

Theoretical design of core modified (oxa and thia) porphyrin based organic dyes with bridging thiophene linkers

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Supporting Information

(51 pages including this page)

Figure S1: Conformational search carried out for **STPP-βN** at the B3LYP/3-21G* level.

Figure S2: Conformational search carried out for **STPP-βP** at the B3LYP/3-21G* level.

Figure S3: Conformational search carried out for **S₂TPP-βN** at the B3LYP/3-21G* level.

Figure S4: Conformational search carried out for **S₂TPP-βN** at the B3LYP/3-21G* level.

Figure S5: The HOMO-LUMO gap (in eV) at B3LYP/6-31G* level of the β-substituted CMP sensitizers in CHCl₃ solvent.

Figure S6: The spatial distribution of the HOMO-LUMO of the sensitizers carried out at the B3LYP/3-21G* level.

Figure S7: The spatial distribution of the HOMOs of the **TPP** and **TPP-βN** carried out at the B3LYP/6-31G* level.

Figure S8: The spatial distribution of the LUMOs of the **TPP** and **TPP-βN** carried out at the B3LYP/6-31G* level.

Figure S9: The spatial distribution of the HOMOs of the **OTPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S10: The spatial distribution of the LUMOs of the **OTPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S11: The spatial distribution of the HOMOs of the **STPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S12: The spatial distribution of the LUMOs of the **STPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S13: The spatial distribution of the HOMOs of the **O₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S14: The spatial distribution of the LUMOs of the **O₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S15: The spatial distribution of the HOMOs of the **S₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S16: The spatial distribution of the LUMOs of the **S₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S17: The spatial distribution of the HOMOs of the **OSTPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S18: The spatial distribution of the LUMOs of the **OSTPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

Figure S19: Total densities of states (TDOS in black) and projected densities of states (PDOS) of dye (in orange) and TiO₂ (in green) of representative dye-(TiO₂)₁₆ complexes at B3LYP/6-311G(d)ULANL2DZ and B3LYP/6-31G(d)ULANL2DZ basis set.

Table S1: The % molecular orbital contribution of the HOMO and LUMO of the core modified porphyrin sensitizers at the B3LYP/6-31G* level.

Table S2: The calculated excitation energies (E in eV), wavelength (λ in nm) oscillator strength (f), and major transition configuration of sensitizers at TD-B3LYP/6-31G* level.

Table S3: The optimized coordinates of the fourteen core modified sensitizers at the B3LYP/6-31G* level.

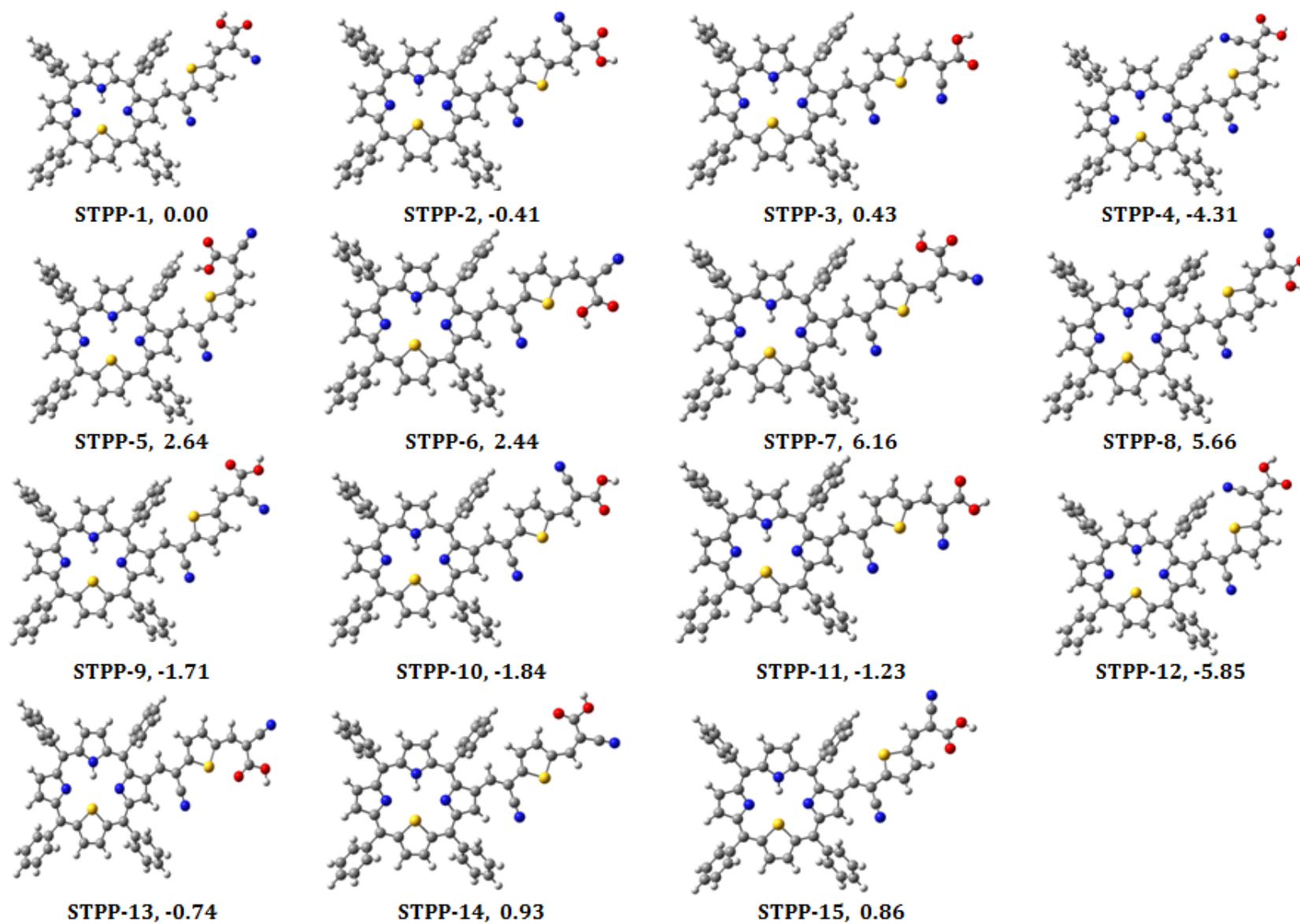


Figure S1: Conformational search carried out for **STPP- β N** at the B3LYP/3-21G* level.

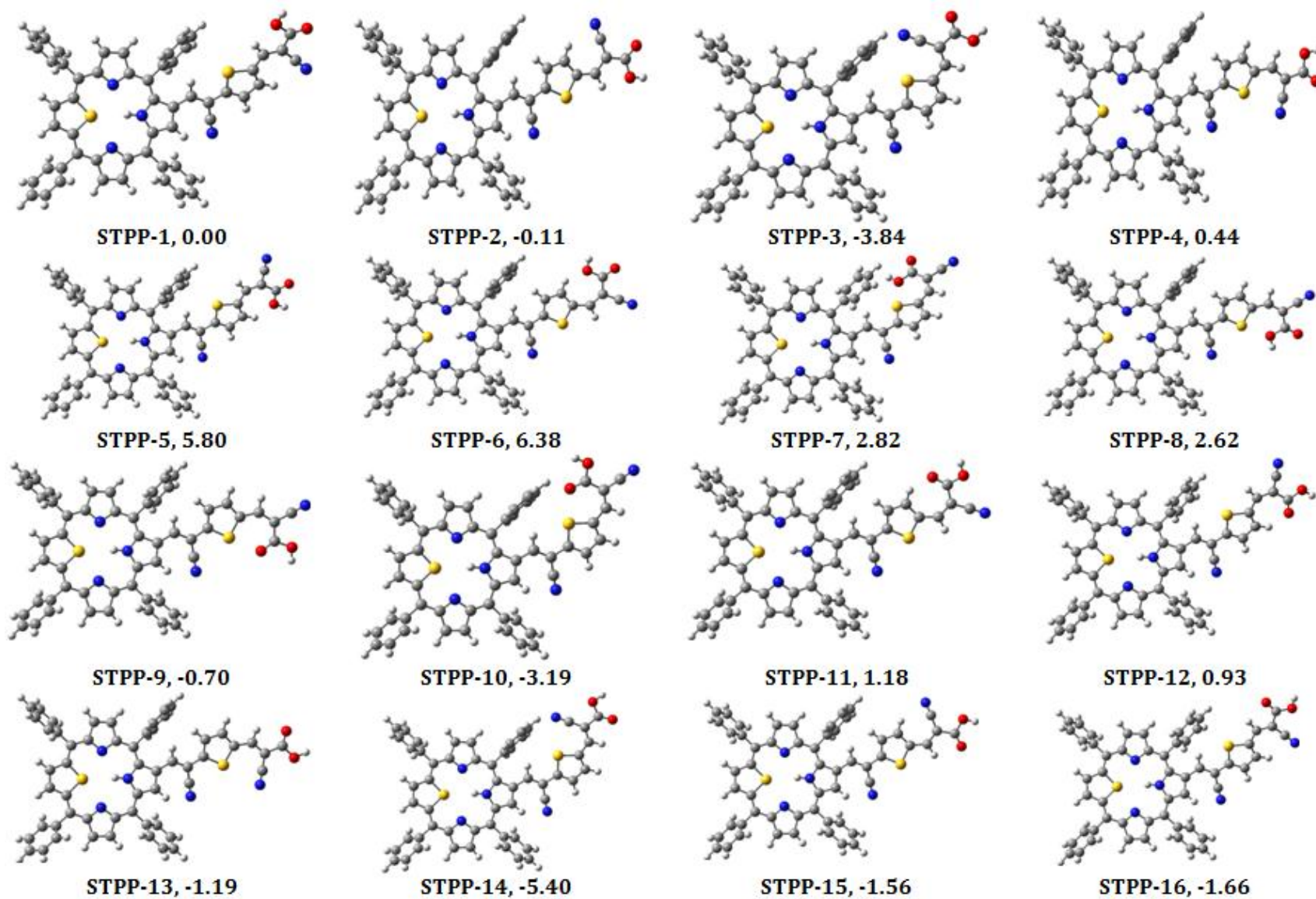


Figure S2: Conformational search carried out for **STPP-βP** at the B3LYP/3-21G* level.

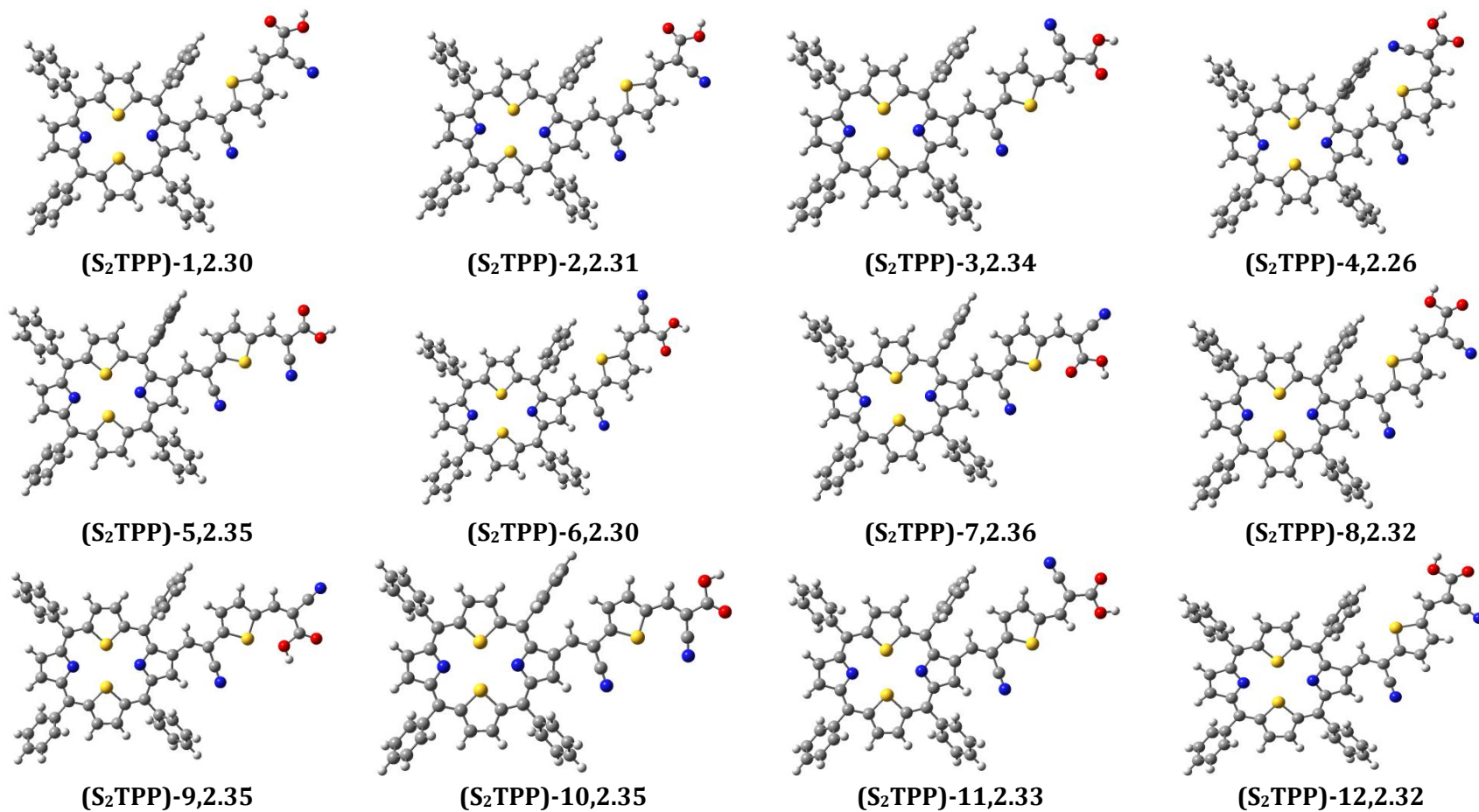


Figure S3: Conformational search carried out for $S_2TPP-\beta N$ at the B3LYP/3-21G* level.

