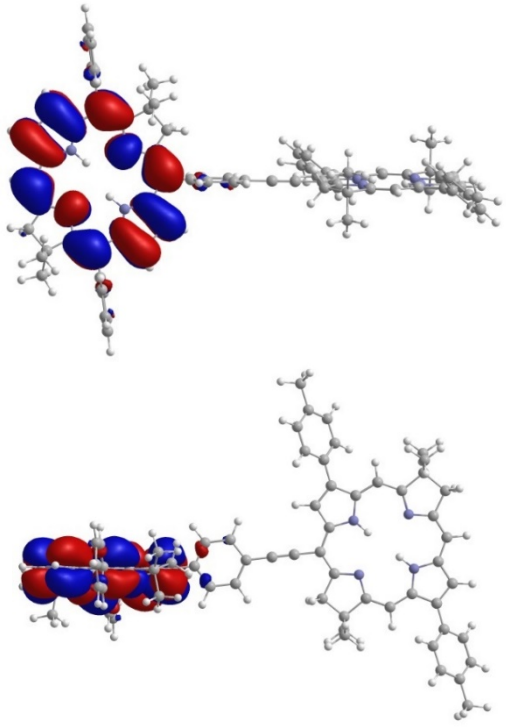
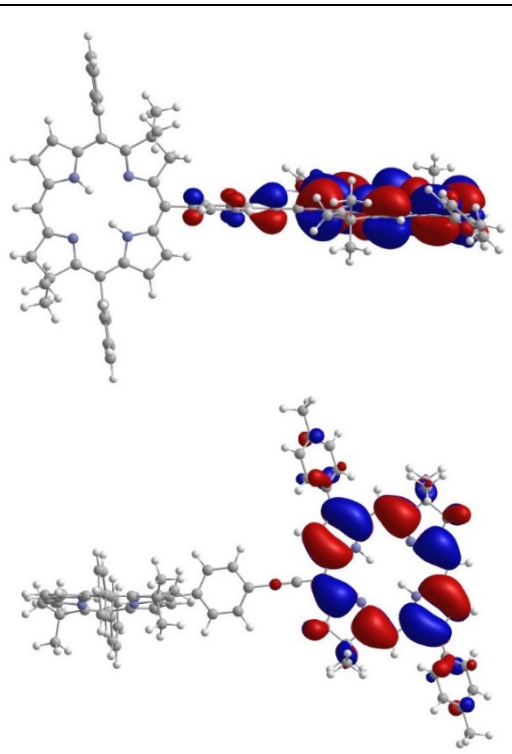
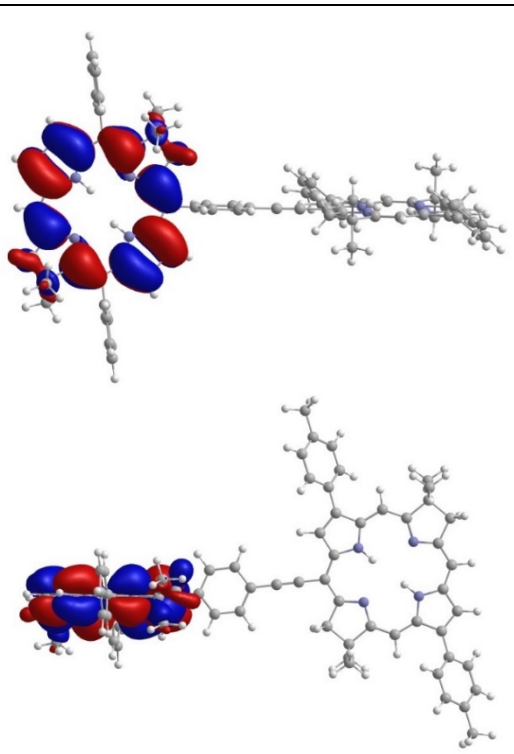
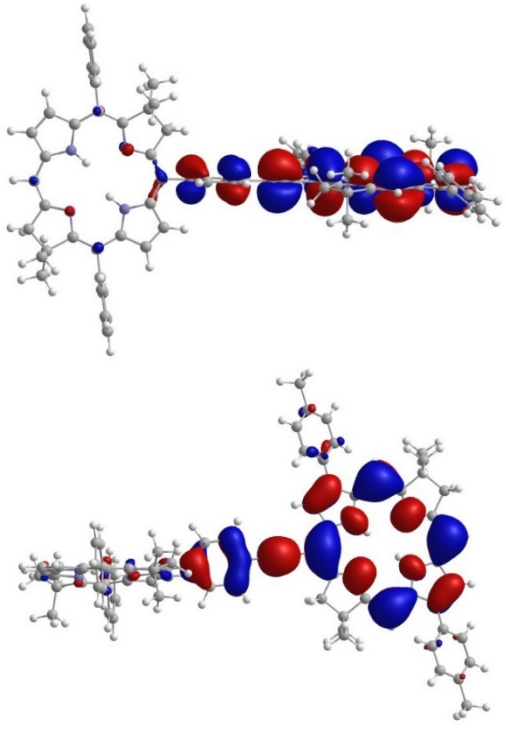
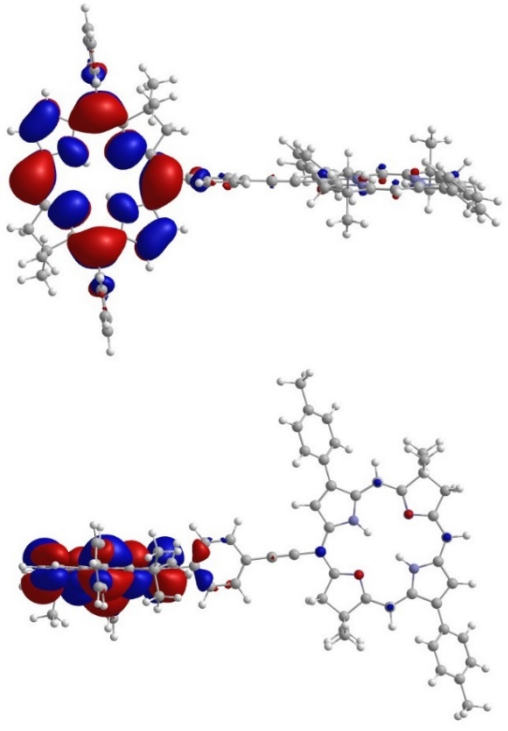
	
HOMO-6 -8.94 eV	HOMO-7 -8.96 eV
	
HOMO-8 -8.97 eV	HOMO-9 -8.99 eV

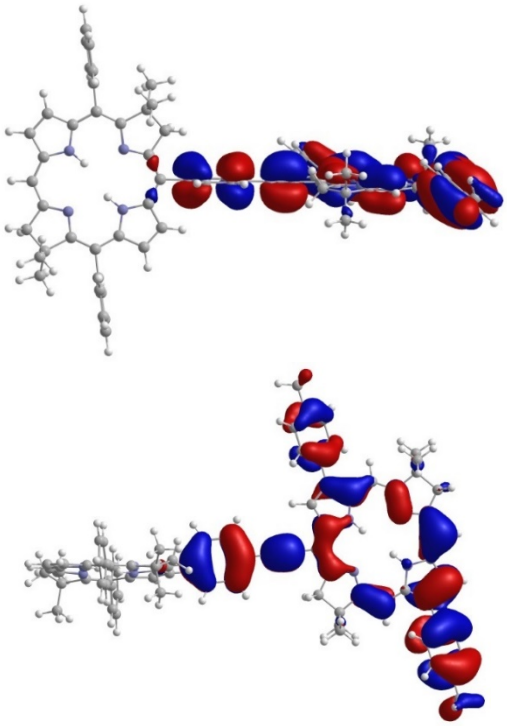
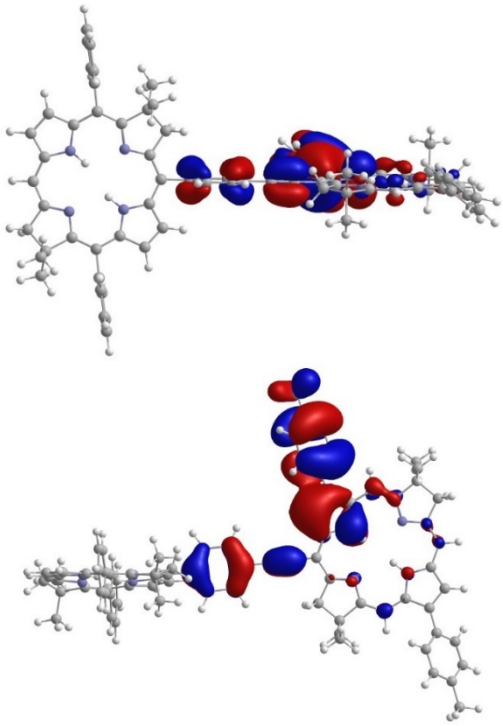
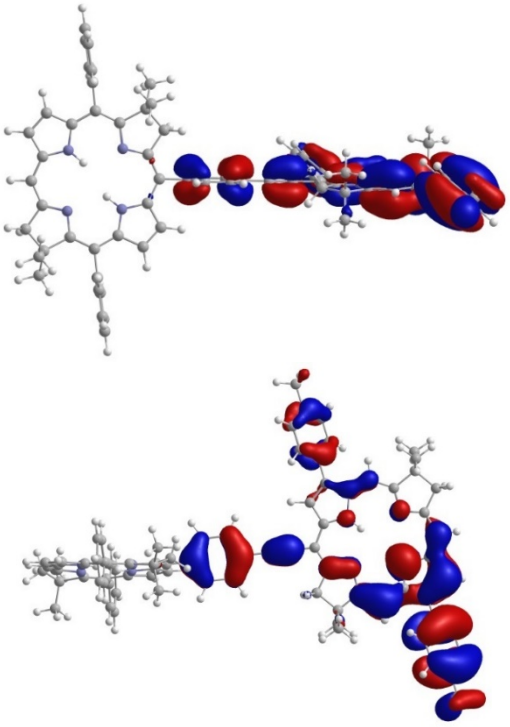
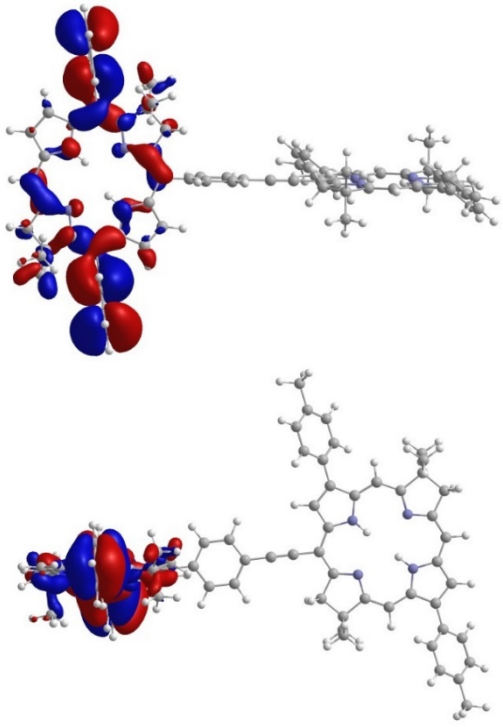
Table S8. MOs for **Dyad-6** in toluene.

	
LUMO+10 +1.19 eV	LUMO+11 +1.26 eV
	
LUMO+8 +1.13 eV	LUMO+9 +1.17 eV

	
LUMO+6 +1.07 eV	LUMO+7 +1.09 eV
	
LUMO+4 +0.76 eV	LUMO+5 +1.02 eV

	
LUMO+2 -0.05 eV	LUMO+3 +0.11 eV
	
LUMO -1.63 eV	LUMO+1 -1.46 eV

	
HOMO #311 -6.13 eV	HOMO-1 -6.16 eV
	
HOMO-2 -6.69 eV	HOMO-3 -6.83 eV

	
HOMO-4 -8.15 eV	HOMO-5 -8.32 eV
	
HOMO-6 -8.43 eV	HOMO-7 -8.91 eV

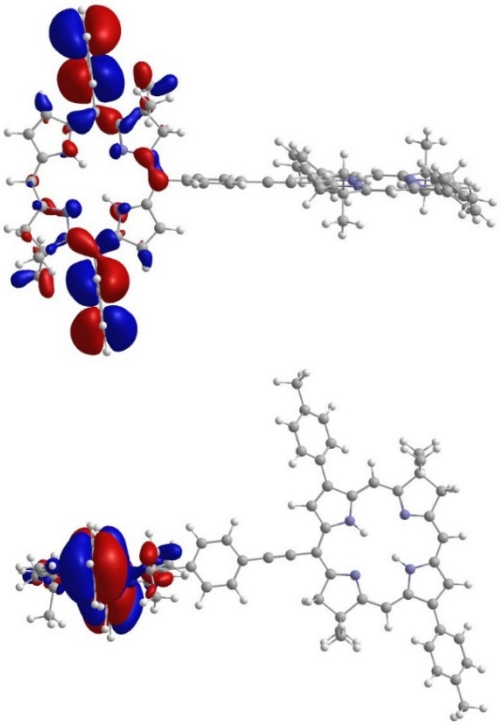
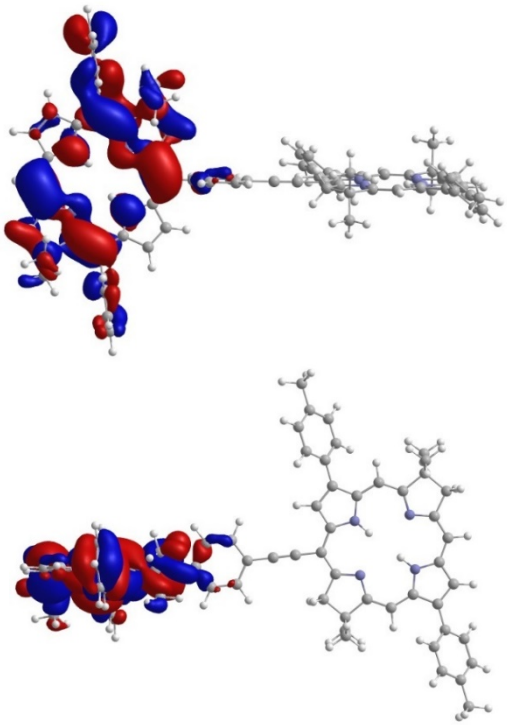
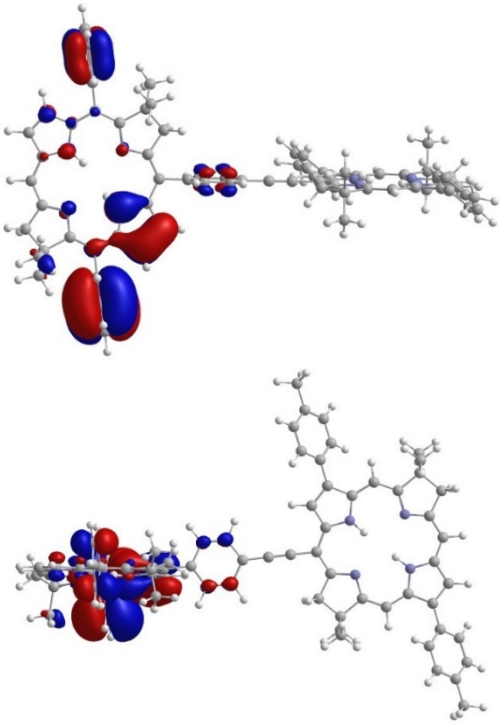
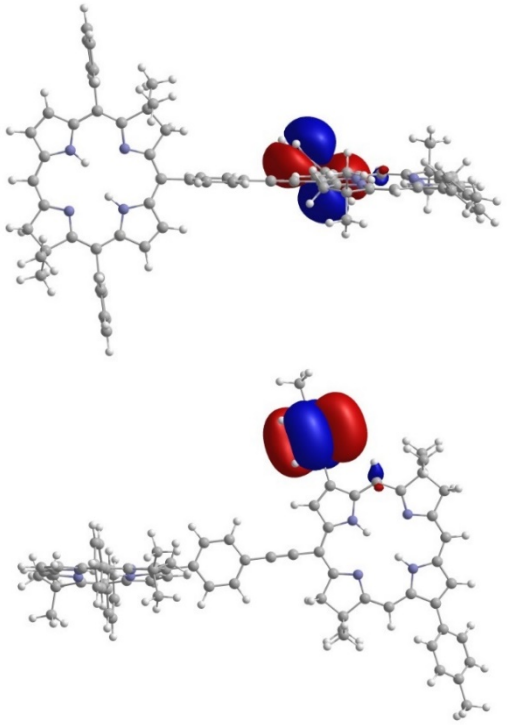
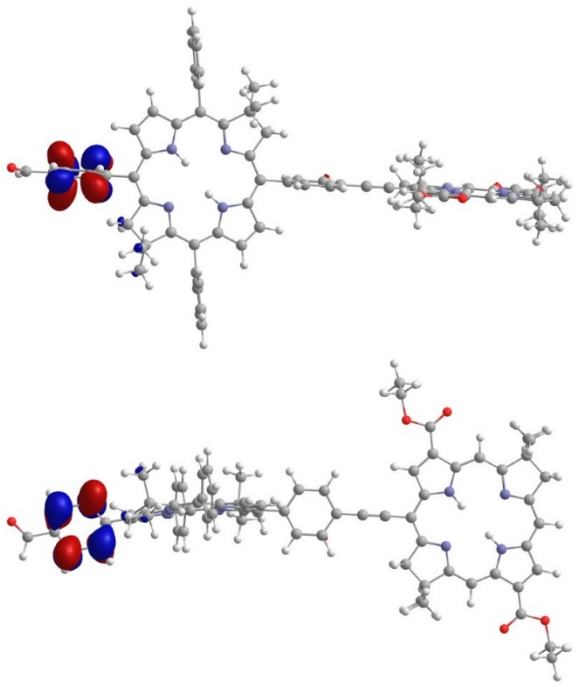
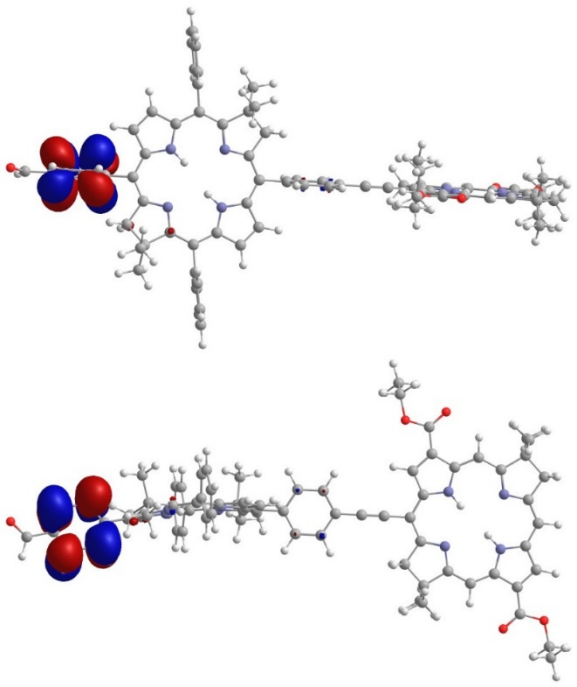
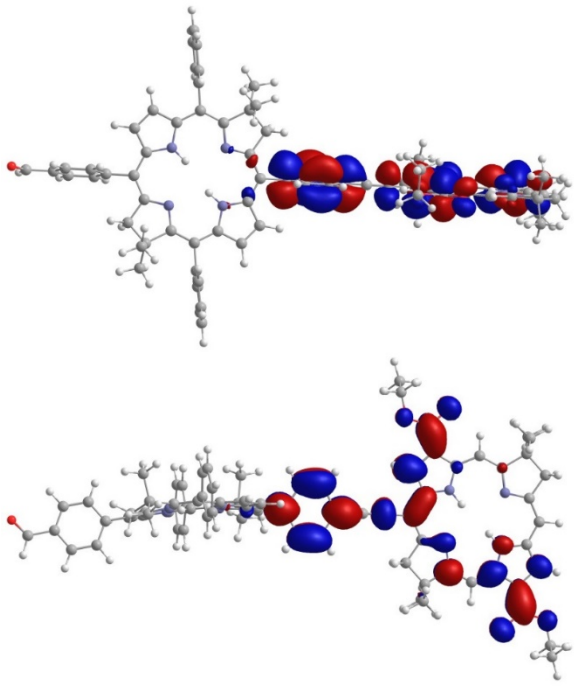
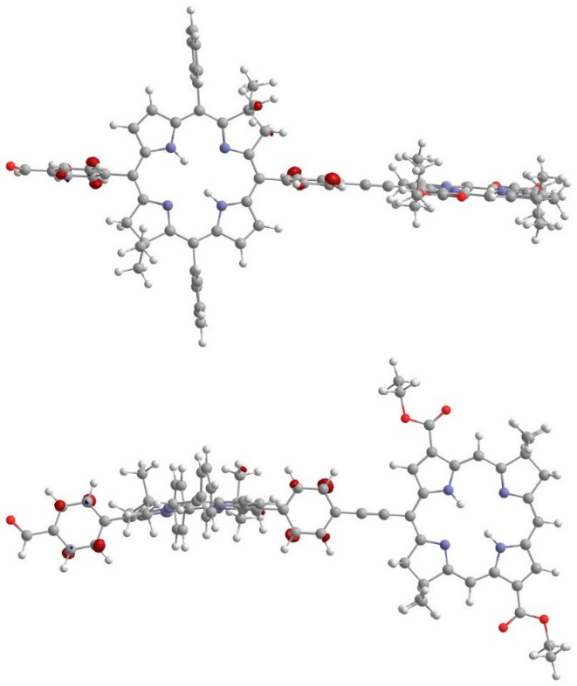
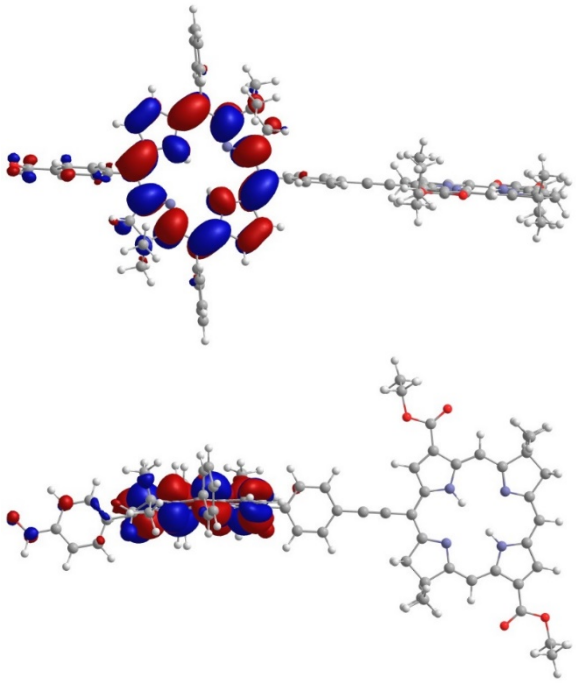
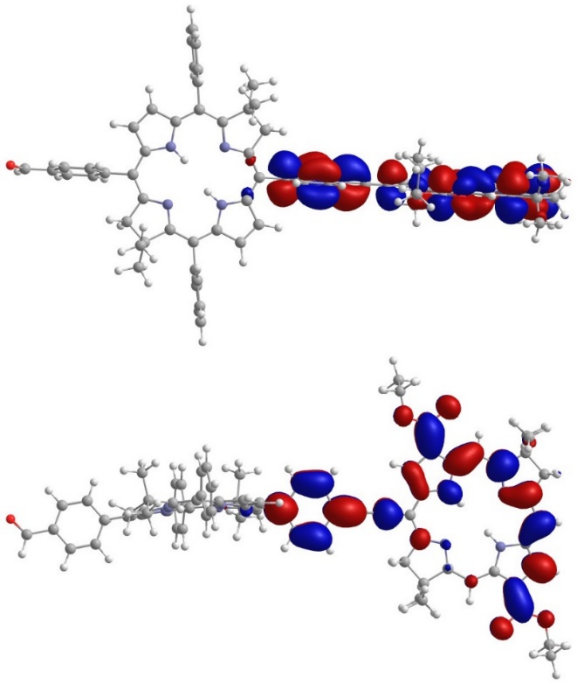
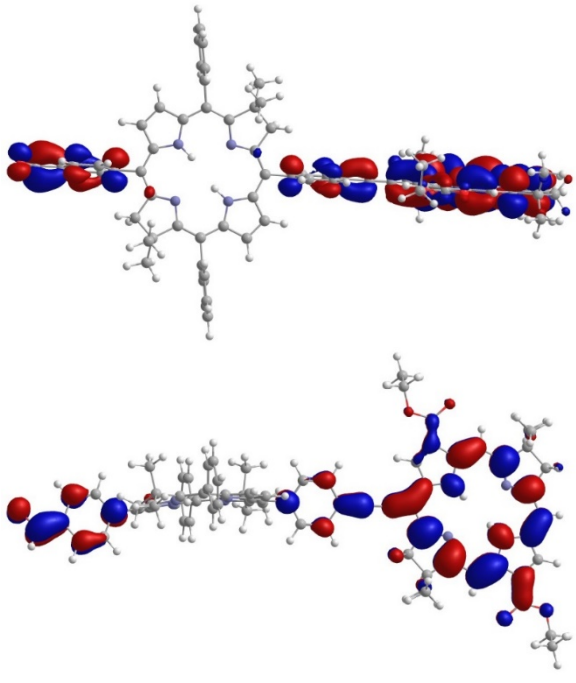
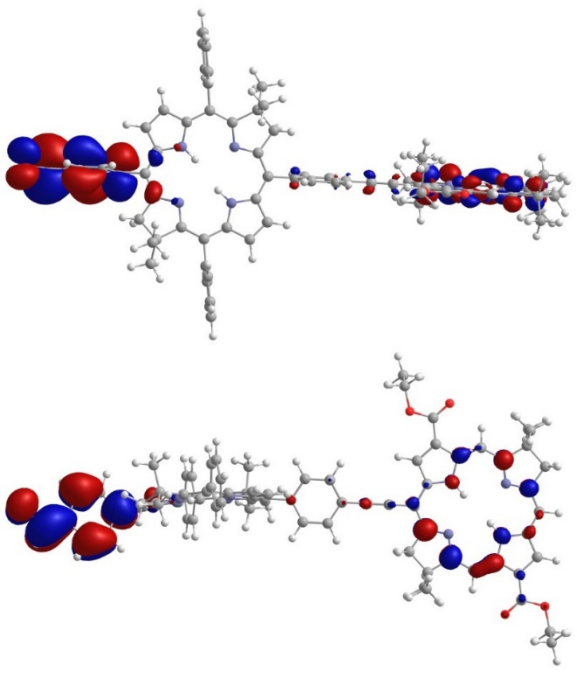
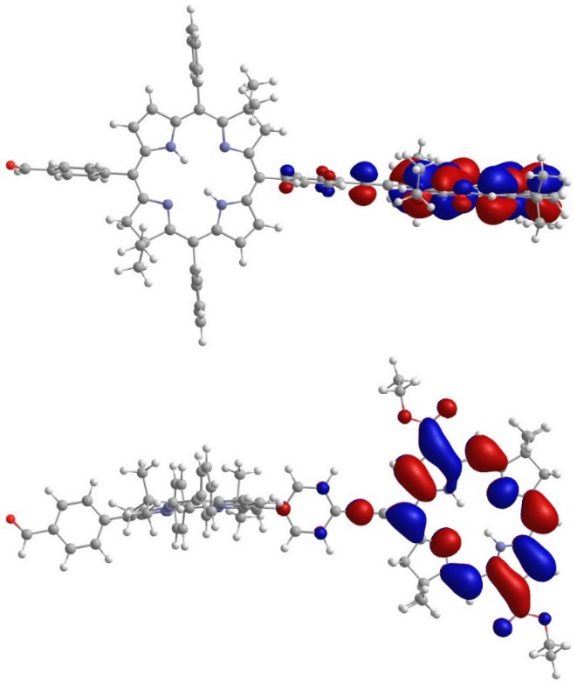
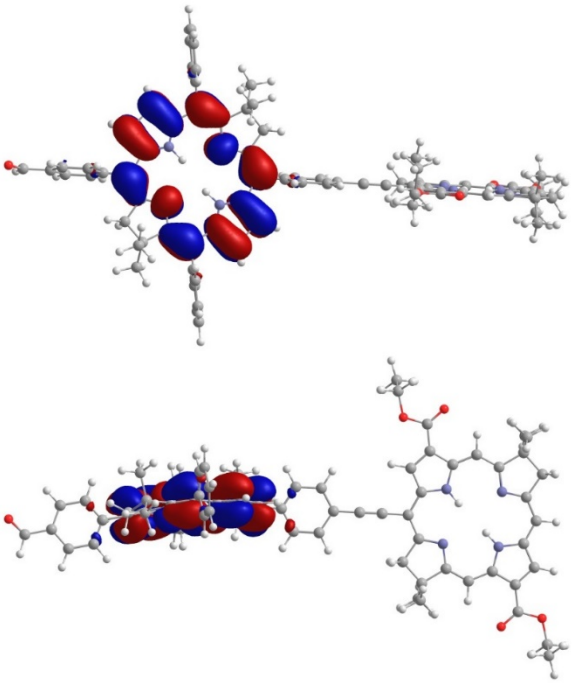
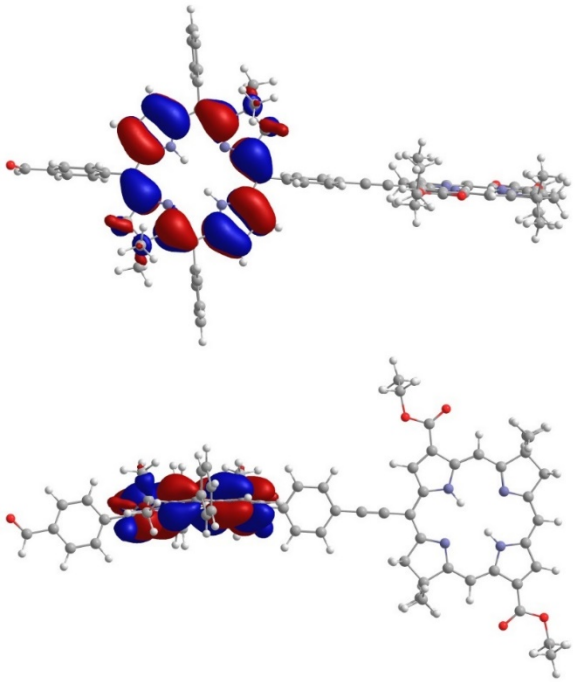
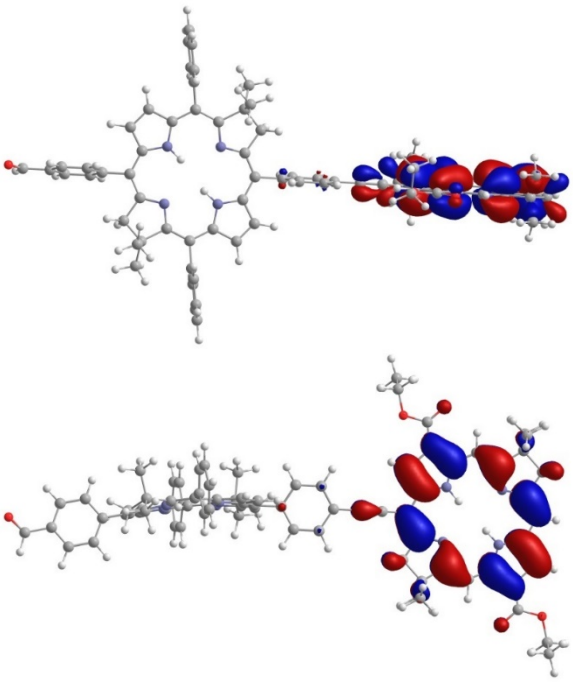
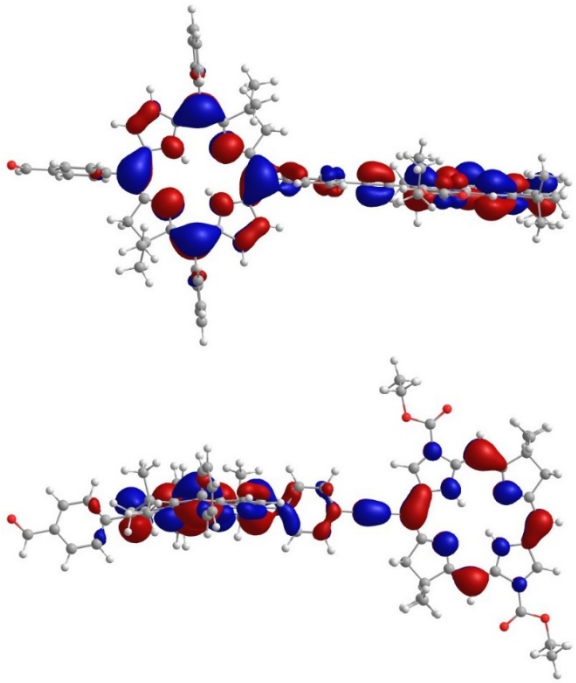
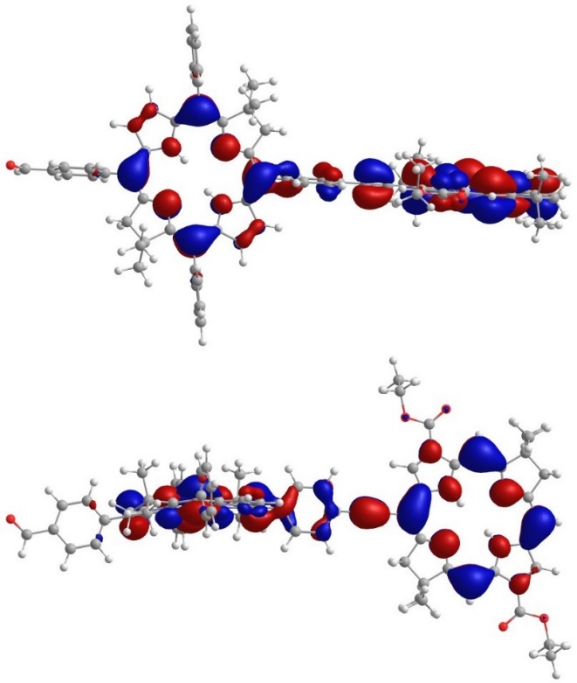
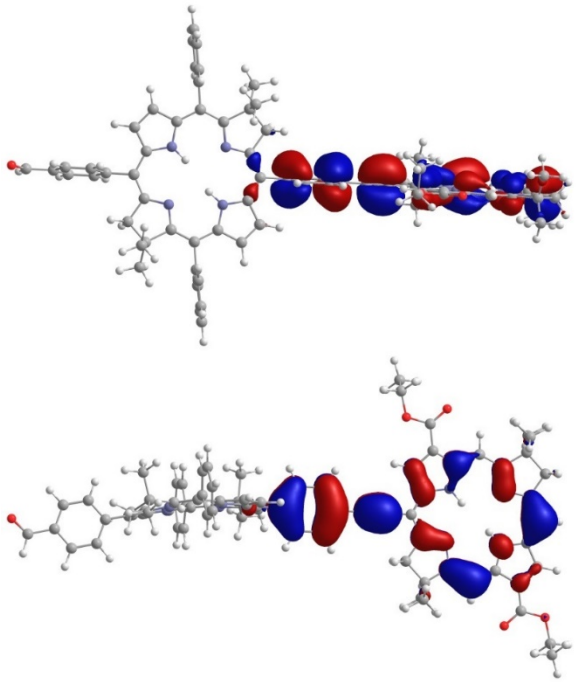
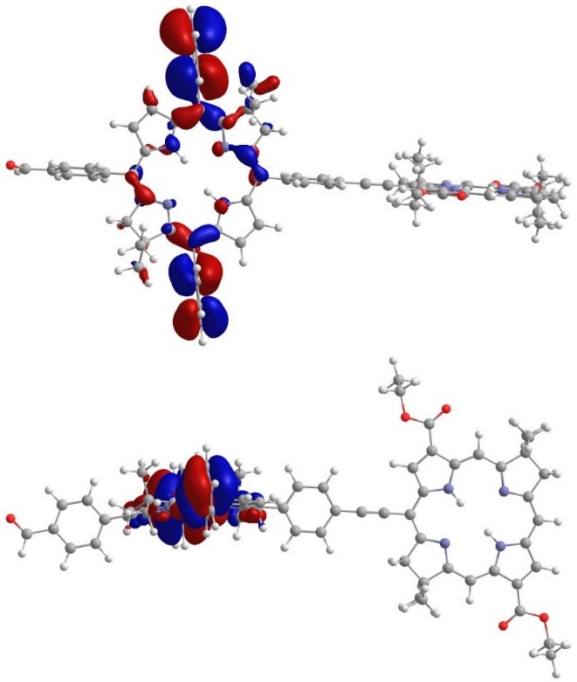
	
HOMO-8 -8.94 eV	HOMO-9 -8.97 eV
	
HOMO-10 -9.04 eV	HOMO-11 -9.08 eV

Table S9. MOs for **Dyad-7** in toluene.

	
LUMO+8 +1.06 eV	LUMO+9 +1.09 eV
	
LUMO+6 +0.84 eV	LUMO+7 +0.97 eV

	
LUMO+4 +0.00 eV	LUMO+5 +0.52 eV
	
LUMO+2 -0.29 eV	LUMO+3 -0.29 eV

	
LUMO -2.05 eV	LUMO+1 -1.58 eV
	
HOMO #328 -6.27 eV	HOMO-1 -6.46 eV

	
HOMO-2 -6.88 eV	HOMO-3 -6.94 eV
	
HOMO-4 -8.42 eV	HOMO-5 -8.96 eV

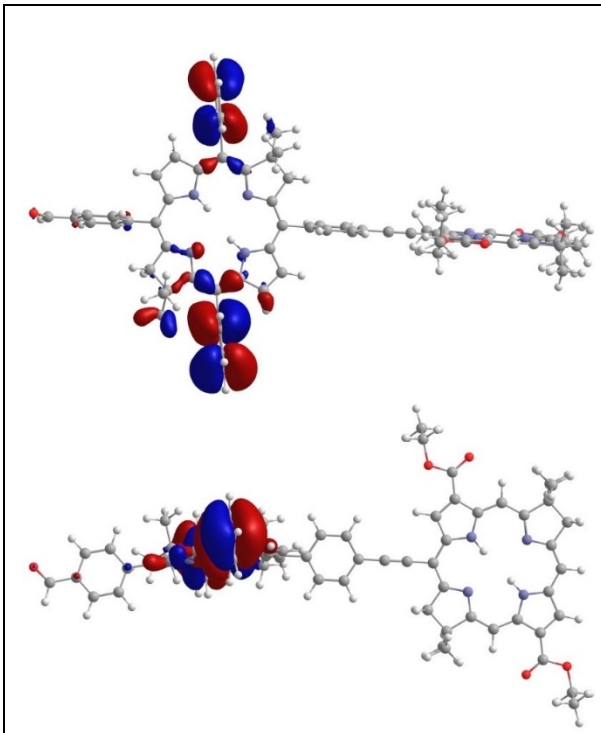
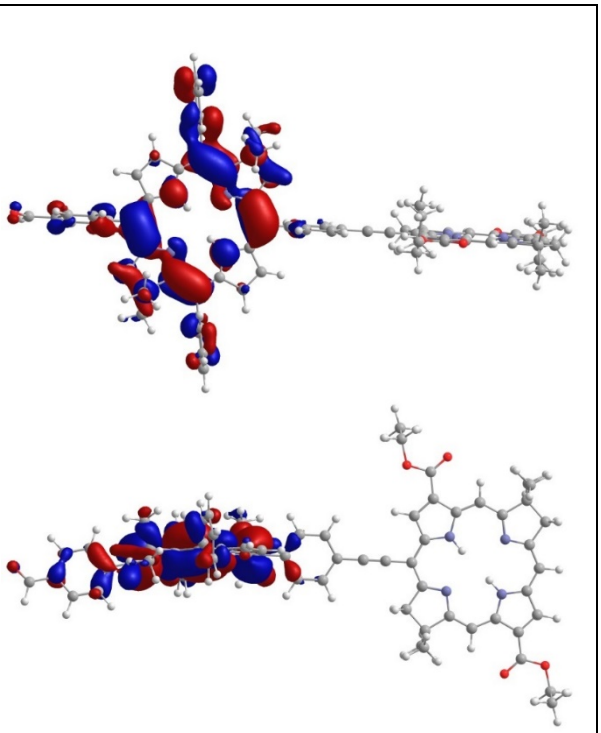
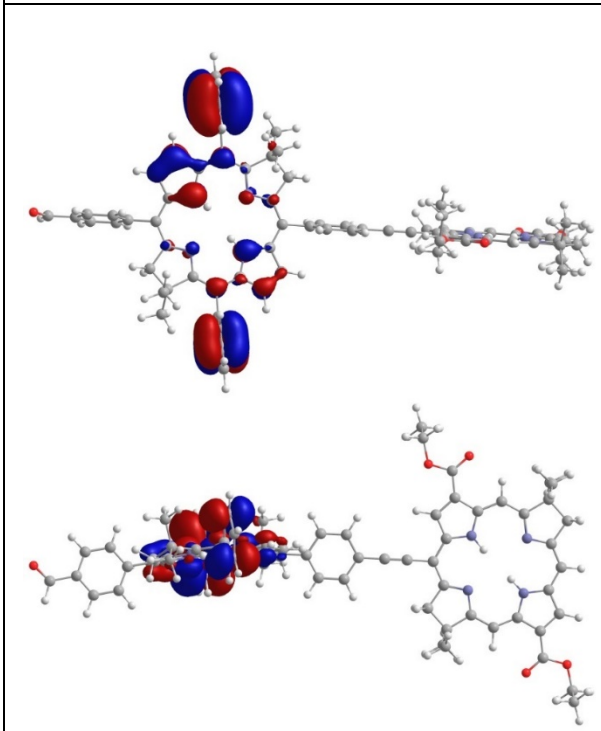
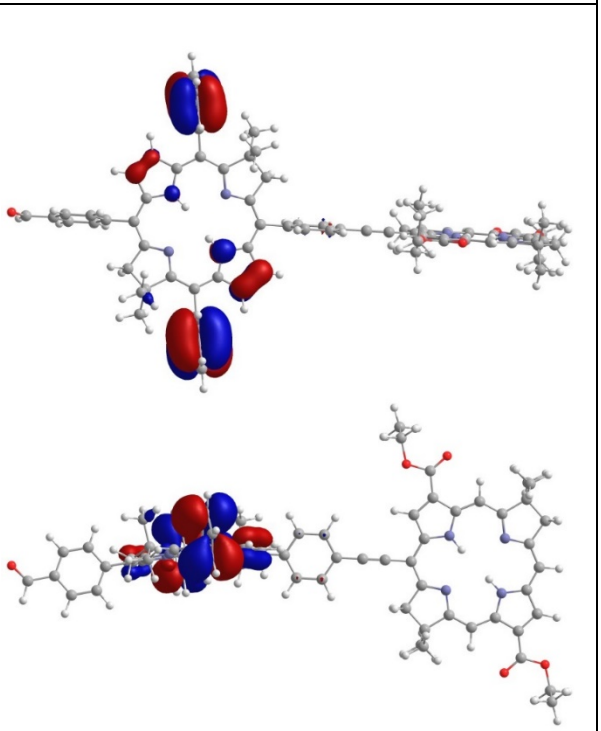
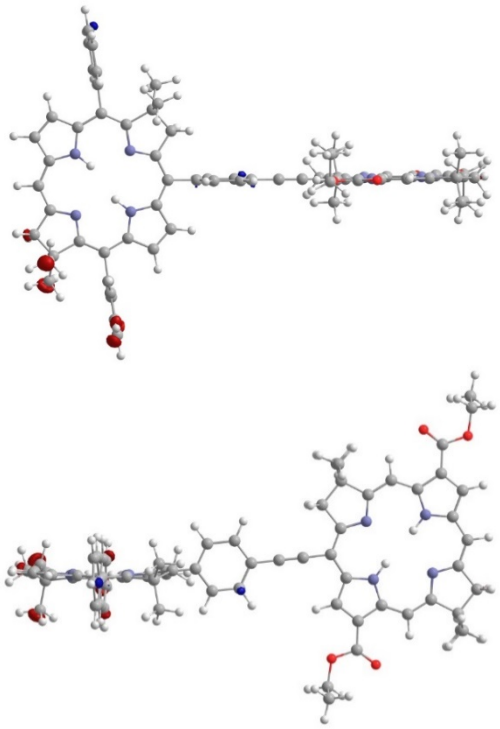
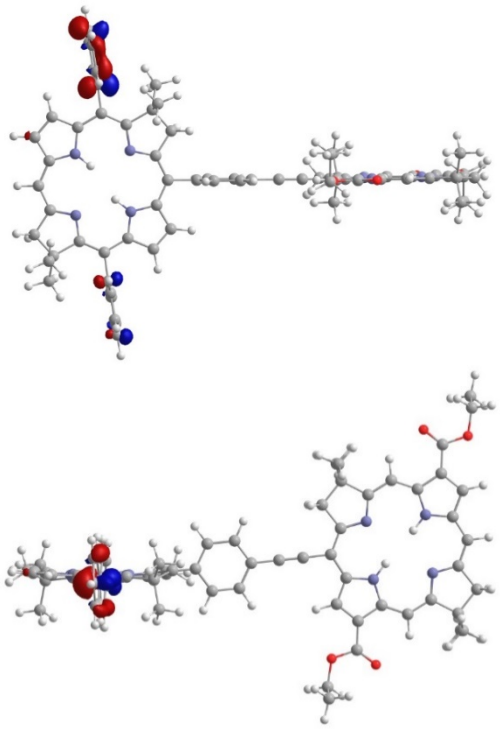
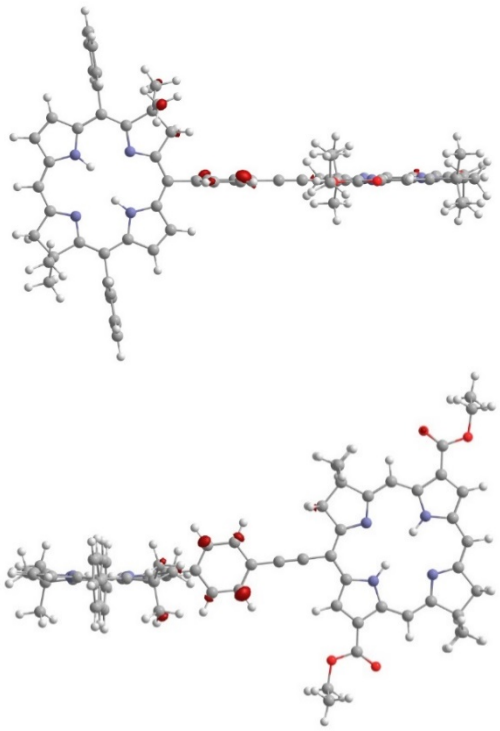
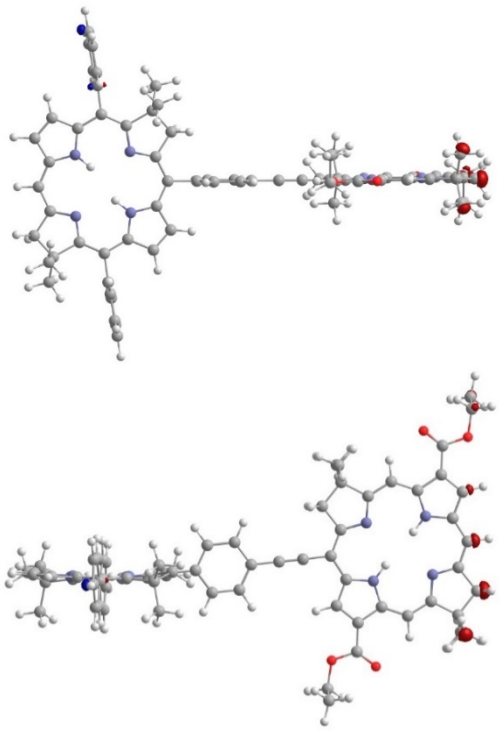
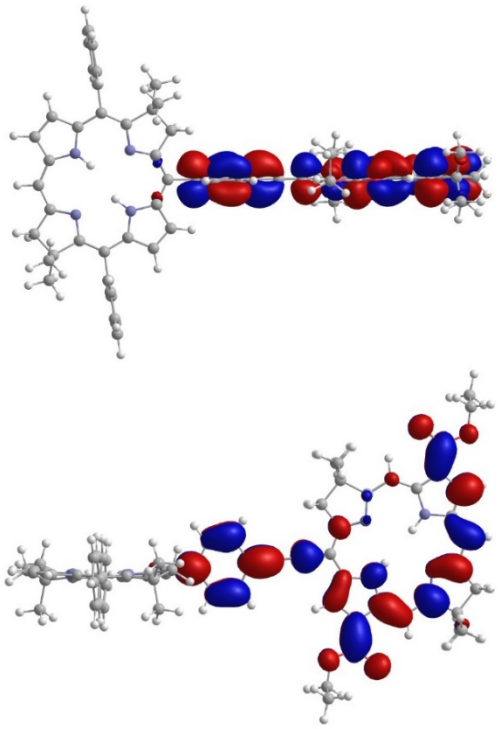
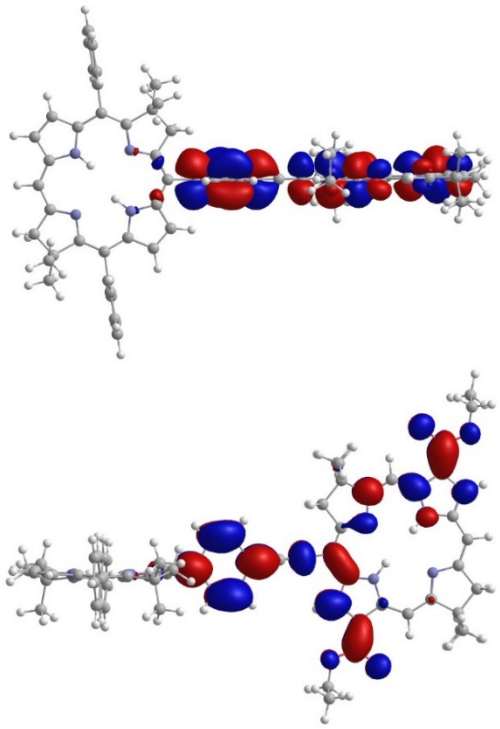
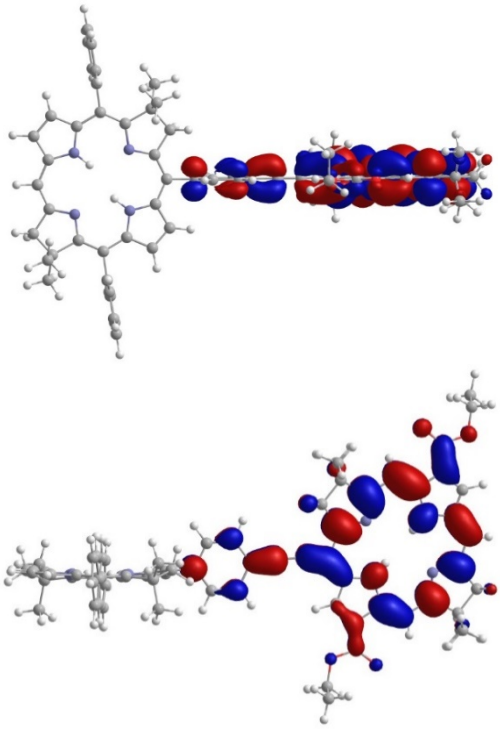
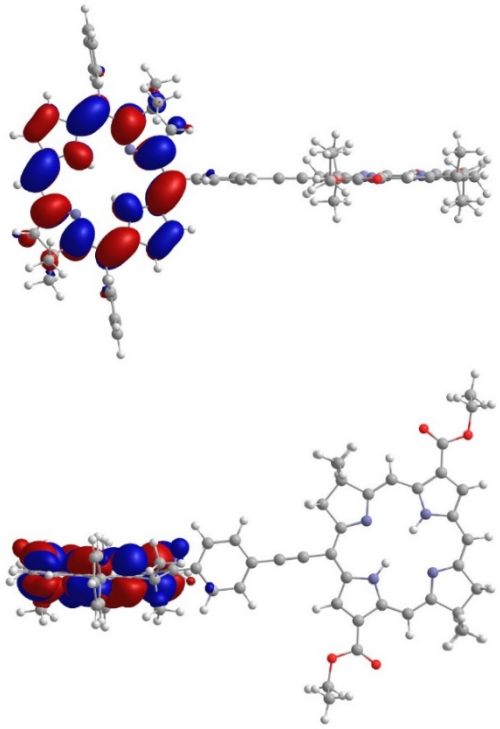
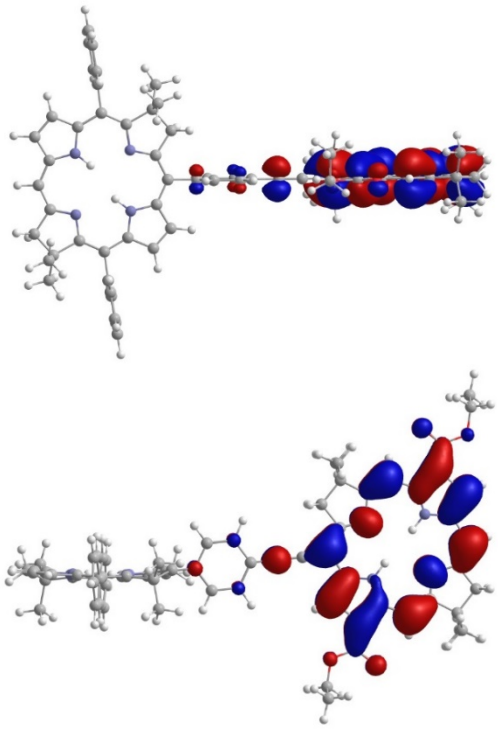
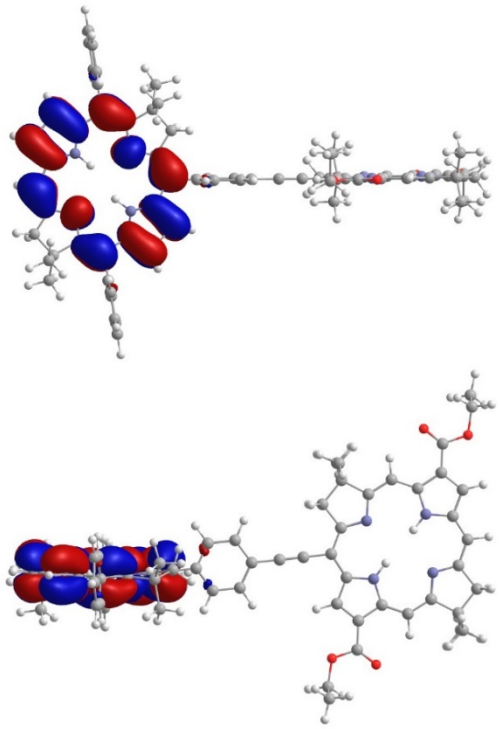
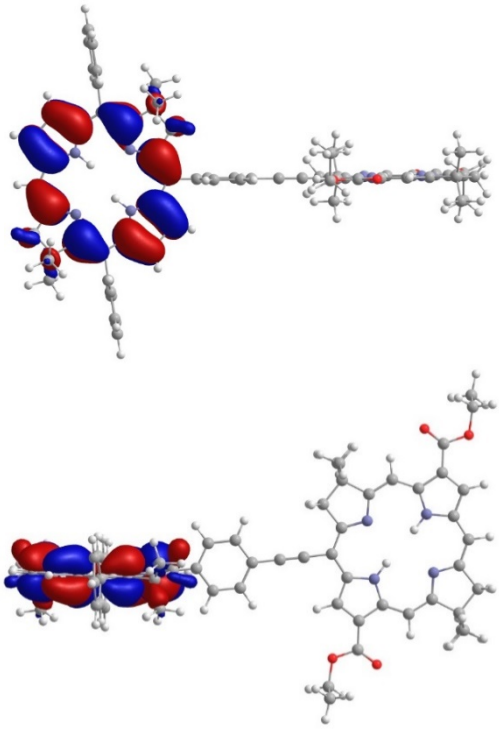
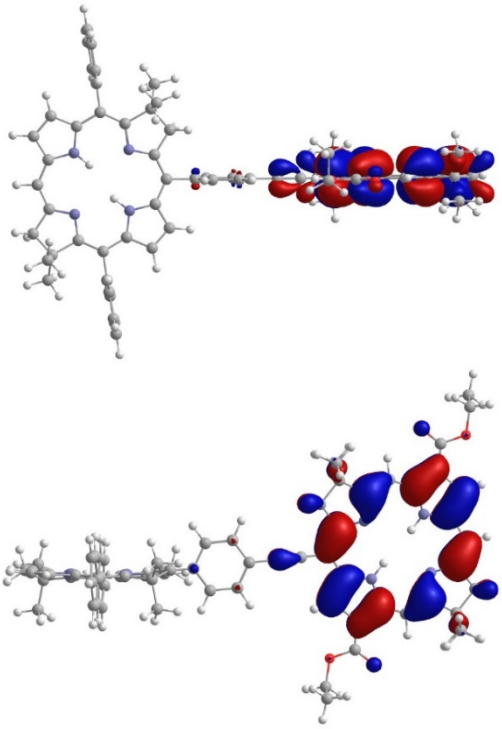
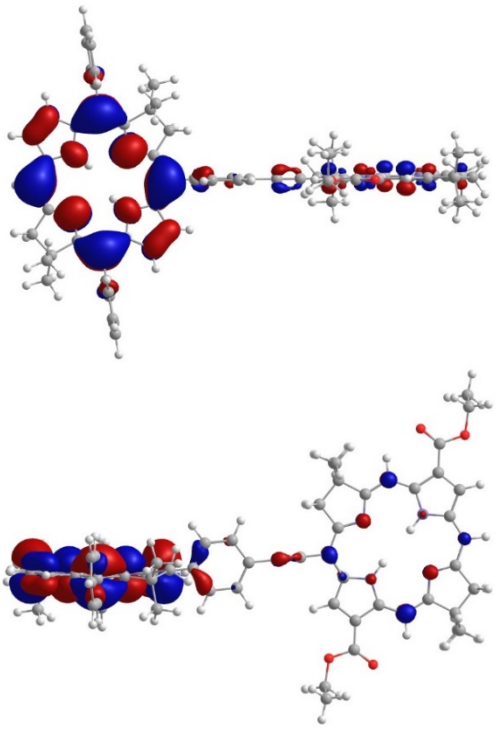
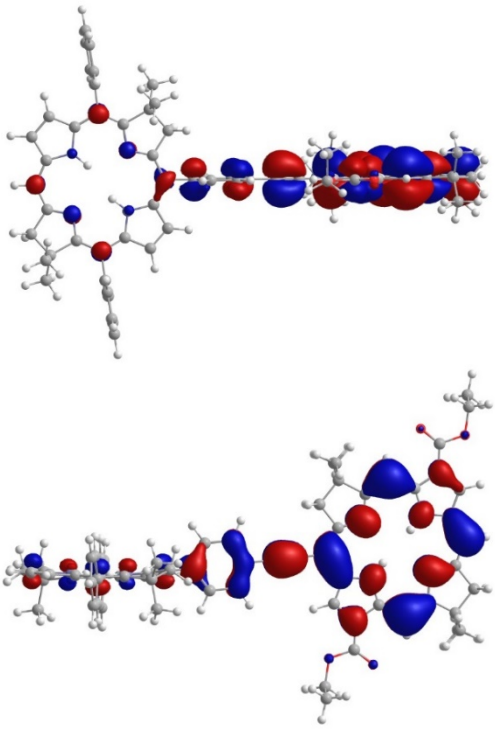
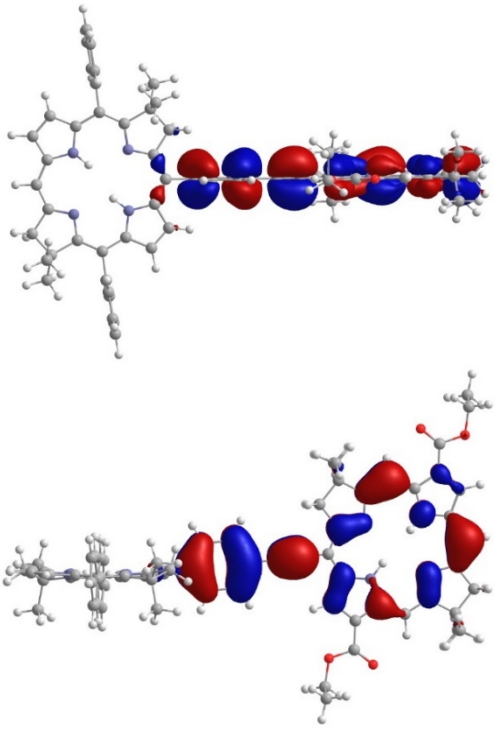
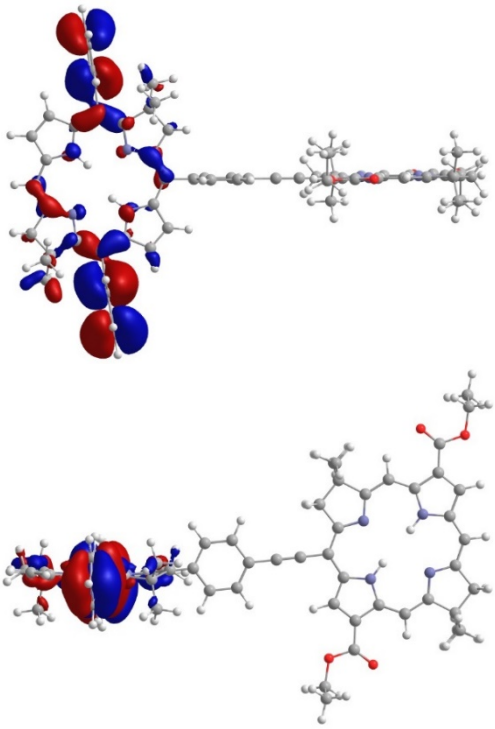
	
HOMO-6 -8.99 eV	HOMO-7 -9.04 eV
	
HOMO-8 -9.10 eV	HOMO-9 -9.12 eV

Table S10. MOs for **Dyad-8** in toluene.

	
LUMO+8 +1.16 eV	LUMO+9 +1.1.17 eV
	
LUMO+6 +1.02 eV	LUMO+7 +1.10 eV

	
LUMO+4 +0.55 eV	LUMO+5 +0.87 eV
	
LUMO+2 -0.27 eV	LUMO+3 +0.09 eV

	
LUMO -2.02 eV	LUMO+1 -1.48 eV
	
HOMO #301 -6.18 eV	HOMO-1 -6.44 eV

	
HOMO-2 -6.84 eV	HOMO-3 -6.90 eV
	
HOMO-4 -8.38 eV	HOMO-5 -8.93 eV

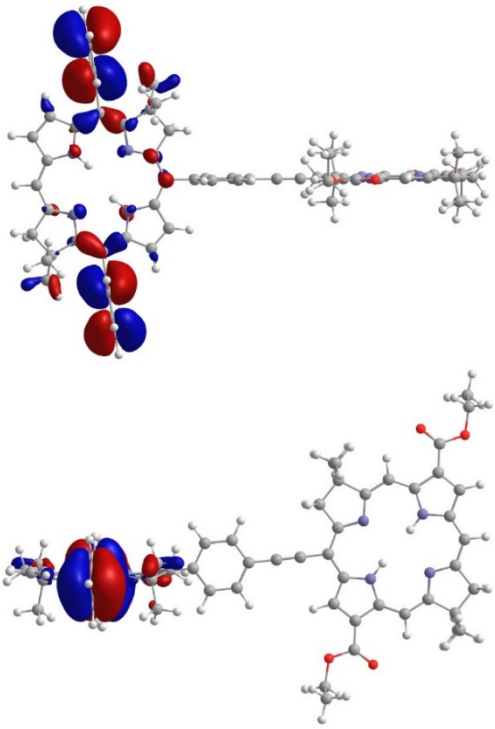
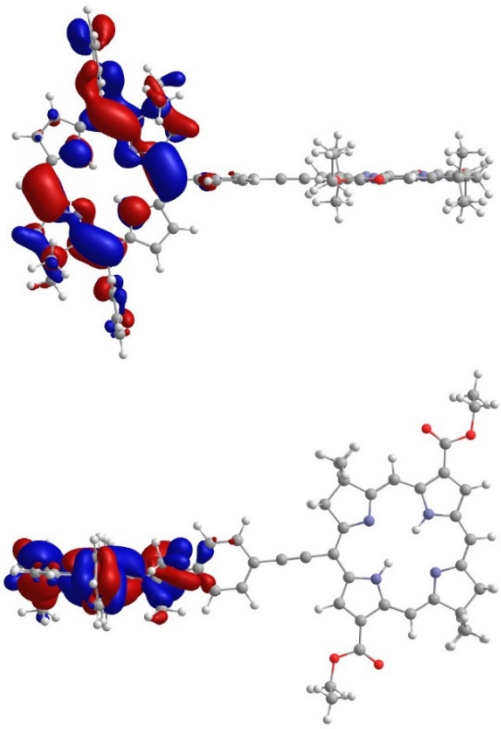
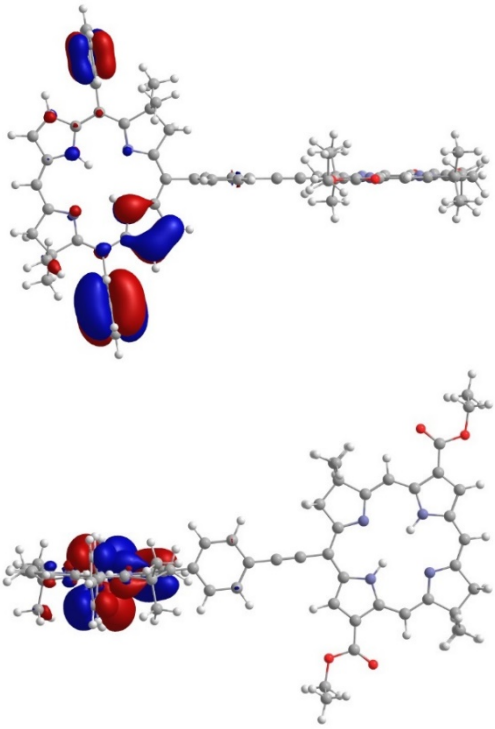
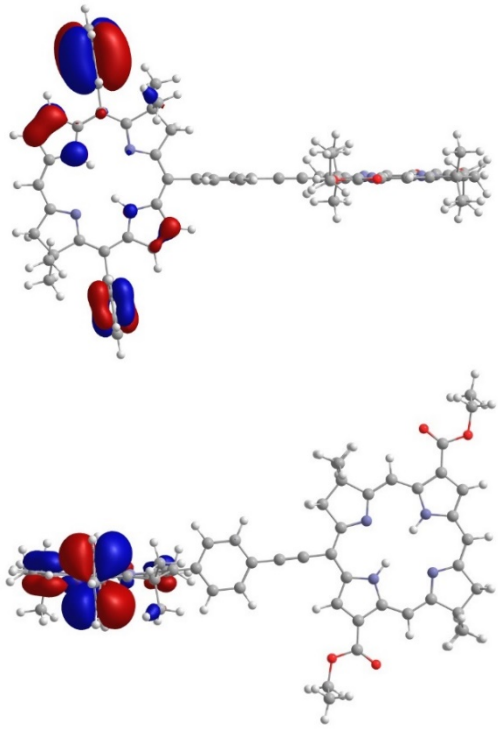
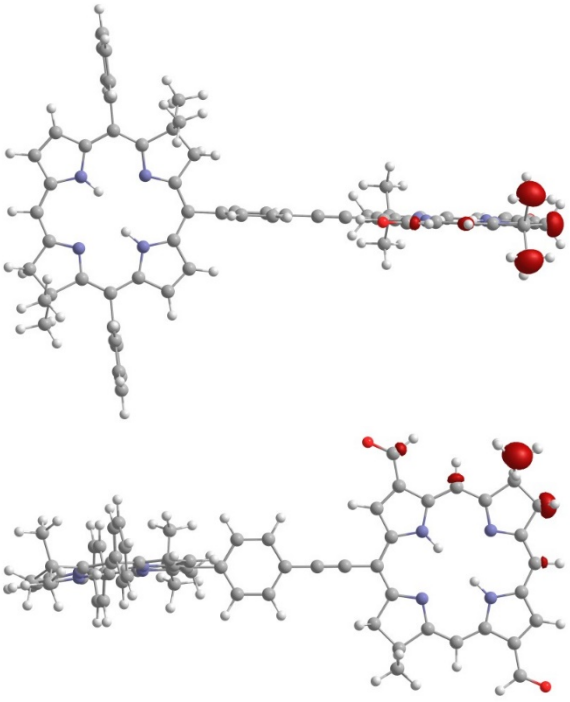
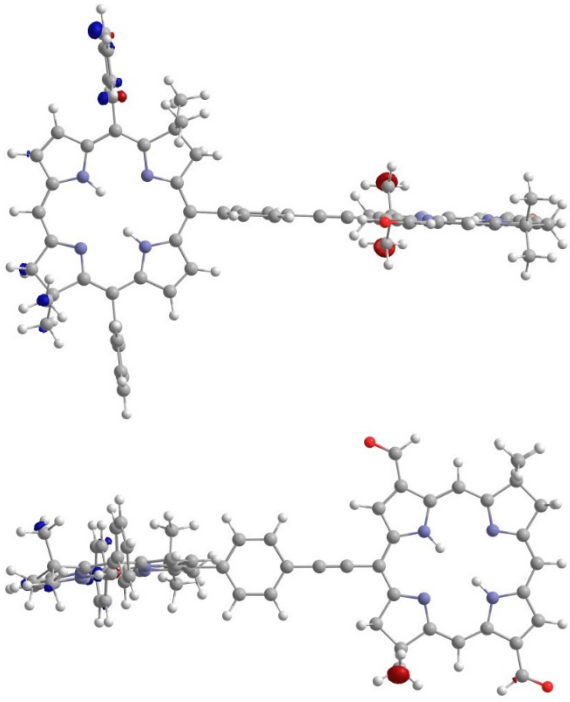
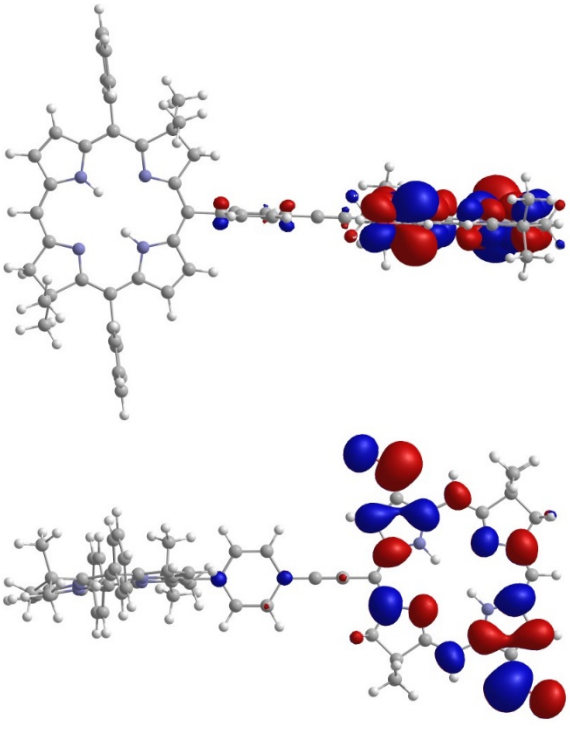
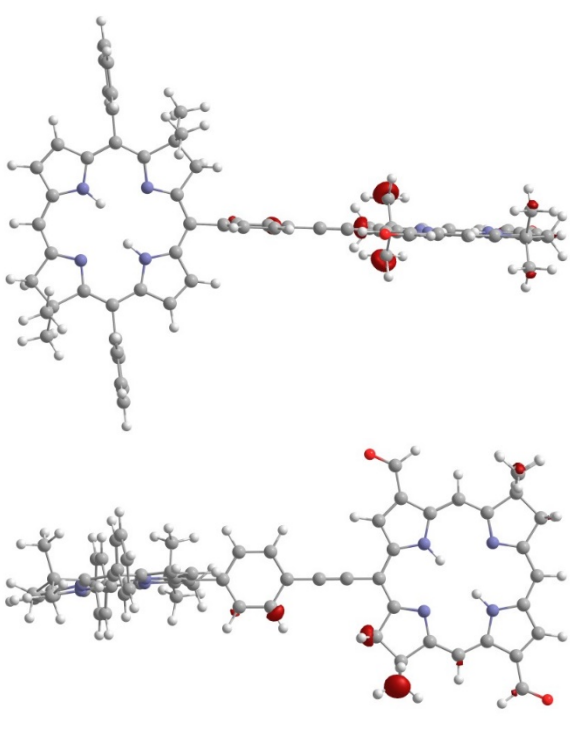
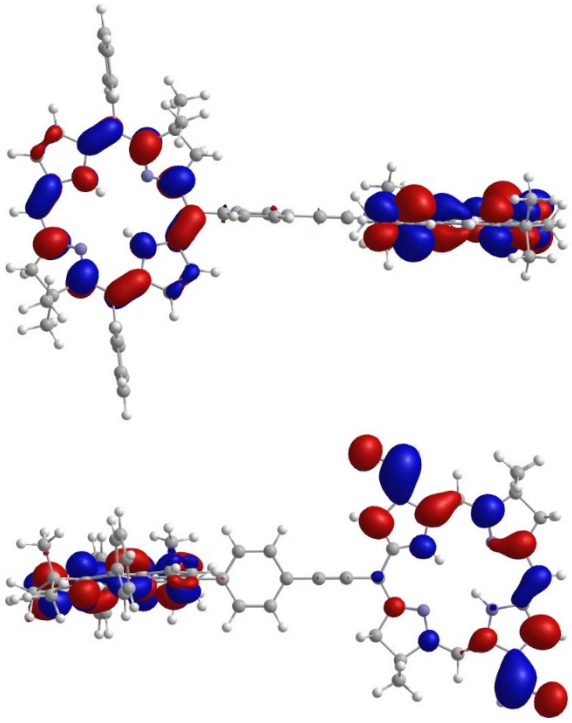
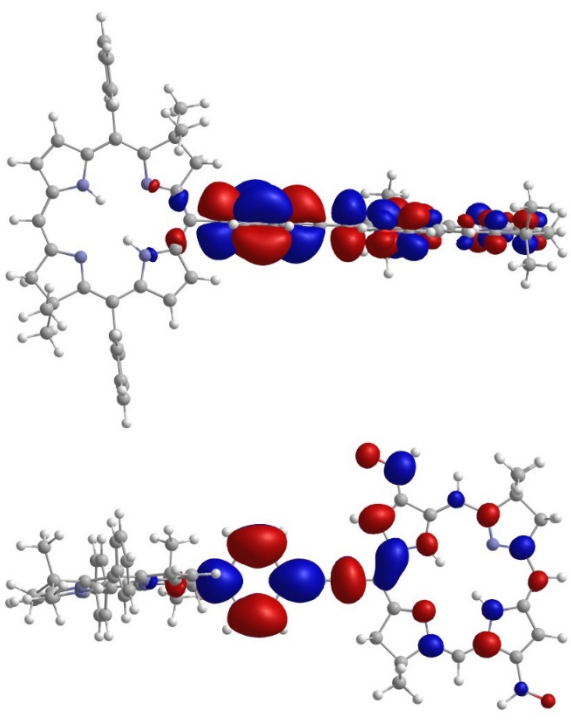
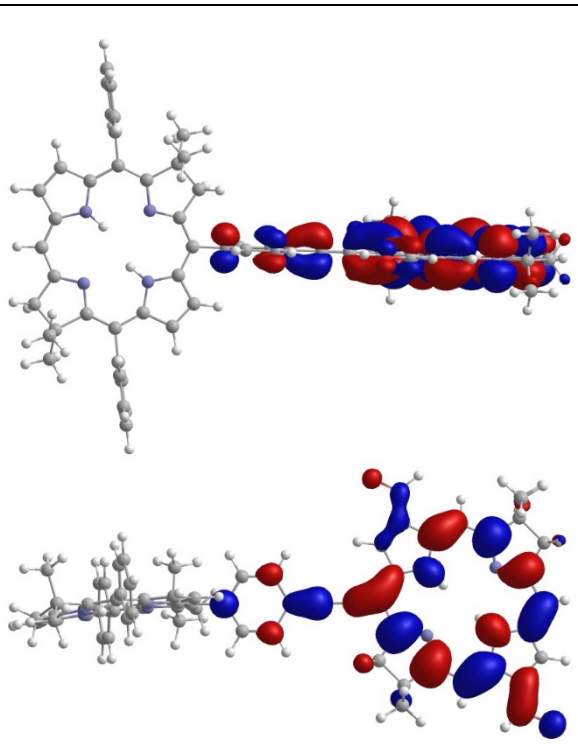
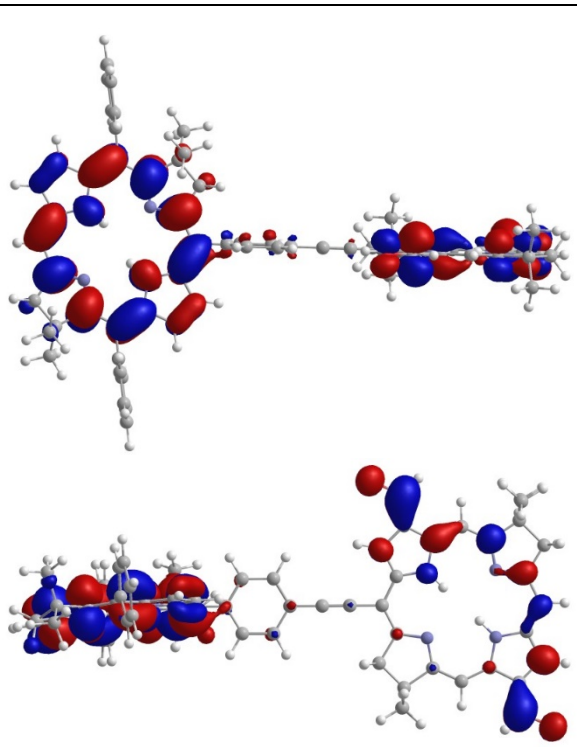
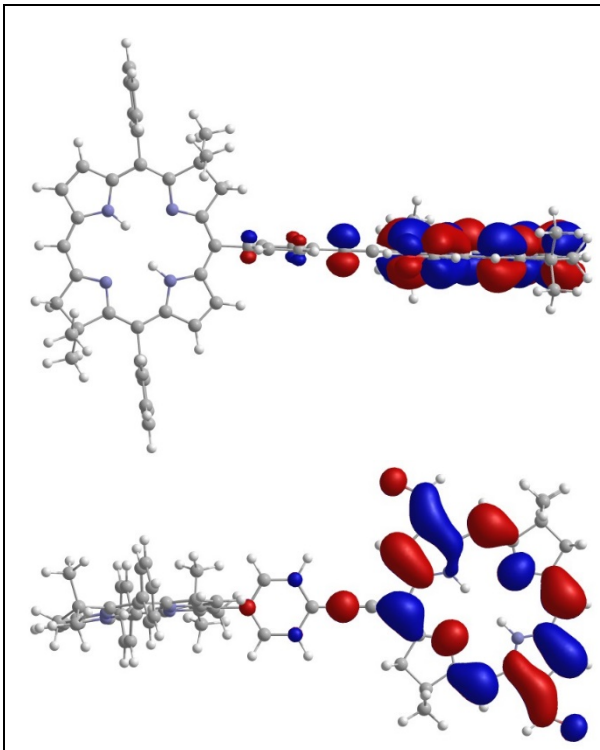
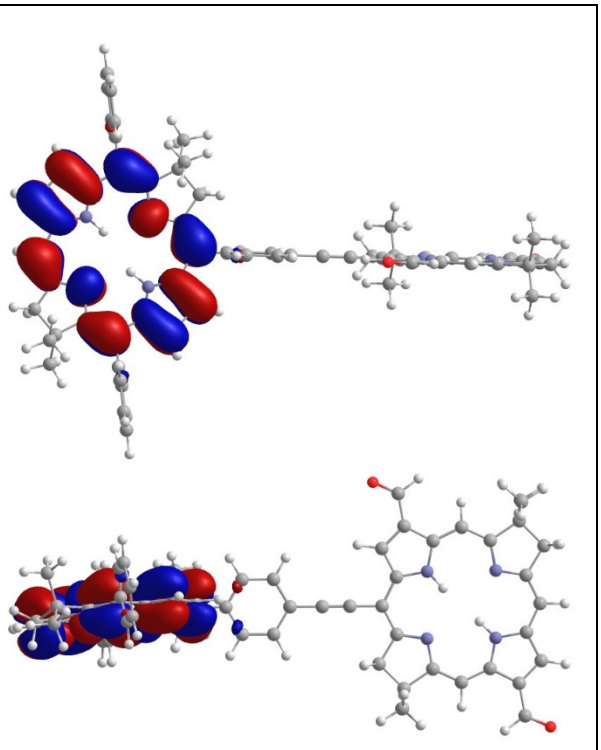
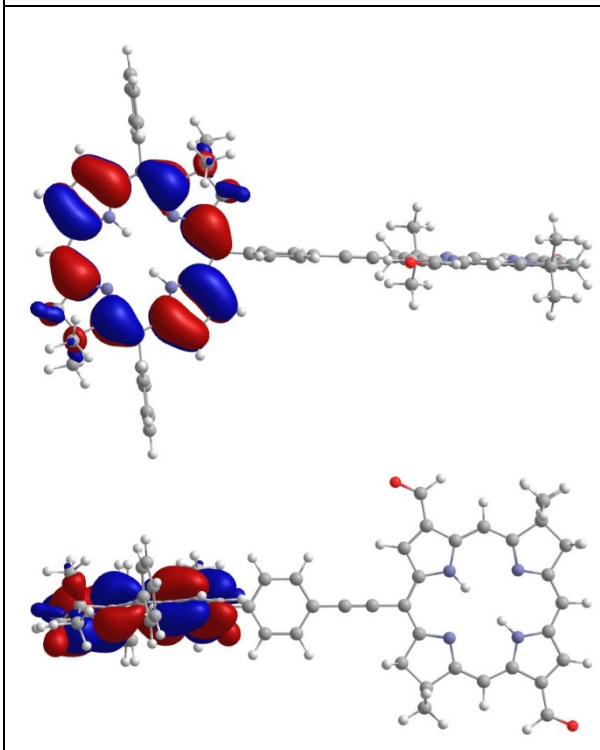
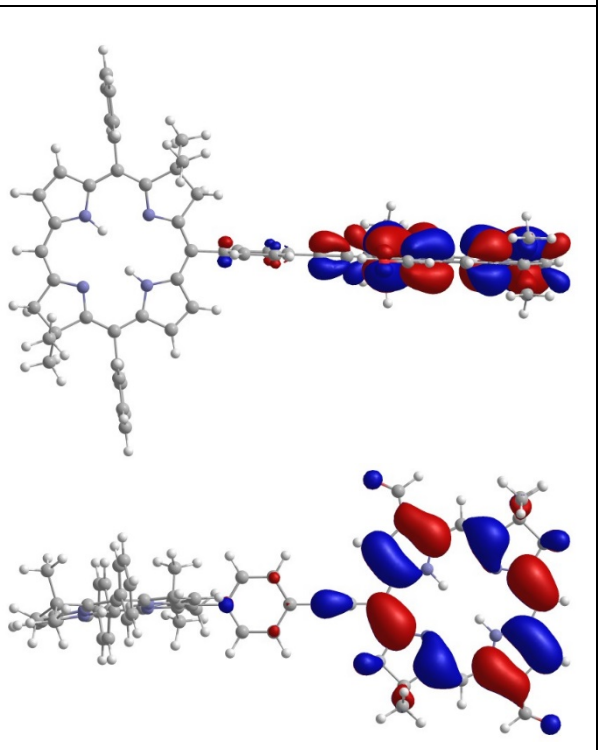
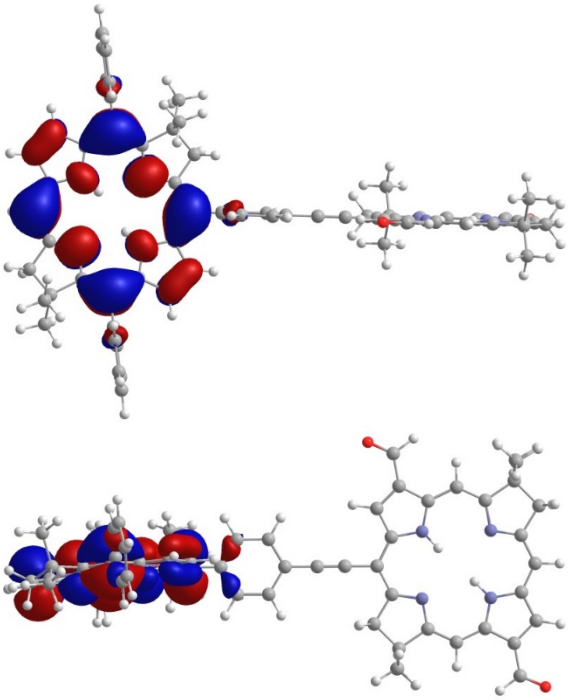
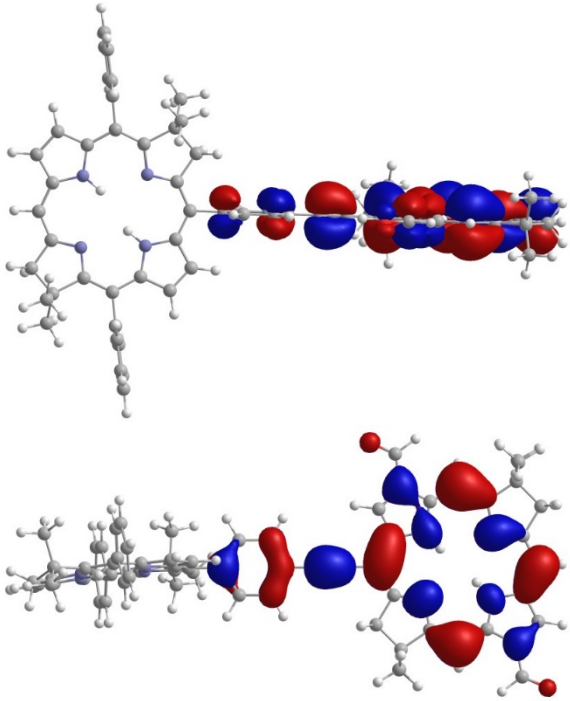
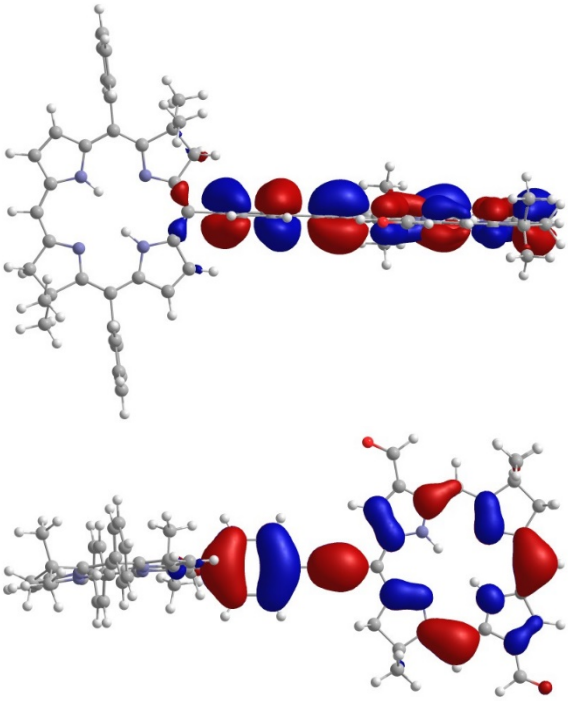
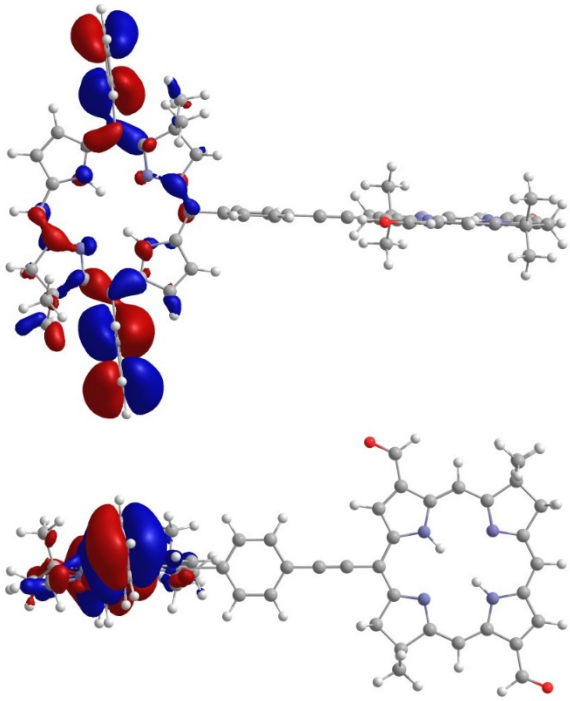
	
HOMO-6 -8.96 eV	HOMO-7 -8.99 eV
	
HOMO-8 -9.05 eV	HOMO-9 -9.08 eV

Table S11. MOs for **Dyad-9** in toluene.

	
LUMO+8 +1.04 eV	LUMO+9 +1.10 eV
	
LUMO+6 +0.73 eV	LUMO+7 +0.98 eV

	
LUMO+4 +0.10 eV	LUMO+5 +0.68 eV
	
LUMO+2 -0.47 eV	LUMO+3 +0.08 eV

	
LUMO -2.30 eV	LUMO+1 -1.48 eV
	
HOMO #277 -6.18 eV	HOMO-1 -6.65 eV

	
HOMO-2 -6.84 eV	HOMO-3 -7.10 eV
	
HOMO-4 -8.52 eV	HOMO-5 -8.93 eV

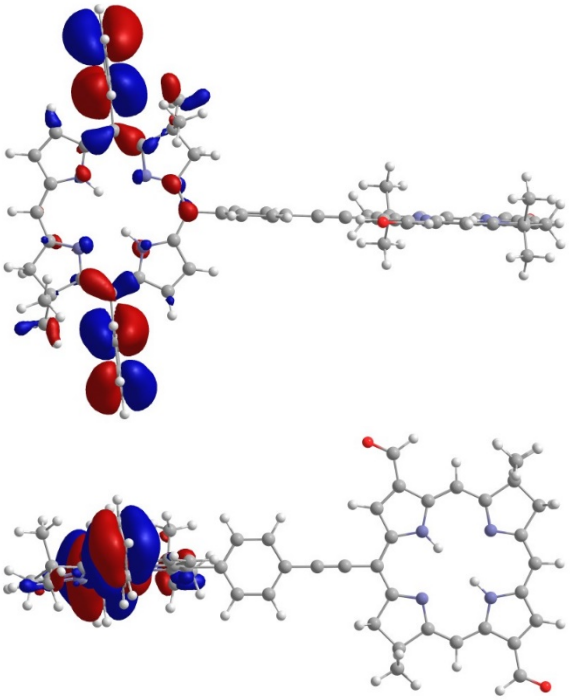
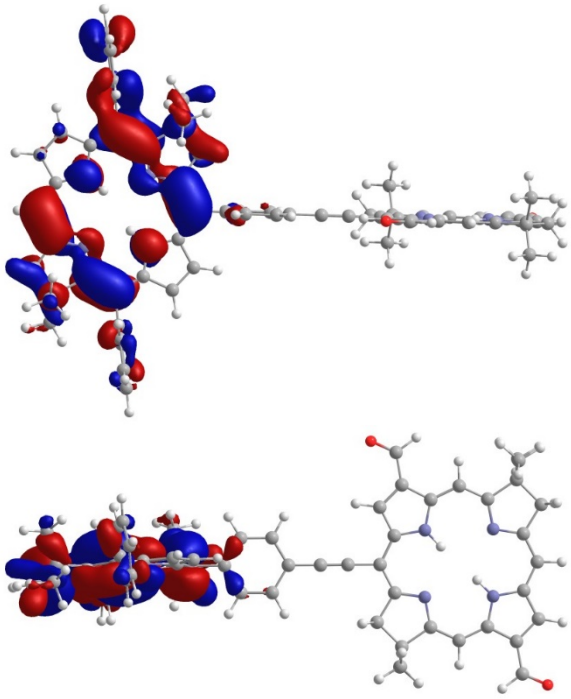
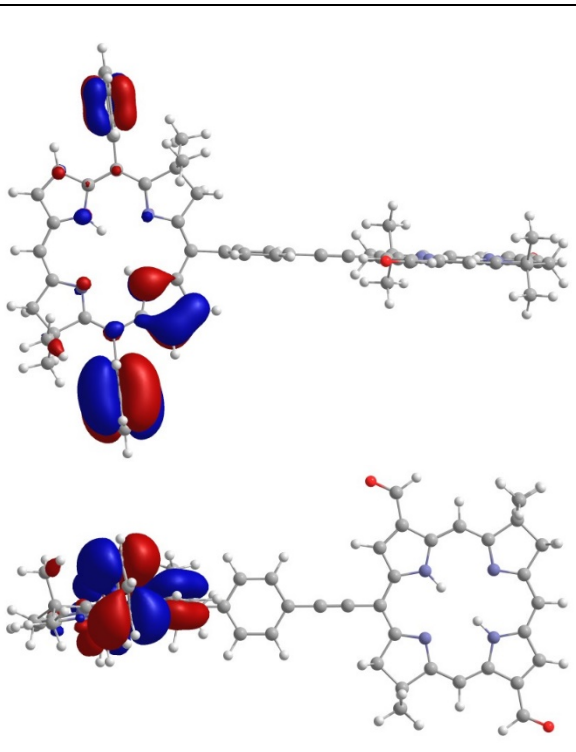
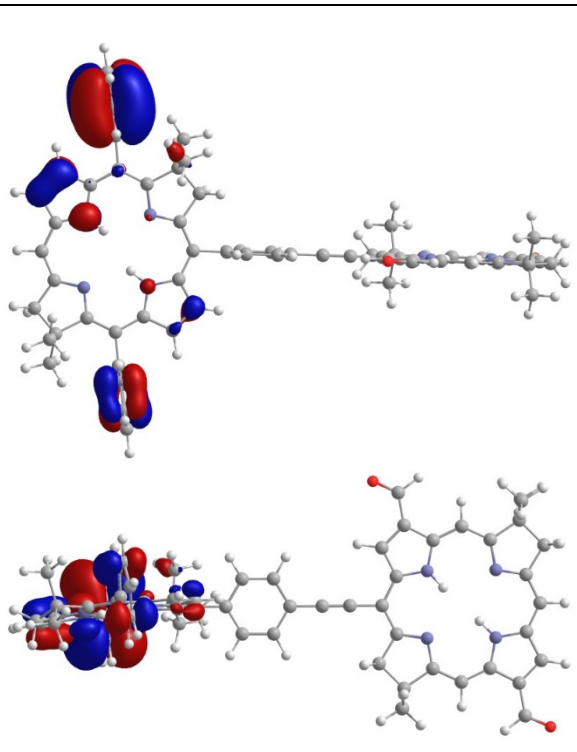
	
HOMO-6 -8.96 eV	HOMO-7 -9.00 eV
	
HOMO-8 -9.05 eV	HOMO-9 -9.08 eV

Table S12. TDDFT results for **Dyad-1**.