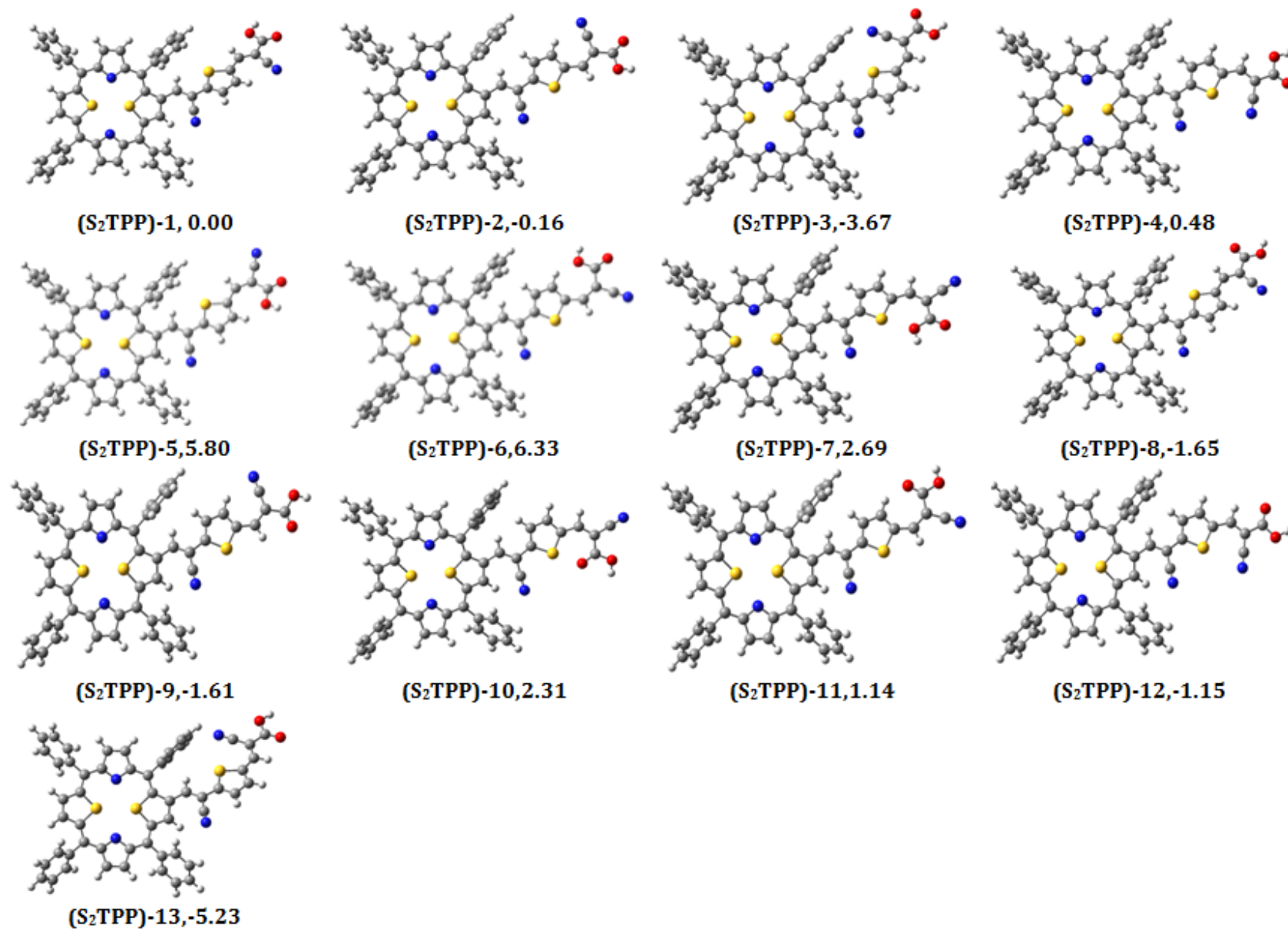


Figure S4: Conformational search carried out for **S₂TPP-βN** at the B3LYP/3-21G* level.

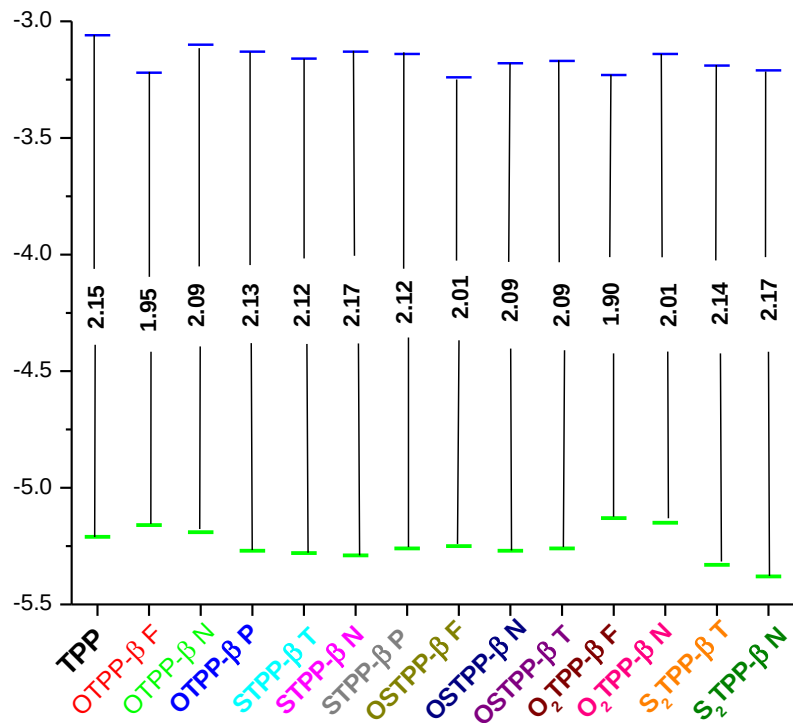
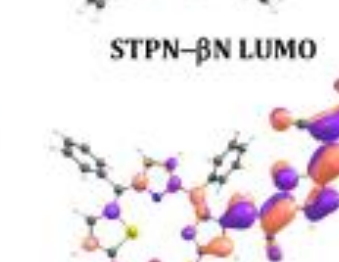
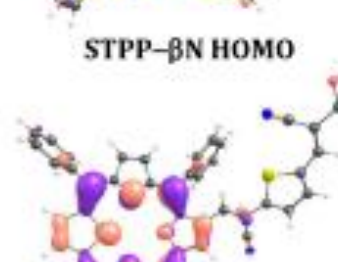
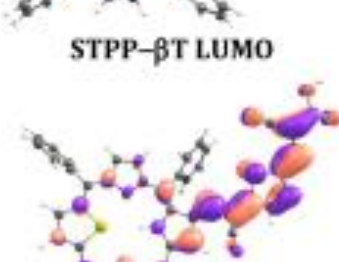
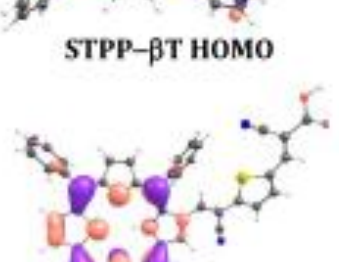
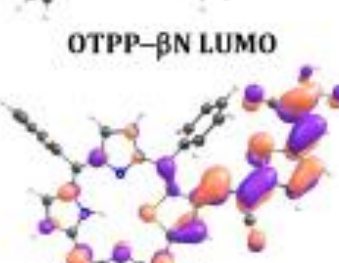
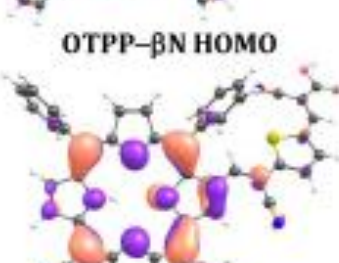
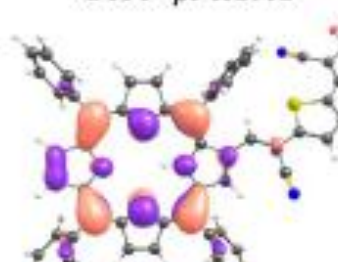
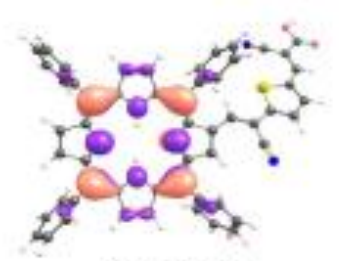


Figure S5: The HOMO-LUMO gap (in eV) at B3LYP/6-31G* level of the β -substituted CMP sensitizers in CHCl_3 solvent.



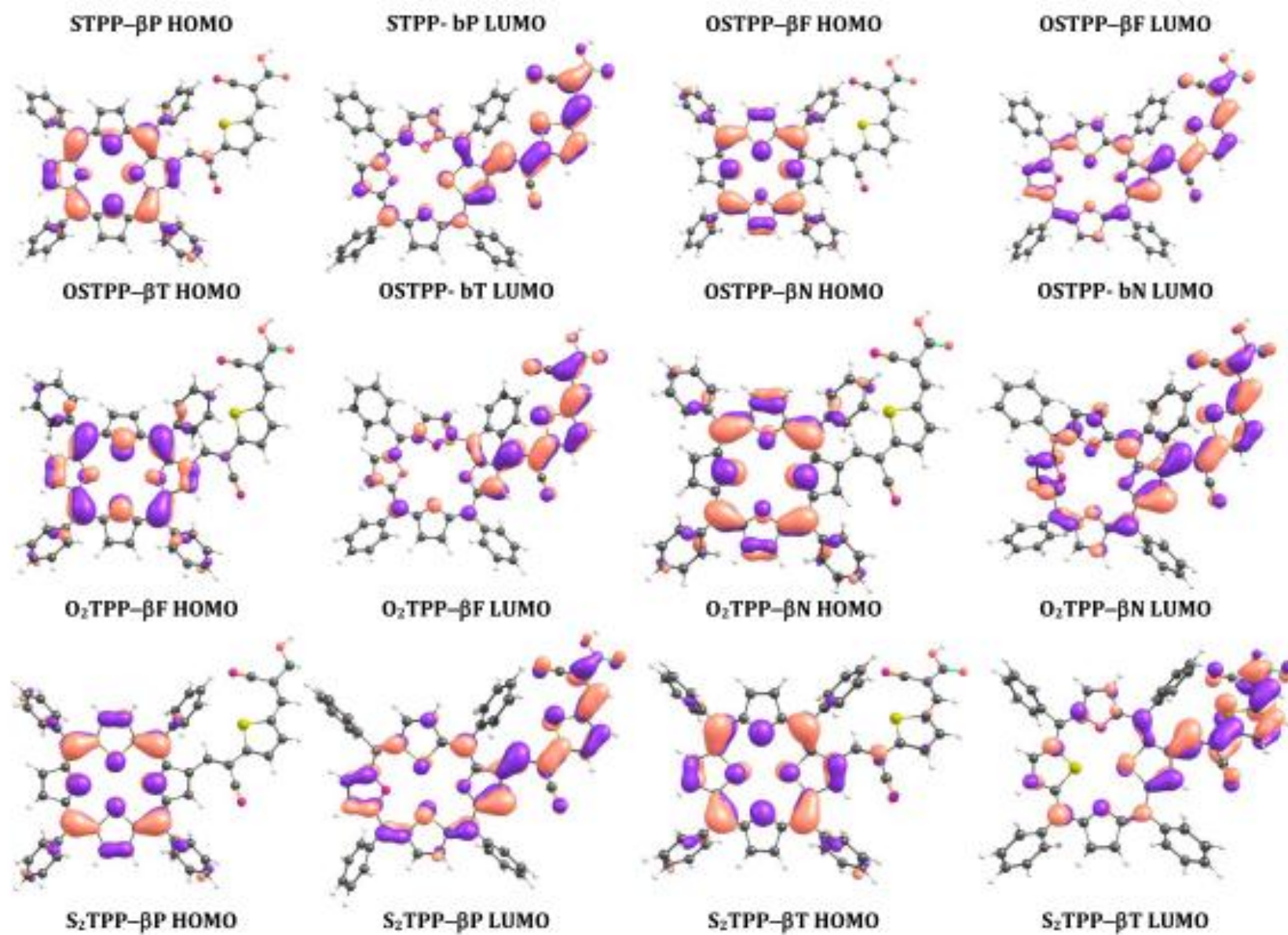


Figure S6: The spatial distribution of the HOMO-LUMO of the sensitizers carried out at the B3LYP/3-21G* level.

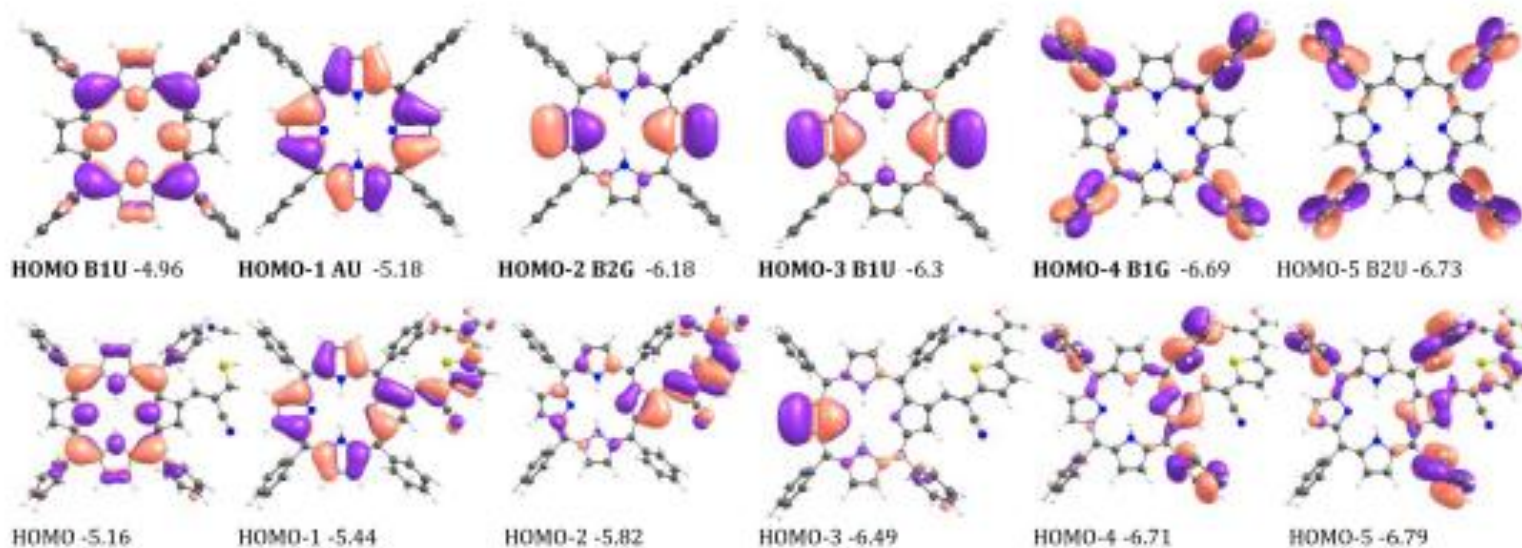


Figure S7: The spatial distribution of the HOMOs of the **TPP** and **TPP- β N** carried out at the B3LYP/6-31G* level.

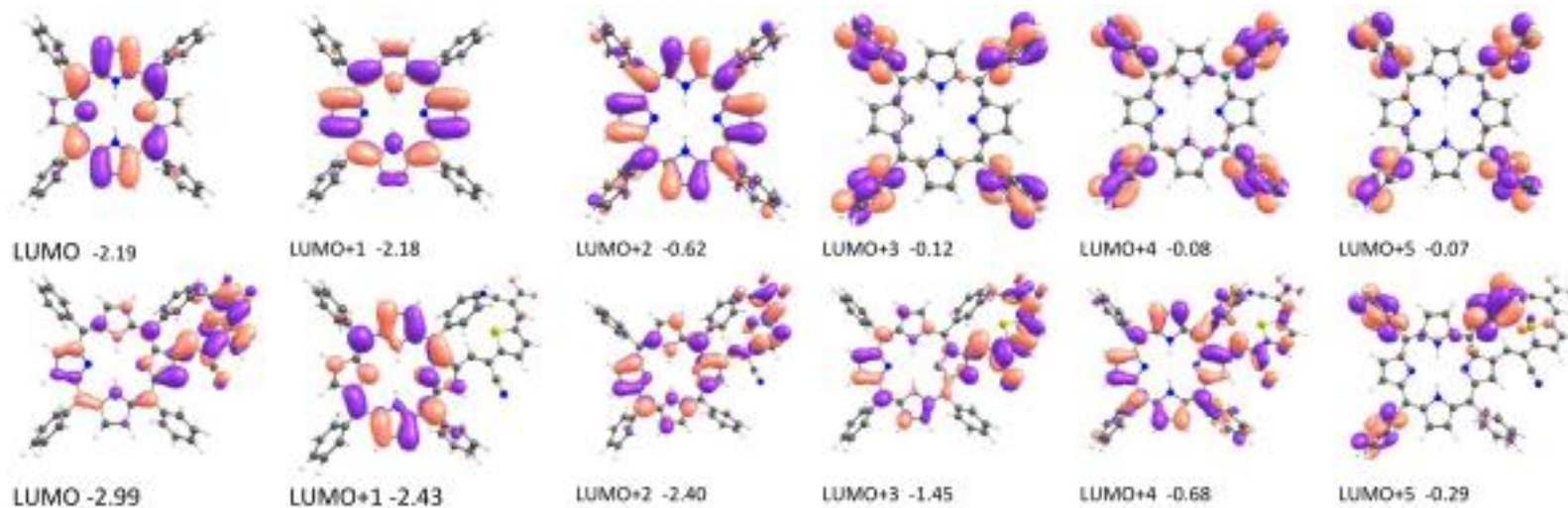


Figure S8: The spatial distribution of the LUMOs of the **TPP** and **TPP- β N** carried out at the B3LYP/6-31G* level.

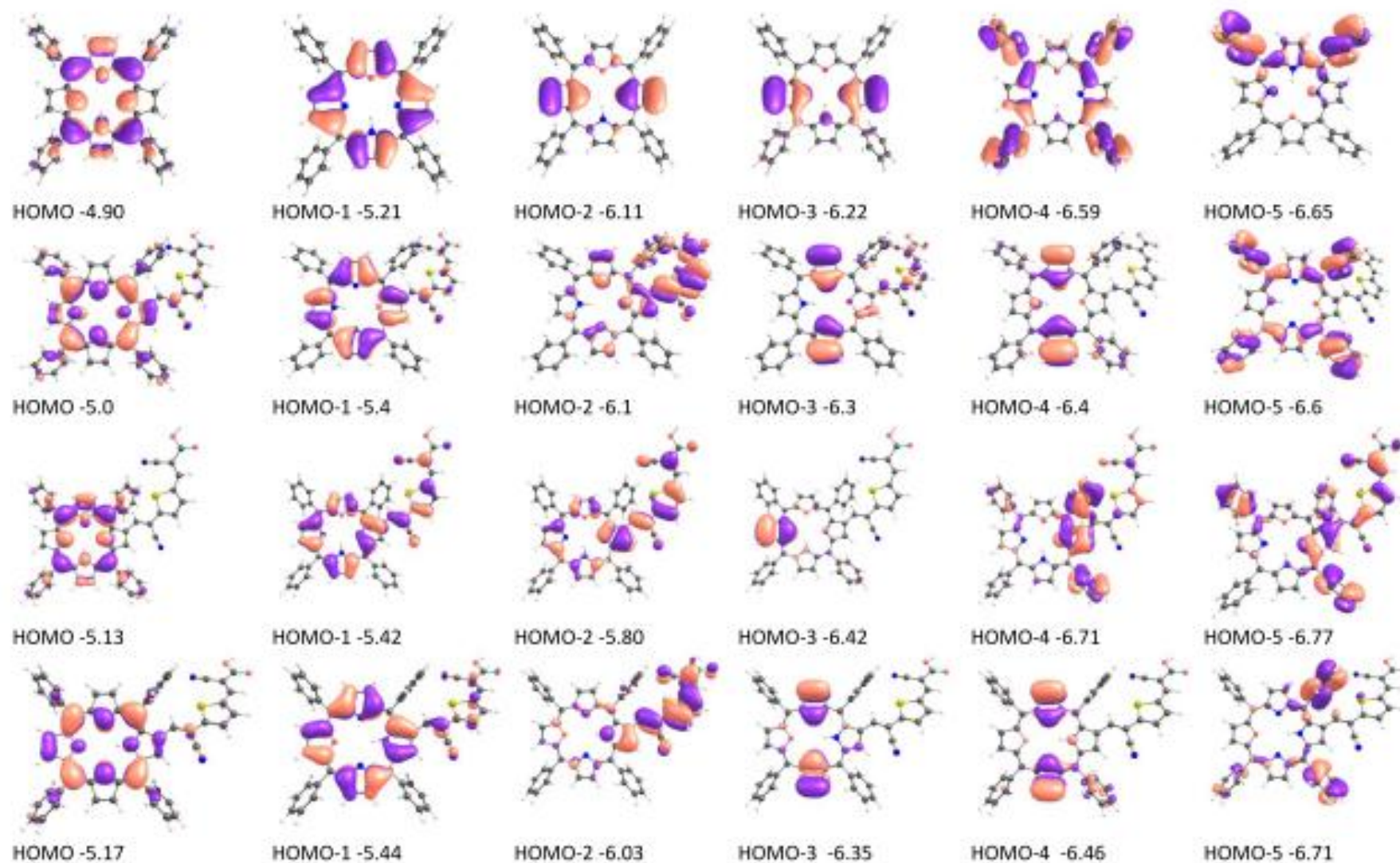


Figure S9: The spatial distribution of the HOMOs of the **OTPP** and **β -substituted analogues** carried out at the B3LYP/6-31G* level.

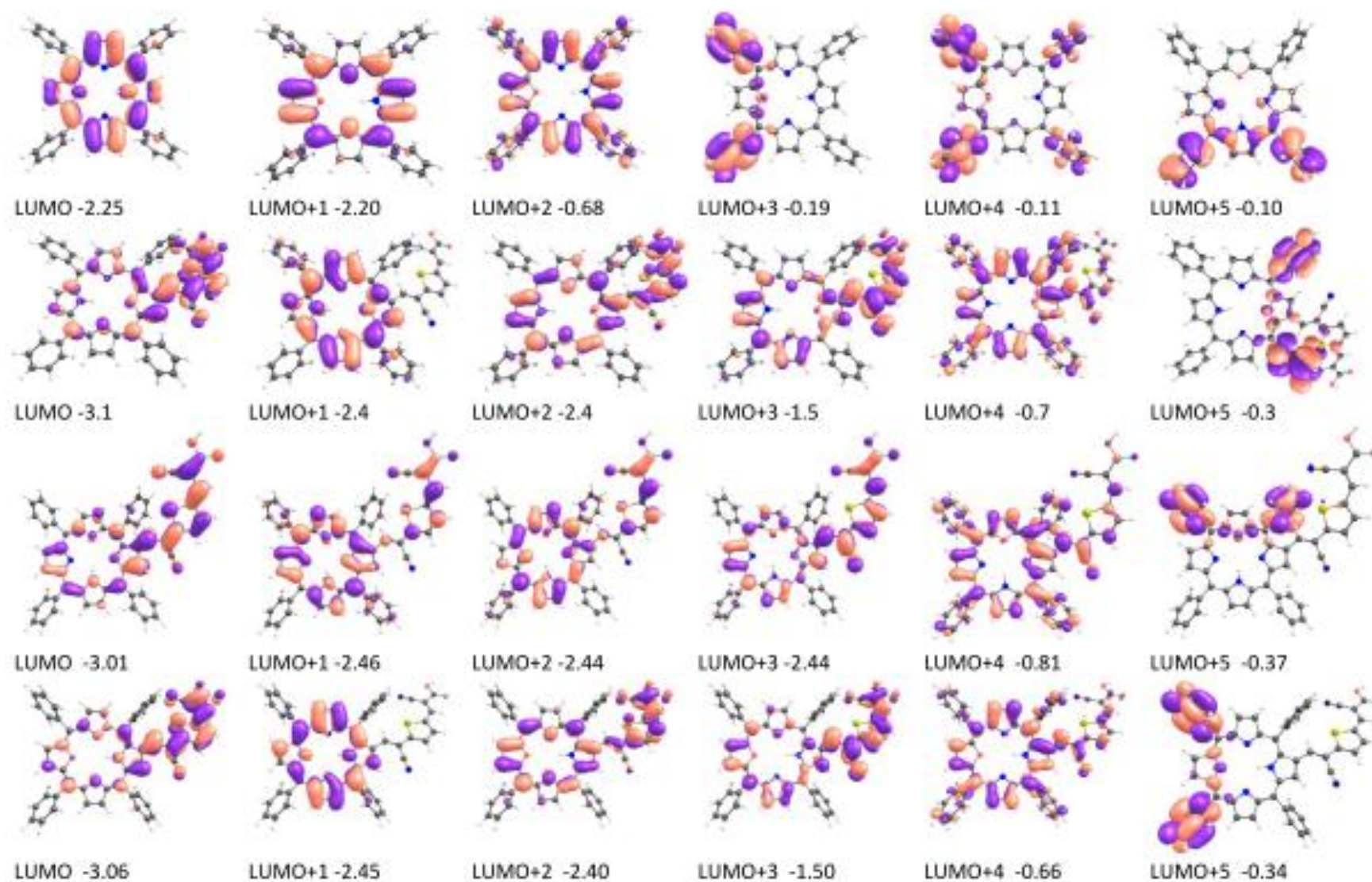


Figure S10: The spatial distribution of the LUMOs of the **OTTP** and **β -substituted analogues** carried out at the B3LYP/6-31G* level.

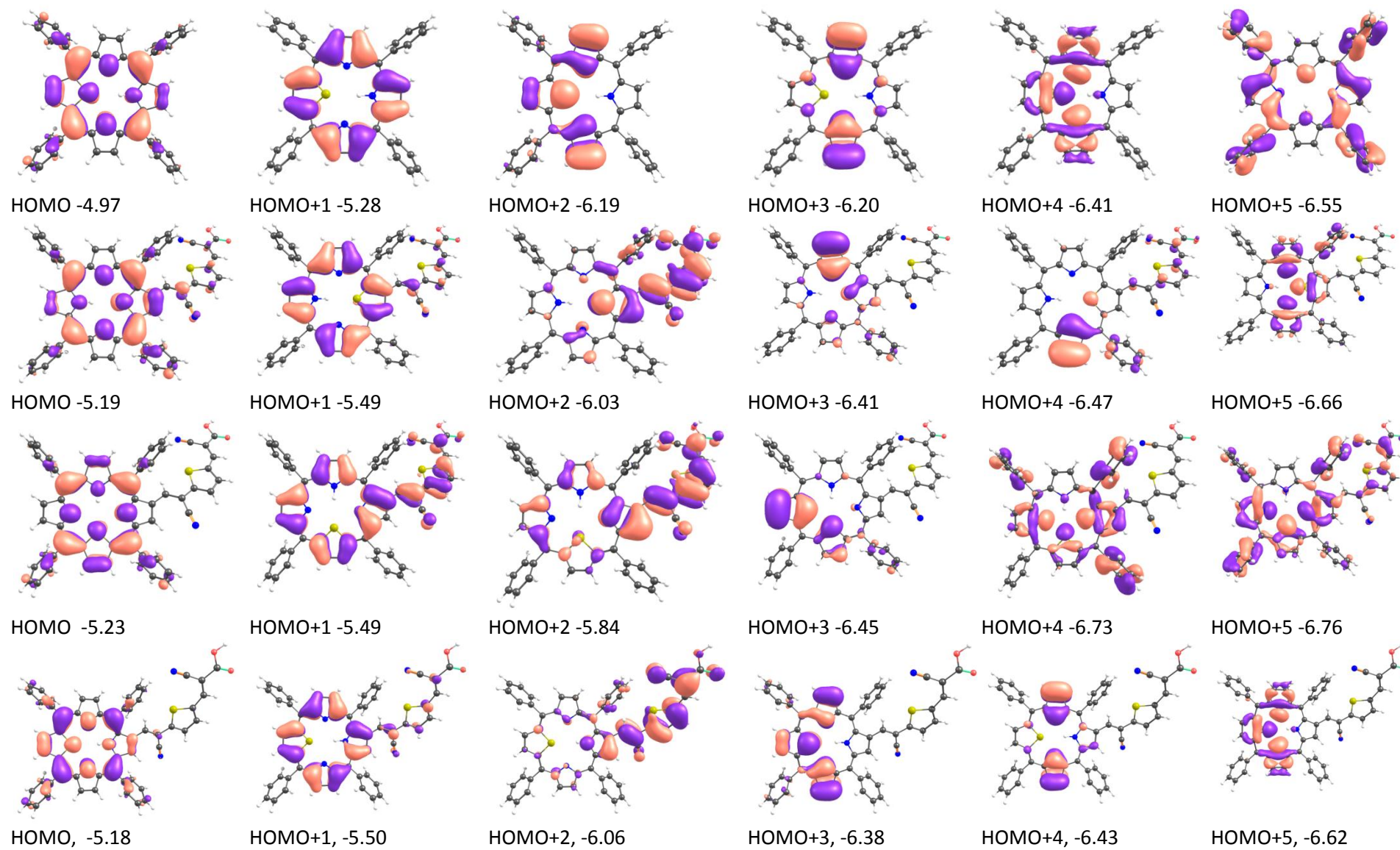


Figure S11: The spatial distribution of the HOMOs of the **STPP** and **β -substituted analogues** carried out at the B3LYP/6-31G* level.