Excited State 1: 1.6308eV 760.28nm f=0.6749
H -2 335 -> L +2 340 0.16008 [5.13%]
H -1 336 -> L 338 0.62910 [79.15%]
H 337 -> L +1 339 -0.24448 [11.95%]
Excited State 2: 1.6602eV 746.78nm f=0.4551
H -3 334 -> L +3 341 -0.17013 [5.79%] **[-> - <- = 5.79 - 2.13 = 4.%
H -1 336 -> L 338 0.24004 [11.52%]
H 337 -> L +1 339 0.63070 [79.56%]
H -3 334 <- L +3 341 -0.10326 [2.13%] ** See -> Component Above
Excited State 3: 2.1240eV 583.74nm f=0.5563
H -3 334 -> L 338 -0.19366 [7.50%]
H -2 335 -> L 338 0.61294 [75.14%]
H -1 336 -> L +2 340 -0.25122 [12.62%]
Excited State 4: 2.3447eV 528.78nm f=0.1512
H -3 334 -> L +1 339 0.56897 [64.75%]
H -2 335 -> L +1 339 0.22224 [9.88%]
H 337 -> L +3 341 0.32963 [21.73%]
Excited State 5: 3.2946eV 376.33nm f=0.0089
H 337 -> L 338 0.68654 [94.27%]
H 337 -> L +5 343 0.10569 [2.23%]
Excited State 6: 3.3594eV 369.07nm f=2.4608
H -5 332 -> L 338 0.17584 [6.18%]
H -2 335 -> L 338 0.23917 [11.44%]
H -2 335 -> L +2 340 0.19109 [7.30%]
H -1 336 -> L +2 340 0.53253 [56.72%]
H -1 336 -> L +5 343 -0.12602 [3.18%]
H 337 -> L +3 341 0.18970 [7.20%]
Excited State 7: 3.4963eV 354.62nm f=1.4514
H -3 334 -> L +1 339 -0.24215 [11.73%]
H -2 335 -> L 338 -0.10599 [2.25%]
H -2 335 -> L +1 339 -0.15778 [4.98%]
H -2 335 -> L +2 340 0.15272 [4.66%]
H -1 336 -> L +2 340 -0.26908 [14.48%]
H 337 -> L +3 341 0.52506 [55.14%]
Excited State 8: 3.6174eV 342.75nm f=1.2243
H -5 332 -> L 338 0.14089 [3.97%]
H -3 334 -> L +1 339 0.16485 [5.44%]
H -3 334 -> L +2 340 -0.14985 [4.49%]
H -3 334 -> L +3 341 0.11198 [2.51%]
H -2 335 -> L +2 340 0.52138 [54.37%]
H -1 336 -> L 338 -0.17422 [6.07%]
H -1 336 -> L +2 340 -0.16696 [5.58%]
H 337 -> L +3 341 -0.23896 [11.42%]
Excited State 9: 3.7617eV 329.60nm f=0.0642
H -5 332 -> L +1 339 -0.12542 [3.15%]
H -3 334 -> L +1 339 0.13534 [3.66%]
H -2 335 -> L +1 339 -0.22198 [9.86%]
H -1 336 -> L +1 339 0.62302 [77.63%]
Excited State 10: 3.7851eV 327.56nm f=0.9883
H -6 331 -> L +1 339 -0.22545 [10.17%]

H -5 332 -> L   338   0.18695 [6.99%]
H -3 334 -> L   338   0.12810 [3.28%]
H -3 334 -> L +2 340   0.14892 [4.44%]
H -3 334 -> L +3 341   0.47419 [44.97%]
H -2 335 -> L +2 340   -0.15825 [5.01%]
H -2 335 -> L +3 341   0.21250 [9.03%]
H   337 -> L +1 339   0.16650 [5.54%]
Excited State 11:   3.8201eV   324.56nm   f=0.8738
H-18 319 -> L   338   -0.12477 [3.11%]
H-16 321 -> L   338   0.15765 [4.97%]
H -6 331 -> L +1 339   0.14450 [4.18%]
H -5 332 -> L   338   0.45094 [40.67%]
H -4 333 -> L   338   -0.19619 [7.70%]
H -3 334 -> L   338   0.14458 [4.18%]
H -3 334 -> L +3 341   -0.24689 [12.19%]
H -2 335 -> L +2 340   -0.16078 [5.17%]
H -1 336 -> L +2 340   -0.12459 [3.10%]
Excited State 12:   3.9121eV   316.92nm   f=0.0023
H-28 309 -> L +1 339   0.16102 [5.19%]
H-10 327 -> L +1 339   -0.15780 [4.98%]
H -5 332 -> L +1 339   0.23032 [10.61%]
H -4 333 -> L +1 339   0.57583 [66.32%]
Excited State 13:   4.0187eV   308.52nm   f=0.0875
H-26 311 -> L +1 339   -0.12412 [3.08%]
H-25 312 -> L +1 339   -0.13051 [3.41%]
H -6 331 -> L +1 339   0.48340 [46.74%]
H -5 332 -> L   338   -0.12425 [3.09%]
H -3 334 -> L   338   0.32411 [21.01%]
H -3 334 -> L +3 341   0.17689 [6.26%]
H -2 335 -> L   338   0.10084 [2.03%]
Excited State 14:   4.0216eV   308.29nm   f=0.0071
H -5 332 -> L +1 339   0.16988 [5.77%]
H -3 334 -> L   338   0.13038 [3.40%]
H -3 334 -> L +1 339   -0.19003 [7.22%]
H -2 335 -> L +1 339   0.54068 [58.47%]
H -1 336 -> L +1 339   0.30385 [18.46%]
Excited State 15:   4.0532eV   305.90nm   f=0.1017
H -6 331 -> L +1 339   -0.29410 [17.30%]
H -3 334 -> L   338   0.48945 [47.91%]
H -3 334 -> L +1 339   0.10911 [2.38%]
H -3 334 -> L +3 341   -0.19683 [7.75%]
H -3 334 -> L +5 343   0.12380 [3.07%]
H -2 335 -> L   338   0.16791 [5.64%]
Excited State 16:   4.1892eV   295.96nm   f=0.0160
H-27 310 -> L   338   -0.19799 [7.84%]
H-26 311 -> L   338   0.12865 [3.31%]
H-25 312 -> L   338   -0.10132 [2.05%]
H-24 313 -> L   338   -0.11231 [2.52%]
H-23 314 -> L   338   -0.55785 [62.24%]
H-16 321 -> L   338   0.12739 [3.25%]
H -9 328 -> L   338   0.15242 [4.65%]

Table S13. TDDFT results for **Dyad-2**.

Excited State 1: 1.6469eV 752.84nm f=0.6237
H -2 328 -> L +3 334 0.17179 [5.90%] **[-> - <- = 5.90 - 2.14 = 4.%
H -1 329 -> L +1 332 0.19454 [7.57%]
H 330 -> L 331 0.64511 [83.23%]
H -2 328 <- L +3 334 0.10348 [2.14%] ** See -> Component Above
Excited State 2: 1.6814eV 737.38nm f=0.3031
H -3 327 -> L +4 335 0.19481 [7.59%] **[-> - <- = 7.59 - 2.61 = 5.%
H -1 329 -> L +1 332 0.64165 [82.34%]
H 330 -> L 331 -0.17469 [6.10%]
H -3 327 <- L +4 335 0.11413 [2.61%] ** See -> Component Above
Excited State 3: 2.1586eV 574.37nm f=0.5110
H -3 327 -> L +1 332 -0.11786 [2.78%]
H -2 328 -> L 331 0.62458 [78.02%]
H 330 -> L +3 334 -0.25780 [13.29%]
Excited State 4: 2.2783eV 544.19nm f=0.2145
H -3 327 -> L +1 332 0.61157 [74.80%]
H -2 328 -> L +1 332 -0.12675 [3.21%]
H -1 329 -> L +4 335 -0.28730 [16.51%]
Excited State 5: 3.3791eV 366.91nm f=2.2850
H -4 326 -> L 331 0.18305 [6.70%]
H -2 328 -> L 331 0.25152 [12.65%]
H -2 328 -> L +3 334 0.17123 [5.86%]
H -1 329 -> L +4 335 -0.18765 [7.04%]
H 330 -> L +3 334 0.54173 [58.69%]
H 330 -> L +5 336 -0.13483 [3.64%]
Excited State 6: 3.4841eV 355.85nm f=1.2201
H -3 327 -> L +1 332 0.23826 [11.35%]
H -1 329 -> L 331 -0.32217 [20.76%]
H -1 329 -> L +2 333 -0.14491 [4.20%]
H -1 329 -> L +3 334 -0.13490 [3.64%]
H -1 329 -> L +4 335 0.48200 [46.46%]
H 330 -> L +3 334 0.17917 [6.42%]
Excited State 7: 3.5154eV 352.69nm f=0.3630
H -3 327 -> L +1 332 0.10669 [2.28%]
H -1 329 -> L 331 0.59982 [71.96%]
H -1 329 -> L +4 335 0.25081 [12.58%]
H -1 329 -> L +5 336 0.11577 [2.68%]
H 330 -> L +3 334 0.11701 [2.74%]
Excited State 8: 3.6075eV 343.68nm f=0.2361
H -4 326 -> L +1 332 -0.12705 [3.23%]
H -3 327 -> L +1 332 -0.12564 [3.16%]
H -2 328 -> L +1 332 -0.22475 [10.10%]
H -2 328 -> L +3 334 -0.18559 [6.89%]
H -1 329 -> L +4 335 -0.11892 [2.83%]
H 330 -> L 331 0.10700 [2.29%]
H 330 -> L +1 332 0.57518 [66.17%]
Excited State 9: 3.6333eV 341.25nm f=1.7401
H -4 326 -> L 331 0.14565 [4.24%]
H -3 327 -> L +4 335 0.15438 [4.77%]
H -2 328 -> L +3 334 0.52328 [54.76%]
H -1 329 -> L +4 335 0.11833 [2.80%]

H 330 -> L 331 -0.13763 [3.79%]
H 330 -> L +1 332 0.24999 [12.50%]
H 330 -> L +3 334 -0.17486 [6.12%]
Excited State 10: 3.7650eV 329.31nm f=0.1575
H -3 327 -> L +2 333 0.18450 [6.81%]
H -3 327 -> L +4 335 -0.23310 [10.87%]
H -2 328 -> L +3 334 0.10426 [2.17%]
H -1 329 -> L +2 333 0.56251 [63.28%]
H -1 329 -> L +4 335 0.16660 [5.55%]
Excited State 11: 3.7983eV 326.42nm f=0.7939
H -3 327 -> L +3 334 -0.12438 [3.09%]
H -3 327 -> L +4 335 0.53905 [58.11%]
H -2 328 -> L +3 334 -0.14527 [4.22%]
H -2 328 -> L +4 335 -0.13177 [3.47%]
H -1 329 -> L +1 332 -0.17988 [6.47%] **[-> - <- = 6.47 - 2.29 = 4.%
H -1 329 -> L +2 333 0.29781 [17.74%]
H -1 329 <- L +1 332 0.10702 [2.29%] ** See -> Component Above
Excited State 12: 3.8838eV 319.24nm f=0.2603
H-18 312 -> L 331 -0.17559 [6.17%]
H-14 316 -> L 331 0.17026 [5.80%]
H -4 326 -> L 331 0.55785 [62.24%]
H -3 327 -> L +4 335 -0.11002 [2.42%]
H -2 328 -> L +3 334 -0.18730 [7.02%]
H 330 -> L +3 334 -0.13833 [3.83%]
Excited State 13: 3.8960eV 318.24nm f=0.0077
H -4 326 -> L +1 332 0.20057 [8.05%]
H -3 327 -> L +1 332 0.10791 [2.33%]
H -2 328 -> L +1 332 0.58183 [67.71%]
H 330 -> L +1 332 0.29676 [17.61%]
Excited State 14: 3.9110eV 317.01nm f=0.0000
H-24 306 -> L +2 333 -0.29385 [17.27%]
H-23 307 -> L +2 333 0.58296 [67.97%]
Excited State 15: 4.1189eV 301.01nm f=0.0041
H -3 327 -> L 331 0.65333 [85.37%]
H -3 327 -> L +5 336 0.13992 [3.92%]
H -2 328 -> L 331 -0.10527 [2.22%]
Excited State 16: 4.1360eV 299.77nm f=0.0098
H-27 303 -> L +1 332 -0.23245 [10.81%]
H-21 309 -> L +1 332 -0.10398 [2.16%]
H-20 310 -> L +1 332 -0.19905 [7.92%]
H-17 313 -> L +1 332 0.18654 [6.96%]
H-10 320 -> L +1 332 0.23301 [10.86%]
H -9 321 -> L +1 332 0.49033 [48.08%]

Table S14. TDDFT results for **Dyad-3**.

Excited State 1: Singlet-A 1.5703 eV 789.58 nm f=0.7667
H-2 297 -> 302 L+2 -0.15459 5%
H-1 298 -> 300 L 0.63956 82%
H 299 -> 301 L+1 -0.19944 8%
Excited State 2: Singlet-A 1.6191 eV 765.77 nm f=0.4379
H-3 296 -> 303 L+3 0.17808 6.34-2.36= 4%
H-1 298 -> 300 L 0.20809 9%
H 299 -> 301 L+1 0.64228 83%
H-3 296 <- 303 L+3 0.10874 2.36%
Excited State 3: Singlet-A 2.0669 eV 599.85 nm f=0.4303
H-3 296 -> 300 L -0.16305 5%
H-3 296 -> 301 L+1 -0.10039 2%
H-2 297 -> 300 L 0.62863 79%
H-1 298 -> 302 L+2 0.22367 10%
Excited State 4: Singlet-A 2.2176 eV 559.09 nm f=0.2088
H-3 296 -> 301 L+1 0.60784 74%
H-2 297 -> 301 L+1 0.20719 9%
H 299 -> 303 L+3 -0.26134 14%
Excited State 5: Singlet-A 3.3029 eV 375.38 nm f=0.0562
H-1 298 -> 302 L+2 0.11117 2%
H 299 -> 300 L 0.67226 90%
Excited State 6: Singlet-A 3.3618 eV 368.80 nm f=1.6055
H-4 295 -> 300 L 0.23849 11%
H-2 297 -> 300 L -0.22017 10%
H-2 297 -> 302 L+2 0.22476 10%
H-1 298 -> 302 L+2 0.50551 51%
H-1 298 -> 304 L+4 0.10921 2%
H 299 -> 300 L -0.12802 3%
H 299 -> 303 L+3 0.12680 3%
Excited State 7: Singlet-A 3.4727 eV 357.03 nm f=0.6849
H-4 295 -> 301 L+1 0.12349 3%
H-2 297 -> 301 L+1 -0.27001 15%
H-2 297 -> 302 L+2 -0.16088 5%
H-1 298 -> 301 L+1 0.45343 41%
H-1 298 -> 302 L+2 0.21016 9%
H 299 -> 303 L+3 -0.31873 20%
Excited State 8: Singlet-A 3.5298 eV 351.25 nm f=0.7823
H-3 296 -> 301 L+1 0.25091 13%
H-1 298 -> 301 L+1 0.38551 30%
H-1 298 -> 302 L+2 -0.14294 4%
H 299 -> 303 L+3 0.48133 46%
Excited State 9: Singlet-A 3.5831 eV 346.02 nm f=1.0444
H-4 295 -> 300 L 0.19964 8%
H-3 296 -> 301 L+1 -0.10877 2%
H-3 296 -> 302 L+2 -0.11009 2%
H-3 296 -> 303 L+3 0.11386 3%
H-2 297 -> 302 L+2 0.46841 44%
H-1 298 -> 300 L 0.13508 4%
H-1 298 -> 301 L+1 0.15054 5%
H-1 298 -> 302 L+2 -0.25130 13%
H 299 -> 303 L+3 -0.24746 12%

Excited State 10: Singlet-A 3.7624 eV 329.54 nm f=0.2611
H-7 292 -> 300 L 0.17826 6%
H-4 295 -> 300 L 0.49415 48%
H-3 296 -> 300 L -0.18670 7%
H-3 296 -> 302 L+2 0.10690 2%
H-2 297 -> 302 L+2 -0.29352 17%
H-1 298 -> 302 L+2 -0.13493 4%
Excited State 11: Singlet-A 3.7933 eV 326.85 nm f=0.0490
H-4 295 -> 301 L+1 -0.18178 7%
H-3 296 -> 301 L+1 -0.17141 6%
H-2 297 -> 301 L+1 0.53001 56%
H-1 298 -> 301 L+1 0.32215 21%
Excited State 12: Singlet-A 3.8262 eV 324.04 nm f=1.3928
H-4 295 -> 300 L -0.15200 5%
H-3 296 -> 302 L+2 0.11765 3%
H-3 296 -> 303 L+3 0.58948 69%
H-2 297 -> 301 L+1 -0.10538 2%
H-2 297 -> 303 L+3 0.19693 8%
H 299 -> 301 L+1 -0.19786 8%
H 299 <- 301 L+1 0.11501 3%
Excited State 13: Singlet-A 3.9594 eV 313.14 nm f=0.0258
H-7 292 -> 300 L 0.10222 2%
H-4 295 -> 300 L 0.14824 4%
H-3 296 -> 300 L 0.62418 78%
H-3 296 -> 303 L+3 0.10265 2%
H-2 297 -> 300 L 0.17025 6%
Excited State 14: Singlet-A 4.1042 eV 302.09 nm f=0.0008
Excited State 15: Singlet-A 4.1292 eV 300.26 nm f=0.0002
Excited State 16: Singlet-A 4.1985 eV 295.30 nm f=0.0247
H-18 281 -> 300 L -0.12572 3%
H-11 288 -> 300 L 0.12177 3%
H-9 290 -> 300 L -0.25473 13%
H-7 292 -> 300 L 0.27284 15%
H-4 295 -> 300 L -0.10192 2%
H-1 298 -> 304 L+4 0.44688 40%
H-1 298 -> 306 L+6 -0.25530 13%

Table S15. TDDFT results for **Dyad-4**.

Excited State 1: 1.6322eV 759.59nm f=0.6269
H -2 354 -> L +3 360 0.17579 [6.18%] **[-> - <- = 6.18 - 2.26 = 4.%
H -1 355 -> L 357 0.65978 [87.06%]
H 356 -> L +1 358 0.13838 [3.83%]
H -2 354 <- L +3 360 0.10641 [2.26%] ** See -> Component Above
Excited State 2: 1.6811eV 737.51nm f=0.3459
H -3 353 -> L +4 361 0.19995 [8.00%] **[-> - <- = 8.00 - 2.75 = 5.%
H -1 355 -> L 357 -0.13610 [3.70%]
H 356 -> L +1 358 0.66110 [87.41%]
H -3 353 <- L +4 361 0.11725 [2.75%] ** See -> Component Above
Excited State 3: 2.1264eV 583.08nm f=0.5838
H -2 354 -> L 357 0.63490 [80.62%]
H -1 355 -> L +3 360 -0.25096 [12.60%]
Excited State 4: 2.2784eV 544.18nm f=0.2258
H -3 353 -> L +1 358 0.62053 [77.01%]
H -2 354 -> L +1 358 -0.10811 [2.34%]
H 356 -> L +4 361 -0.29059 [16.89%]
Excited State 5: 3.3674eV 368.19nm f=2.3922
H -4 352 -> L 357 0.18362 [6.74%]
H -2 354 -> L 357 0.24012 [11.53%]
H -2 354 -> L +3 360 0.18094 [6.55%]
H -1 355 -> L +3 360 0.55043 [60.59%]
H -1 355 -> L +6 363 -0.13234 [3.50%]
H 356 -> L +4 361 -0.15993 [5.12%]
Excited State 6: 3.4575eV 358.60nm f=0.1777
H -3 353 -> L +1 358 -0.10028 [2.01%]
H 356 -> L 357 0.64860 [84.14%]
H 356 -> L +4 361 -0.18452 [6.81%]
H 356 -> L +6 363 0.10400 [2.16%]
Excited State 7: 3.4935eV 354.90nm f=1.4799
H -3 353 -> L +1 358 0.24952 [12.45%]
H -2 354 -> L +3 360 -0.11592 [2.69%]
H -1 355 -> L +3 360 0.21119 [8.92%]
H 356 -> L 357 0.23256 [10.82%]
H 356 -> L +2 359 -0.19523 [7.62%]
H 356 -> L +4 361 0.51321 [52.68%]
Excited State 8: 3.6127eV 343.19nm f=1.7459
H -4 352 -> L 357 0.15568 [4.85%]
H -3 353 -> L +1 358 0.11551 [2.67%]
H -3 353 -> L +4 361 0.13867 [3.85%]
H -2 354 -> L +3 360 0.54692 [59.82%]
H -1 355 -> L 357 -0.17659 [6.24%]
H -1 355 -> L +1 358 -0.10060 [2.02%]
H -1 355 -> L +3 360 -0.18107 [6.56%]
H 356 -> L +4 361 0.16004 [5.12%]
Excited State 9: 3.6464eV 340.02nm f=0.1028
H -4 352 -> L +1 358 -0.14621 [4.28%]
H -2 354 -> L +1 358 -0.26615 [14.17%]
H -2 354 -> L +3 360 0.12204 [2.98%]
H -1 355 -> L +1 358 0.61287 [75.12%]
Excited State 10: 3.7671eV 329.12nm f=0.1766

H -3 353 -> L +2 359   0.20724 [8.59%]
H -3 353 -> L +4 361   -0.26206 [13.74%]
H -2 354 -> L +3 360   0.12136 [2.95%]
H   356 -> L +1 358   0.10679 [2.28%]
H   356 -> L +2 359   0.52900 [55.97%]
H   356 -> L +4 361   0.19759 [7.81%]
Excited State 11:   3.7922eV   326.94nm   f=0.5802
H -4 352 -> L   357   0.14585 [4.25%]
H -3 353 -> L +4 361   0.49554 [49.11%]
H -2 354 -> L +3 360   -0.16127 [5.20%]
H -2 354 -> L +4 361   -0.10343 [2.14%]
H   356 -> L +1 358   -0.16345 [5.34%]
H   356 -> L +2 359   0.33105 [21.92%]
H   356 -> L +4 361   0.12058 [2.91%]
Excited State 12:   3.8334eV   323.43nm   f=0.6014
H-20 336 -> L   357   -0.13963 [3.90%]
H-15 341 -> L   357   0.17605 [6.20%]
H -4 352 -> L   357   0.54481 [59.36%]
H -3 353 -> L +4 361   -0.21712 [9.43%]
H -2 354 -> L +3 360   -0.15500 [4.81%]
H -1 355 -> L +3 360   -0.12553 [3.15%]
Excited State 13:   3.9092eV   317.16nm   f=0.0001
H-25 331 -> L +2 359   -0.64196 [82.42%]
H-25 331 -> L +4 361   -0.12289 [3.02%]
Excited State 14:   3.9106eV   317.05nm   f=0.0048
H -4 352 -> L +1 358   0.18961 [7.19%]
H -2 354 -> L +1 358   0.57663 [66.50%]
H -1 355 -> L +1 358   0.32307 [20.87%]
Excited State 15:   4.0727eV   304.43nm   f=0.0030
H -3 353 -> L   357   0.66386 [88.14%]
H -3 353 -> L +6 363   0.13651 [3.73%]
Excited State 16:   4.1369eV   299.70nm   f=0.0098
H-28 328 -> L +1 358   0.23392 [10.94%]
H-23 333 -> L +1 358   -0.12541 [3.15%]
H-21 335 -> L +1 358   -0.20236 [8.19%]
H-19 337 -> L +1 358   0.13955 [3.89%]
H-17 339 -> L +1 358   0.13025 [3.39%]
H-11 345 -> L +1 358   -0.24382 [11.89%]
H-10 346 -> L +1 358   0.48417 [46.88%]

Table S16. TDDFT results for **Dyad-5**.

Excited State 1: Singlet-A 1.6482 eV 752.22 nm f=0.5486
H-2 301 -> 306 L+2 0.17918 6.42-2.31= 4%
H-1 302 -> 304 L 0.66363 88%
H 303 -> 305 L+1 -0.12854 3%
H-2 301 <- 306 L+2 0.10750 2.31%
Excited State 2: Singlet-A 1.6989 eV 729.81 nm f=0.3466
H-3 300 -> 307 L+3 0.20807 8.66-2.94= 6%
H-1 302 -> 304 L 0.12230 3%
H 303 -> 305 L+1 0.66500 88%
H-3 300 <- 307 L+3 0.12123 2.94%
Excited State 3: Singlet-A 2.1584 eV 574.43 nm f=0.4739
H-2 301 -> 304 L 0.63178 80%
H-1 302 -> 306 L+2 -0.26358 14%
Excited State 4: Singlet-A 2.3112 eV 536.45 nm f=0.1881
H-3 300 -> 305 L+1 0.61901 77%
H 303 -> 307 L+3 -0.31256 20%
Excited State 5: Singlet-A 3.3814 eV 366.67 nm f=2.0730
H-4 299 -> 304 L 0.18608 7%
H-2 301 -> 304 L 0.25553 13%
H-2 301 -> 306 L+2 0.16614 6%
H-1 302 -> 306 L+2 0.56182 63%
H-1 302 -> 308 L+4 0.13103 3%
H 303 -> 307 L+3 -0.14715 4%
Excited State 6: Singlet-A 3.4250 eV 362.00 nm f=0.0152
H 303 -> 304 L 0.68577 94%
H 303 -> 308 L+4 -0.12053 3%
Excited State 7: Singlet-A 3.5167 eV 352.55 nm f=1.7535
H-3 300 -> 305 L+1 0.28550 16%
H-2 301 -> 306 L+2 -0.14021 4%
H-1 302 -> 306 L+2 0.19596 8%
H 303 -> 307 L+3 0.58194 68%
H-3 300 <- 305 L+1 -0.10416 2.17%
Excited State 8: Singlet-A 3.6325 eV 341.32 nm f=1.8157
H-4 299 -> 304 L 0.16245 5%
H-3 300 -> 305 L+1 0.11195 3%
H-3 300 -> 307 L+3 -0.13900 4%
H-2 301 -> 306 L+2 0.56308 63%
H-1 302 -> 304 L -0.17642 6%
H-1 302 -> 306 L+2 -0.17593 6%
H 303 -> 307 L+3 0.18582 7%
Excited State 9: Singlet-A 3.7035 eV 334.77 nm f=0.0124
H-4 299 -> 305 L+1 -0.14230 4%
H-2 301 -> 305 L+1 -0.25793 13%
H-1 302 -> 305 L+1 0.63337 80%
Excited State 10: Singlet-A 3.8317 eV 323.57 nm f=0.8318
H-4 299 -> 304 L -0.12046 3%
H-3 300 -> 307 L+3 0.61012 74%
H-2 301 -> 306 L+2 0.18603 7%
H-2 301 -> 307 L+3 0.10987 2%
H 303 -> 305 L+1 -0.20450 8%
H 303 <- 305 L+1 0.11954 3%

Excited State 11: Singlet-A 3.8838 eV 319.23 nm f=0.3849
H-17 286 -> 304 L -0.17260 6%
H-15 288 -> 304 L -0.18140 7%
H-4 299 -> 304 L 0.55095 61%
H-3 300 -> 307 L+3 0.19312 7%
H-2 301 -> 306 L+2 -0.16983 6%
H-1 302 -> 306 L+2 -0.13682 4%
Excited State 12: Singlet-A 3.9868 eV 310.99 nm f=0.0021
Excited State 13: Singlet-A 4.0781 eV 304.02 nm f=0.0025
Excited State 14: Singlet-A 4.1806 eV 296.57 nm f=0.0069
Excited State 15: Singlet-A 4.2052 eV 294.83 nm f=0.0126
H-26 277 -> 304 L -0.10271 2%
H-25 278 -> 304 L 0.24560 12%
H-23 280 -> 304 L 0.52538 55%
H-22 281 -> 304 L 0.19126 7%
H-21 282 -> 304 L 0.11443 3%
H-15 288 -> 304 L 0.14861 4%
H-9 294 -> 304 L 0.12812 3%
H-7 296 -> 304 L 0.11393 3%
Excited State 16: Singlet-A 4.2718 eV 290.24 nm f=0.0250
H-20 283 -> 305 L+1 0.65747 86%
H-6 297 -> 305 L+1 0.14433 4%

Table S17. TDDFT results for **Dyad-6**.

Excited State 1: 1.6113eV 769.46nm f=0.6553
H -2 309 -> L +2 314 0.17435 [6.08%] **[-> - <- = 6.08 - 2.24 = 4.%
H 311 -> L 312 0.67785 [91.90%]
H -2 309 <- L +2 314 0.10584 [2.24%] ** See -> Component Above
Excited State 2: 1.6980eV 730.19nm f=0.4032
H -3 308 -> L +3 315 -0.21047 [8.86%] **[-> - <- = 8.86 - 3.01 = 6.%
H -1 310 -> L +1 313 0.67462 [91.02%]
H -3 308 <- L +3 315 -0.12277 [3.01%] ** See -> Component Above
Excited State 3: 2.2007eV 563.40nm f=0.4518
H -3 308 -> L +1 313 0.11041 [2.44%]
H -2 309 -> L 312 0.62353 [77.76%]
H 311 -> L +2 314 -0.27320 [14.93%]
Excited State 4: 2.3118eV 536.30nm f=0.1721
H -3 308 -> L +1 313 0.61378 [75.35%]
H -2 309 -> L +1 313 -0.10126 [2.05%]
H -1 310 -> L +3 315 0.31058 [19.29%]
Excited State 5: 3.3356eV 371.70nm f=2.2521
H -4 307 -> L 312 -0.15311 [4.69%]
H -2 309 -> L 312 0.26431 [13.97%]
H -2 309 -> L +2 314 -0.18218 [6.64%]
H -1 310 -> L +3 315 -0.12888 [3.32%]
H 311 -> L +2 314 0.55971 [62.66%]
H 311 -> L +4 316 0.12284 [3.02%]
Excited State 6: 3.4487eV 359.51nm f=0.0304
H -1 310 -> L 312 0.68105 [92.77%]
H -1 310 -> L +4 316 0.11834 [2.80%]
Excited State 7: 3.5208eV 352.14nm f=1.5063
H -3 308 -> L +1 313 -0.29361 [17.24%] **[-> - <- = 17.24 - 2.29 = 15.%
H -2 309 -> L +2 314 0.10015 [2.01%]
H -1 310 -> L +3 315 0.59507 [70.82%]
H 311 -> L +2 314 0.16027 [5.14%]
H -3 308 <- L +1 313 0.10702 [2.29%] ** See -> Component Above
Excited State 8: 3.6373eV 340.87nm f=1.8401
H -5 306 -> L 312 0.13320 [3.55%]
H -3 308 -> L +3 315 0.11022 [2.43%]
H -2 309 -> L +2 314 0.57242 [65.53%]
H -1 310 -> L +3 315 -0.13723 [3.77%]
H 311 -> L 312 -0.17662 [6.24%]
H 311 -> L +2 314 0.18459 [6.81%]
Excited State 9: 3.6749eV 337.38nm f=0.0247
H -2 309 -> L +1 313 0.17629 [6.22%]
H 311 -> L +1 313 0.67130 [90.13%]
Excited State 10: 3.7981eV 326.44nm f=0.2791
H-26 285 -> L 312 -0.12023 [2.89%]
H -5 306 -> L 312 0.49016 [48.05%]
H -4 307 -> L 312 -0.31482 [19.82%]
H -3 308 -> L +3 315 -0.27308 [14.91%]
Excited State 11: 3.8340eV 323.38nm f=0.8410
H -6 305 -> L 312 0.12487 [3.12%]
H -5 306 -> L 312 0.24243 [11.75%]
H -4 307 -> L 312 -0.12716 [3.23%]

H -3 308 -> L +3 315   0.56120 [62.99%]
H -2 309 -> L +2 314   -0.11963 [2.86%]
H -2 309 -> L +3 315   -0.10314 [2.13%]
H -1 310 -> L +1 313   0.18929 [7.17%] **[-> - <- =   7.17 - 2.44 =   5.%
H -1 310 <- L +1 313   -0.11041 [2.44%] ** See -> Component Above
Excited State 12:   3.9143eV   316.75nm   f=0.0052
H -6 305 -> L +1 313   -0.10062 [2.02%]
H -4 307 -> L +1 313   -0.17933 [6.43%]
H -3 308 -> L +1 313   0.10271 [2.11%]
H -2 309 -> L +1 313   0.61180 [74.86%]
H   311 -> L +1 313   -0.20775 [8.63%]
Excited State 13:   3.9394eV   314.73nm   f=0.0676
H-25 286 -> L   312   -0.21268 [9.05%]
H -6 305 -> L   312   0.47831 [45.76%]
H -5 306 -> L   312   -0.19242 [7.41%]
H -4 307 -> L   312   -0.33216 [22.07%]
H -2 309 -> L +2 314   0.17416 [6.07%]
Excited State 14:   3.9456eV   314.23nm   f=0.1735
H-15 296 -> L   312   -0.17965 [6.45%]
H -6 305 -> L   312   0.36095 [26.06%]
H -5 306 -> L   312   0.21882 [9.58%]
H -4 307 -> L   312   0.41574 [34.57%]
H -3 308 -> L   312   0.10163 [2.07%]
H -3 308 -> L +3 315   -0.14566 [4.24%]
H -2 309 -> L +4 316   -0.10385 [2.16%]
H   311 -> L +2 314   0.14592 [4.26%]
Excited State 15:   4.1033eV   302.16nm   f=0.0018
H -3 308 -> L   312   0.66024 [87.18%]
H -3 308 -> L +4 316   0.13961 [3.90%]
Excited State 16:   4.1816eV   296.50nm   f=0.0066
H-20 291 -> L +1 313   0.24304 [11.81%]
H-19 292 -> L +1 313   0.11674 [2.73%]
H-17 294 -> L +1 313   0.15428 [4.76%]
H-16 295 -> L +1 313   -0.22566 [10.18%]
H-10 301 -> L +1 313   0.19405 [7.53%]
H -9 302 -> L +1 313   0.50808 [51.63%]
H -8 303 -> L +1 313   0.10446 [2.18%]

Table S18. TDDFT results for **Dyad-7**.

Excited State 1: Singlet-A 1.5731 eV 788.17 nm f=0.6565
H-3 325 -> 331 L+2 0.12245 3%
H-1 327 -> 329 L 0.67530 91%
Excited State 2: Singlet-A 1.6800 eV 737.98 nm f=0.4273
H-3 325 -> 333 L+4 0.12434 3%
H-2 326 -> 333 L+4 0.16766 6%
H 328 -> 330 L+1 0.67266 90%
Excited State 3: Singlet-A 2.0663 eV 600.04 nm f=0.4459
H-3 325 -> 329 L 0.51599 53%
H-2 326 -> 329 L -0.40347 33%
H-1 327 -> 331 L+2 -0.20673 9%
Excited State 4: Singlet-A 2.2779 eV 544.28 nm f=0.2446
H-3 325 -> 330 L+1 0.37532 28%
H-2 326 -> 330 L+1 0.51069 52%
Excited State 5: Singlet-A 3.1771 eV 390.24 nm f=0.0020
Excited State 6: Singlet-A 3.3579 eV 369.23 nm f=1.8305
H-4 324 -> 329 L -0.25160 13%
H-3 325 -> 329 L 0.13351 4%
H-3 325 -> 331 L+2 -0.15095 5%
H-2 326 -> 329 L -0.16509 5%
H-2 326 -> 331 L+2 0.14871 44%
H-1 327 -> 331 L+2 0.47183 45%
H-1 327 -> 332 L+3 -0.22178 10%
H-1 327 -> 334 L+5 0.10697 2%
H 328 -> 333 L+4 0.15180 5%
Excited State 7: Singlet-A 3.4849 eV 355.77 nm f=1.7514
H-3 325 -> 330 L+1 0.13760 4%
H-3 325 -> 331 L+2 -0.11652 3%
H-2 326 -> 330 L+1 0.22783 10%
H-1 327 -> 331 L+2 -0.23684 11%
H-1 327 -> 332 L+3 0.10941 2%
H 328 -> 332 L+3 -0.11532 3%
H 328 -> 333 L+4 0.54256 59%
Excited State 8: Singlet-A 3.5809 eV 346.24 nm f=1.2919
H-4 324 -> 329 L 0.21005 9%
H-3 325 -> 329 L 0.10256 2%
H-3 325 -> 331 L+2 0.33420 22%
H-3 325 -> 332 L+3 -0.17584 6%
H-2 326 -> 330 L+1 0.10486 2%
H-2 326 -> 331 L+2 -0.29029 17%
H-2 326 -> 332 L+3 0.10845 2%
H-1 327 -> 329 L -0.14697 4%
H-1 327 -> 331 L+2 0.23452 11%
H-1 327 -> 332 L+3 -0.10846 2%
H 328 -> 333 L+4 0.24335 12%
Excited State 9: Singlet-A 3.7513 eV 330.51 nm f=0.1949
H-13 315 -> 329 L -0.14411 4%
H-4 324 -> 329 L 0.39895 32%
H-3 325 -> 329 L 0.24214 12%
H-3 325 -> 331 L+2 -0.25874 13%
H-2 326 -> 329 L 0.29227 17%

H-2 326 -> 331 L+2 0.12922 3%
H-2 326 -> 333 L+4 0.12088 3%
H-1 327 -> 331 L+2 0.10704 2%
Excited State 10: Singlet-A 3.7740 eV 328.52 nm f=0.2758
H-4 324 -> 329 L 0.11963 3%
H-4 324 -> 330 L+1 0.11412 3%
H-3 325 -> 330 L+1 -0.16327 5%
H-3 325 -> 333 L+4 -0.13897 4%
H-2 326 -> 330 L+1 0.11973 3%
H-2 326 -> 332 L+3 0.10562 2%
H-2 326 -> 333 L+4 -0.19624 8%
H-1 327 -> 330 L+1 -0.36543 27%
H 328 -> 331 L+2 0.16976 6%
H 328 -> 332 L+3 0.37993 29%
Excited State 11: Singlet-A 3.7785 eV 328.13 nm f=0.1473
H-4 324 -> 330 L+1 -0.13789 4%
H-3 325 -> 330 L+1 0.22263 10%
H-2 326 -> 330 L+1 -0.11850 3%
H-2 326 -> 333 L+4 -0.11164 2%
H-1 327 -> 330 L+1 0.46330 43%
H 328 -> 331 L+2 0.14128 4%
H 328 -> 332 L+3 0.32479 21%
H 328 -> 333 L+4 0.11411 3%
Excited State 12: Singlet-A 3.8003 eV 326.25 nm f=0.9498
H-13 315 -> 329 L 0.10308 2%
H-4 324 -> 329 L -0.24565 12%
H-3 325 -> 329 L 0.12447 3%
H-3 325 -> 333 L+4 0.28276 16%
H-2 326 -> 329 L 0.15407 5%
H-2 326 -> 333 L+4 0.38074 29%
H 328 -> 330 L+1 -0.15201 5%
H 328 -> 331 L+2 0.13085 3%
H 328 -> 332 L+3 0.29848 18%
Excited State 13: Singlet-A 3.8181 eV 324.73 nm f=0.1879
H-13 315 -> 329 L 0.10182 2%
H-4 324 -> 329 L -0.22913 11%
H-3 325 -> 329 L 0.32827 22%
H-3 325 -> 333 L+4 -0.15779 5%
H-2 326 -> 329 L 0.42567 36%
H-2 326 -> 333 L+4 -0.23159 11%
Excited State 14: Singlet-A 3.9104 eV 317.06 nm f=0.0000
Excited State 15: Singlet-A 4.0707 eV 304.58 nm f=0.0027
Excited State 16: Singlet-A 4.1400 eV 299.48 nm f=0.0006

Table S19. TDDFT results for **Dyad-8**.

Excited State 1: Singlet-A 1.5742 eV 787.59 nm f=0.6397
H-3 298 -> 304 L+2 0.16530 5.46-2.08= 3%
H-1 300 -> 302 L 0.67667 92%
H-3 298 <- 304 L+2 0.10190 2.08%
Excited State 2: Singlet-A 1.6988 eV 729.83 nm f=0.4091
H-2 299 -> 305 L+3 0.20505 8.41-2.85= 6%
H 301 -> 303 L+1 0.67394 91%
H-2 299 <- 305 L+3 0.11946 2.85%
Excited State 3: Singlet-A 2.0648 eV 600.46 nm f=0.4298
H-3 298 -> 302 L 0.62791 79%
H-2 299 -> 302 L 0.18962 7%
H-1 300 -> 304 L+2 -0.22892 10%
Excited State 4: Singlet-A 2.3107 eV 536.56 nm f=0.2021
H-3 298 -> 303 L+1 -0.17258 6%
H-2 299 -> 303 L+1 0.60573 73%
H 301 -> 305 L+3 -0.31380 20%
Excited State 5: Singlet-A 3.0968 eV 400.36 nm f=0.0011
Excited State 6: Singlet-A 3.3592 eV 369.09 nm f=1.6397
H-4 297 -> 302 L 0.25706 13%
H-3 298 -> 302 L 0.19343 7%
H-3 298 -> 304 L+2 0.21553 9%
H-1 300 -> 304 L+2 0.53171 57%
H-1 300 -> 306 L+4 -0.10162 2%
H 301 -> 305 L+3 0.12483 3%
Excited State 7: Singlet-A 3.5059 eV 353.64 nm f=1.8479
H-3 298 -> 302 L -0.10476 2%
H-3 298 -> 304 L+2 0.21078 9%
H-2 299 -> 303 L+1 0.26000 14%
H-1 300 -> 304 L+2 -0.25768 13%
H 301 -> 305 L+3 0.54093 59%
Excited State 8: Singlet-A 3.5864 eV 345.71 nm f=1.3046
H-4 297 -> 302 L 0.20731 9%
H-3 298 -> 304 L+2 0.44969 40%
H-2 299 -> 303 L+1 -0.16285 5%
H-2 299 -> 304 L+2 0.14328 4%
H-2 299 -> 305 L+3 0.10349 2%
H-1 300 -> 302 L -0.14286 4%
H-1 300 -> 304 L+2 -0.24349 12%
H 301 -> 305 L+3 -0.30307 18%
Excited State 9: Singlet-A 3.7441 eV 331.15 nm f=0.1361
H-4 297 -> 302 L 0.28658 16%
H-3 298 -> 302 L -0.16964 6%
H-3 298 -> 304 L+2 -0.23597 11%
H-2 299 -> 302 L 0.53416 57%
Excited State 10: Singlet-A 3.7780 eV 328.17 nm f=0.2204
H-12 289 -> 302 L -0.15661 5%
H-4 297 -> 302 L 0.45155 41%
H-3 298 -> 302 L 0.10946 2%
H-3 298 -> 304 L+2 -0.20715 9%
H-2 299 -> 302 L -0.38077 29%
H-2 299 -> 304 L+2 -0.10421 2%

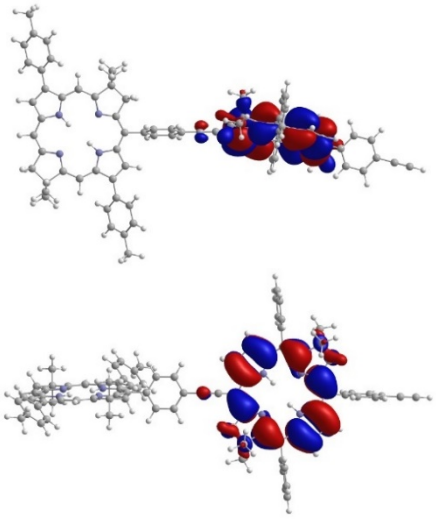
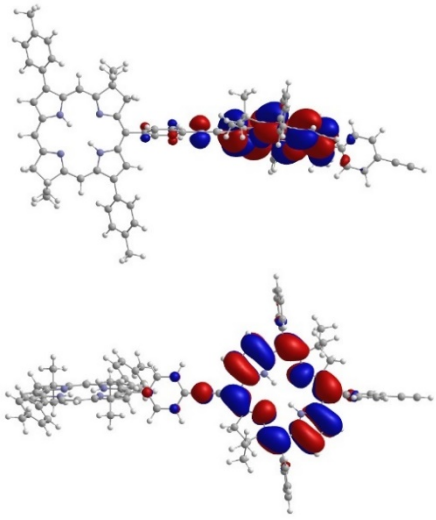
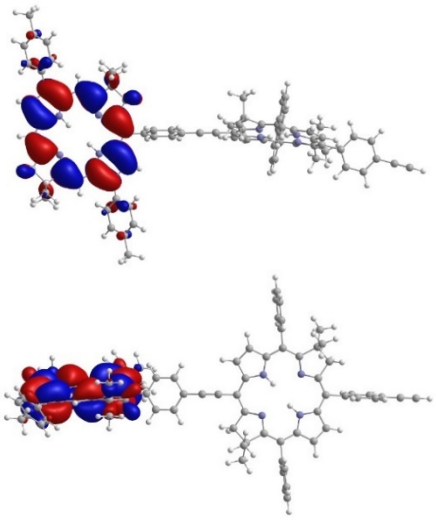
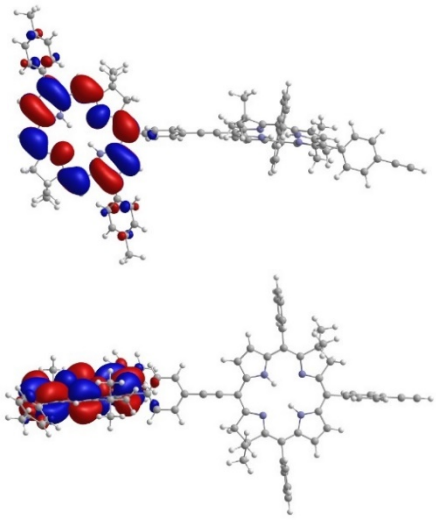
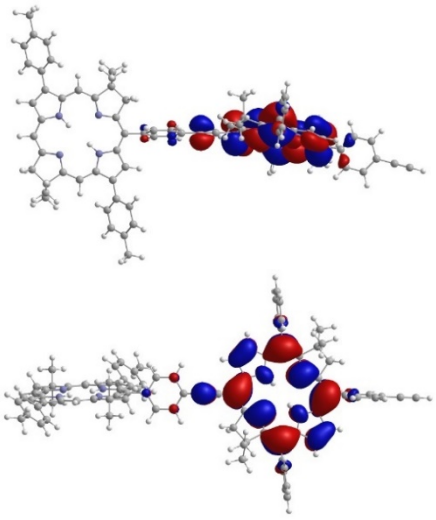
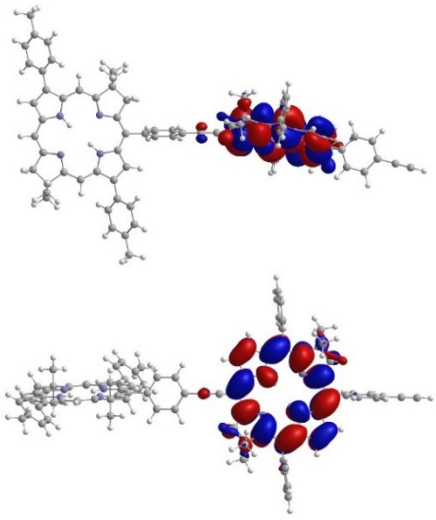
H-1 300 -> 304 L+2 -0.11719 3%
Excited State 11: Singlet-A 3.8371 eV 323.12 nm f=1.2784
H-3 298 -> 305 L+3 -0.17310 6%
H-2 299 -> 305 L+3 0.62748 79%
H 301 -> 303 L+1 -0.21472 9%
H 301 <- 303 L+1 0.12557 3%
Excited State 12: Singlet-A 3.8660 eV 320.71 nm f=0.0081
Excited State 13: Singlet-A 4.1330 eV 299.99 nm f=0.0002
Excited State 14: Singlet-A 4.1614 eV 297.94 nm f=0.0009
Excited State 15: Singlet-A 4.1812 eV 296.52 nm f=0.0012
Excited State 16: Singlet-A 4.1959 eV 295.49 nm f=0.0216
H-22 279 -> 302 L 0.13734 4%
H-18 283 -> 302 L 0.11860 3%
H-17 284 -> 302 L 0.27447 15%
H-12 289 -> 302 L 0.24163 12%
H-11 290 -> 302 L -0.13862 4%
H-1 300 -> 306 L+4 0.45361 41%
H-1 300 -> 307 L+5 -0.23311 11%

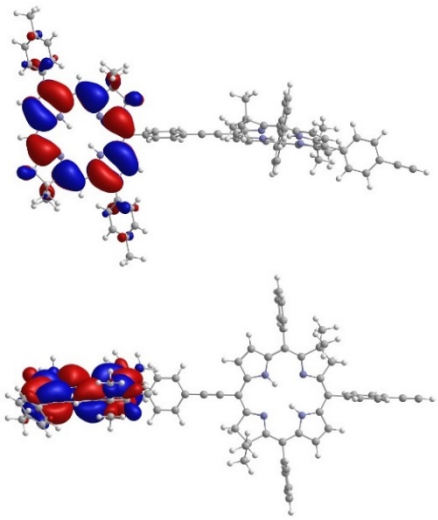
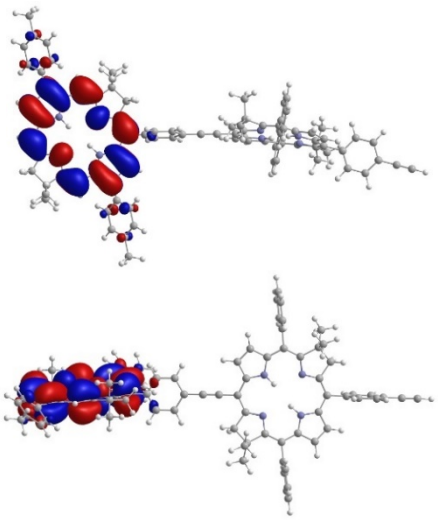
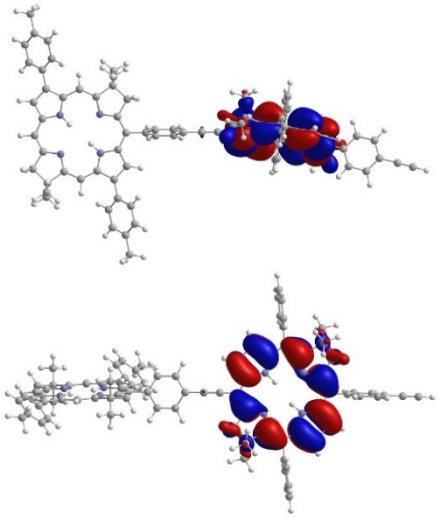
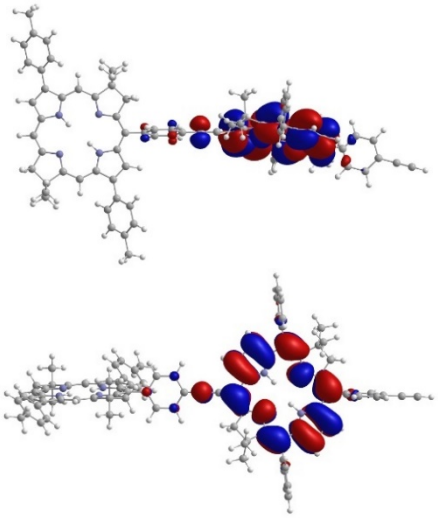
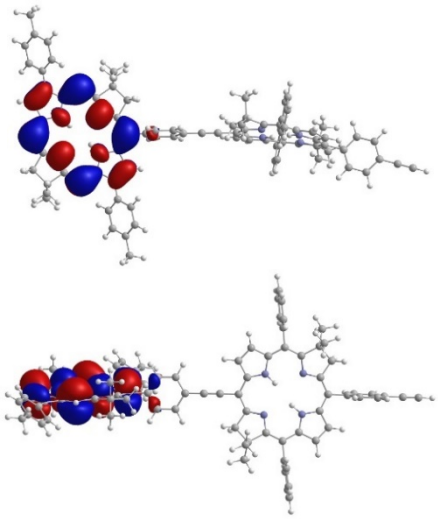
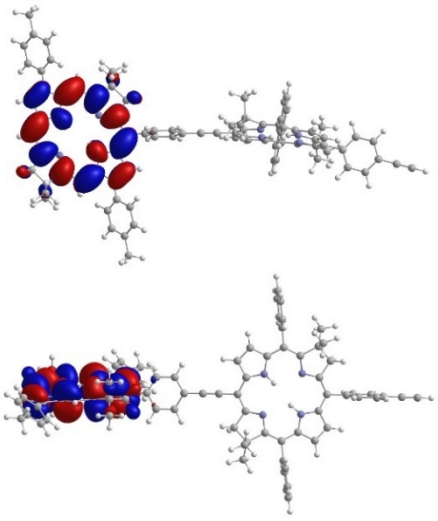
Table S20. TDDFT results for **Dyad-9**.

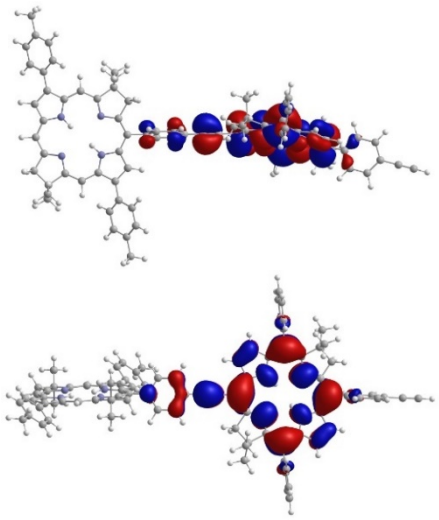
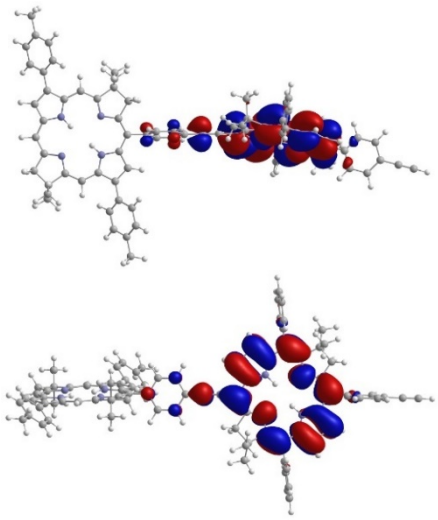
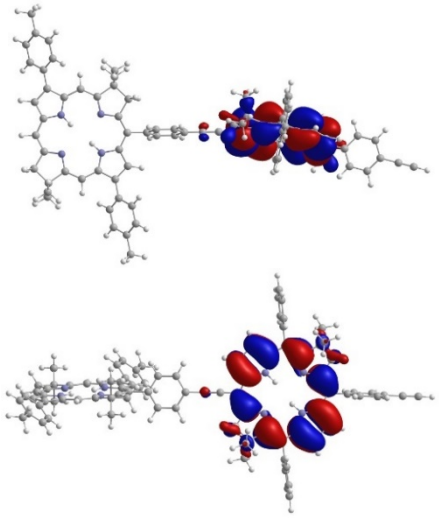
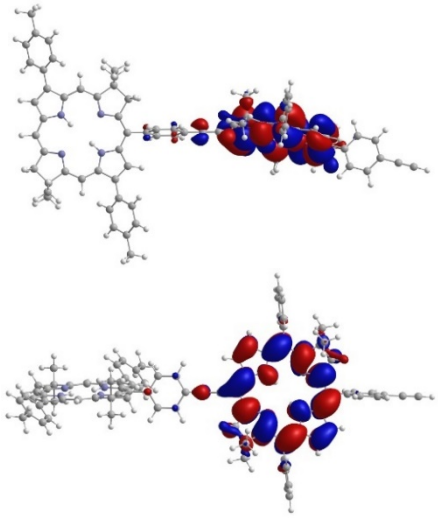
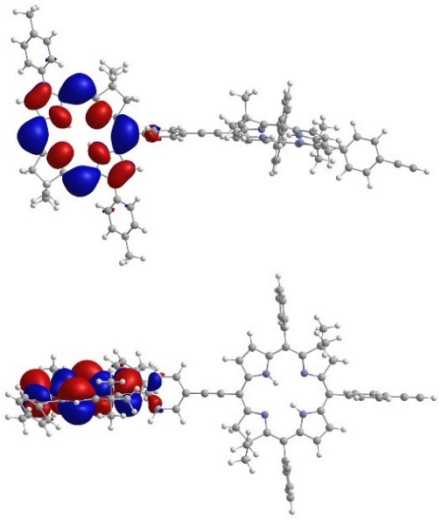
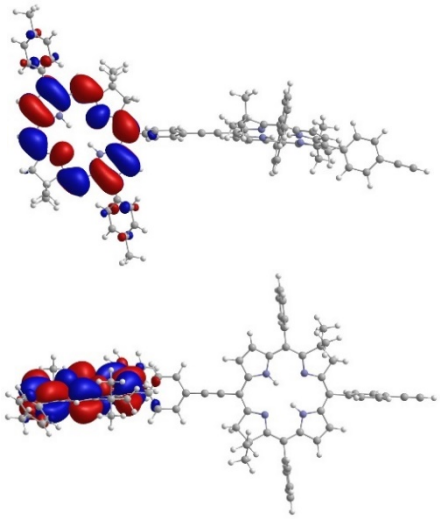
Excited State 1: Singlet-A 1.5563 eV 796.64 nm f=0.6797
H-3 274 -> 280 L+2 0.16492 5.44-2.14= 3%
H-1 276 -> 278 L 0.67571 91%
H-3 274 <- 280 L+2 0.10350 2.14%
Excited State 2: Singlet-A 1.6993 eV 729.62 nm f=0.4063
H-2 275 -> 281 L+3 0.17344 6.02-2.04= 4%
H-2 275 -> 282 L+4 -0.12300 3%
H 277 -> 279 L+1 0.67394 91%
H-2 275 <- 281 L+3 0.10105 2.04%
Excited State 3: Singlet-A 2.0404 eV 607.65 nm f=0.4220
H-3 274 -> 278 L 0.65530 86%
H-1 276 -> 280 L+2 -0.21716 9%
Excited State 4: Singlet-A 2.3108 eV 536.55 nm f=0.2037
H-2 275 -> 279 L+1 0.62779 79%
H 277 -> 281 L+3 -0.25680 13%
H 277 -> 282 L+4 0.18080 7%
Excited State 5: Singlet-A 2.8334 eV 437.58 nm f=0.0005
Excited State 6: Singlet-A 3.3416 eV 371.03 nm f=1.3315
H-4 273 -> 278 L -0.33350 22%
H-3 274 -> 278 L 0.17846 6%
H-3 274 -> 280 L+2 -0.22459 10%
H-2 275 -> 278 L 0.12277 3%
H-1 276 -> 280 L+2 0.48304 4%
H-1 276 -> 283 L+5 -0.10212 2%
Excited State 7: Singlet-A 3.4914 eV 355.11 nm f=0.4218
H-3 274 -> 278 L -0.14832 4%
H-3 274 -> 280 L+2 -0.12326 3%
H-2 275 -> 278 L 0.56487 64%
H-1 276 -> 280 L+2 -0.27155 15%
H 277 -> 281 L+3 0.16416 5%
H 277 -> 282 L+4 -0.11902 3%
Excited State 8: Singlet-A 3.5039 eV 353.84 nm f=1.5553
H-3 274 -> 280 L+2 -0.21190 9%
H-2 275 -> 278 L -0.36081 26%
H-2 275 -> 279 L+1 0.23336 11%
H-1 276 -> 280 L+2 -0.18810 7%
H 277 -> 281 L+3 0.38557 30%
H 277 -> 282 L+4 -0.26850 14%
Excited State 9: Singlet-A 3.5729 eV 347.01 nm f=1.0979
H-4 273 -> 278 L 0.24370 12%
H-3 274 -> 280 L+2 0.39362 31%
H-2 275 -> 278 L 0.12215 3%
H-2 275 -> 279 L+1 0.19223 7%
H-1 276 -> 278 L -0.11176 2%
H-1 276 -> 280 L+2 0.25846 13%
H 277 -> 281 L+3 0.28960 17%
H 277 -> 282 L+4 -0.20375 8%
Excited State 10: Singlet-A 3.6693 eV 337.90 nm f=0.0001
Excited State 11: Singlet-A 3.7016 eV 334.95 nm f=0.0001
Excited State 12: Singlet-A 3.7258 eV 332.77 nm f=0.6896
H-18 259 -> 278 L -0.13194 3%

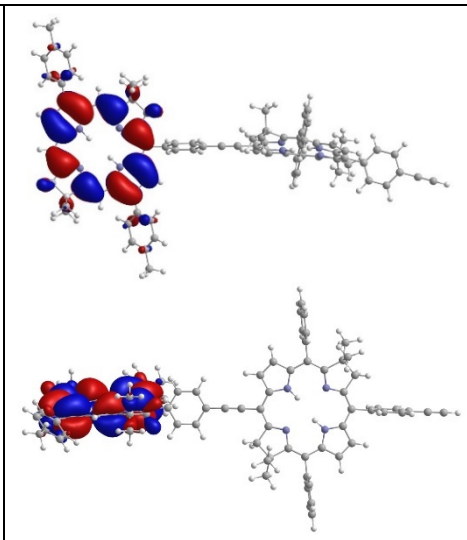
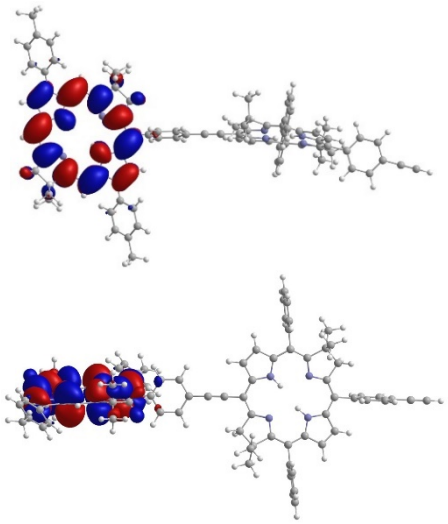
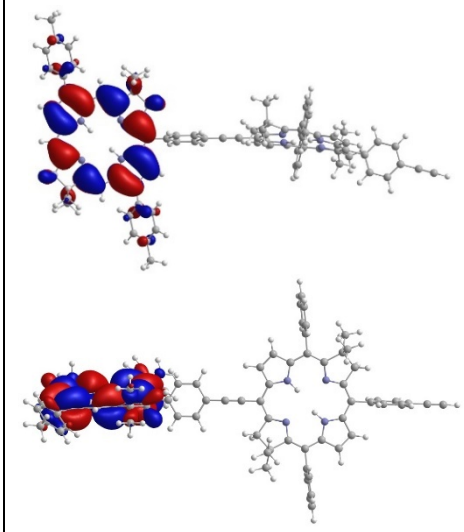
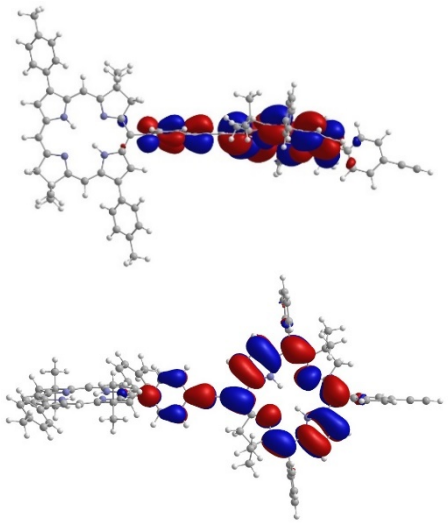
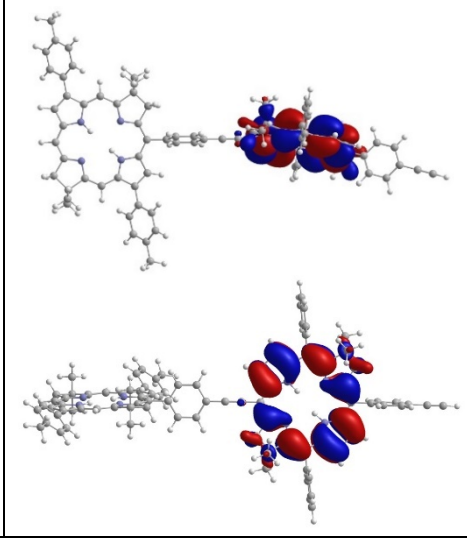
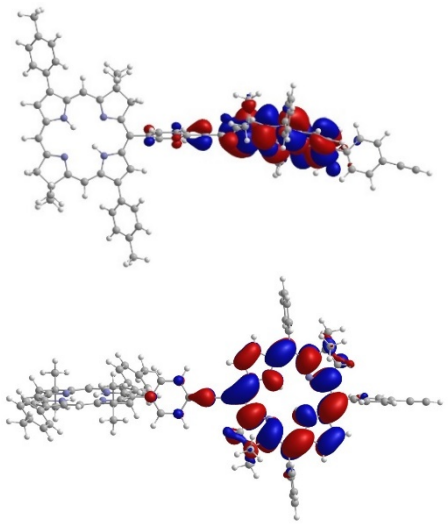
H-14 263 -> 278 L -0.11457 3%
H-4 273 -> 278 L 0.47325 45%
H-3 274 -> 280 L+2 -0.38707 30%
H-1 276 -> 278 L 0.10193 2%
H-1 276 -> 280 L+2 0.16801 6%
Excited State 13: Singlet-A 3.8354 eV 323.26 nm f=1.2760
H-3 274 -> 280 L+2 0.10624 2%
H-2 275 -> 281 L+3 0.53500 57%
H-2 275 -> 282 L+4 -0.37698 28%
H 277 -> 279 L+1 -0.21646 9%
H 277 <- 279 L+1 0.12650 3%
Excited State 14: Singlet-A 3.9977 eV 310.14 nm f=0.0346
H-19 258 -> 278 L -0.10667 2%
H-1 276 -> 281 L+3 0.37756 29%
H-1 276 -> 282 L+4 0.53539 57%
Excited State 15: Singlet-A 4.0218 eV 308.28 nm f=0.0017
Excited State 16: Singlet-A 4.1211 eV 300.85 nm f=0.0006

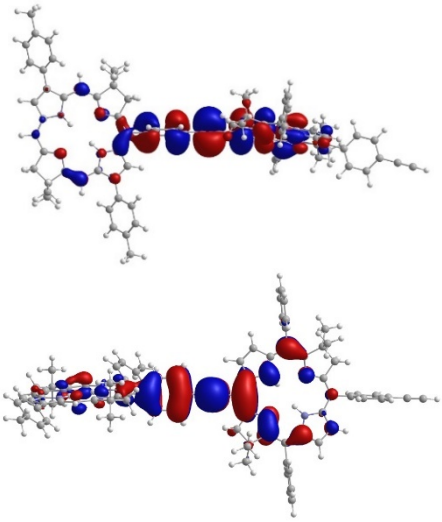
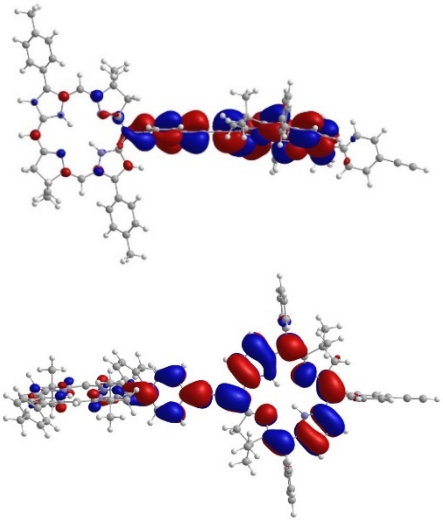
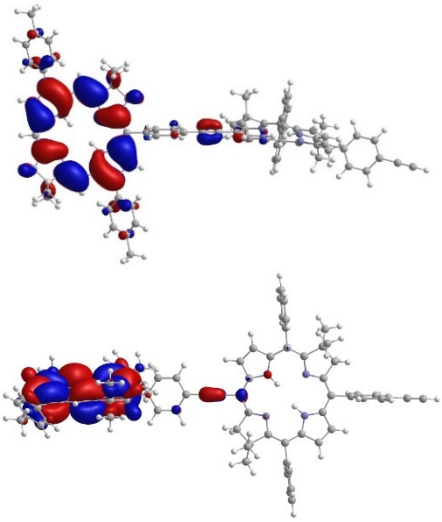
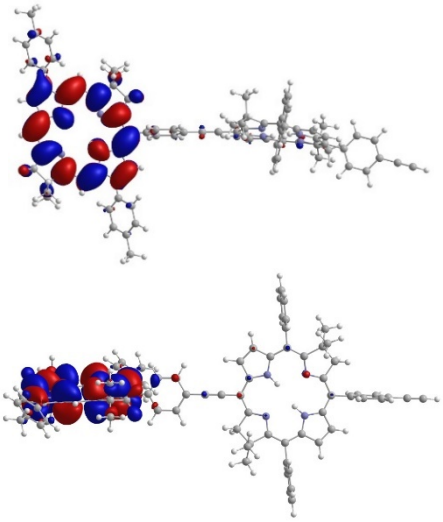
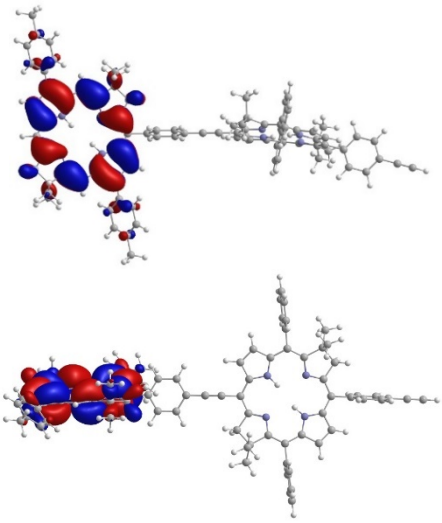
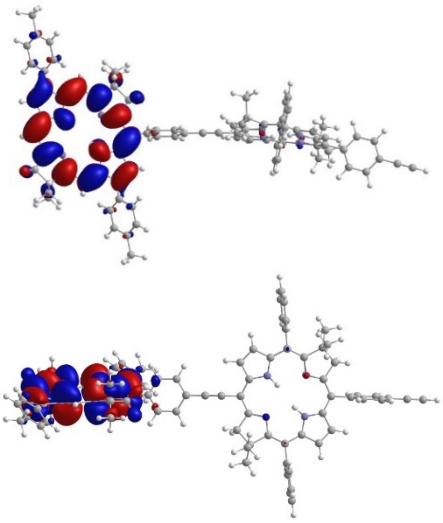
Table S21. NTOs for **Dyad-1**.

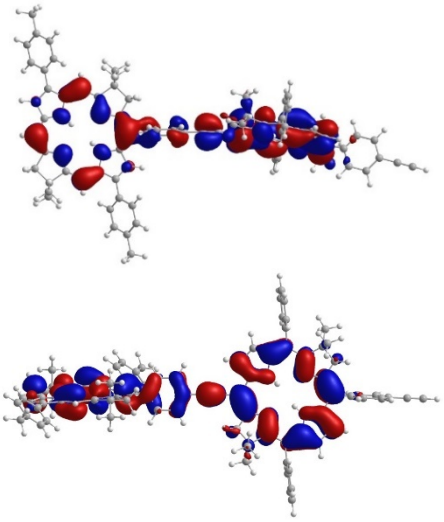
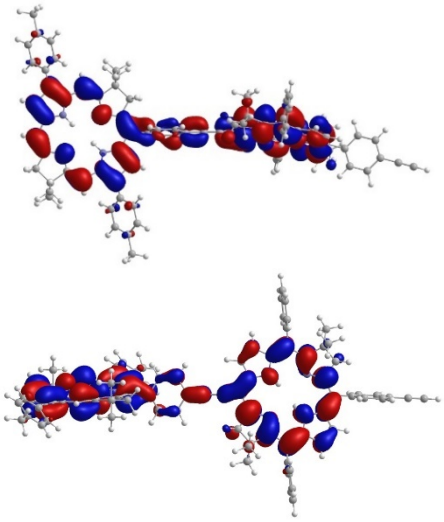
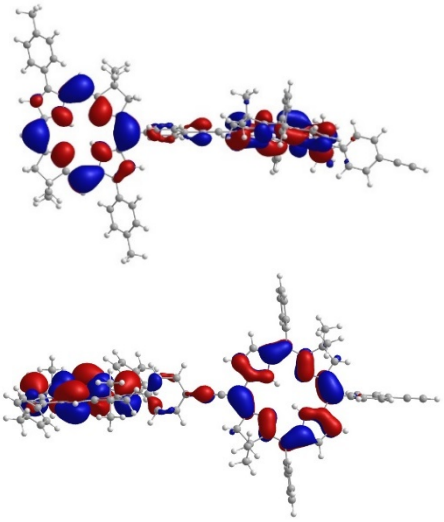
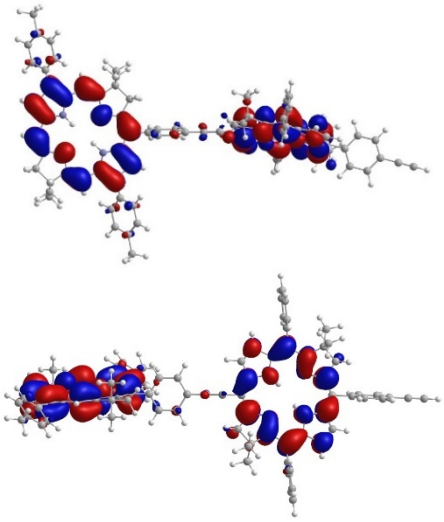
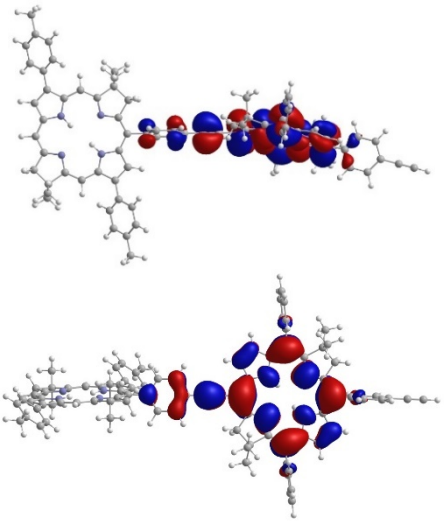
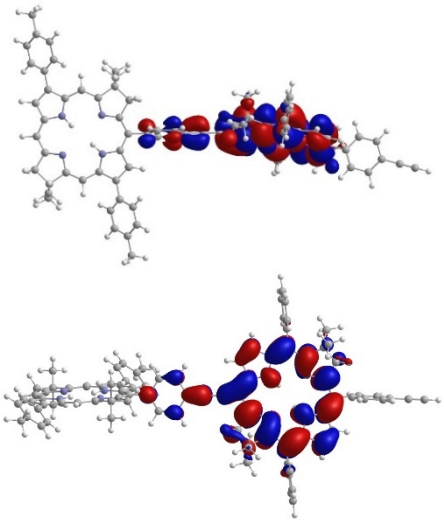
S#	Eigenvalue	From (NTO)	To (NTO)
S1	0.80966		
S1	0.12252		
S1	0.07429		

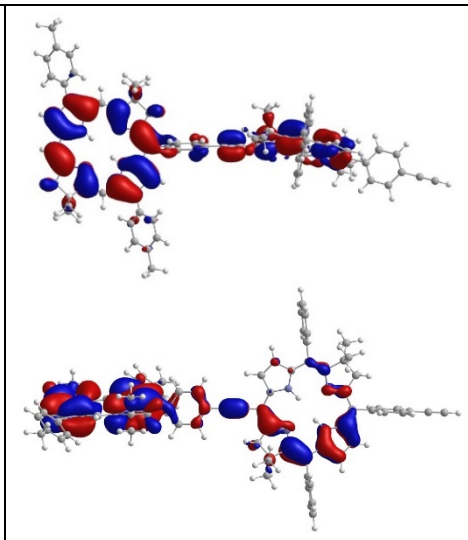
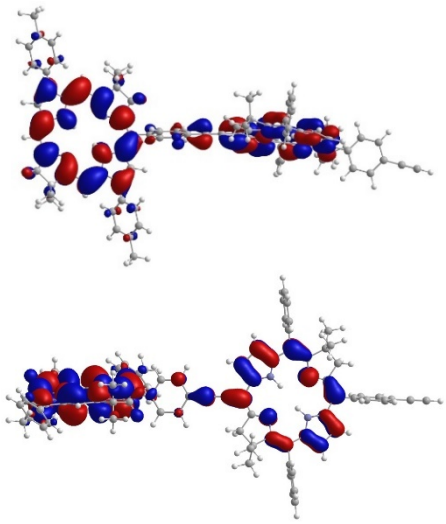
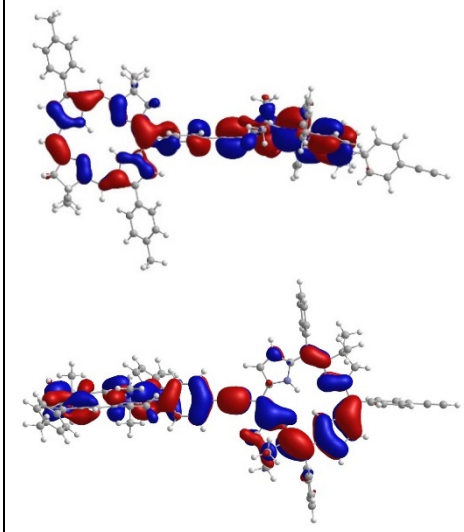
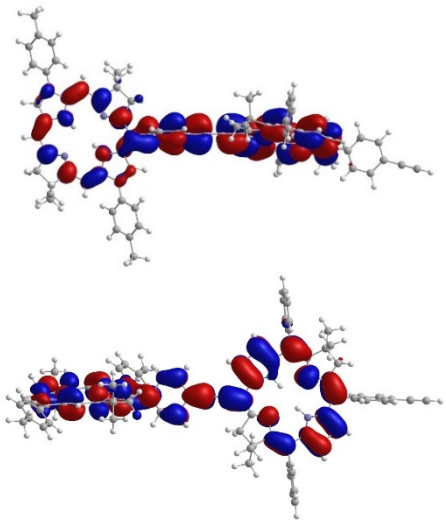
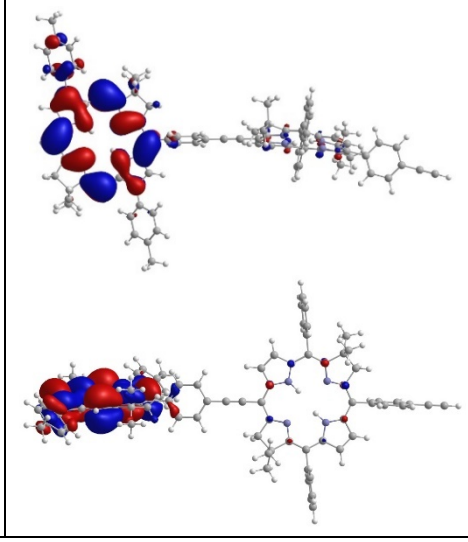
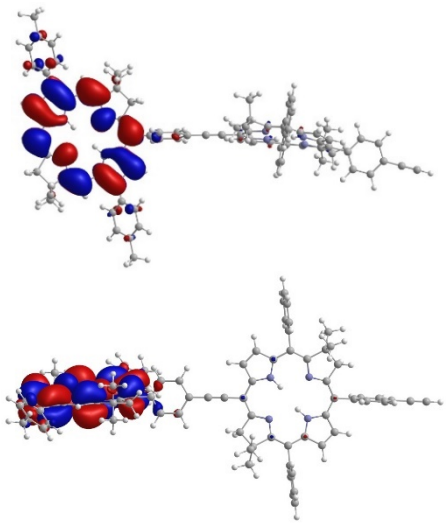
S2	0.80680		
S2	0.12101		
S2	0.07476		

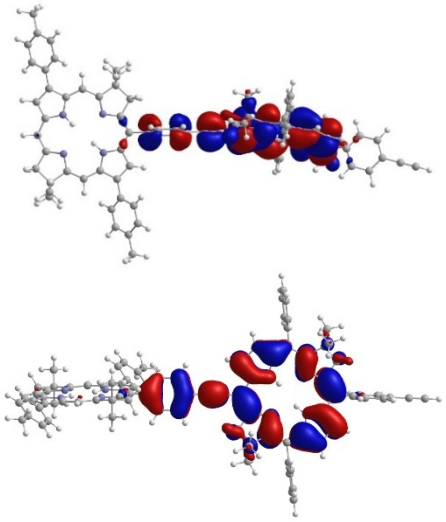
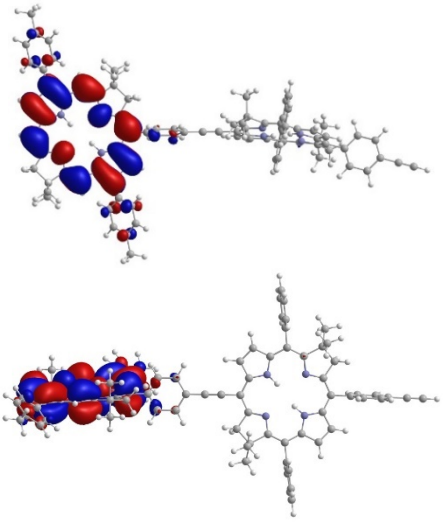
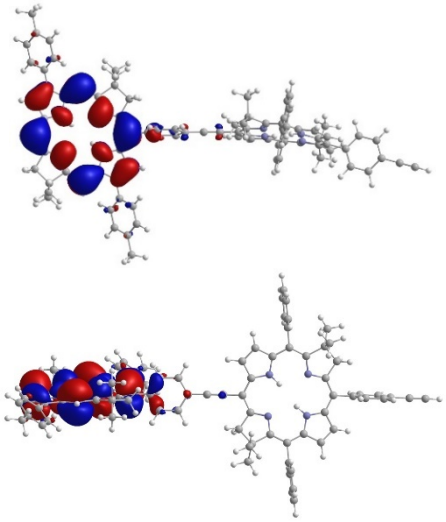
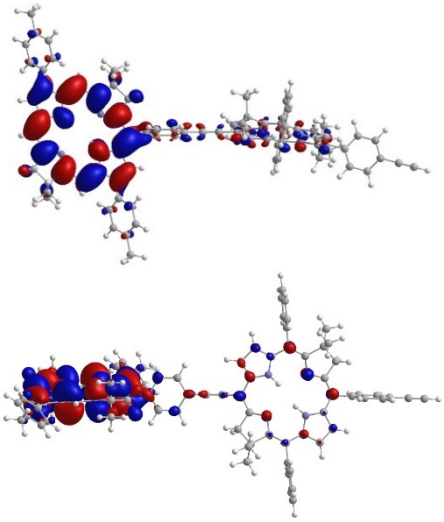
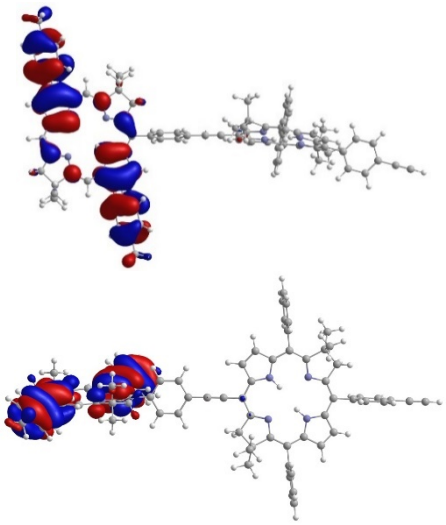
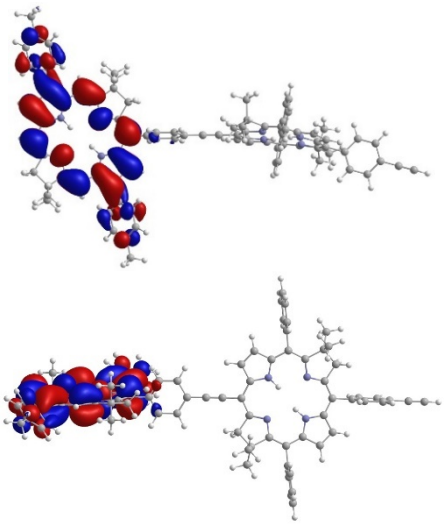
S3	0.85476		
S3	0.13429		
S4	0.76638		

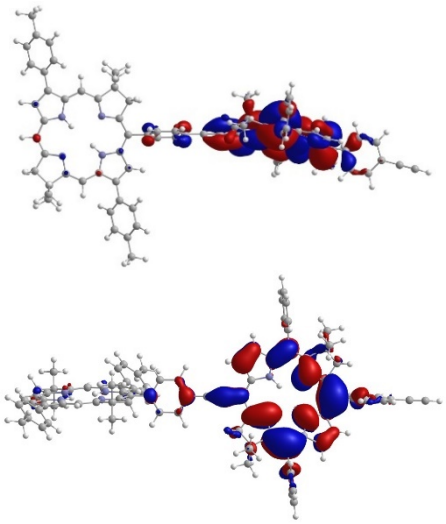
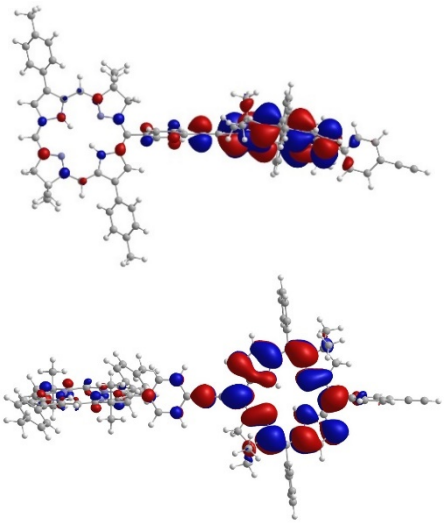
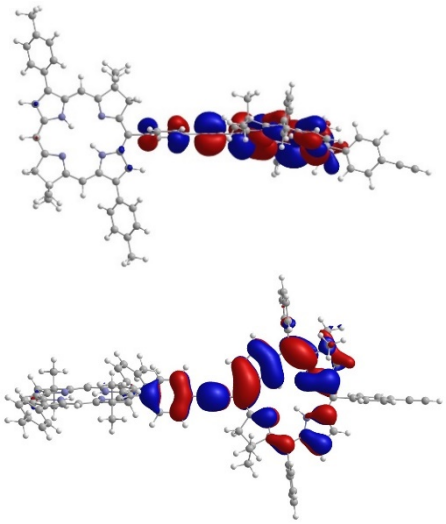
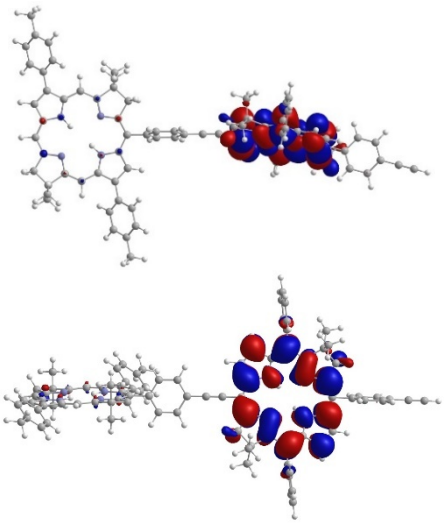
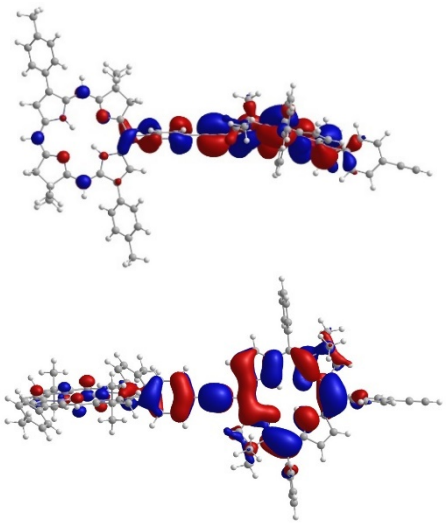
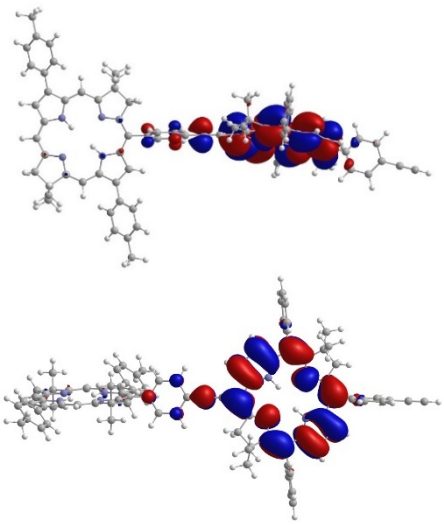
S4	0.22819		
S5	0.99299		
S6	0.68987		

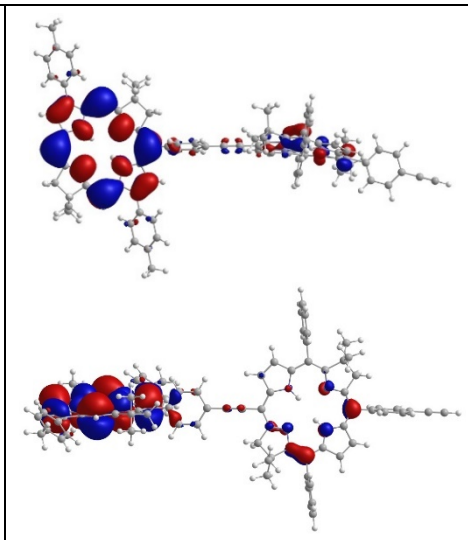
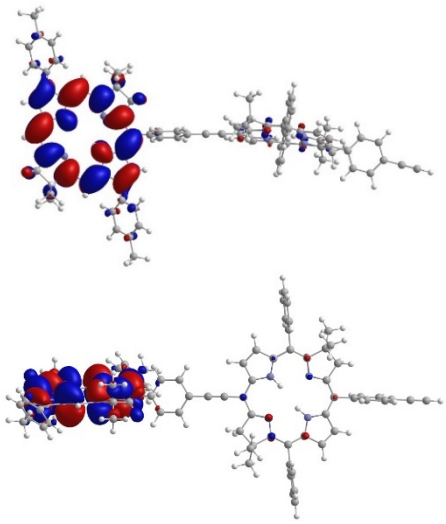
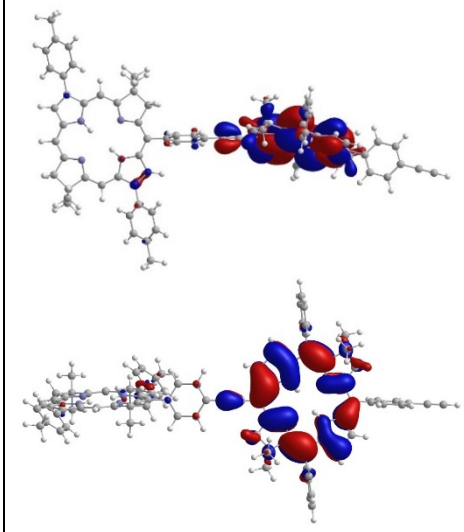
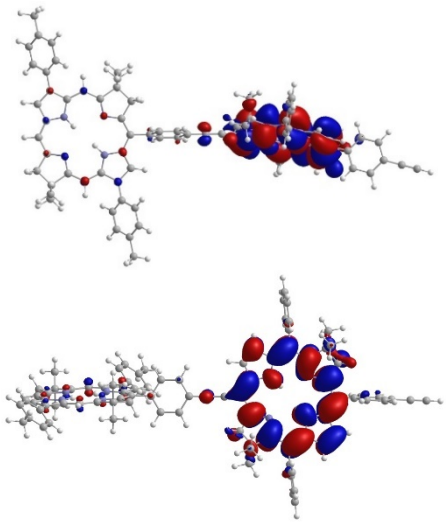
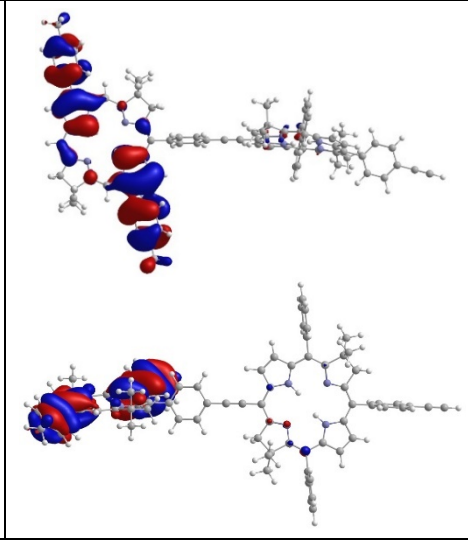
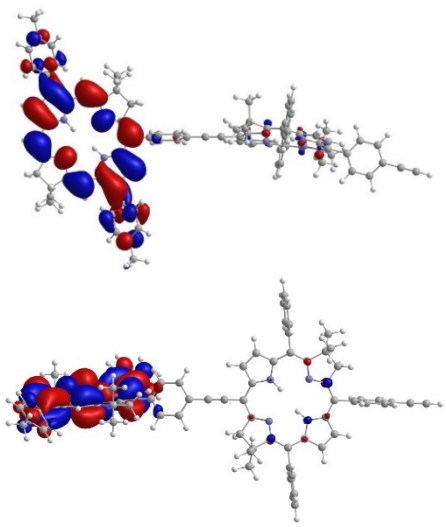
S6	0.22002		
S6	0.08013		
S7	0.58561		

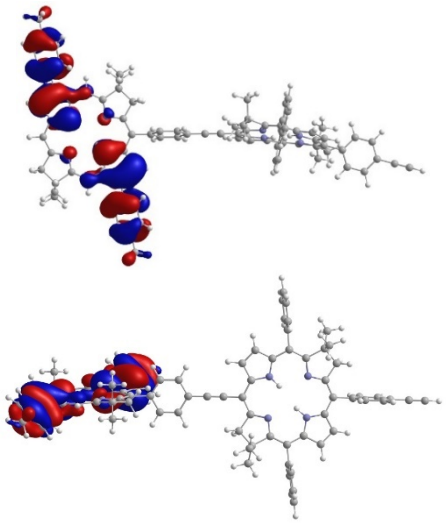
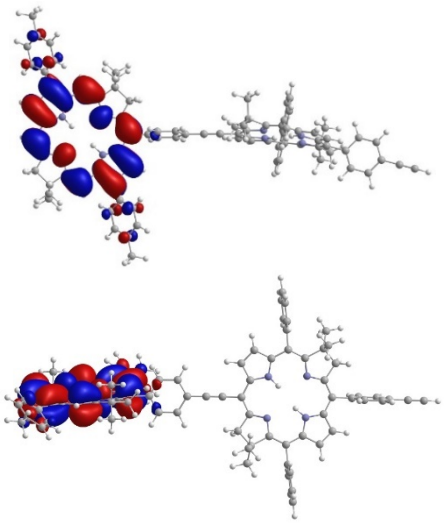
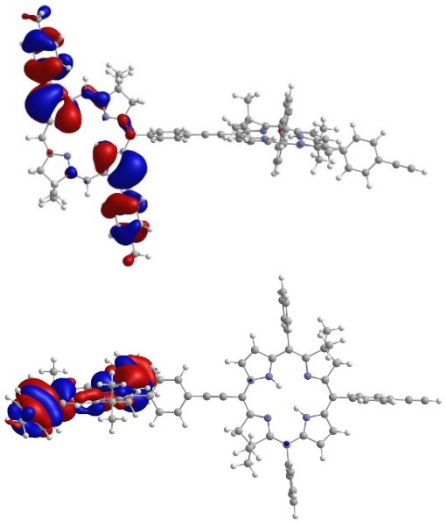
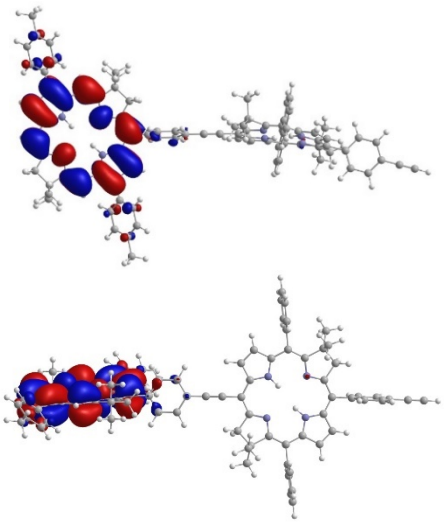
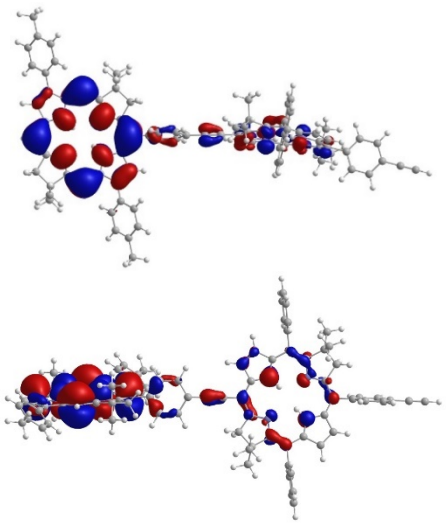
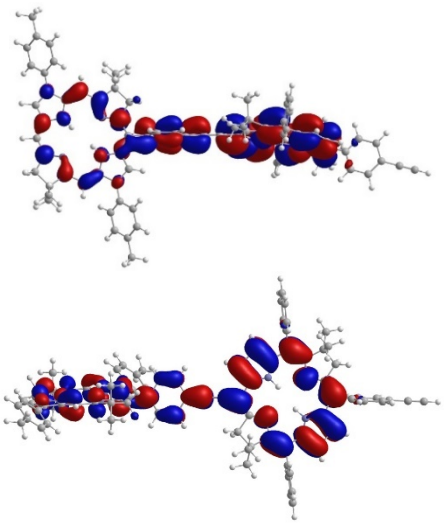
S7	0.25059		
S7	0.13696		
S8	0.67001		

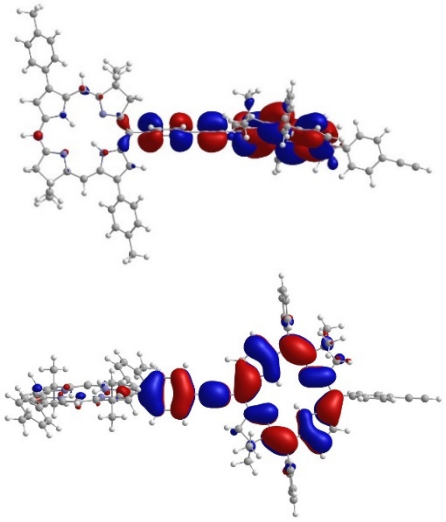
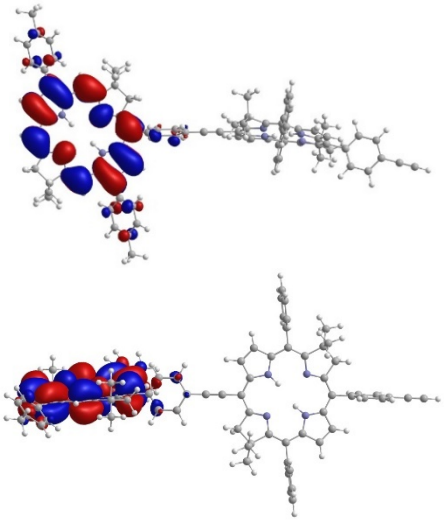
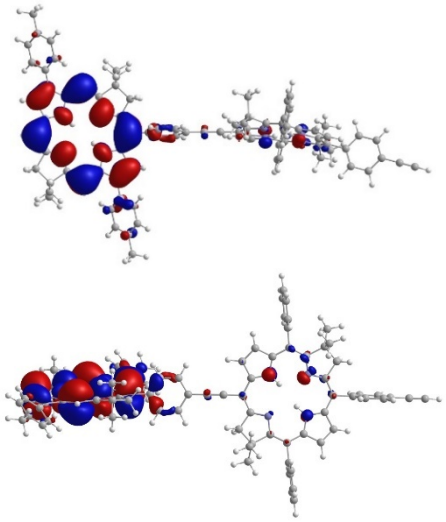
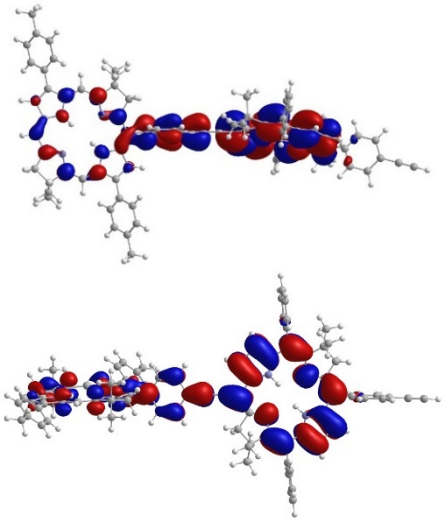
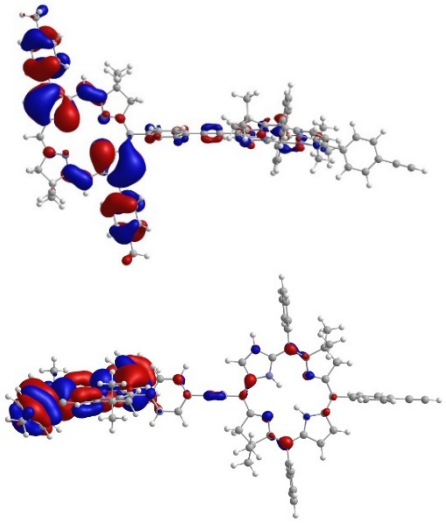
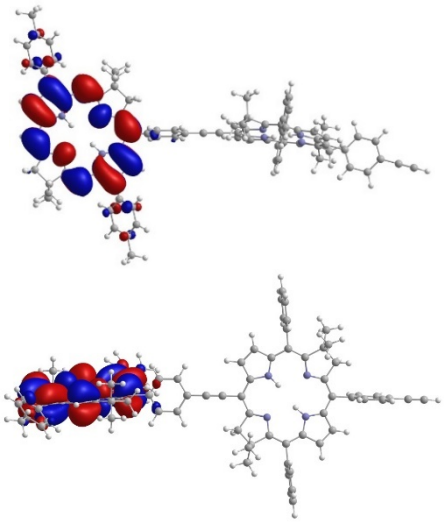
S8	0.14607		
S8	0.13673		
S8	0.05118		

S9	0.97608		
S10	0.60103		
S10	0.18323		

S10	0.11423		
S10	0.09216		
S11	0.68062		

S11	0.12808		
S11	0.09755		
S11	0.07443		

S12	0.94757		
S13	0.58460		
S13	0.36735		

S14	0.95781		
S15	0.72481		
S15	0.24890		

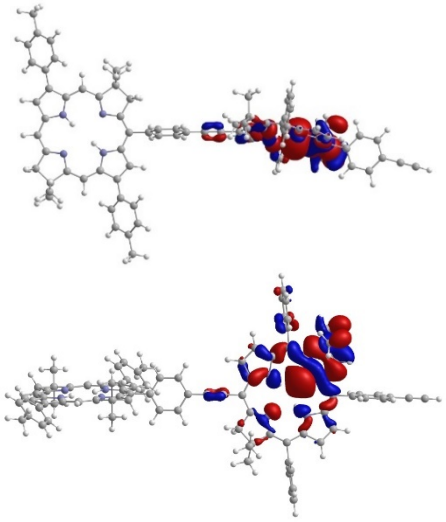
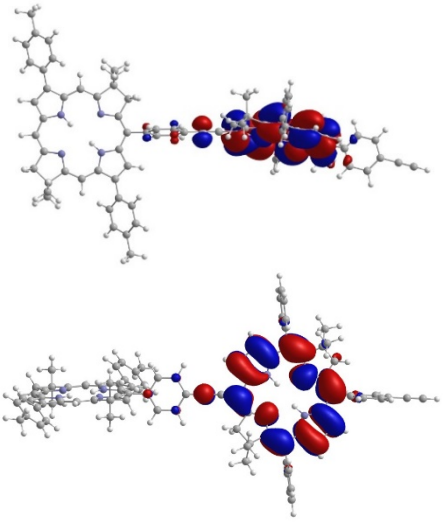
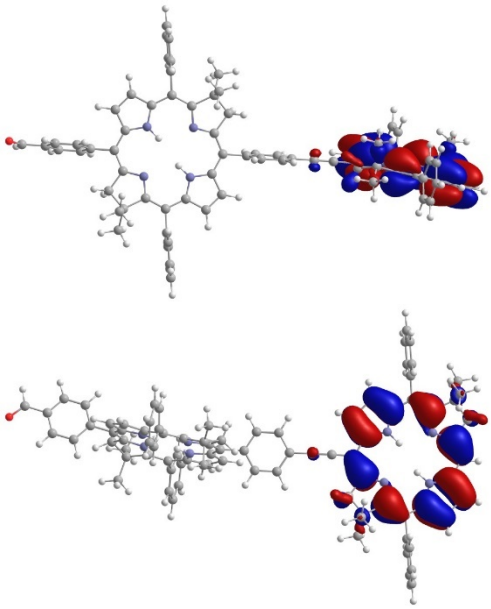
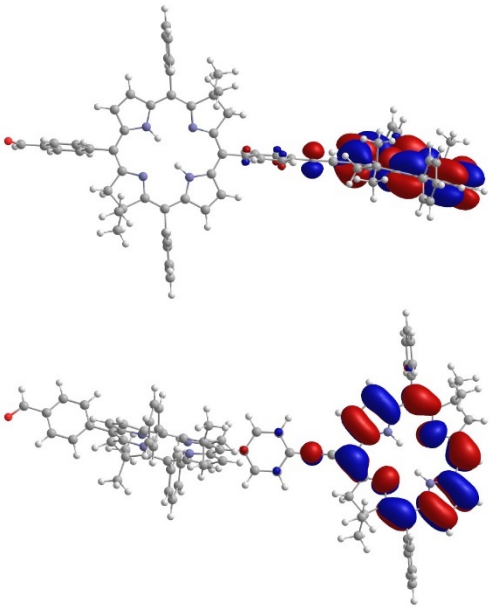
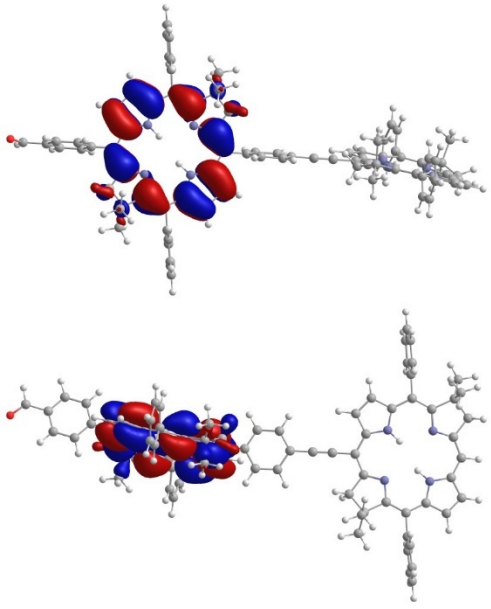
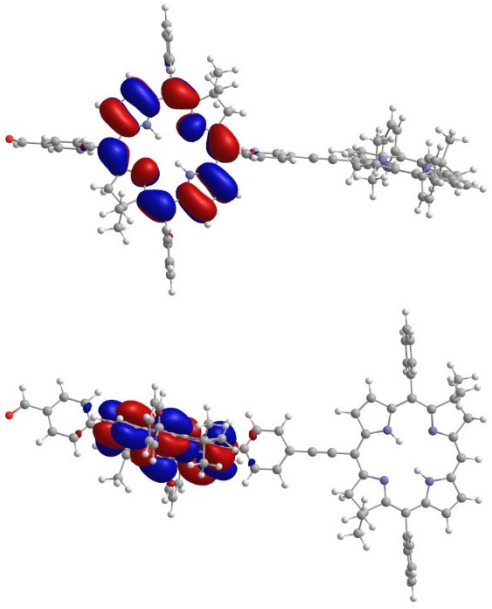
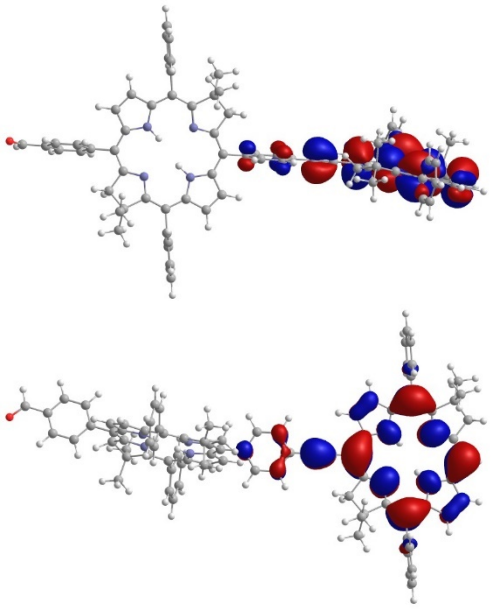
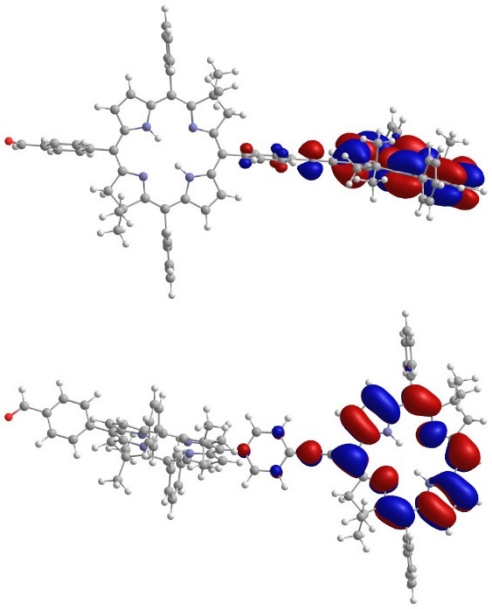
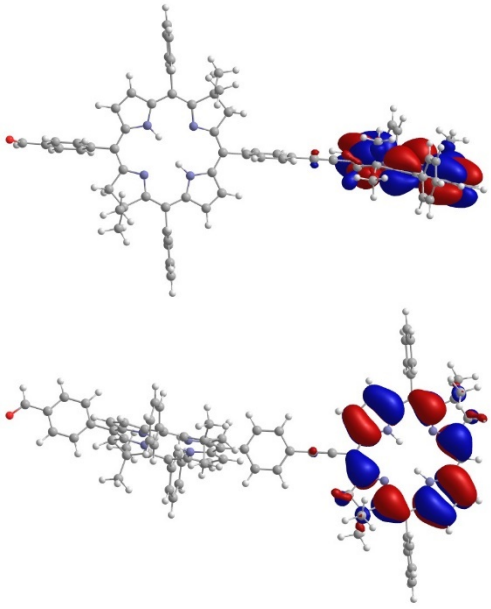
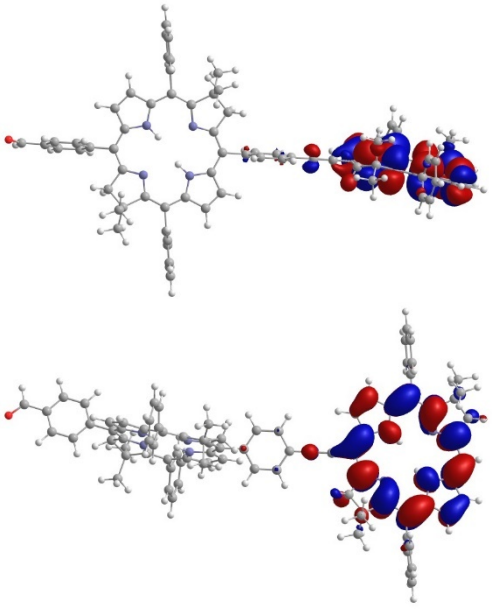
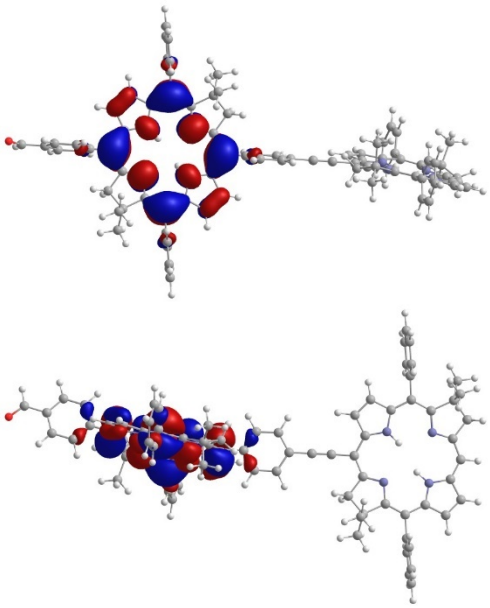
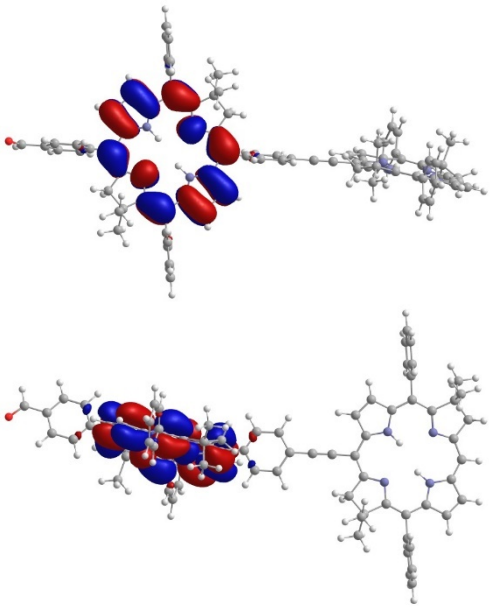
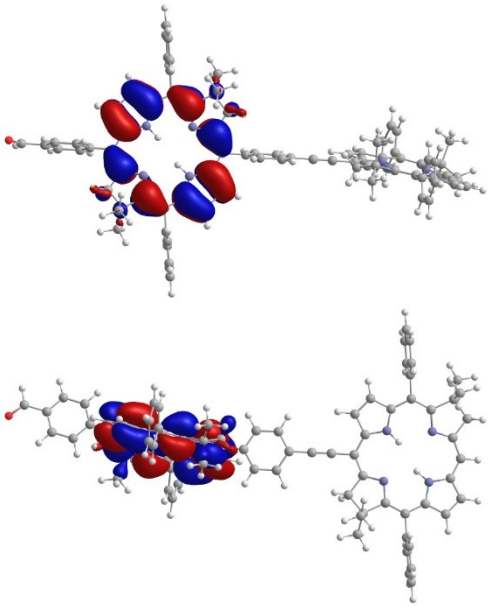
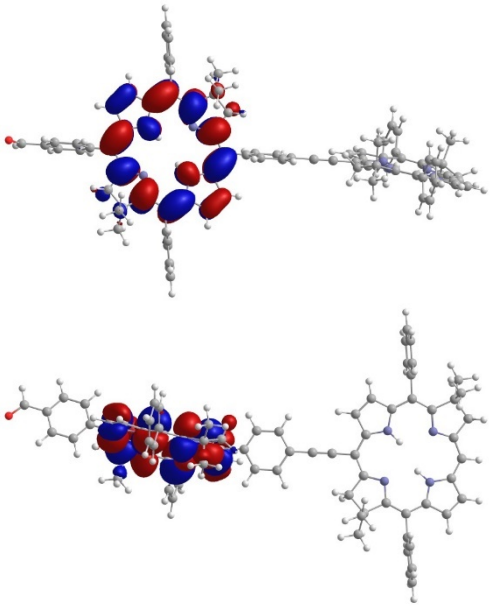
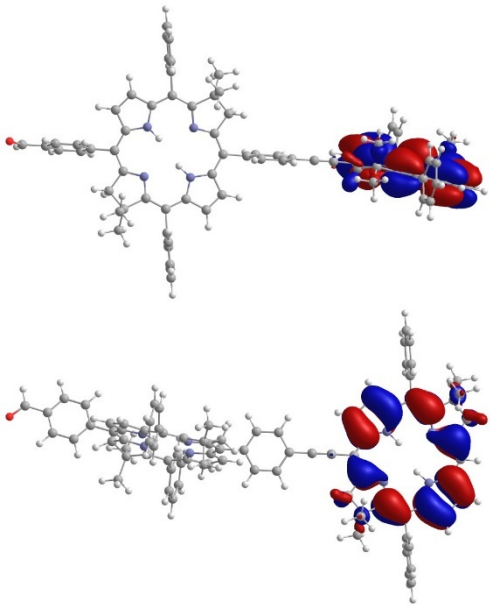
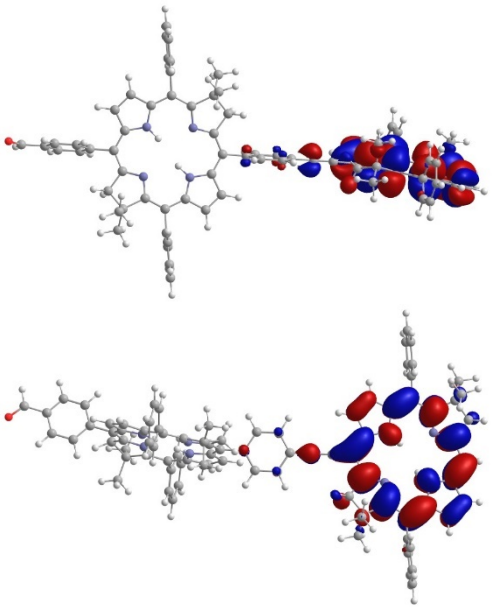
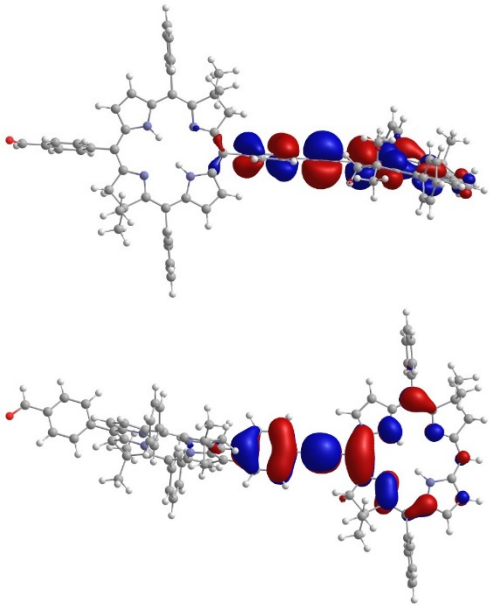
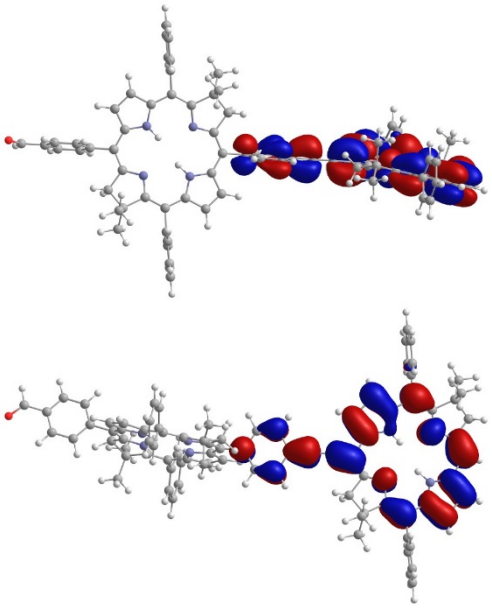
S16	0.98379		

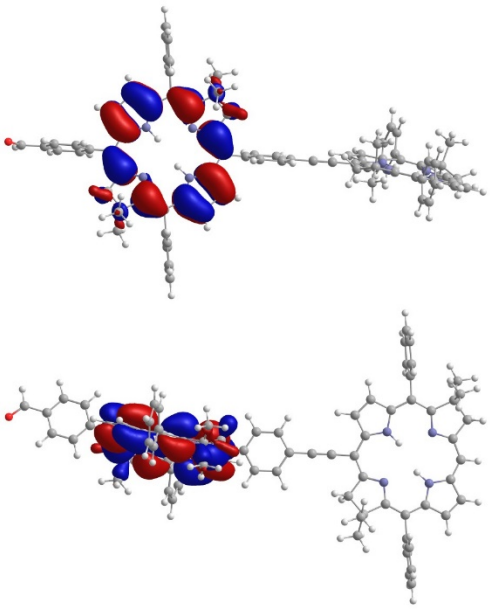
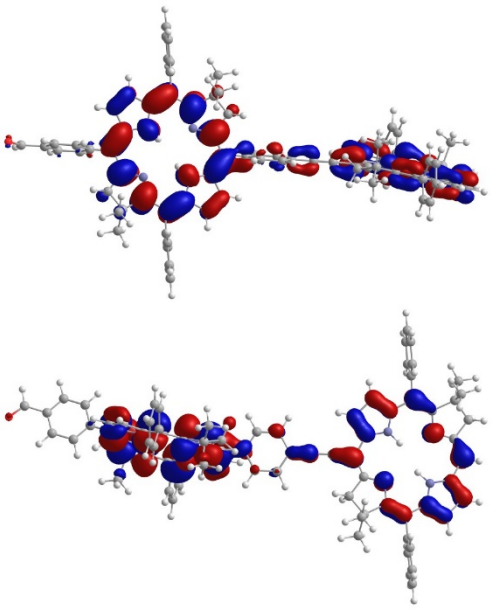
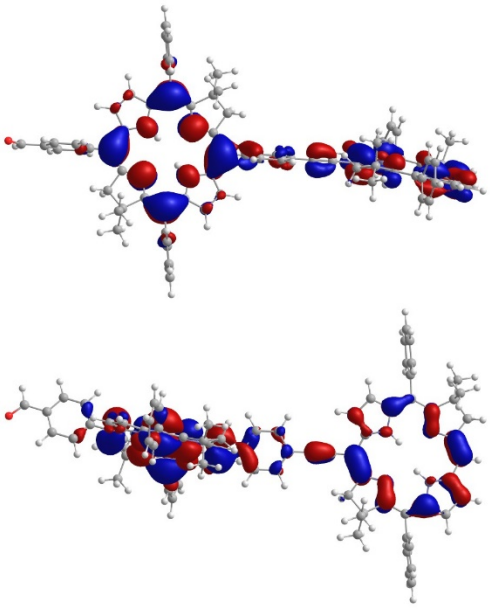
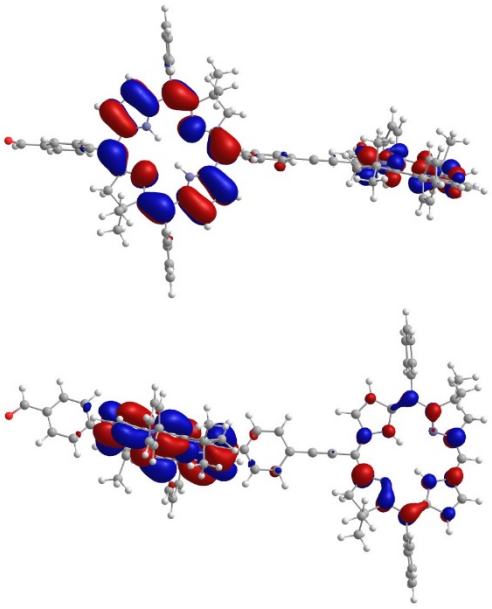
Table S22. NTOs for **Dyad-2**.

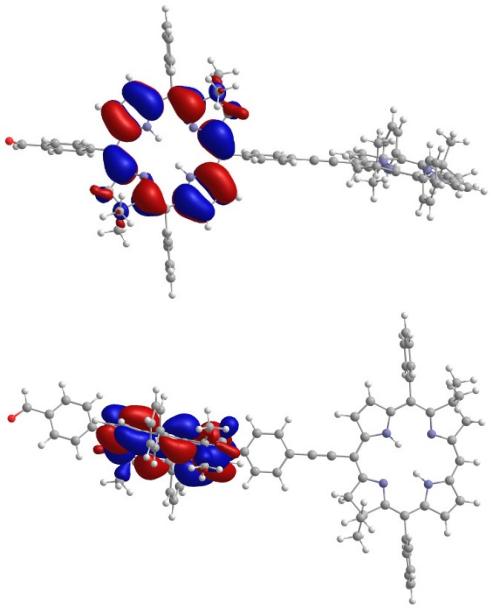
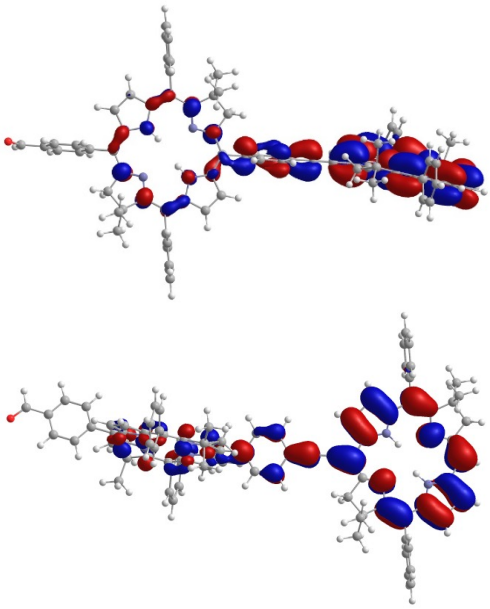
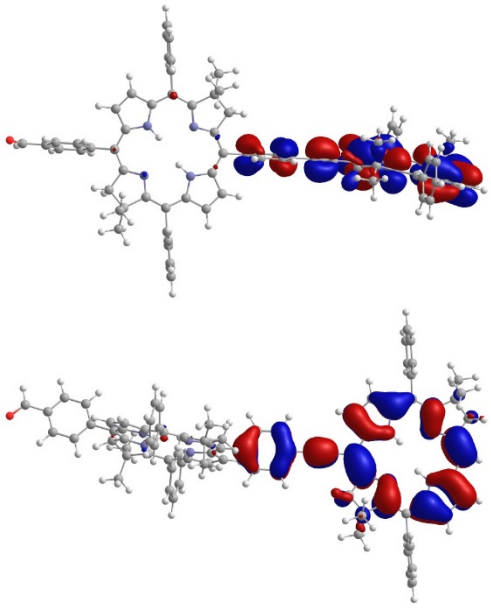
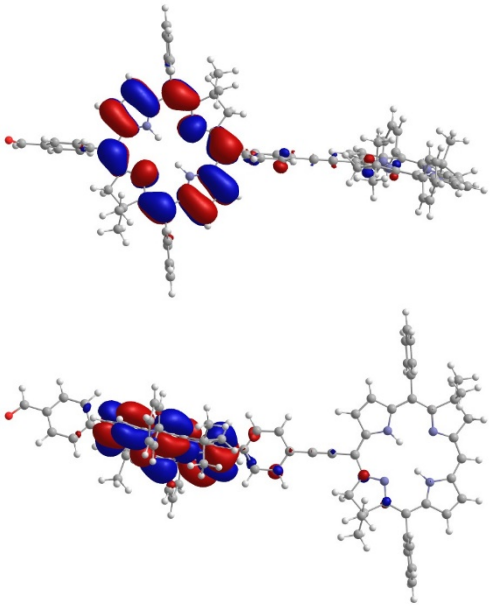
S#	Eigenvalue	From	To
S1	0.85700		
S2	0.84937		

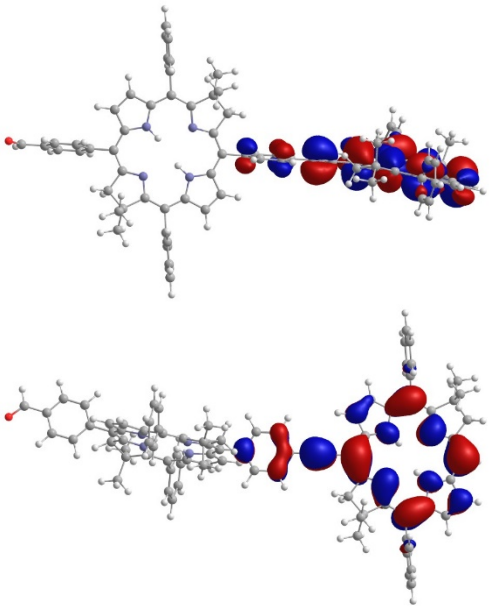
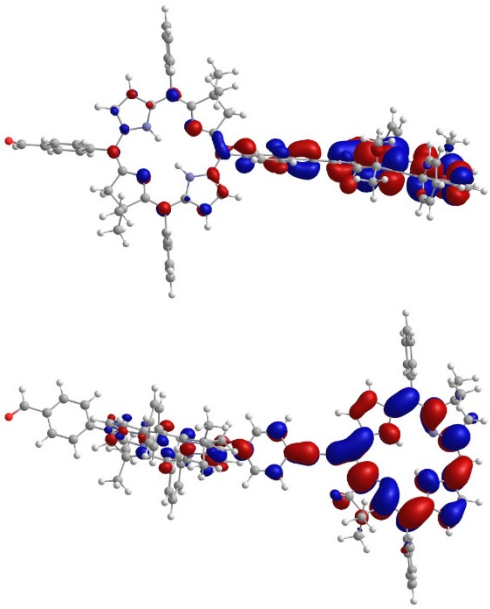
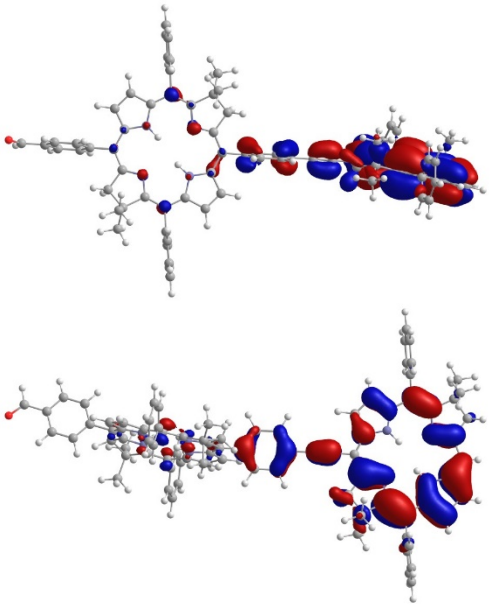
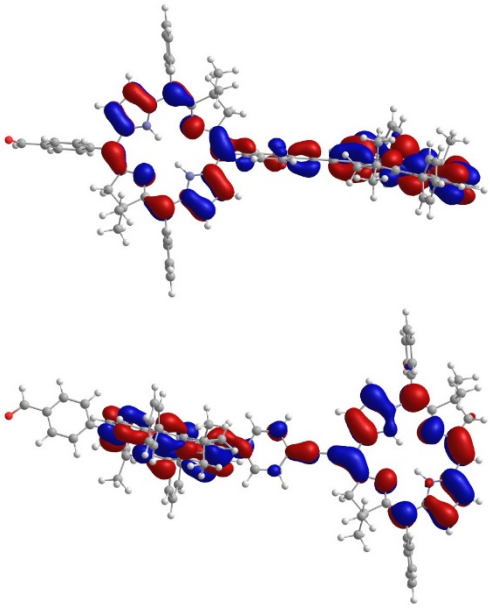
S3	0.82656		
S3	0.14348		

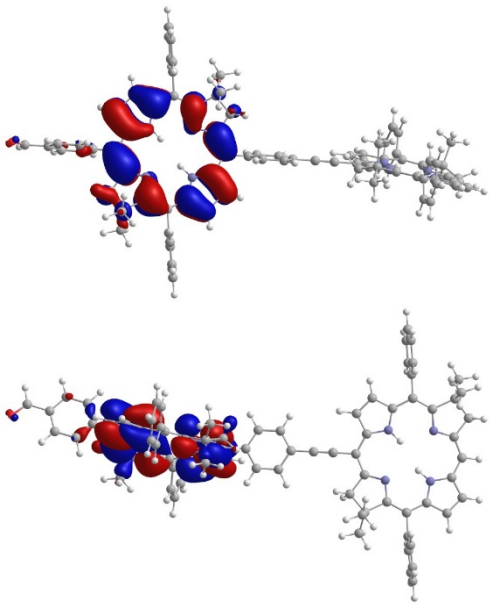
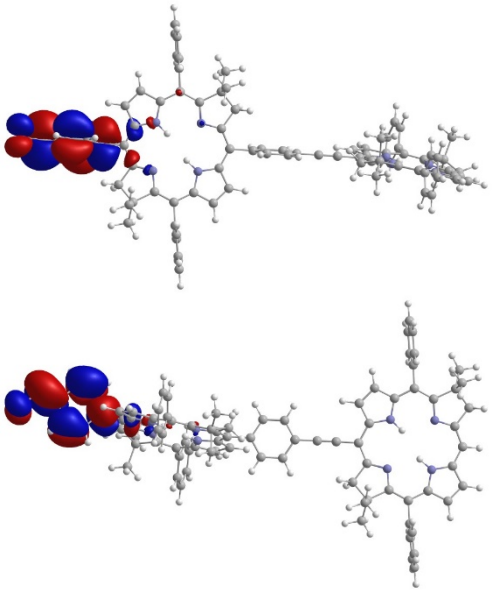
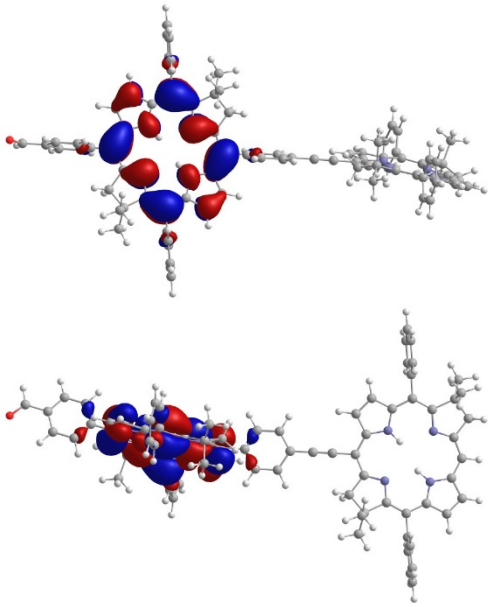
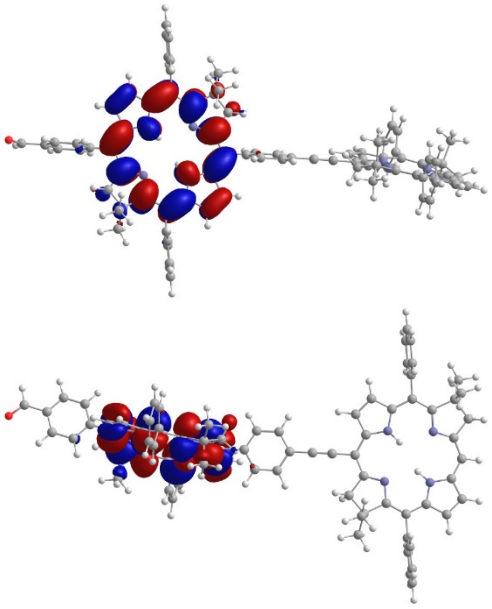
S4	0.79376		
S4	0.18224		

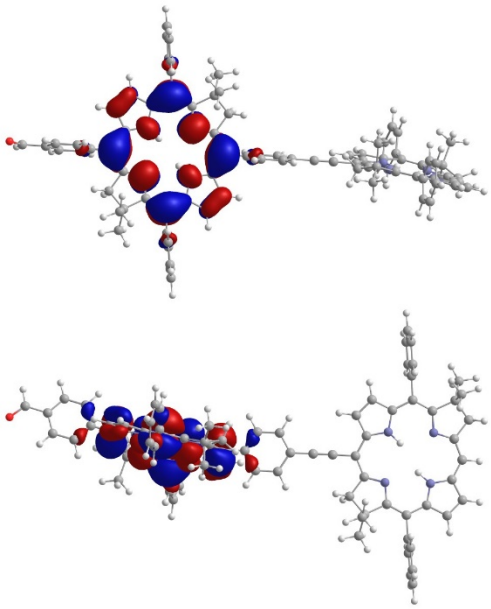
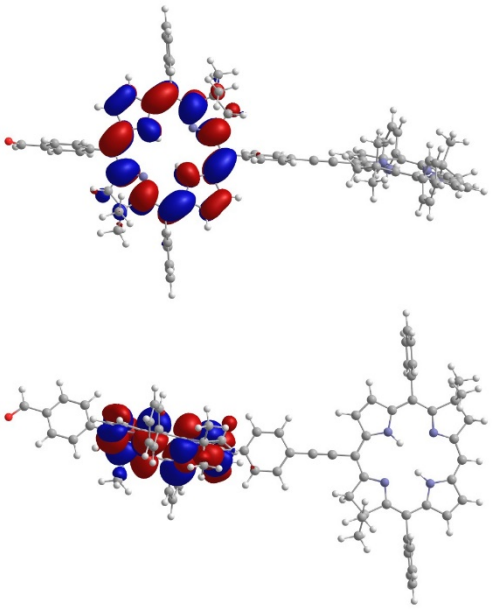
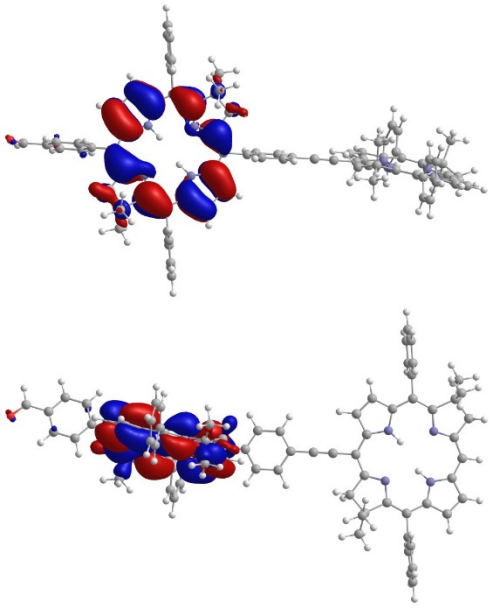
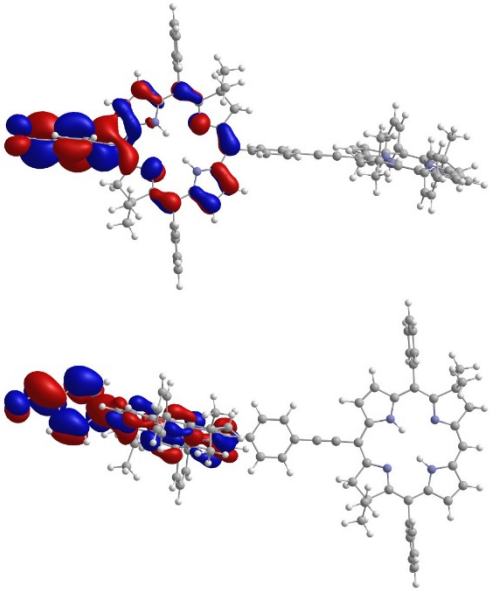
S5	0.70288		
S5	0.21480		

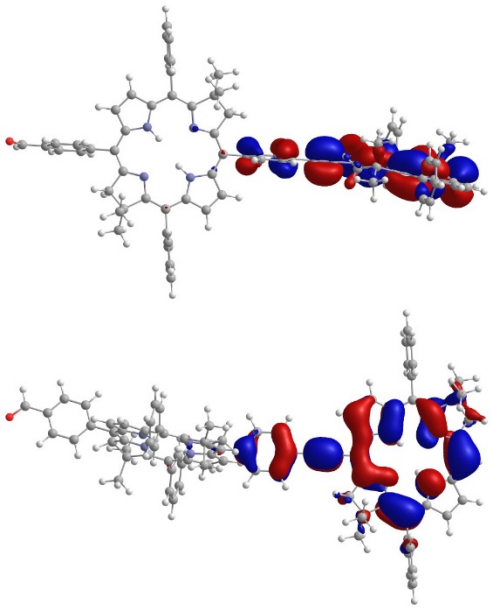
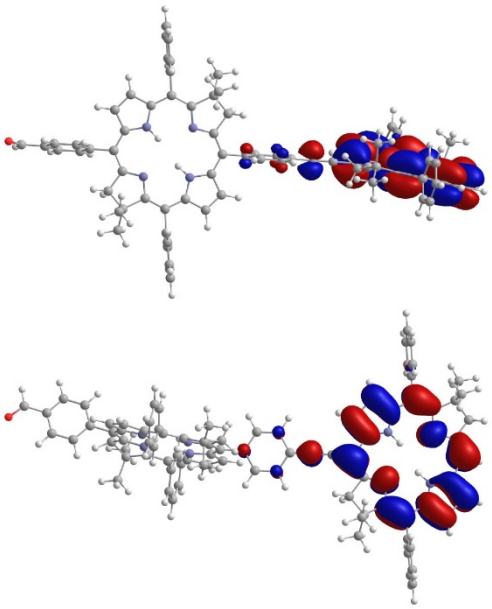
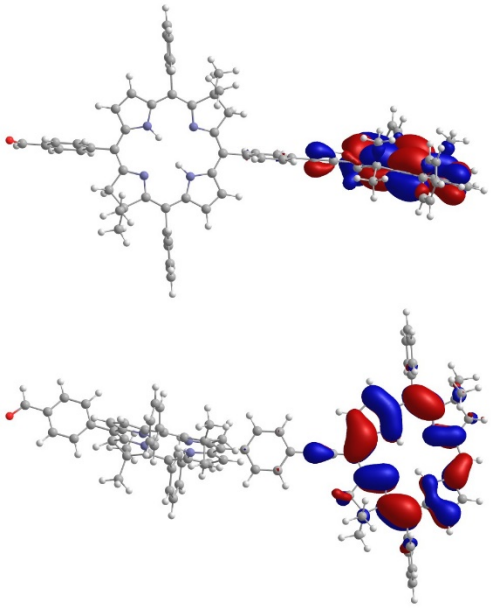
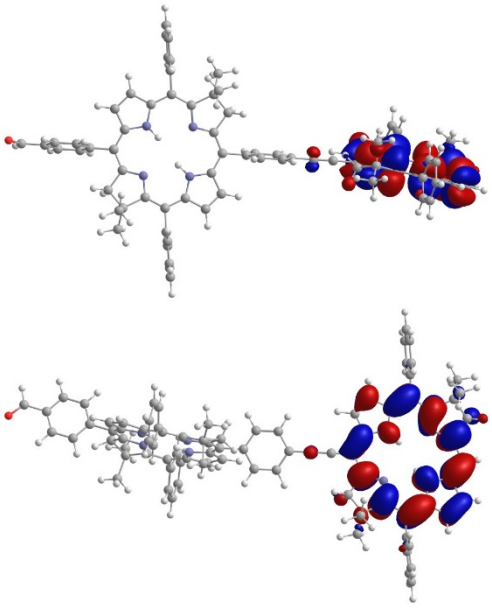
S6	0.76247		
S6	0.15152		

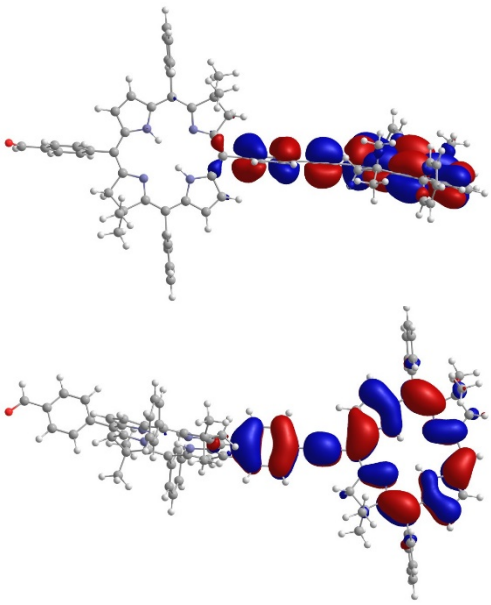
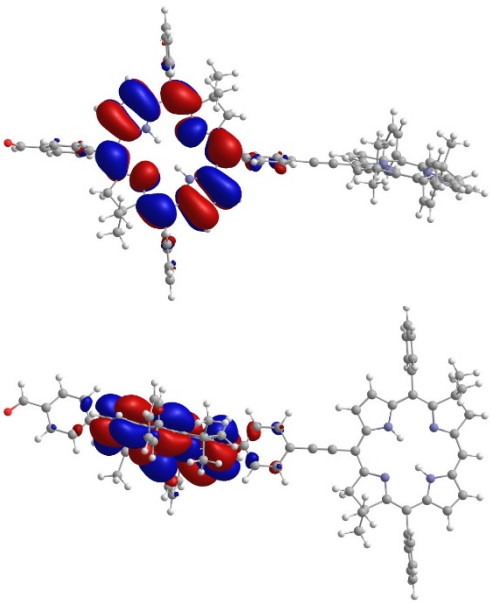
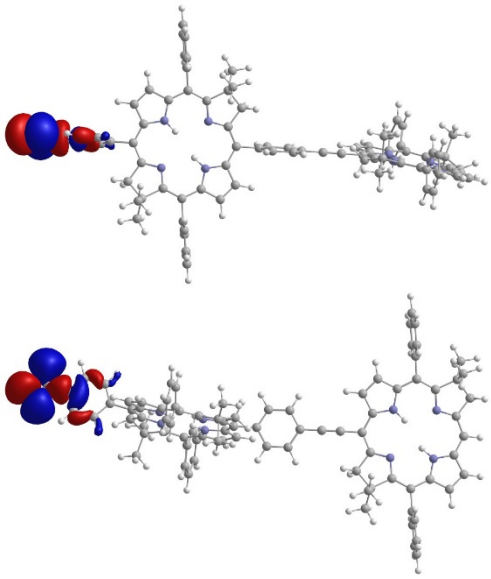
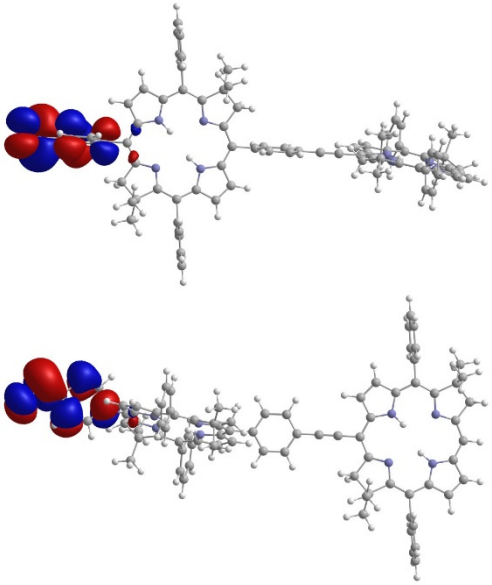
S7	0.92265		
S8	0.89399		

S9	0.68809		
S9	0.20888		

S10	0.80765		
S10	0.16076		

S11	0.65909		
S11	0.27093		

S12	0.82302		
S12	0.13295		

S13	0.99428		
S14	0.99851		

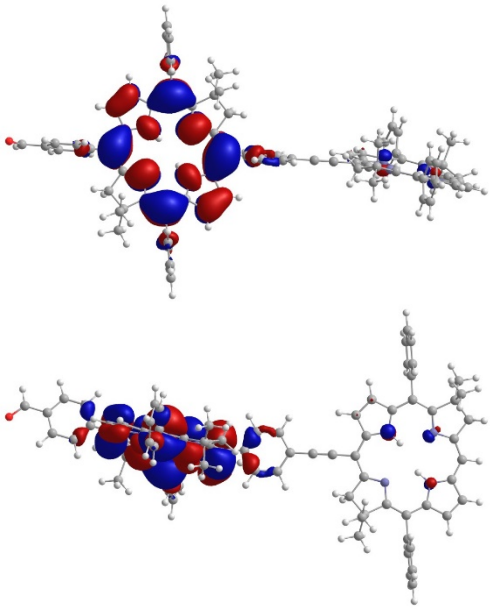
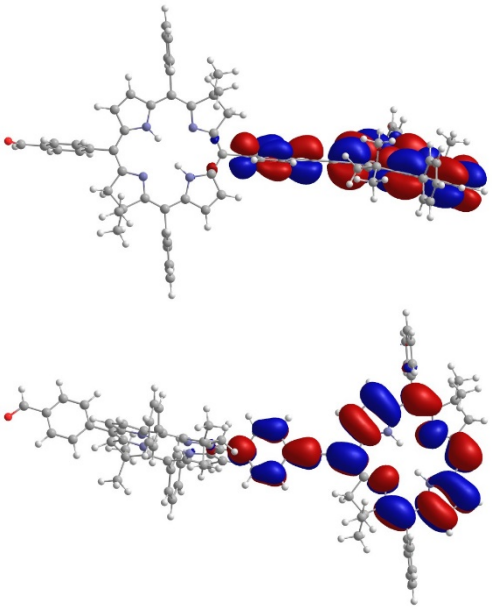
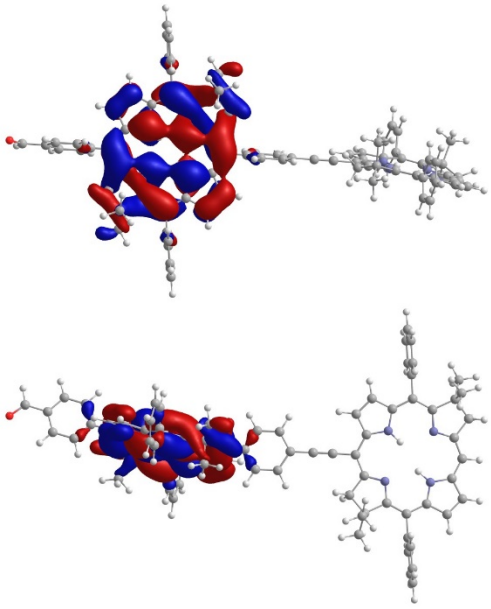
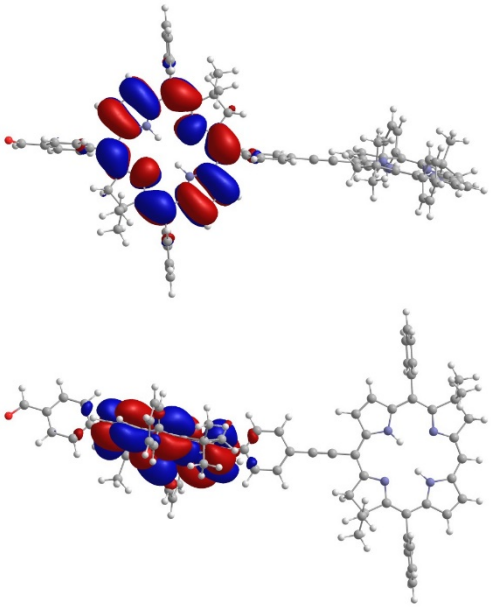
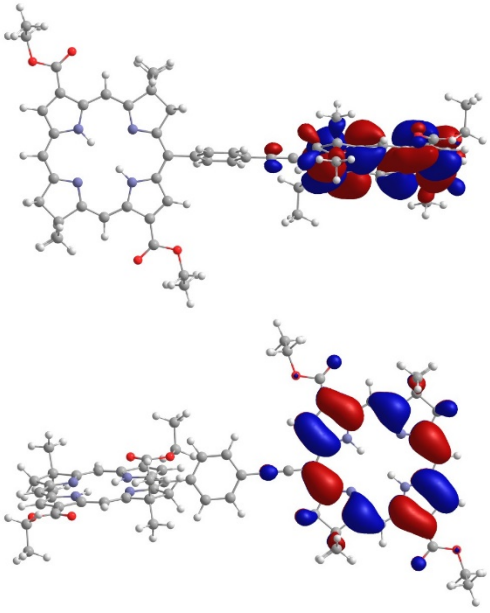
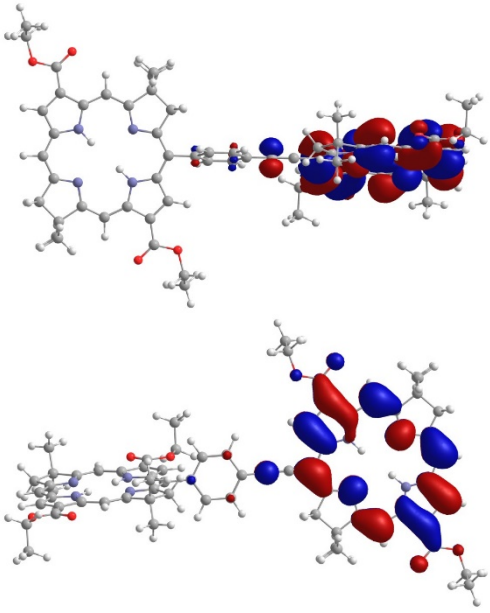
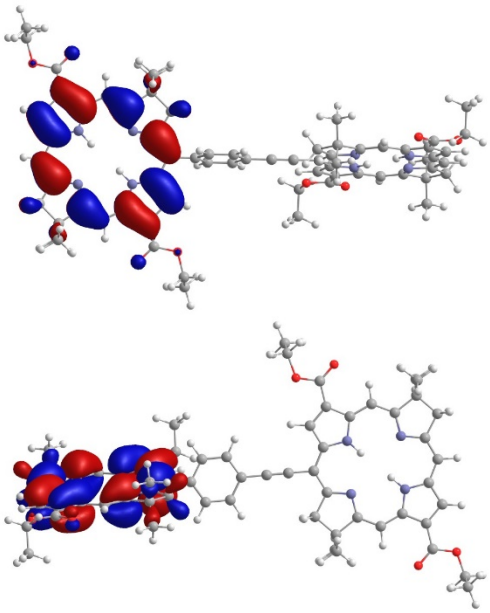
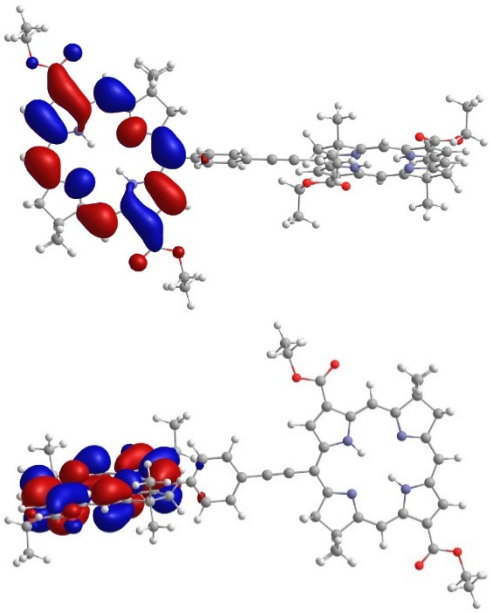
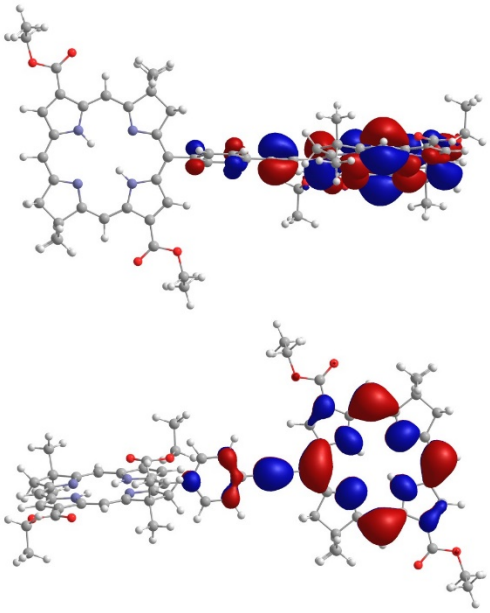
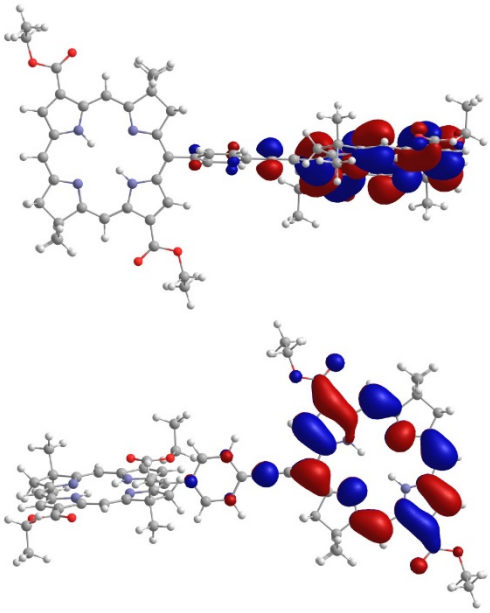
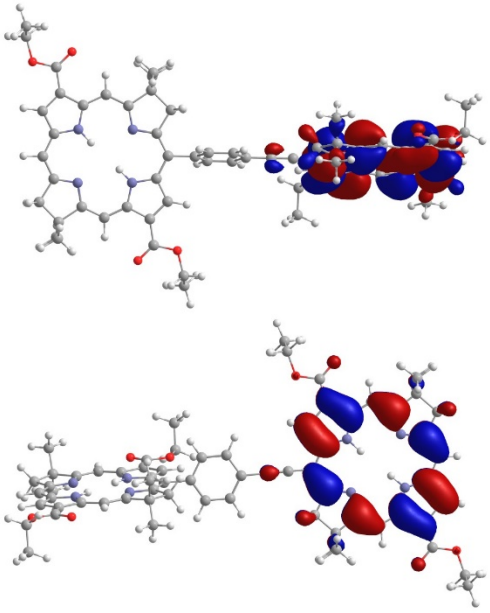
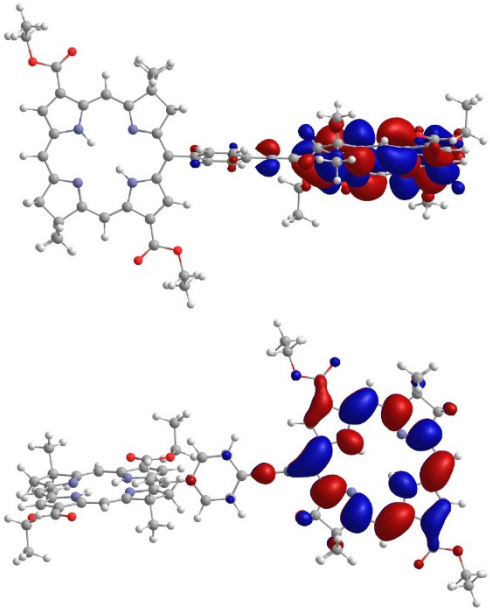
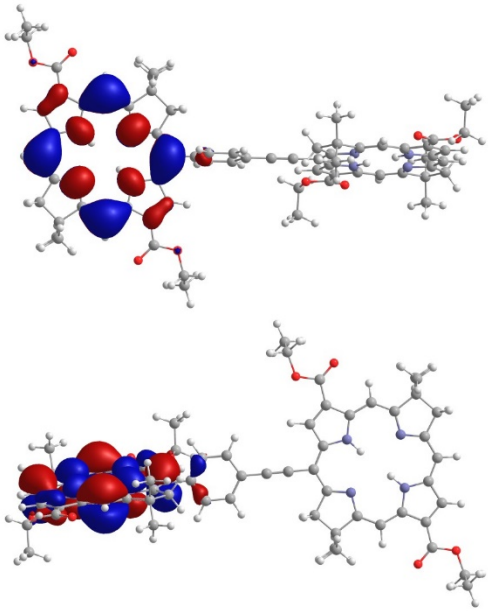
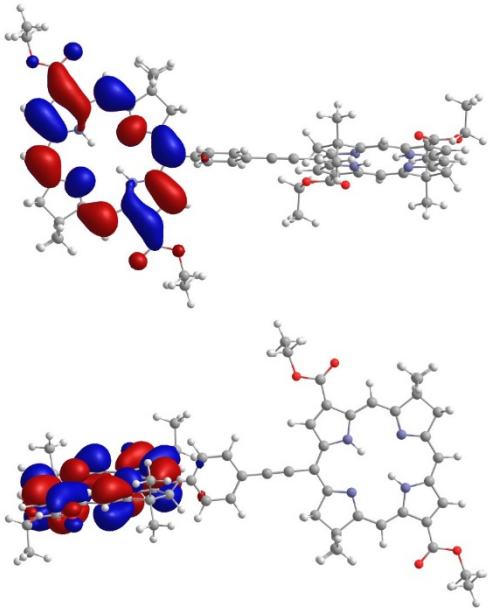
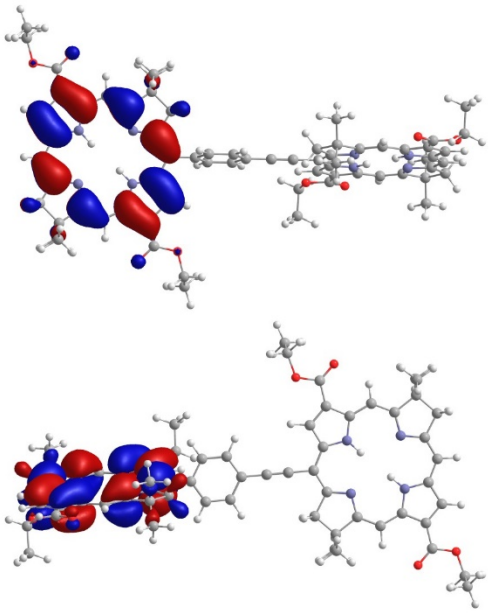
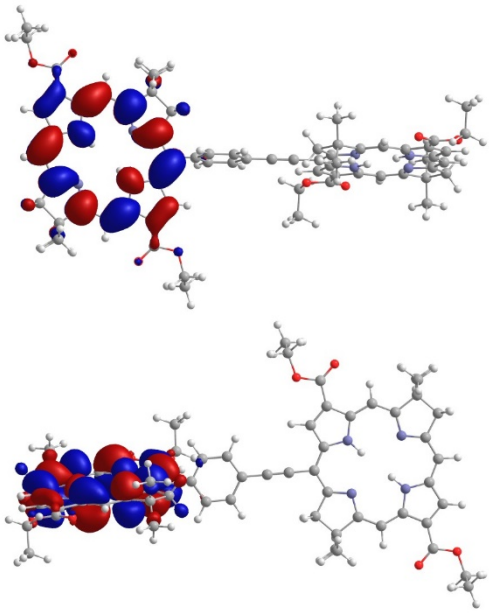
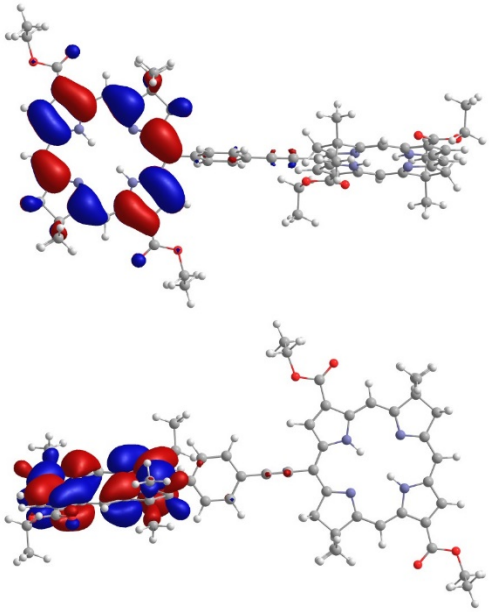
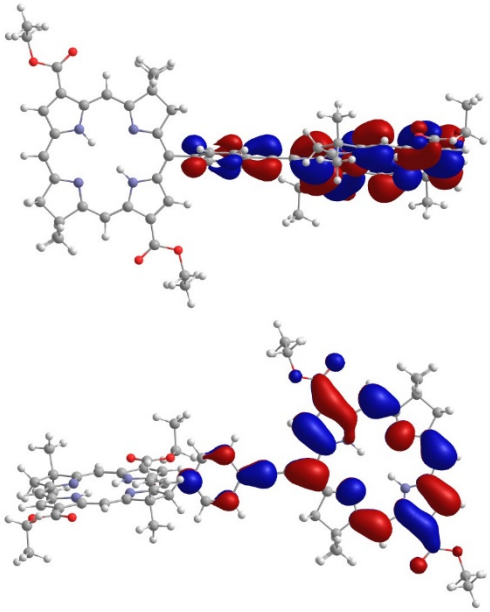
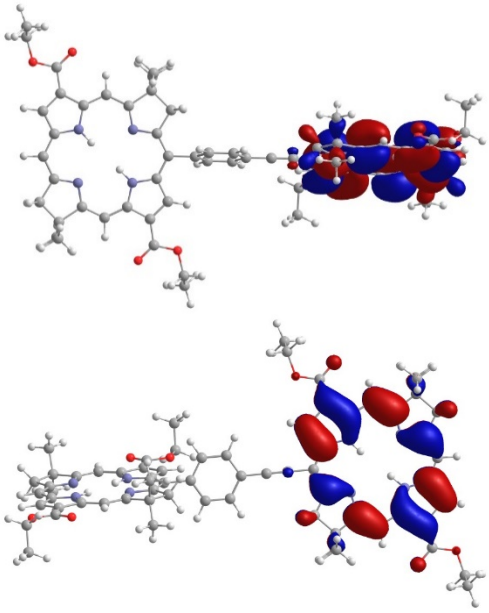
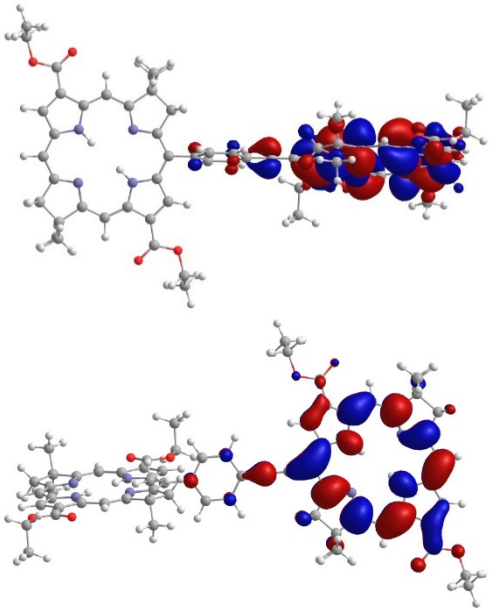
S15	0.98565		
S16	0.95377		

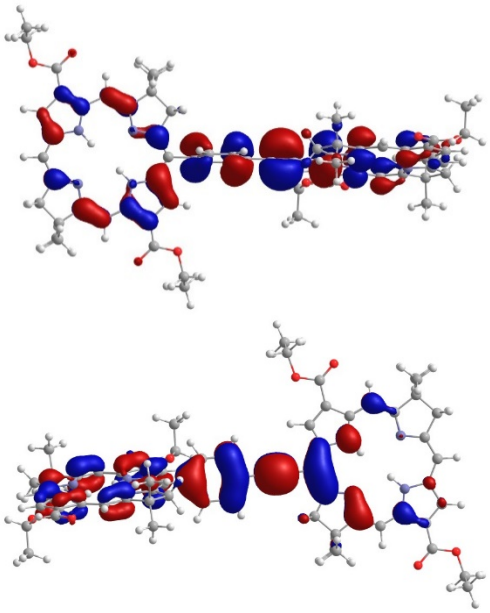
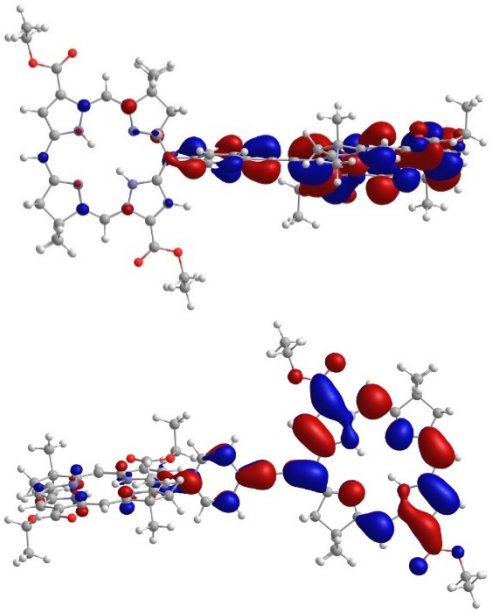
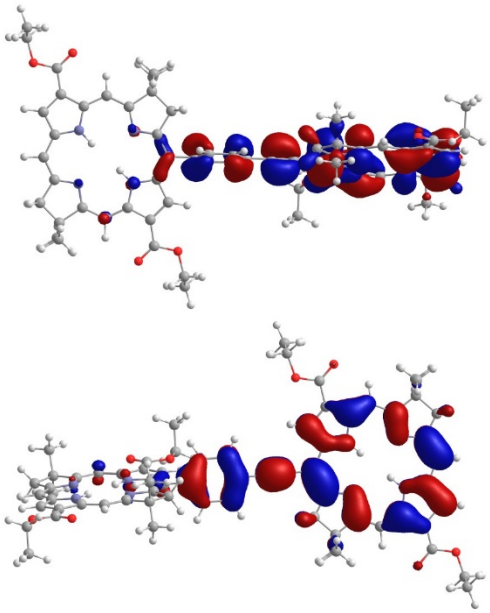
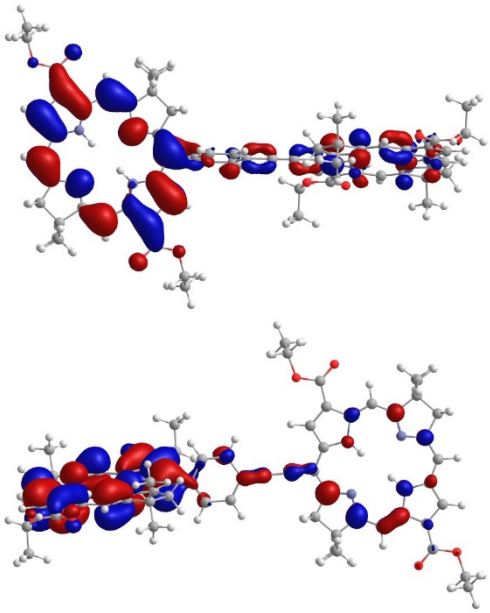
Table S23. NTOs for **Dyad-3**.