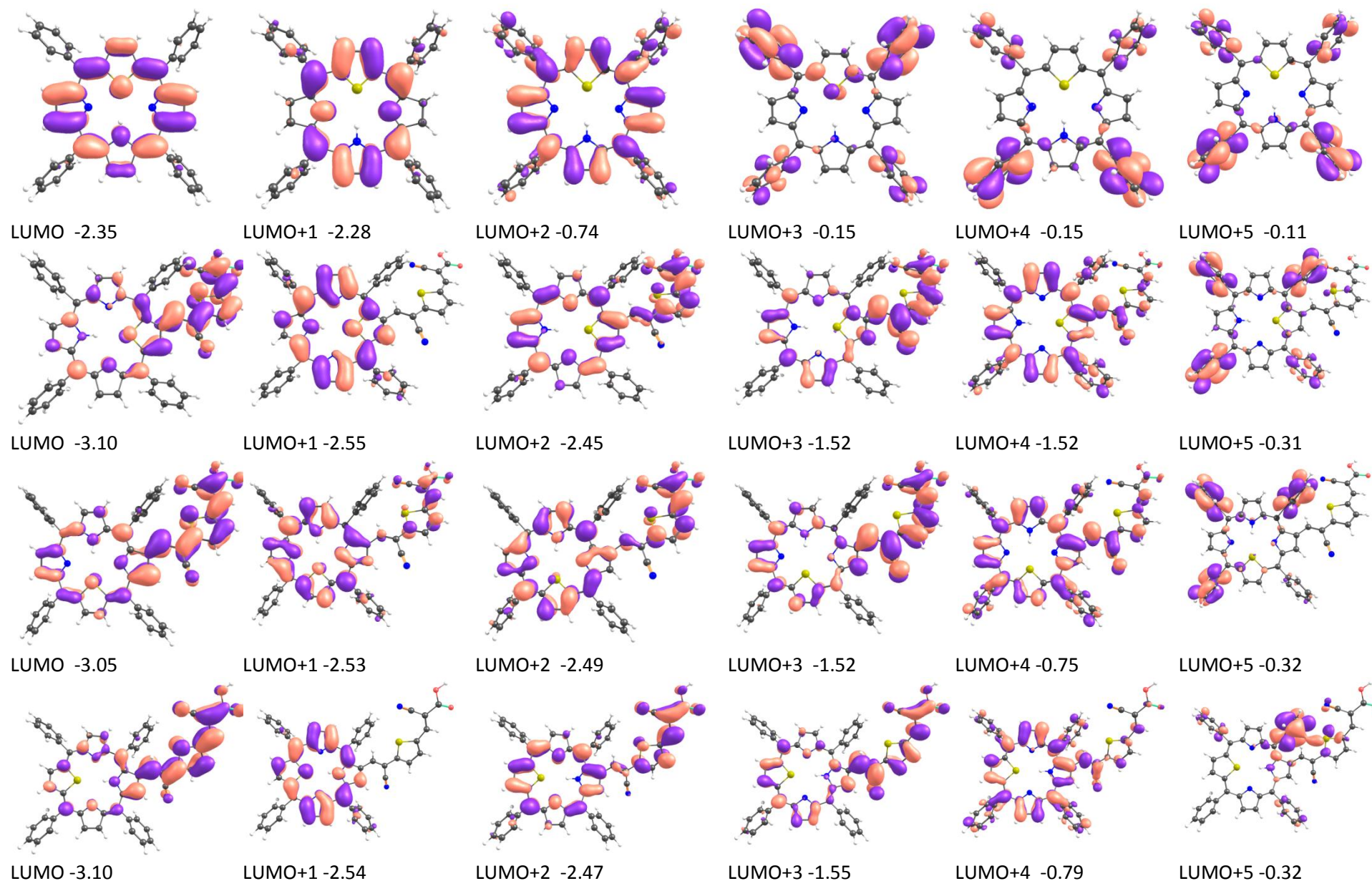


Figure S12: The spatial distribution of the LUMOs of the **STPP** and **β -substituted analogues** carried out at the B3LYP/6-31G* level.

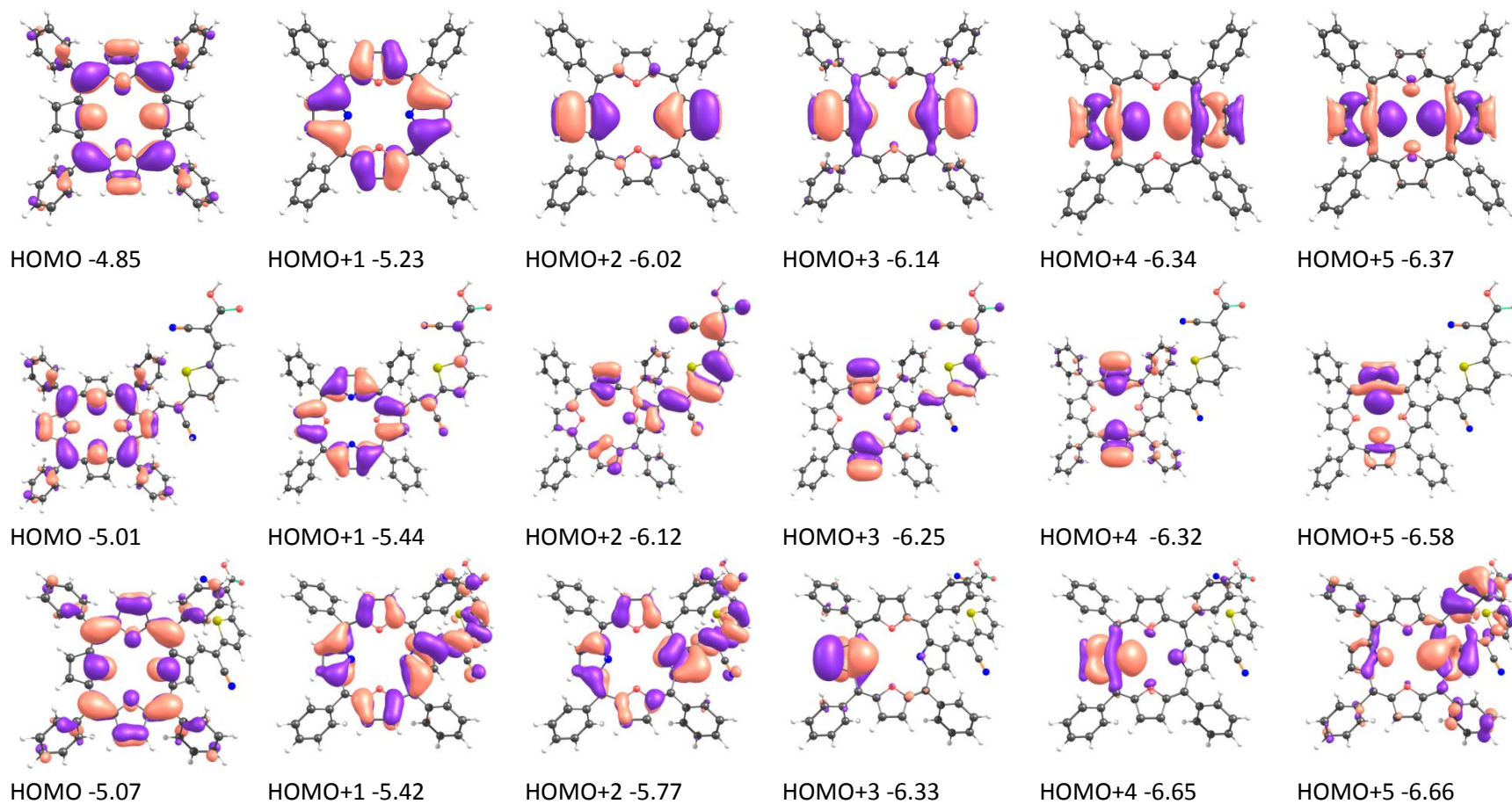


Figure S13: The spatial distribution of the HOMOs of the **O₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

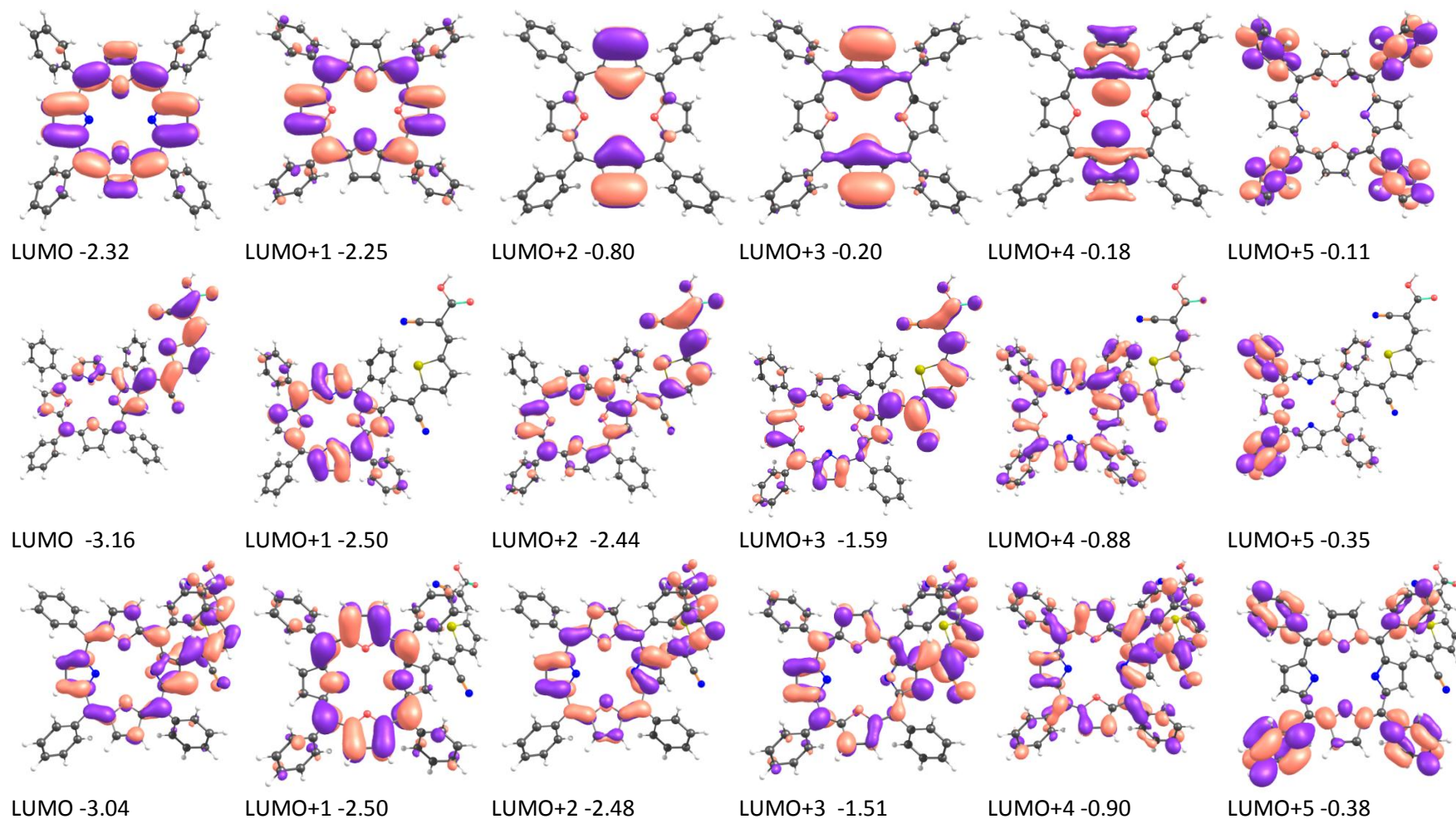


Figure S14: The spatial distribution of the LUMOs of the **O₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

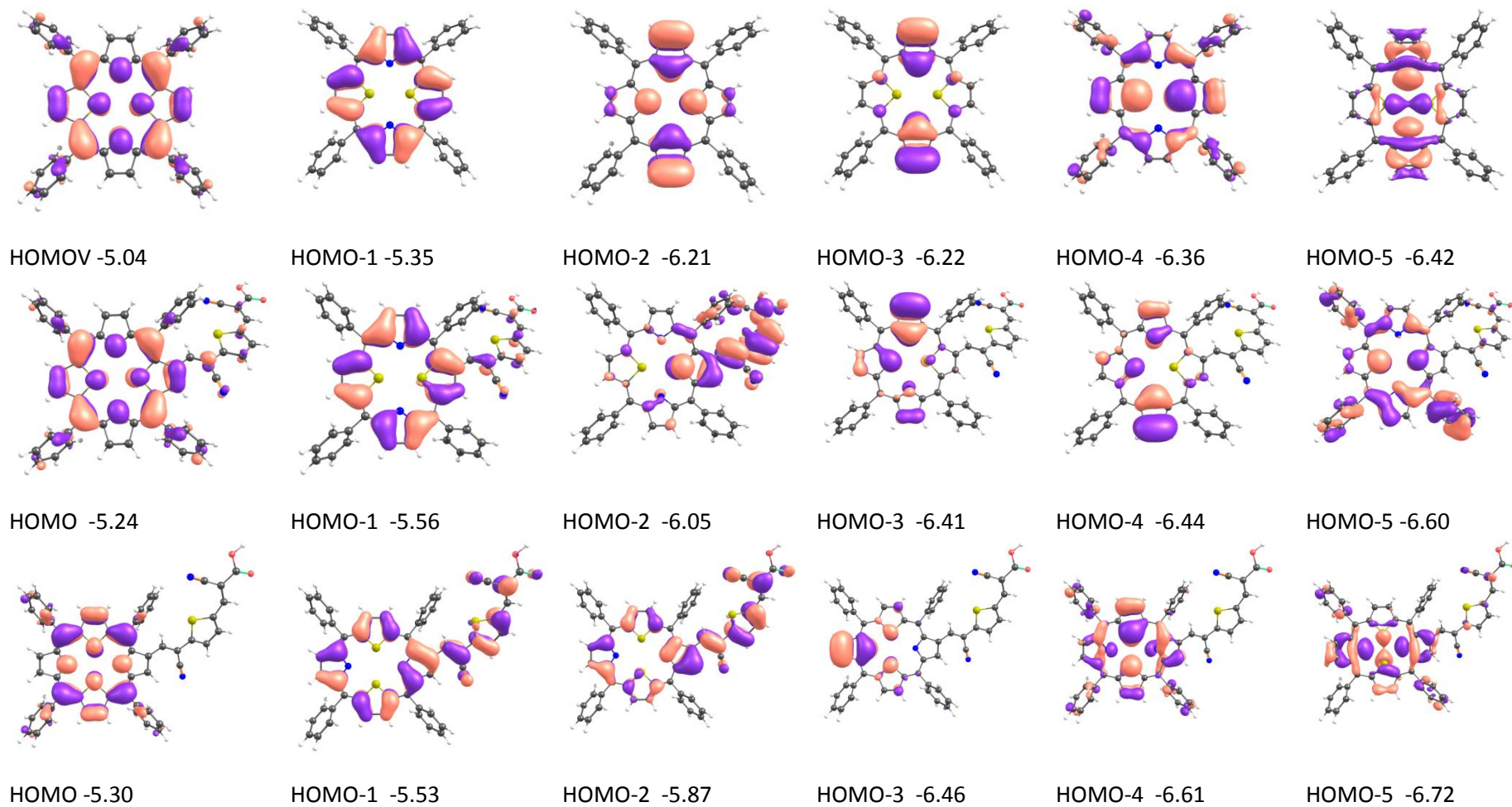


Figure S15: The spatial distribution of the HOMOs of the **S₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

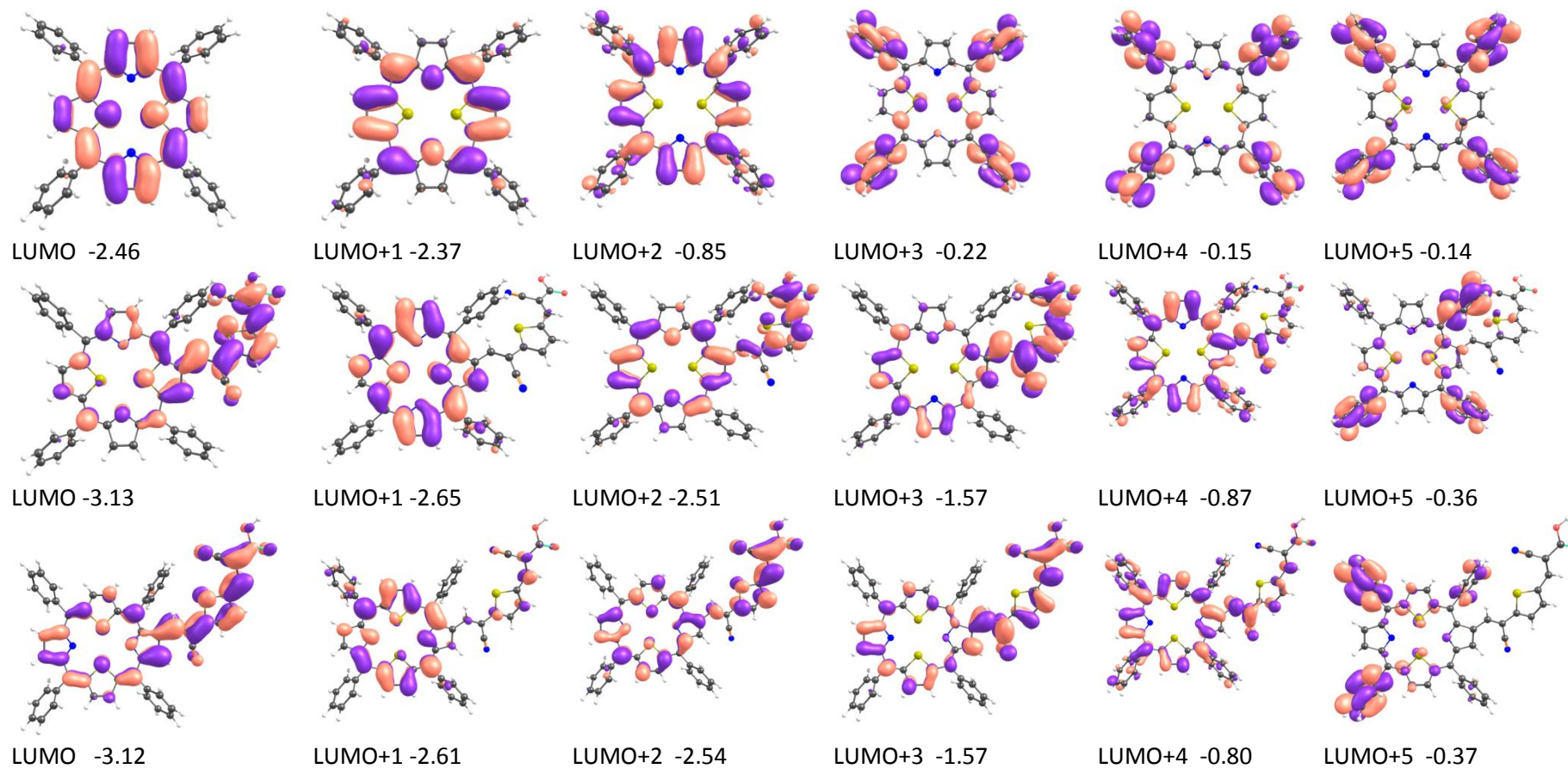


Figure S16: The spatial distribution of the LUMOs of the **S₂TPP** and **β-substituted analogues** carried out at the B3LYP/6-31G* level.

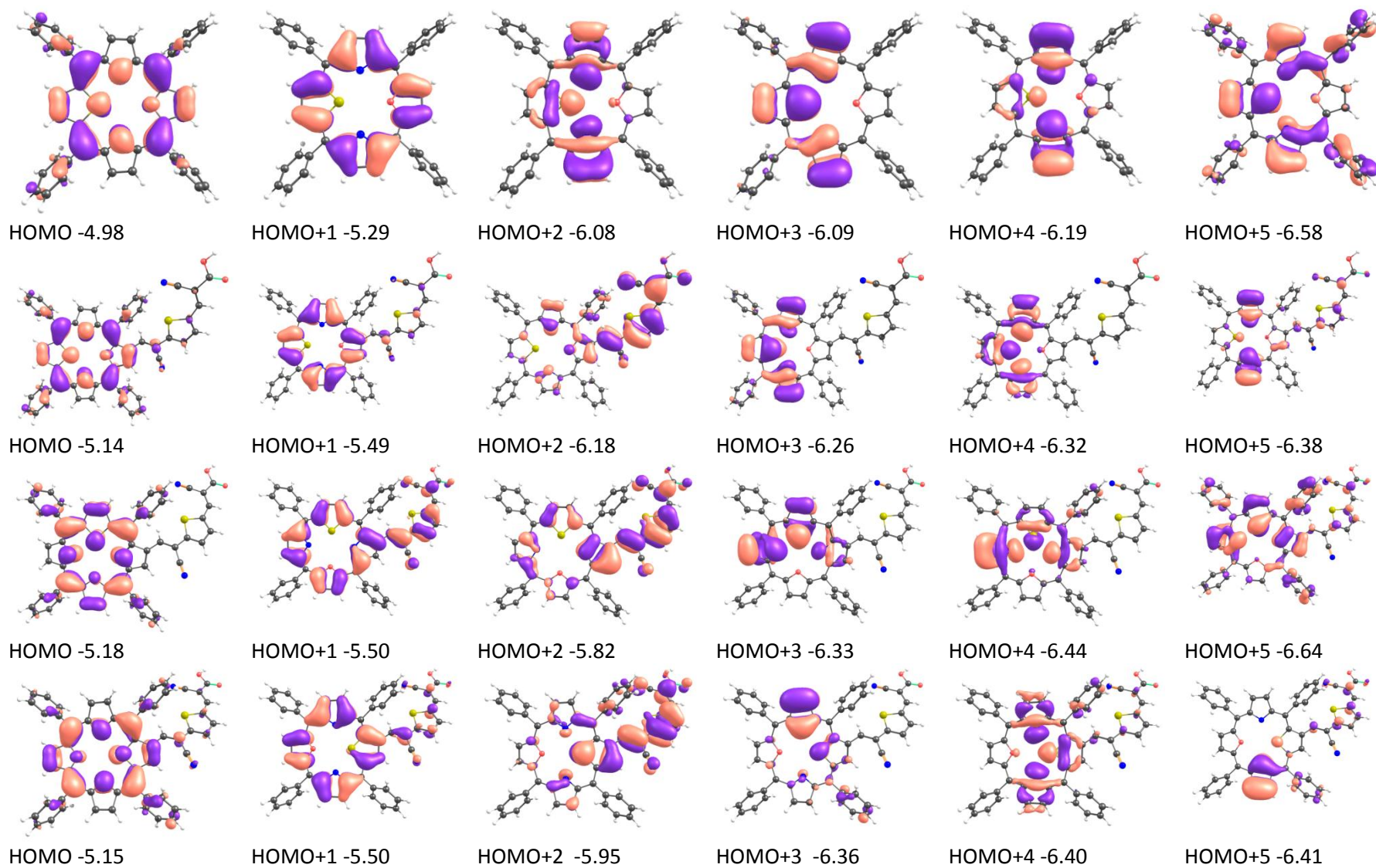


Figure S17: The spatial distribution of the HOMOs of the **OSTPP** and **β -substituted analogues** carried out at the B3LYP/6-31G* level.