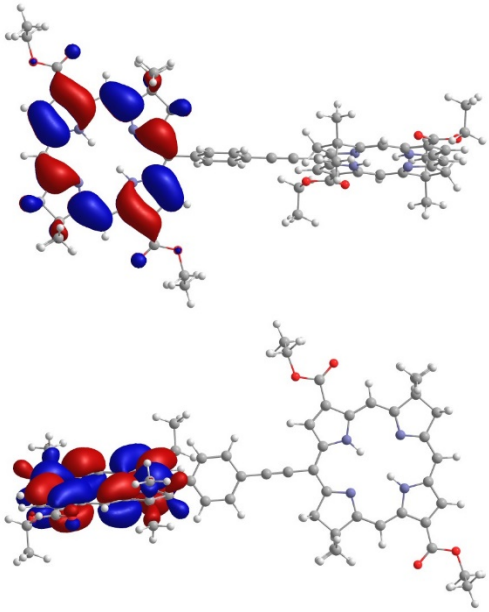
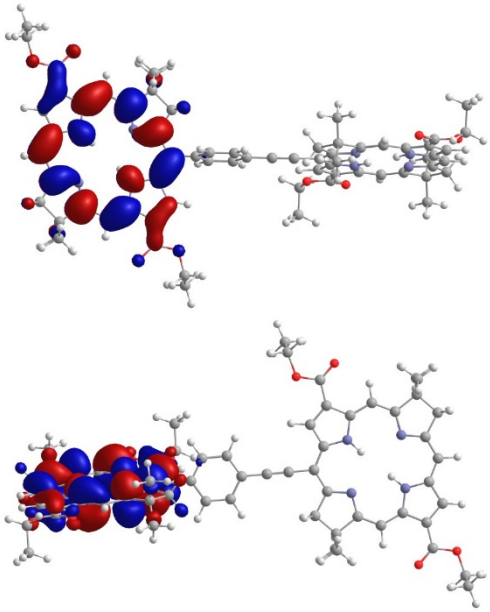
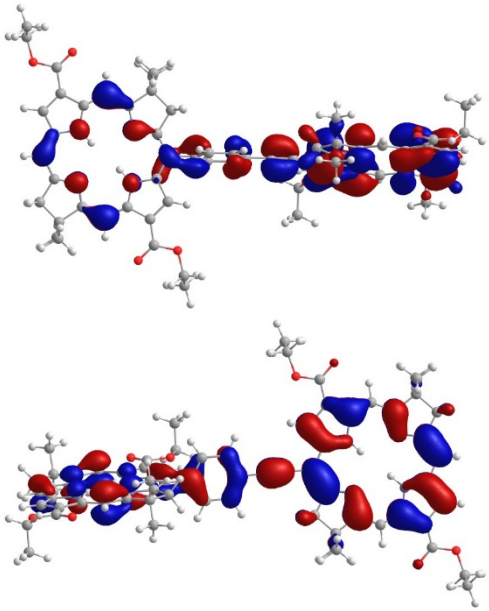
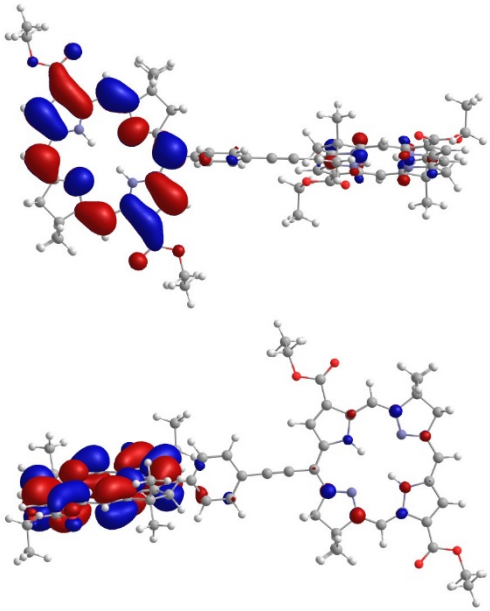
S#	Eigenvalue	From	To
S1	0.85028		
S2	0.84304		

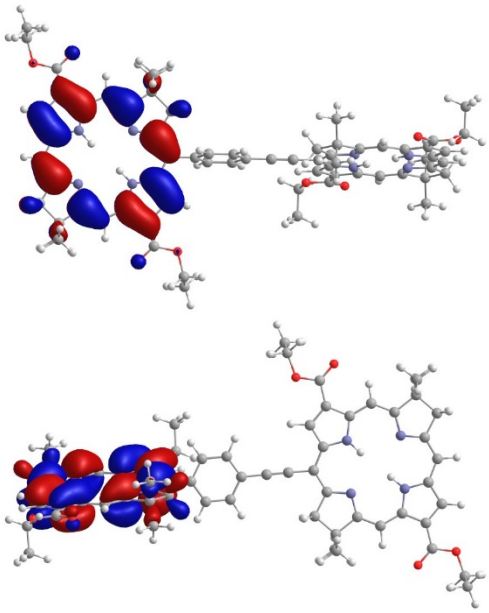
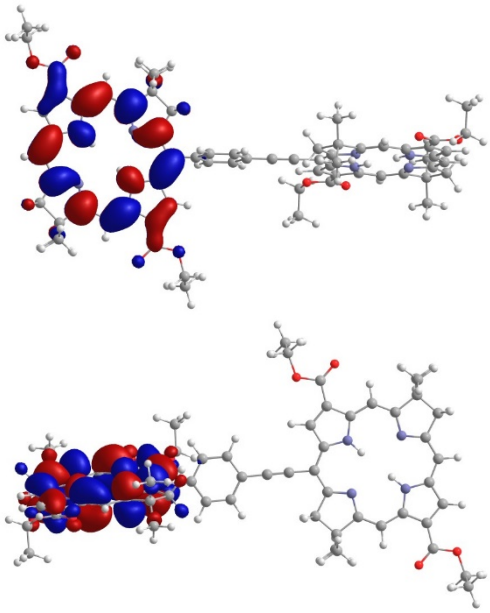
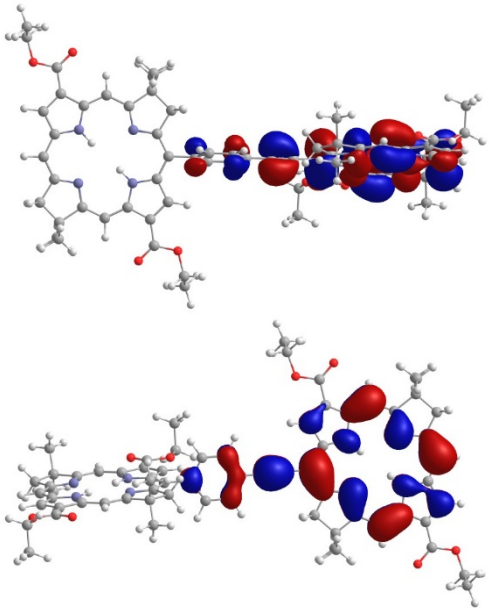
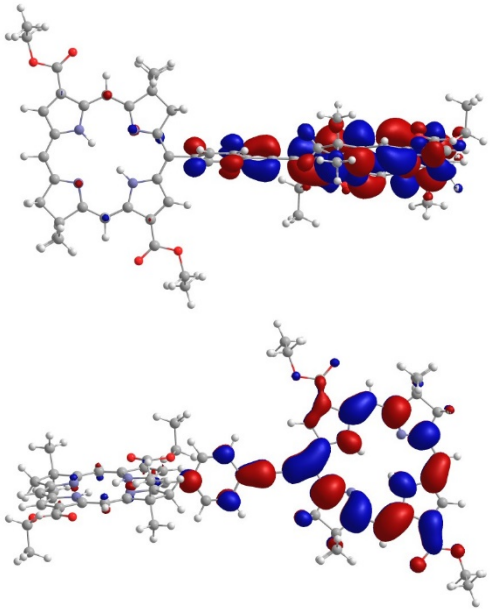
S3	0.86981		
S3	0.11065		

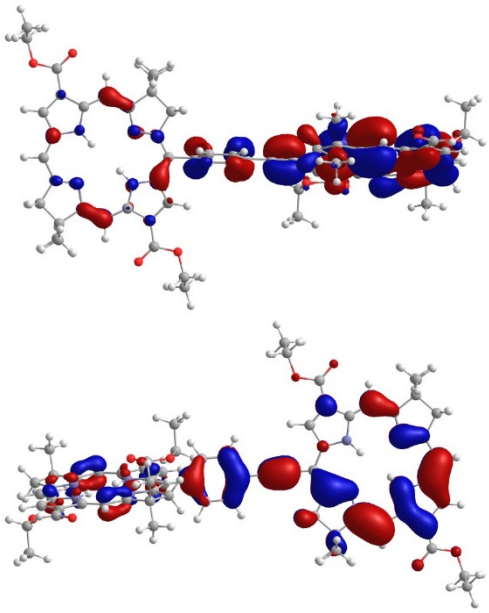
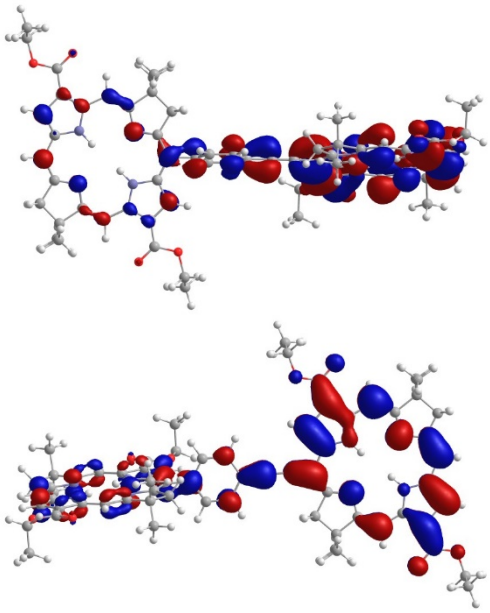
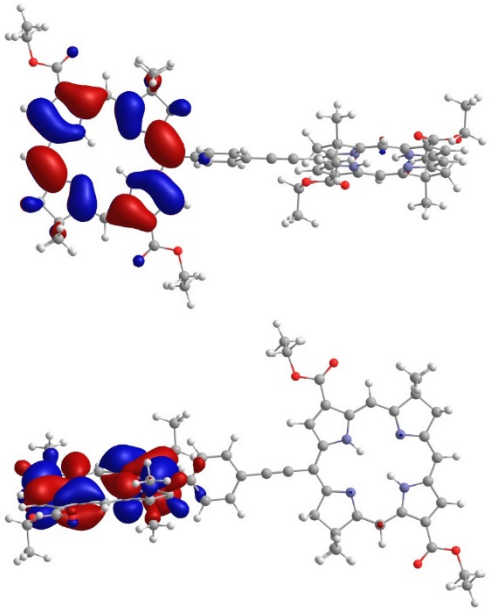
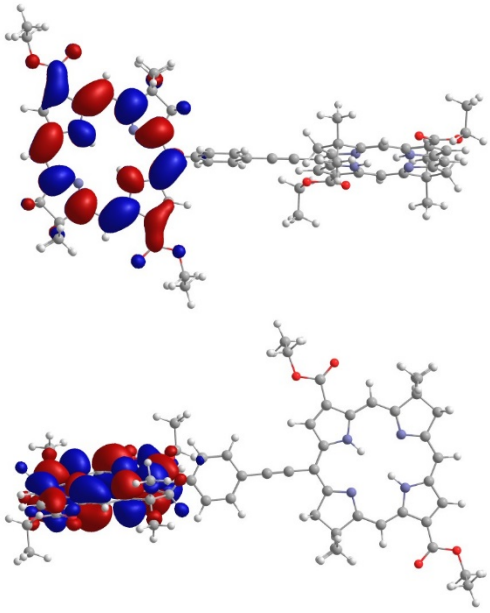
S4	0.84304		
S4	0.14324		

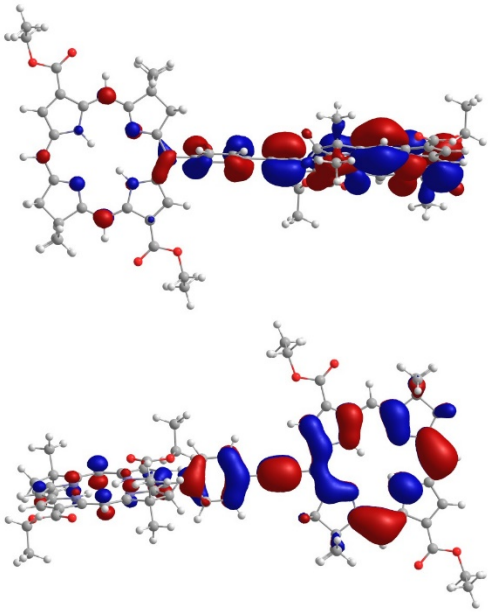
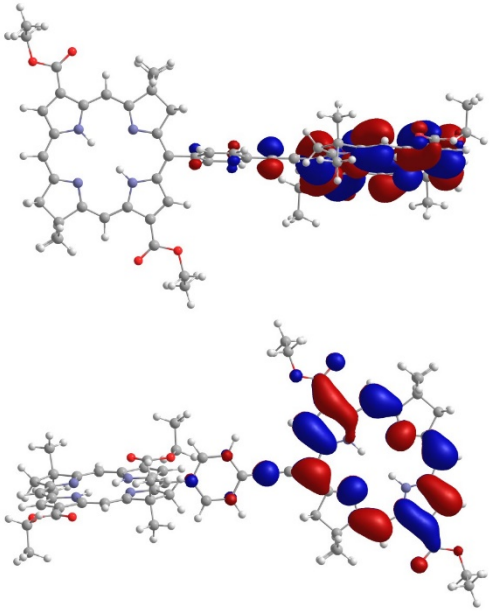
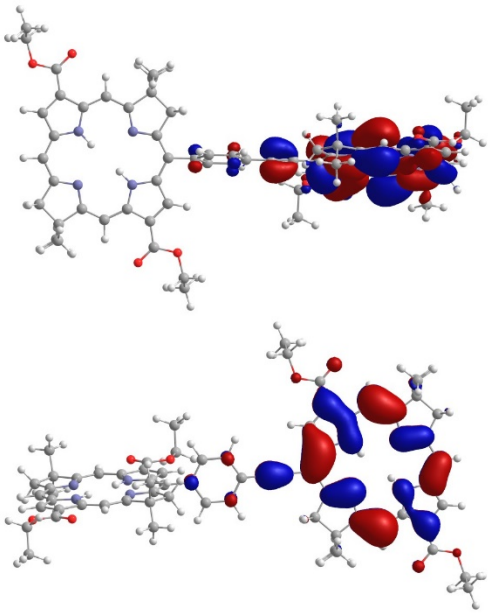
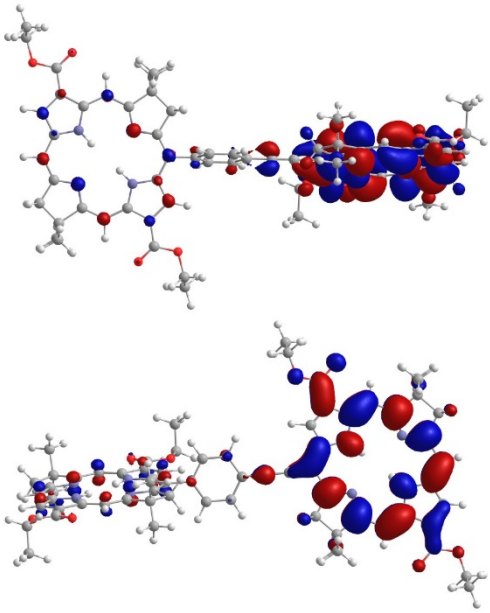
S5	0.96689		
S6	0.67227		

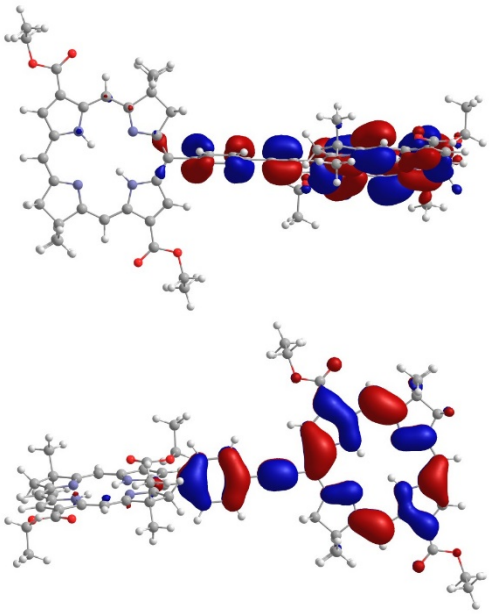
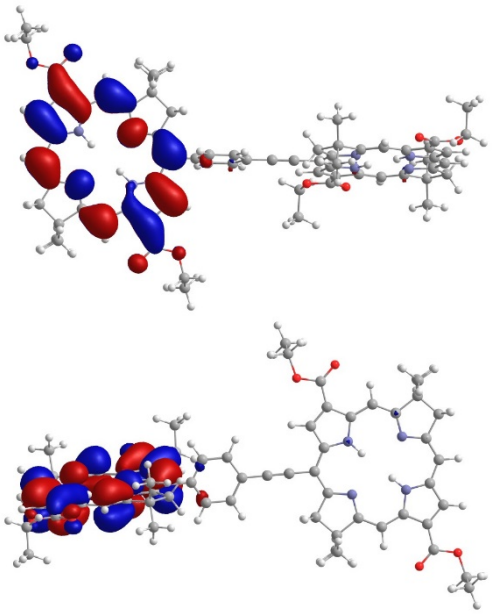
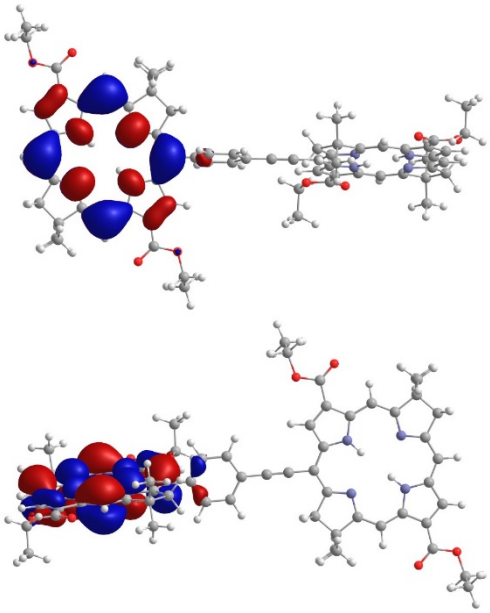
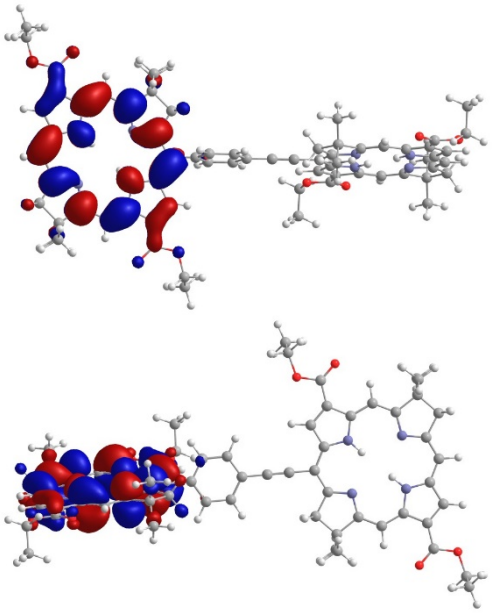
S6	0.28474		
S7	0.74207		

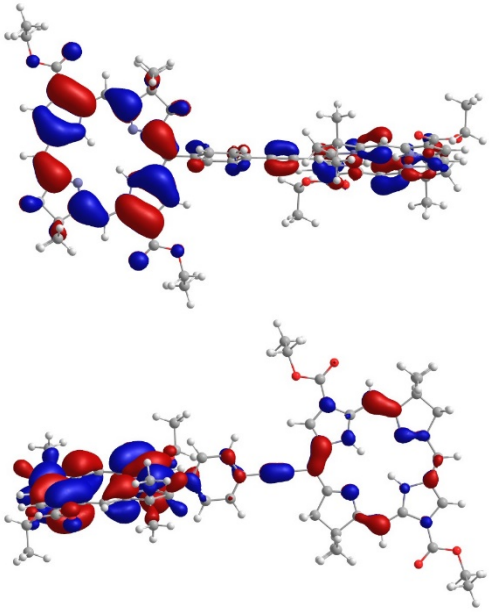
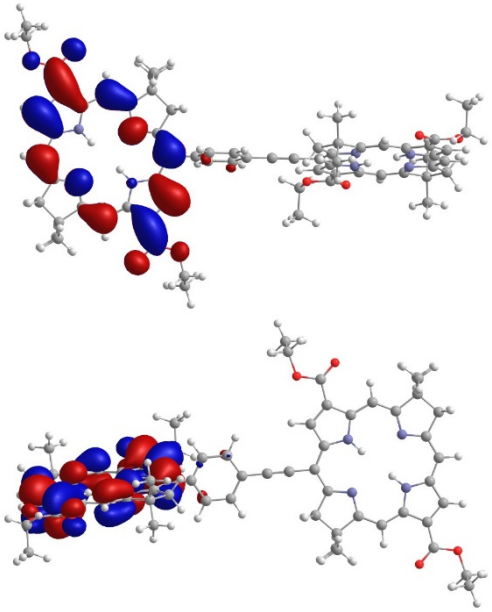
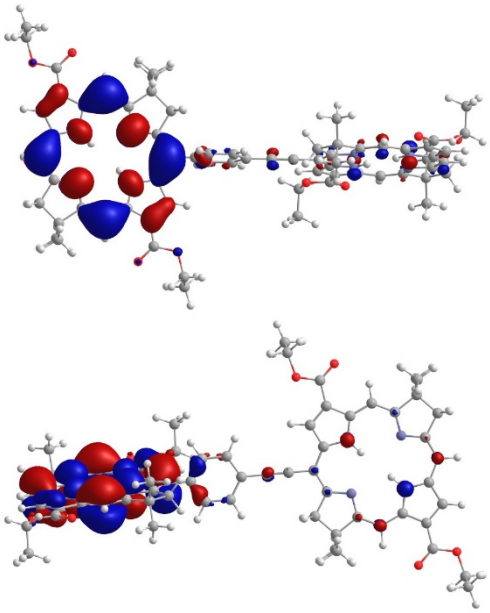
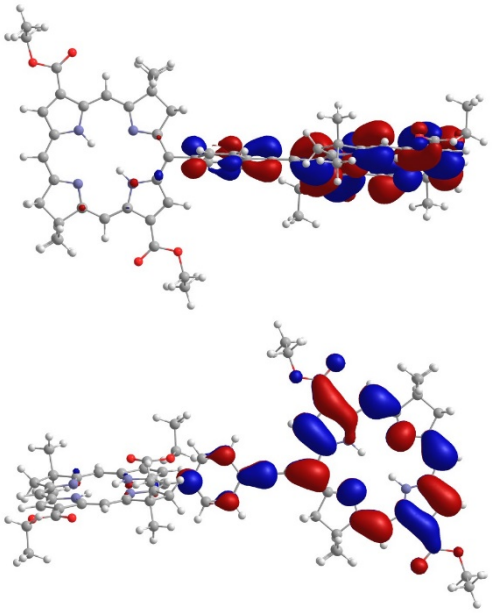
S7	0.21652		
S8	0.50495		

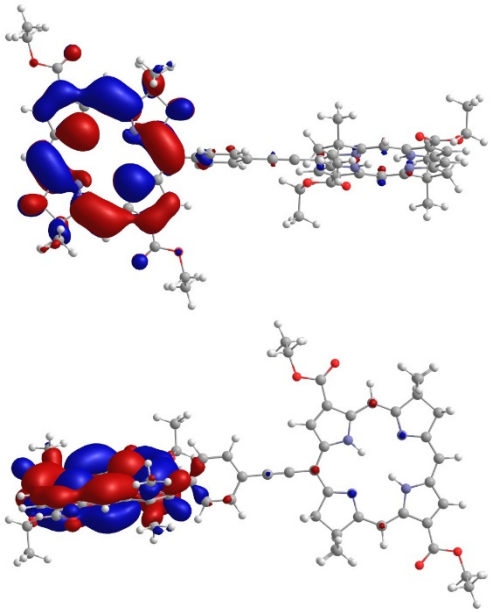
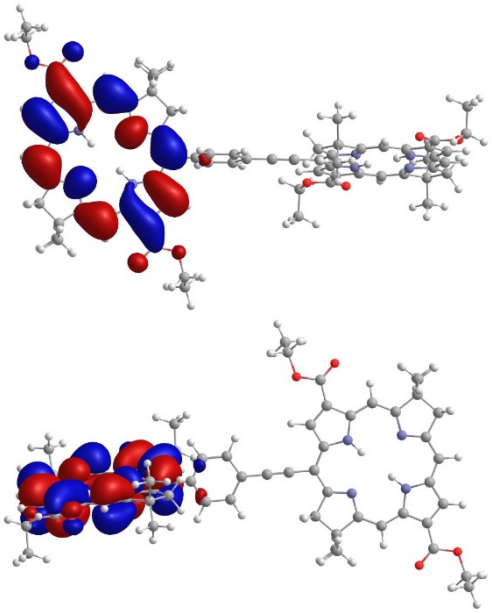
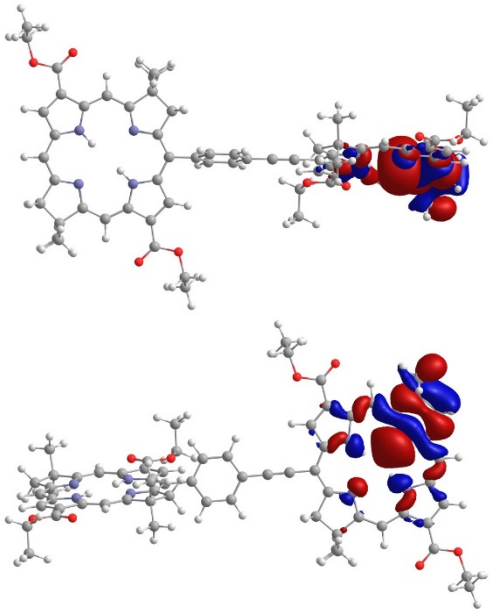
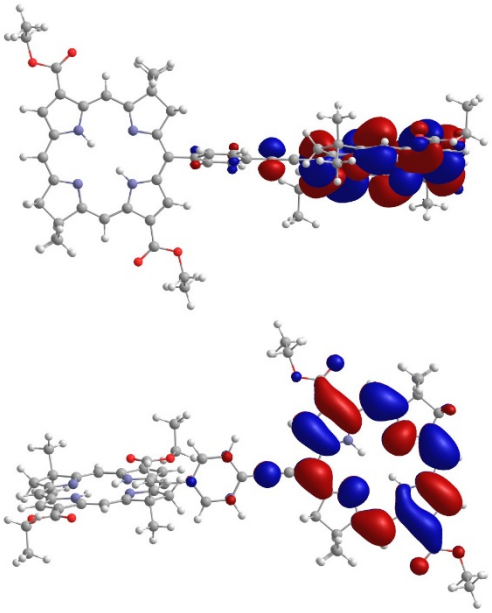
S8	0.48130		
S9	0.63144		

S9	0.19184		
S9	0.15411		

S10	0.68951		
S10	0.28764		

S11	0.95805		
S12	0.81060		

S12	0.12256		
S13	0.98148		

S14	0.92897		
S15	0.99741		

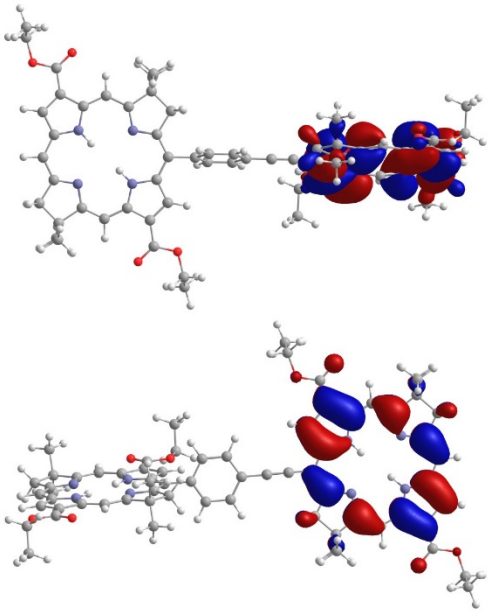
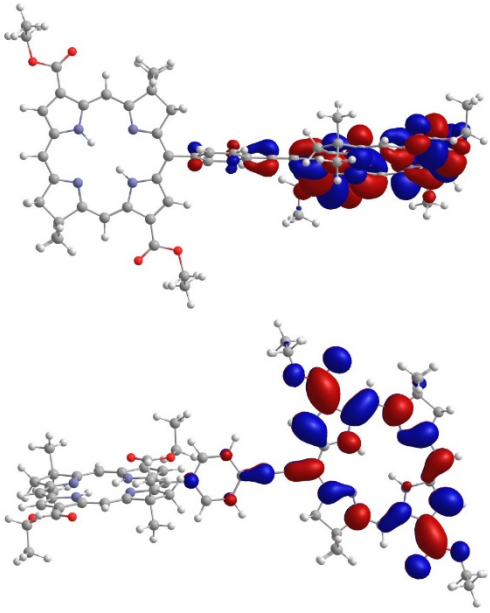
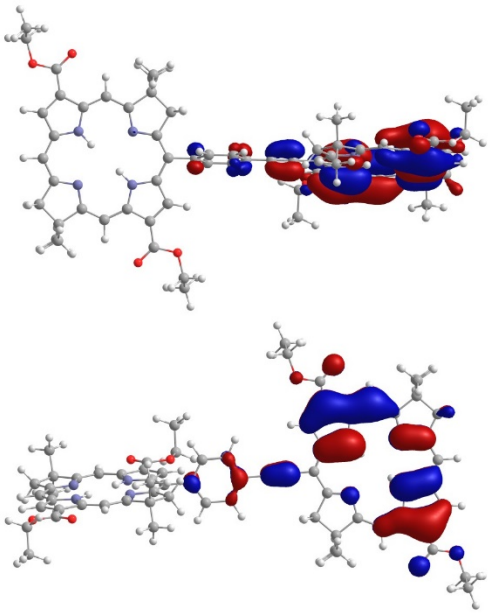
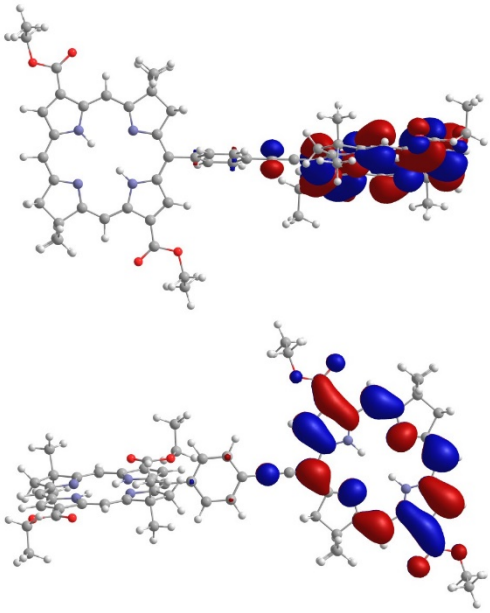
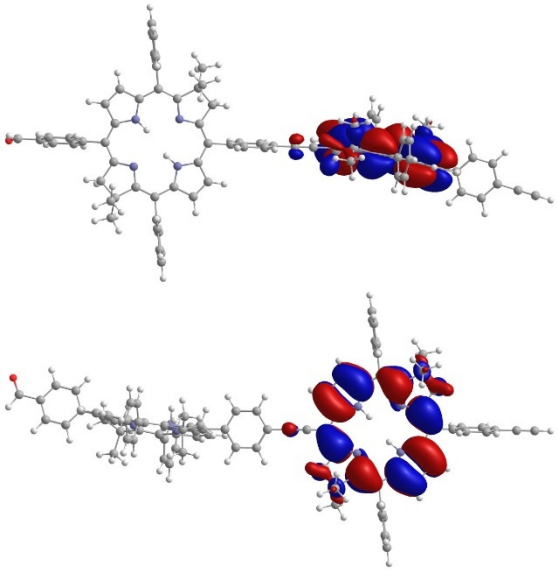
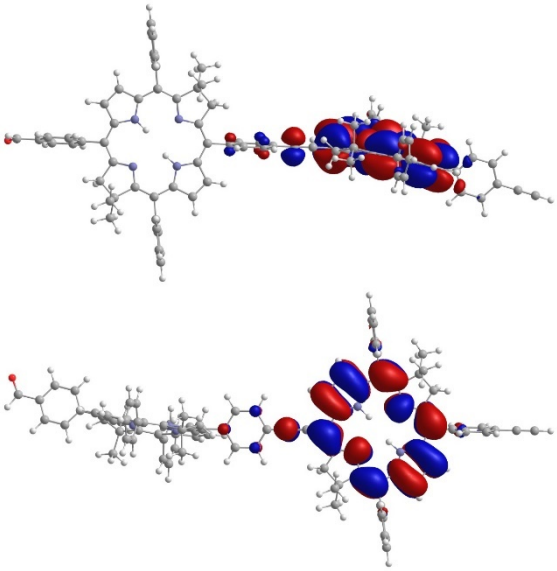
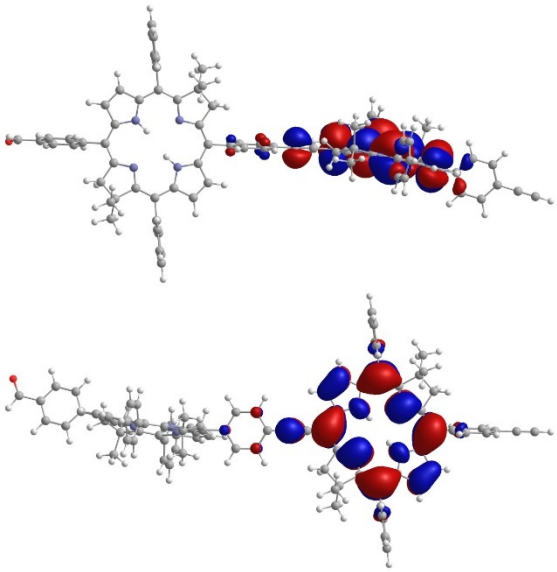
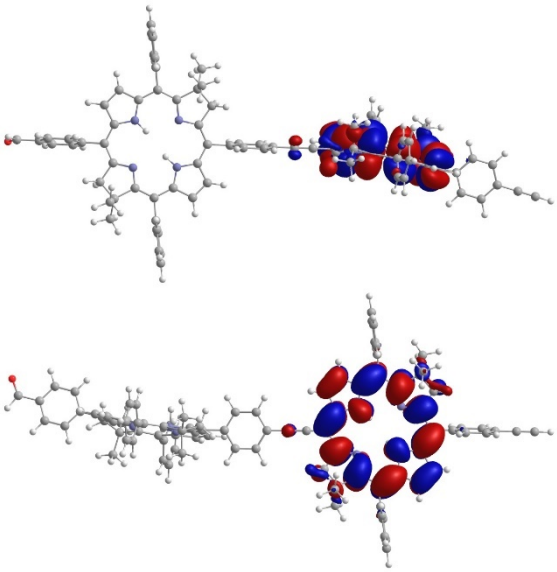
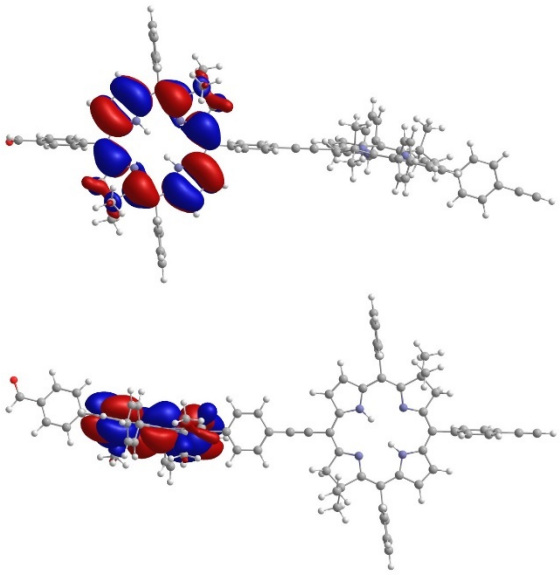
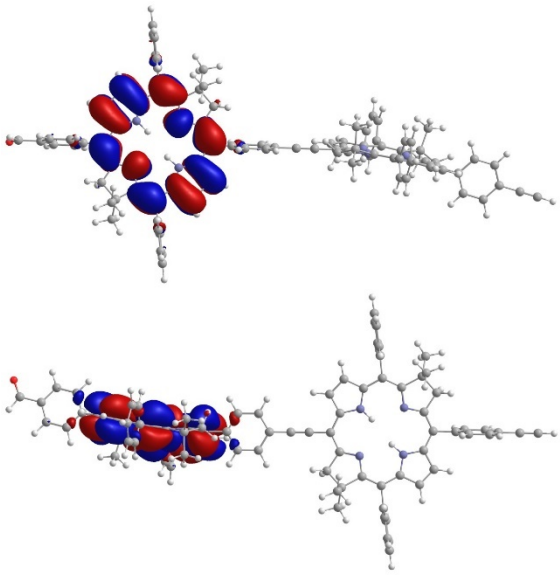
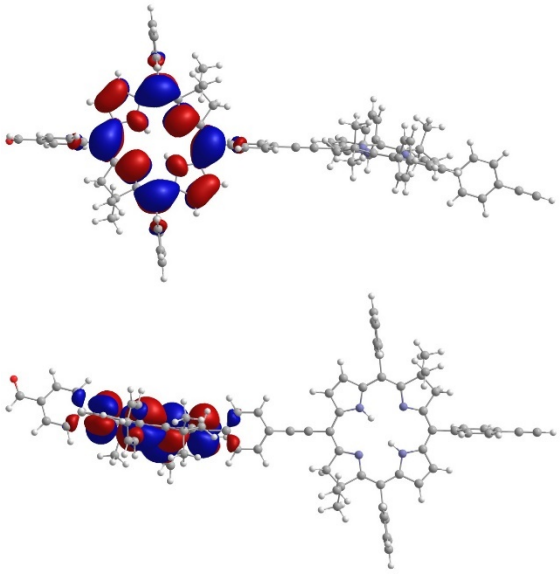
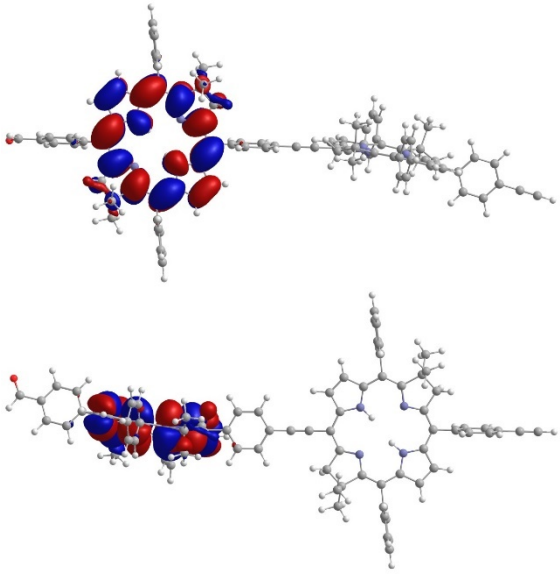
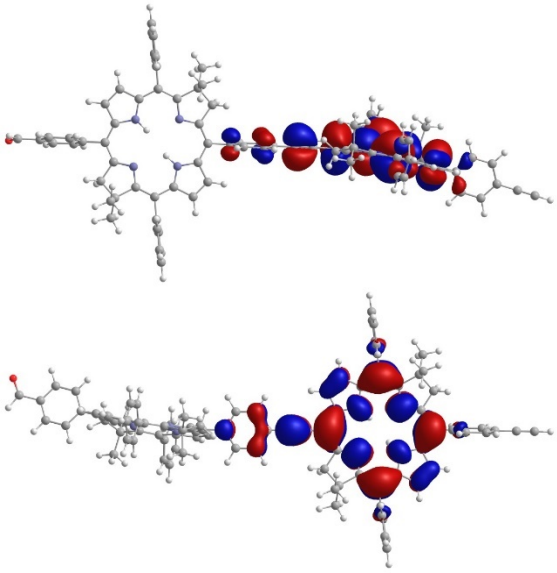
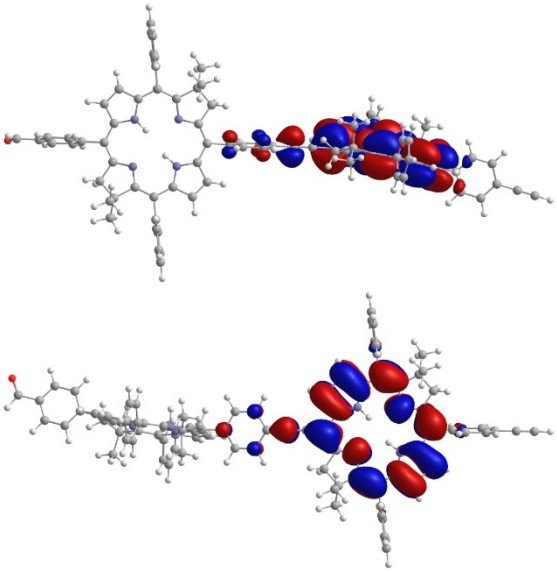
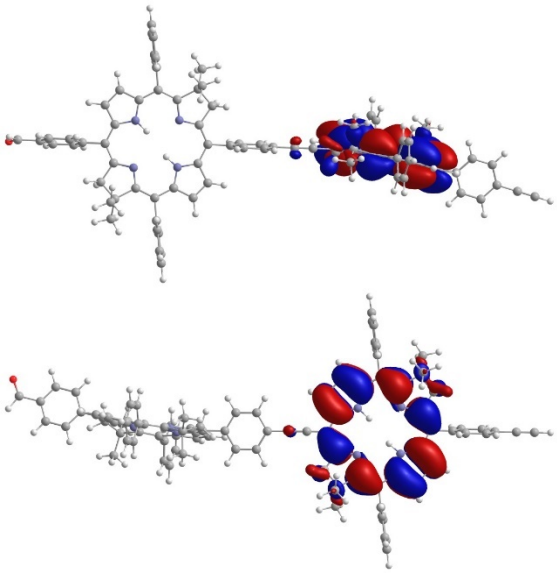
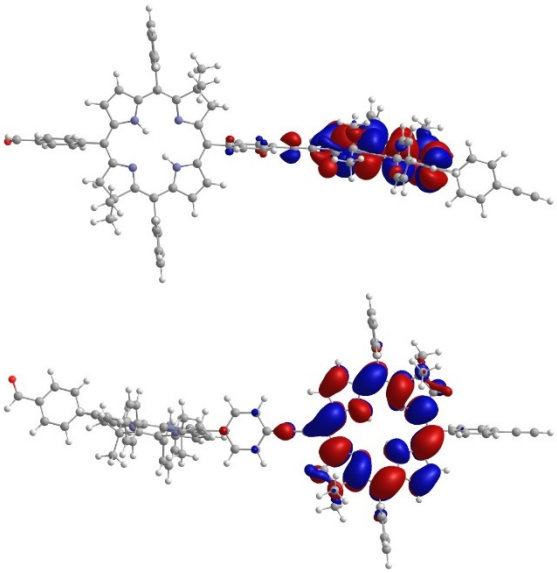
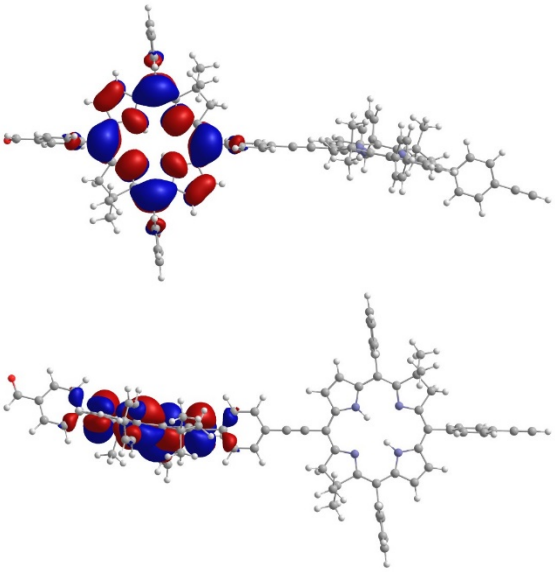
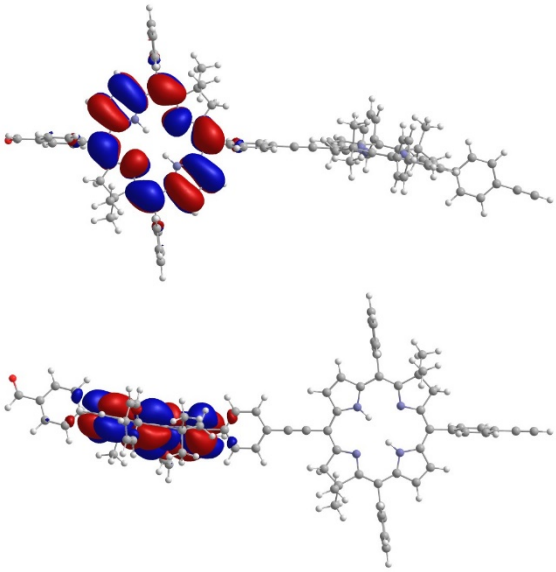
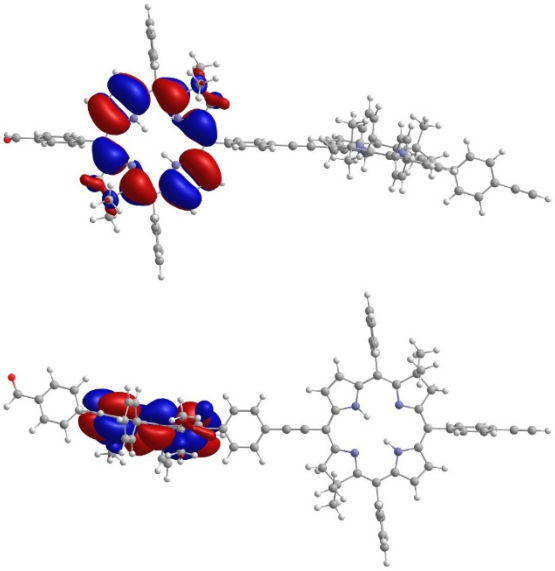
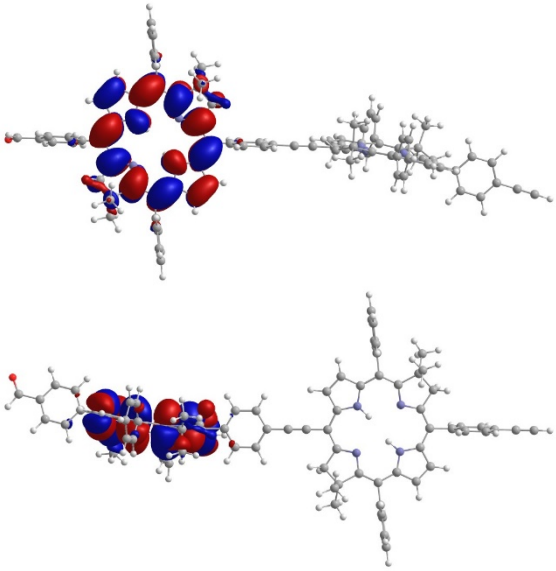
S16	0.59295		
S16	0.38599		

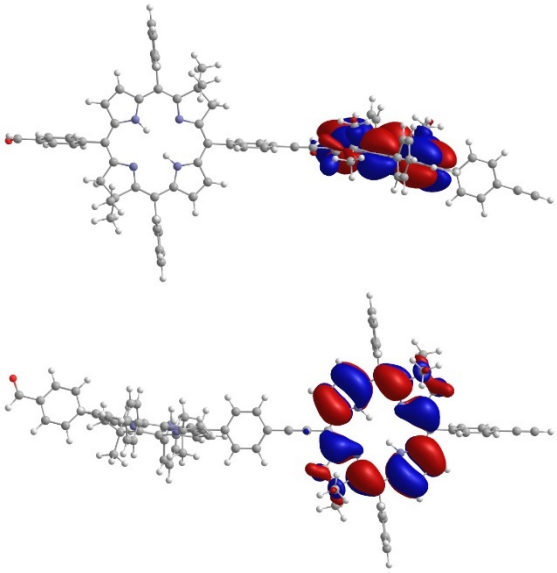
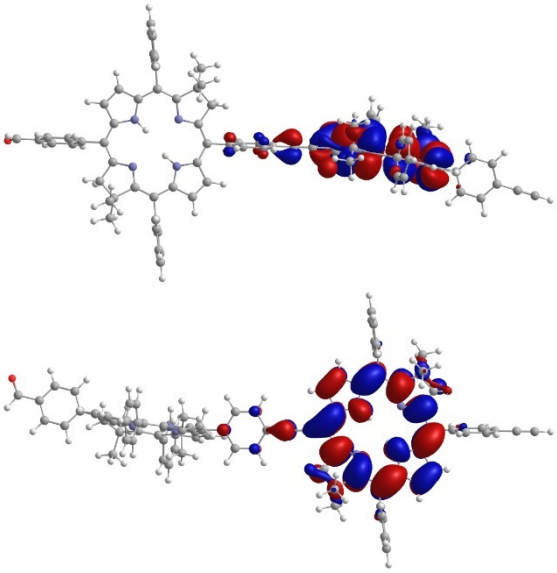
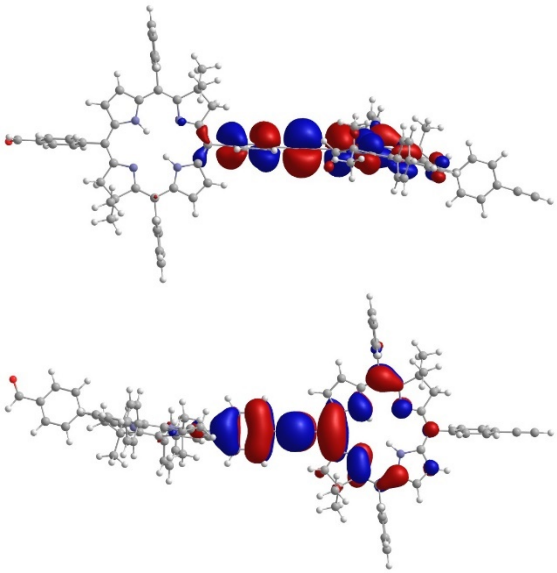
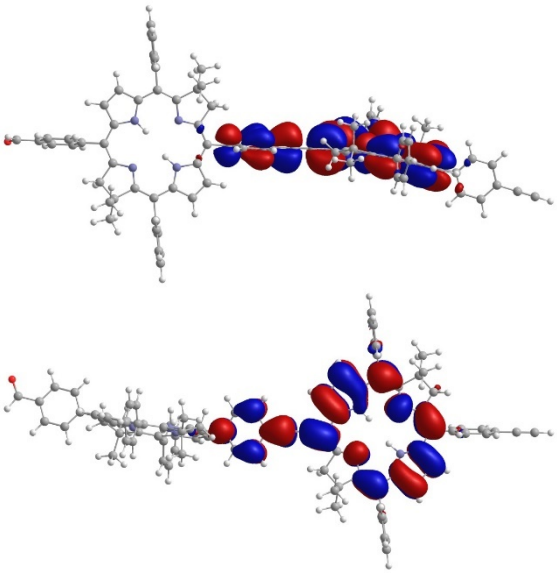
Table S24. NTOs for **Dyad-4**.

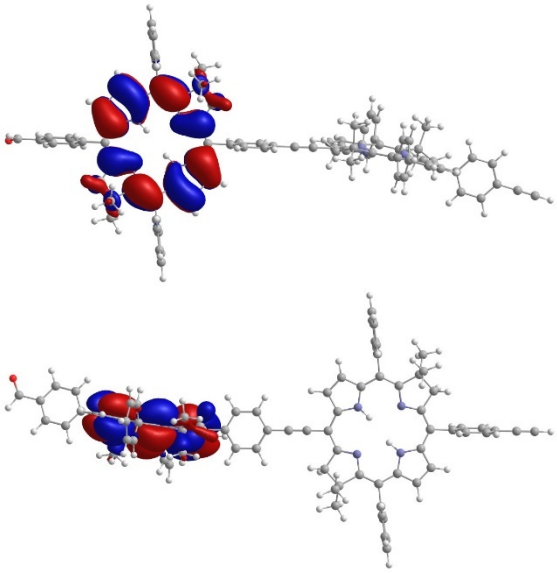
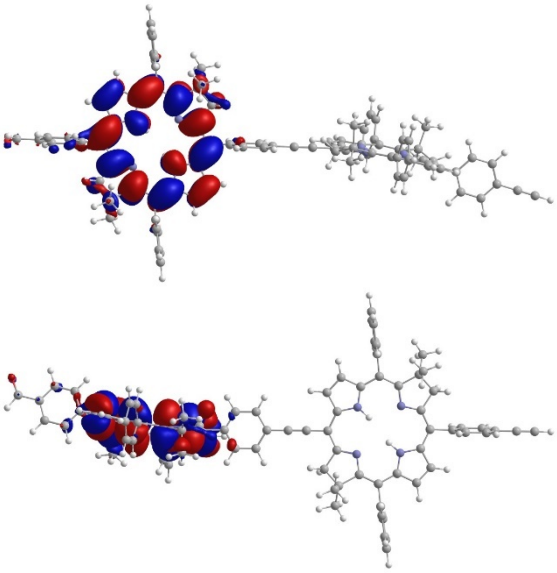
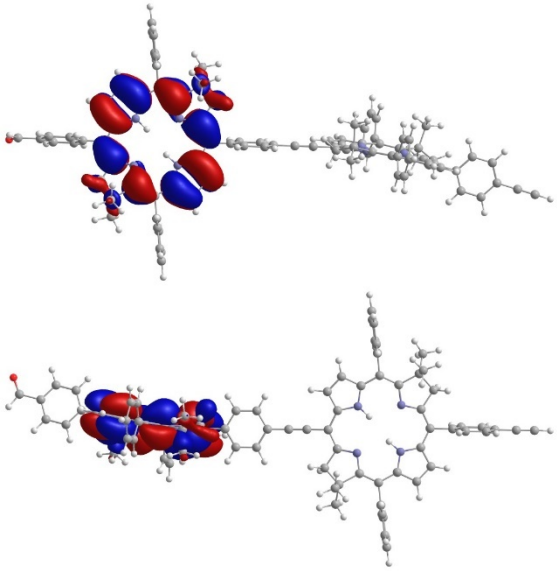
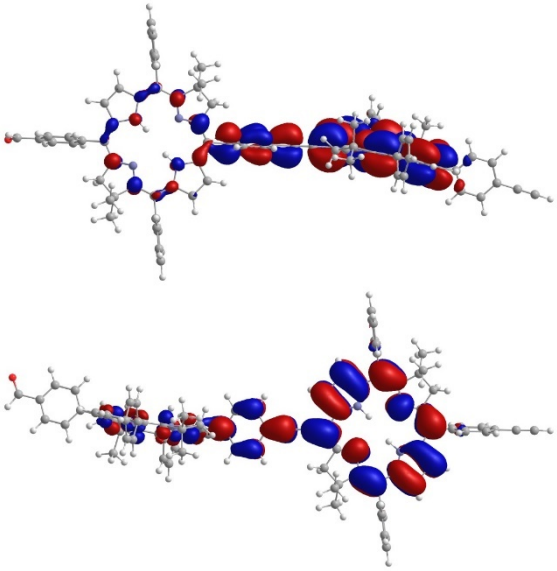
S#	Eigenvalue	From (NTO)	To (NTO)
S1	0.89087		
S1	0.08259		

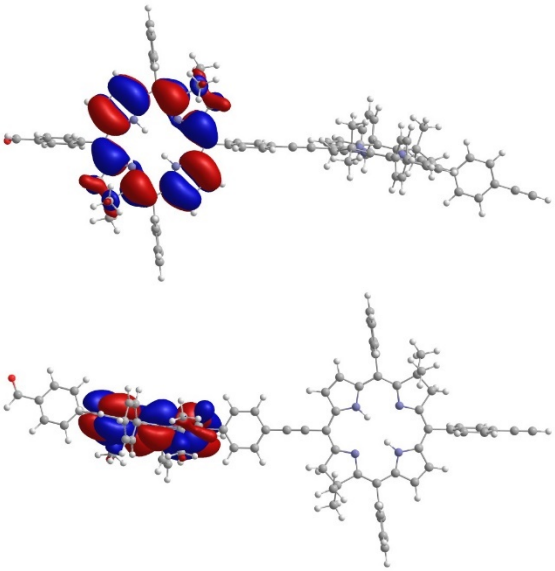
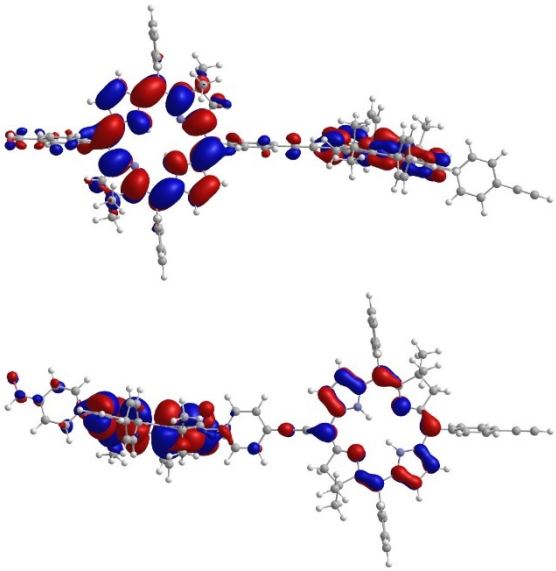
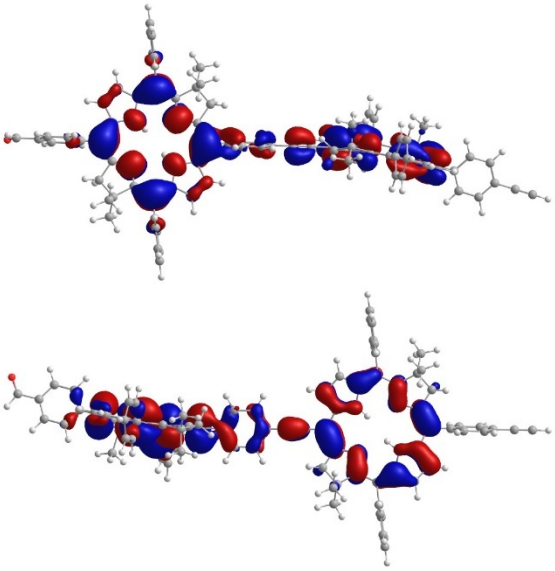
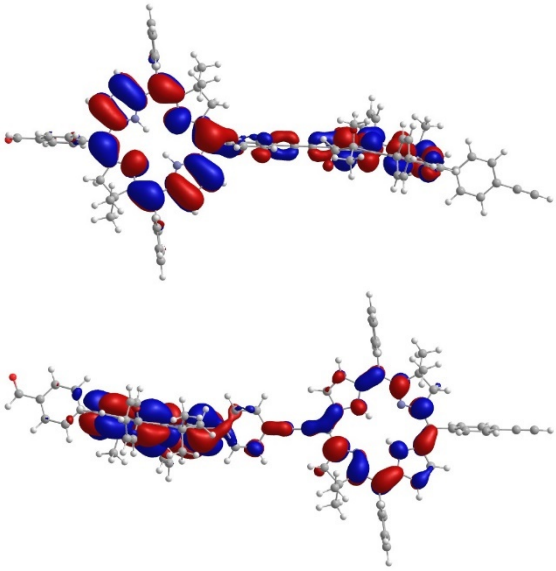
S2	0.88170		
S2	0.09019		

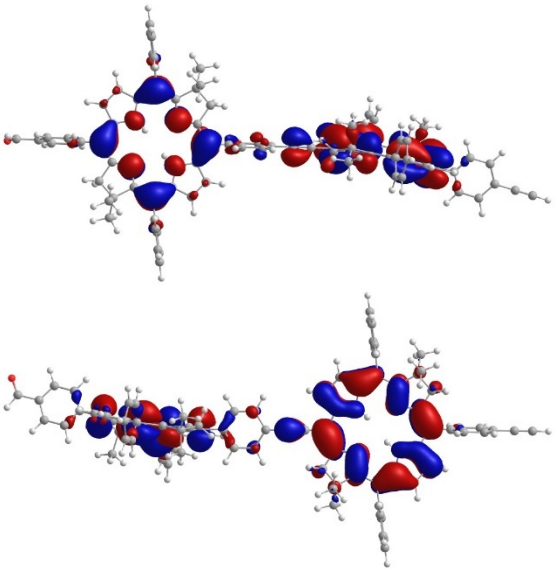
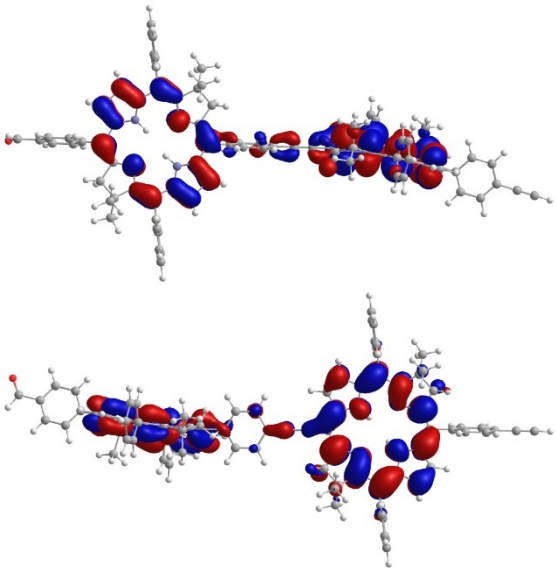
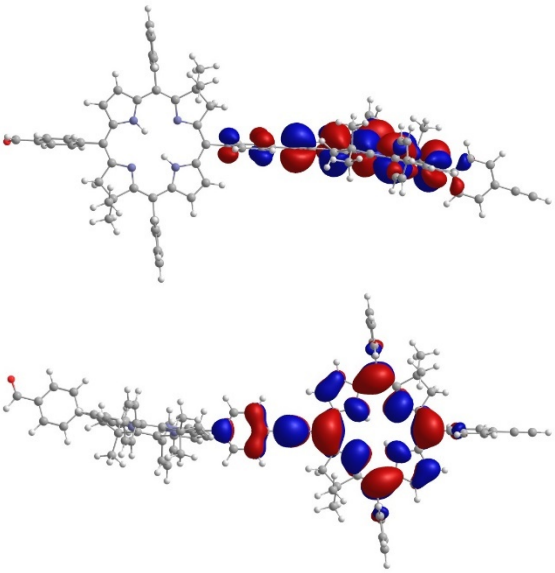
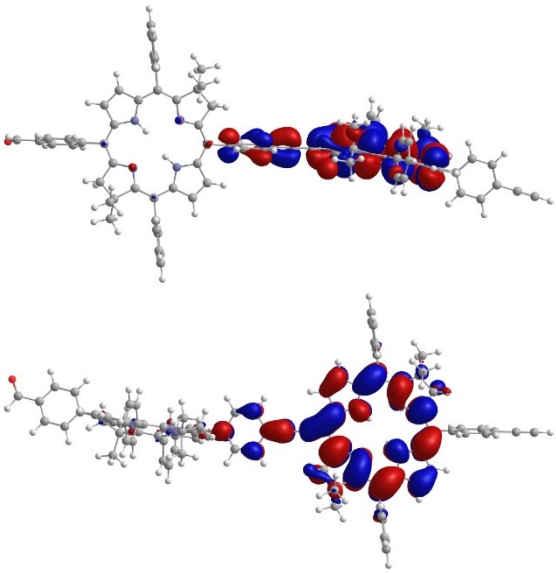
S3	0.84584		
S3	0.13381		

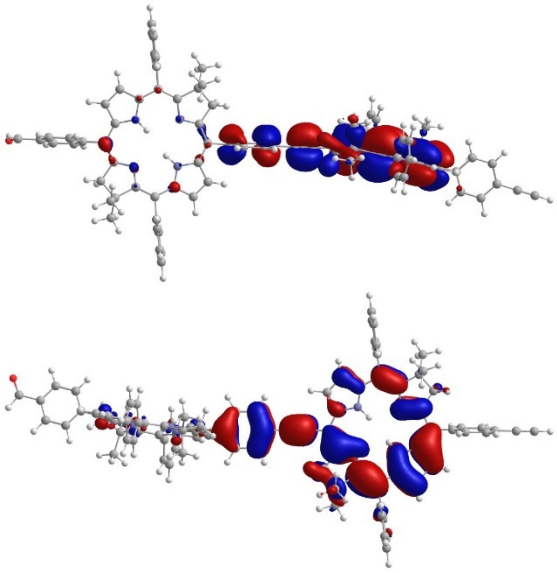
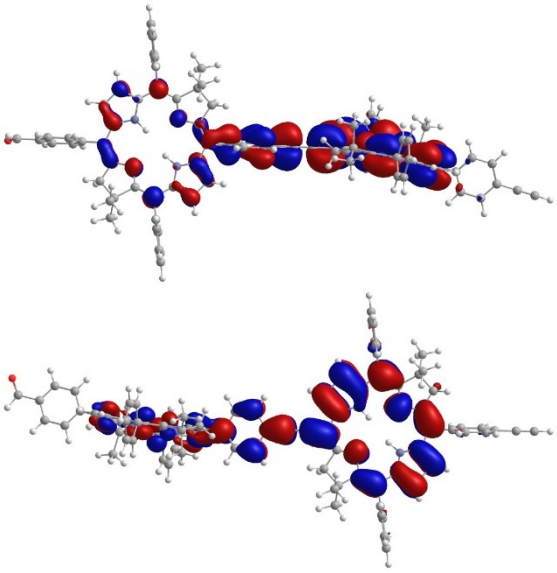
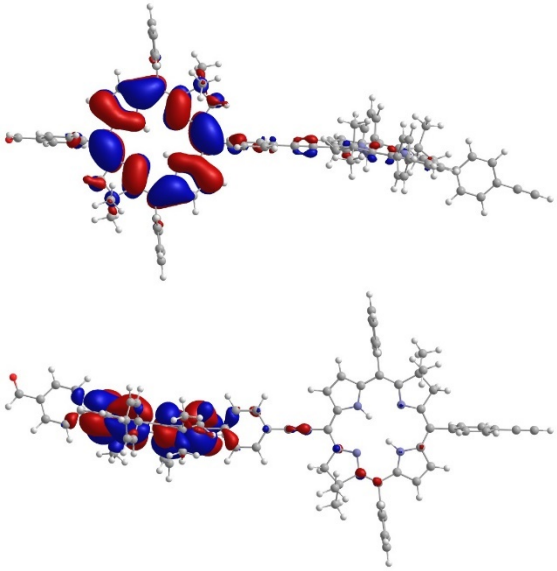
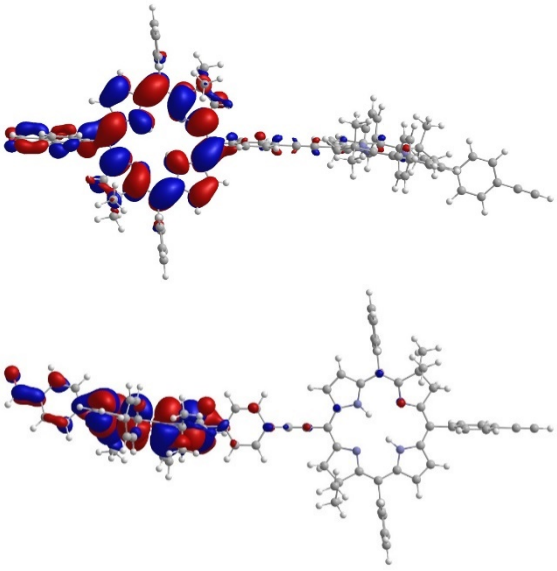
S4	0.80214		
S4	0.18425		

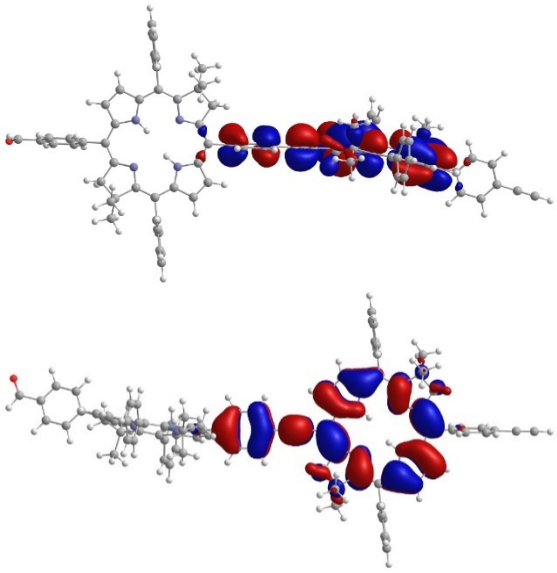
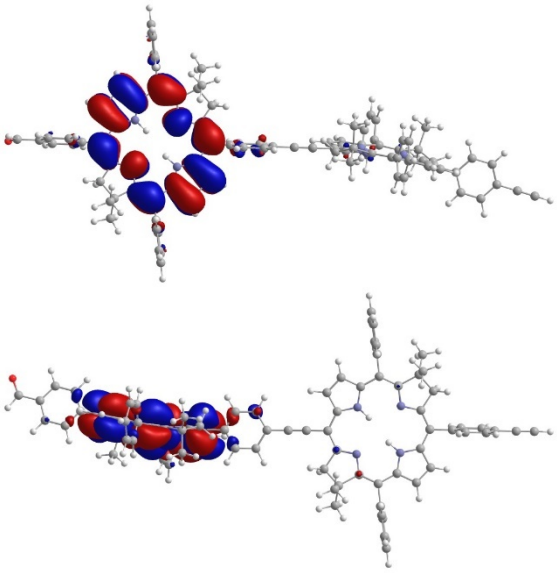
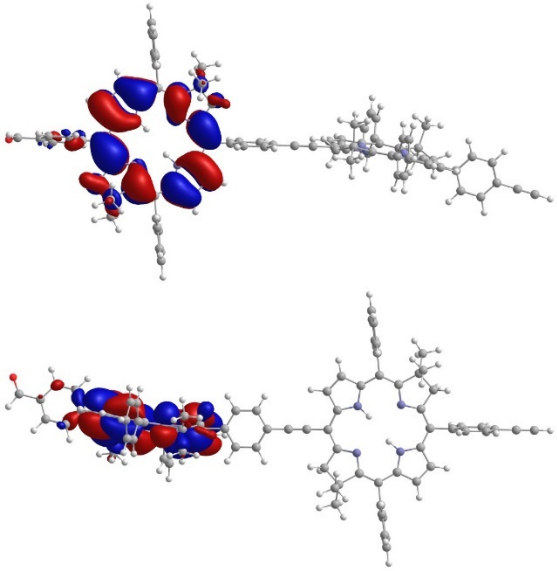
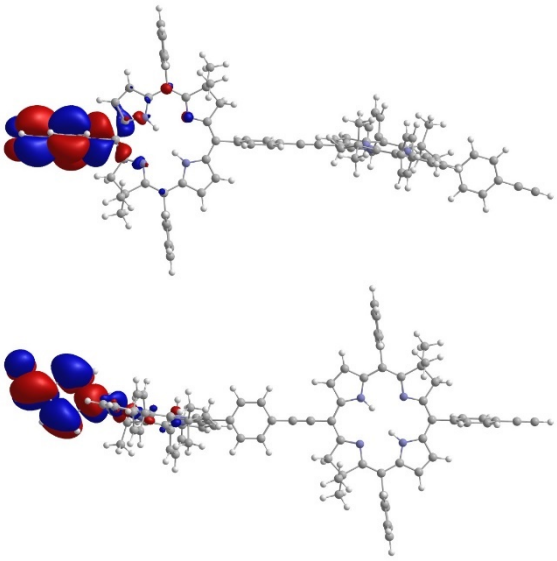
S5	0.72110		
S5	0.20611		

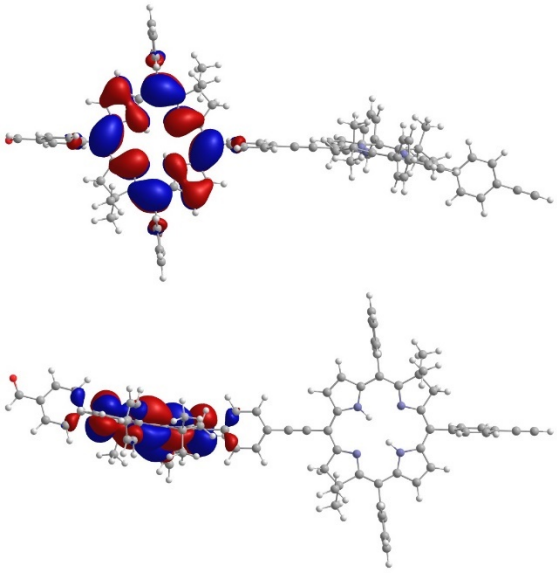
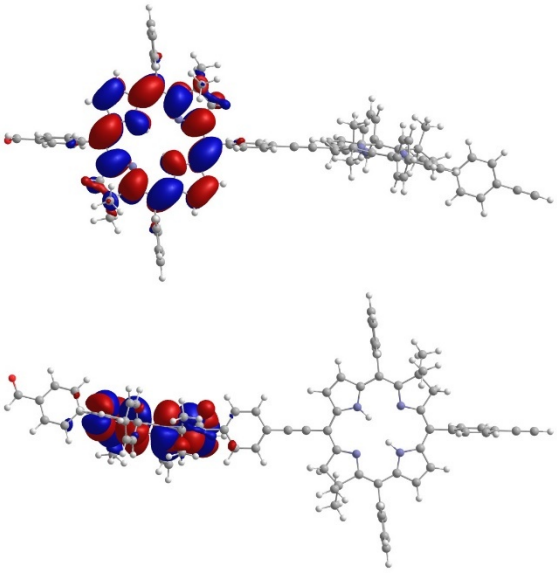
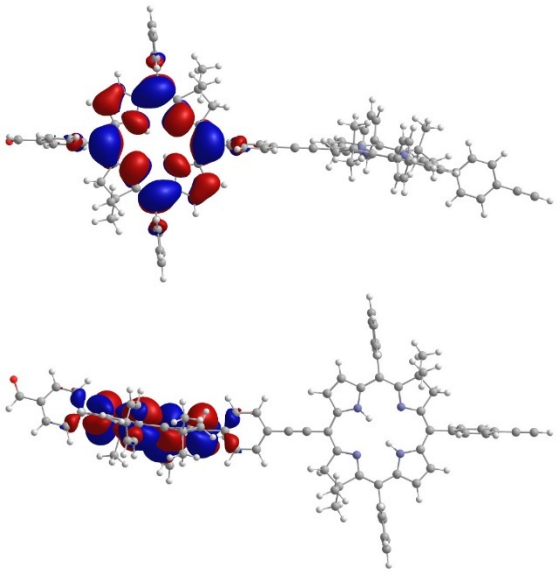
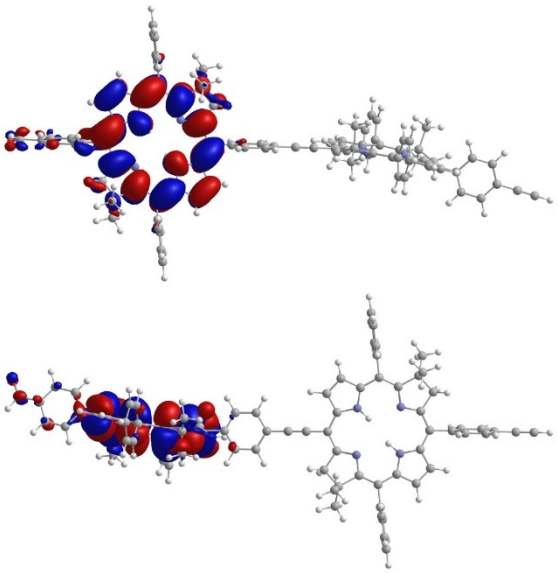
S5	0.06869		
S6	0.96710		

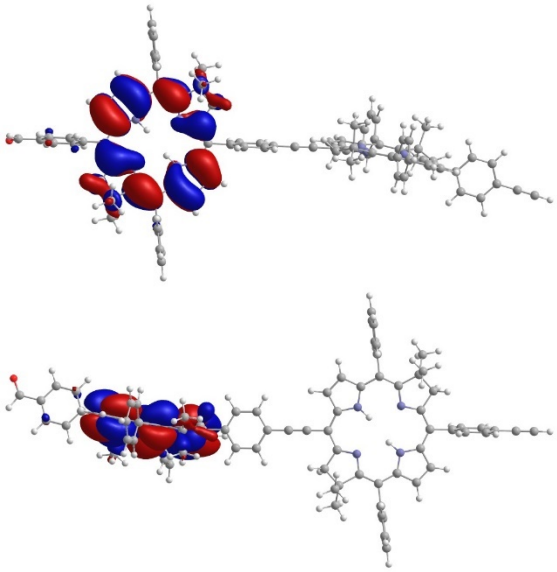
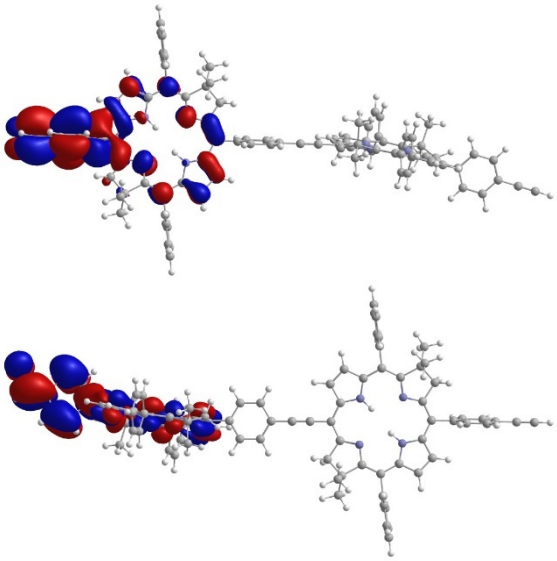
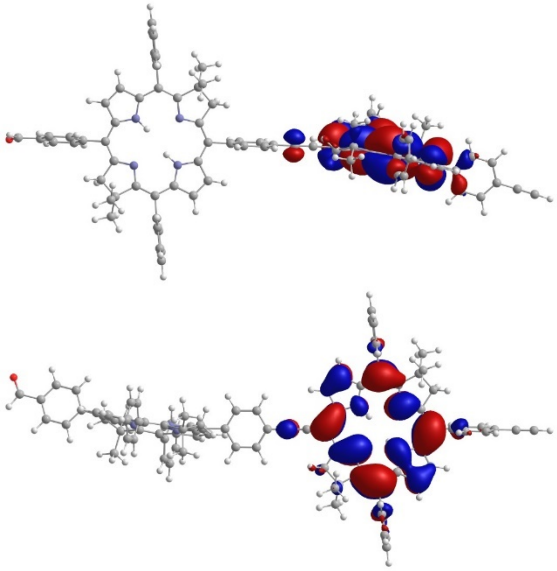
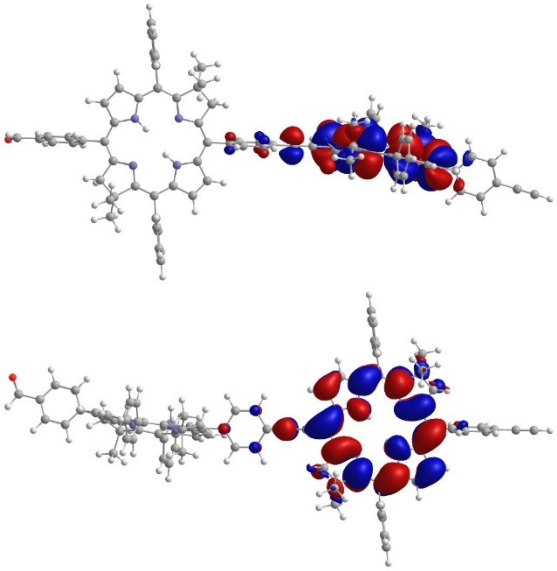
S7	0.72559		
S7	0.16261		

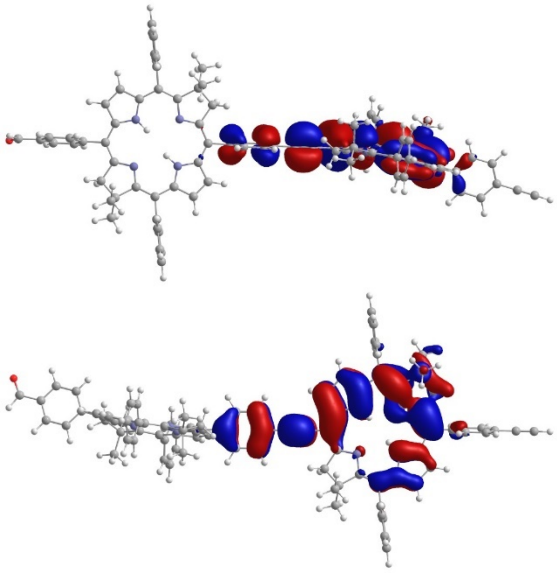
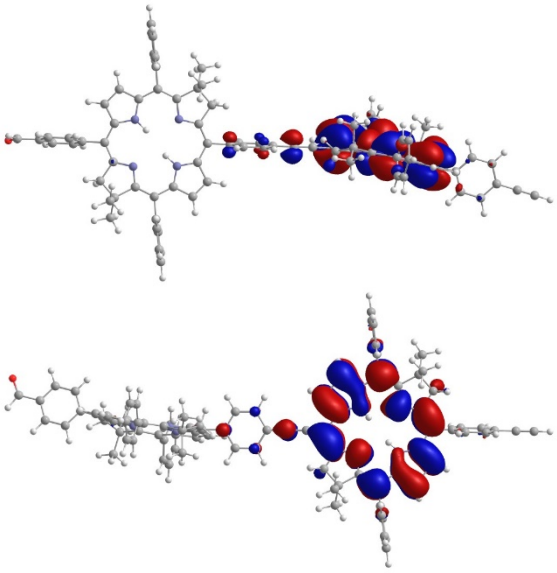
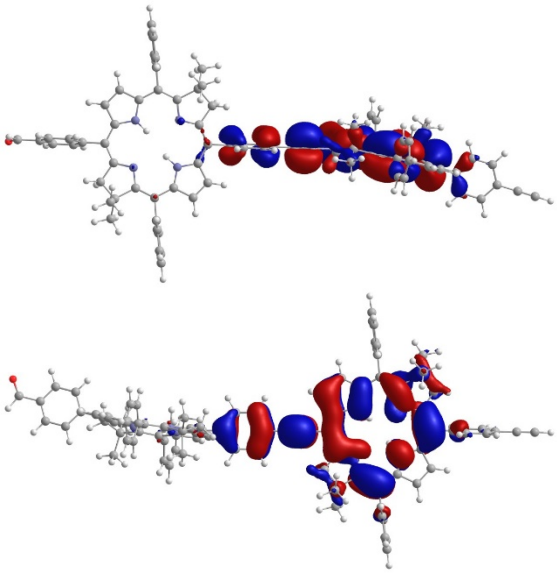
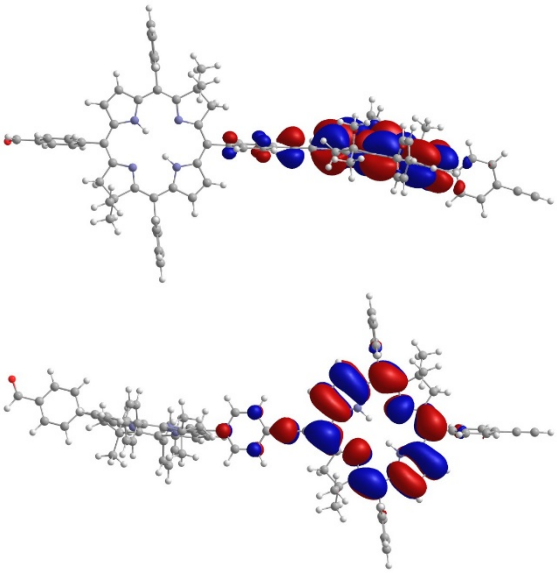
S7	0.10060		
S8	0.70480		

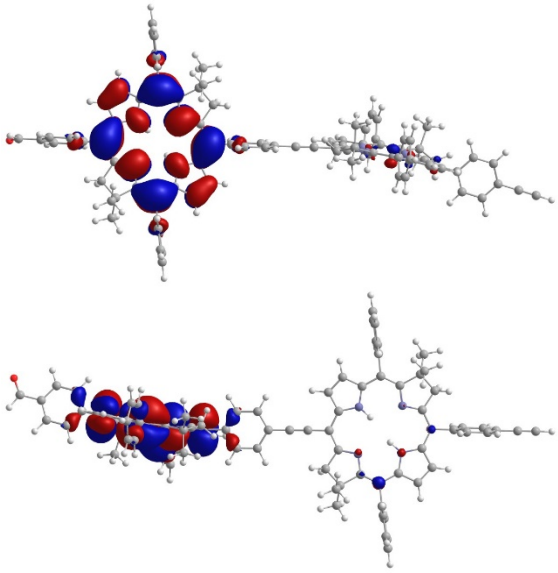
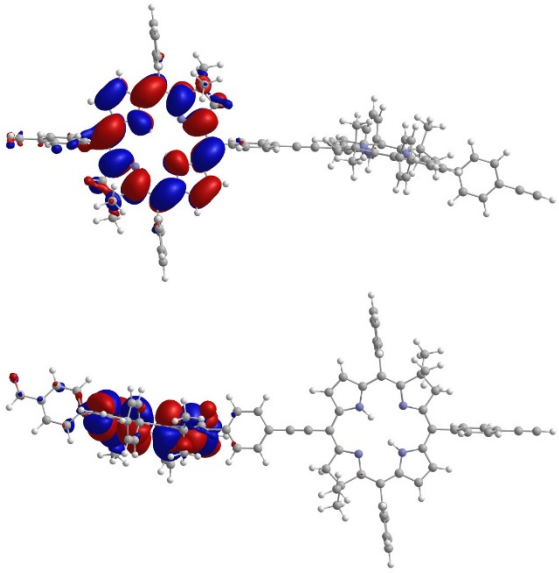
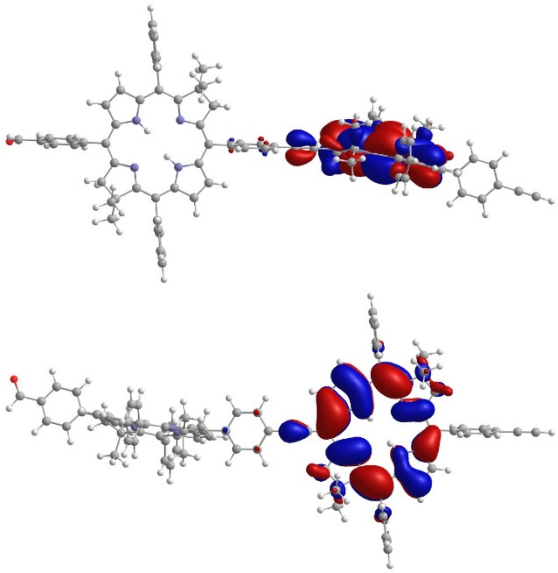
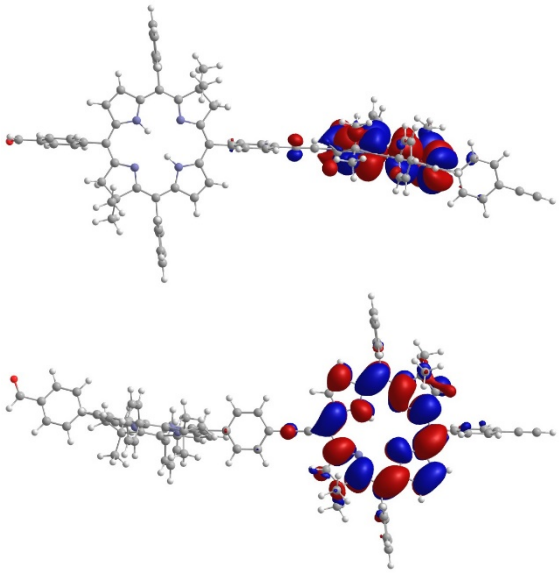
S8	0.15228		
S8	0.11212		

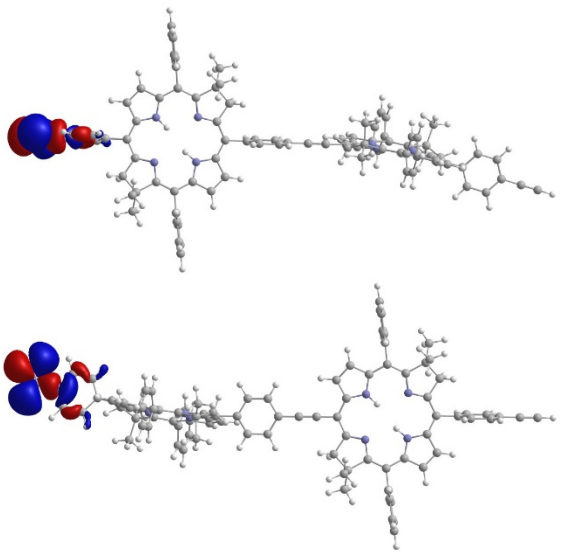
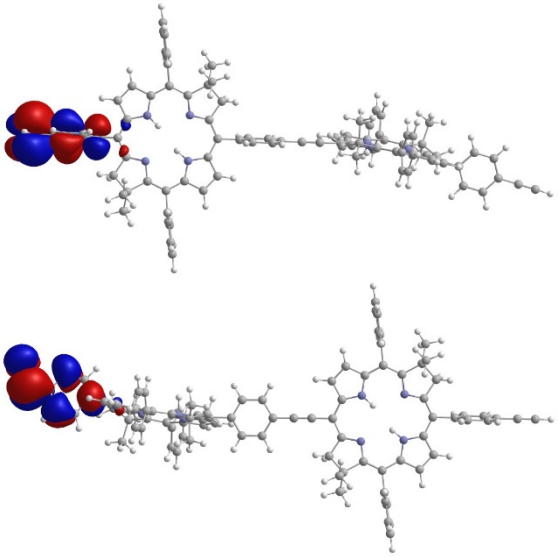
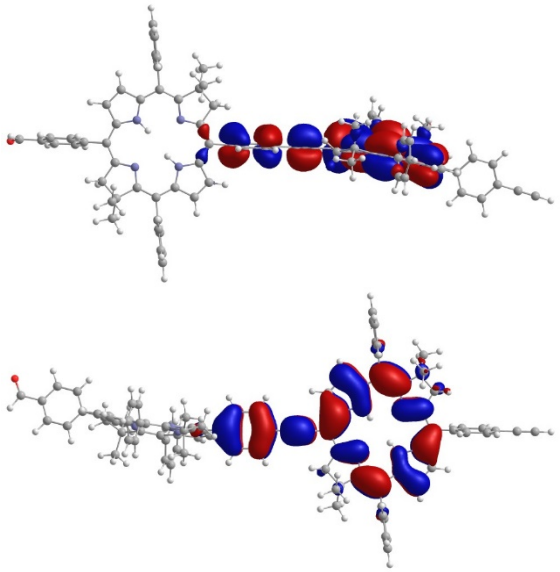
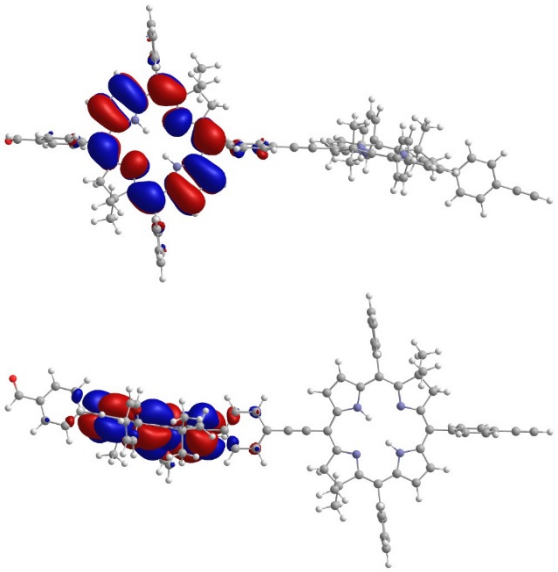
S9	0.97285		
S10	0.74743		

S10	0.20660		
S11	0.55971		

S11	0.31020		
S11	0.07689		

S11	0.05537		
S12	0.76385		

S12	0.10573		
S12	0.09545		

S13	0.99724		
S14	0.99344		

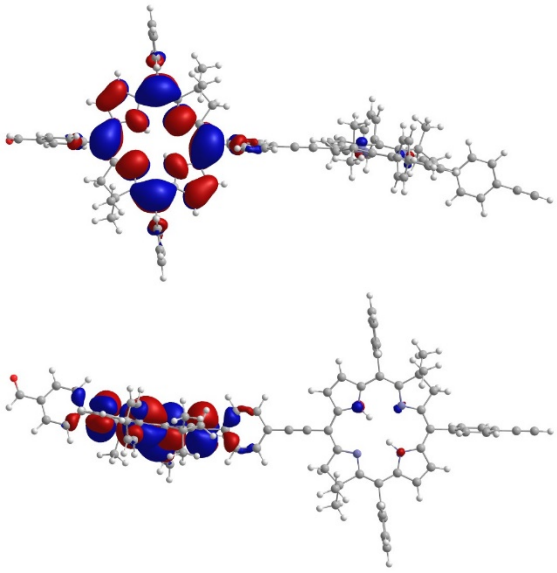
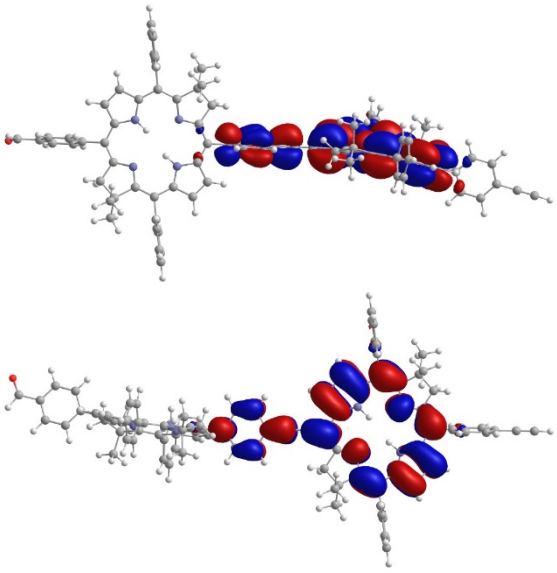
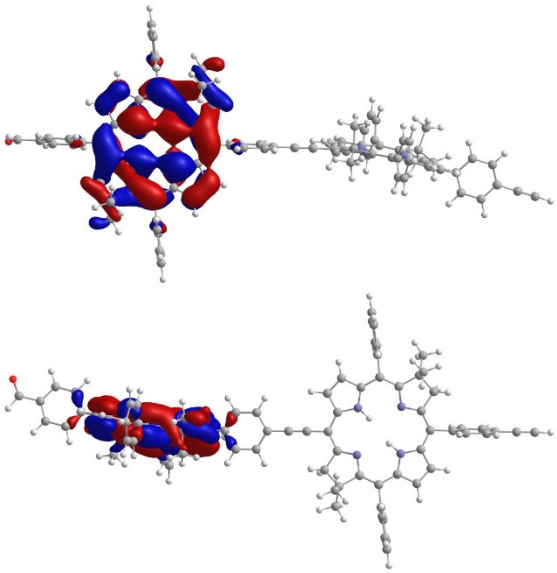
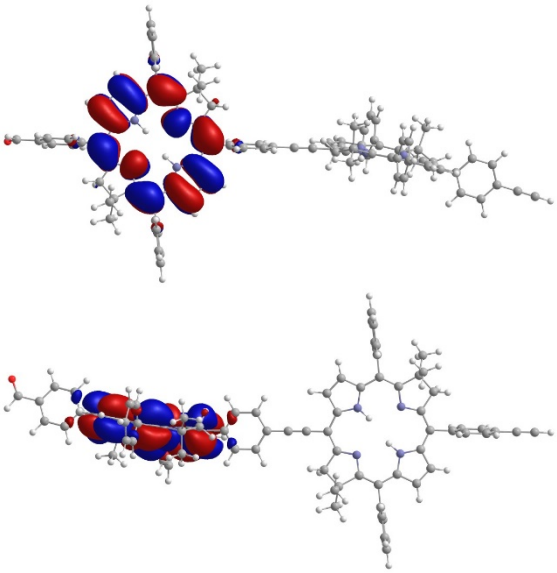
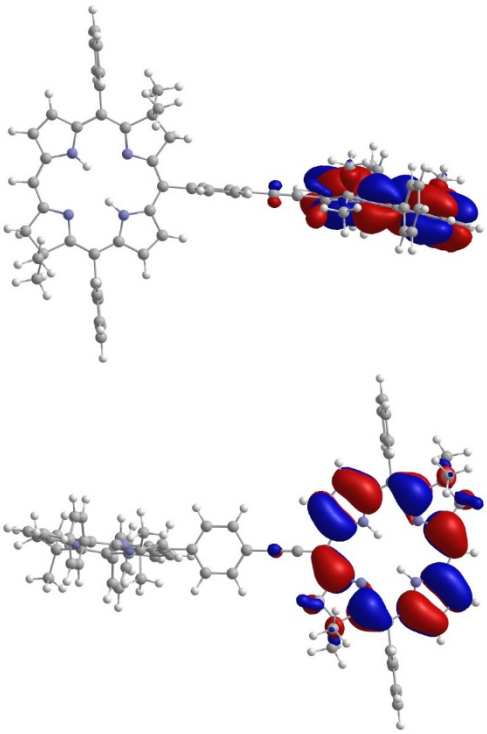
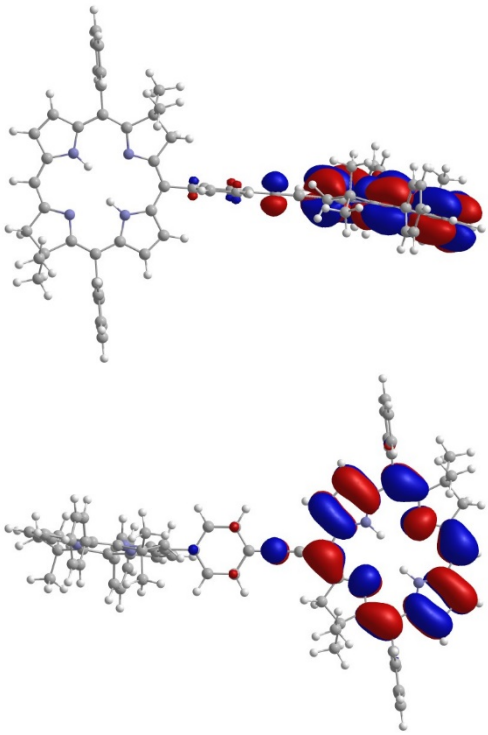
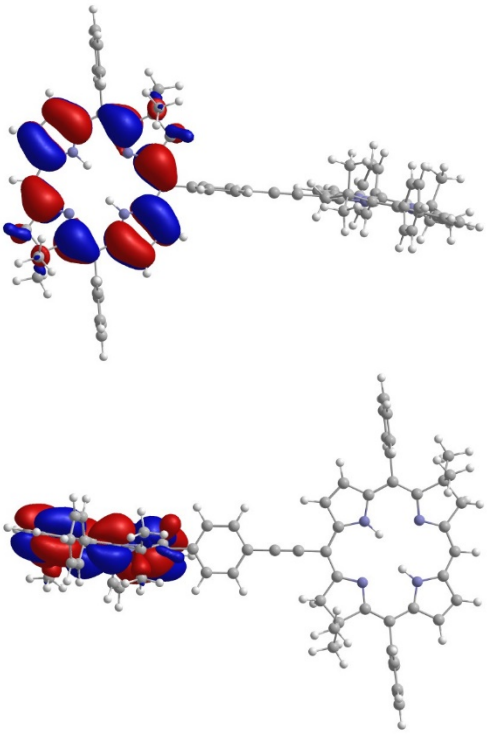
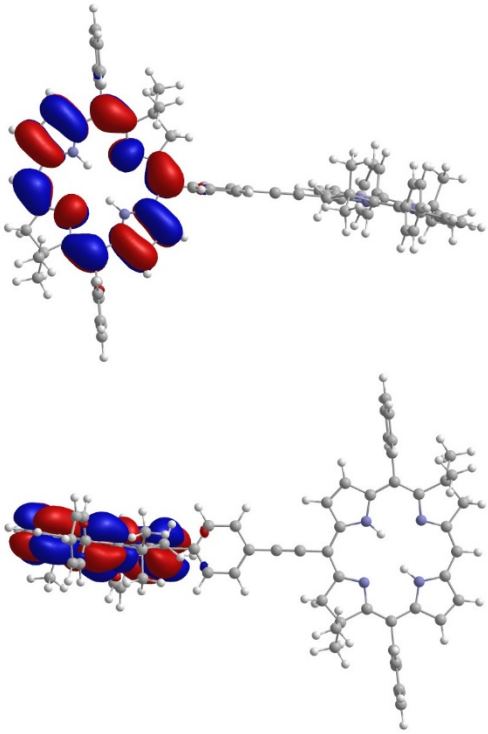
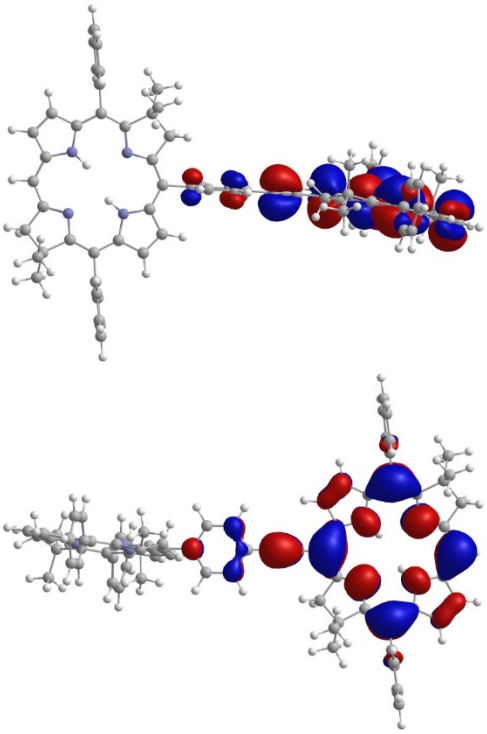
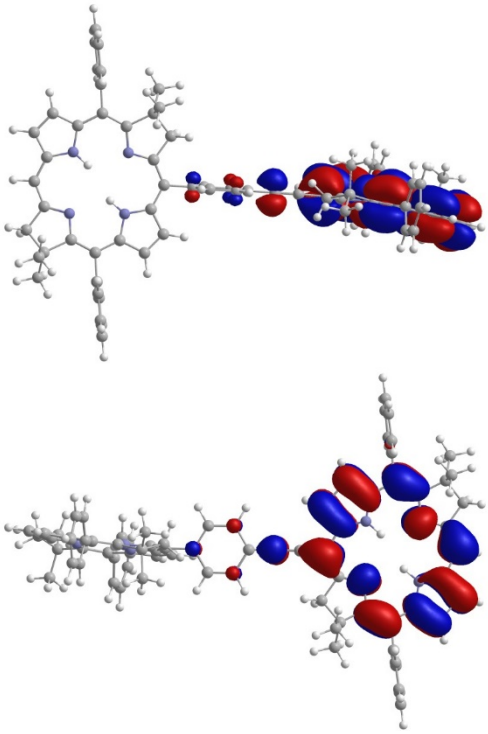
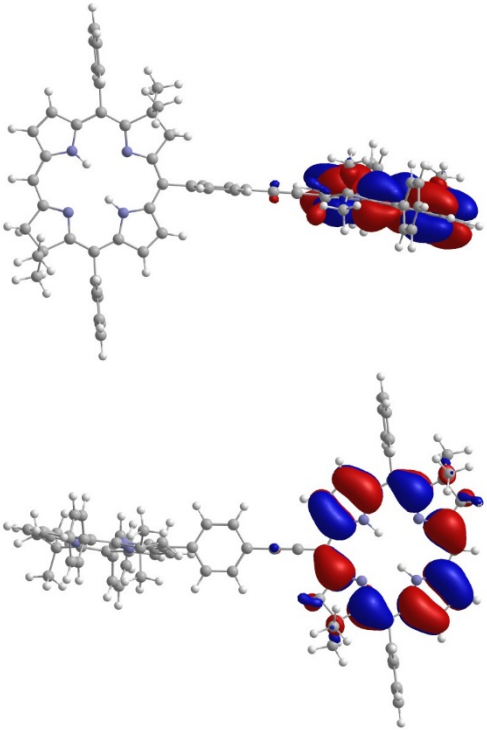
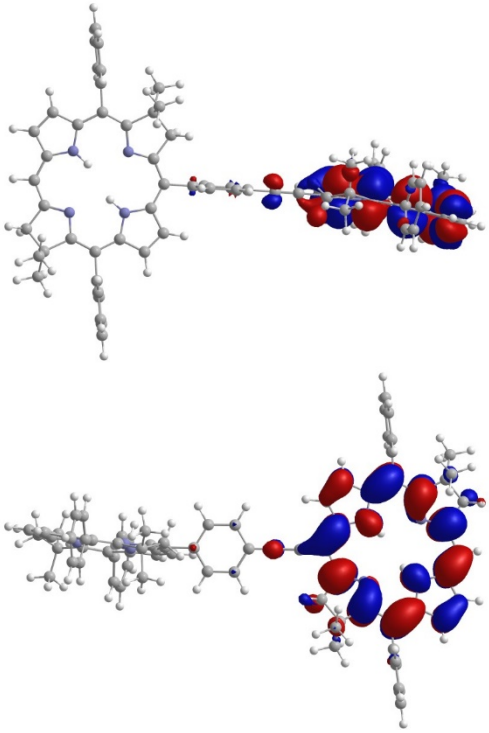
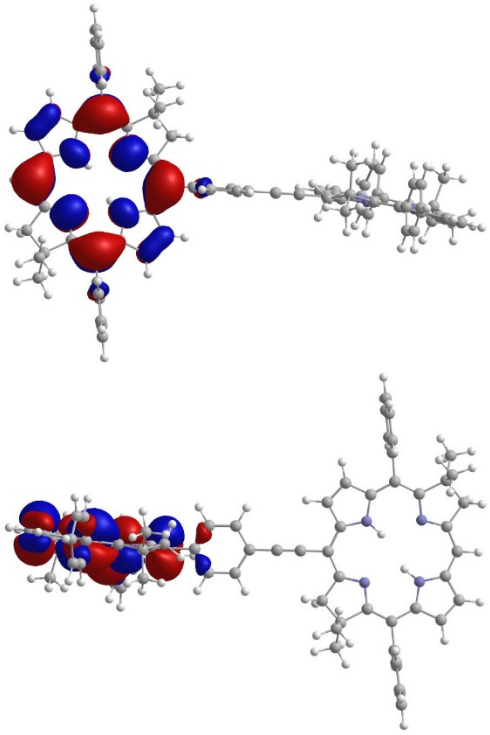
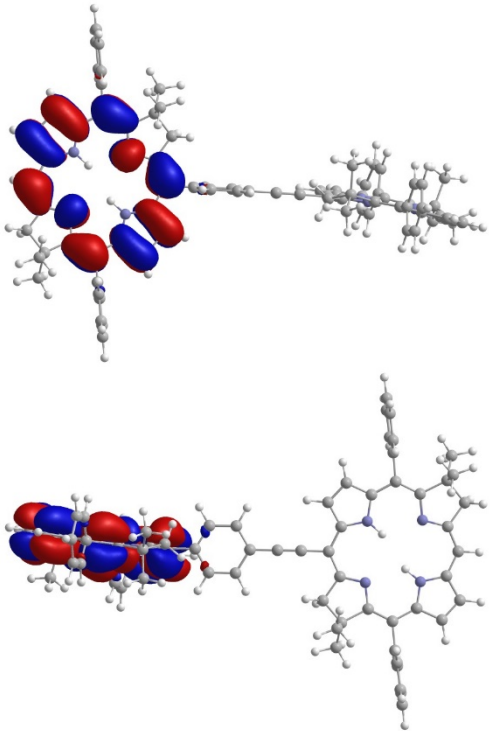
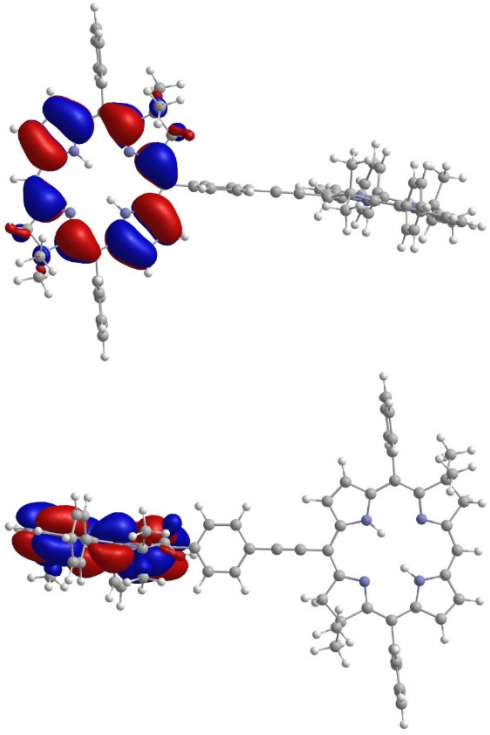
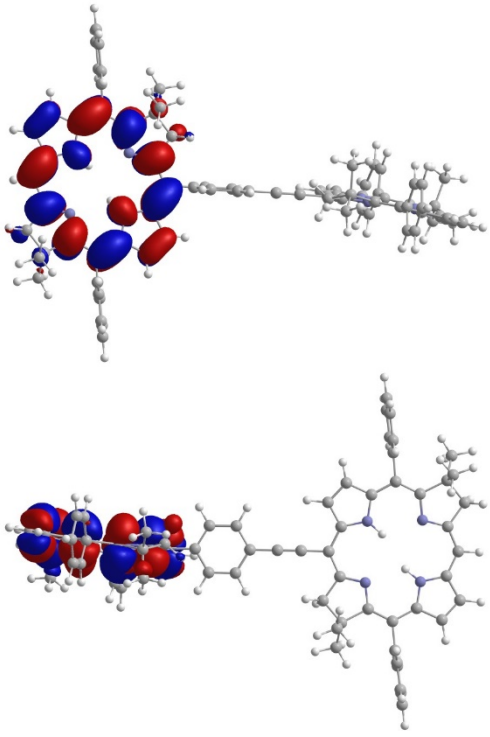
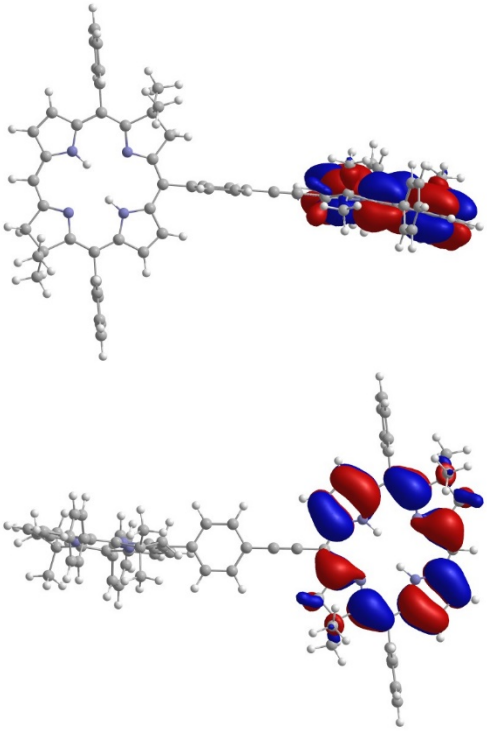
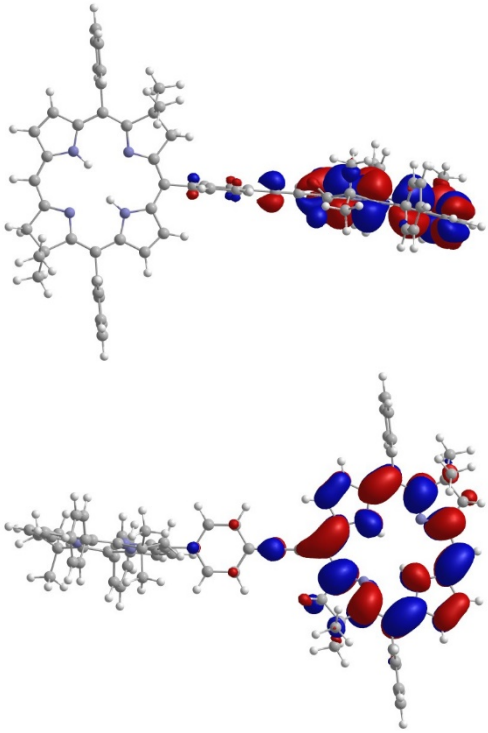
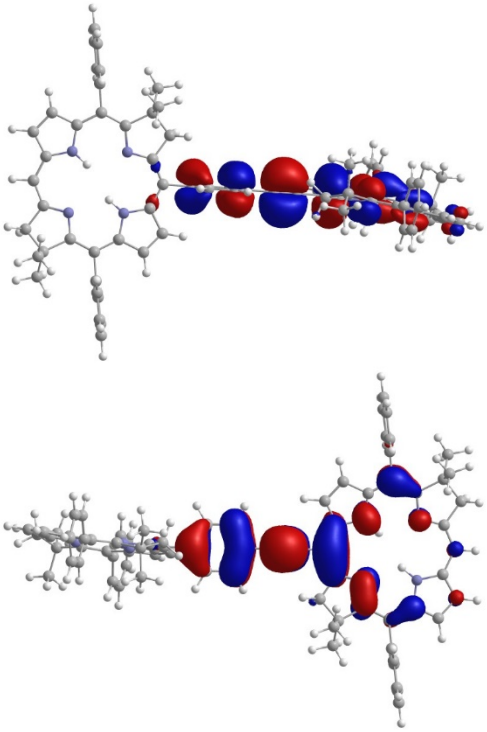
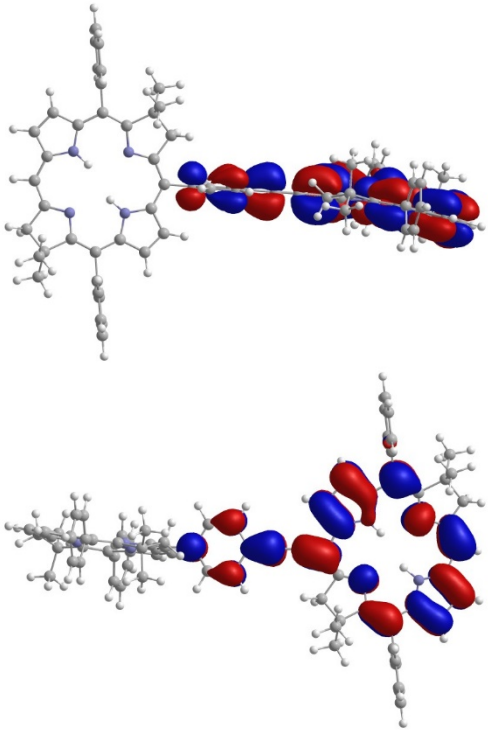
S15	0.98853		
S16	0.95200		