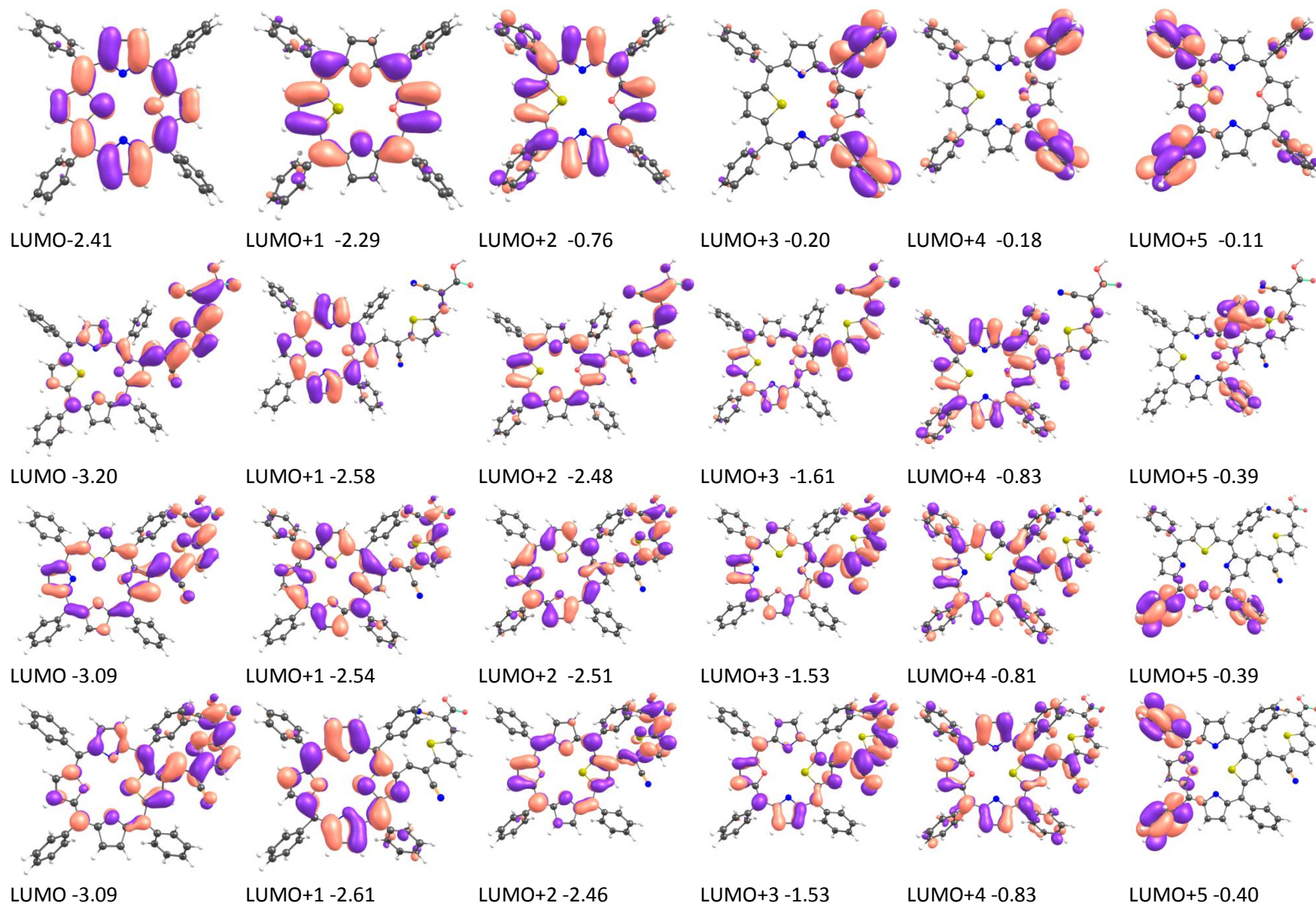
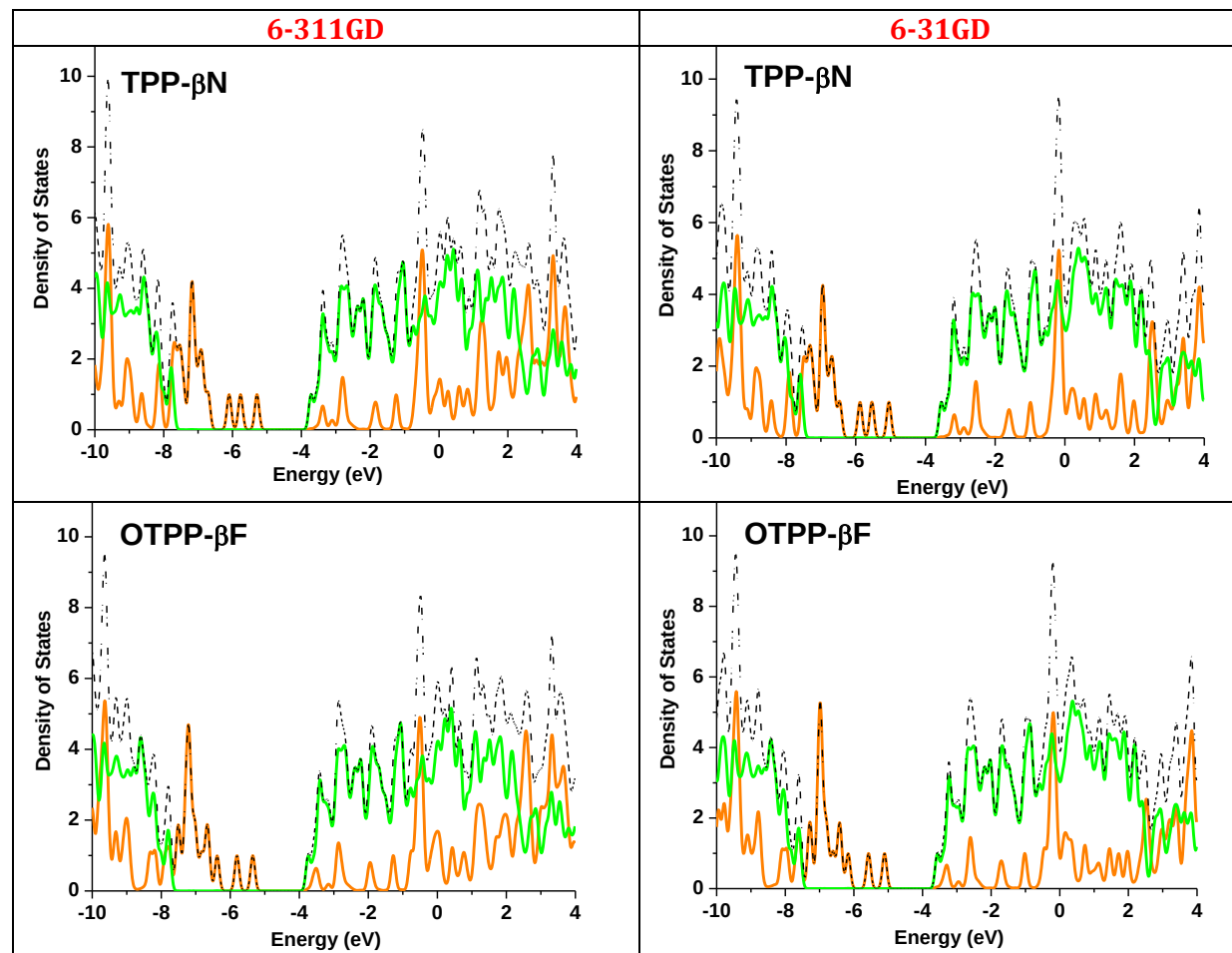
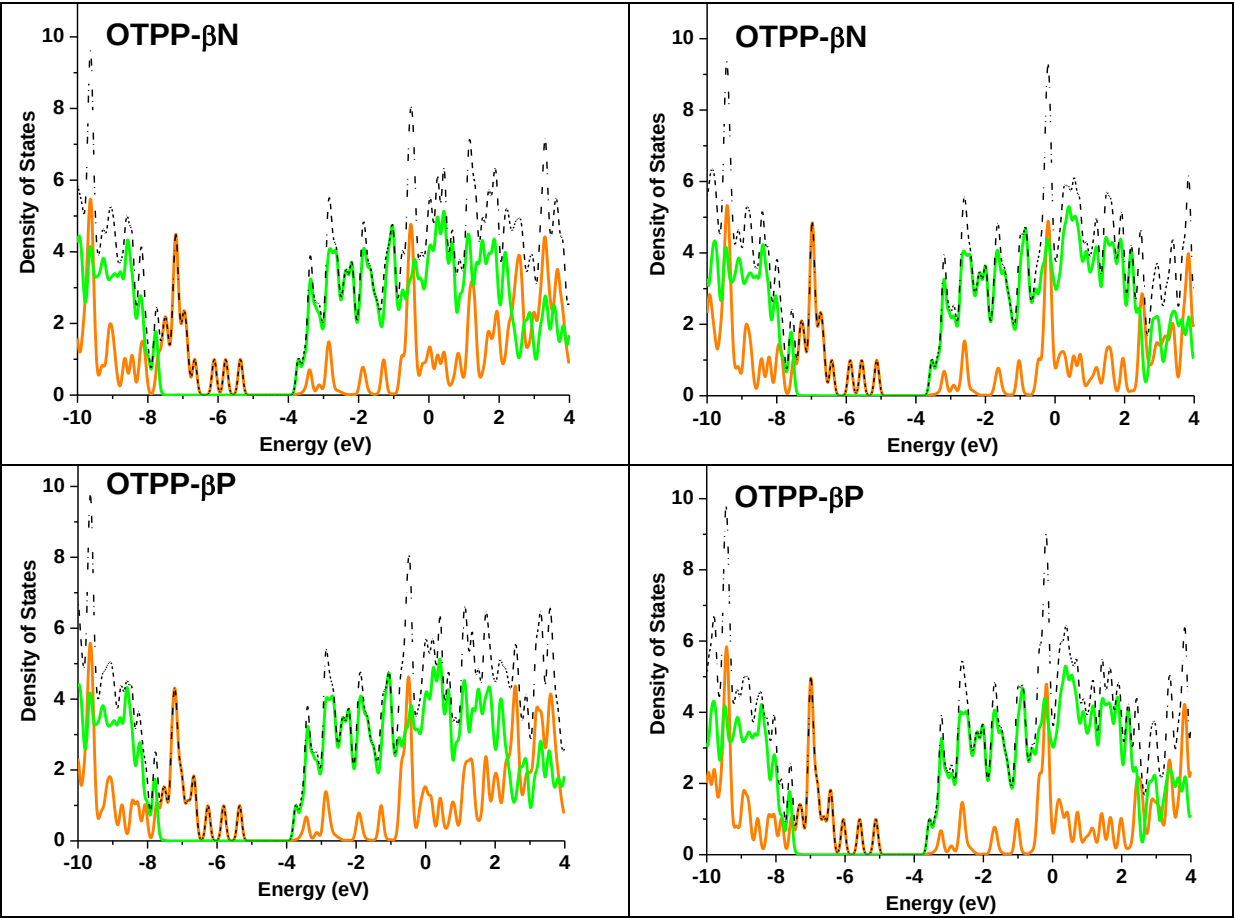
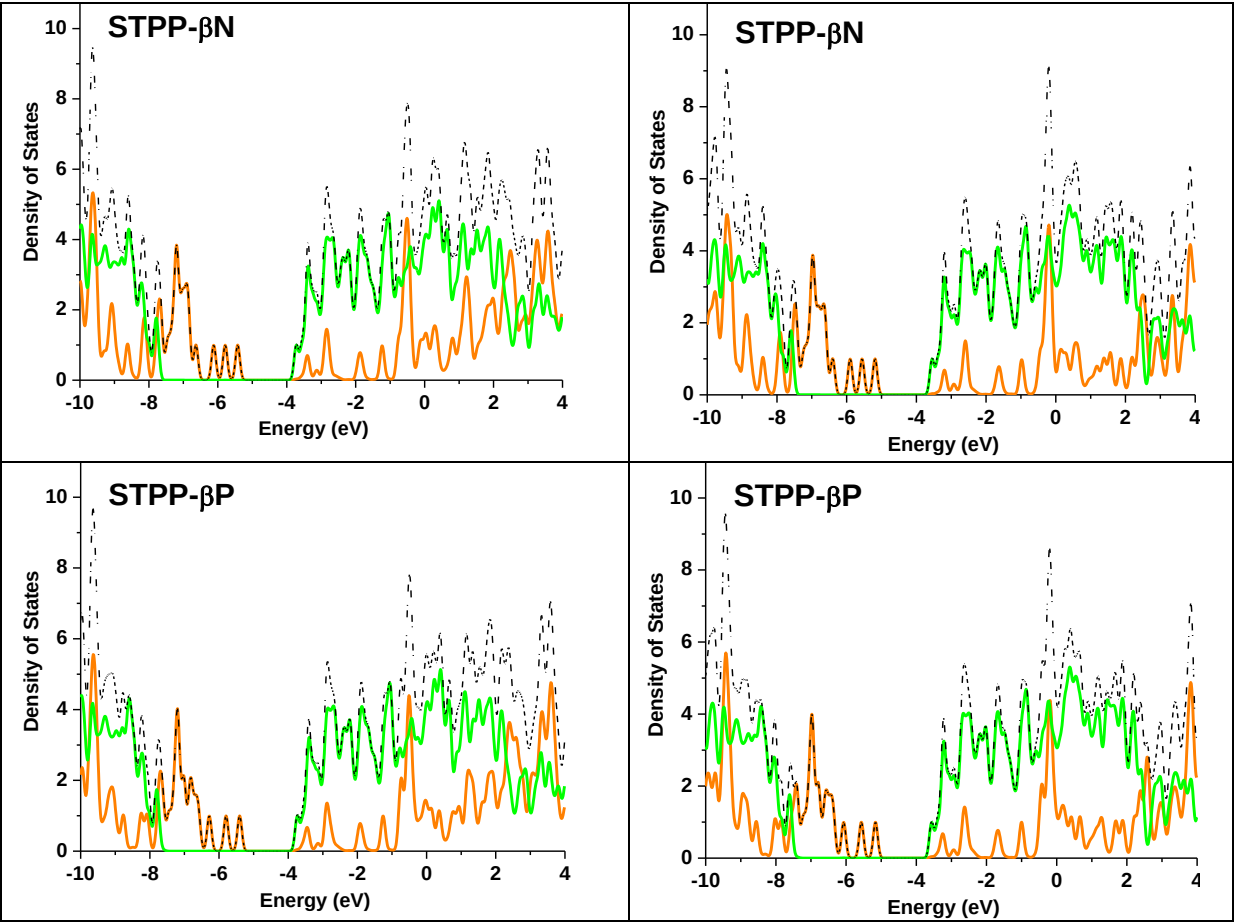


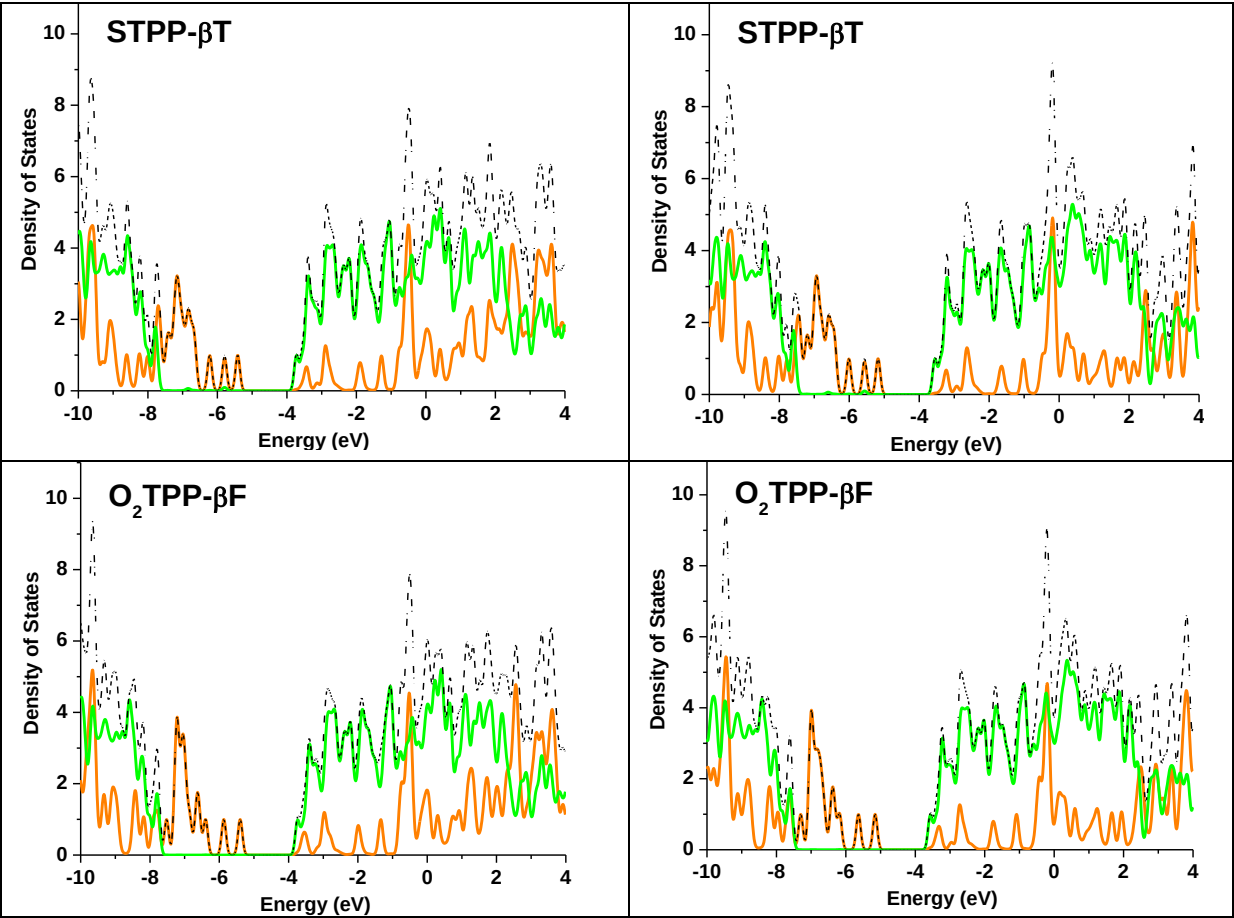
Figure S18: The spatial distribution of the LUMOs of the **OSTTP** and **β -substituted analogues** carried out at the B3LYP/6-31G* level.

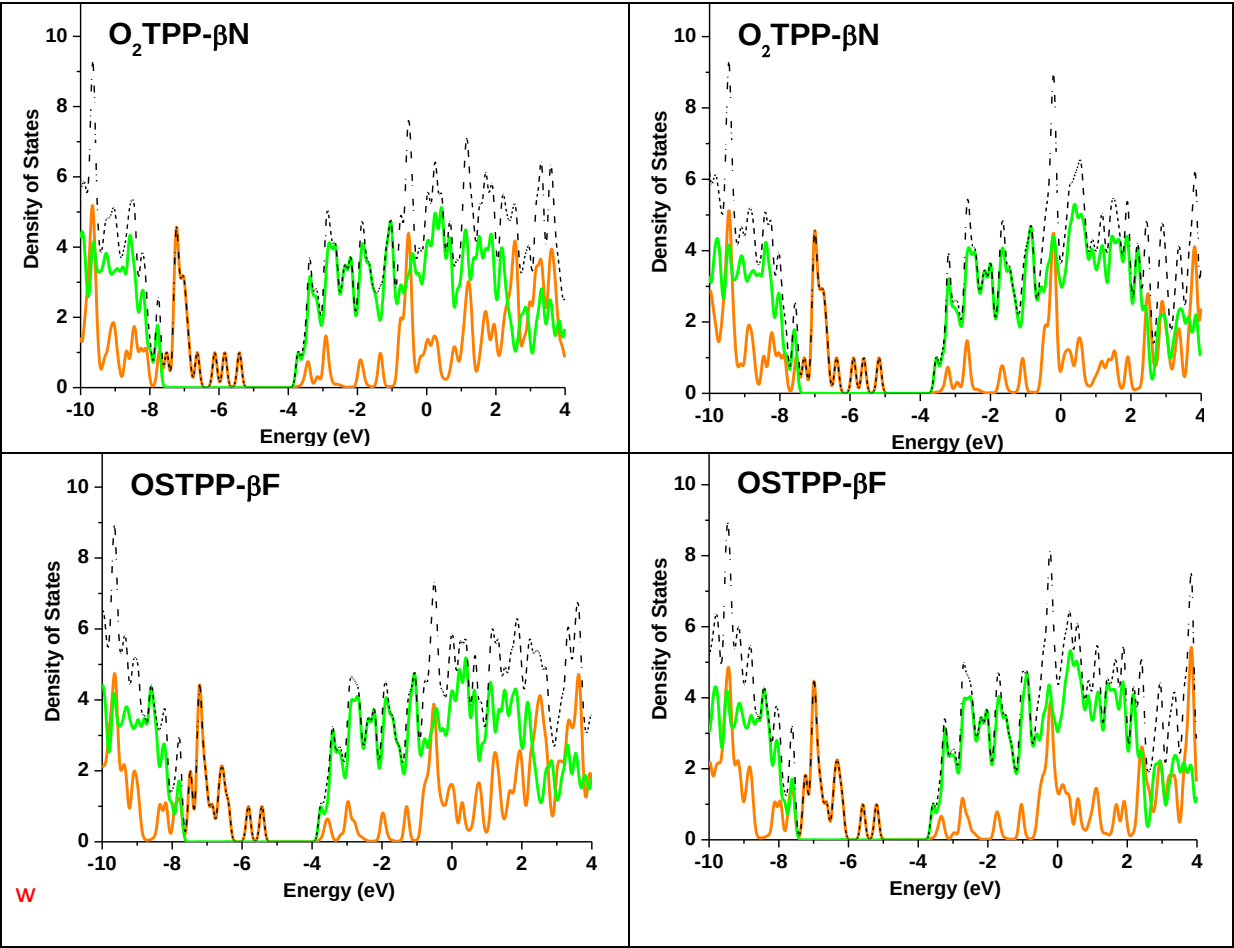
Figure S19: : Total densities of states (TDOS in black) and projected densities of states (PDOS) of dye (in orange) and TiO₂ (in green) of representative dye-(TiO₂)₁₆ complexes at B3LYP/6-311G(d)ULANL2DZ and B3LYP/6-31G(d)ULANL2DZ basis set.

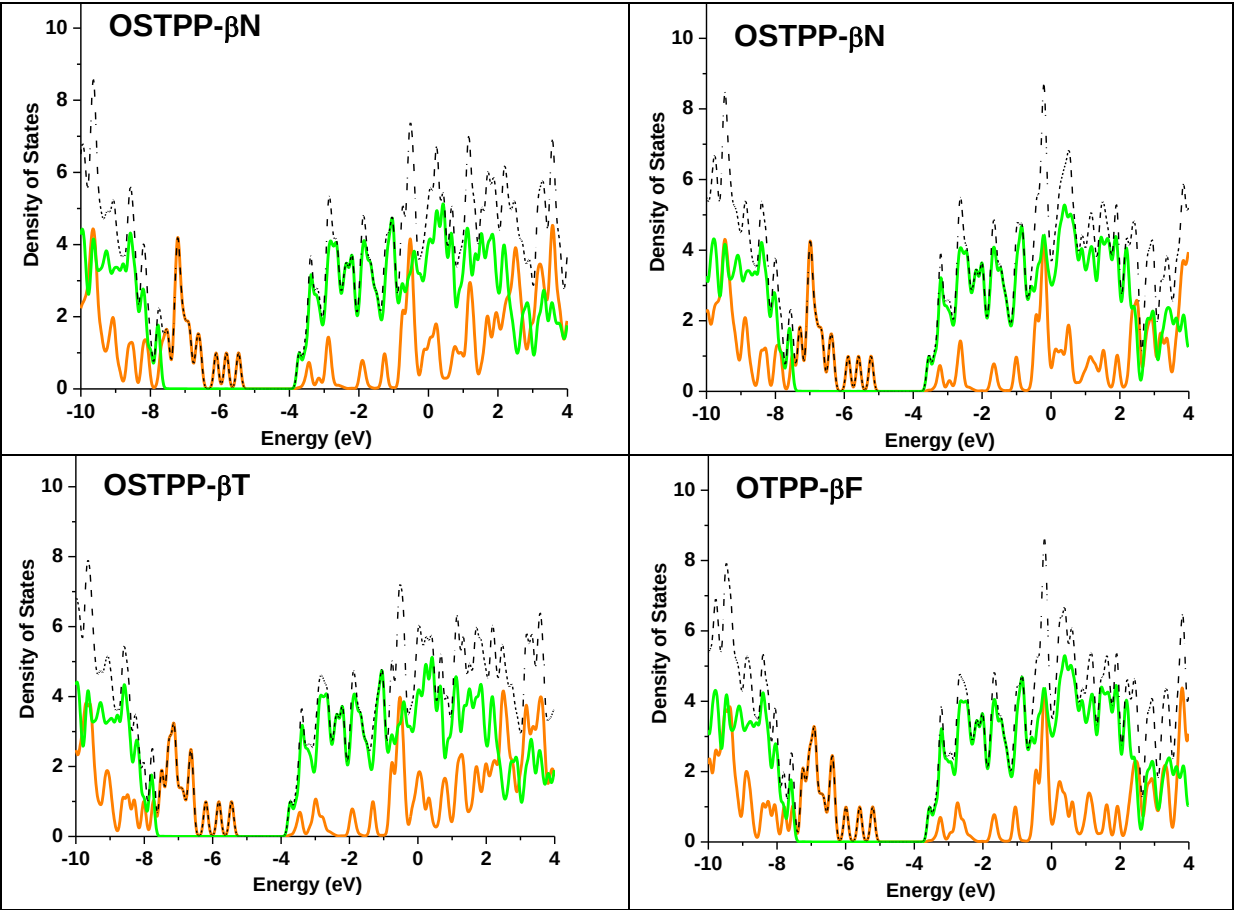












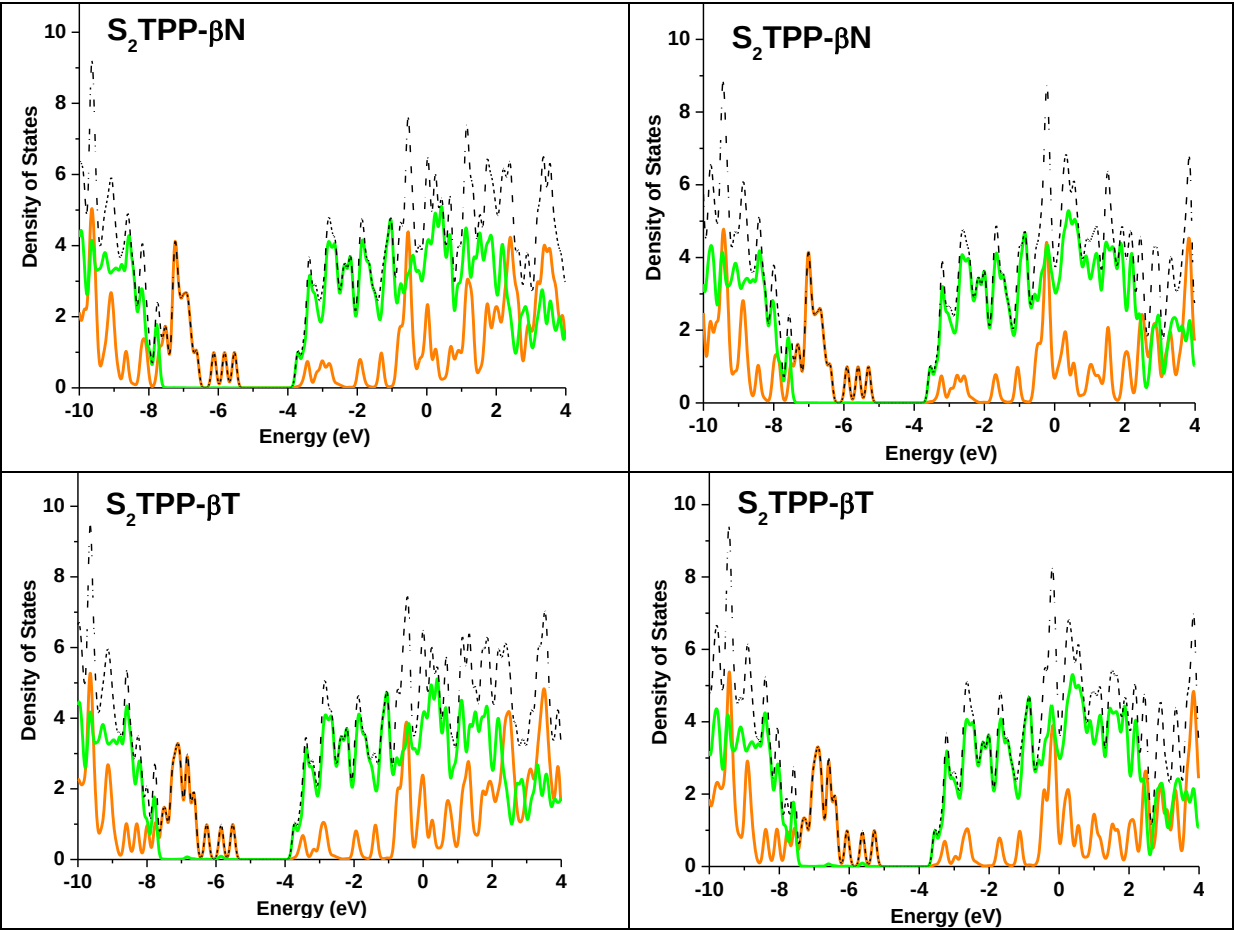


Table S1: The % molecular orbital contribution of the HOMO and LUMO of the core modified porphyrin sensitizers at the B3LYP/6-31G* level.

	MO	E	(%)CMP	(%) <i>meso</i>	(%) β		LUMO	-3.02	41.67	6.27	52.06
TPP	LUMO+4	-0.69	-3.00	19.77	19.64		HOMO	-5.13	80.57	18.85	0.58
	LUMO+3	-1.46	36.55	4.99	58.46		HOMO-1	-5.42	68.04	5.28	26.68
	LUMO+2	-2.41	56.18	7.20	36.62		HOMO-2	-5.80	51.35	4.72	43.94
	LUMO+1	-2.44	83.87	12.25	3.88		HOMO-3	-6.43	93.65	6.03	0.32
	LUMO	-3.00	34.66	4.62	60.72		HOMO-4	-6.72	41.07	49.73	9.20
	HOMO	-5.17	82.16	17.51	0.34	OTPP- β P	LUMO+4	-0.67	59.49	20.73	19.78
	HOMO-1	-5.44	76.56	3.89	19.55		LUMO+3	-1.50	35.26	4.70	60.04
	HOMO-2	-5.83	42.48	3.47	54.05		LUMO+2	-2.41	55.15	7.88	36.97
	HOMO-3	-6.49	93.41	6.03	0.56		LUMO+1	-2.46	87.49	10.48	2.03
	HOMO-4	-6.71	28.56	67.58	3.86		LUMO	-3.07	30.26	3.93	65.81
OTPP- β F	LUMO+4	-0.78	57.03	28.44	14.53		HOMO	-5.18	81.48	14.92	3.60
	LUMO+3	-1.56	36.41	7.34	56.25		HOMO-1	-5.44	84.74	4.68	10.59
	LUMO+2	-2.42	49.62	8.69	41.69		HOMO-2	-6.03	29.09	3.82	67.09
	LUMO+1	-2.45	85.48	13.08	1.44		HOMO-3	-6.35	96.65	1.59	1.77
	LUMO	-3.18	29.74	4.83	65.44		HOMO-4	-6.46	90.84	8.96	0.20
	HOMO	-5.07	77.56	17.51	4.93	STPP- β T	LUMO+4	-0.79	63.74	19.62	16.64
	HOMO-1	-5.43	85.47	7.19	7.34		LUMO+3	-1.52	33.75	4.87	61.38
	HOMO-2	-6.16	27.68	5.84	66.48		LUMO+2	-2.46	53.44	8.08	38.48
	HOMO-3	-6.34	86.50	4.47	9.02		LUMO+1	-2.55	87.00	10.20	2.80
	HOMO-4	-6.41	89.61	10.22	0.17		LUMO	-3.11	32.63	4.48	62.89
OTPP- β N	LUMO+4	-0.82	51.88	27.05	21.07		HOMO	-5.20	78.18	15.81	6.01
	LUMO+3	-1.49	38.81	7.25	53.94		HOMO-1	-5.50	86.81	5.42	7.77
	LUMO+2	-2.45	64.38	11.37	24.25		HOMO-2	-6.04	37.57	4.38	58.04
	LUMO+1	-2.46	66.91	11.23	21.86		HOMO-3	-6.42	94.58	4.71	0.71