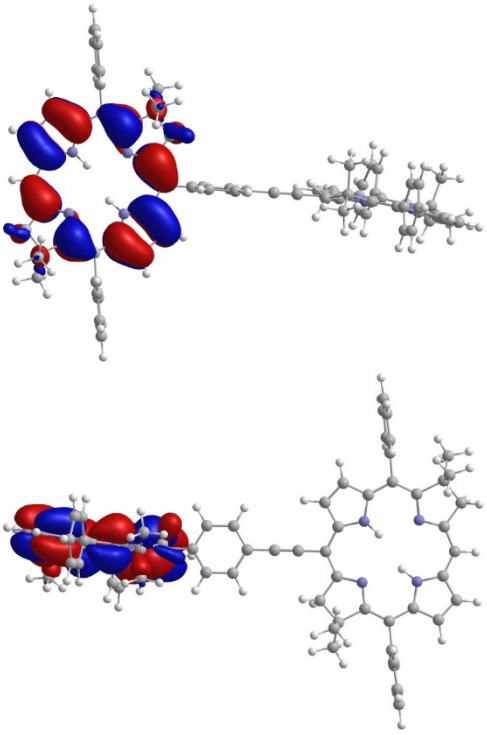
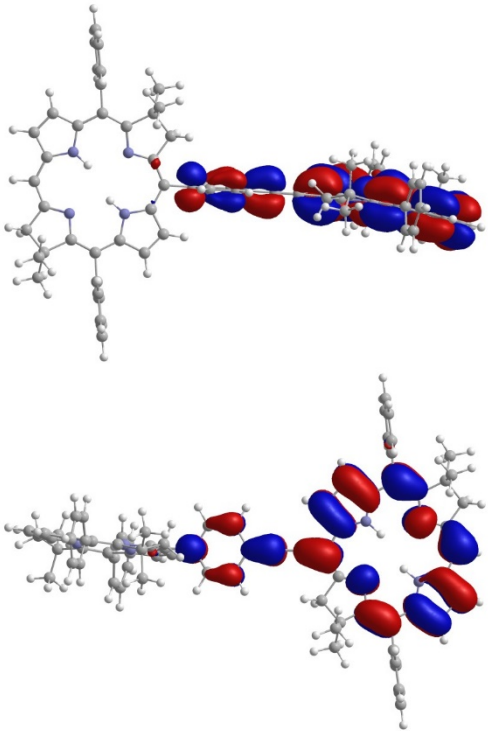
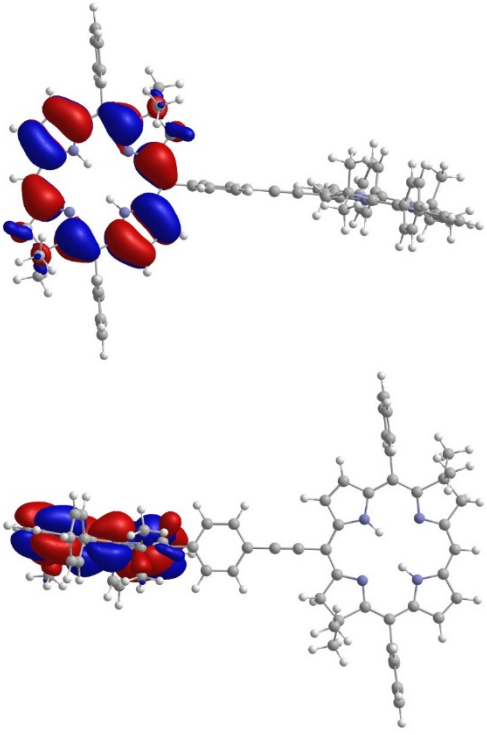
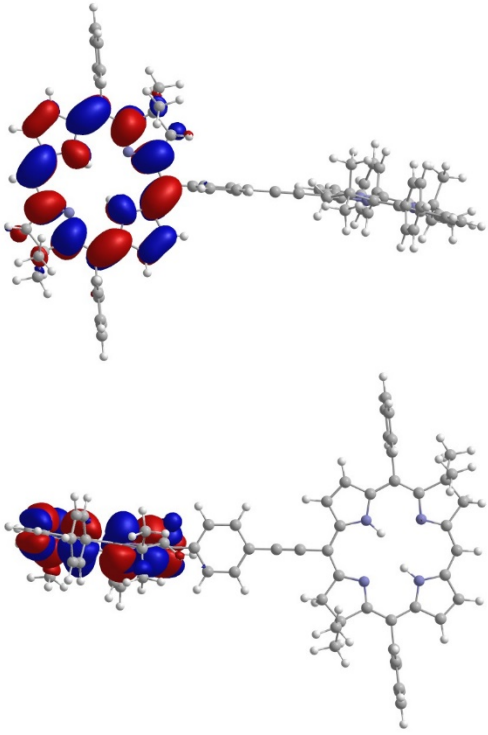
Table S25. NTOs for **Dyad-5**.

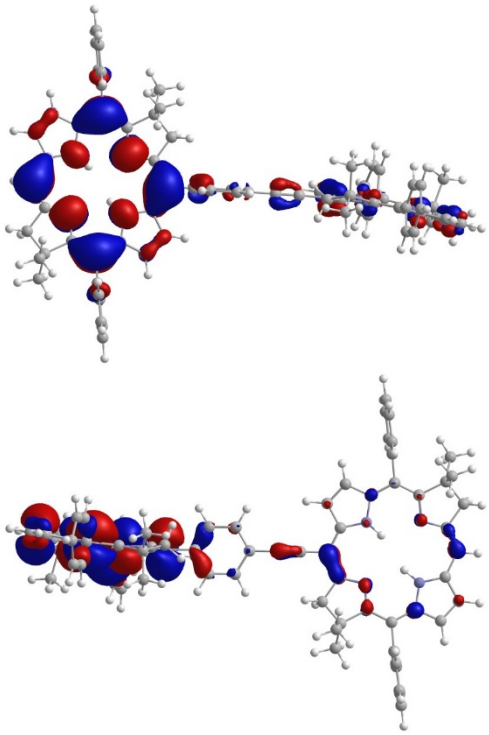
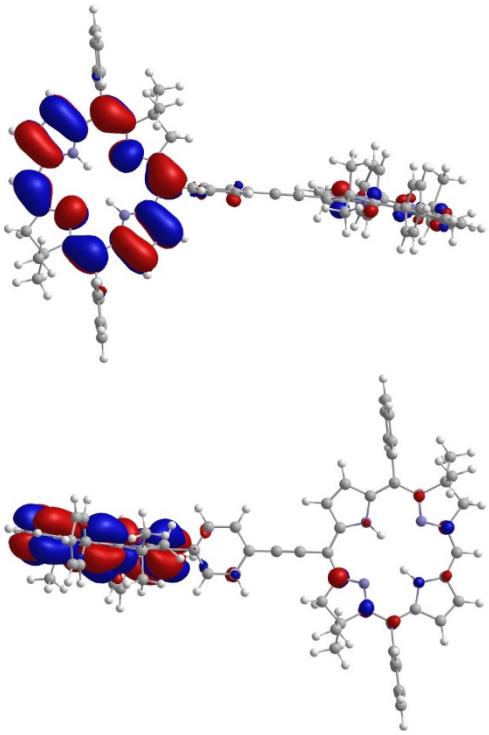
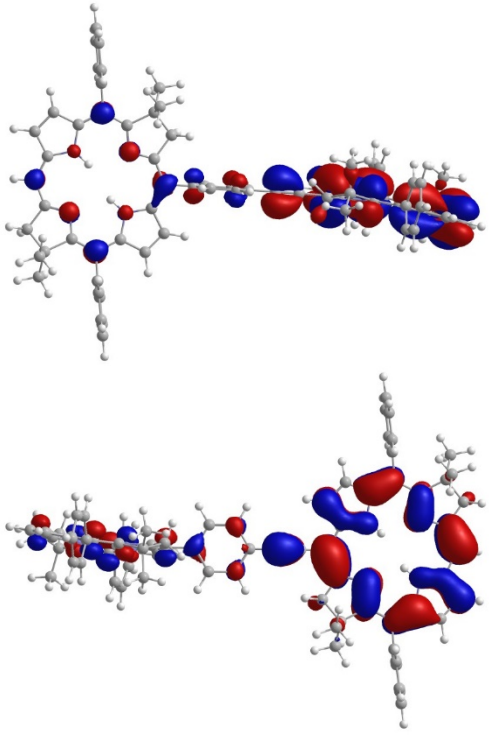
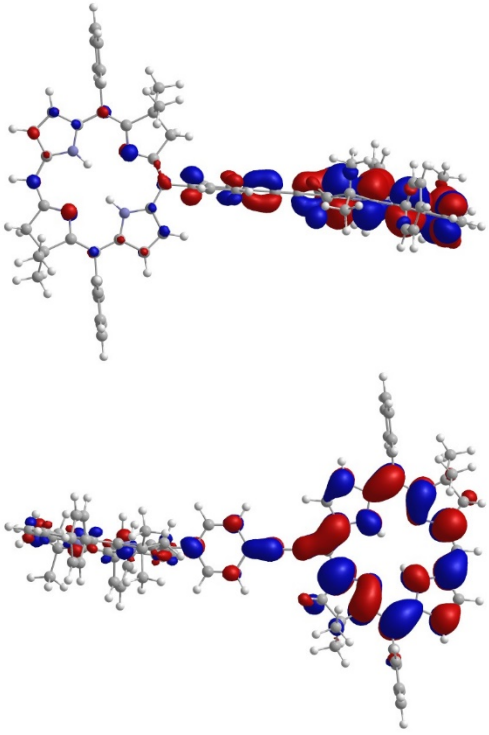
S#	Eigenvalue	From	To
S1	0.89569		
S2	0.88748		

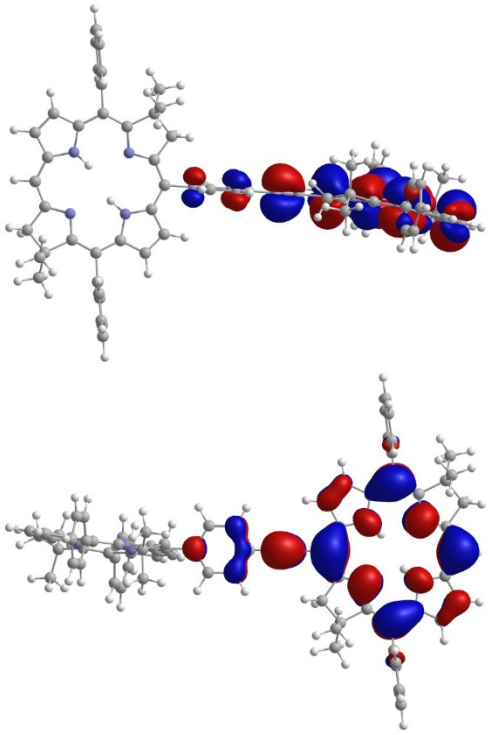
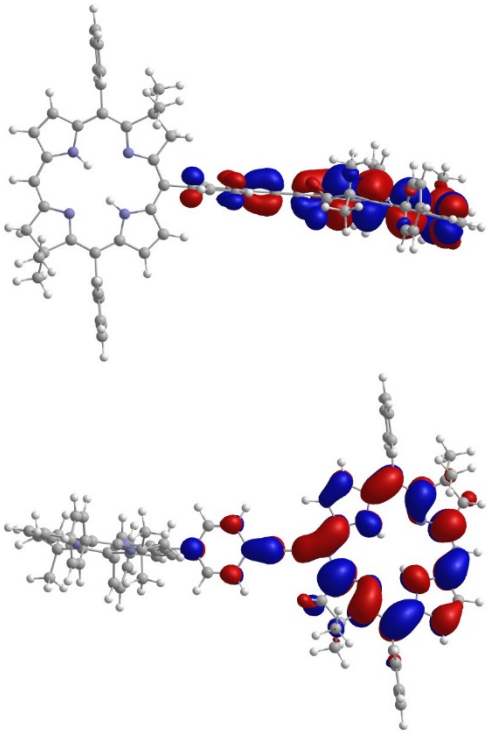
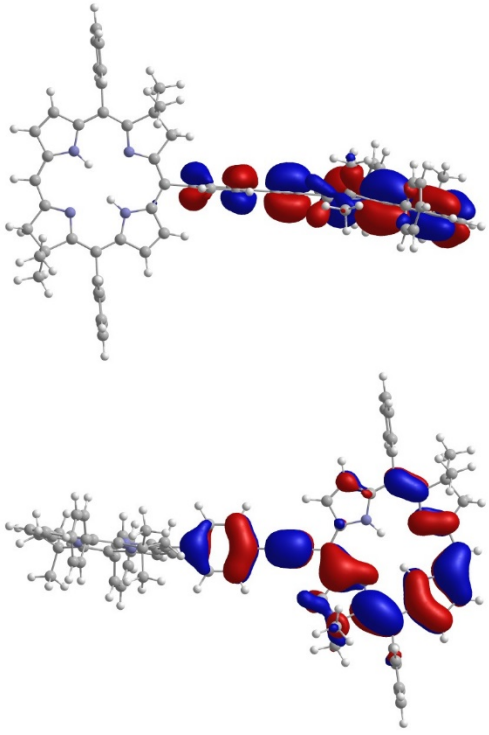
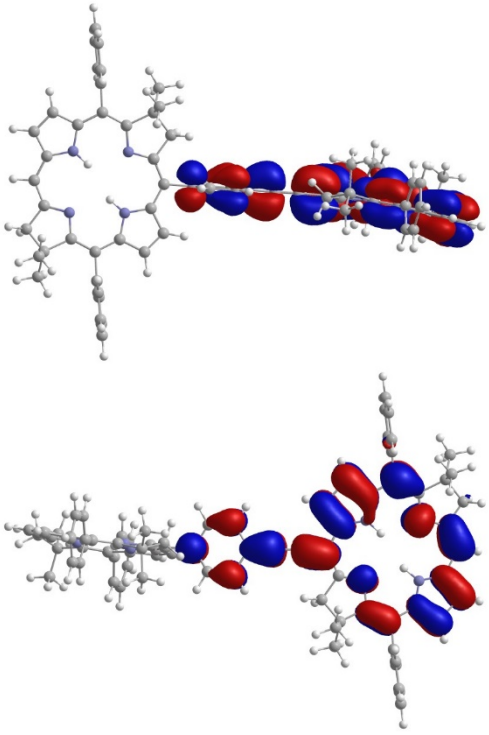
S3	0.83825		
S3	0.14539		

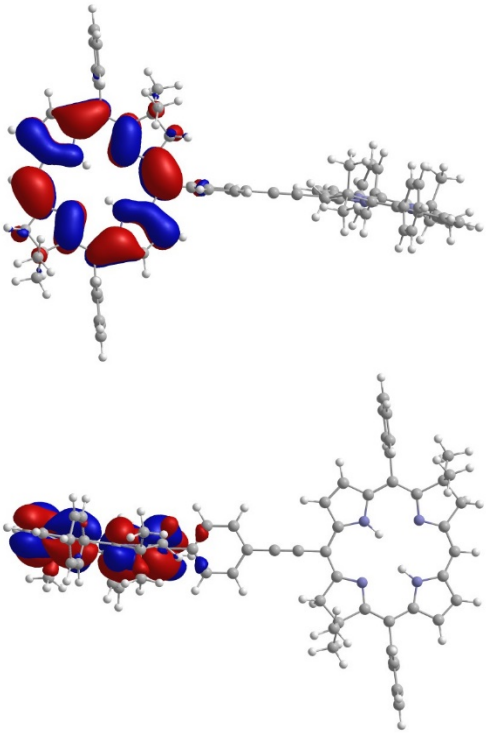
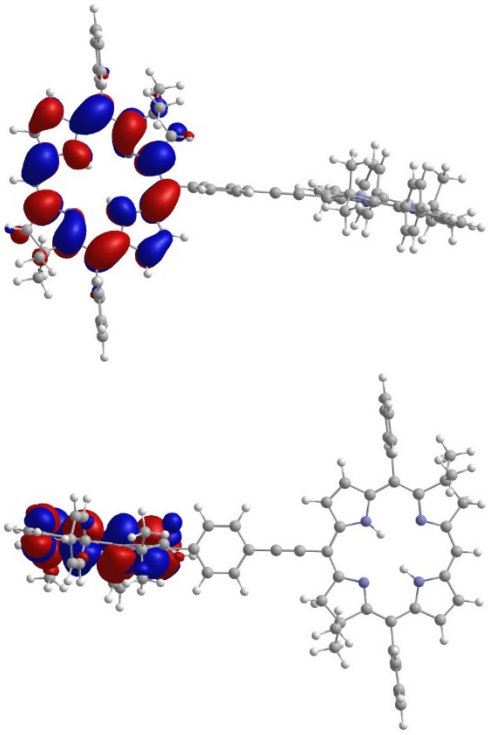
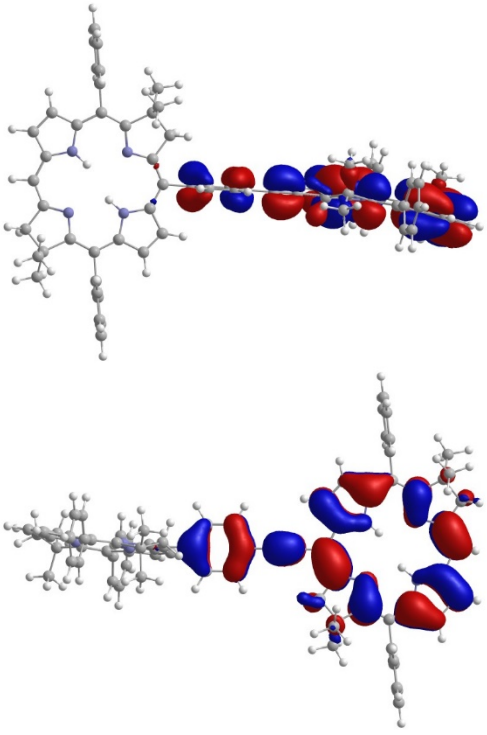
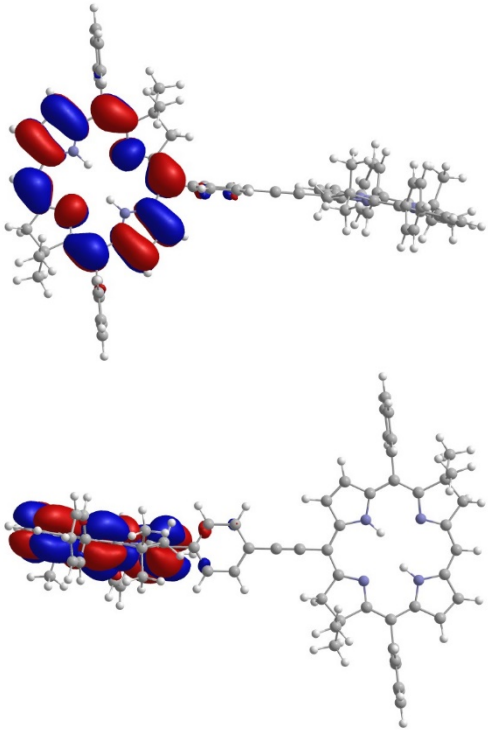
S4	0.79130		
S4	0.19880		

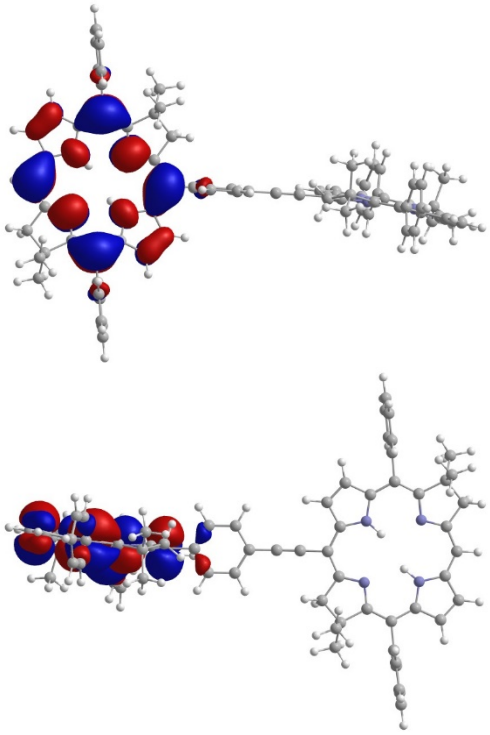
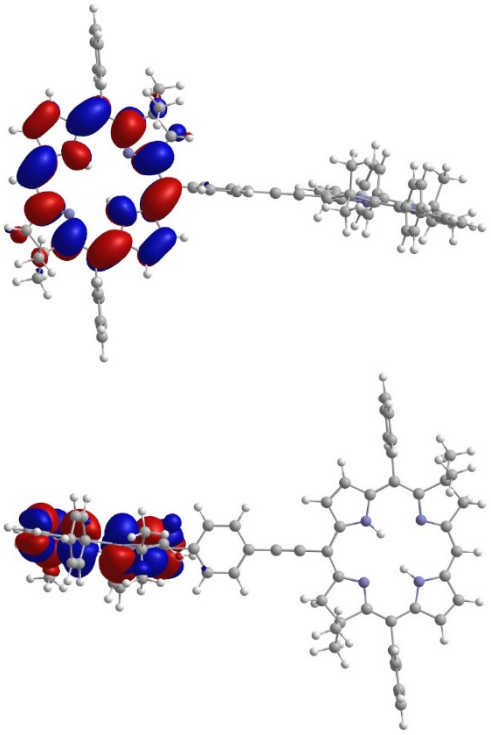
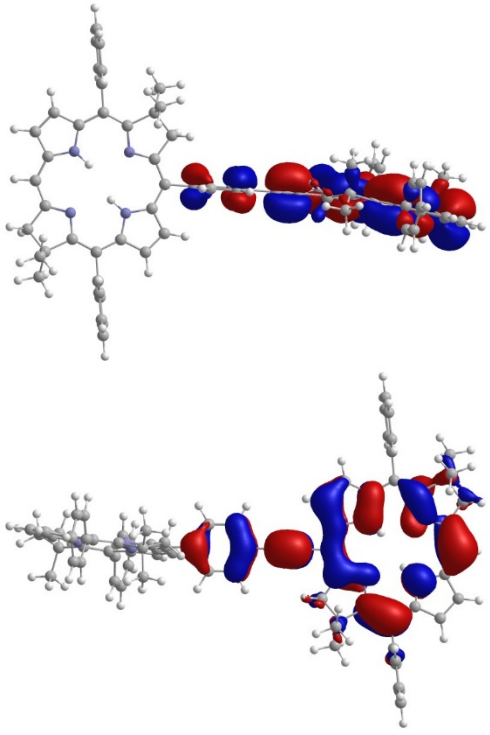
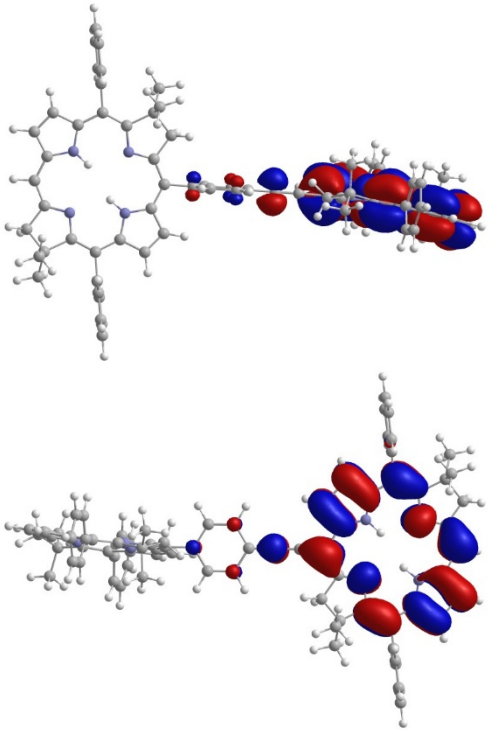
S5	0.72845		
S5	0.22109		

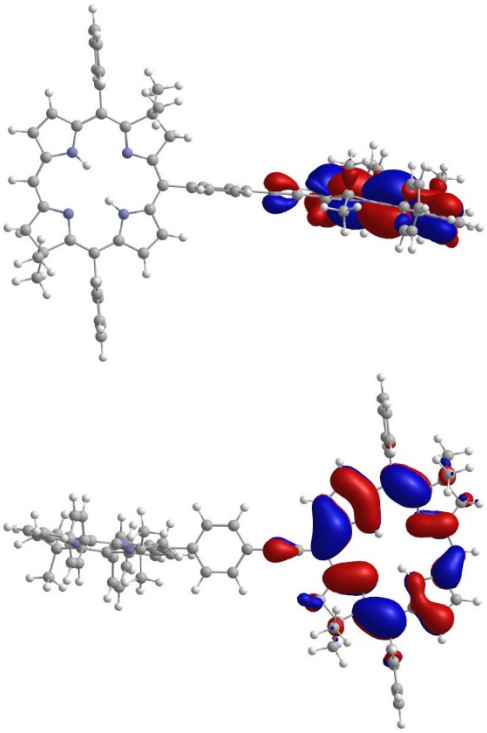
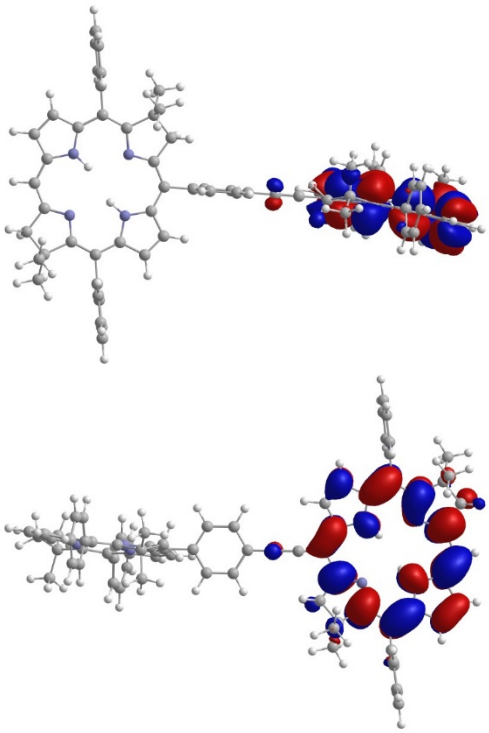
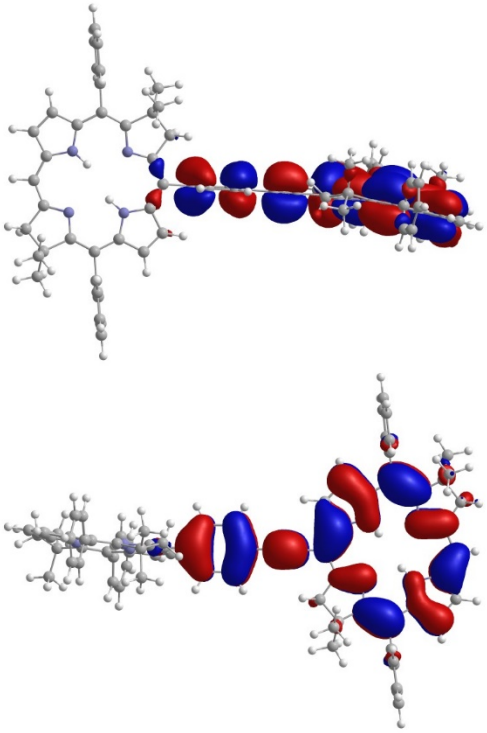
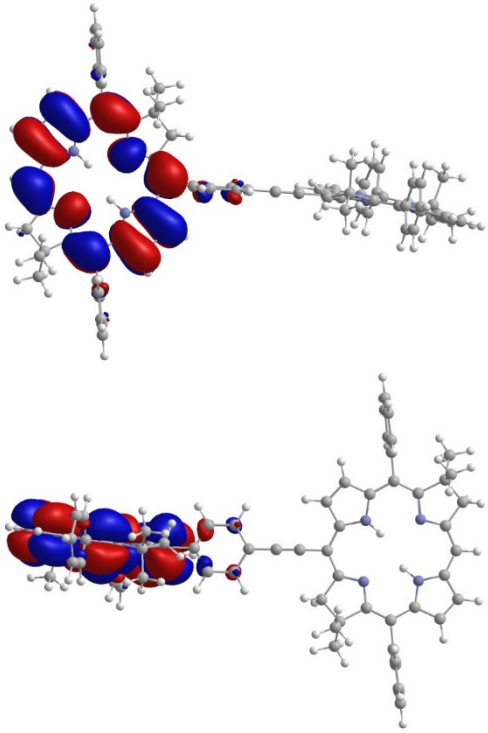
S6	0.99466		
S7	0.69407		

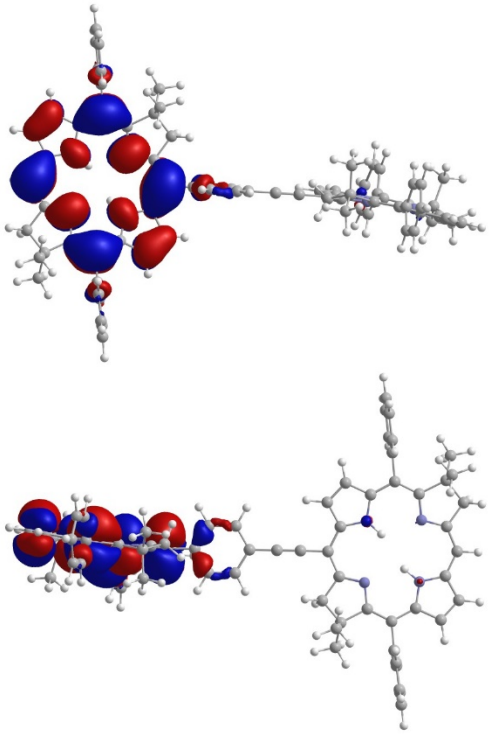
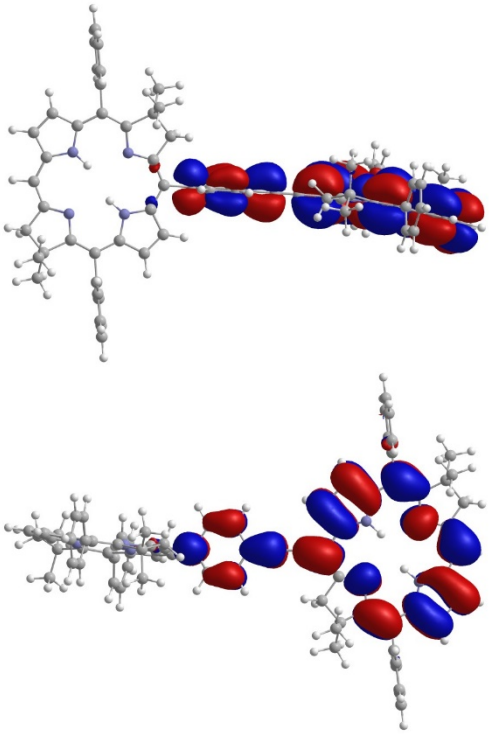
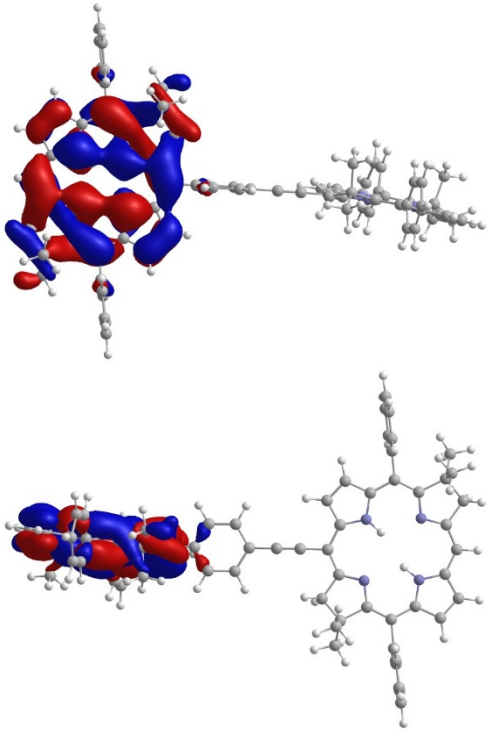
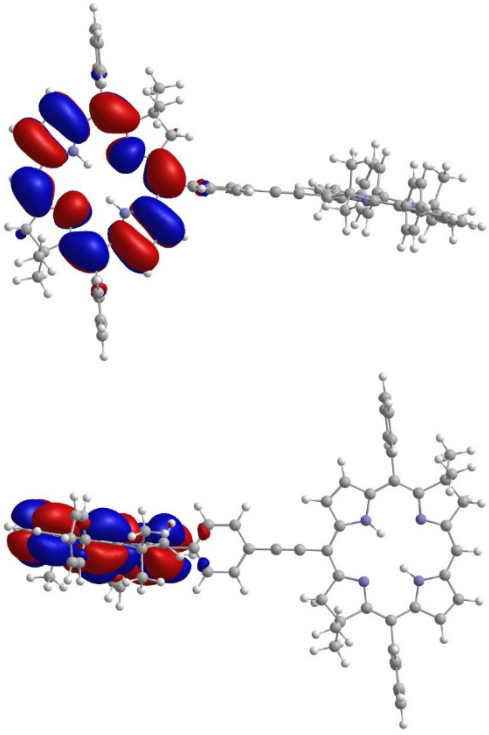
S7	0.18155		
S7	0.11436		

S8	0.71686		
S8	0.14776		

S8	0.11083		
S9	0.99528		

S10	0.78451		
S11	0.78854		

S11	0.11334		
S12	0.99545		

S13	0.98609		
S14	0.95336		

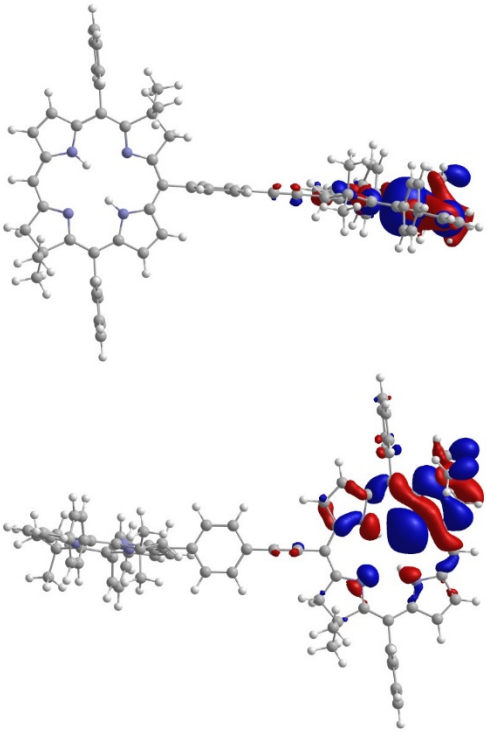
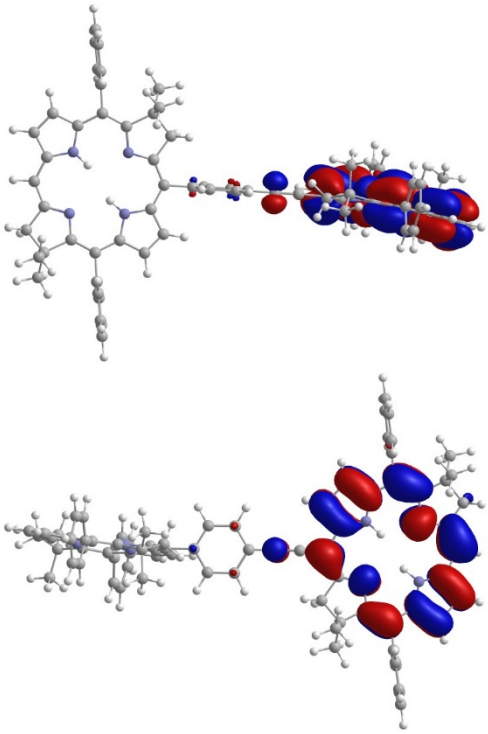
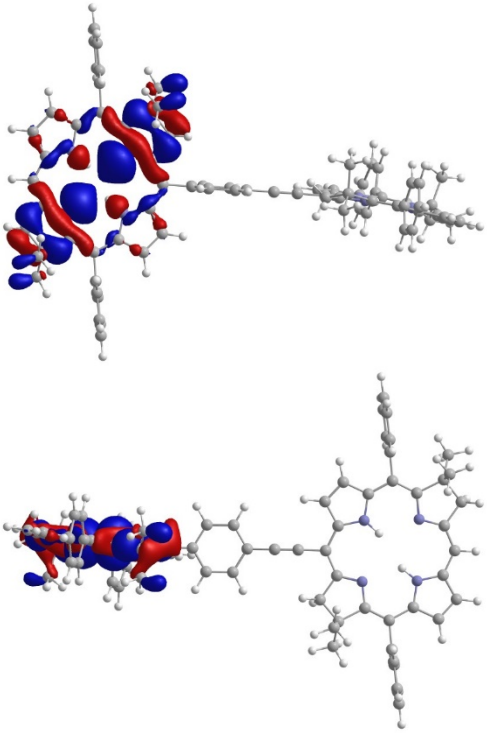
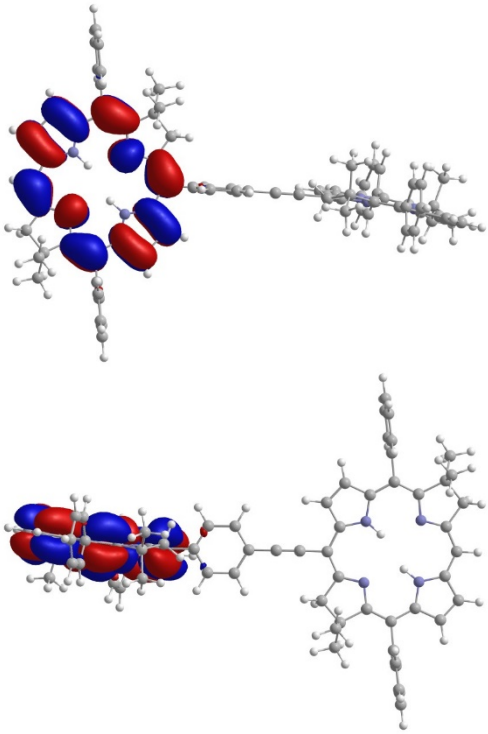
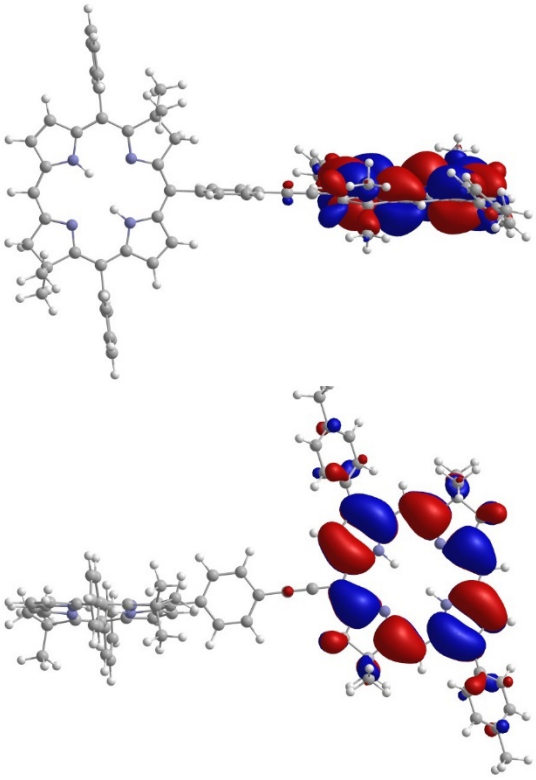
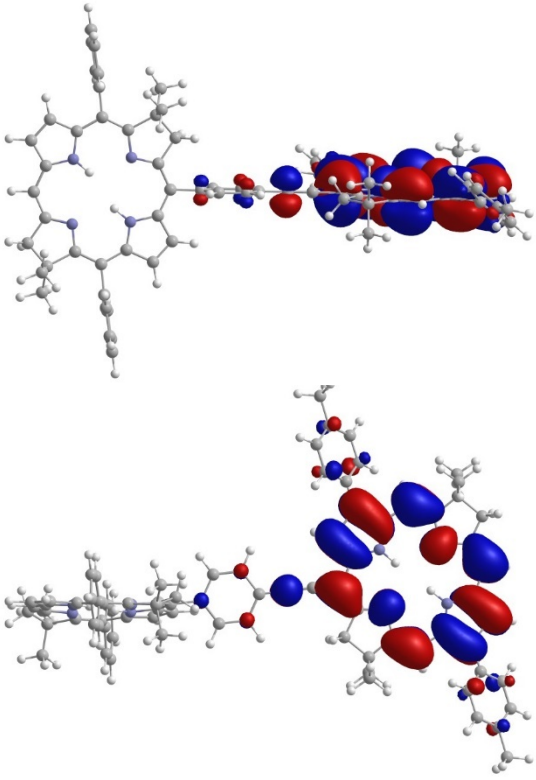
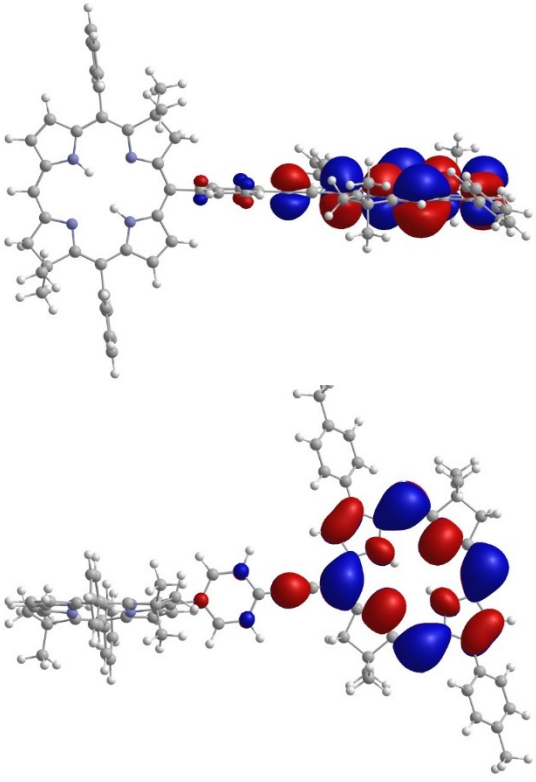
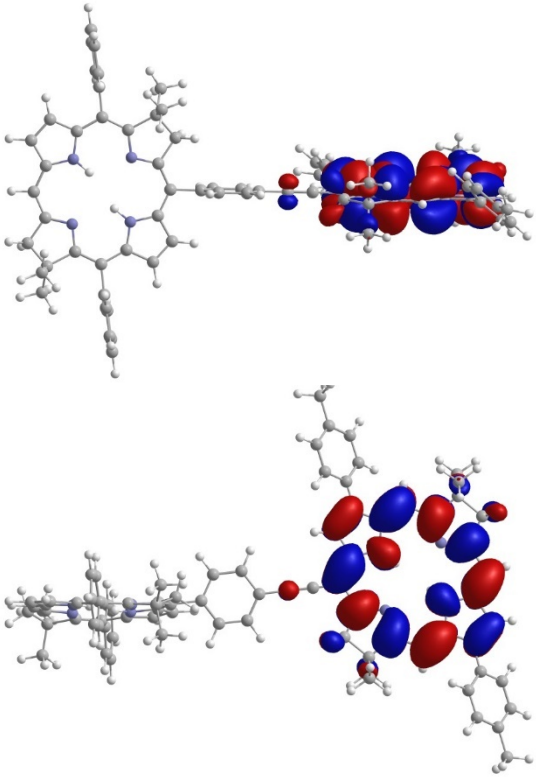
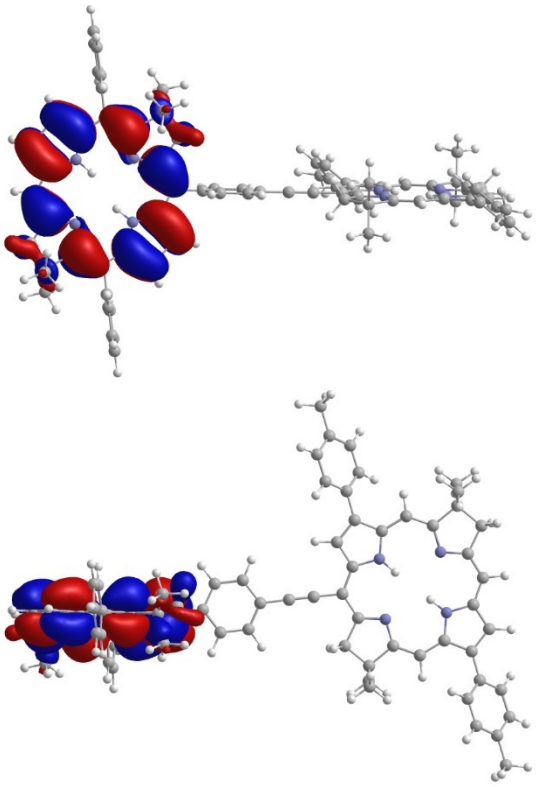
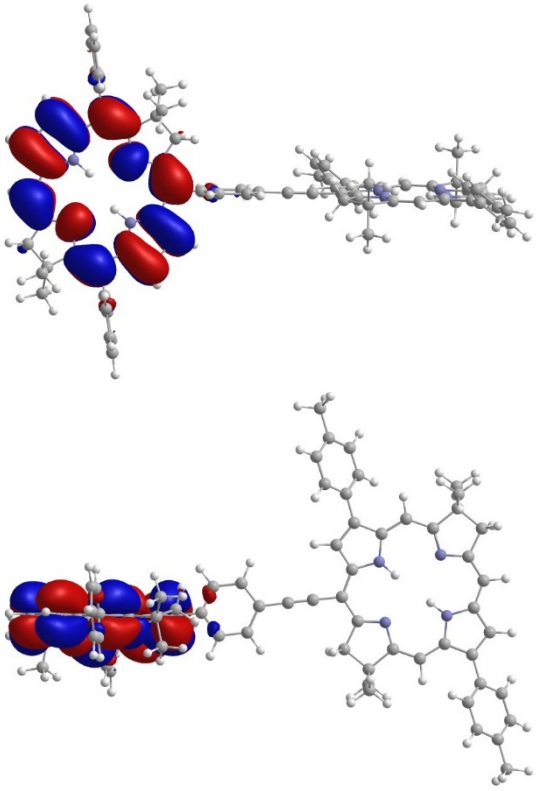
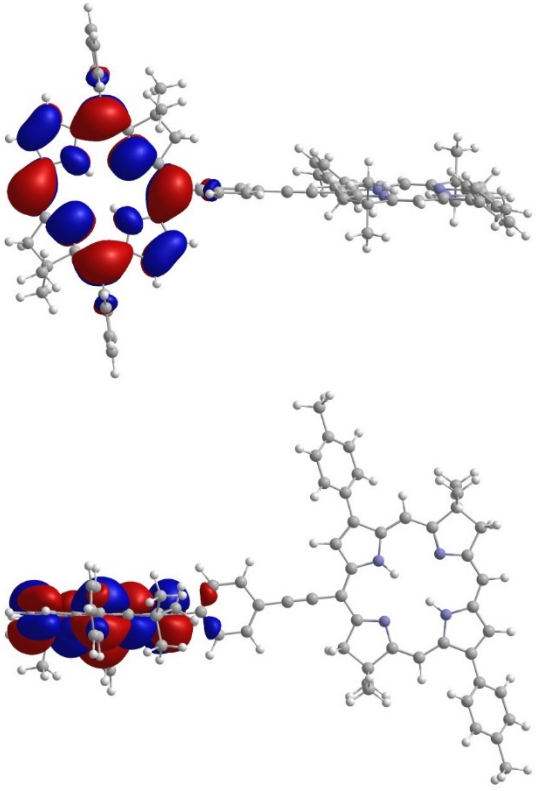
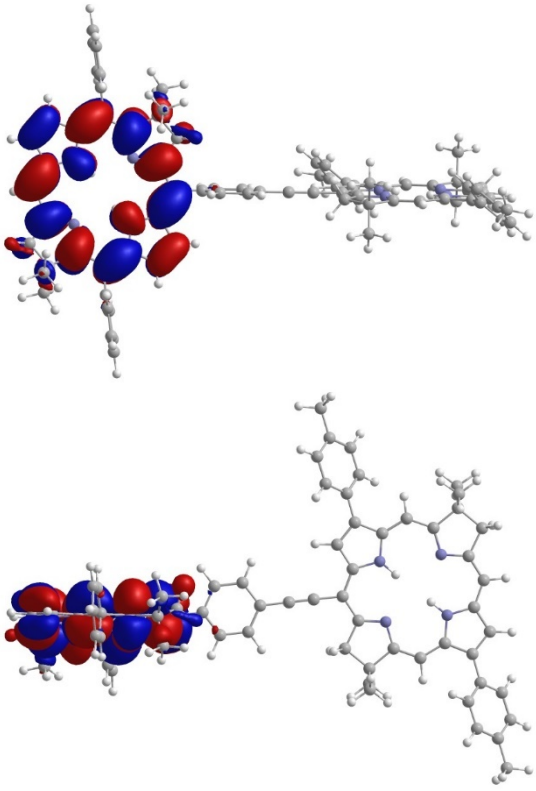
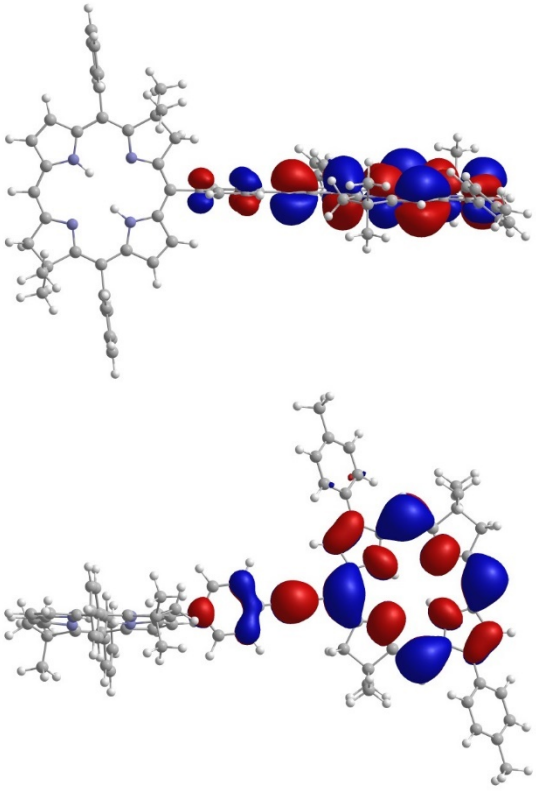
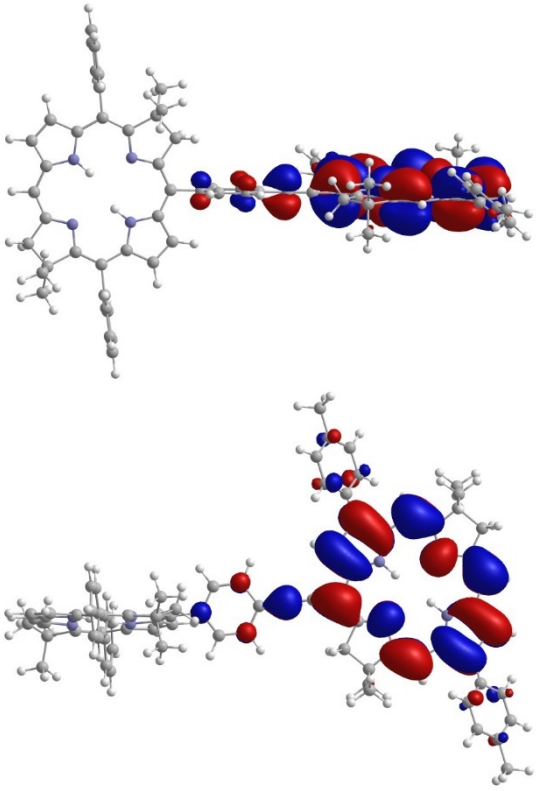
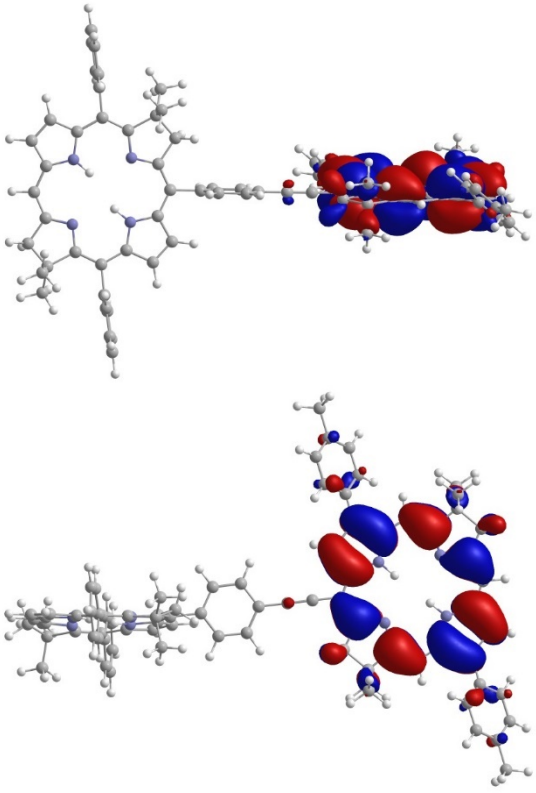
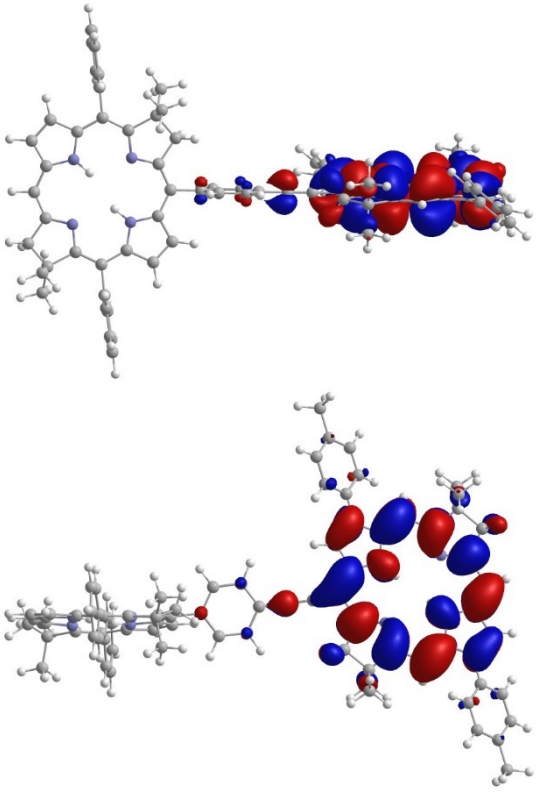
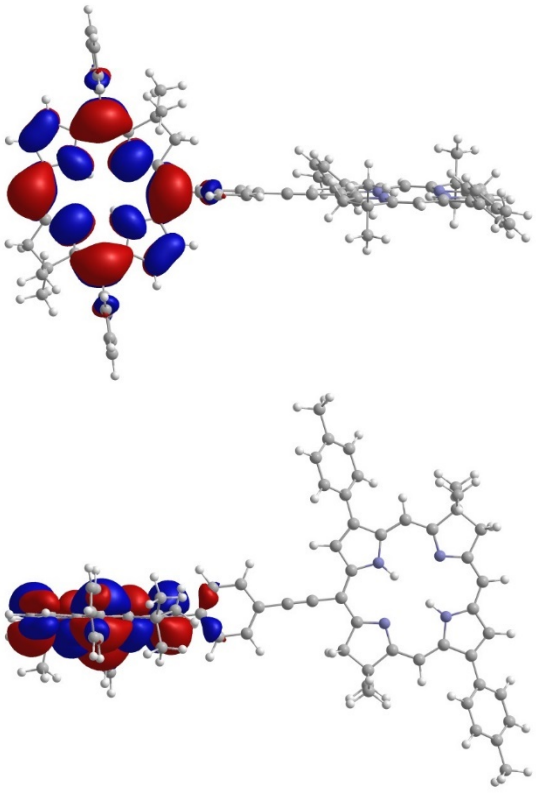
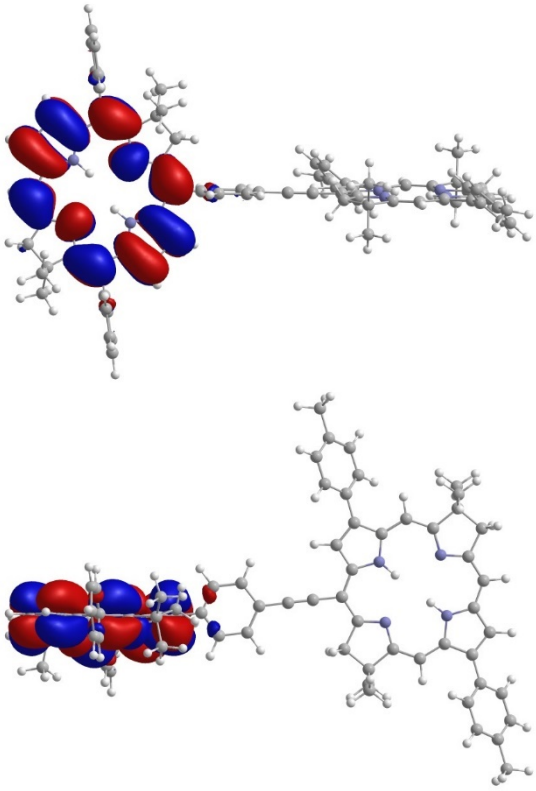
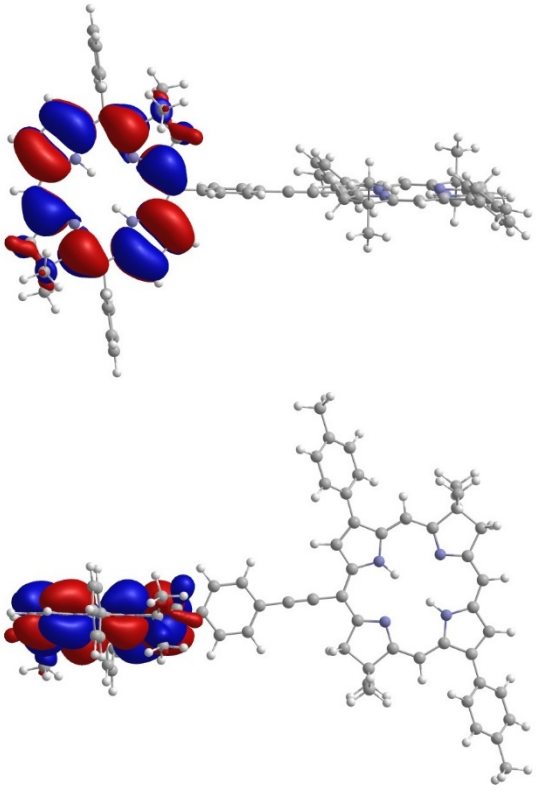
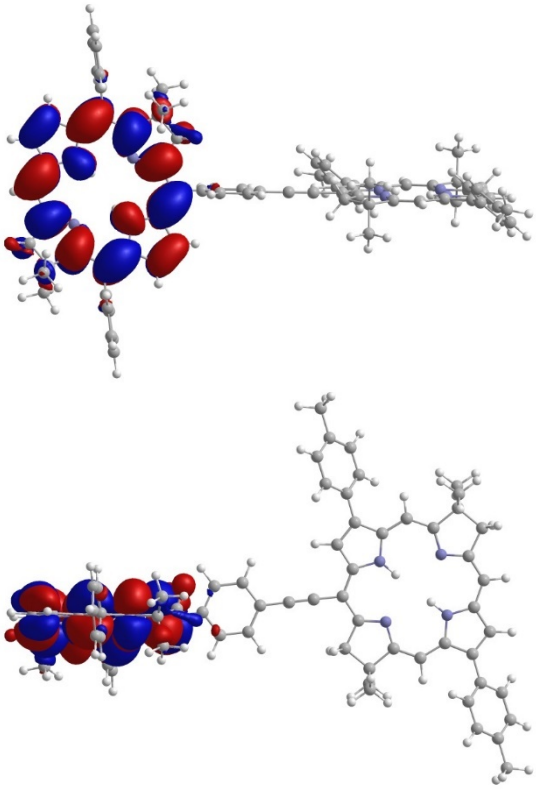
S15	0.98518		
S16	0.95692		

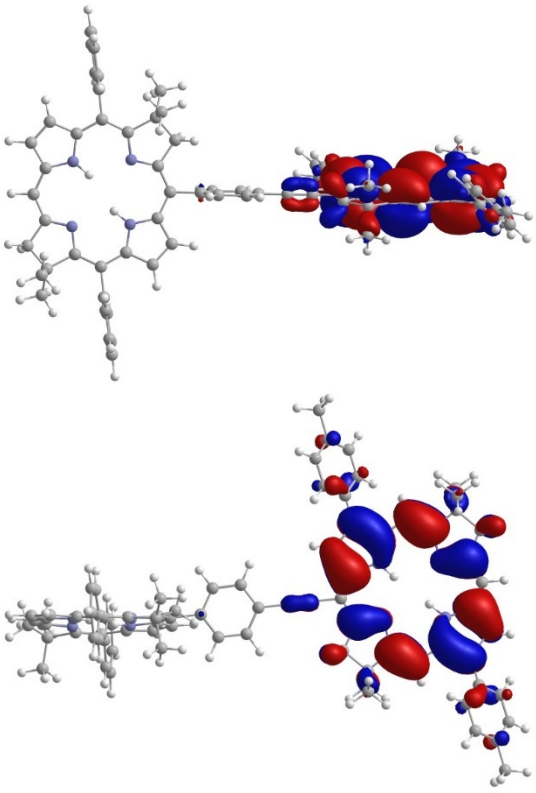
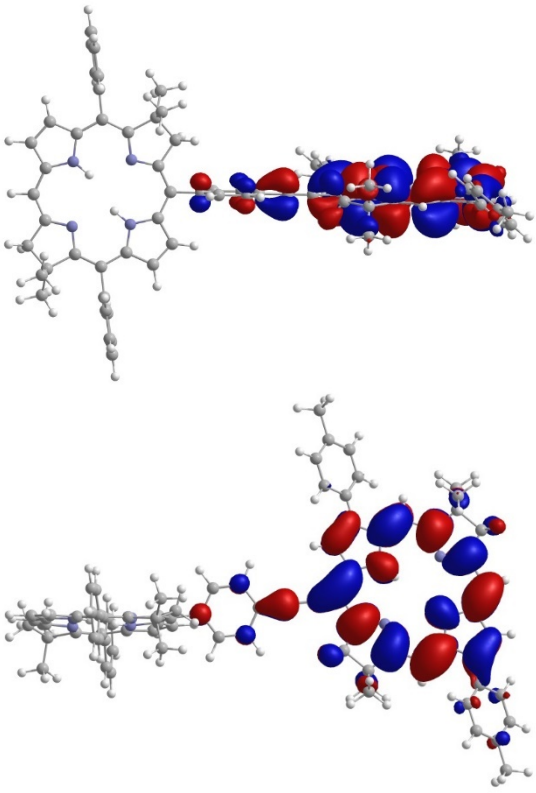
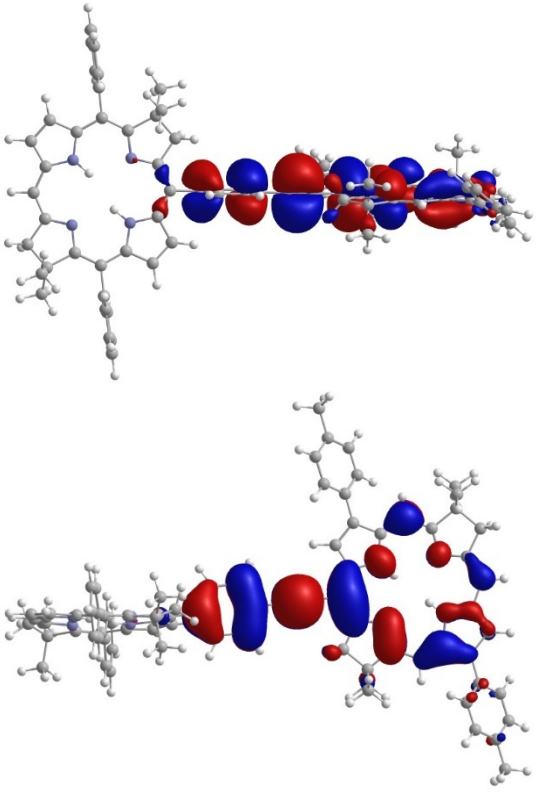
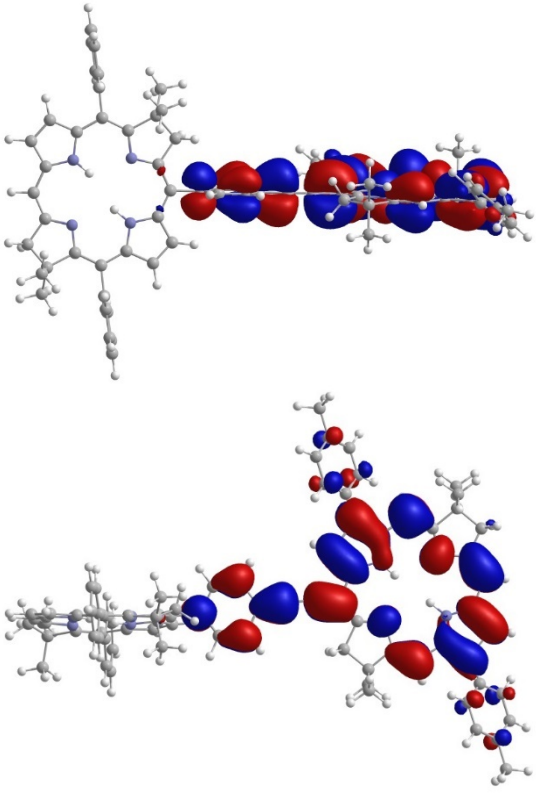
Table S26. NTOs for **Dyad-6**.

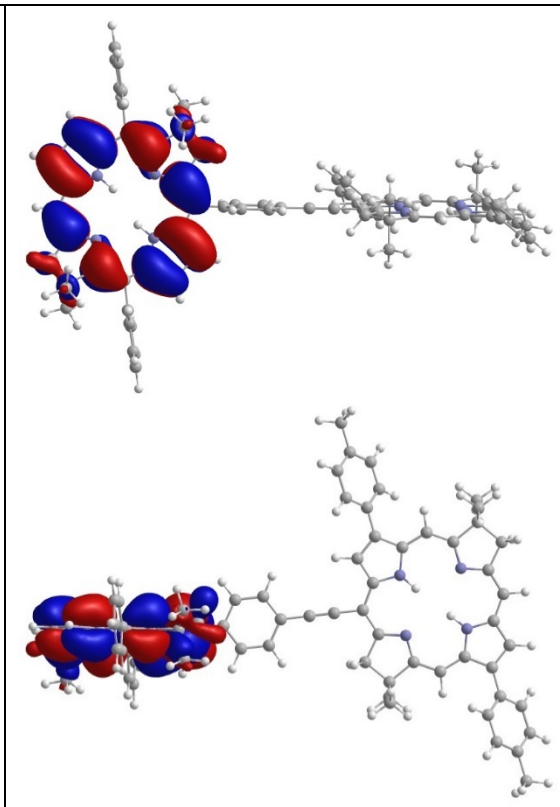
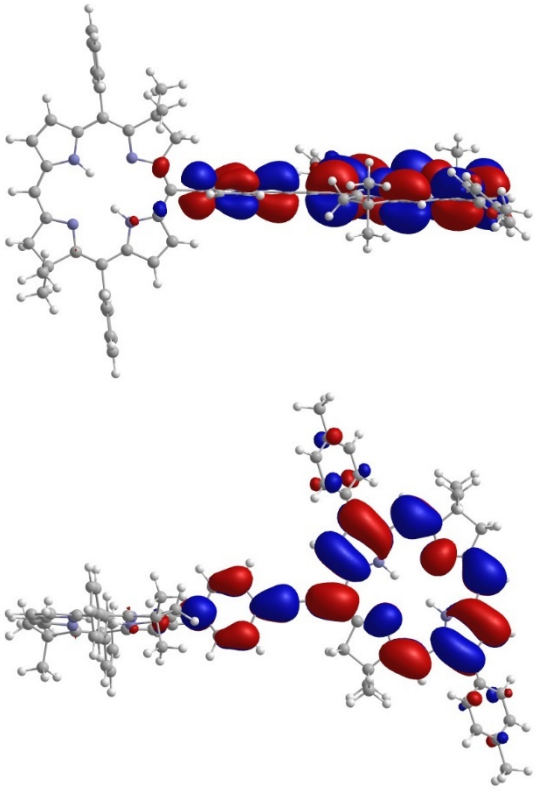
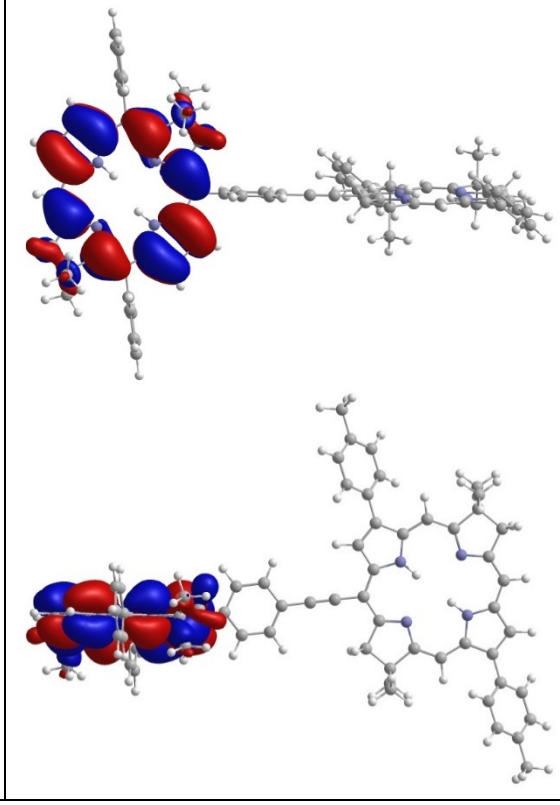
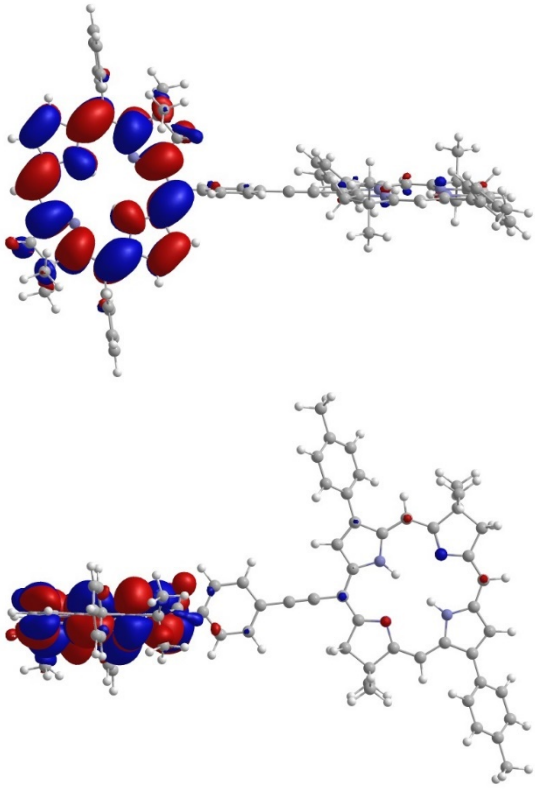
S#	Eigenvalue	From (NTO)	To (NTO)
S1	0.92690		
S1	0.08105		

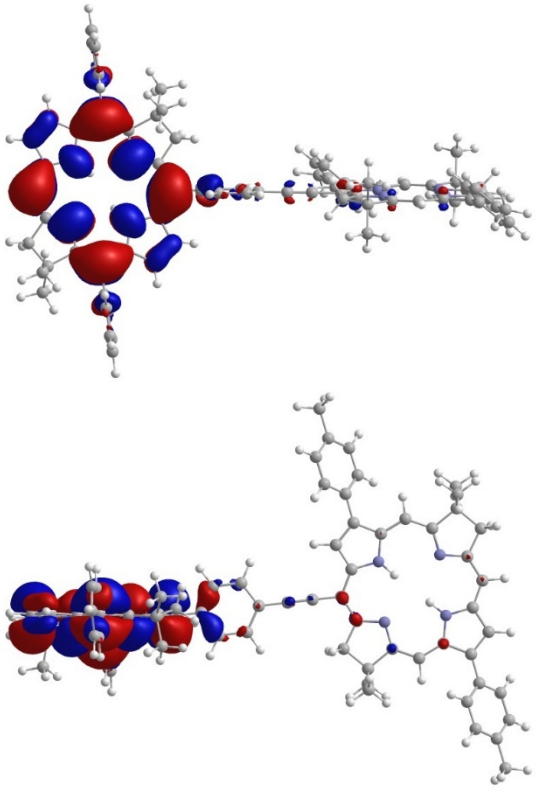
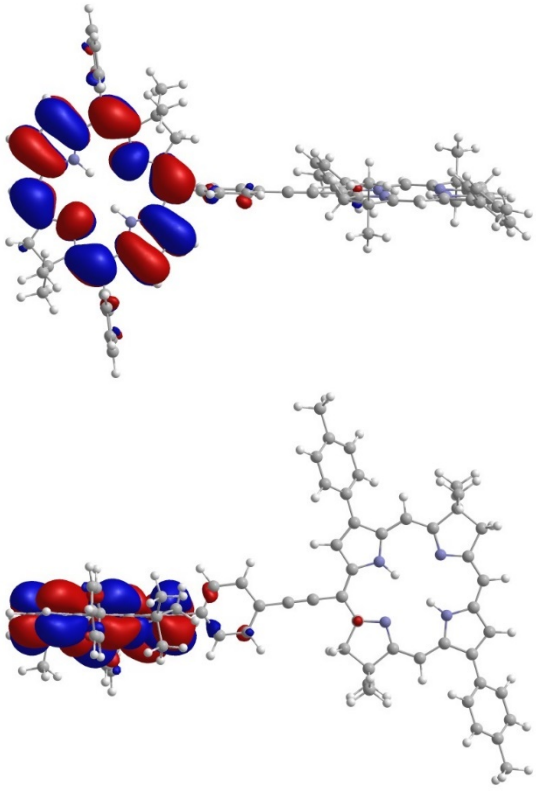
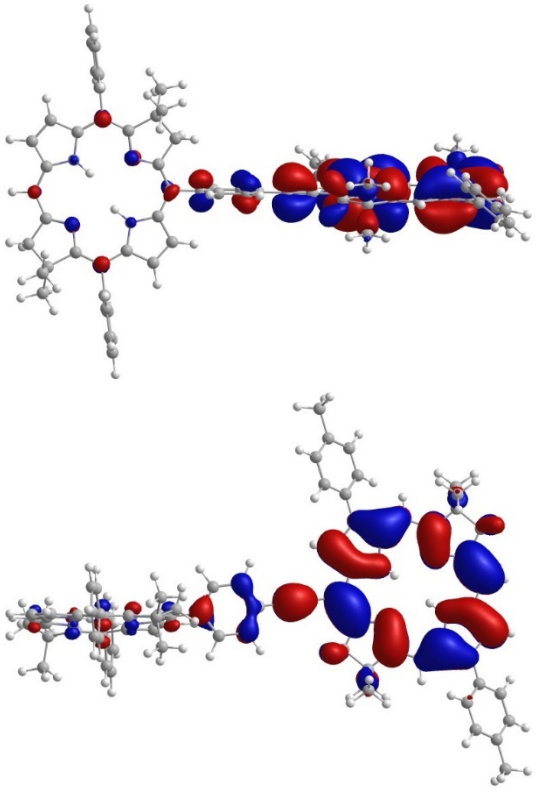
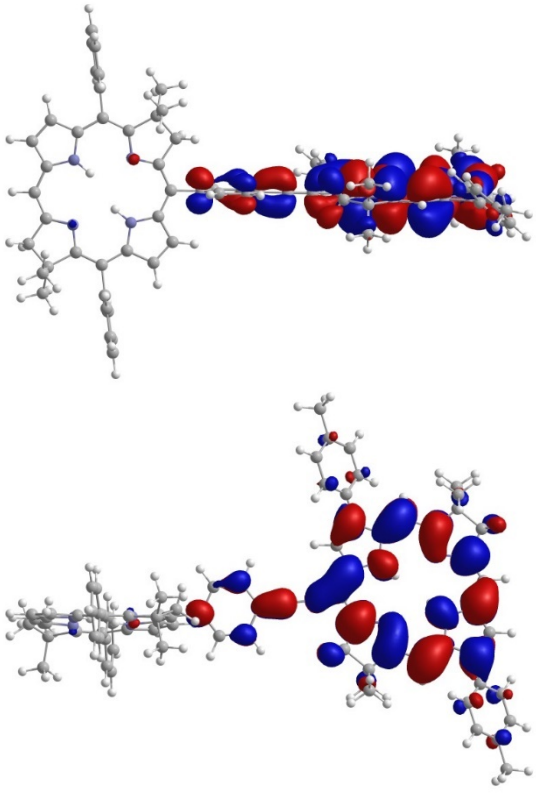
S2	0.91362		
S2	0.09429		

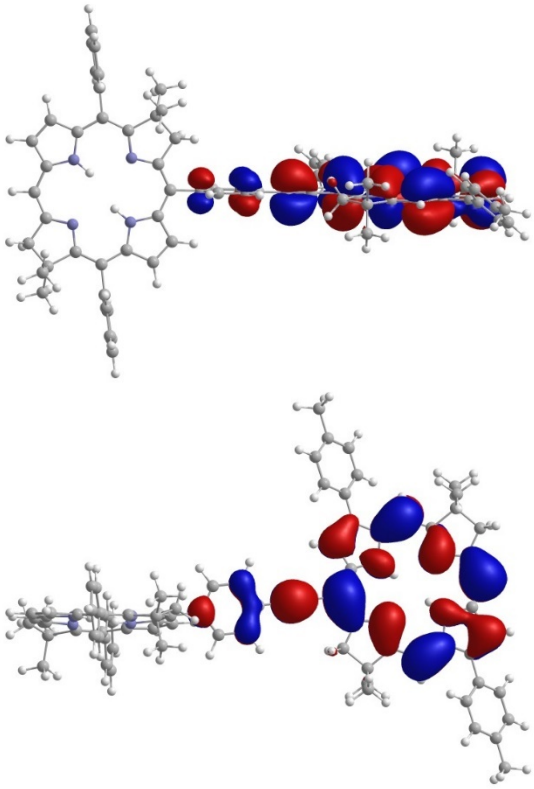
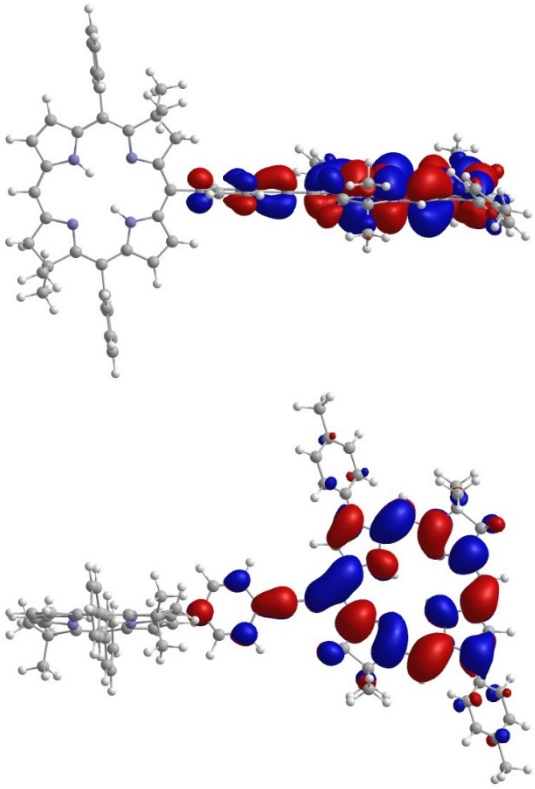
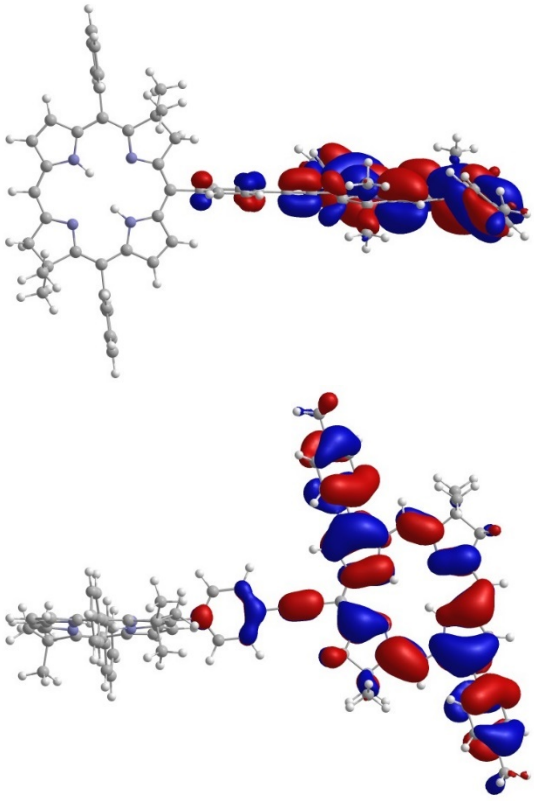
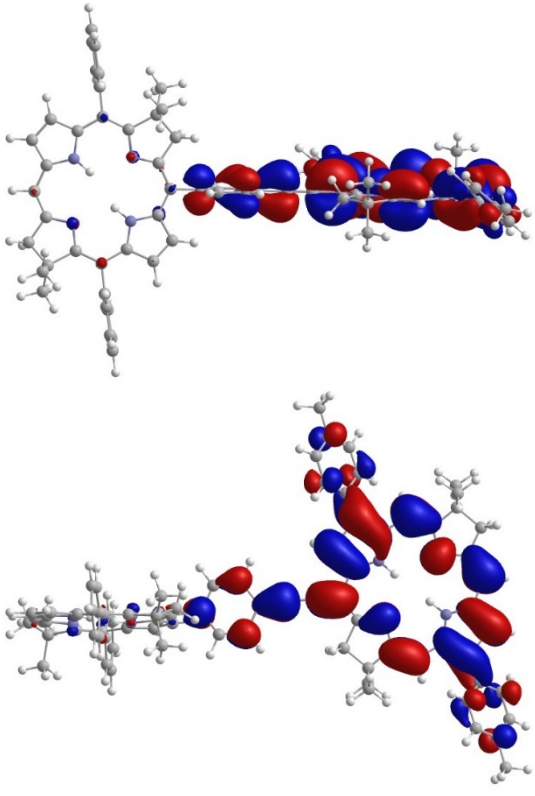
S3	0.80835		
S3	0.16135		

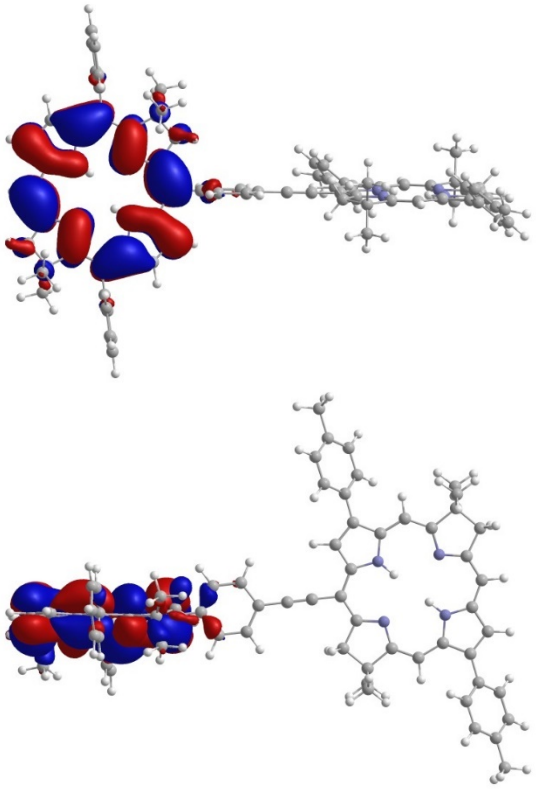
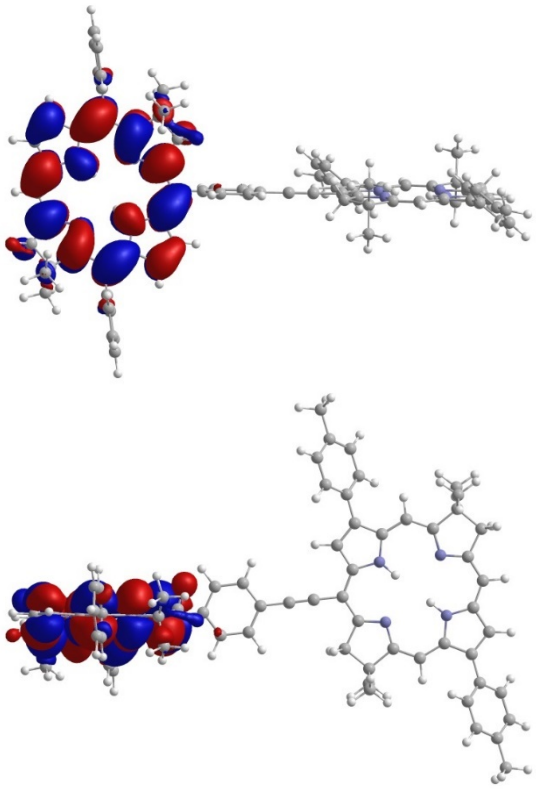
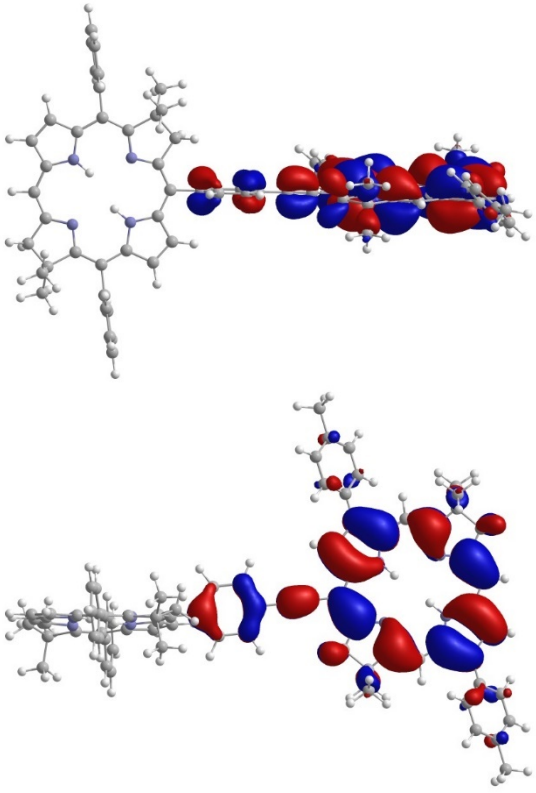
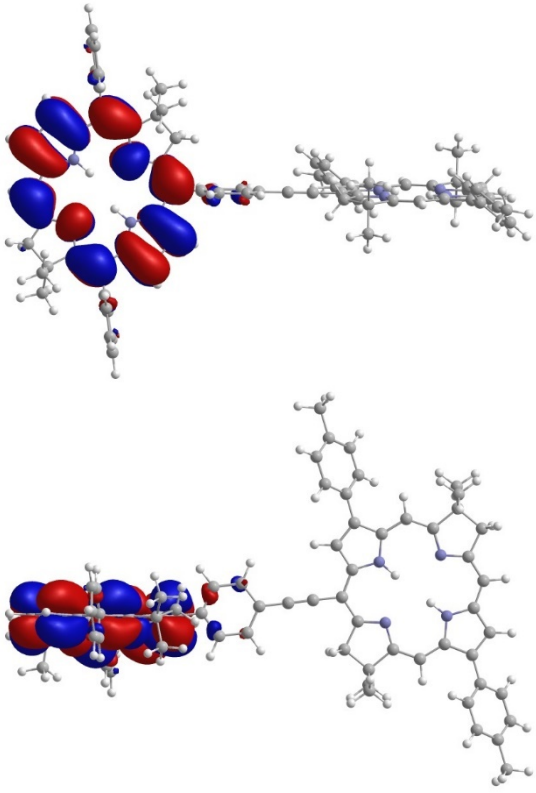
S4	0.78016		
S4	0.19688		

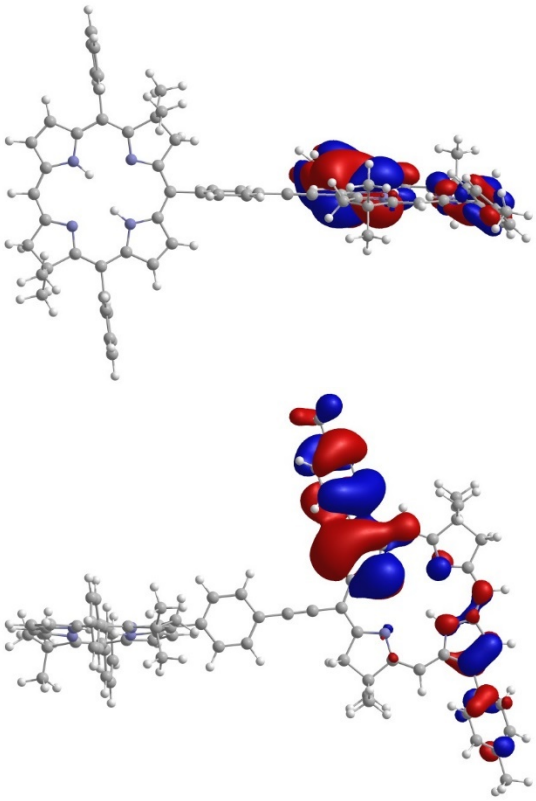
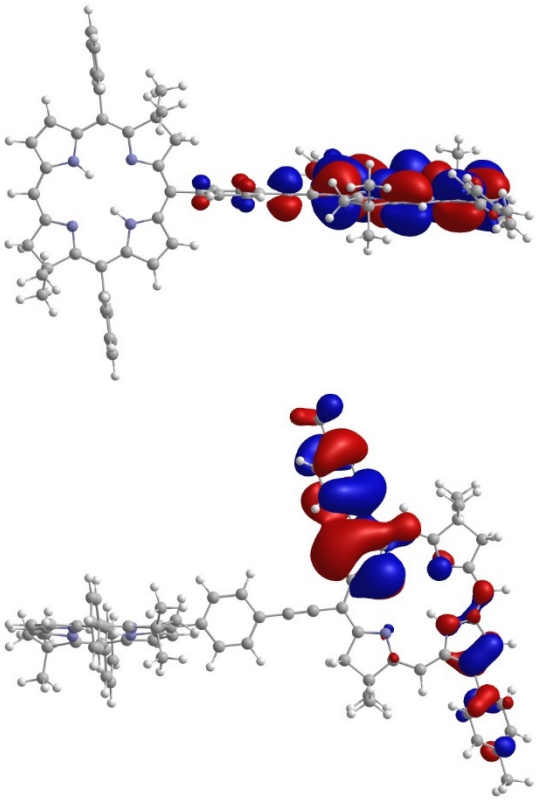
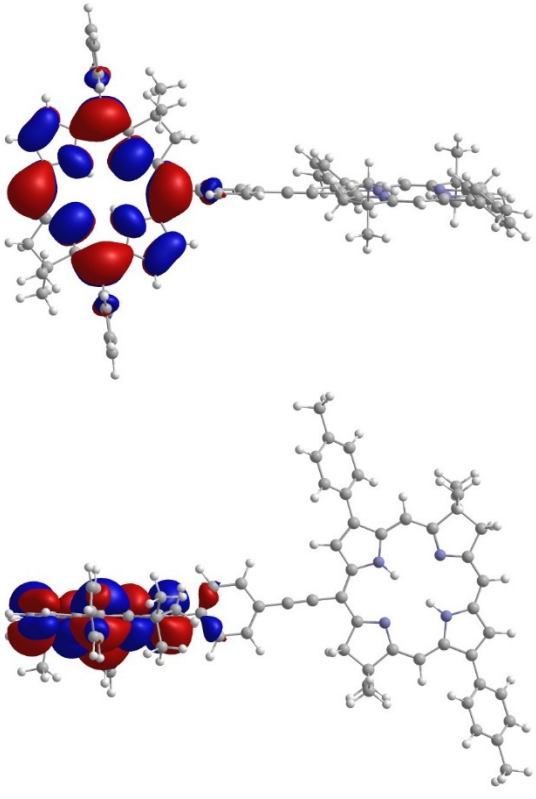
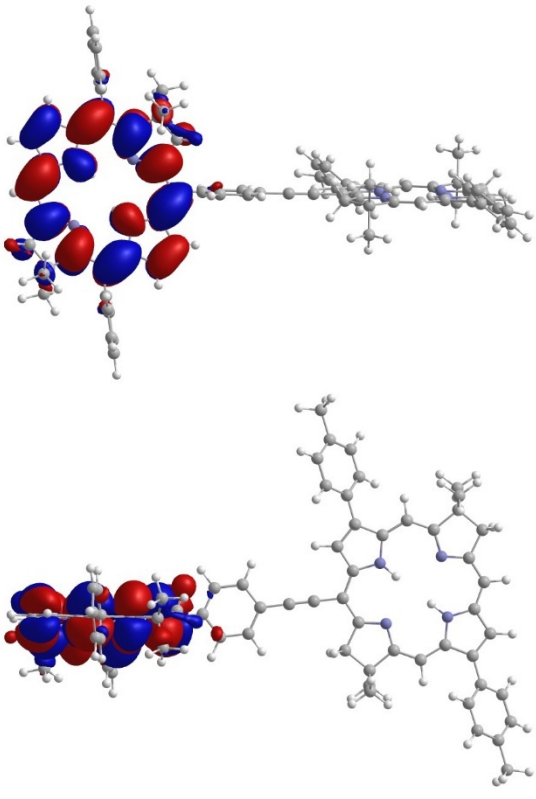
S5	0.73411		
S5	0.22630		

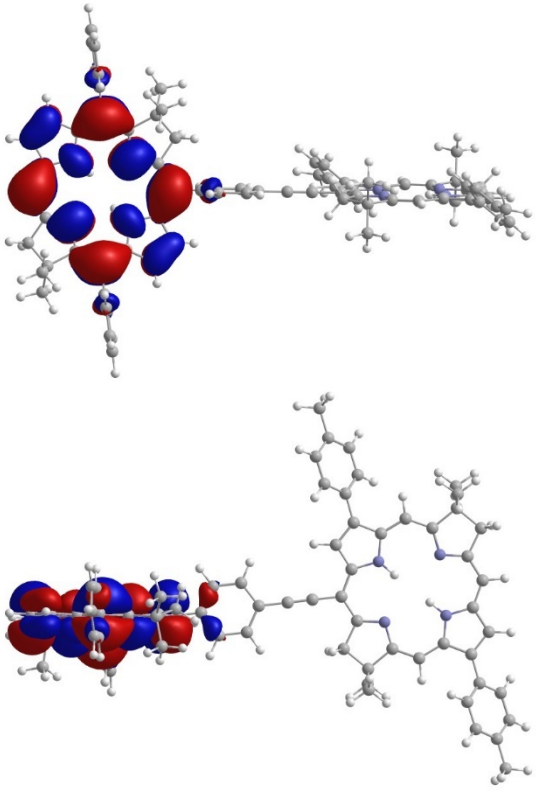
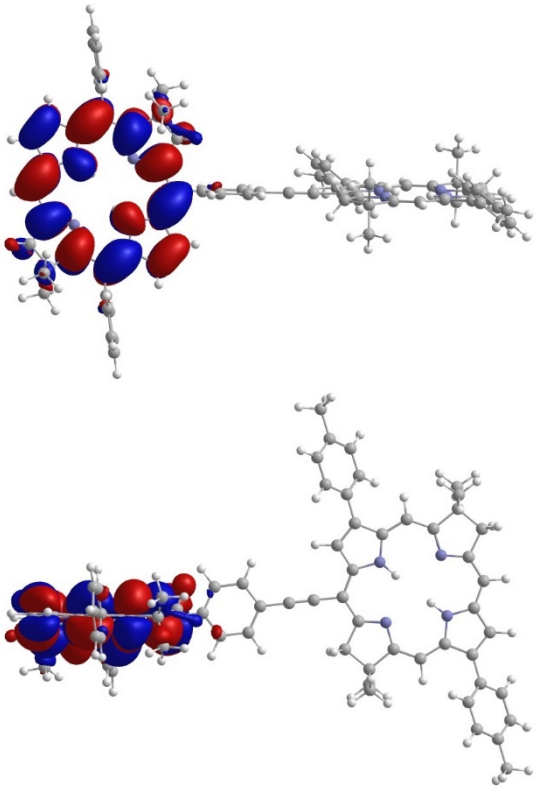
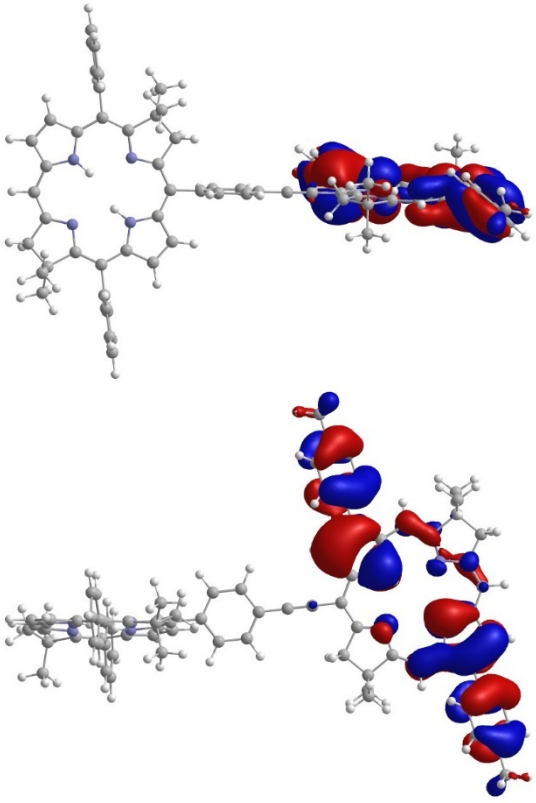
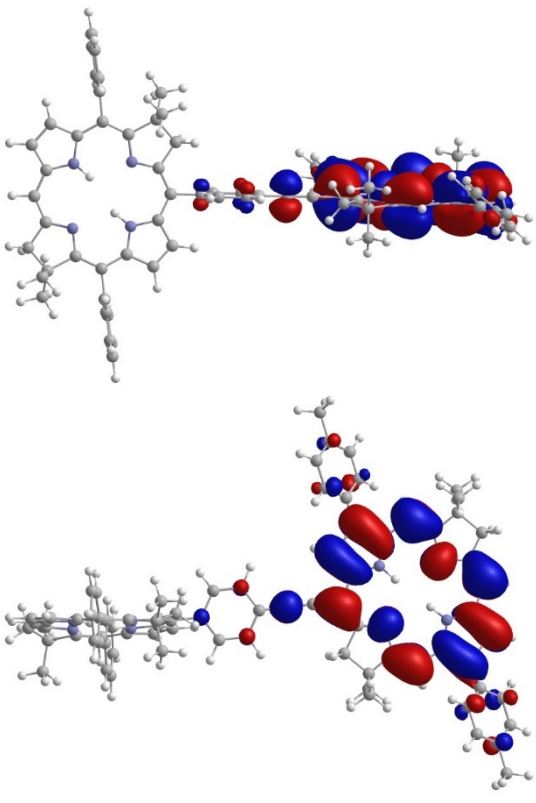
S6	0.99277		
S7	0.73700		

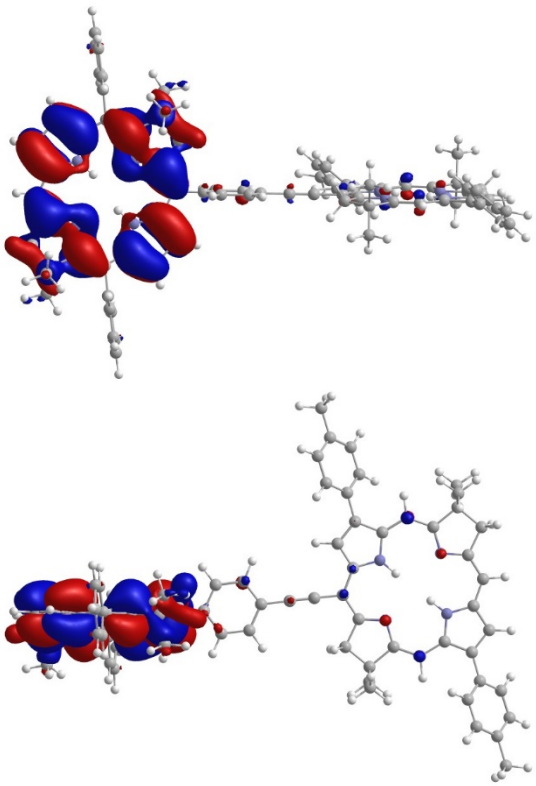
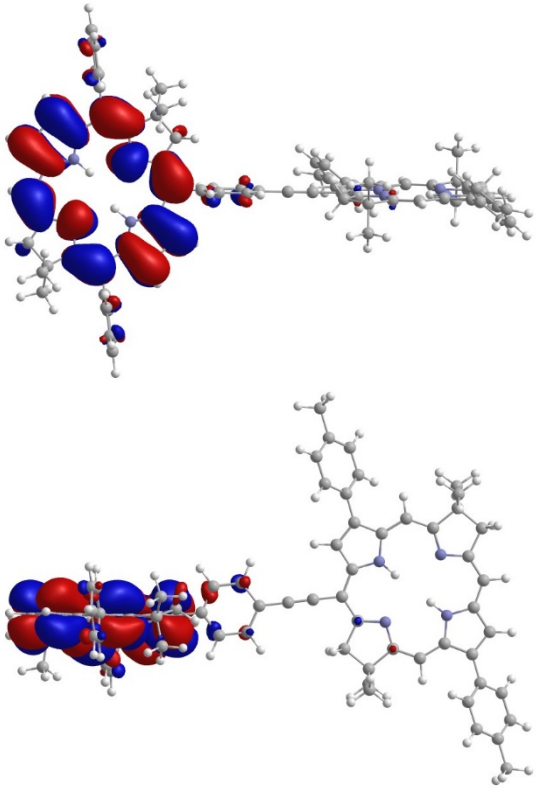
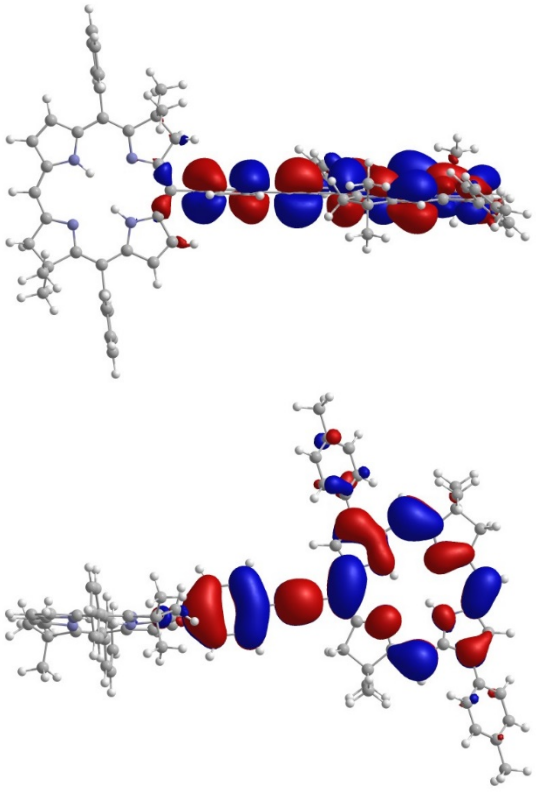
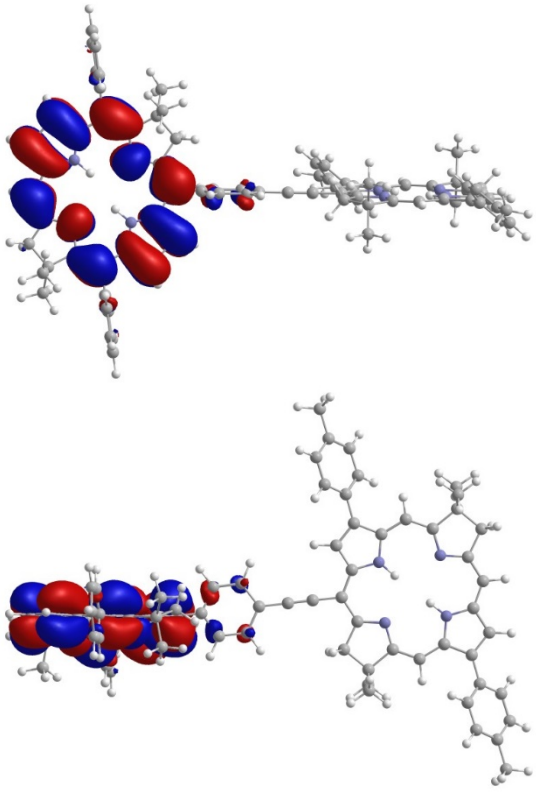
S7	0.18879		
S7	0.07311		

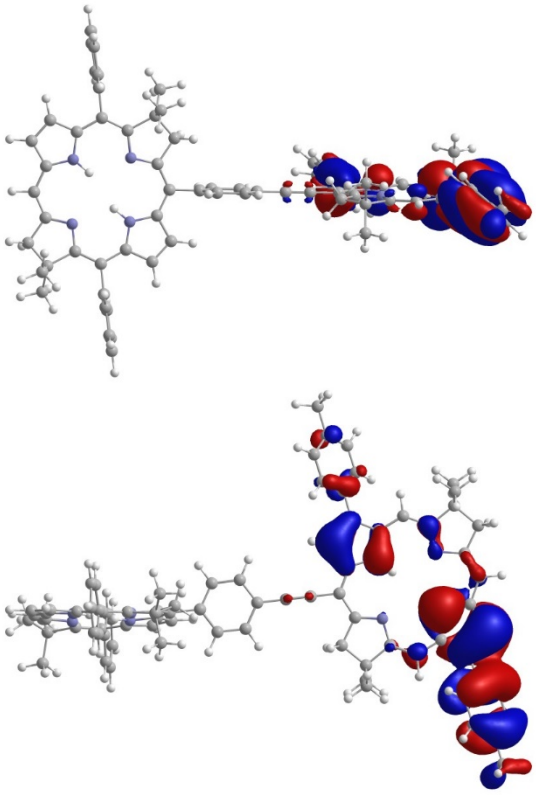
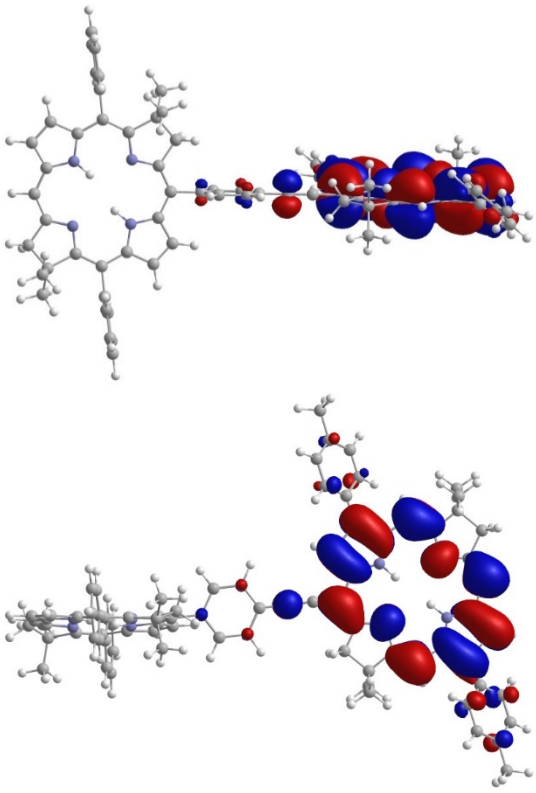
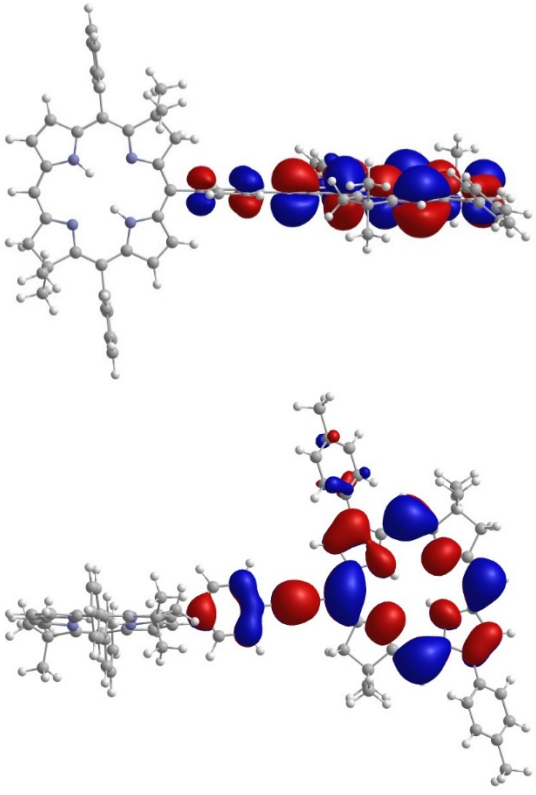
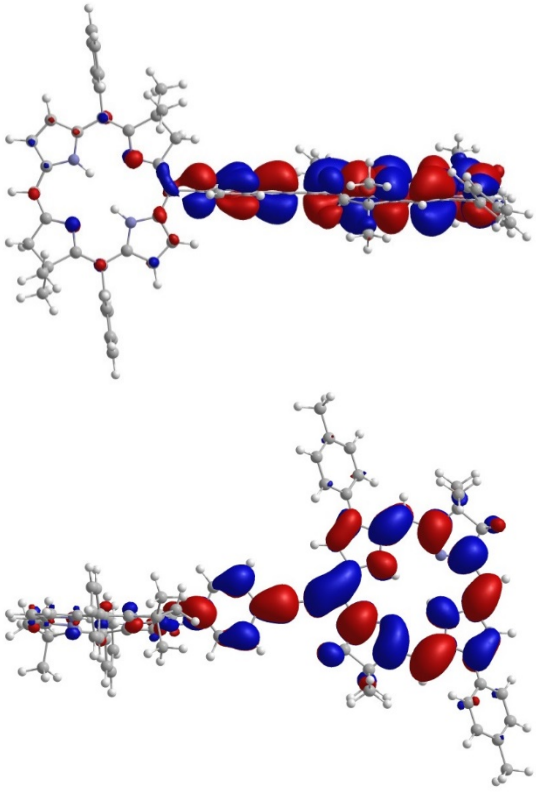
S8	0.75817		
S8	0.15402		

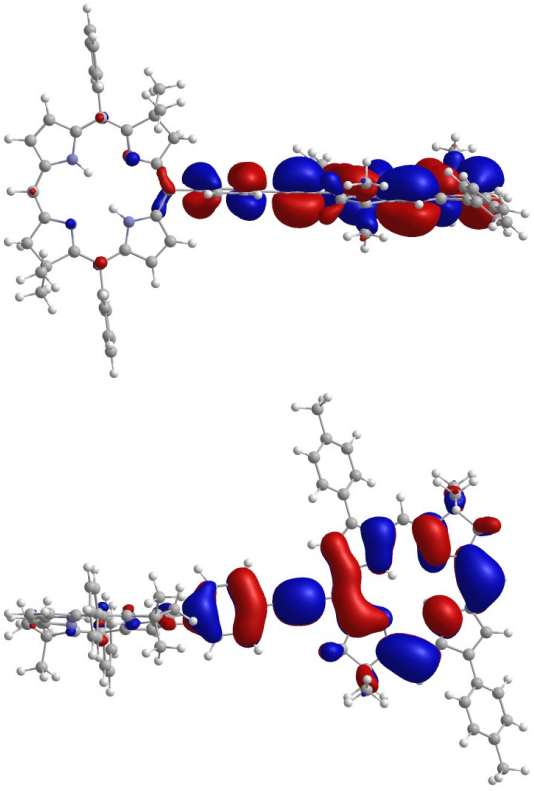
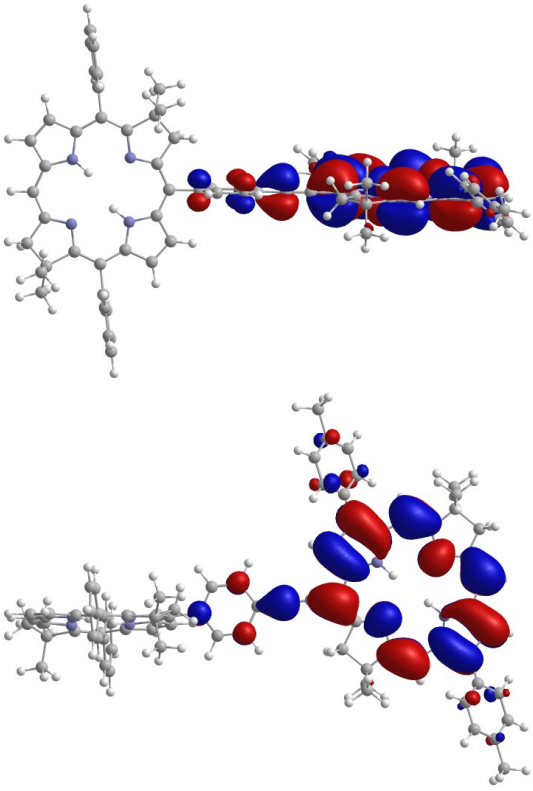
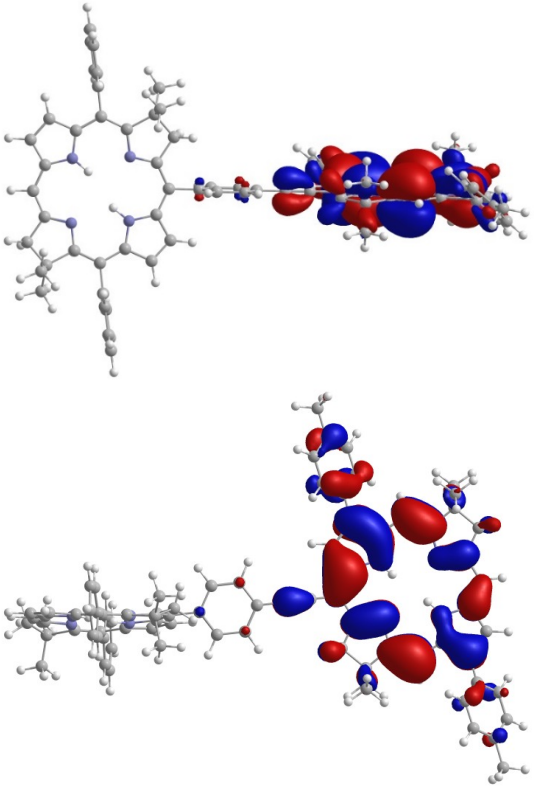
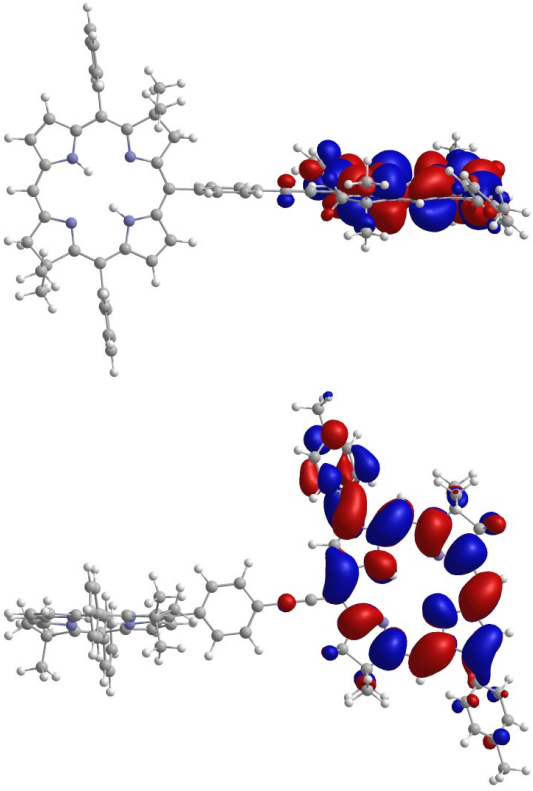
S8	0.06291		
S9	0.99133		

S10	0.79121		
S10	0.15760		

S11	0.66647		
S11	0.21632		

S11	0.07934		
S12	0.99041		

S13	0.89466		
S13	0.06988		

S14	0.83174		
S14	0.08328		

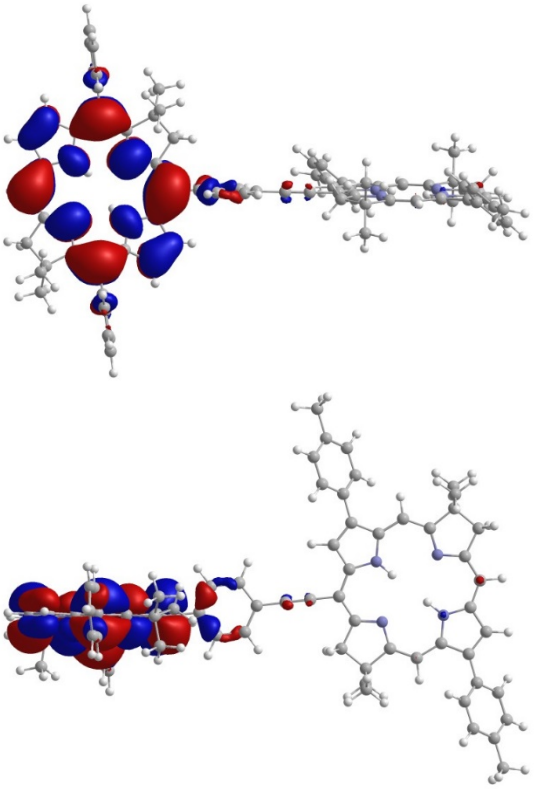
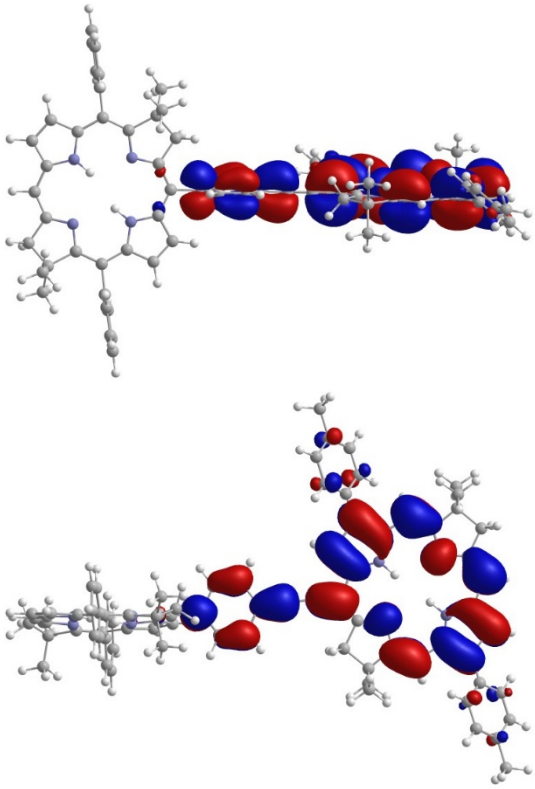
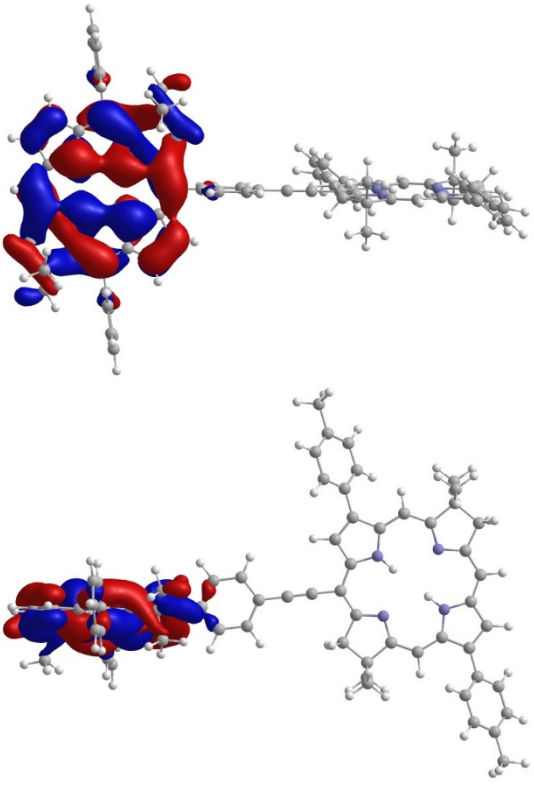
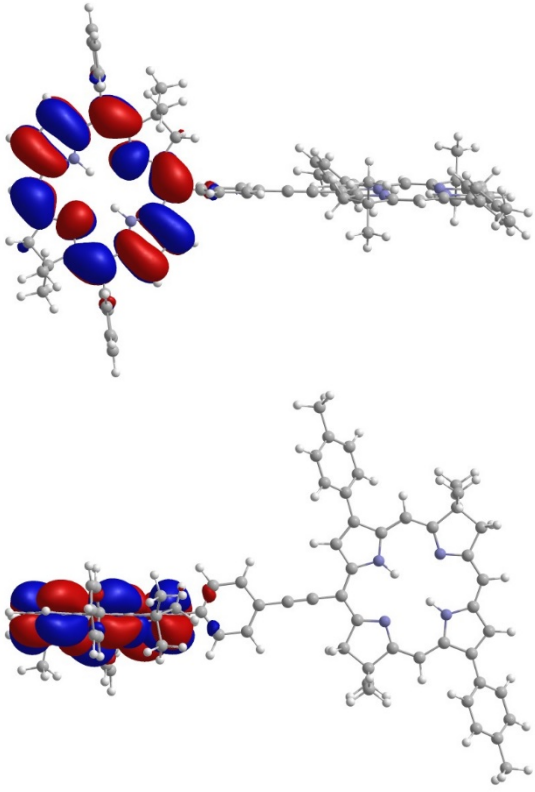
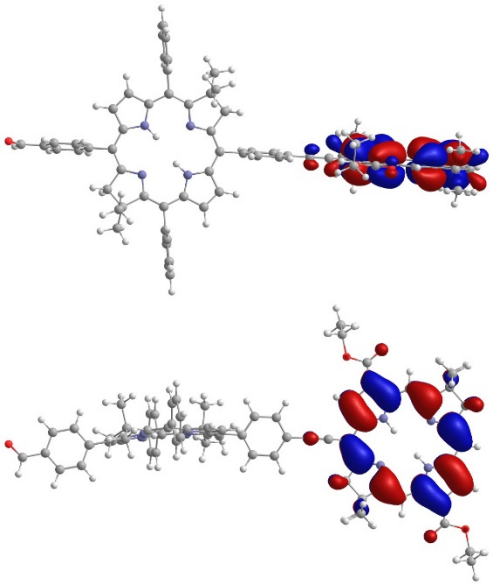
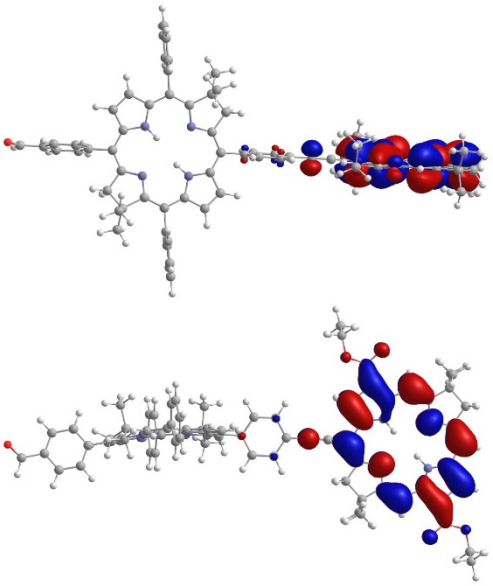
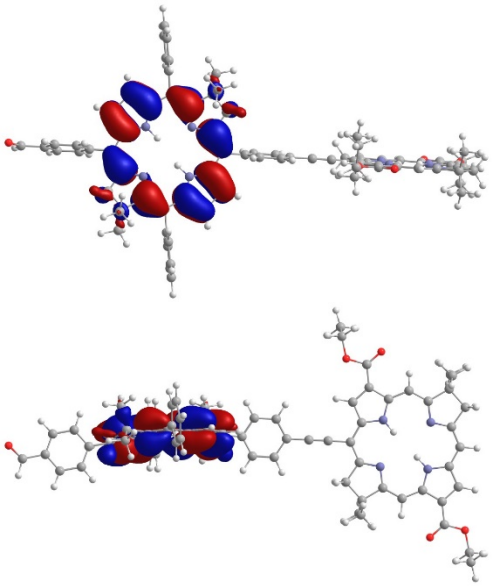
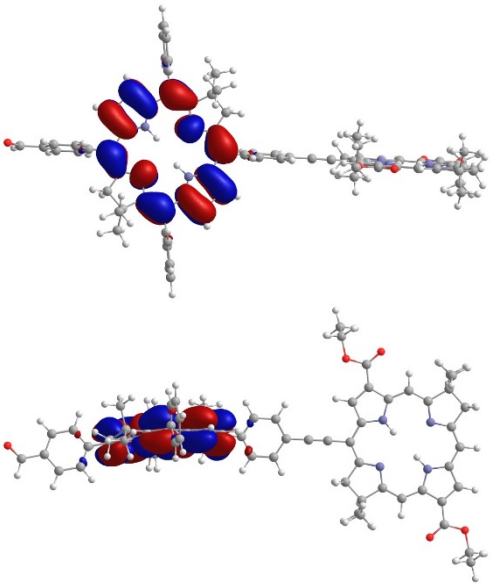
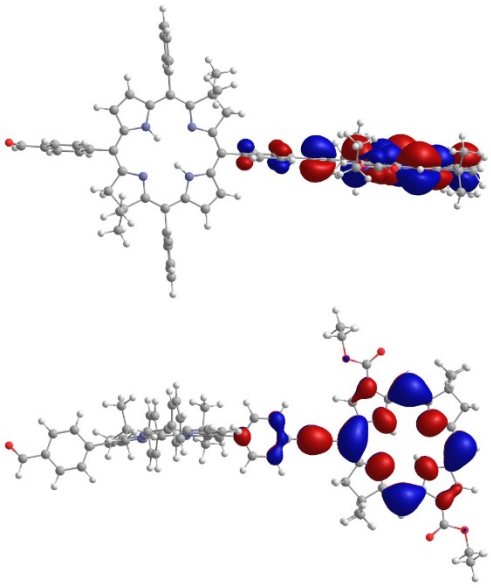
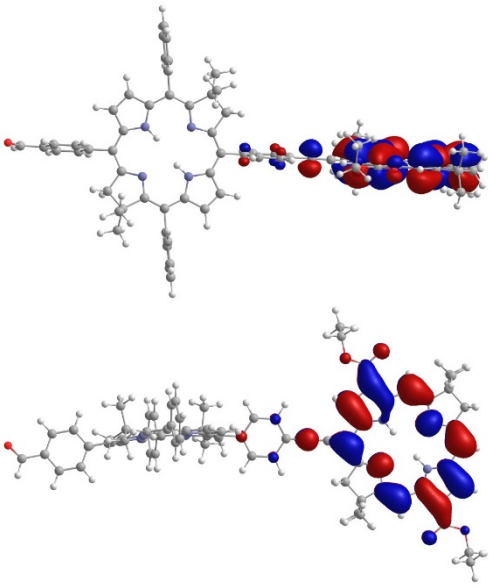
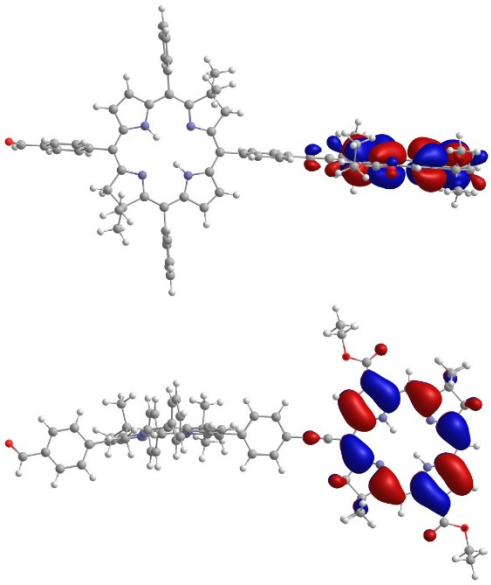
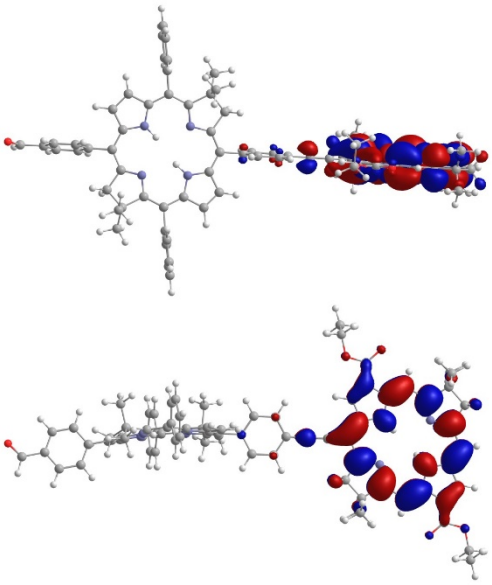
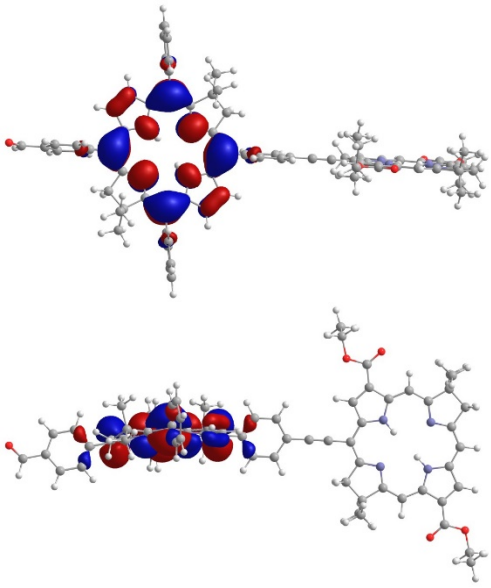
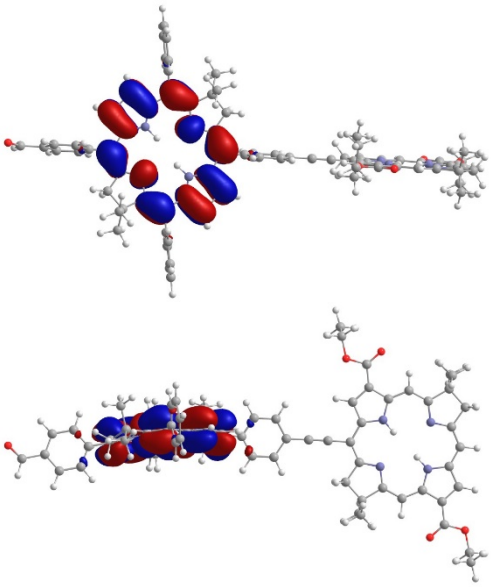
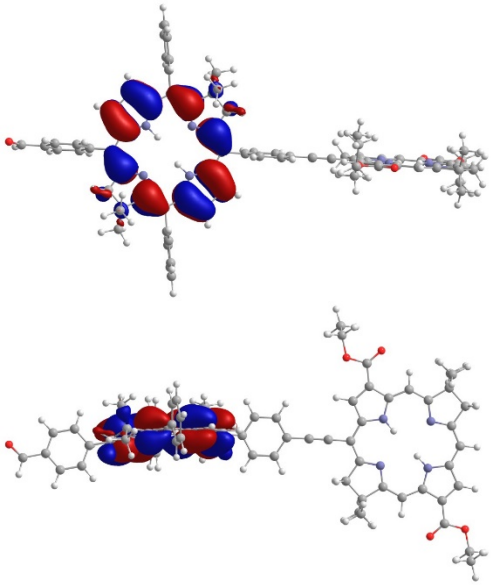
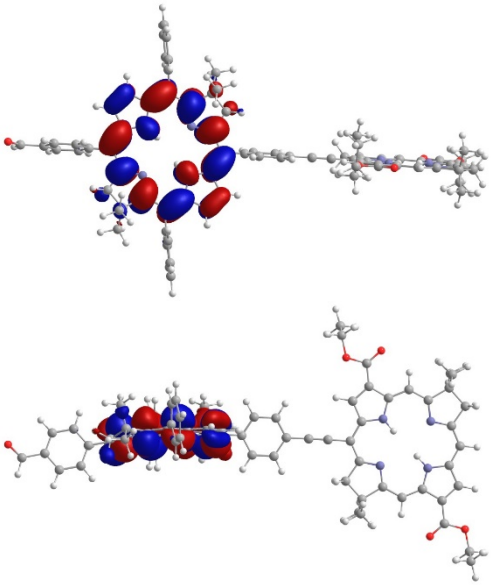
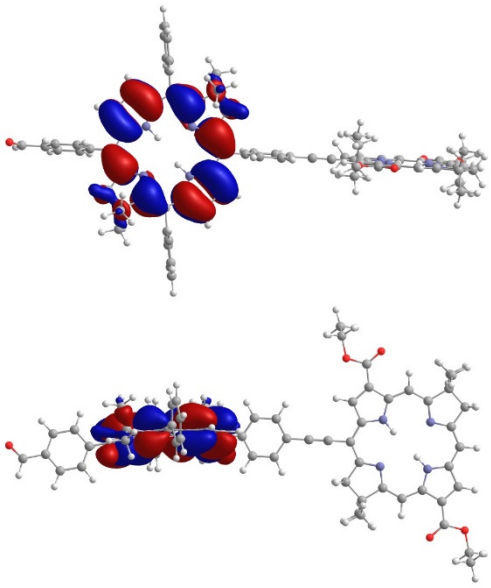
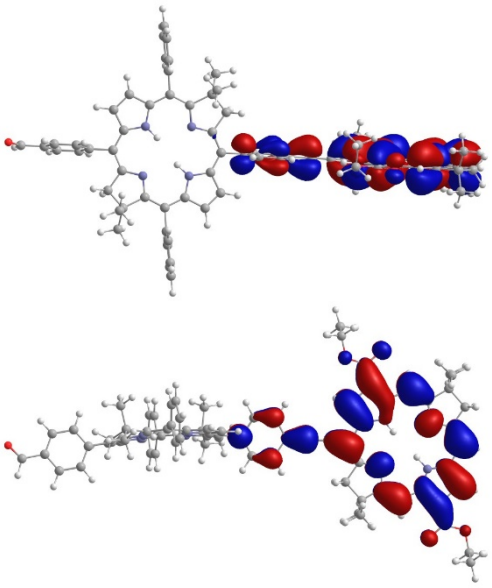
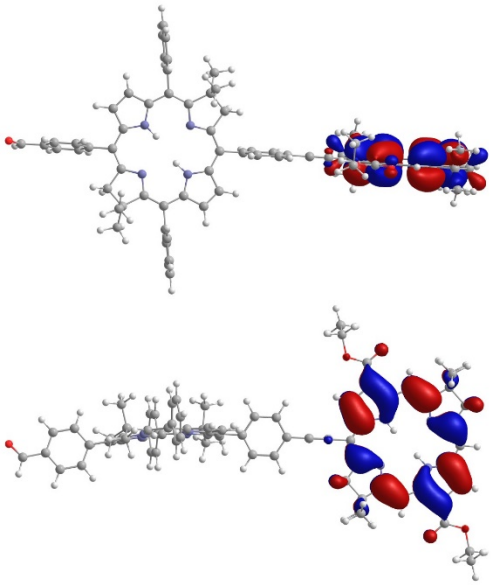
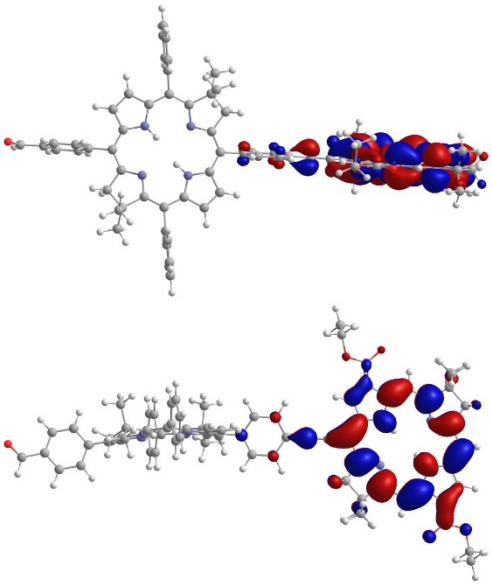
S15	0.98259		
S16	0.95773		

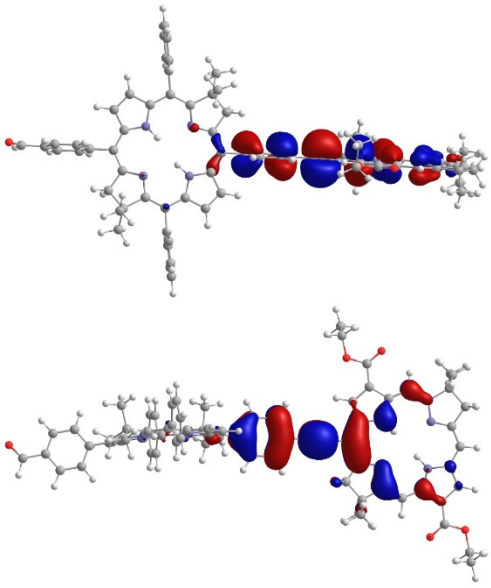
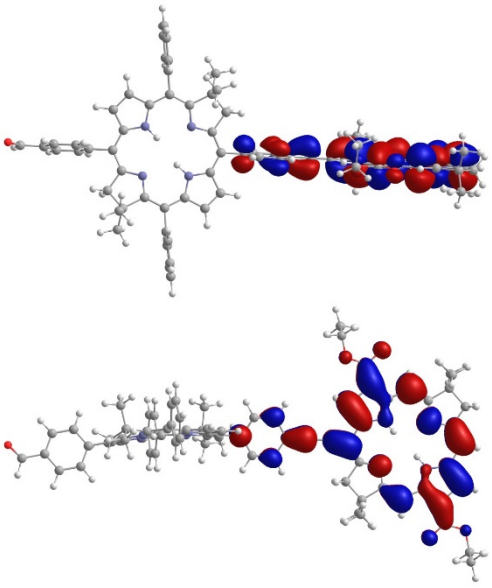
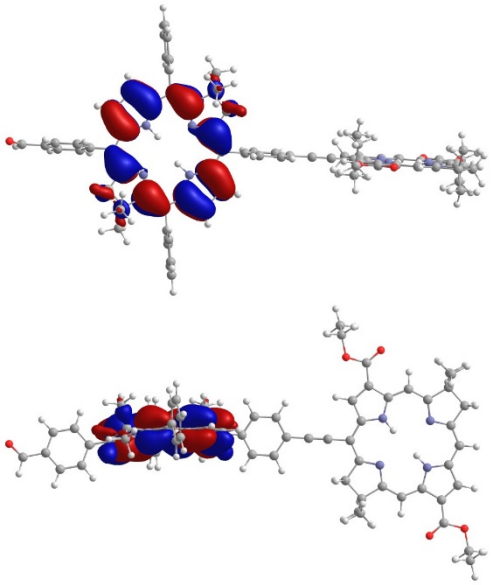
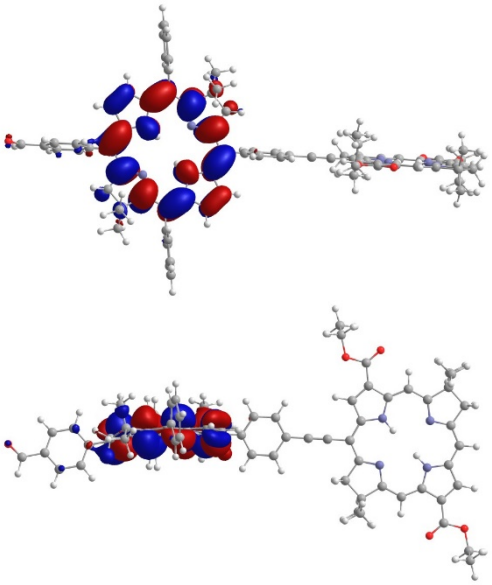
Table S27. NTOs for **Dyad-7**.

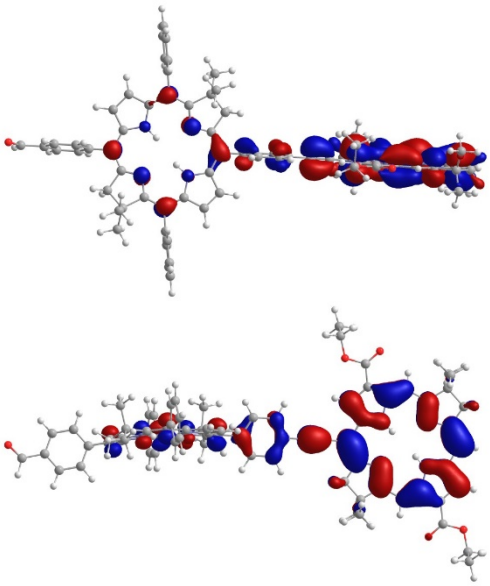
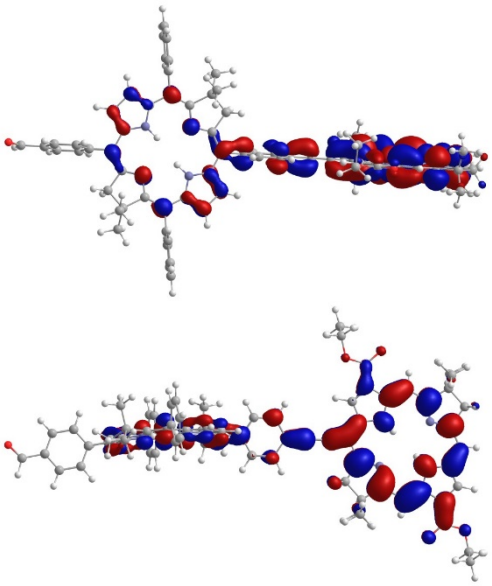
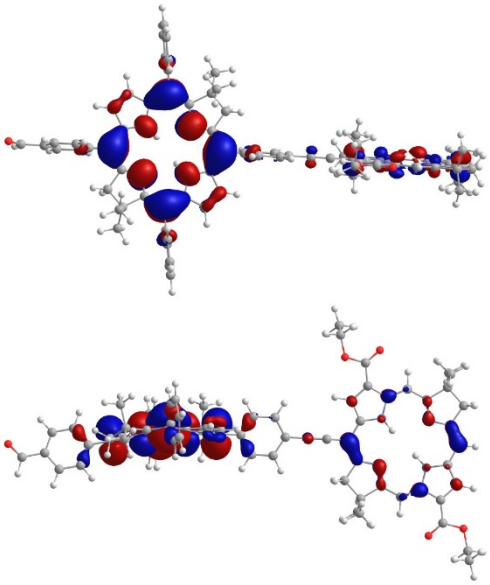
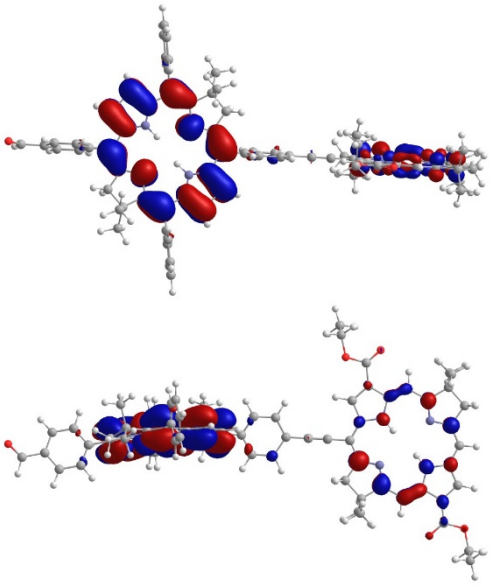
S#	Eigenvalue	From	To
S1	0.92327		
S2	0.90816		

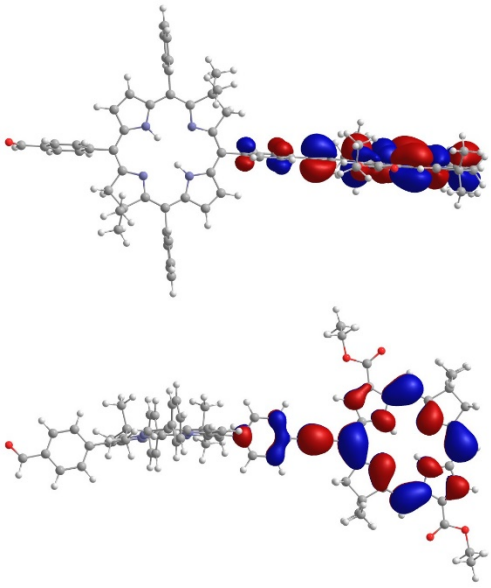
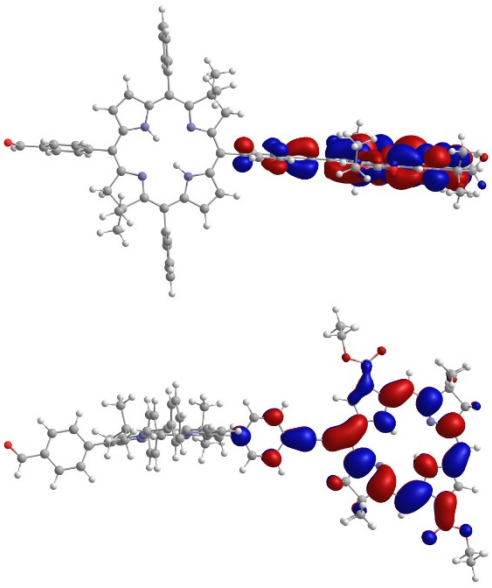
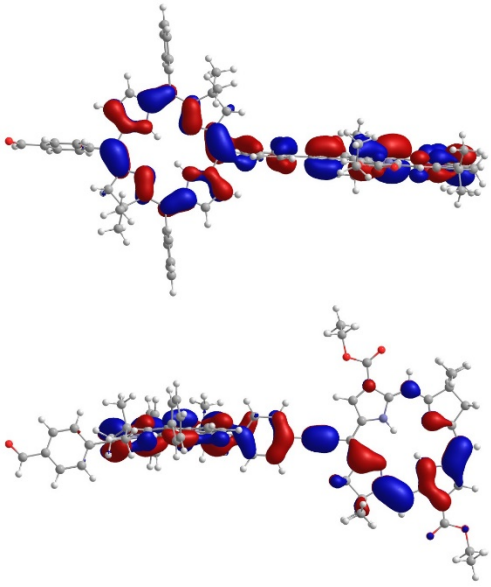
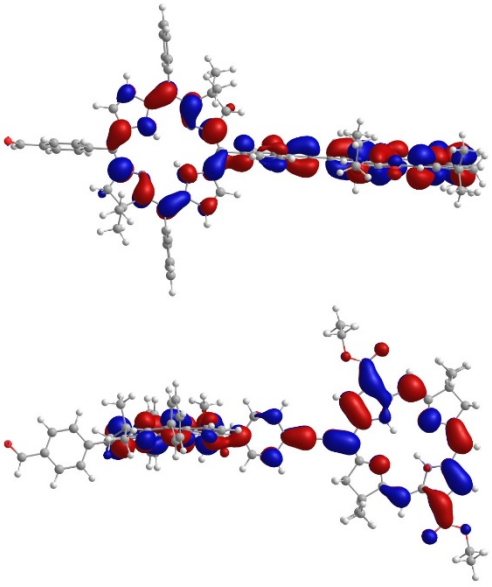
S3	0.87836		
S3	0.11135		

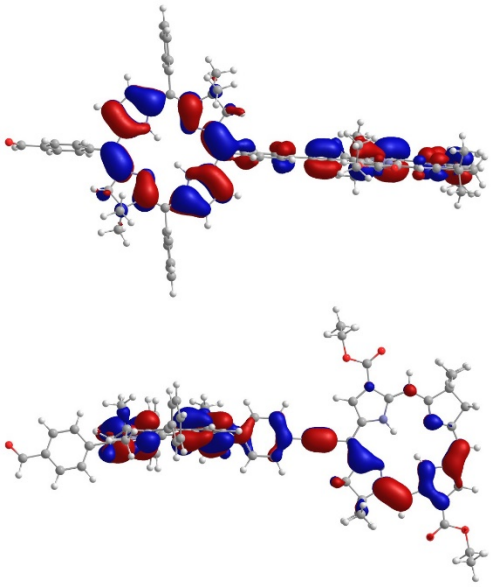
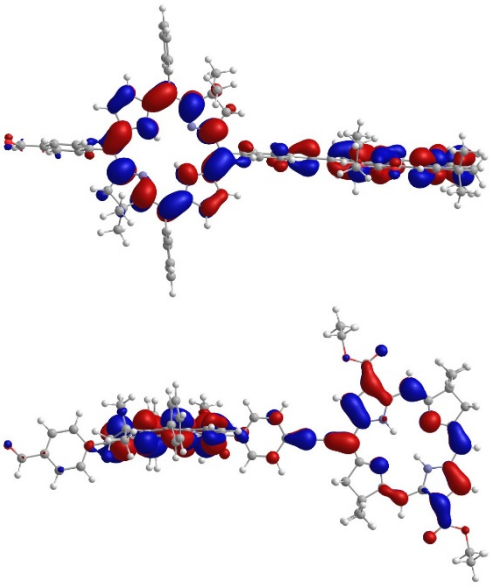
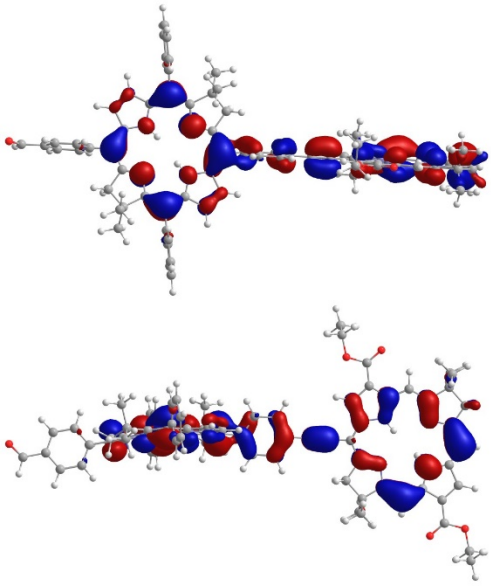
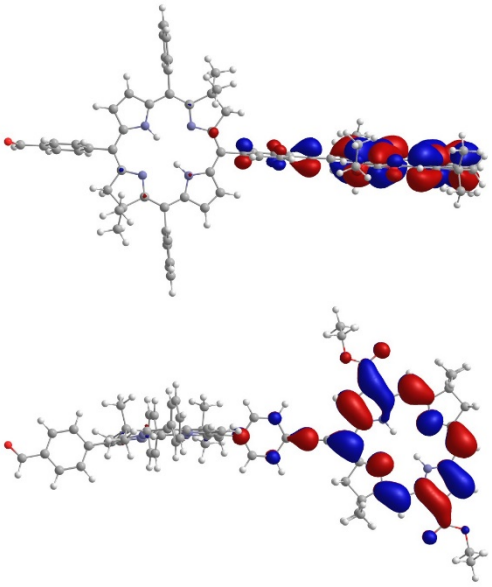
S4	0.81035		
S4	0.18505		

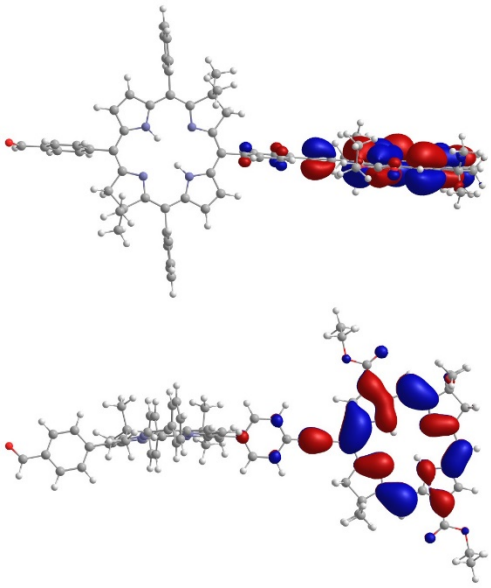
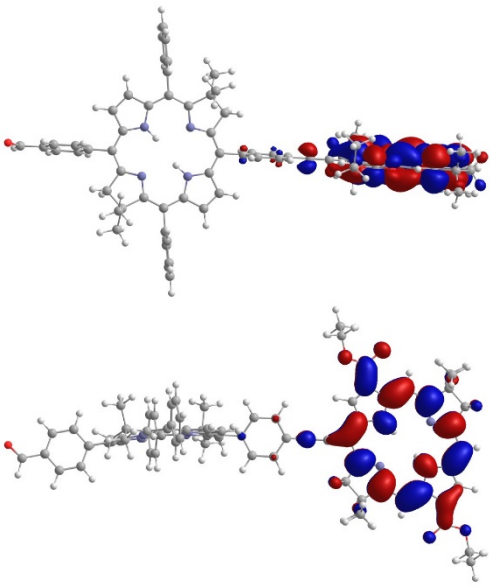
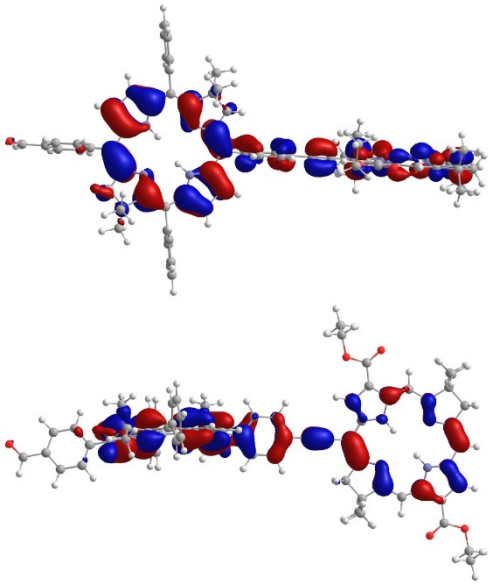
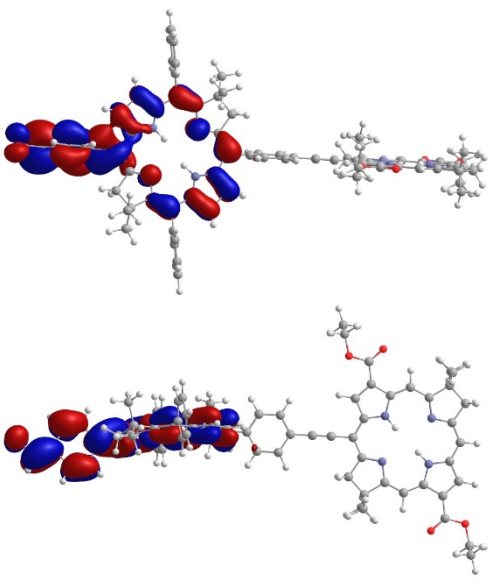
S5	0.99854		
S6	0.68871		

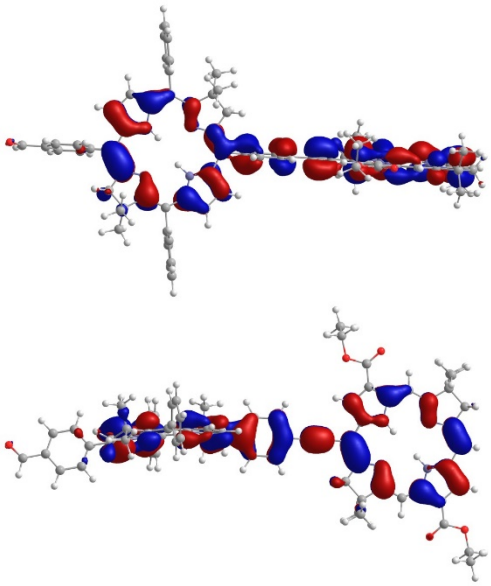
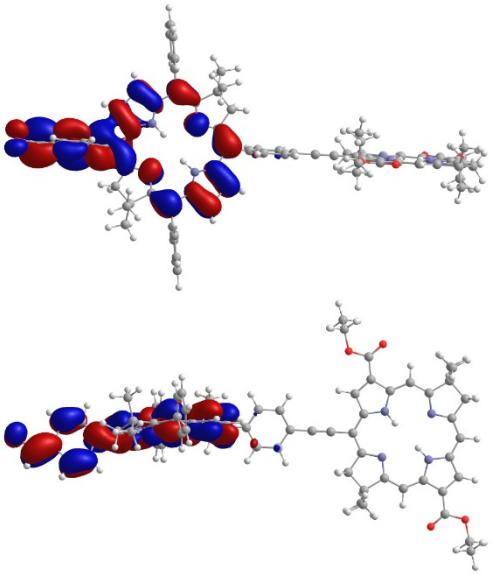
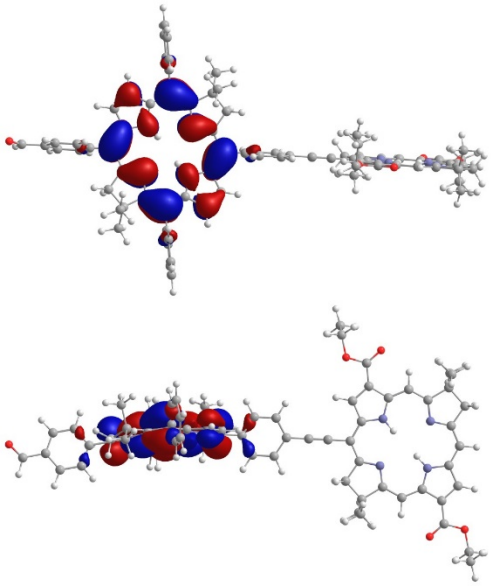
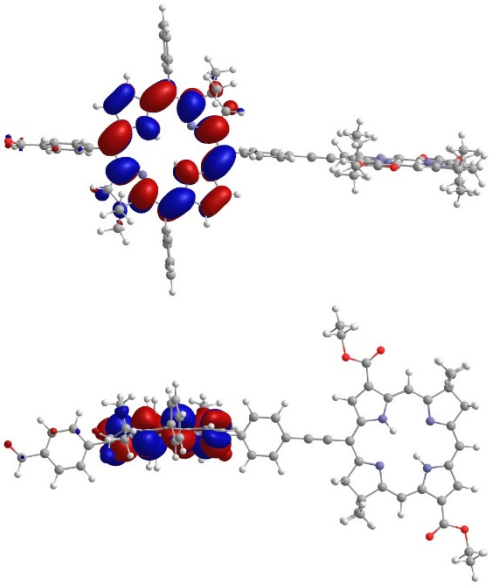
S6	0.24762		
S7	0.64002		

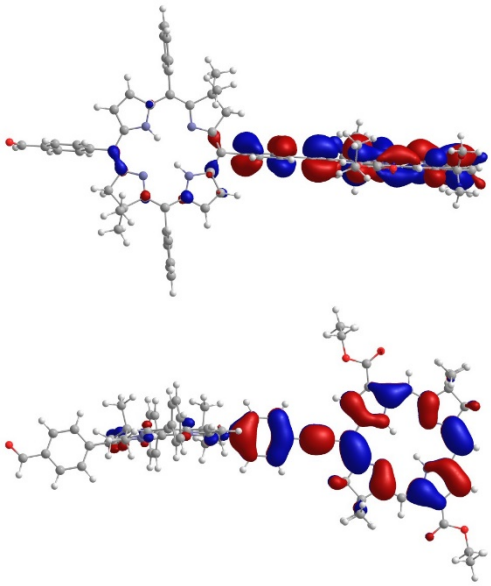
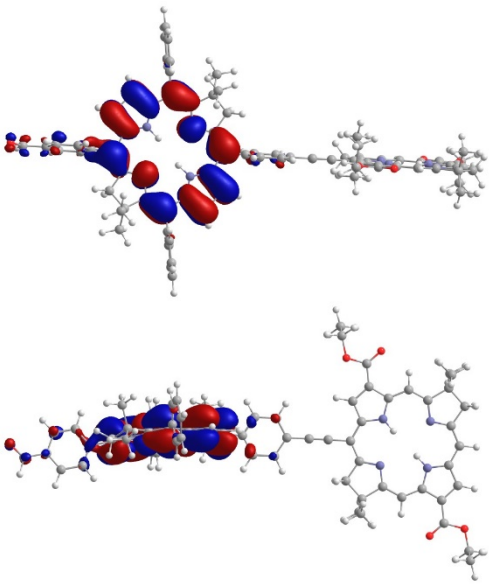
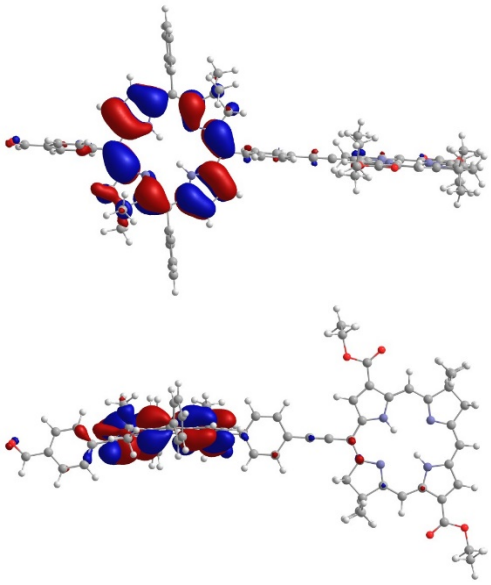
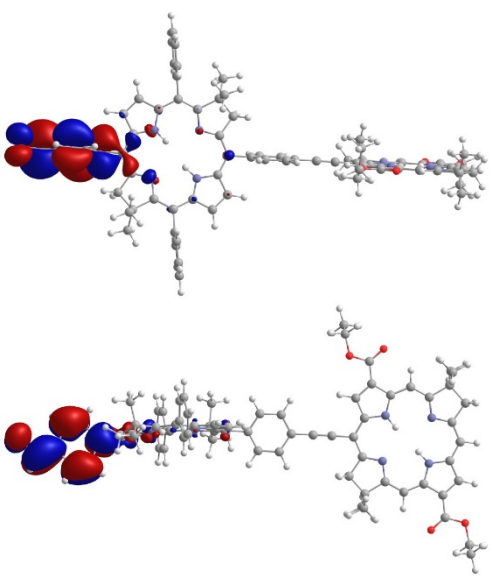
S7	0.20298		
S7	0.13555		

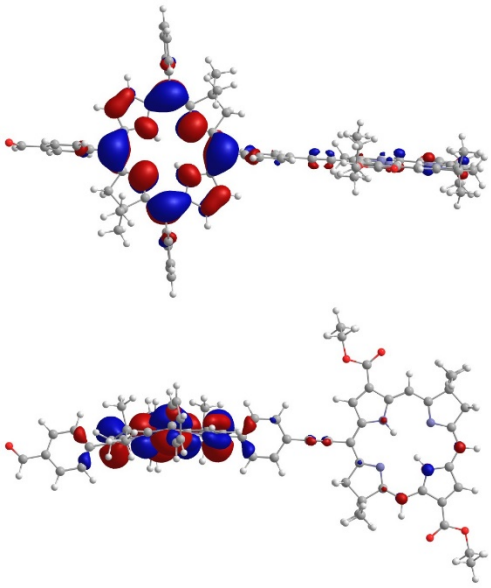
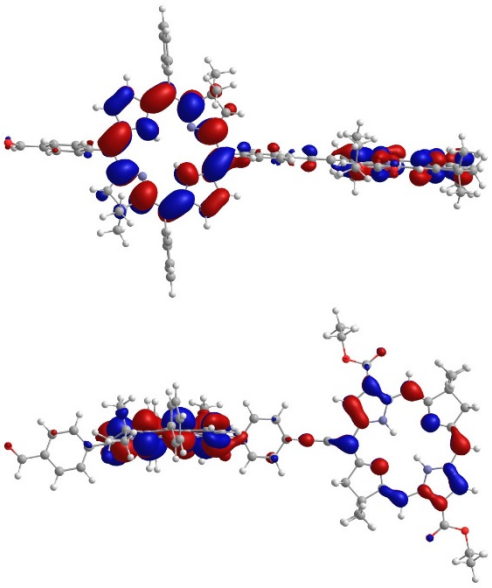
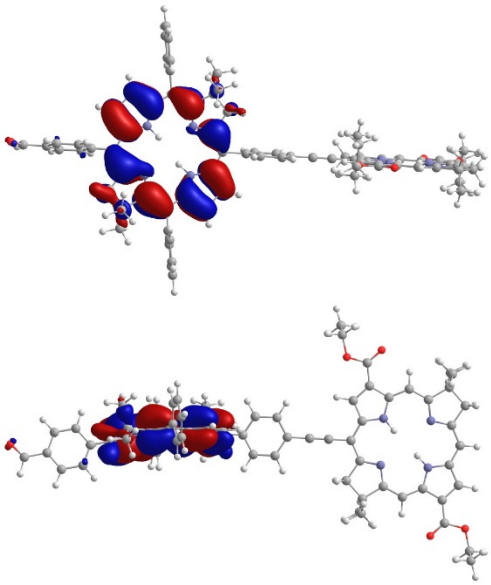
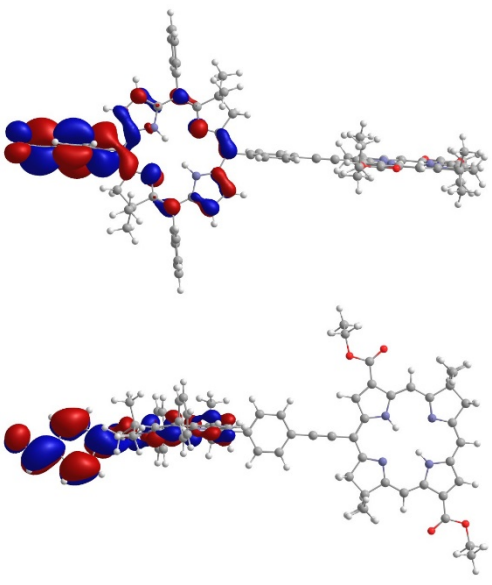
S8	0.61773		
S8	0.18409		

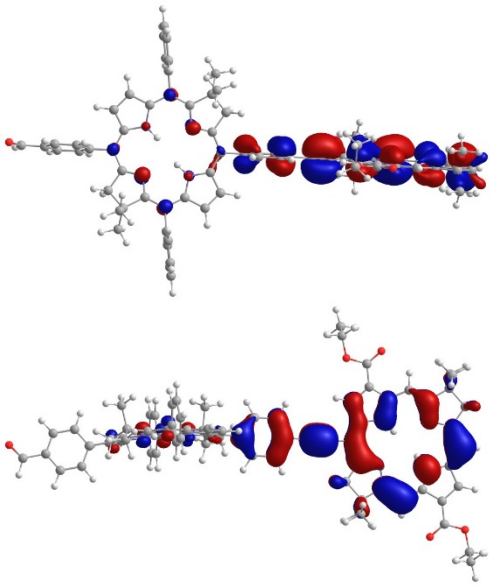
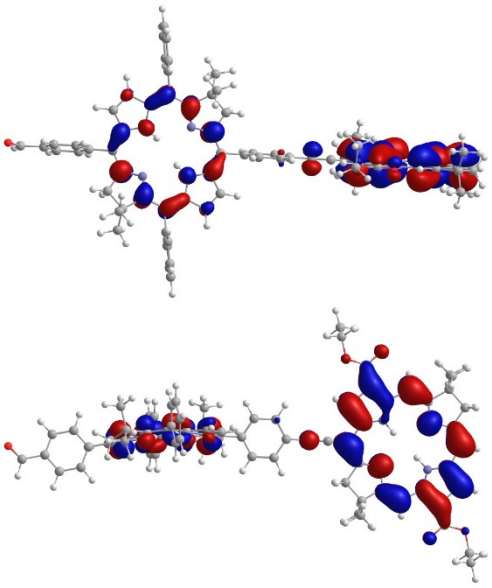
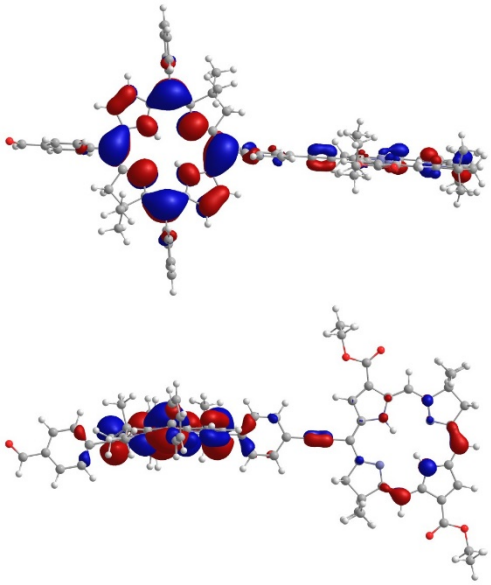
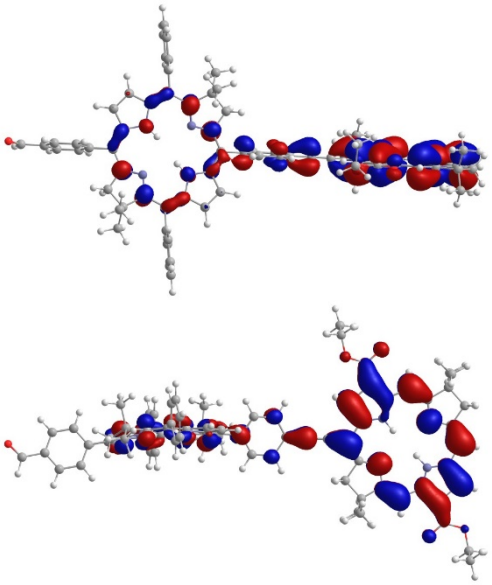
S8	0.16022		
S9	0.70387		

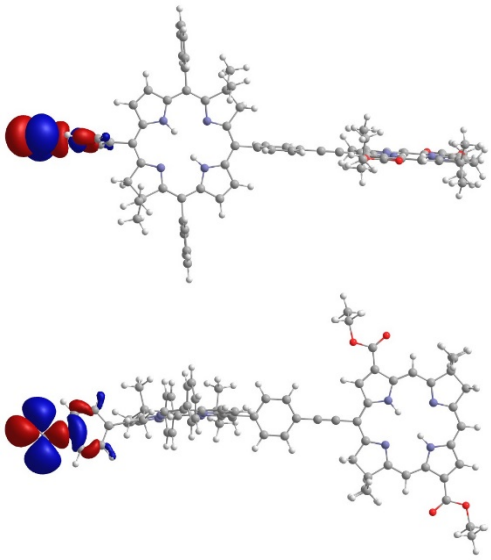
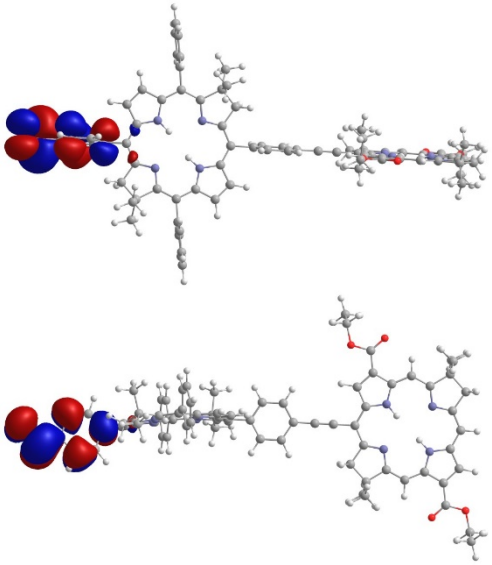
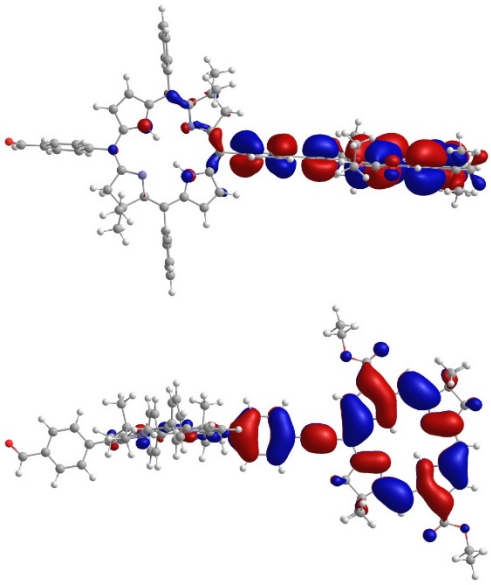
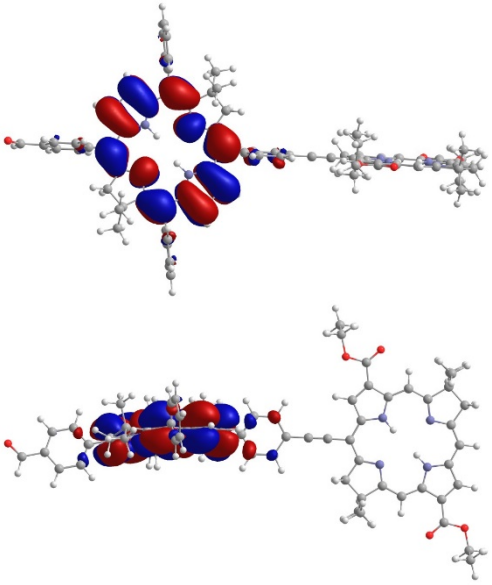
S9	0.24766		
S10	0.48904		

S10	0.33869		
S10	0.13770		

S11	0.61916		
S11	0.30218		

S12	0.57789		
S12	0.28568		

S12	0.12330		
S13	0.87583		

S14	0.99848		
S15	0.99317		

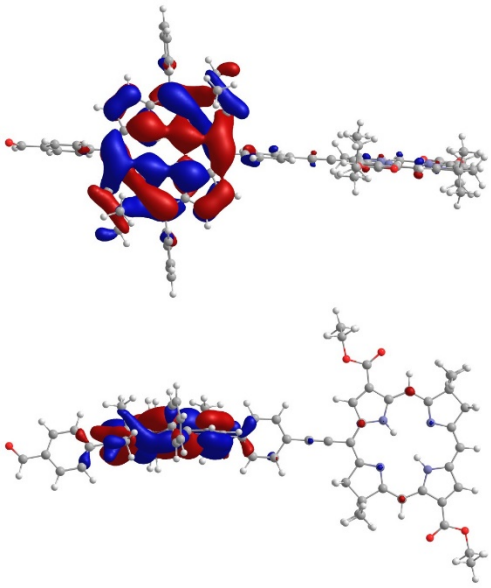
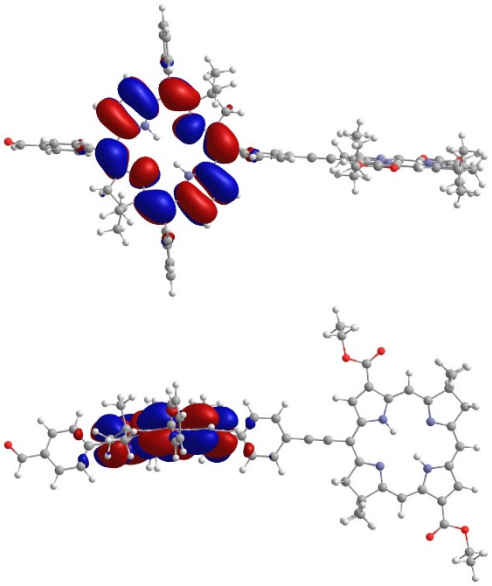
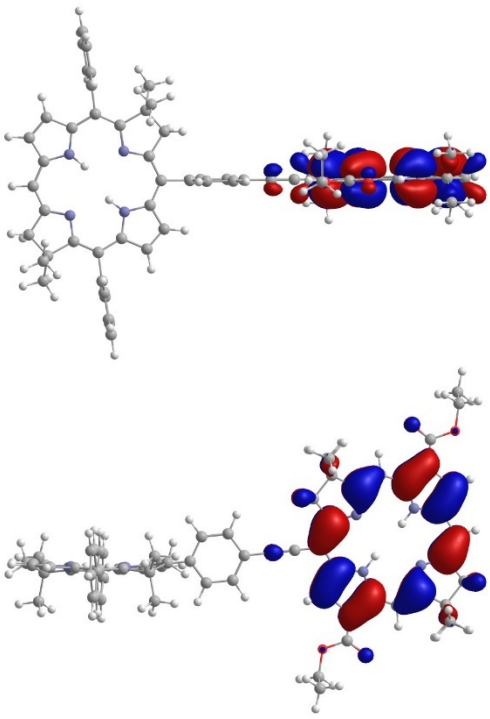
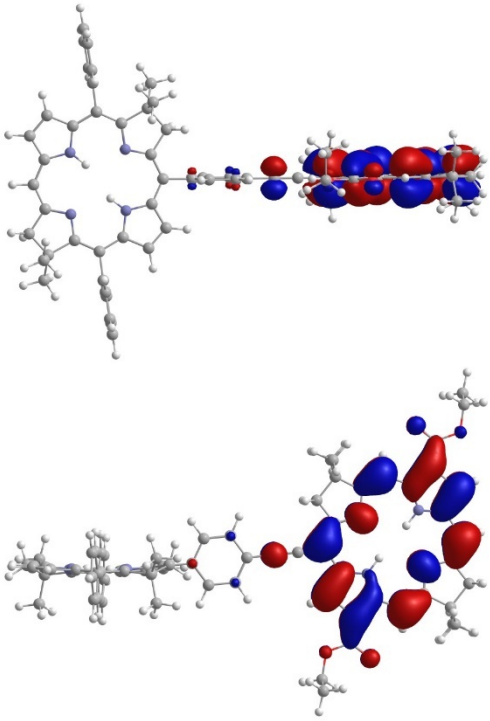
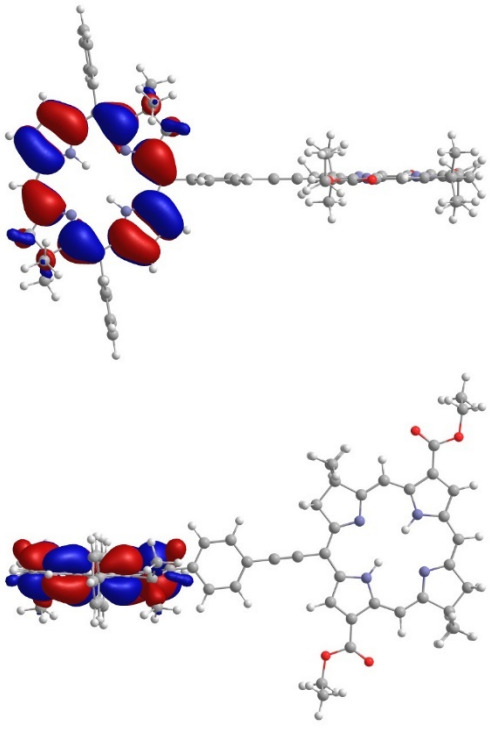
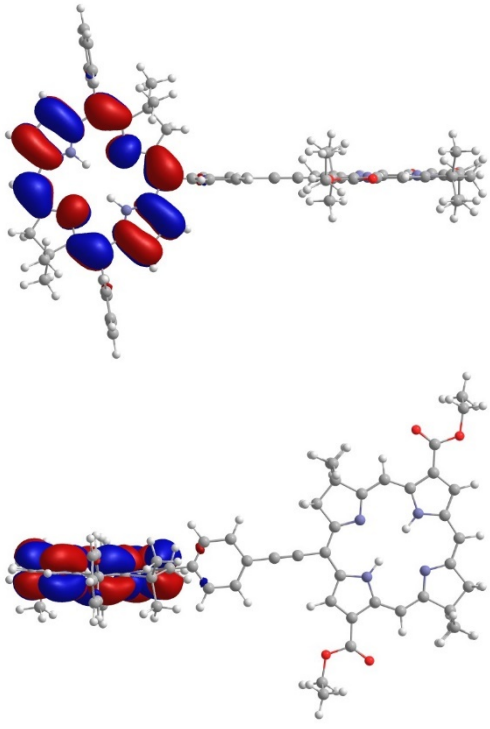
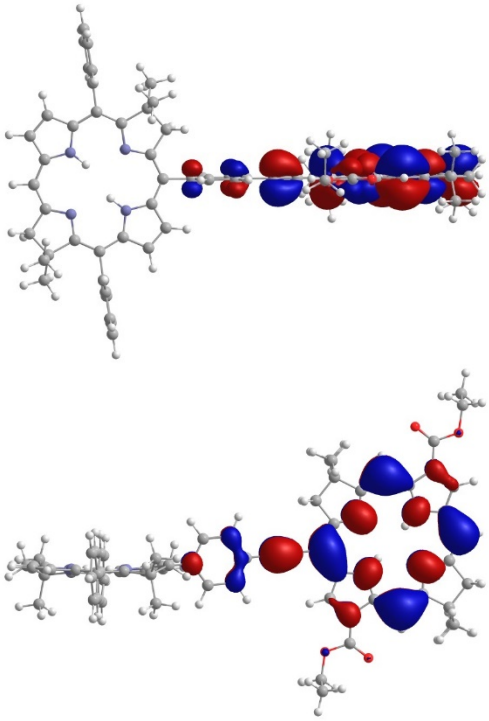
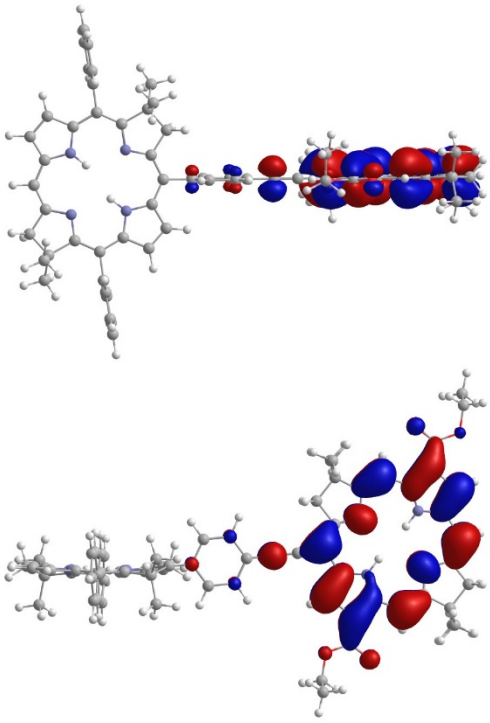
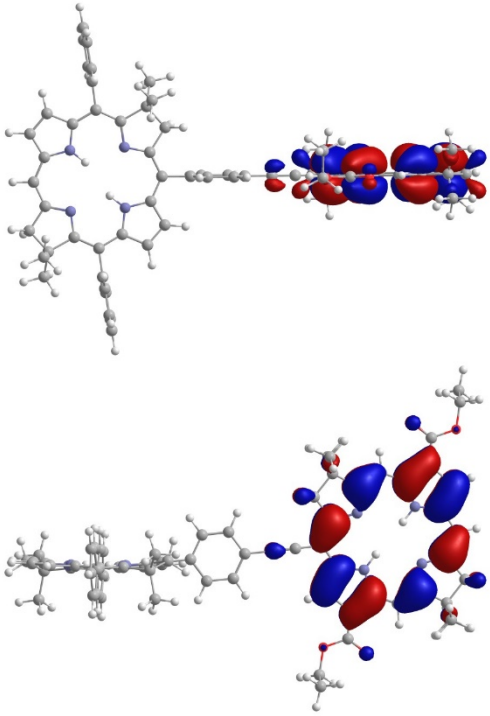
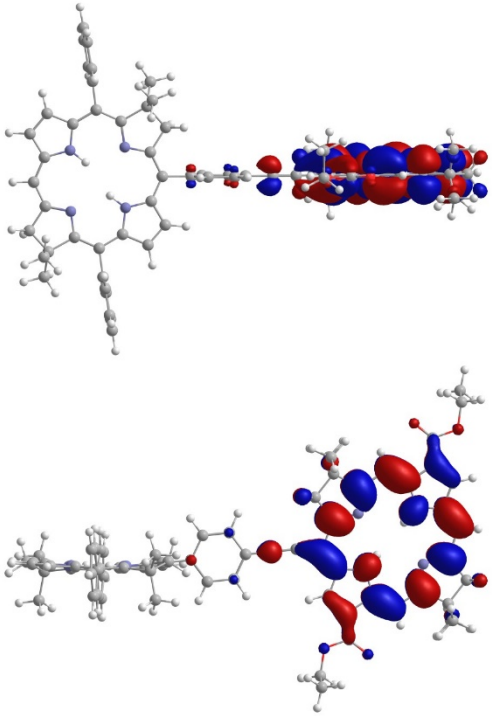
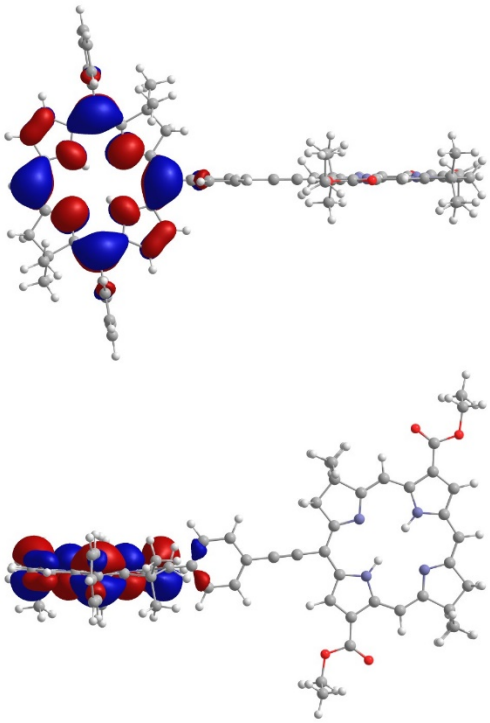
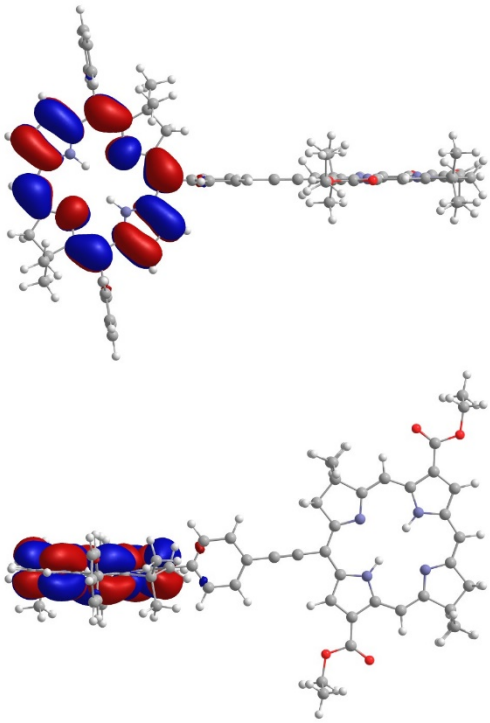
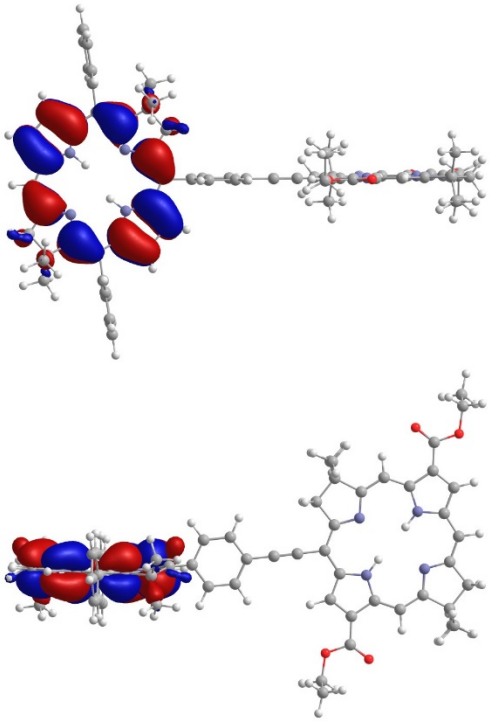
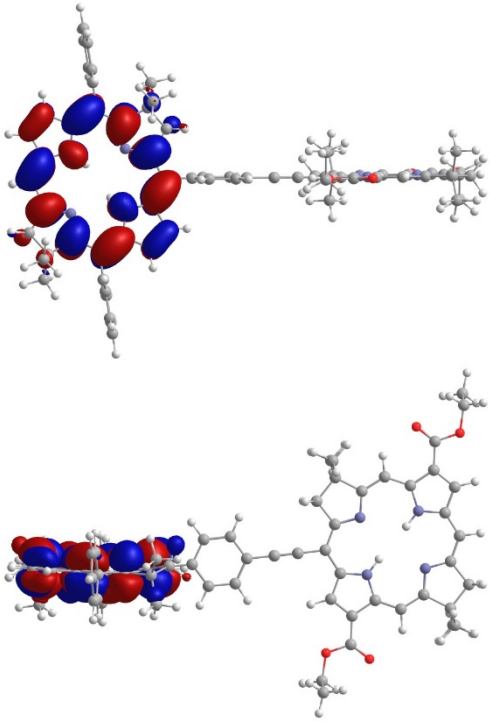
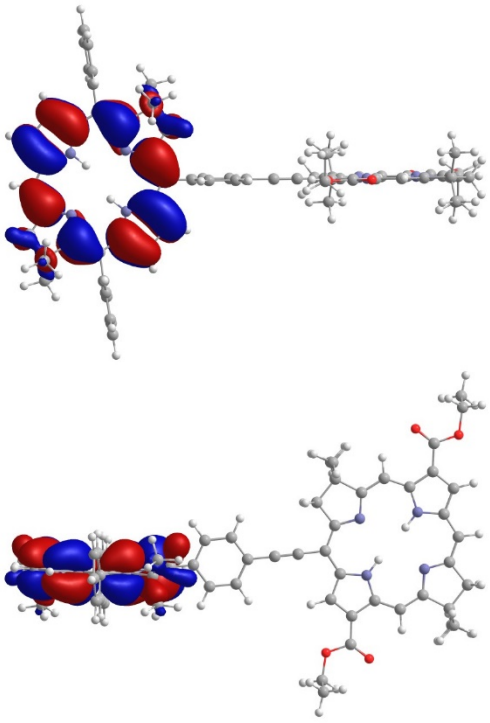
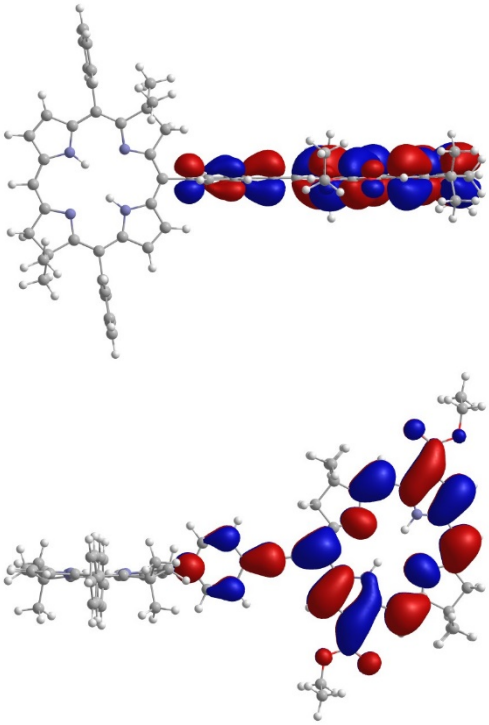
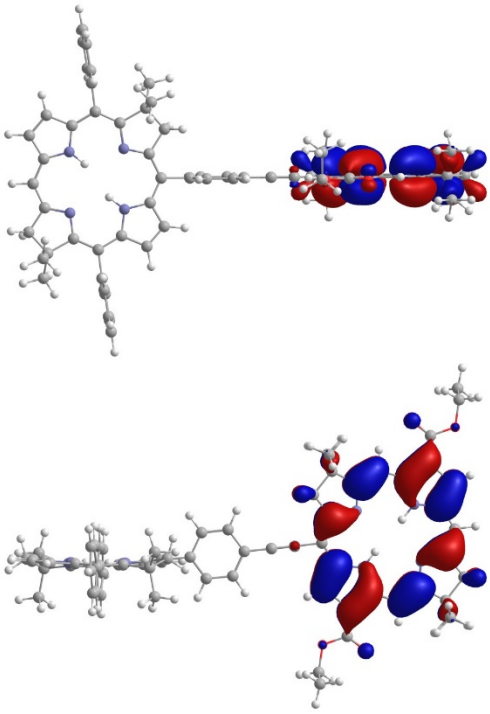
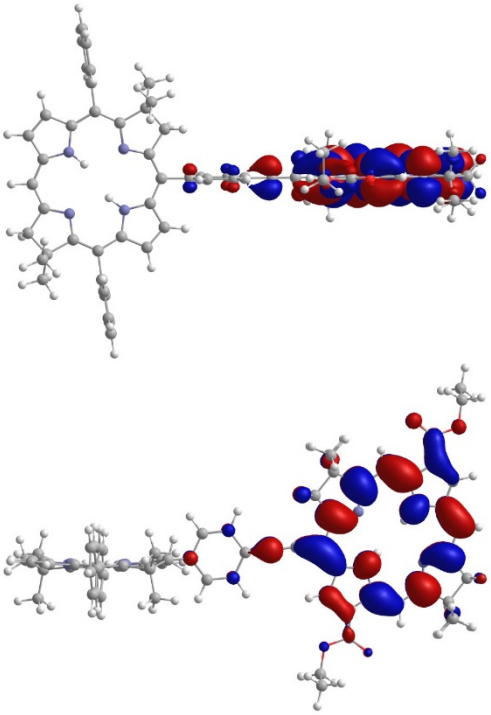
S16	0.95414		

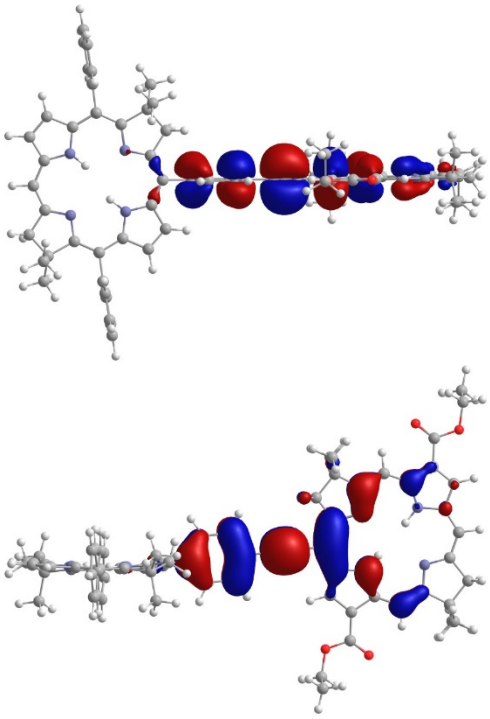
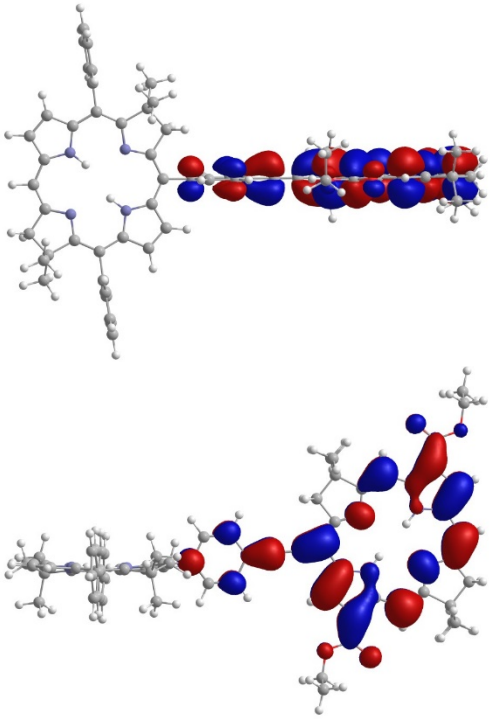
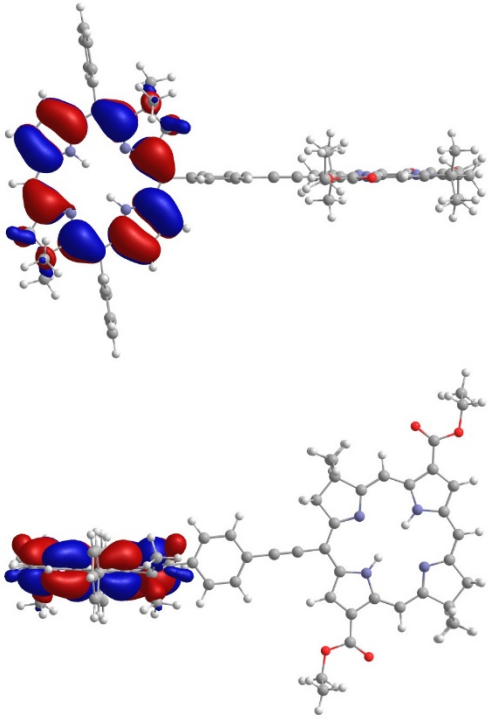
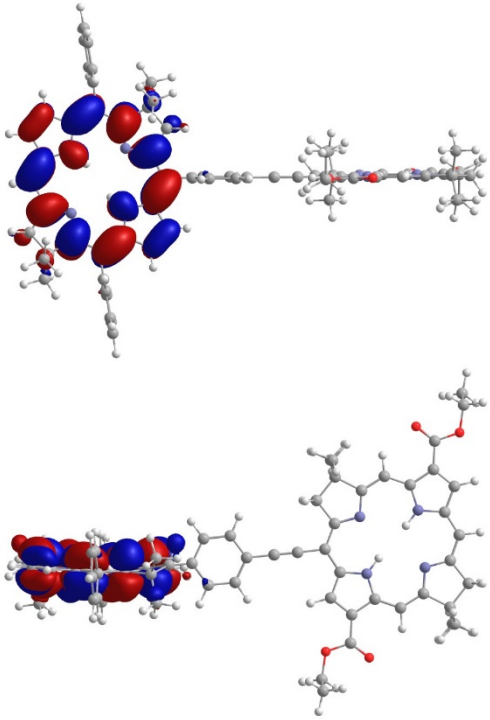
Table S28. NTOs for **Dyad-8**.

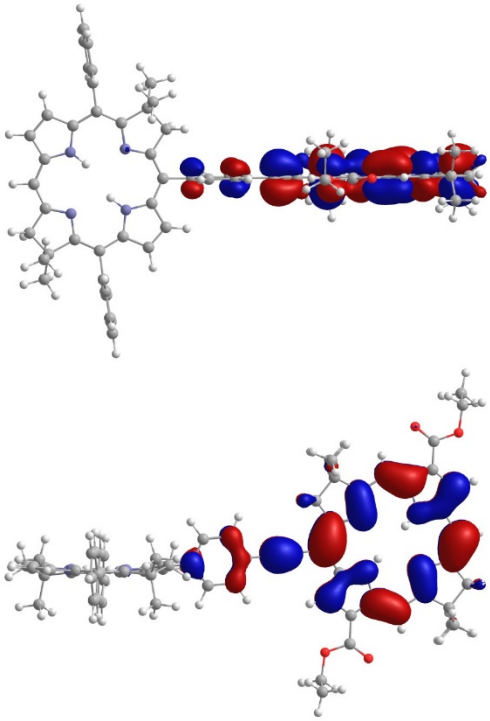
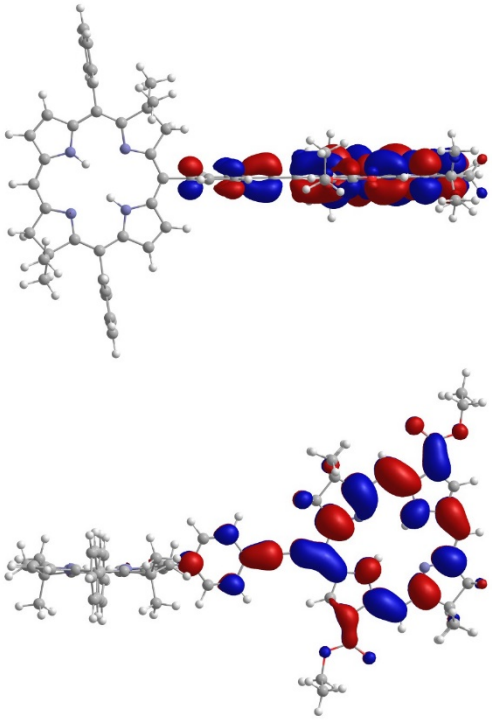
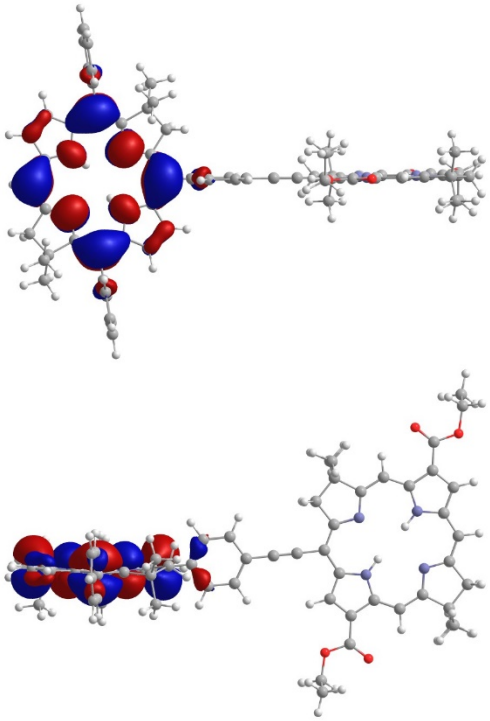
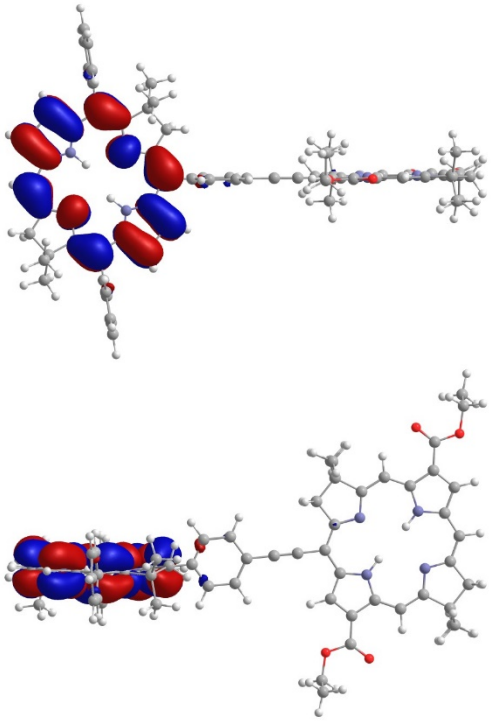
S#	Eigenvalue	From	To
S1	0.92686		
S2	0.91091		

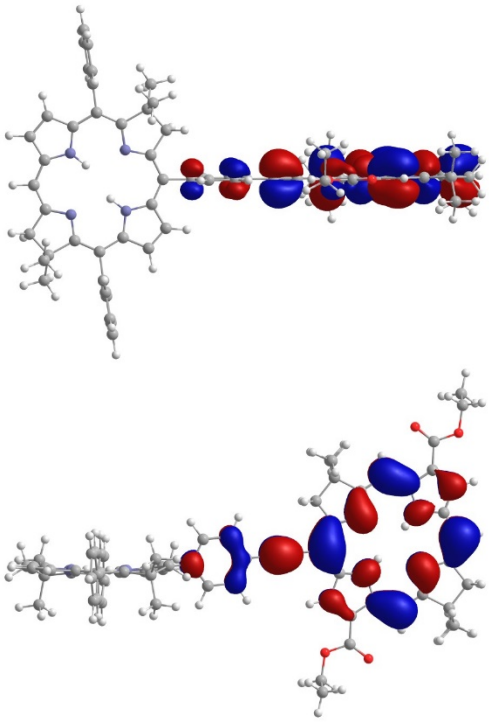
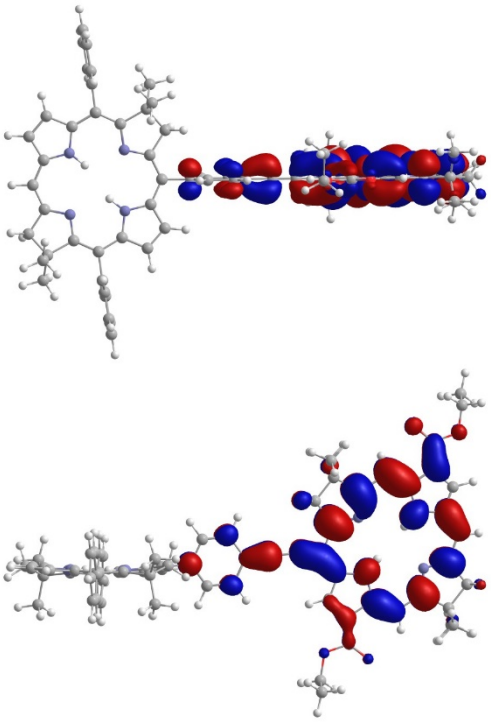
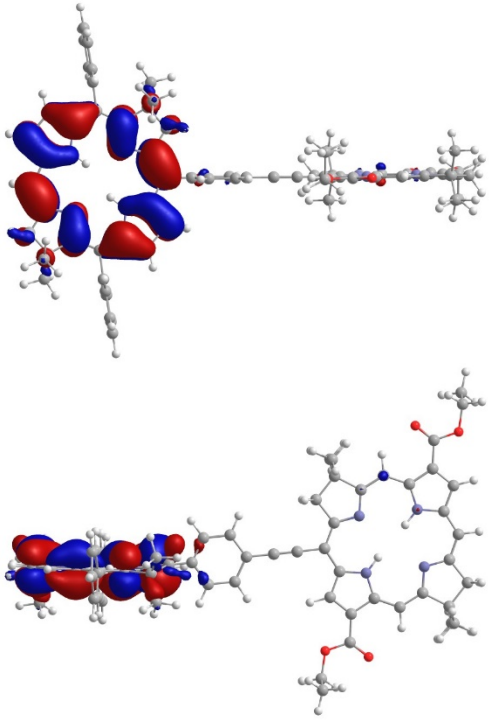
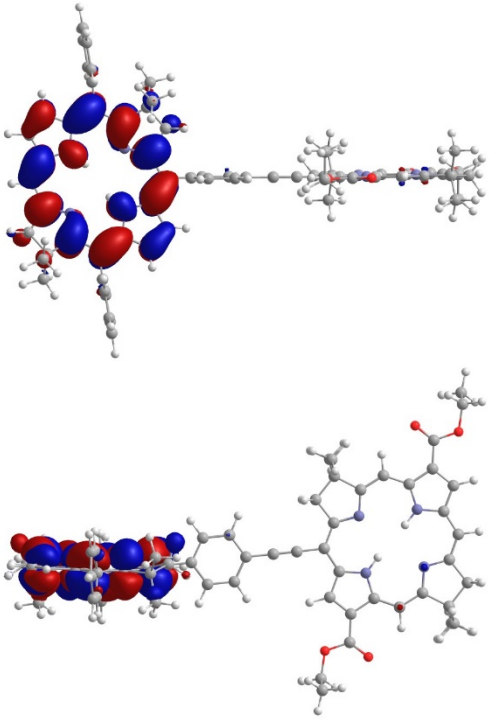
S3	0.88135		
S3	0.11134		

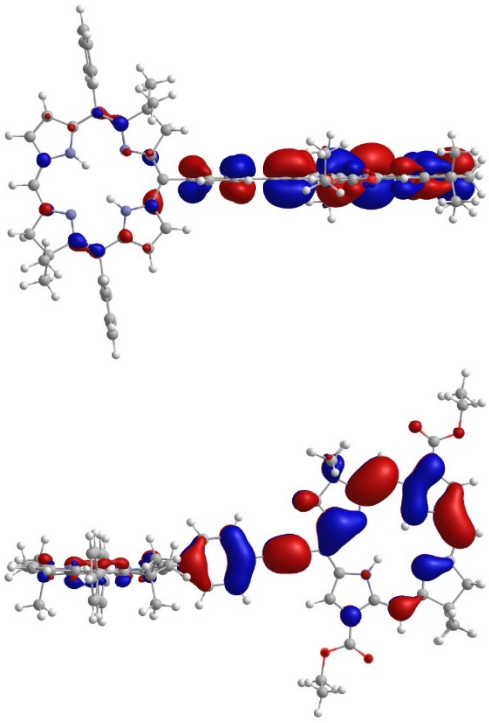
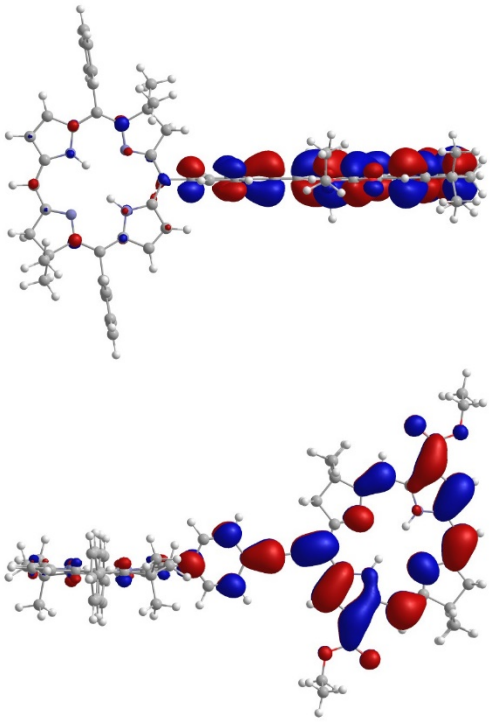
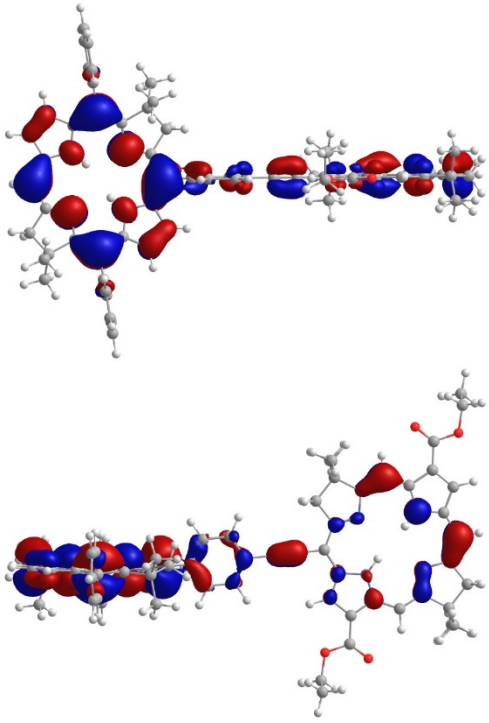
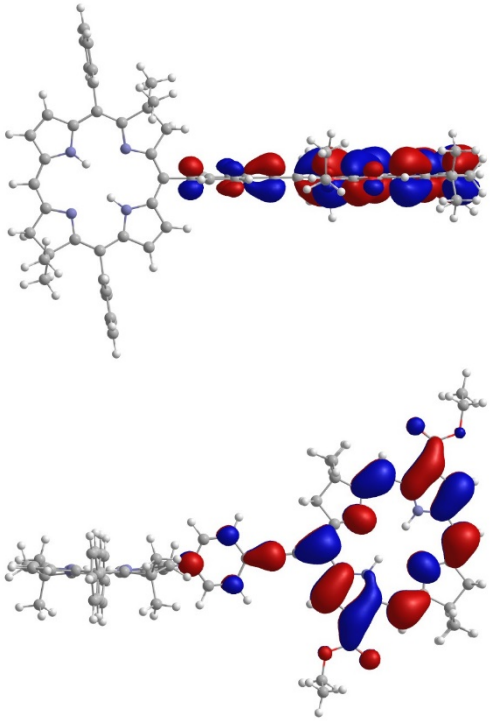
S4	0.79935		
S4	0.19970		

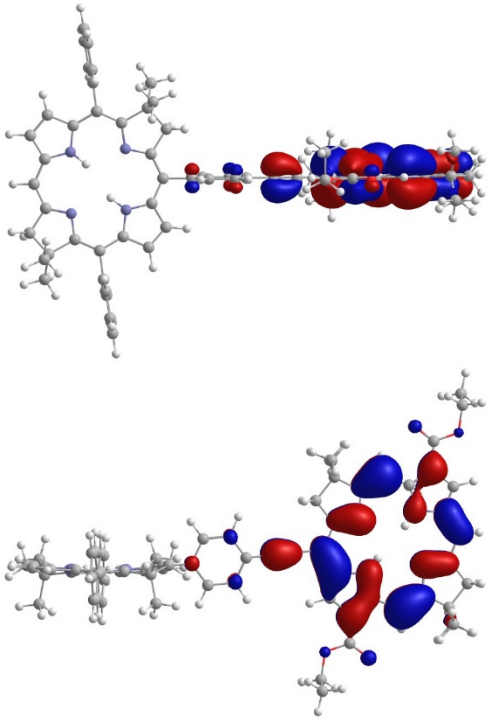
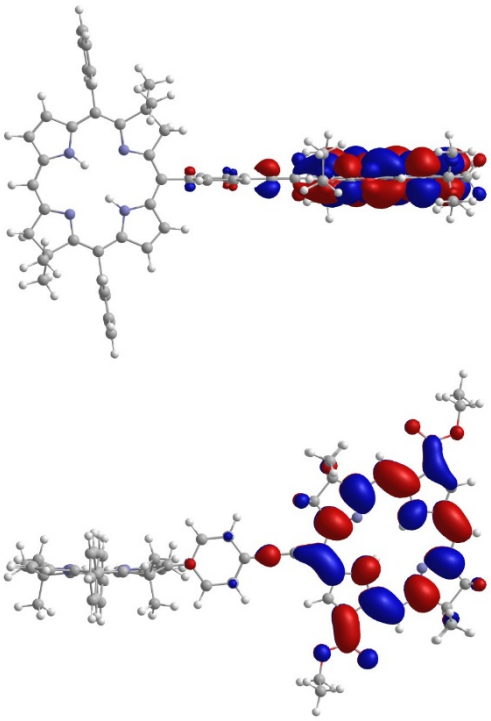
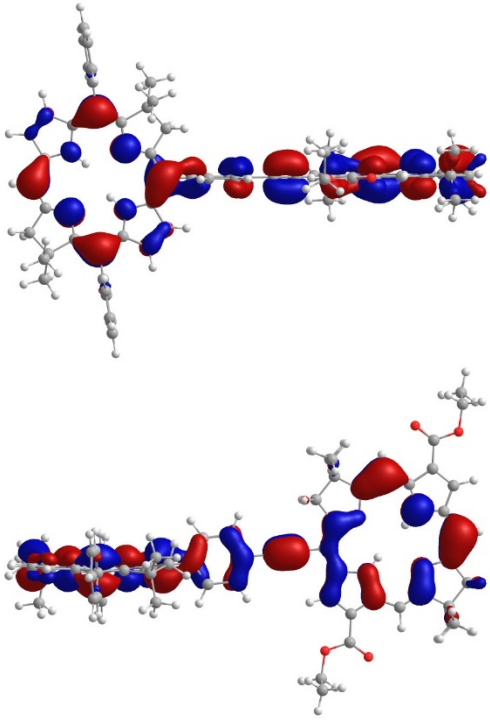
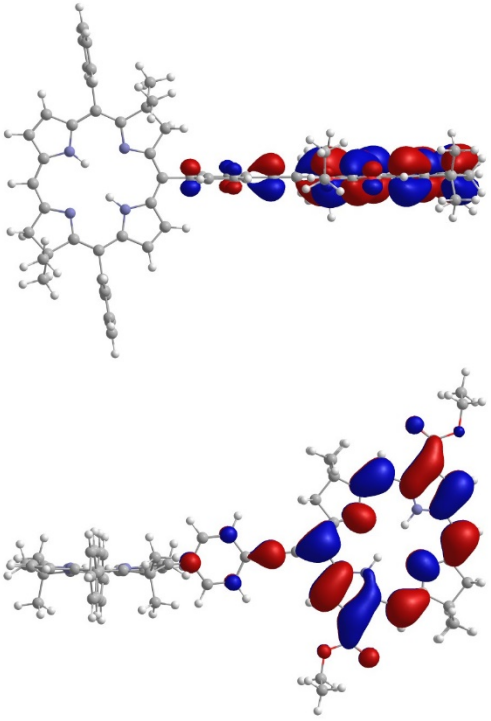
S5	0.99886		
S6	0.70455		

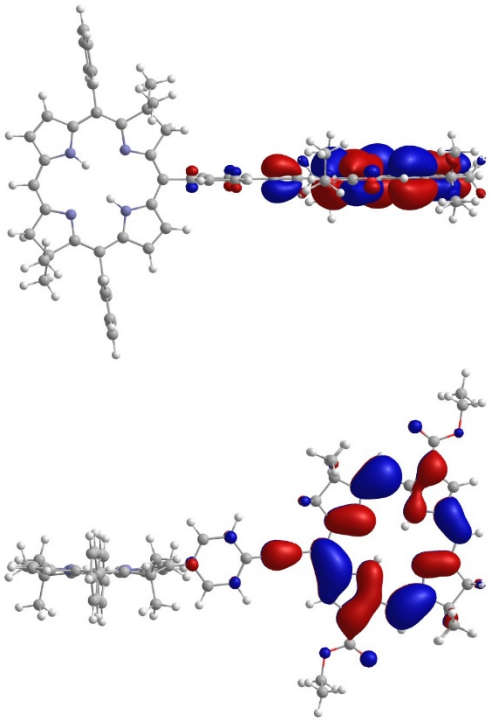
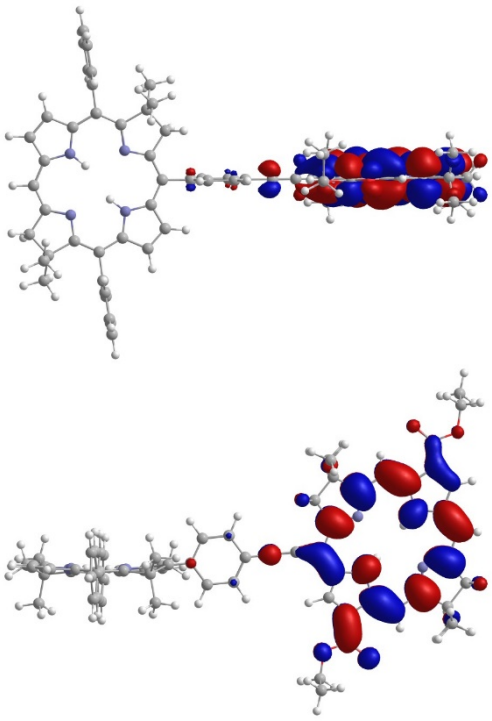
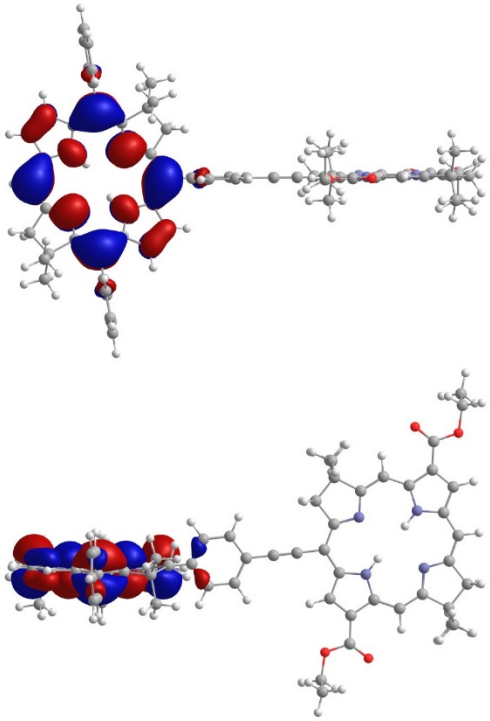
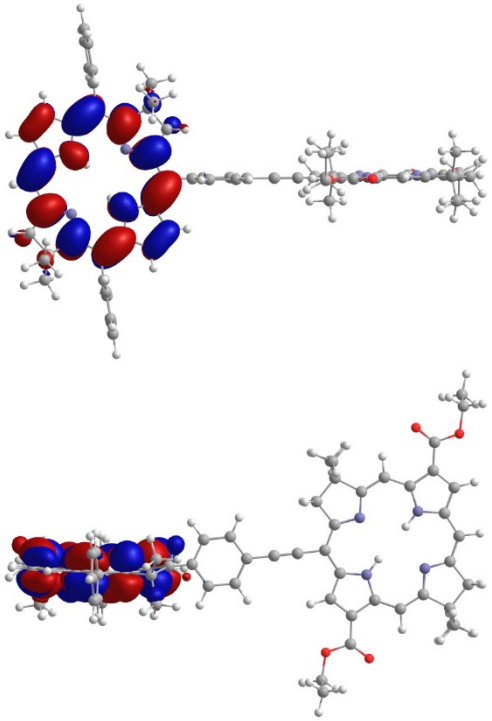
S6	0.25327		
S7	0.59143		

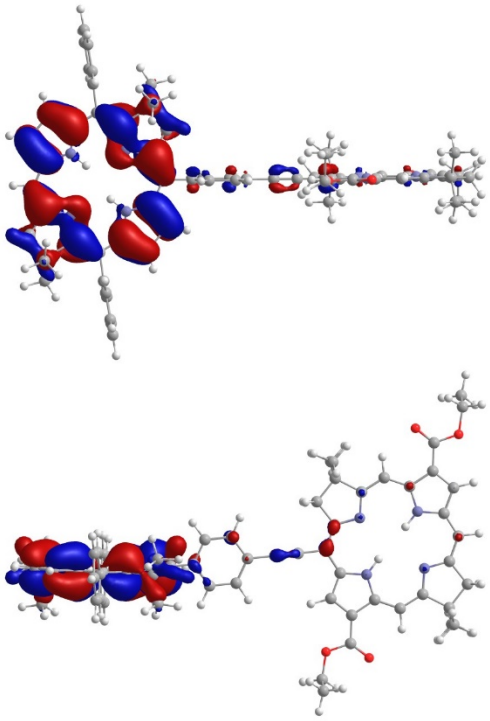
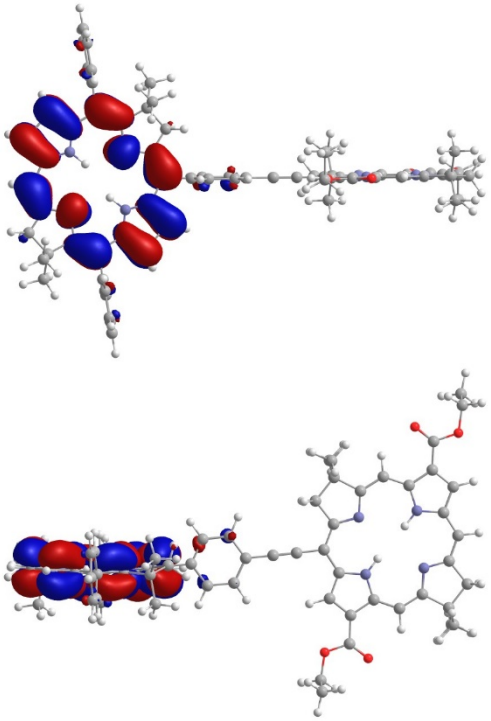
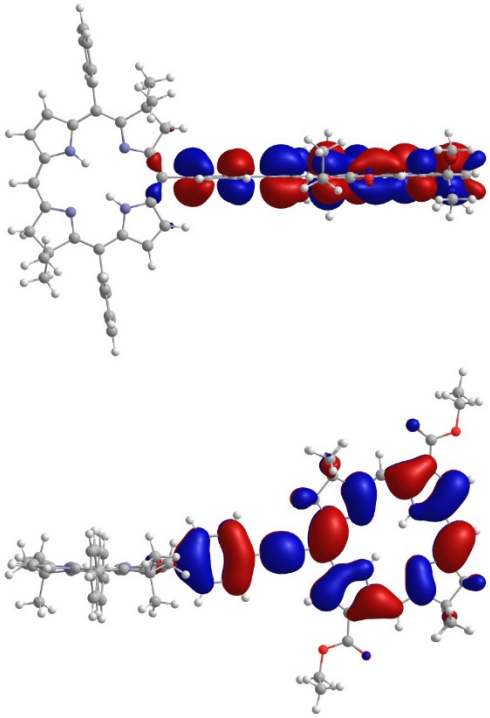
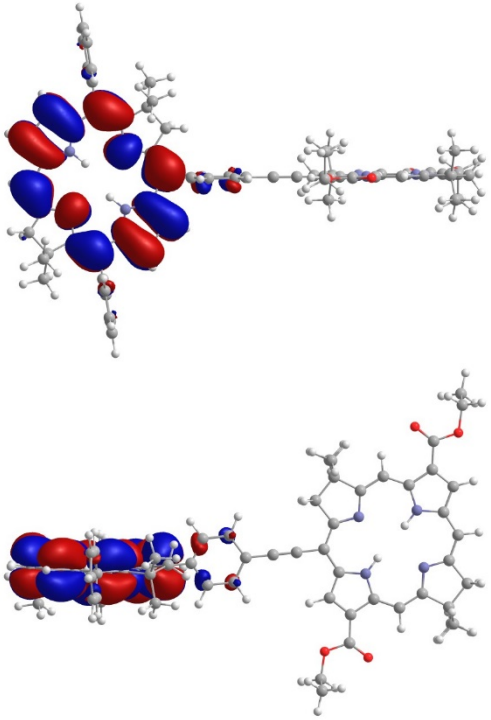
S7	0.23383		
S7	0.14471		

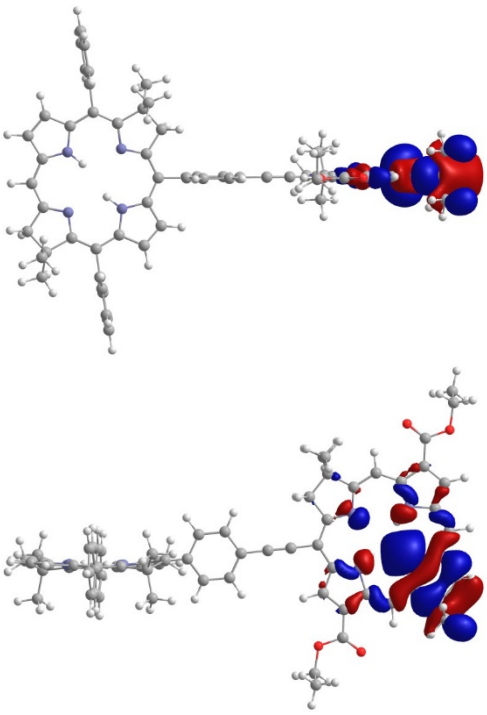
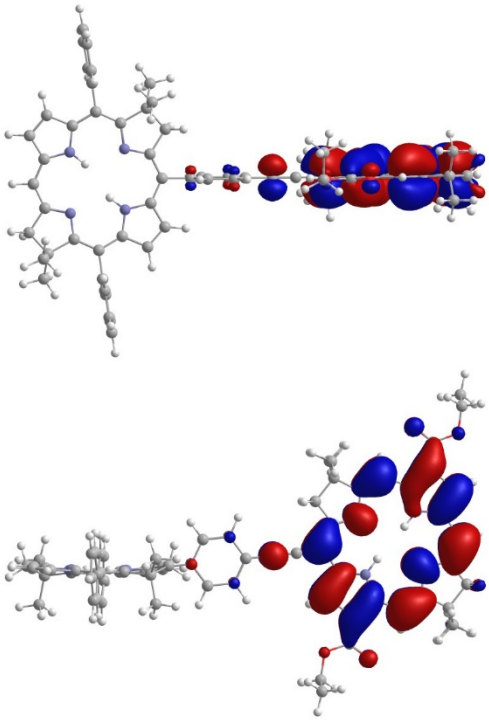
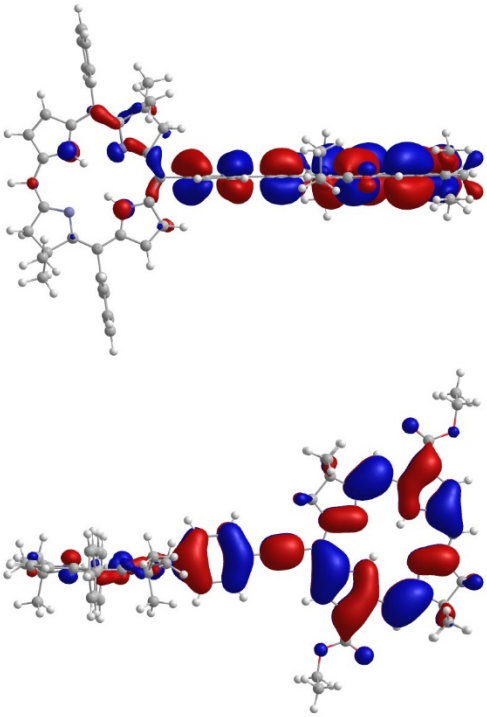
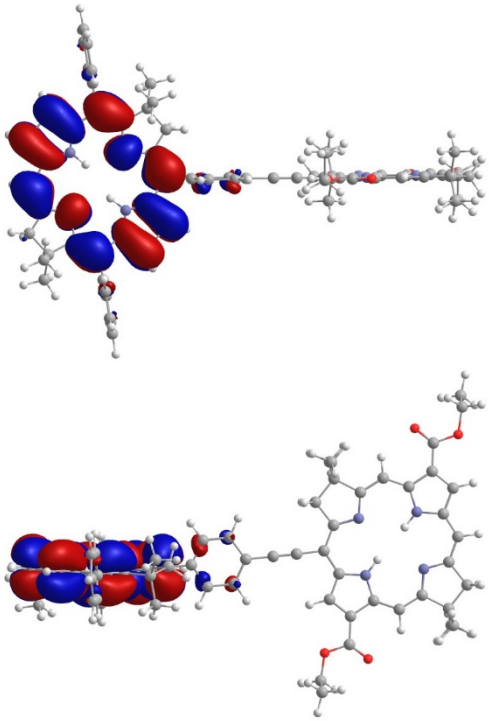
S8	0.57139		
S8	0.21407		

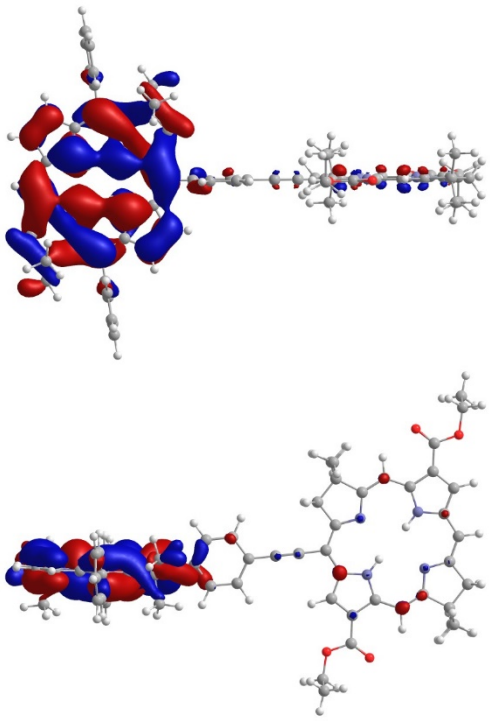
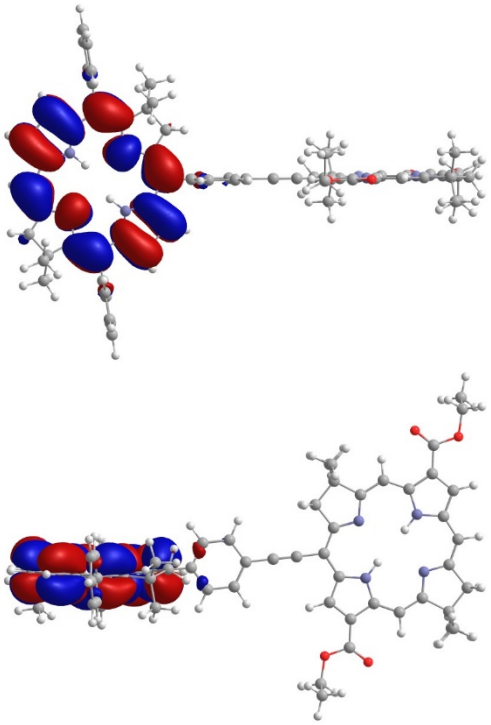
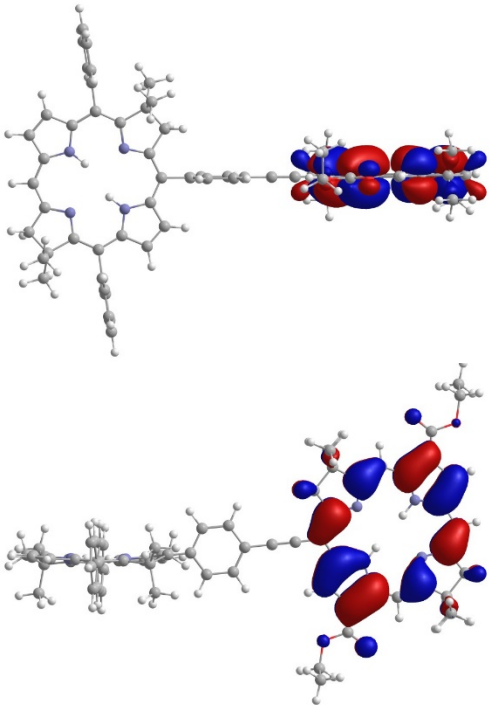
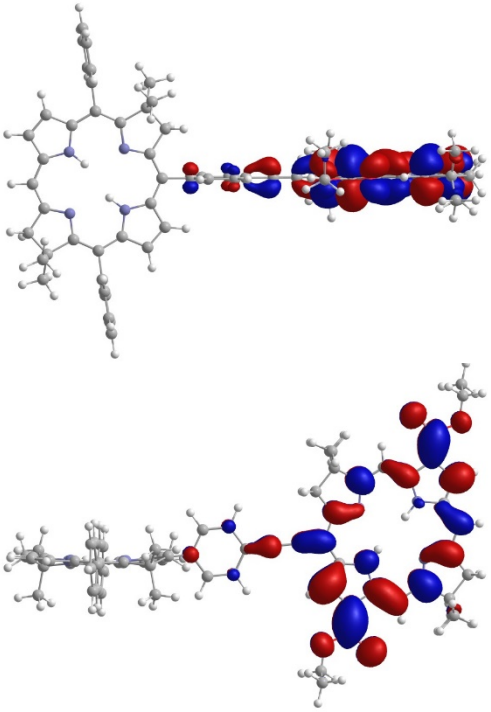
S8	0.16403		
S9	0.85246		

S9	0.13323		
S10	0.83004		

S10	0.15226		
S11	0.86842		

S11	0.10714		
S12	0.99148		

S13	0.99679		
S14	0.99227		

S15	0.94307		
S16	0.56318		

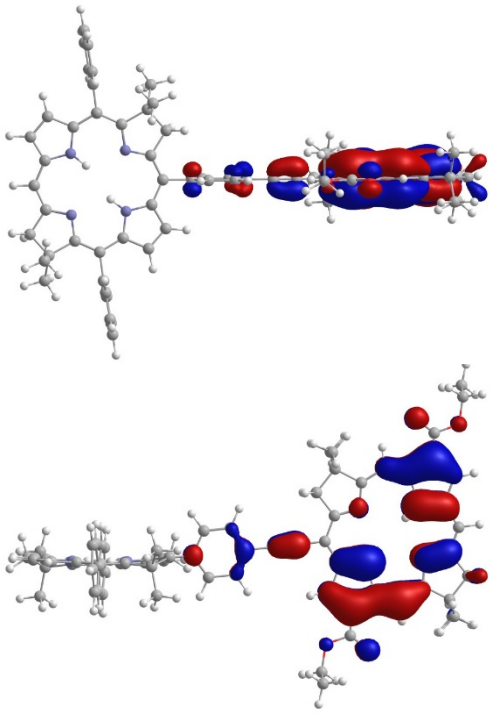
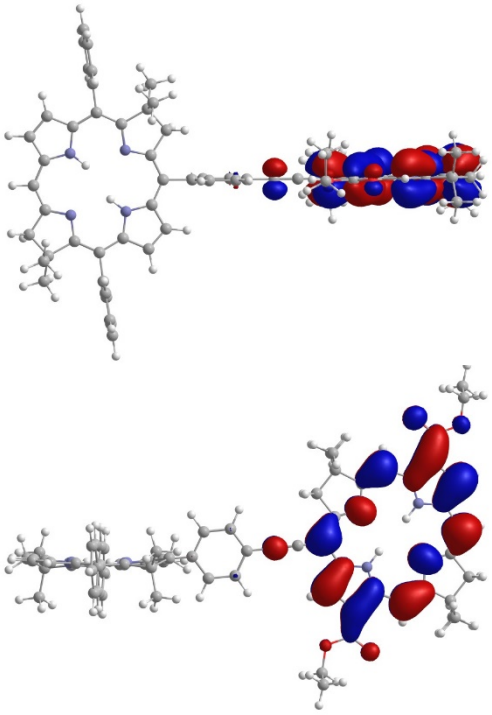
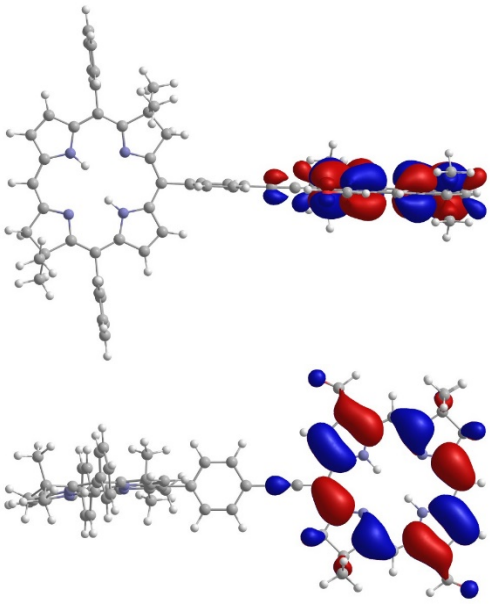
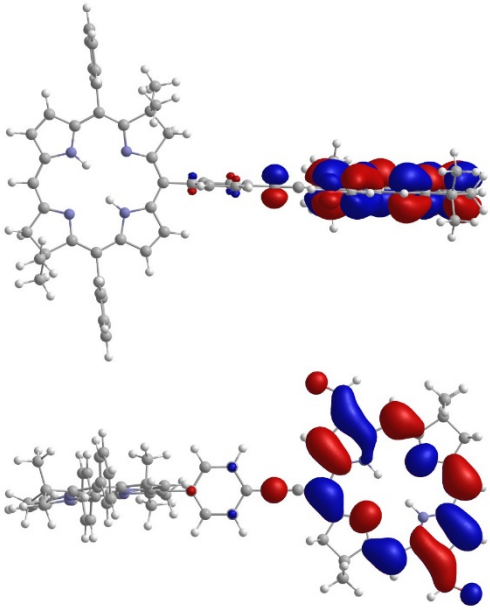
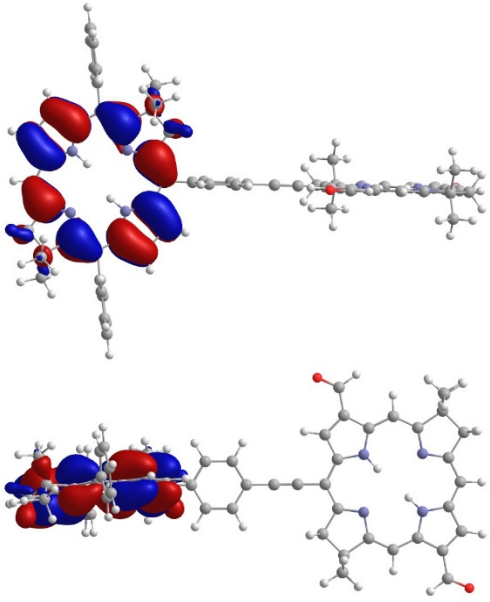
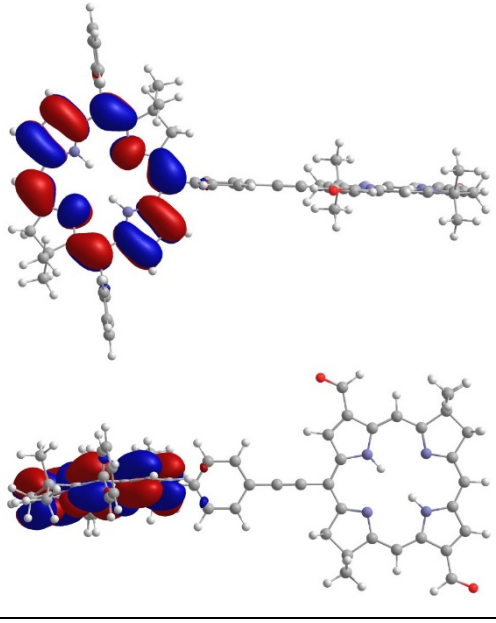
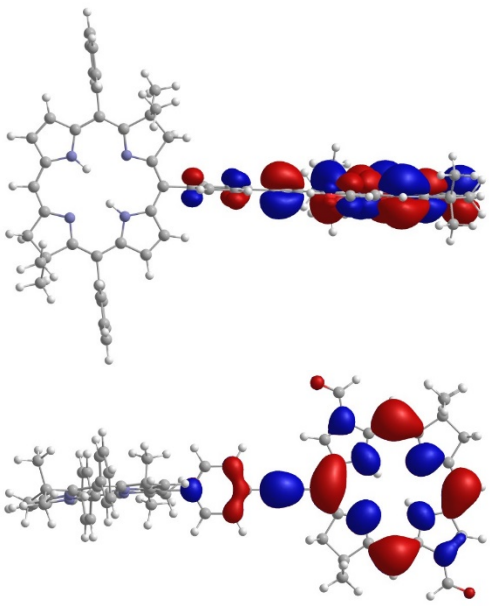
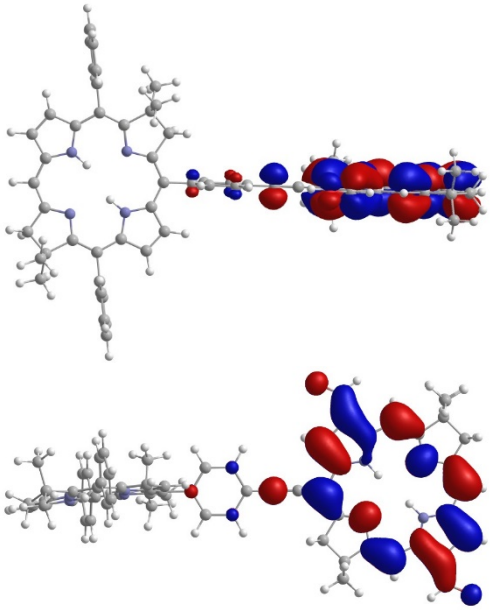
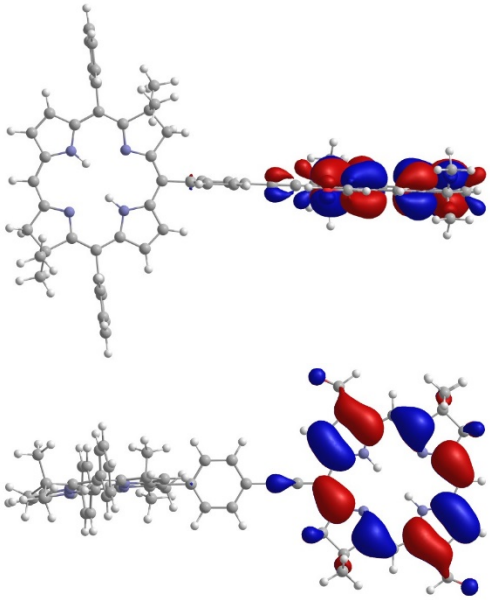
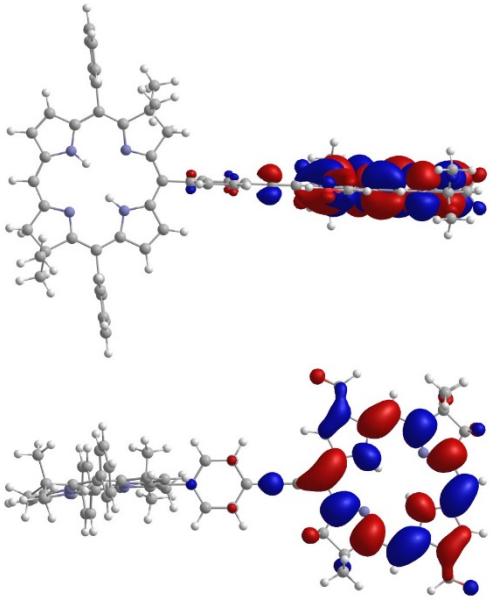
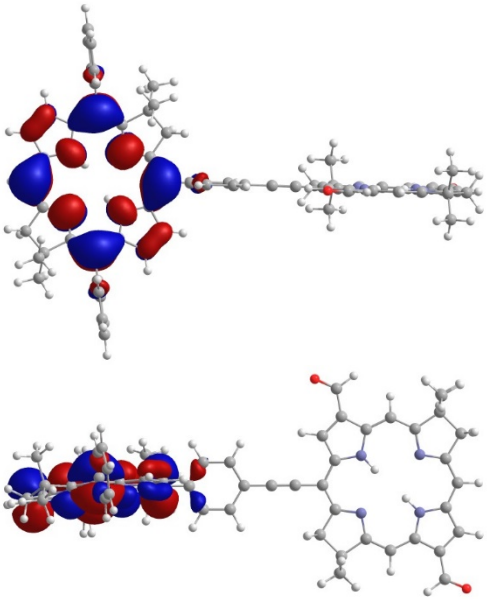
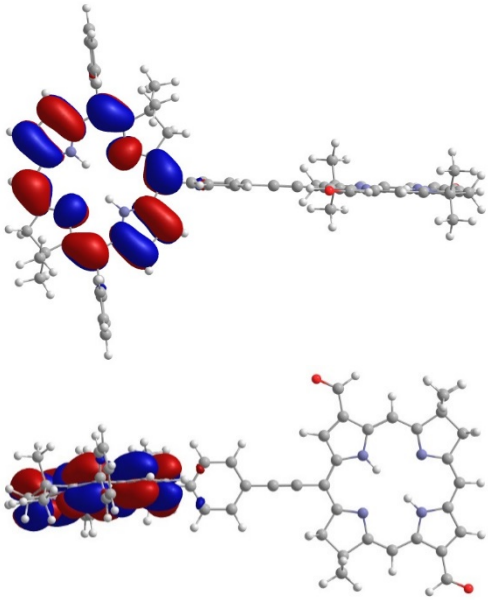
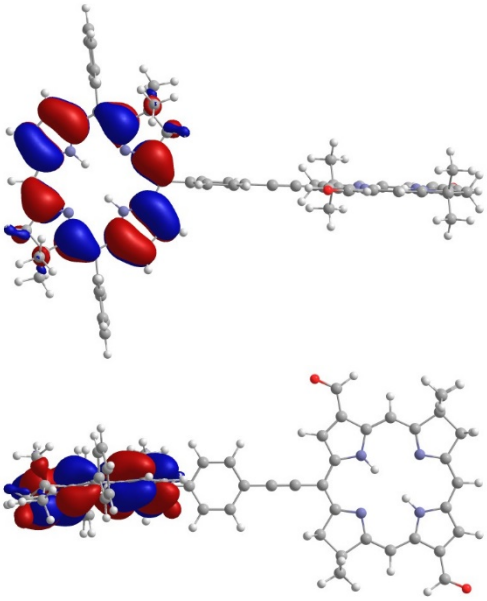
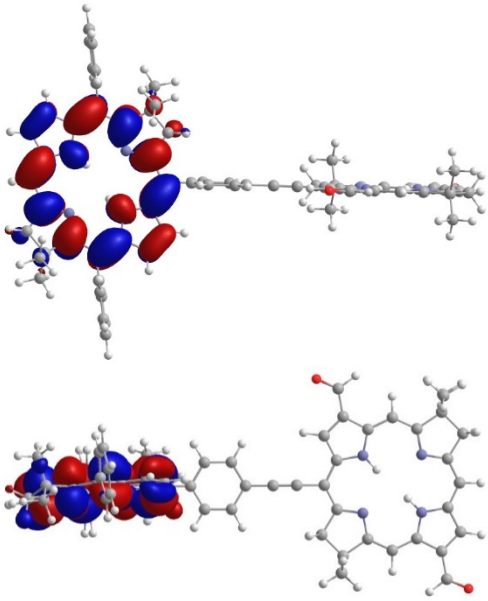
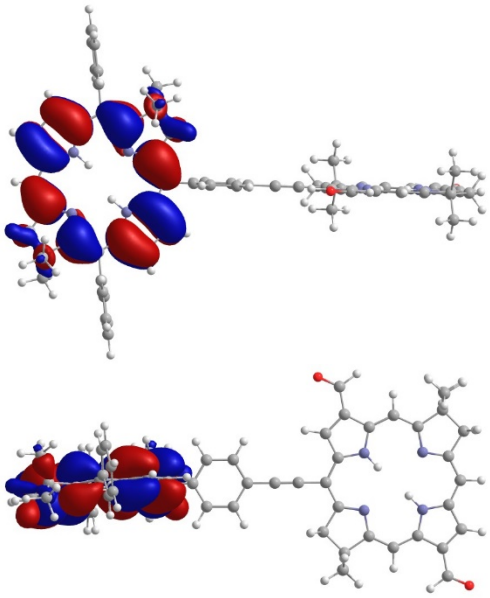
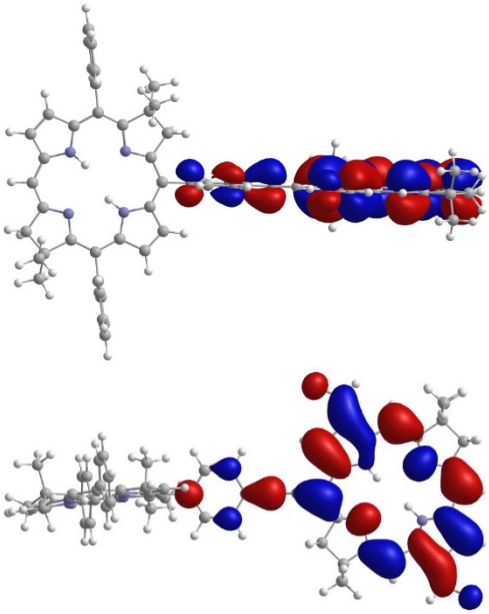
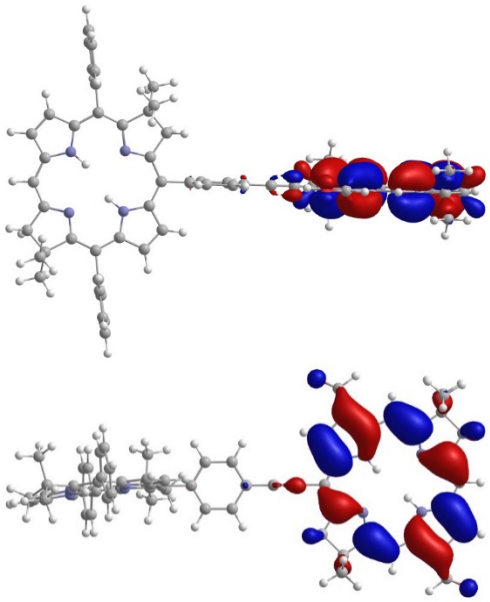
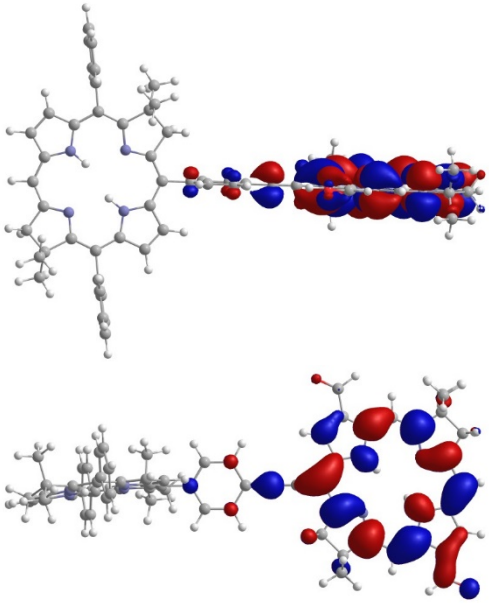
S16	0.40568		

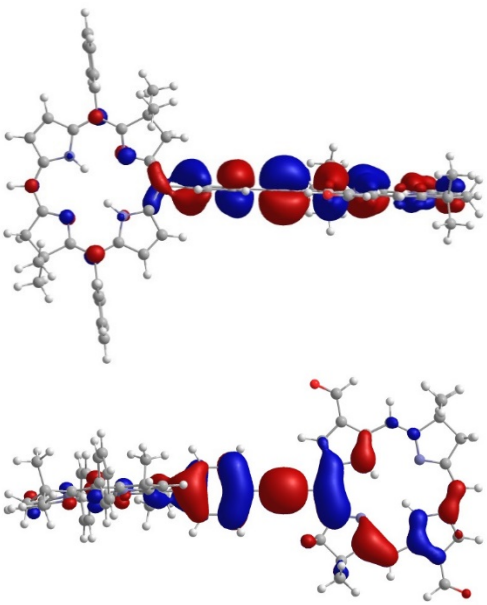
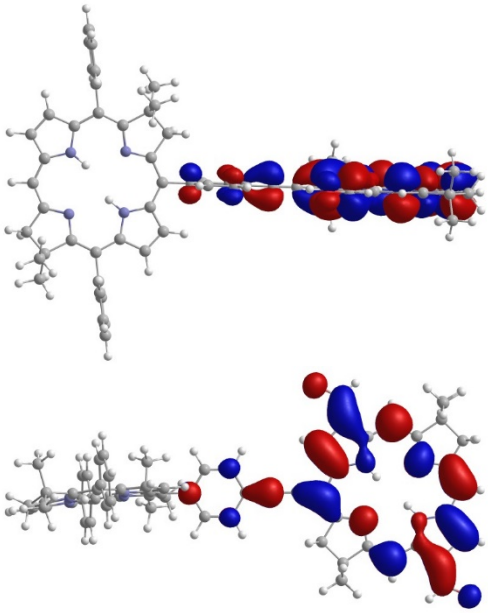
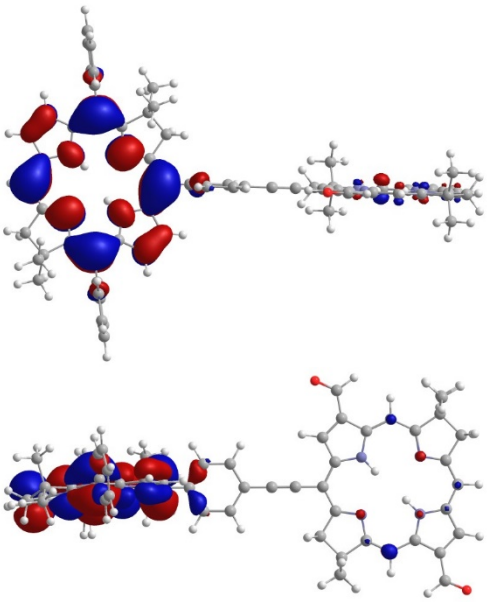
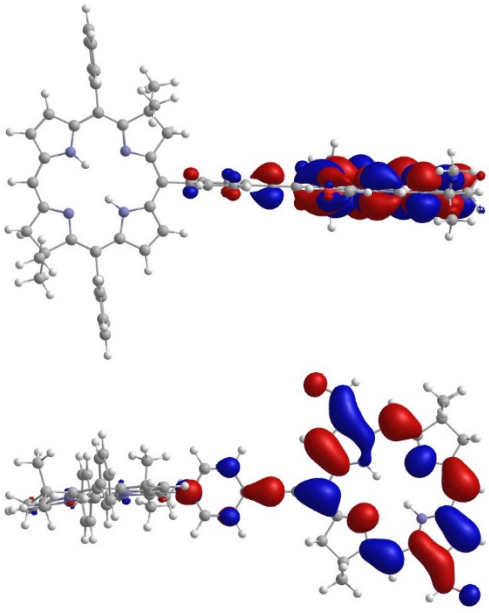
Table S29. NTOs for **Dyad-9**.

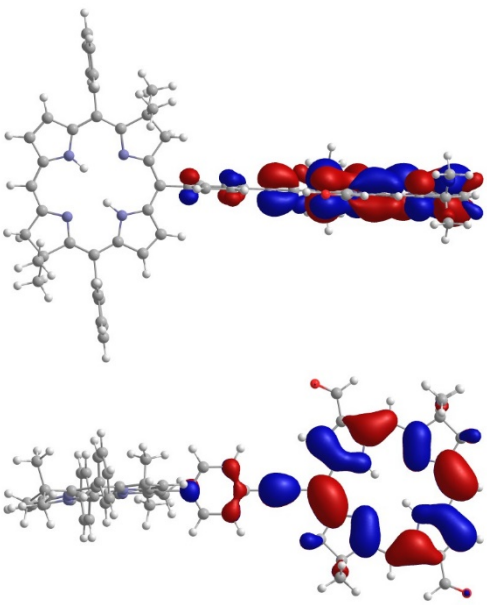
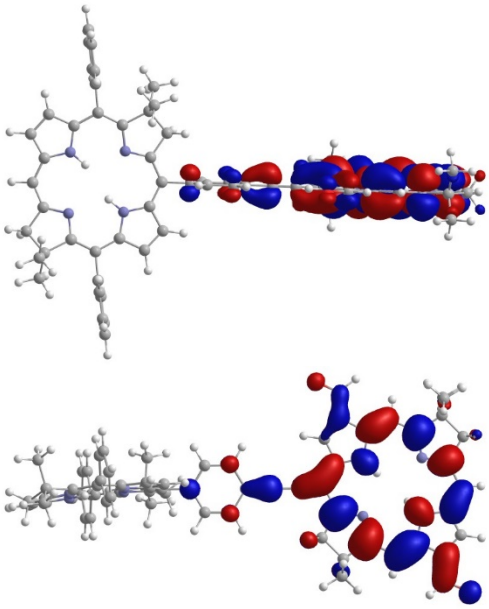
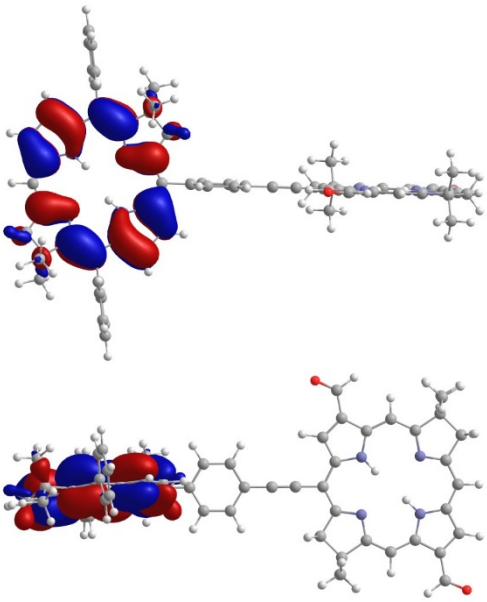
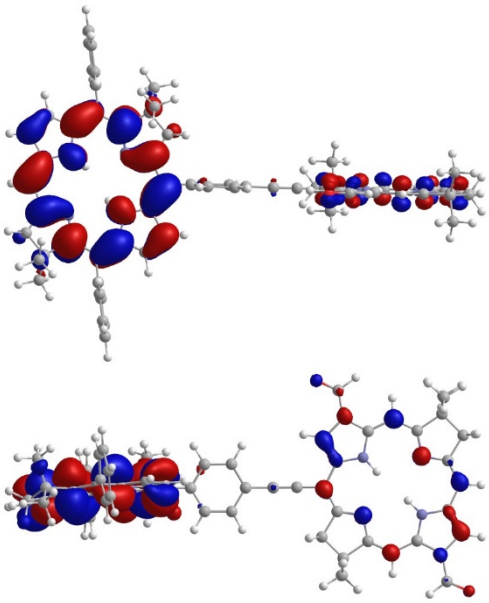
S#	Eigenvalue	From	To
S1	0.93060		
S2	0.91095		

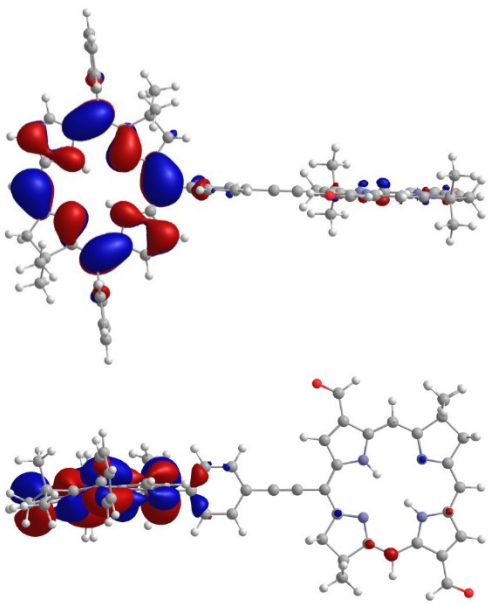
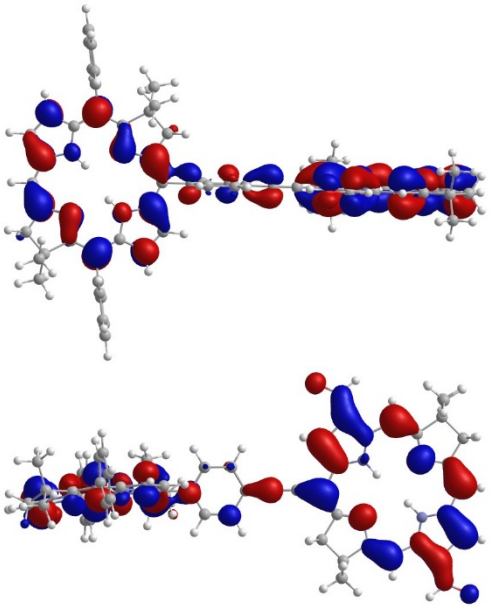
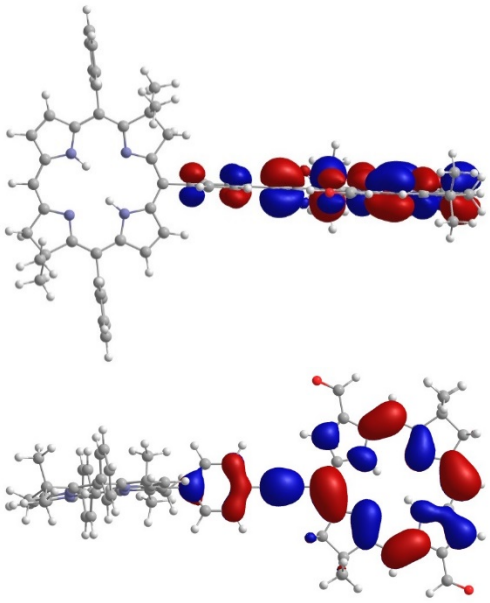
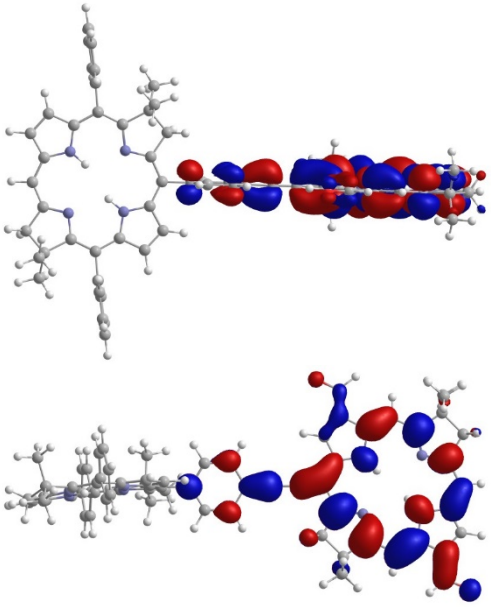
S3	0.89222		
S3	0.10050		

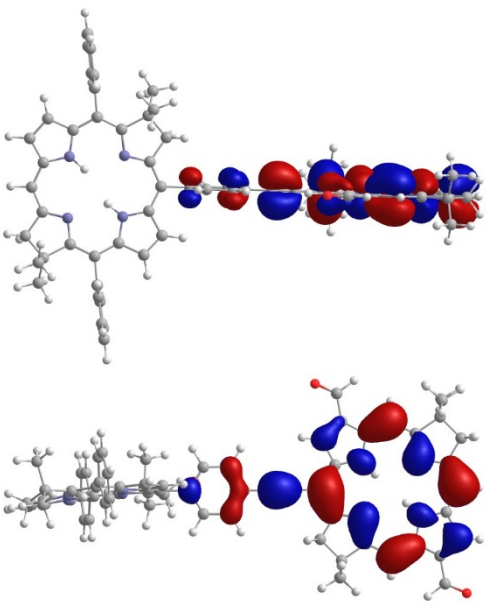
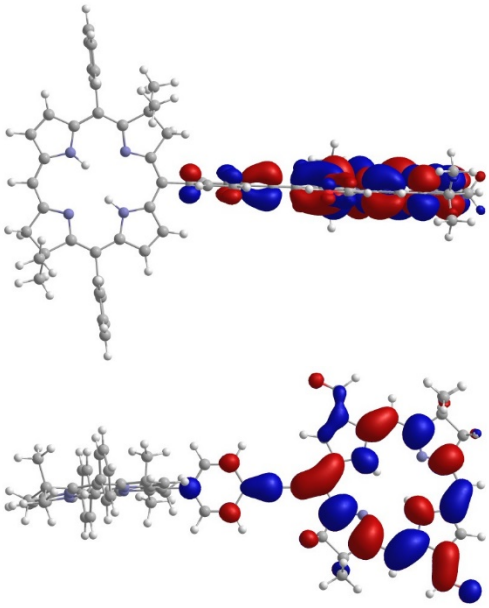
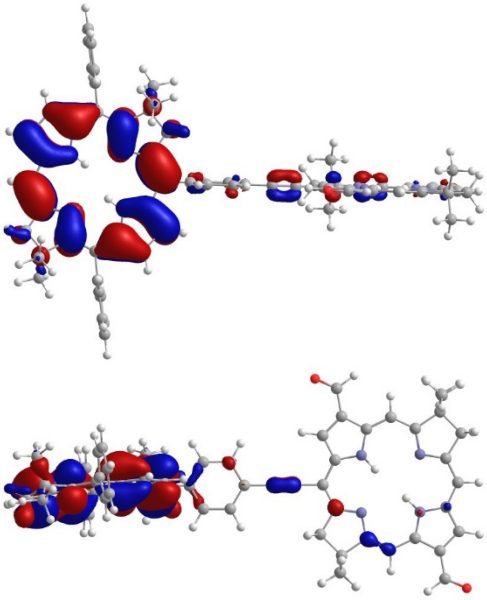
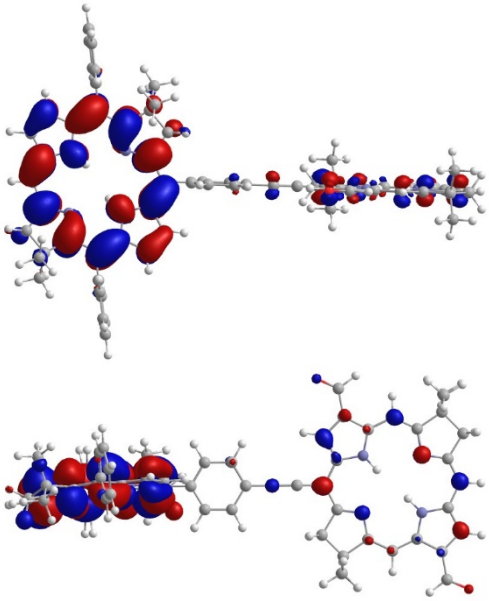
S4	0.79966		
S4	0.20006		

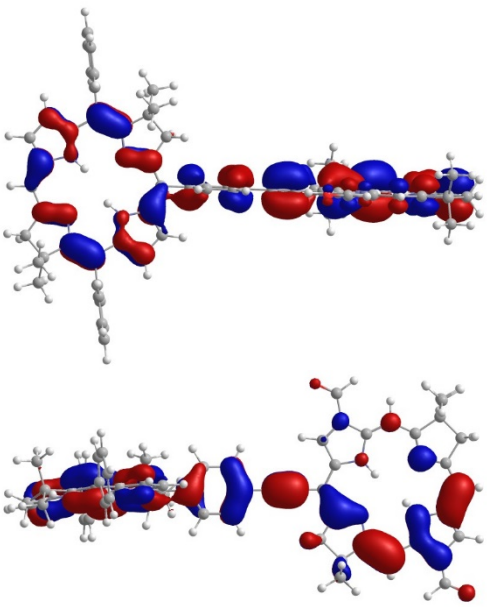
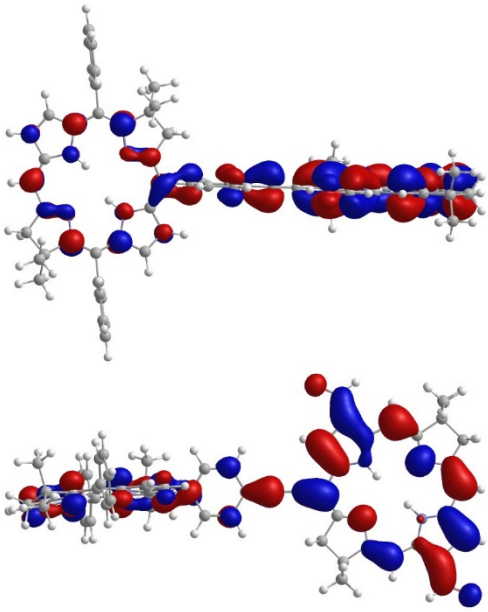
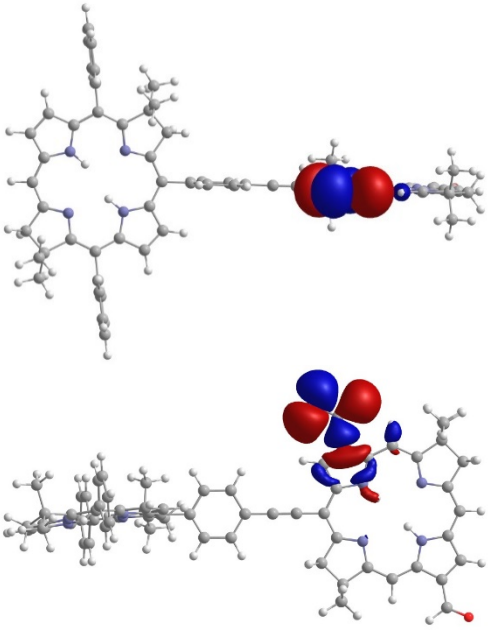
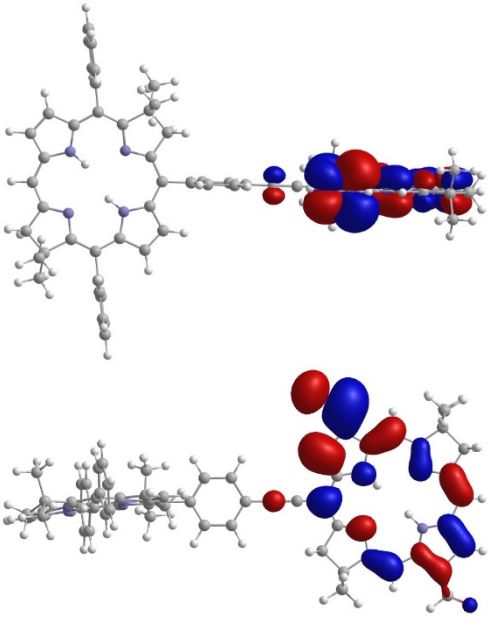
S5	0.99914		
S6	0.60145		

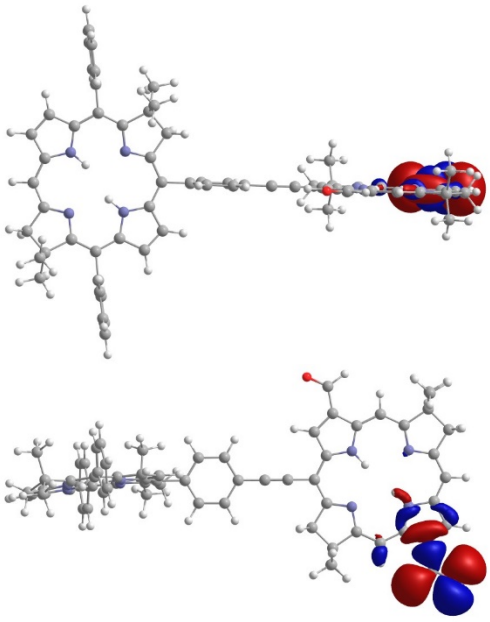
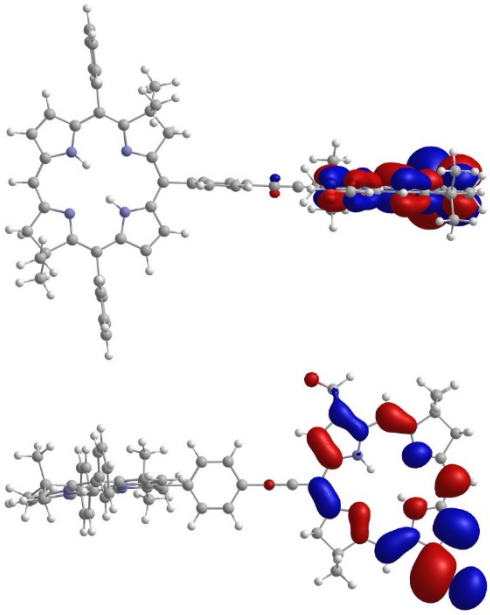
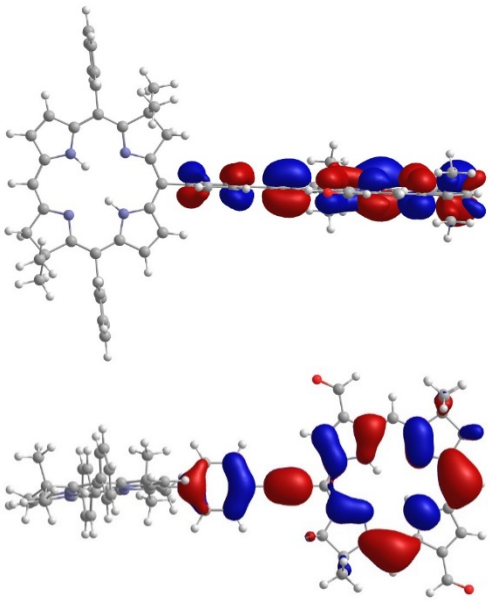
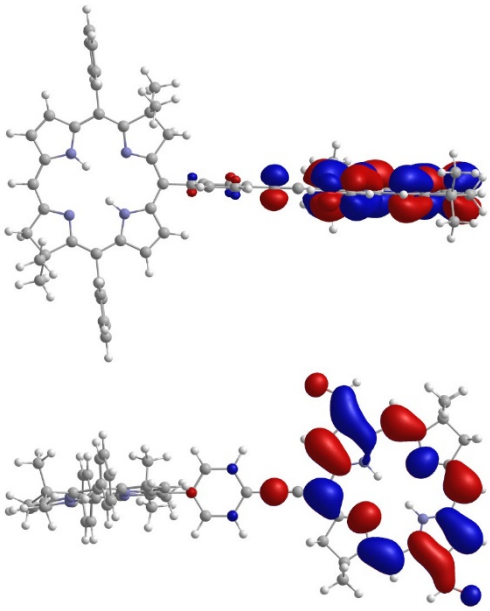
S6	0.35389		
S7	0.73657		

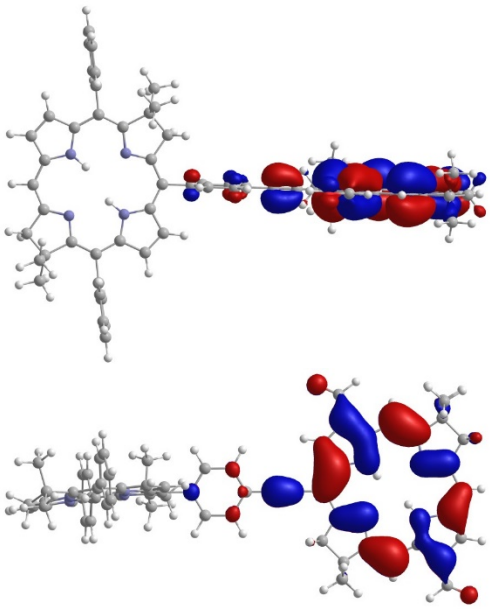
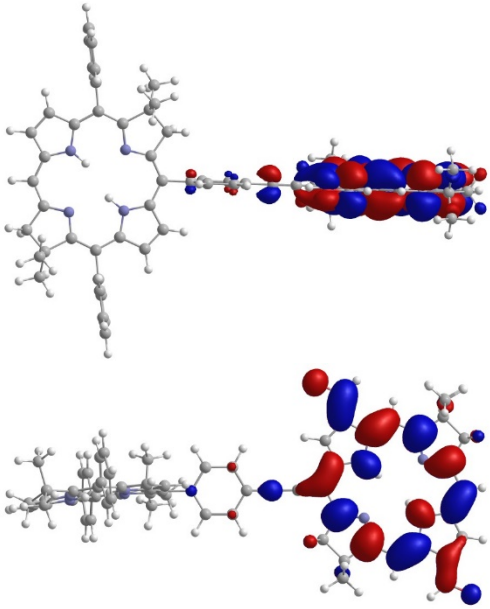
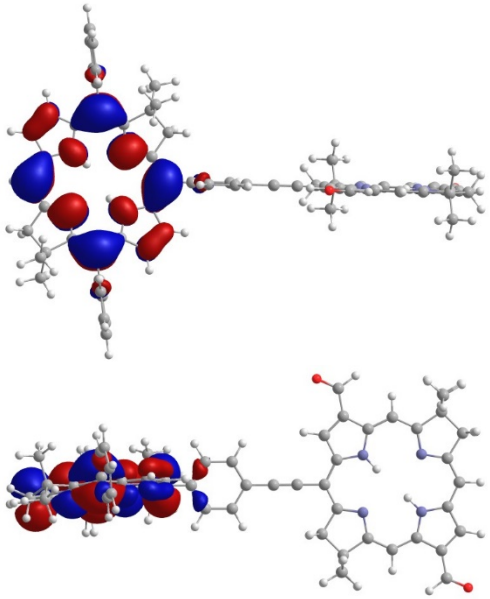
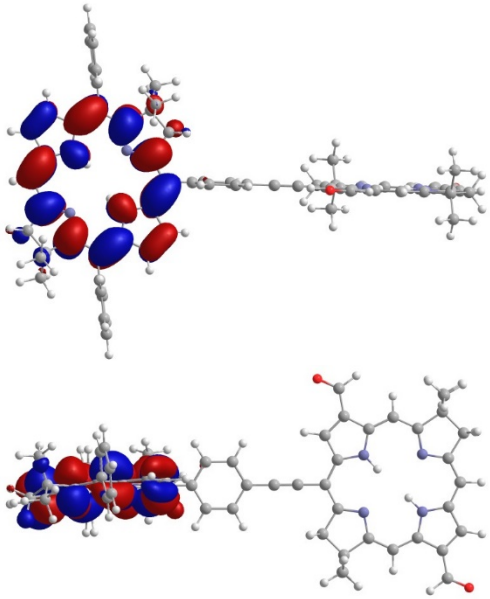
S7	0.17997		
S8	0.45994		

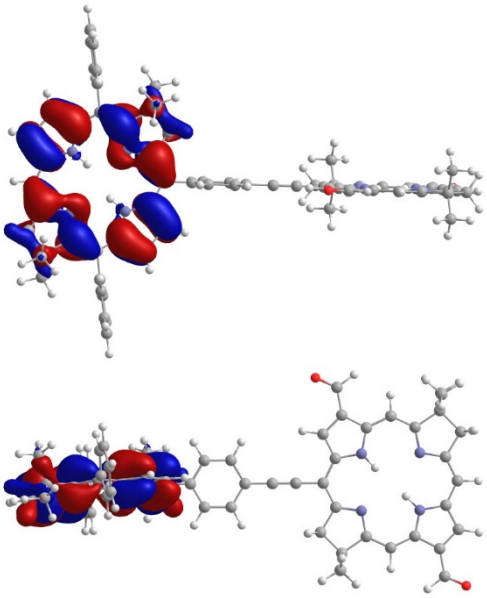
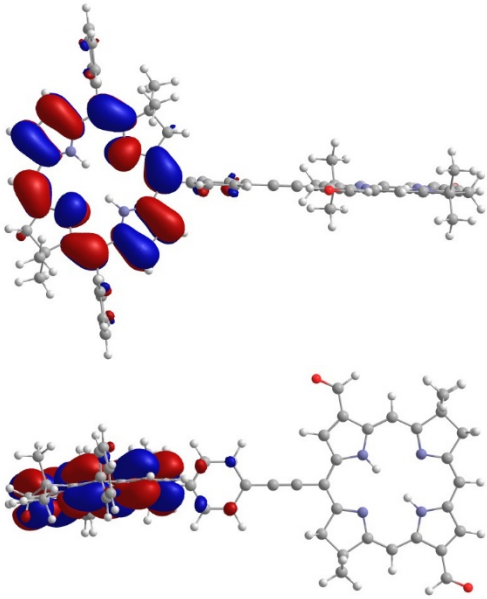
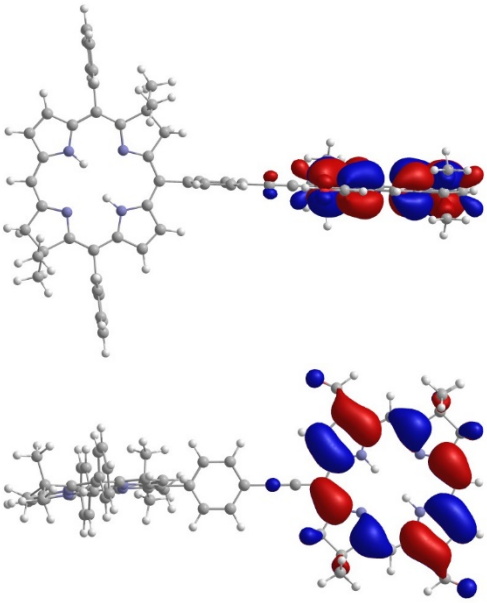
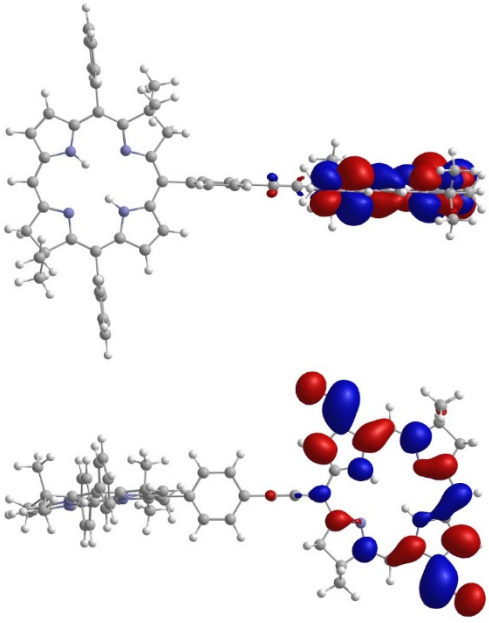
S8	0.37264		
S8	0.16294		

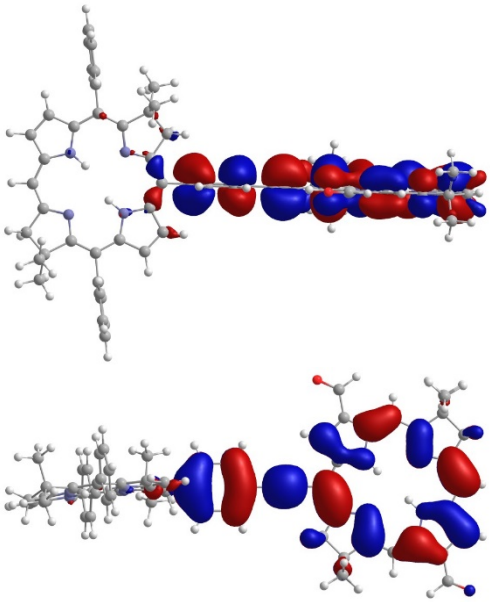
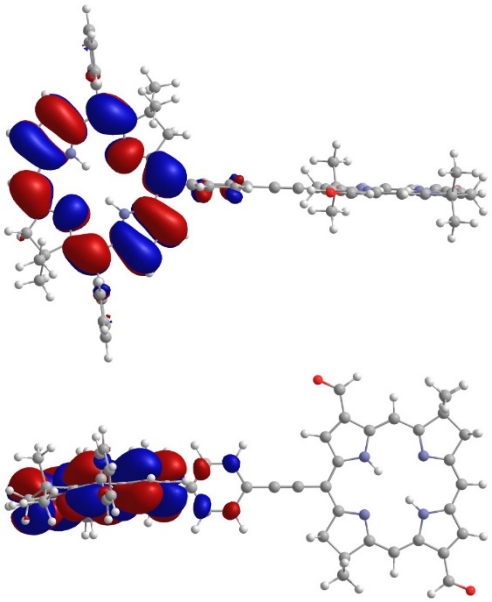
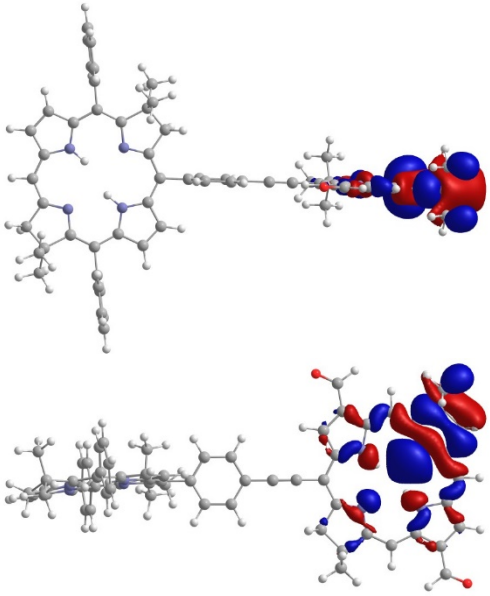
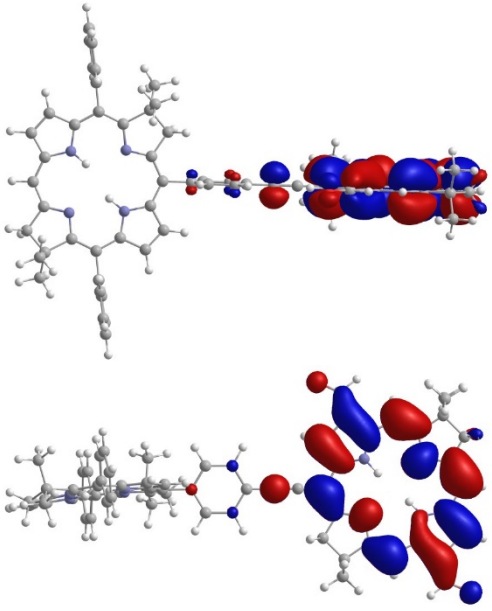
S9	0.45237		
S9	0.27926		

S9	0.20761		
S10	0.99698		

S11	0.99690		
S12	0.57679		

S12	0.40308		
S13	0.87295		

S13	0.10251		
S14	0.89899		

S15	0.99440		
S16	0.99099		

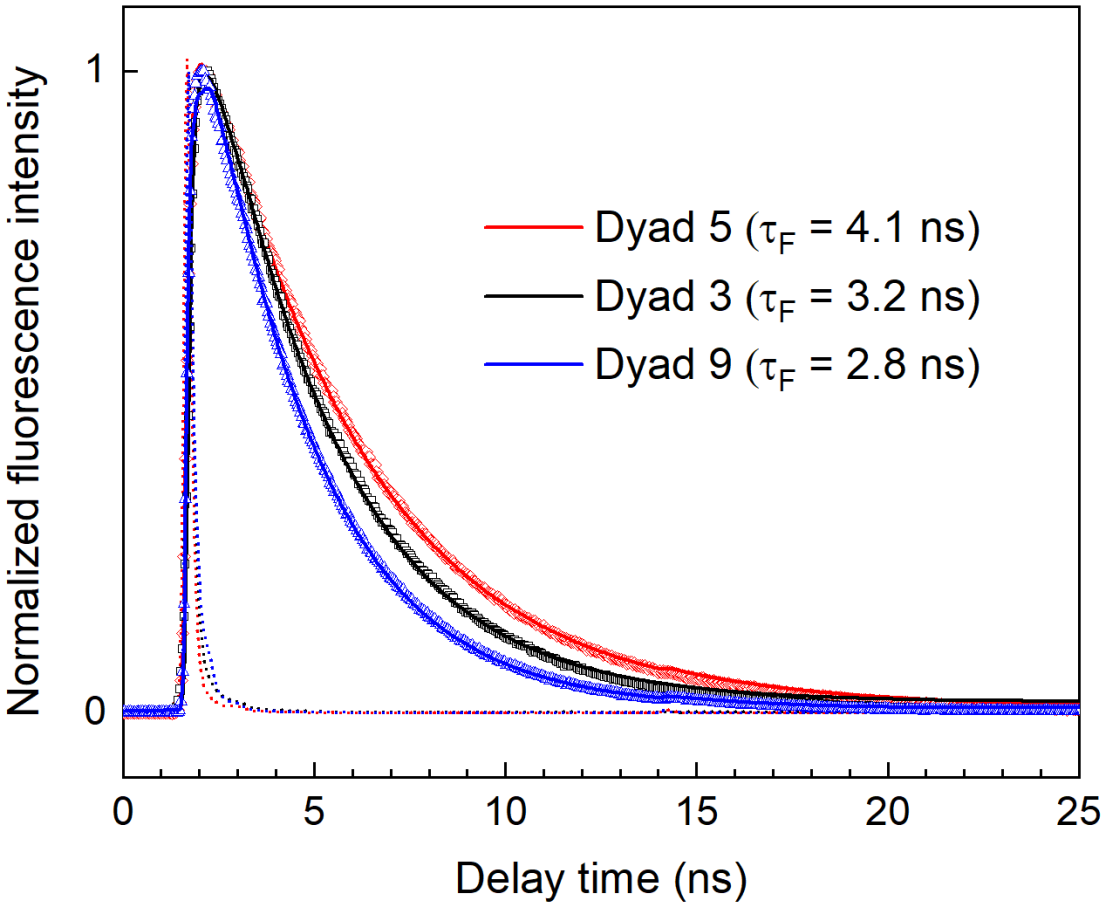
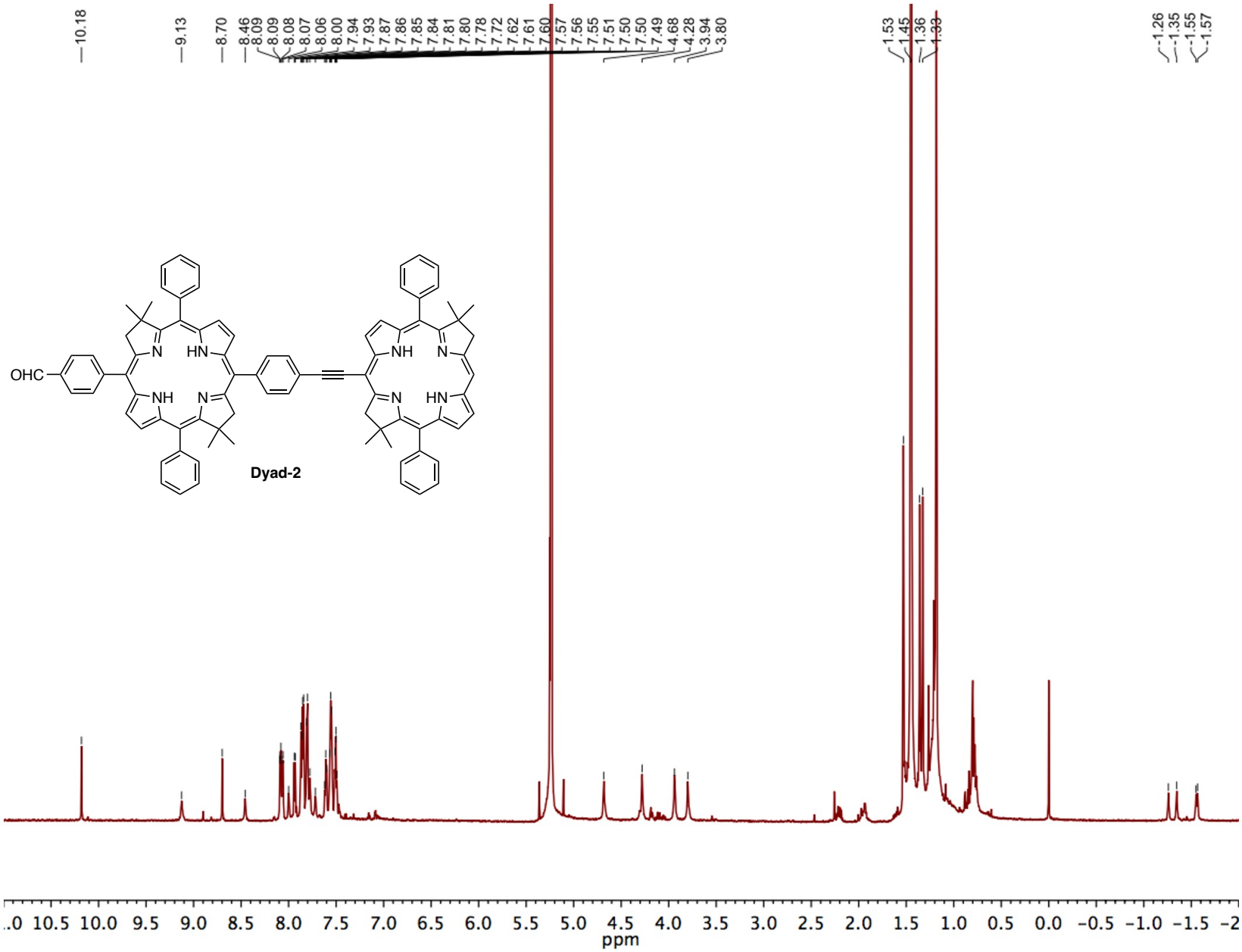


Figure S10. Kinetic traces (symbols) recorded using TCSPC and fits (solid lines) of **Dyad-5** (red), **Dyad-3** (black) and **Dyad-9** (blue) with corresponding S_1 lifetimes obtained from fitting by deconvolution with the instrument response function (IRF, dashed lines).

NMR
Spectra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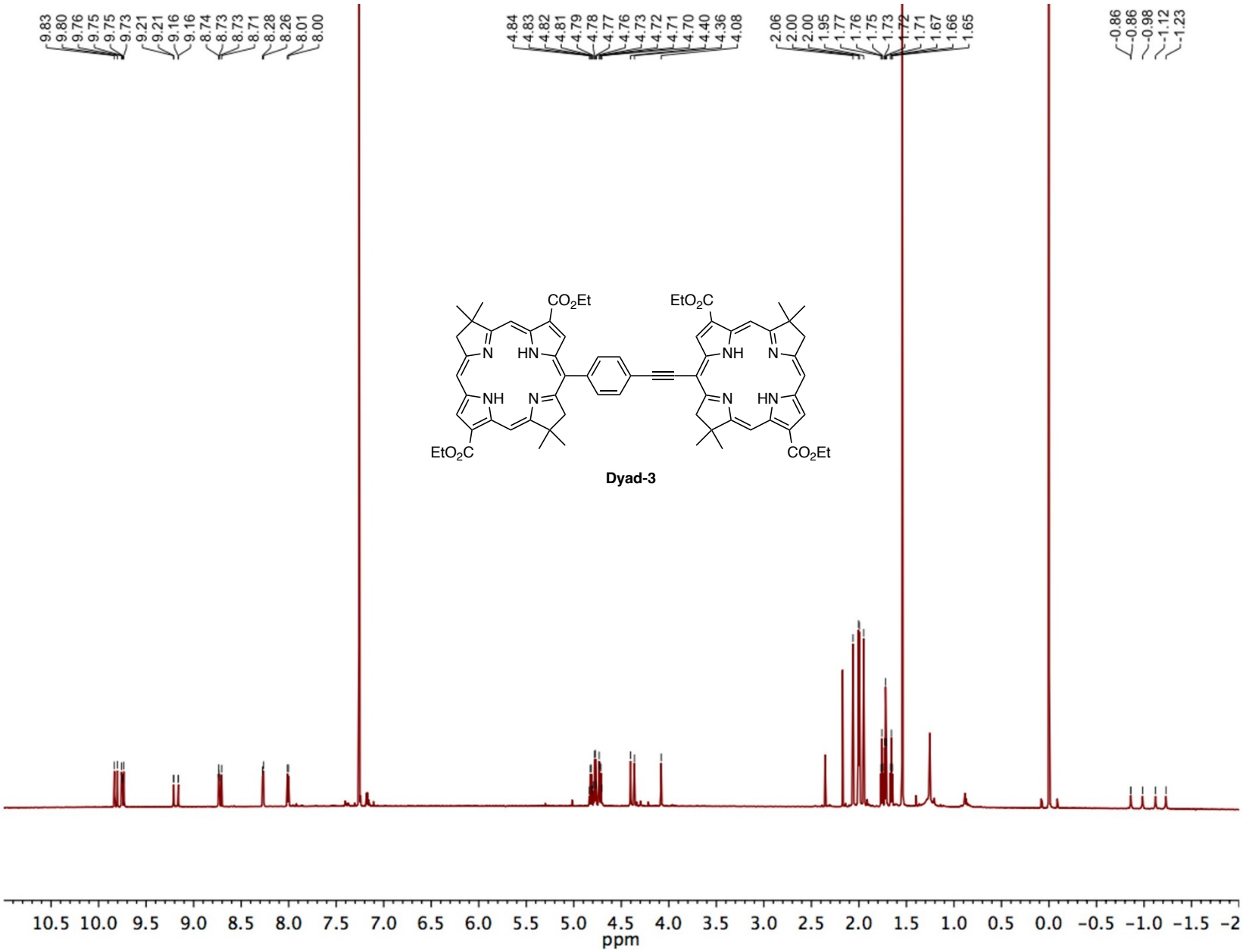
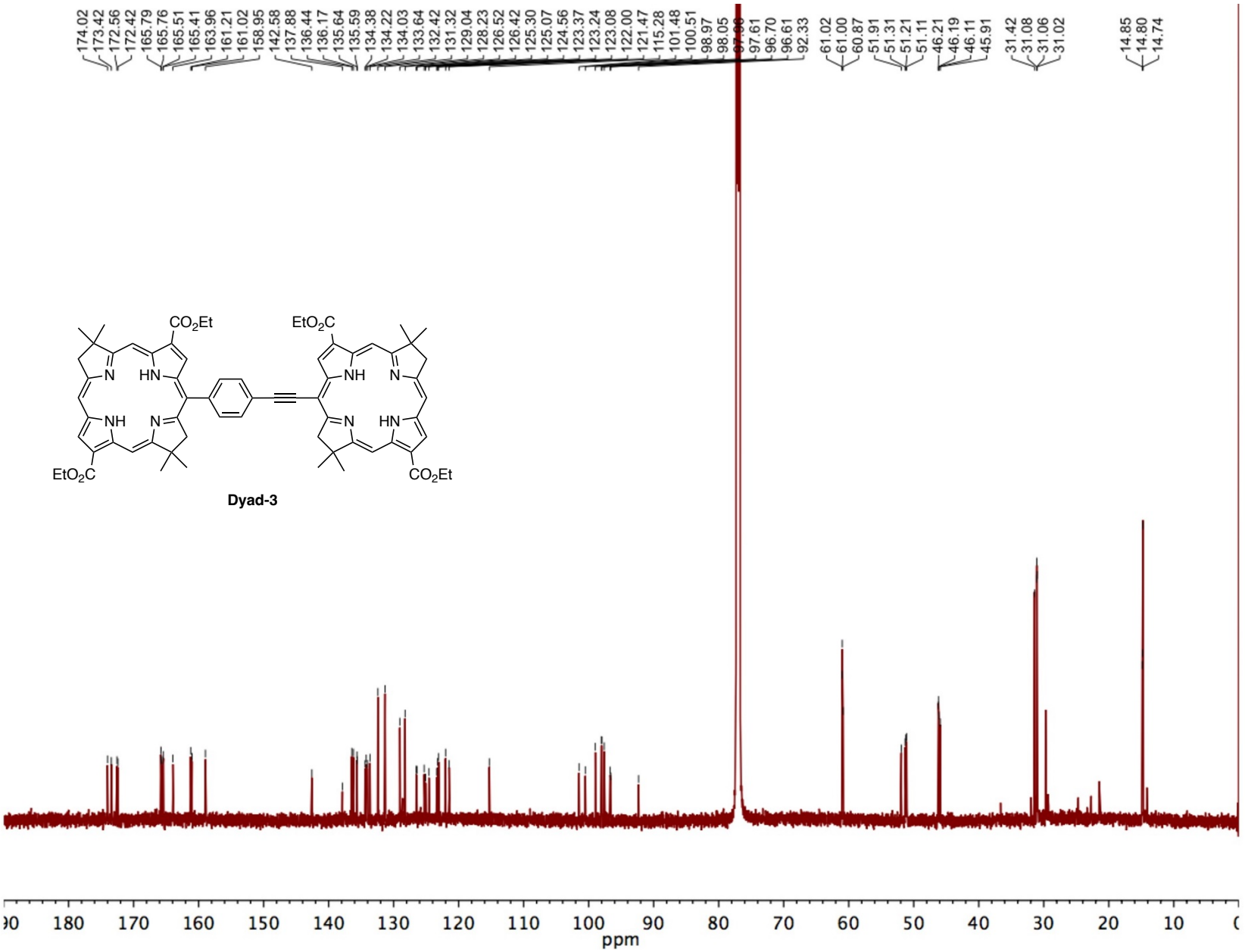
9.13
8.70
8.46
8.09
8.09
8.08
8.07
8.06
8.00
7.94
7.93
7.87
7.86
7.85
7.84
7.81
7.80
7.78
7.72
7.62
7.61
7.60
7.57
7.56
7.55
7.51
7.50
7.50
7.49
4.68
4.28
3.94
3.80
1.53
1.45
1.36
1.33
-1.26
-1.35
-1.55
-1.57
OHC
N
HN
NH
N
NH
N
N
HN
Dyad-2
ppm


9.83
9.80
9.76
9.75
9.75
9.73
9.21
9.21
9.16
9.16
8.74
8.73
8.73
8.71
8.28
8.26
8.01
8.00
4.84
4.83
4.82
4.81
4.79
4.78
4.77
4.76
4.73
4.72
4.71
4.70
4.40
4.36
4.08
2.06
2.00
2.00
1.95
1.77
1.76
1.75
1.73
1.72
1.71
1.67
1.66
1.65
0.86
0.86
0.98
1.12
1.23
CO2Et
EtO2C
N
HN
NH
N
NH
N
N
HN
EtO2C
CO2Et
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2
ppm

Dyad-3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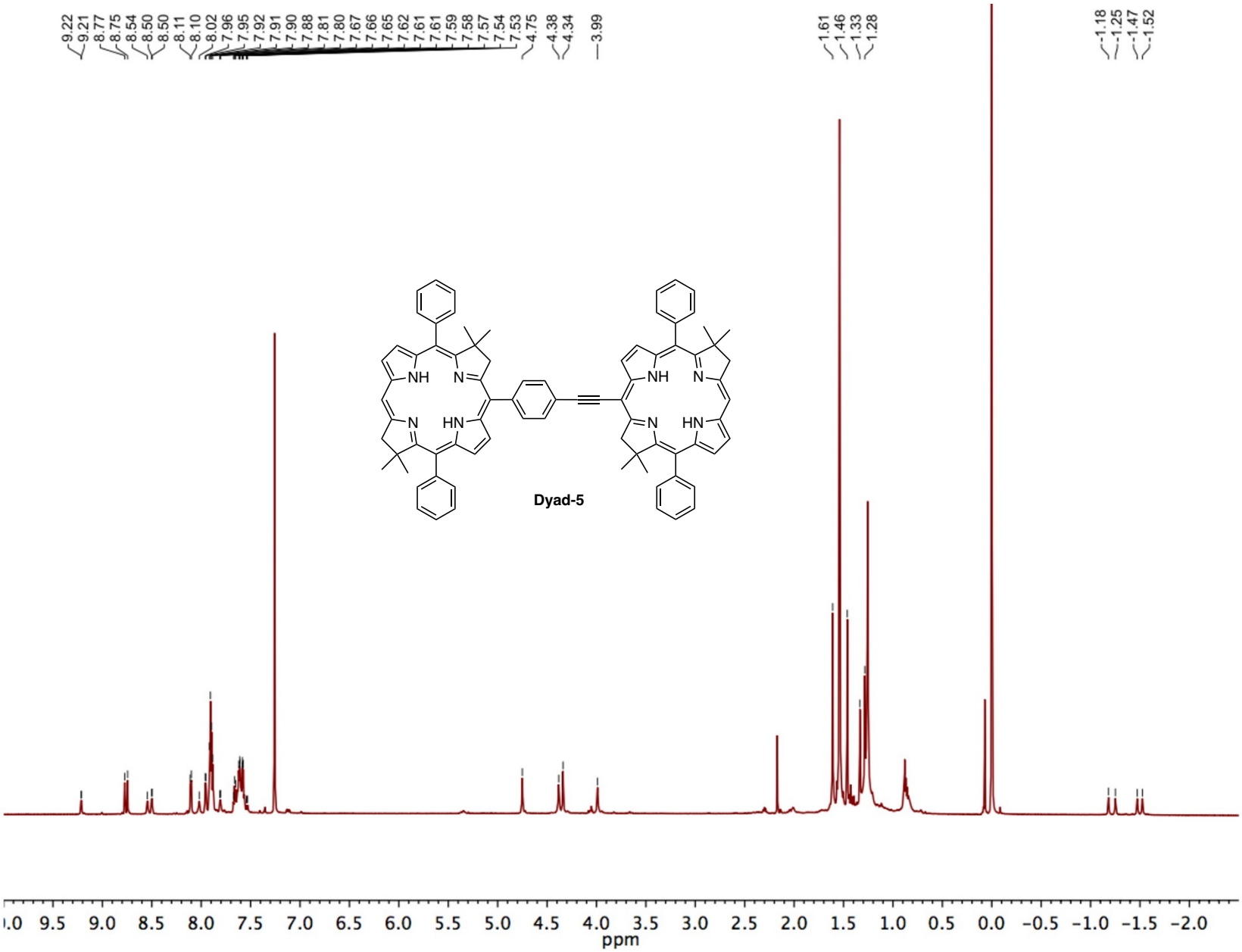
173.42
172.56
172.42
165.79
165.76
165.51
165.41
163.96
161.21
161.02
158.95
142.58
137.88
136.44
136.17
135.64
135.59
134.38
134.22
134.03
133.64
132.42
131.32
129.04
128.23
126.52
126.42
125.30
125.07
124.56
123.37
123.24
123.08
122.00
121.47
115.28
101.48
100.51
98.97
98.05
97.61
96.70
96.61
92.33
61.02
61.00
60.87
51.91
51.31
51.21
51.11
46.21
46.19
46.11
45.91
31.42
31.08
31.06
31.02
14.85
14.80
14.74
CO2Et
EtO2C
N
HN
NH
N
NH
N
N
HN
EtO2C
CO2Et
Dyad-3
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


9.22
9.21
8.77
8.75
8.54
8.50
8.50
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7.54
7.53
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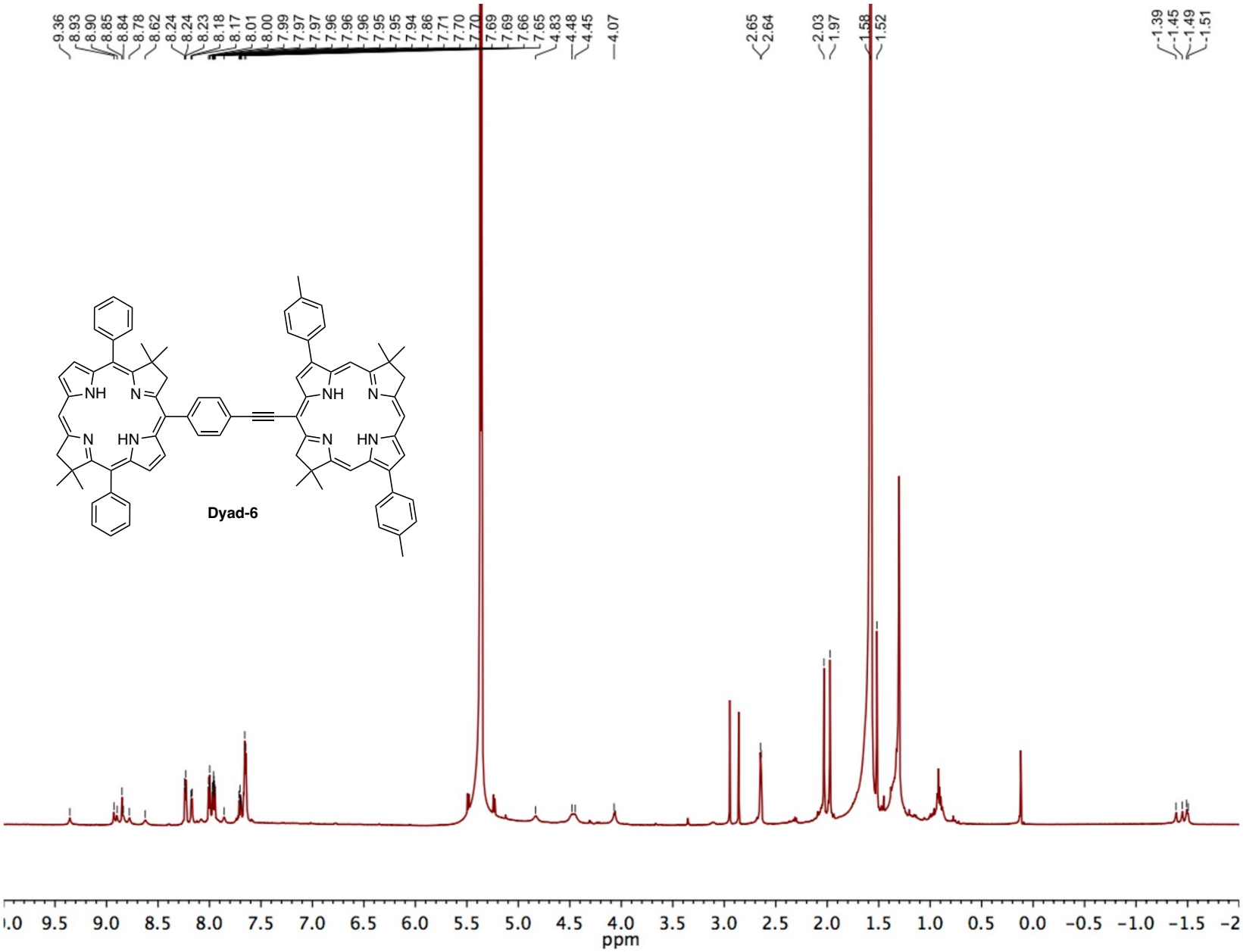
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4.83
4.48
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2.64
2.03
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1.58
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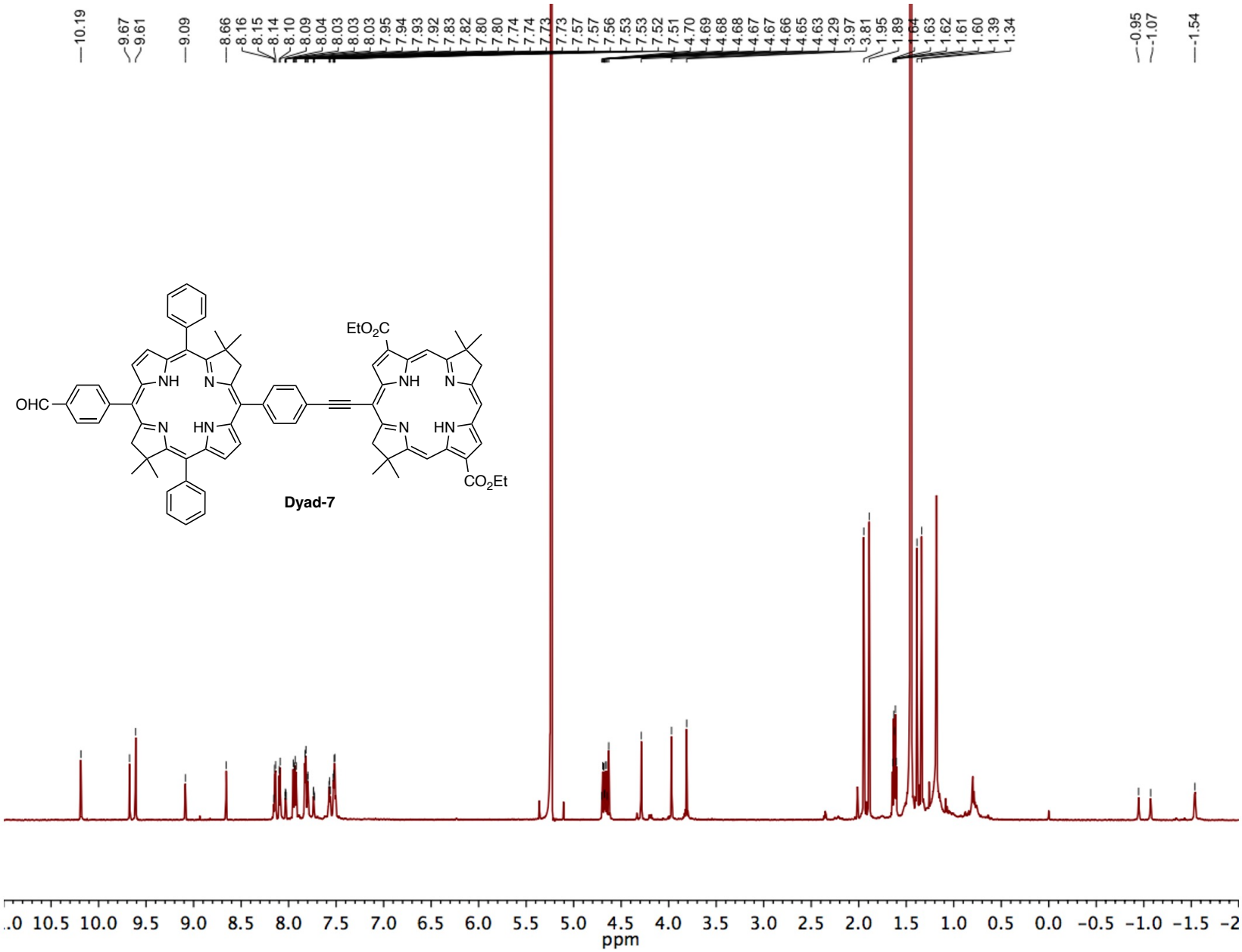
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7.80
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7.73
7.73
7.57
7.57
7.56
7.53
7.53
7.52
7.51
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4.68
4.68
4.67
4.67
4.66
4.65
4.63
4.29
3.97
3.81
1.95
1.89
1.64
1.63
1.62
1.61
1.60
1.39
1.34
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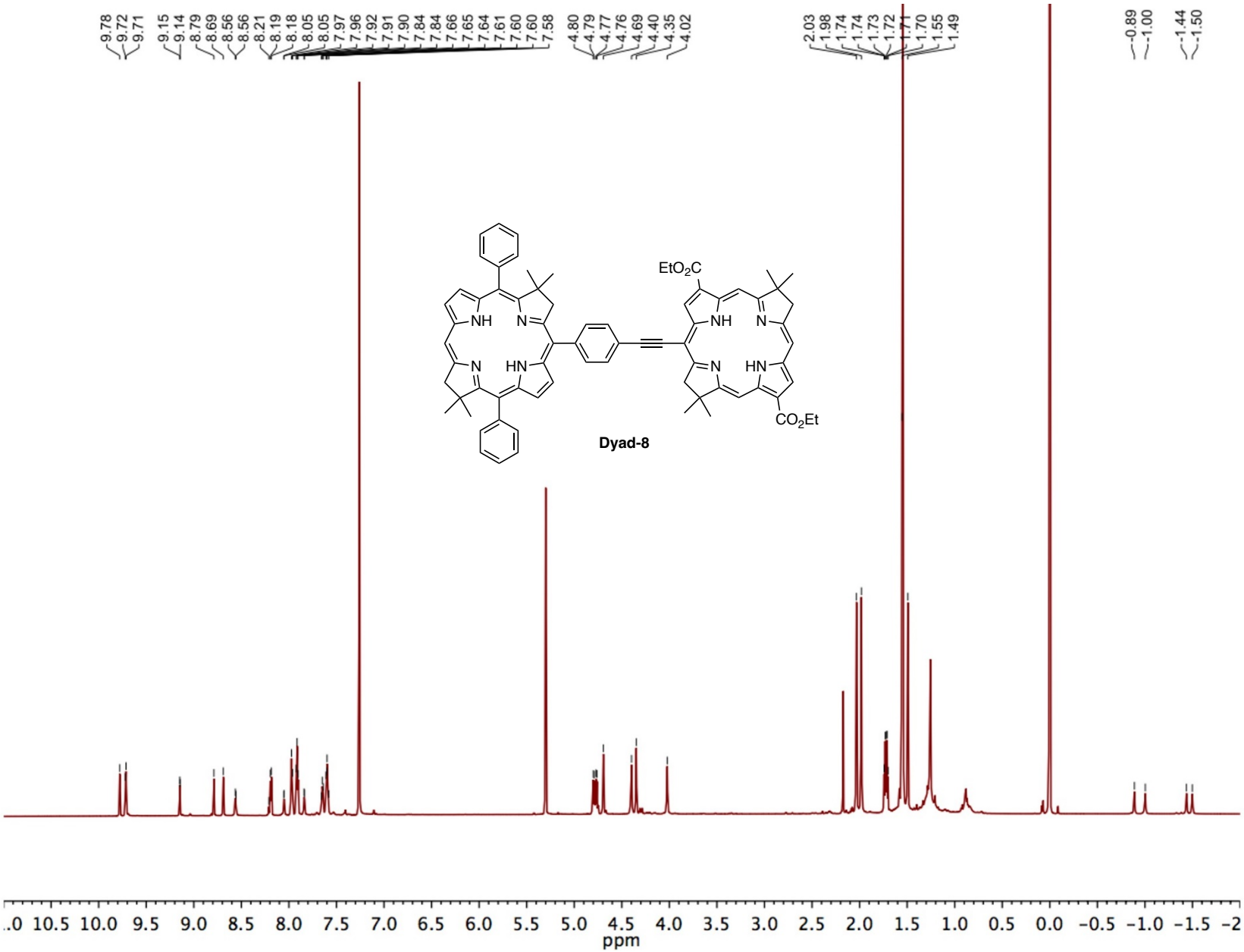
HN
CO2Et
Dyad-7
ppm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8.05
7.97
7.96
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7.91
7.90
7.84
7.84
7.66
7.65
7.64
7.61
7.60
7.60
7.58
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4.76
4.69
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2.03
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1.74
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1.44
1.50
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NH
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HN
NH
N
N
HN
CO2Et
Dyad-8
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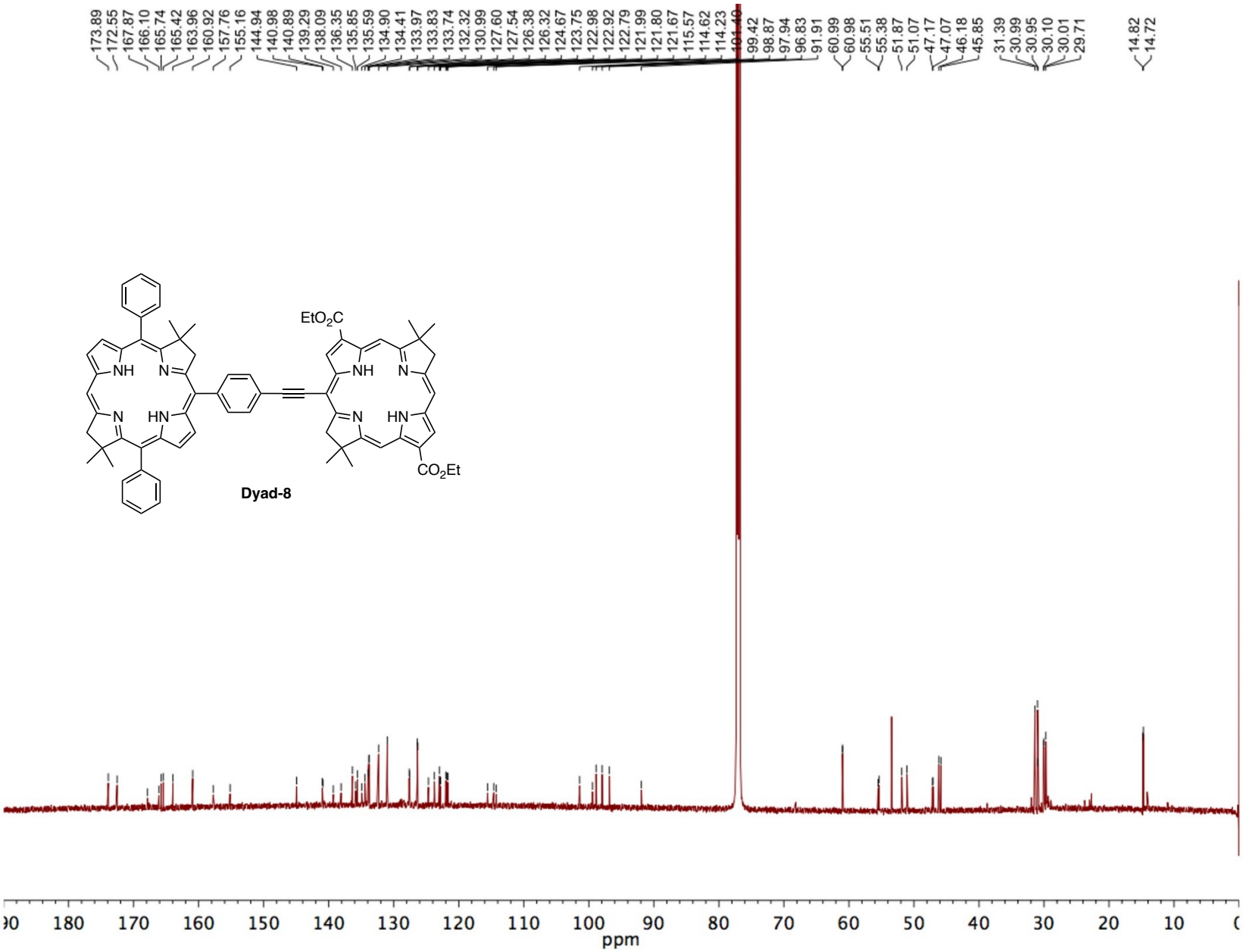
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126.32
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121.67
115.57
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91.91
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60.98
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55.38
51.87
51.07
47.17
47.07
46.18
45.85
31.39
30.99
30.95
30.10
30.01
29.71
14.82
14.72
EtO2C
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NH
N
N
HN
N
HN
CO2Et
Dyad-8
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140
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100
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10
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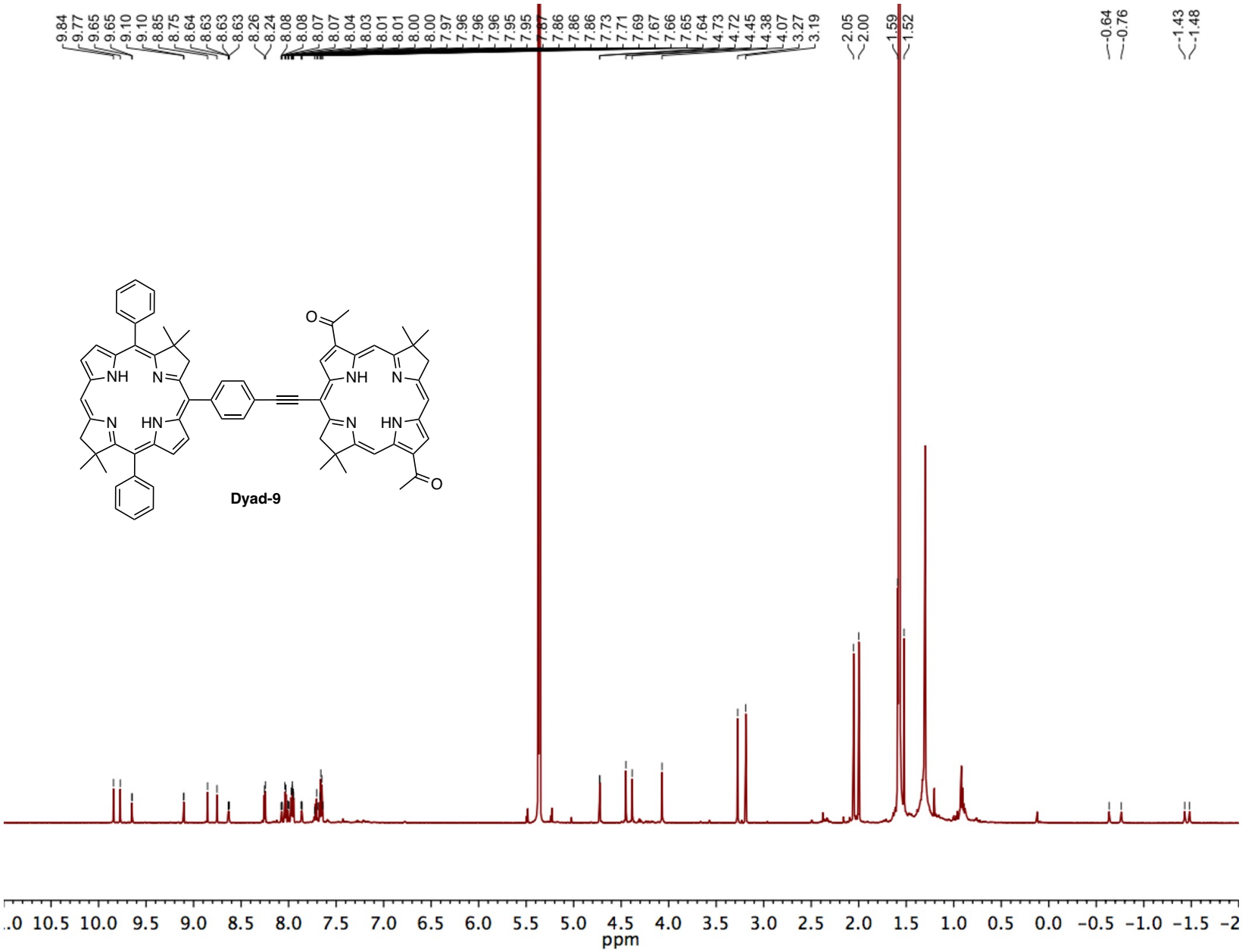
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8.08
8.07
8.07
8.04
8.03
8.01
8.01
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8.00
7.97
7.96
7.96
7.96
7.95
7.95
7.87
7.86
7.86
7.86
7.73
7.71
7.69
7.67
7.66
7.65
7.64
4.73
4.72
4.45
4.38
4.07
3.27
3.19
2.05
2.00
1.59
1.52
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-0.76
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HN
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Dyad-9
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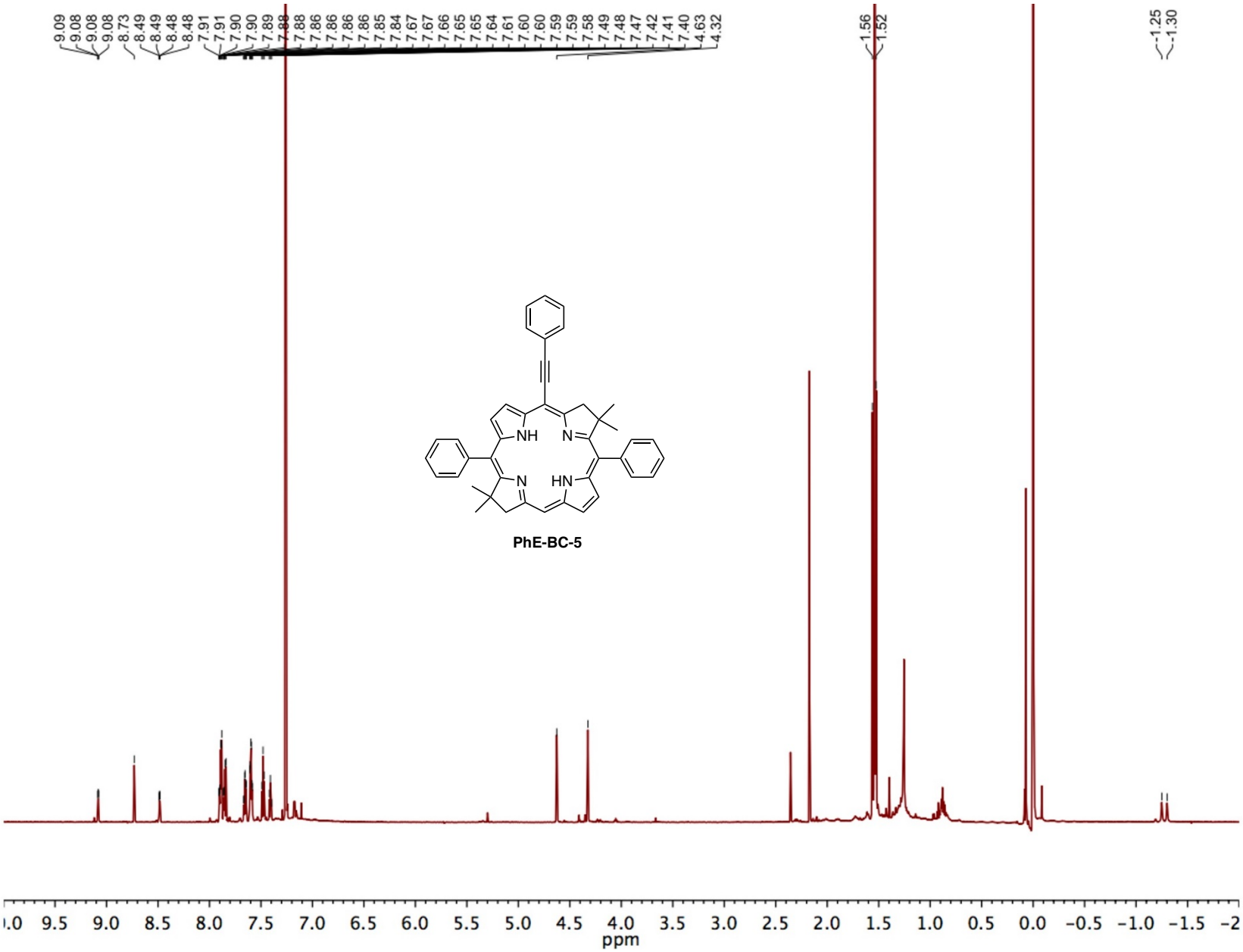
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7.47
7.42
7.41
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4.32
1.56
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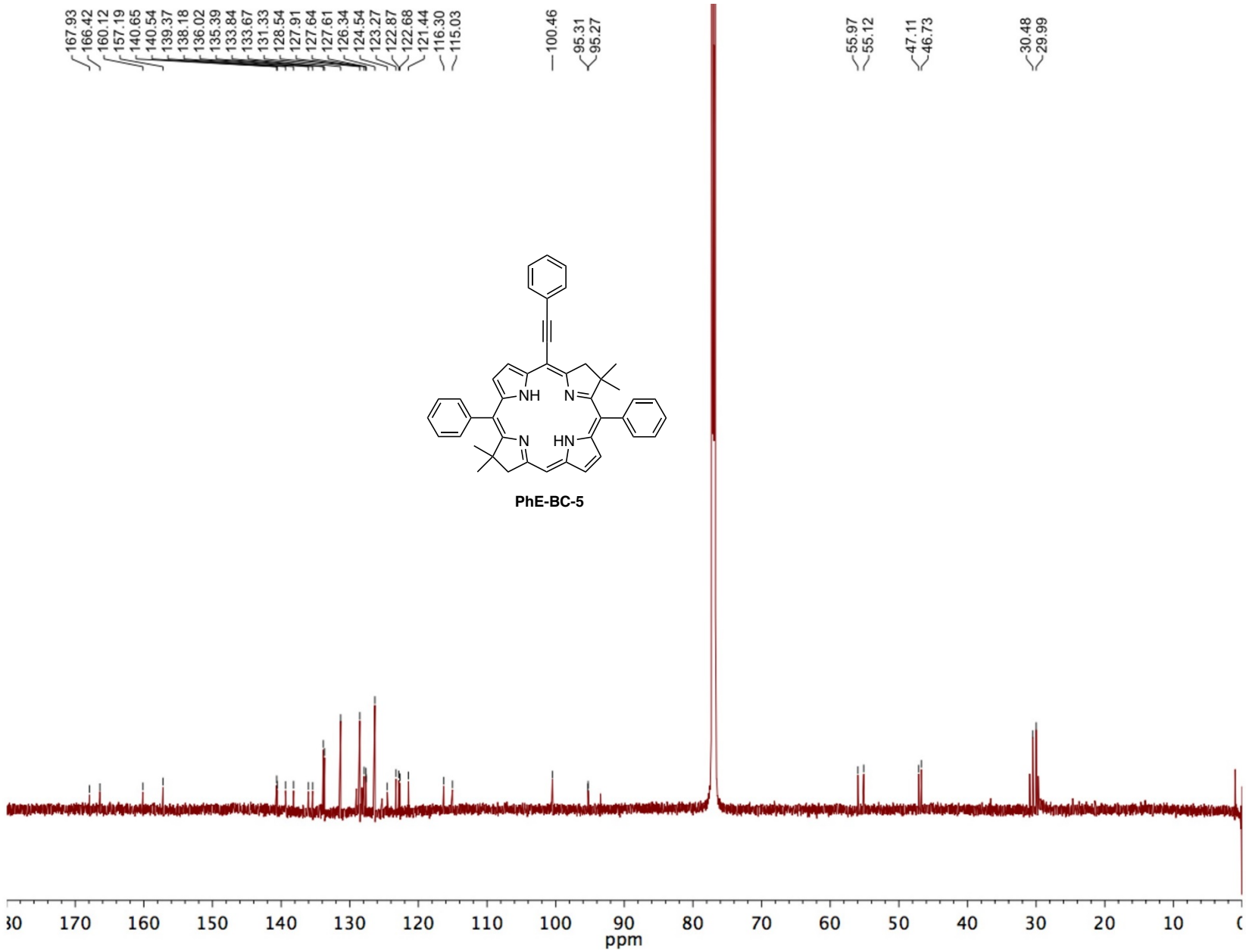
PhE-BC-5
ppm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133.84
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128.54
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127.64
127.61
126.34
124.54
123.27
122.87
122.68
121.44
116.30
115.03
100.46
95.31
95.27
55.97
55.12
47.11
46.73
30.48
29.99
NH
N
N
HN
PhE-BC-5
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150
140
130
120
110
100
90
80
70
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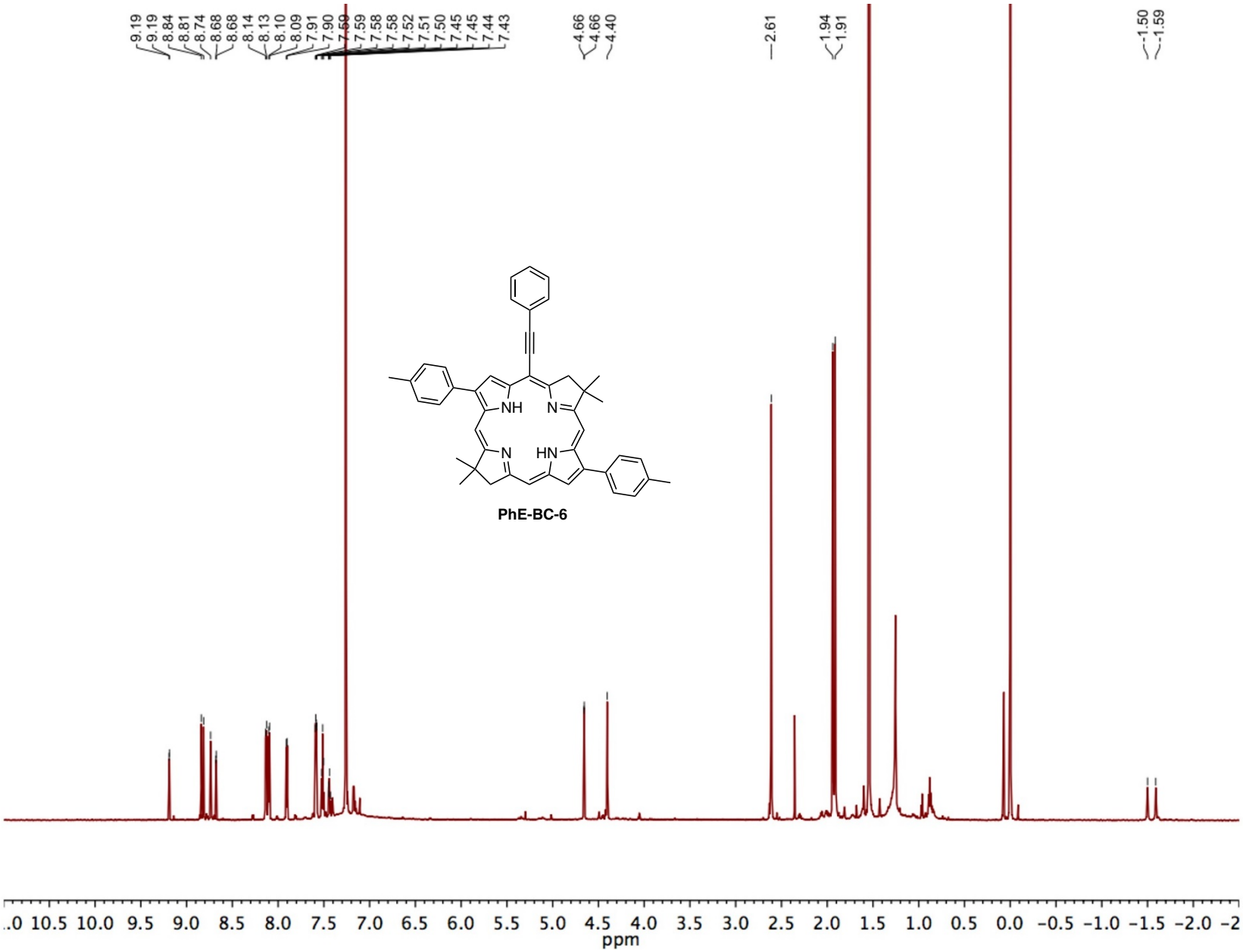
30
20
10
ppm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8.10
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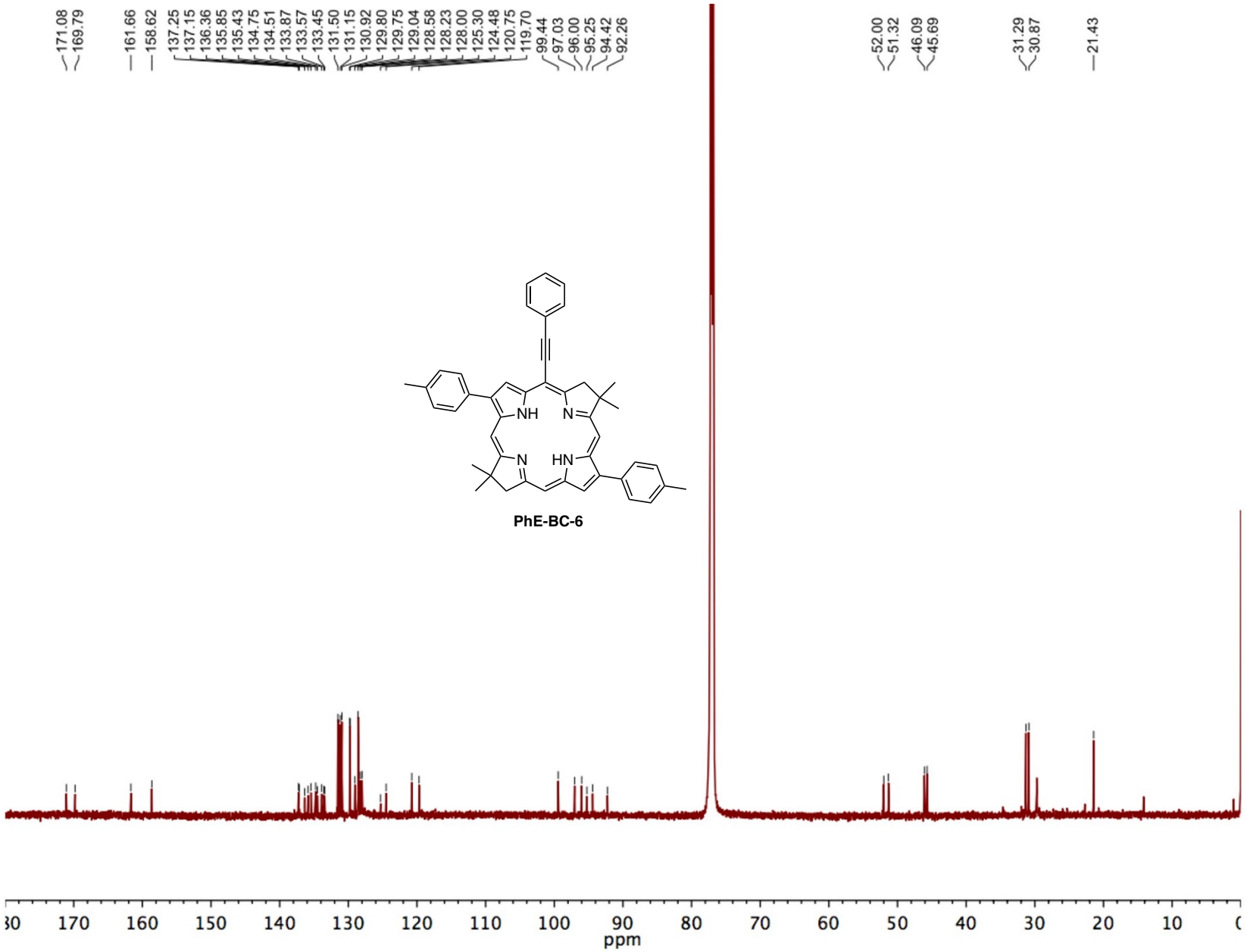
7.59
7.59
7.58
7.58
7.52
7.51
7.50
7.45
7.45
7.44
7.43
4.66
4.66
4.40
2.61
1.94
1.91
-1.50
-1.59
NH
N
N
HN
PhE-BC-6
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2.0 -2
ppm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131.15
130.92
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129.75
129.04
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128.23
128.00
125.30
124.48
120.75
119.70
99.44
97.03
96.00
95.25
94.42
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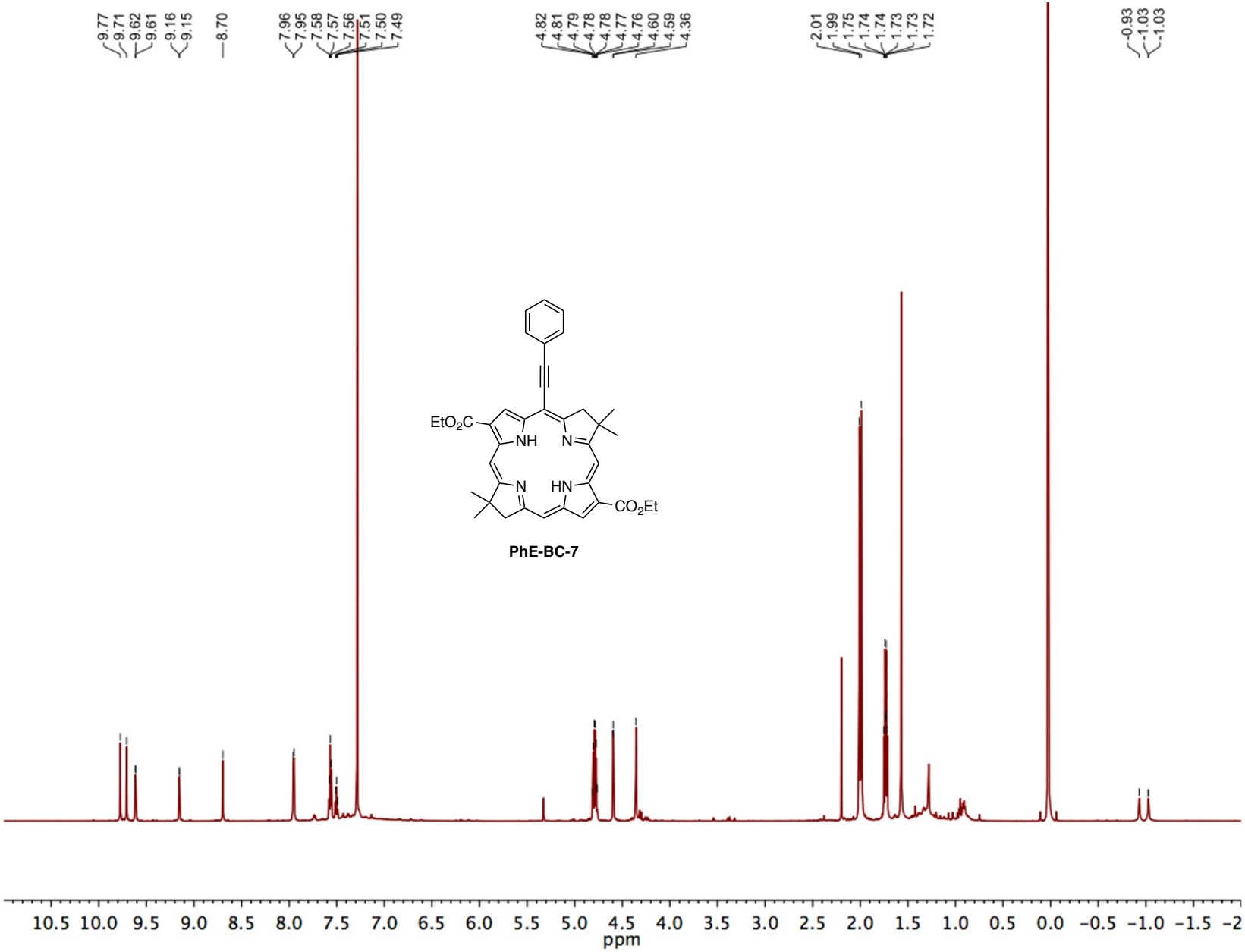
PhE-BC-6
ppm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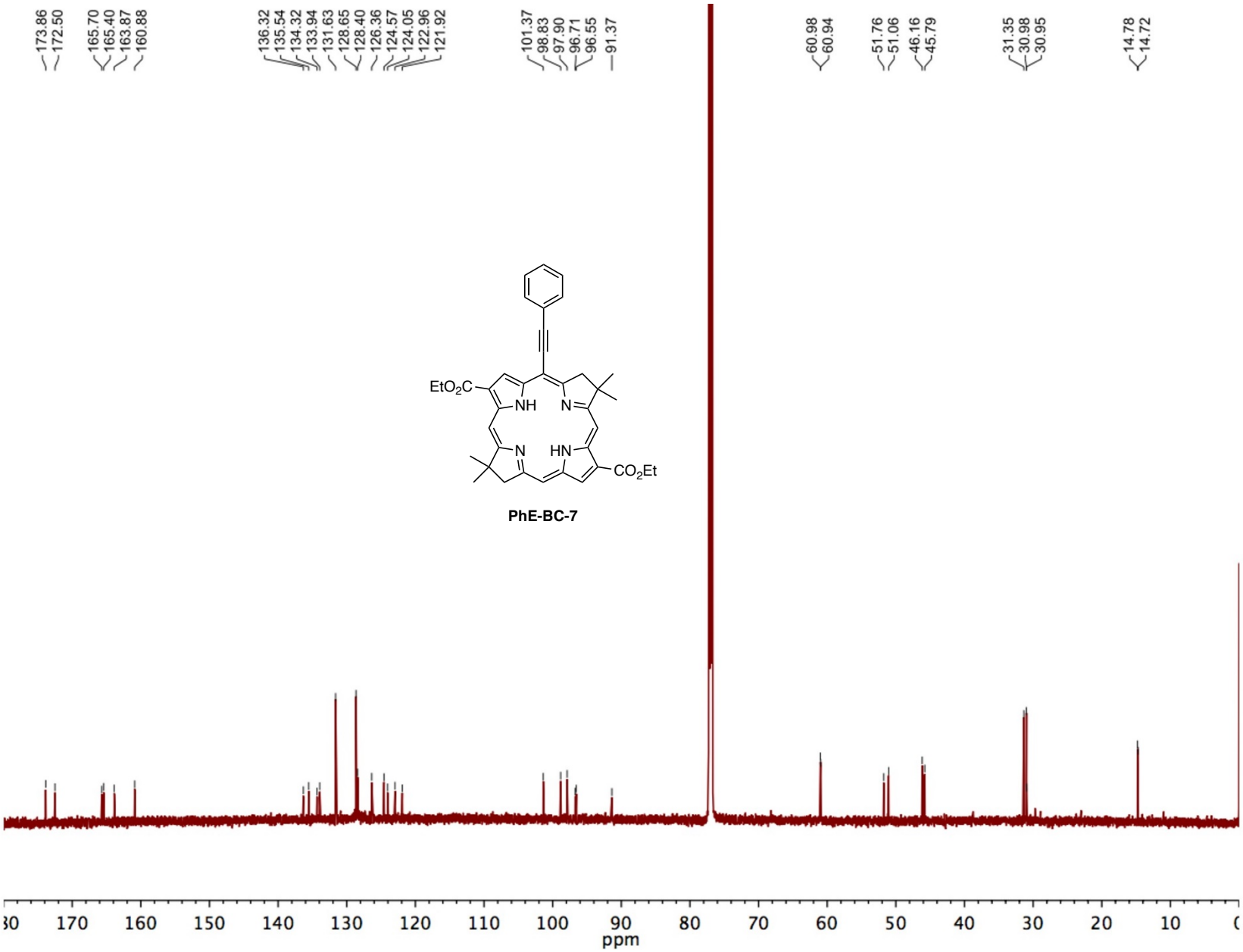
7.58
7.57
7.56
7.51
7.50
7.49
4.82
4.81
4.79
4.78
4.78
4.77
4.76
4.60
4.59
4.36
2.01
1.99
1.75
1.74
1.74
1.73
1.73
1.72
0.93
1.03
1.03
EtO2C
NH
N
N
HN
CO2Et
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5 -2
ppm

PhE-BC-7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128.40
126.36
124.57
124.05
122.96
121.92
101.37
98.83
97.90
96.71
96.55
91.37
60.98
60.94
51.76
51.06
46.16
45.79
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14.78
14.72
EtO2C
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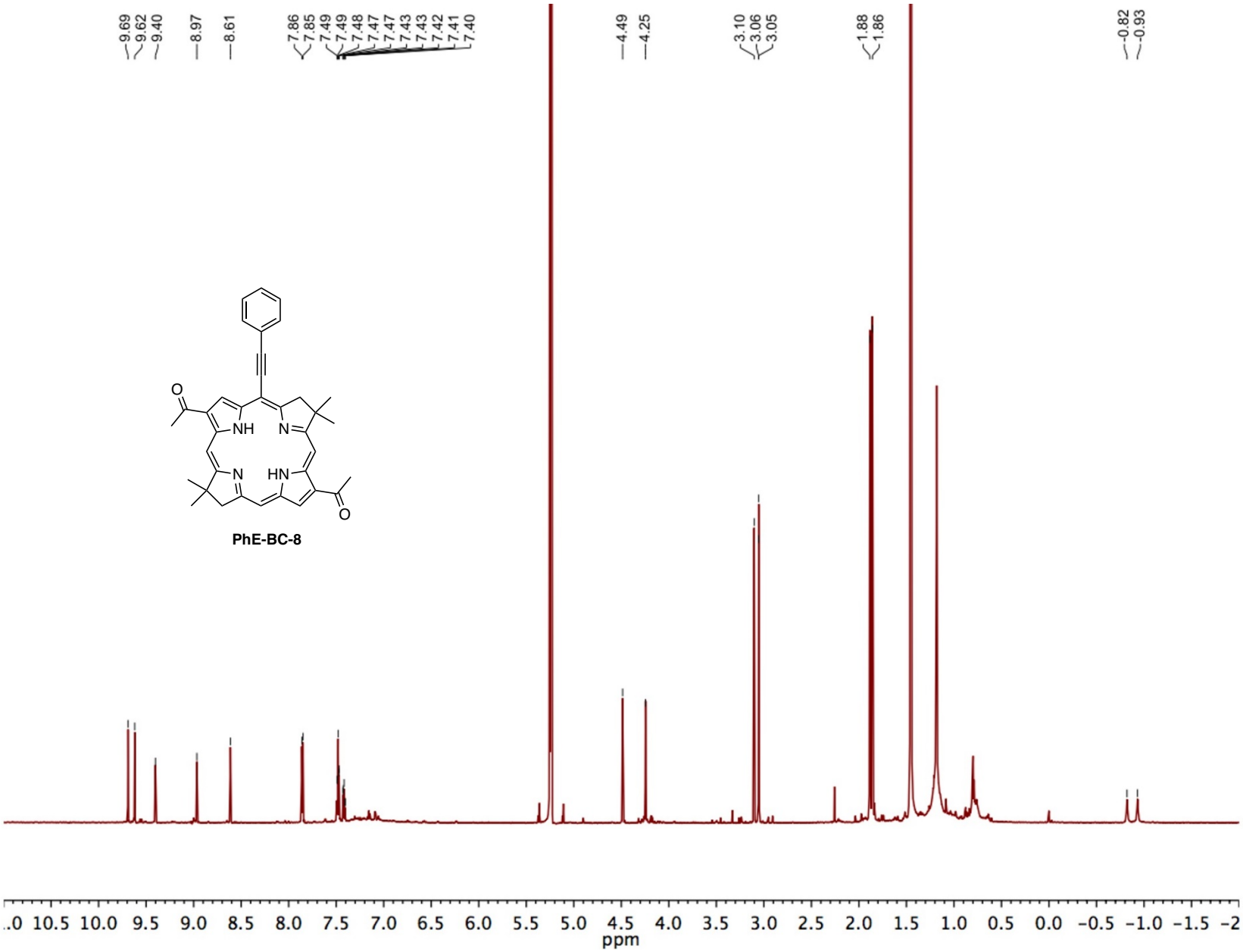
CO2Et
PhE-BC-7
ppm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7.85
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7.48
7.47
7.47
7.43
7.43
7.42
7.41
7.40
4.49
4.25
3.10
3.06
3.05
1.88
1.86
-0.82
-0.93
O
NH
N
N
HN
O
PhE-BC-8
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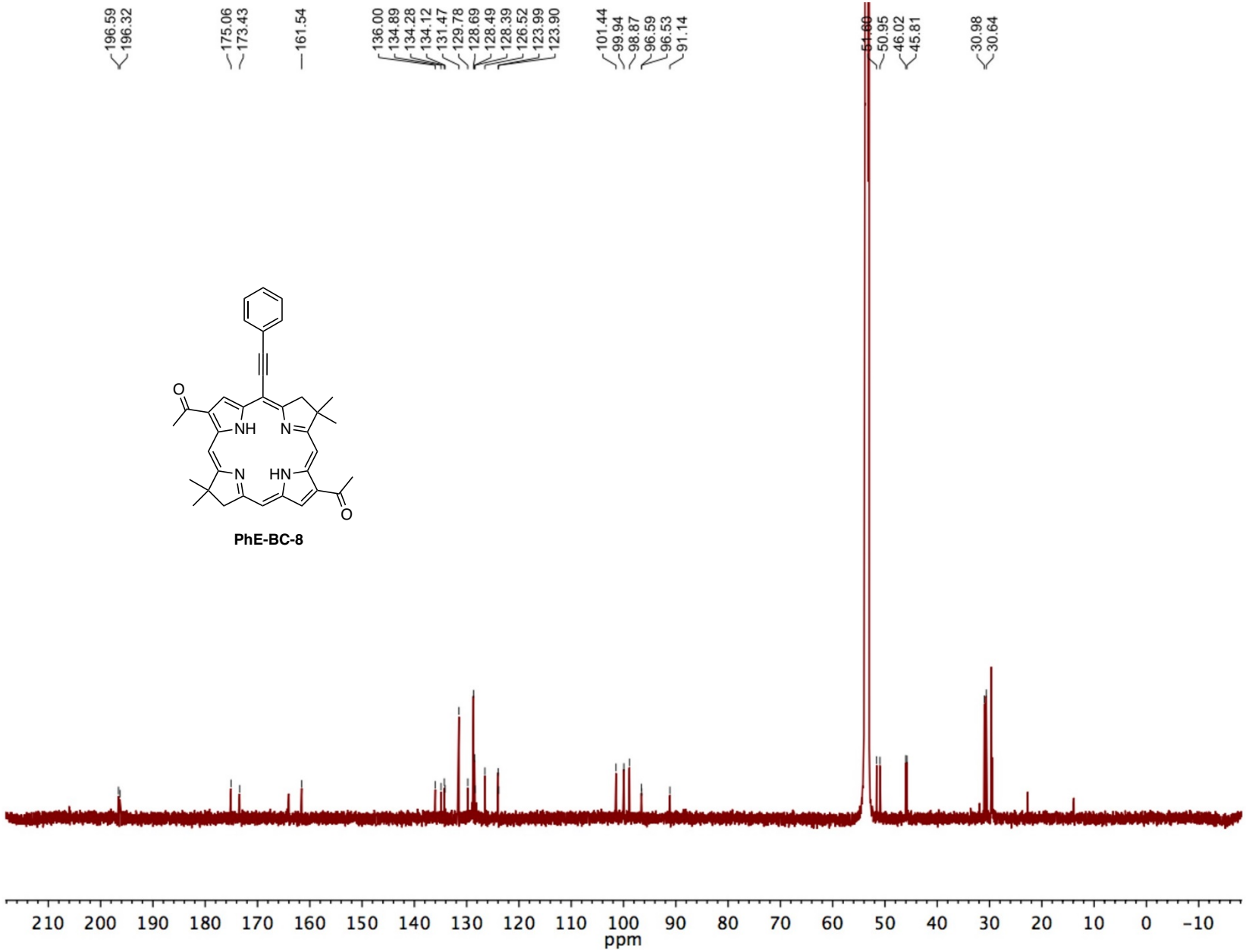
ppm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129.78
128.69
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128.39
126.52
123.99
123.90
101.44
99.94
98.87
96.59
96.53
91.14
51.60
50.95
46.02
45.81
30.98
30.64
O
NH
N
N
HN
O
PhE-BC-8
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
ppm