STPP- β N	HOMO-4	-6.47	86.47	6.56	6.96	OSTPP- β N	HOMO	-5.15	78.34	17.03	4.63
	LUMO+4	-0.76	56.61	21.28	22.11		HOMO-1	-5.49	86.26	6.88	6.86
	LUMO+3	-1.52	37.48	4.73	57.79		HOMO-2	-6.18	26.89	6.50	66.61
	LUMO+2	-2.50	61.82	8.83	29.35		HOMO-3	-6.27	94.54	5.16	0.30
	LUMO+1	-2.53	72.99	10.46	16.55		HOMO-4	-6.32	98.99	0.93	0.08
	LUMO	-3.06	42.65	5.09	52.26		LUMO+4	-0.81	53.28	32.55	14.17
	HOMO	-5.24	82.08	17.67	0.24		LUMO+3	-1.54	38.73	16.62	44.65
	HOMO-1	-5.50	71.26	3.87	24.87		LUMO+2	-2.52	61.98	12.01	26.01
	HOMO-2	-5.85	49.57	3.76	46.67		LUMO+1	-2.55	66.62	12.70	20.68
	HOMO-3	-6.45	94.29	5.53	0.19		LUMO	-3.09	47.60	14.50	37.90
STPP- β P	HOMO-4	-6.73	60.69	37.20	2.10		HOMO	-5.19	81.99	17.32	0.68
	LUMO+4	-0.80	60.23	22.21	17.56		HOMO-1	-5.50	69.74	6.80	23.47
	LUMO+3	-1.56	33.35	5.71	60.94		HOMO-2	-5.83	51.35	9.41	39.24
	LUMO+2	-2.47	55.33	9.11	35.55		HOMO-3	-6.34	97.61	2.12	0.27
	LUMO+1	-2.55	86.40	10.51	3.09		HOMO-4	-6.45	95.55	4.13	0.32
	LUMO	-3.10	30.71	4.78	64.52		LUMO+4	-0.84	58.38	23.29	18.33
	HOMO	-5.18	79.90	17.47	2.63		LUMO+3	-1.53	35.34	5.84	58.82
	HOMO-1	-5.50	84.57	5.84	9.60		LUMO+2	-2.47	51.31	8.76	39.93
	HOMO-2	-6.06	25.63	5.74	68.64		LUMO+1	-2.61	85.68	10.86	3.46
	HOMO-3	-6.38	93.78	6.05	0.17		LUMO	-3.10	35.87	5.46	58.67
OSTPP- β F	HOMO-4	-6.43	95.80	2.54	1.66	OSTPP- β T	HOMO	-5.16	79.23	16.55	4.22
	LUMO+4	-0.83	60.06	24.45	15.49		HOMO-1	-5.51	82.97	6.11	10.92
	LUMO+3	-1.61	34.29	6.61	59.11		HOMO-2	-5.96	45.14	4.43	50.44
	LUMO+2	-2.49	54.02	9.55	36.43		HOMO-3	-6.36	92.00	6.44	1.56
	LUMO+1	-2.59	83.81	10.28	5.91		HOMO-4	-6.41	93.60	3.39	3.00
	LUMO	-3.20	30.79	4.87	64.33						

O₂TPP- βF	LUMO+4	-0.89	53.26	30.81	15.93	S₂TPP- βT	LUMO+4	-0.88	61.48	20.50	18.03
	LUMO+3	-1.60	36.39	8.50	55.11		LUMO+3	-1.58	33.35	5.30	61.34
	LUMO+2	-2.45	49.71	9.84	40.45		LUMO+2	-2.52	52.92	8.54	38.55
	LUMO+1	-2.50	84.25	14.43	1.31		LUMO+1	-2.65	86.48	9.70	3.81
	LUMO	-3.17	30.96	5.64	63.39		LUMO	-3.14	35.20	4.96	59.85
	HOMO	-5.02	78.11	18.41	3.48		HOMO	-5.24	78.13	16.34	5.52
	HOMO-1	-5.44	82.14	8.62	9.24		HOMO-1	-5.56	85.45	5.93	8.63
	HOMO-2	-6.13	36.56	5.55	57.90		HOMO-2	-6.06	35.86	4.96	59.18
	HOMO-3	-6.25	79.95	4.76	15.28		HOMO-3	-6.42	94.99	4.49	0.52
	HOMO-4	-6.33	87.82	11.31	0.86		HOMO-4	-6.45	95.25	3.38	1.37
O₂TPP- βN	LUMO+4	-0.90	45.98	27.76	26.26	S₂TPP- βN	LUMO+4	-0.81	55.10	21.38	23.52
	LUMO+3	-1.52	42.32	9.63	48.05		LUMO+3	-1.58	39.16	4.67	56.17
	LUMO+2	-2.48	43.97	7.51	48.52		LUMO+2	-2.55	51.45	6.24	42.31
	LUMO+1	-2.50	80.48	16.50	3.01		LUMO+1	-2.61	78.76	12.07	9.17
	LUMO	-3.05	48.18	7.78	44.05		LUMO	-3.13	49.58	5.16	45.26
	HOMO	-5.08	79.32	19.06	1.62		HOMO	-5.31	83.17	16.65	0.18
	HOMO-1	-5.43	62.75	6.51	30.75		HOMO-1	-5.54	65.17	3.29	31.54
	HOMO-2	-5.78	58.42	5.89	35.69		HOMO-2	-5.88	55.72	3.92	40.35
	HOMO-3	-6.34	93.15	6.30	0.54		HOMO-3	-6.47	95.29	4.62	0.09
	HOMO-4	-6.65	96.80	2.71	0.49		HOMO-4	-6.62	87.02	12.62	0.36

Table S2: The calculated excitation energies (E in eV), wavelength (λ in nm) oscillator strength (f), and major transition configuration of sensitizers at TD-B3LYP/6-31G* level.

System	λ (nm)	E (eV)	f	% Contribution
TPP	696.0	1.78	0.062	H-0→L+0(+94%)
	606.6	2.04	0.496	H-1→L+0(+88%) H-0→L+1(+9%)
	543.9	2.28	0.055	H-0→L+2(+41%) H-0→L+1(+29%) H-1→L+1(14%) H-1→L+2(+8%)
	521.3	2.38	0.814	H-0→L+1(+29%) H-0→L+2(27%) H-2→L+0(+21%) H-1→L+1(+9%) H-1→L+0(7%) H-1→L+2(+5%)
	490.8	2.53	0.115	H-2→L+0(+62%) H-1→L+2(26%) H-1→L+1(6%)
	426.6	2.91	0.511	H-1→L+1(+38%) H-2→L+1(13%) H-2→L+2(+13%) H-1→L+2(12%) H-0→L+2(+11%)
	417.5	2.97	0.329	H-2→L+1(+50%) H-2→L+2(+19%) H-1→L+2(13%)
OTPP- β F	759.6	1.63	0.367	H-0→L+0(+95%)
	653.8	1.90	0.246	H-1→L+0(+74%) H-0→L+1(+22%)
	552.1	2.25	0.355	H-0→L+1(+40%) H-0→L+2(+19%) H-1→L+0(19%) H-1→L+2(+14%)
	531.5	2.33	0.210	H-0→L+2(+55%) H-1→L+1(22%) H-0→L+1(14%)
	477.2	2.60	0.679	H-2→L+0(+80%) H-1→L+2(13%)
	445.8	2.78	0.023	H-3→L+0(+69%) H-4→L+0(15%)
	427.5	2.90	0.010	H-4→L+0(+69%) H-3→L+0(+21%)
	425.1	2.92	0.669	H-1→L+1(+41%) H-0→L+2(+17%) H-0→L+3(+14%) H-1→L+2(+11%) H-4→L+0(8%)
	416.8	2.97	0.545	H-1→L+2(+39%) H-5→L+0(+13%) H-0→L+1(11%) H-7→L+0(+9%) H-2→L+0(+8%)
OTPP- β N	721.2	1.72	0.071	H-0→L+0(+93%)
	620.0	2.00	0.542	H-1→L+0(+88%) H-0→L+2(6%)
	559.6	2.22	0.060	H-0→L+1(+69%) H-1→L+2(+13%) H-0→L+2(+6%)
	531.1	2.33	0.816	H-0→L+2(+55%) H-2→L+0(23%) H-1→L+1(12%) H-1→L+0(+6%)
	498.5	2.49	0.024	H-2→L+0(+53%) H-1→L+1(27%) H-1→L+2(14%)
	442.3	2.80	0.410	H-1→L+2(+41%) H-2→L+2(18%) H-1→L+1(18%) H-0→L+1(6%)
	427.0	2.90	0.445	H-2→L+1(+65%) H-2→L+0(8%) H-1→L+1(8%) H-1→L+2(6%)
	420.7	2.95	0.035	H-3→L+0(+81%) H-2→L+2(+8%) H-3→L+1(+7%)
OTPP- β P	687.9	1.80	0.242	H-0→L+0(+92%)
	627.5	1.98	0.326	H-1→L+0(+70%) H-0→L+1(23%)

	537.8	2.31	0.521	H-0→L+1(+46%) H-1→L+0(+24%) H-1→L+2(17%) H-0→L+2(7%)
	515.6	2.40	0.151	H-0→L+2(+59%) H-1→L+1(+33%)
	474.8	2.61	0.581	H-2→L+0(+77%) H-1→L+2(19%)
	427.0	2.90	0.063	H-3→L+0(+58%) H-4→L+0(+16%) H-1→L+1(8%)
	417.4	2.97	0.580	H-1→L+1(+38%) H-0→L+2(21%) H-3→L+0(+15%) H-2→L+1(10%) H-0→L+3(6%)
STPP-βT	697.7	1.78	0.366	H-0→L+0(+92%)
	631.5	1.96	0.194	H-1→L+0(+63%) H-0→L+1(+29%)
	540.2	2.30	0.317	H-0→L+1(+35%) H-1→L+0(26%) H-0→L+2(+18%) H-1→L+2(+12%)
	522.0	2.38	0.355	H-0→L+2(+48%) H-1→L+1(29%) H-0→L+1(10%) H-1→L+0(+6%)
	483.1	2.57	0.492	H-2→L+0(+79%) H-1→L+2(15%)
	432.0	2.87	0.130	H-3→L+0(+57%) H-1→L+1(19%) H-0→L+2(9%)
	428.6	2.89	0.482	H-3→L+0(+33%) H-1→L+1(+29%) H-0→L+2(+14%) H-2→L+1(8%)
	417.1	2.97	0.576	H-1→L+2(+49%) H-0→L+1(15%) H-7→L+0(10%) H-2→L+0(+7%)
STPP-βN	693.2	1.79	0.071	H-0→L+0(+91%)
	607.4	2.04	0.559	H-1→L+0(+88%) H-0→L+1(+8%)
	546.9	2.27	0.086	H-0→L+1(+45%) H-0→L+2(26%) H-1→L+2(9%) H-1→L+1(8%)
	526.9	2.35	0.813	H-0→L+2(+38%) H-2→L+0(+34%) H-0→L+1(+13%) H-1→L+1(+8%) H-1→L+0(5%)
	494.6	2.51	0.034	H-2→L+0(+44%) H-1→L+2(+27%) H-1→L+1(16%) H-0→L+1(5%)
	440.9	2.81	0.227	H-1→L+1(+36%) H-2→L+1(21%) H-1→L+2(+16%) H-2→L+2(10%) H-0→L+2(8%)
	427.3	2.90	0.529	H-2→L+1(+39%) H-2→L+2(25%) H-1→L+2(+15%) H-2→L+0(7%)
	422.8	2.93	0.012	H-3→L+0(+80%) H-2→L+1(9%)
STPP-βP	696.6	1.78	0.241	H-0→L+0(+92%)
	627.5	1.98	0.191	H-1→L+0(+60%) H-0→L+1(32%)
	545.3	2.27	0.525	H-0→L+1(+37%) H-1→L+0(+31%) H-0→L+2(13%) H-1→L+2(12%)
	526.2	2.36	0.236	H-0→L+2(+55%) H-1→L+1(+29%) H-0→L+1(+7%)
	478.8	2.59	0.528	H-2→L+0(+79%) H-1→L+2(17%)
	430.3	2.88	0.197	H-3→L+0(+42%) H-1→L+1(21%) H-4→L+0(11%) H-0→L+2(+11%)
	426.2	2.91	0.653	H-1→L+1(+28%) H-4→L+0(21%) H-0→L+2(13%) H-1→L+2(11%) H-3→L+0(+9%)
	420.1	2.95	0.143	H-3→L+0(+41%) H-4→L+0(+26%) H-1→L+2(+7%) H-1→L+1(+6%)
OSTPP-βF	738.5	1.68	0.359	H-0→L+0(+92%)
	650.8	1.91	0.191	H-1→L+0(+60%) H-0→L+1(32%)
	556.3	2.23	0.348	H-0→L+1(+39%), H-1→L+0(+30%), H-0→L+2(14%), H-1→L+2(12%)

	530.6	2.34	0.262	H-0→L+2(+54%), H-1→L+1(+30%), H-0→L+1(+7%), H-1→L+0(+6%)
	479.9	2.58	0.662	H-2→L+0(+81%), H-1→L+2(12%)
	466.0	2.66	0.017	H-4→L+0(+38%), H-5→L+0(+24%), H-3→L+0(+23%)
	455.4	2.72	0.001	H-3→L+0(+55%), H-4→L+0(34%)
	439.2	2.82	0.068	H-5→L+0(+56%), H-4→L+0(13%), H-3→L+0(11%), H-1→L+2(9%)
	433.0	2.86	0.771	H-1→L+1(+51%), H-0→L+2(25%), H-0→L+3(5%)
	422.2	2.94	0.333	H-1→L+2(+33%), H-4→L+1(+14%), H-3→L+1(+9%), H-5→L+0(+8%), H-0→L+1(+7%), H-2→L+0(+7%)
	414.9	2.99	0.217	H-4→L+1(+30%), H-5→L+1(+29%), H-1→L+2(12%)
OSTPP-βP	724.2	1.71	0.073	H-0→L+0(+91%)
	613.8	2.02	0.517	H-1→L+0(+86%) H-0→L+1(+8%)
	557.5	2.22	0.038	H-0→L+1(+49%) H-0→L+2(28%) H-1→L+2(7%) H-1→L+1(6%)
	536.9	2.31	0.865	H-2→L+0(+41%) H-0→L+2(+32%) H-0→L+1(+11%) H-1→L+0(7%) H-1→L+1(+6%)
	501.4	2.47	0.127	H-2→L+0(+39%) H-1→L+2(+26%) H-1→L+1(15%) H-0→L+2(9%) H-0→L+1(8%)
	457.4	2.71	0.014	H-4→L+0(+54%) H-3→L+0(32%)
	447.3	2.77	0.190	H-1→L+1(+29%) H-3→L+0(+21%) H-1→L+2(+16%) H-2→L+1(10%) H-2→L+2(9%)
	438.9	2.82	0.017	H-3→L+0(+31%) H-4→L+0(+22%) H-2→L+1(+20%) H-1→L+1(12%)
	429.5	2.89	0.616	H-2→L+1(+44%) H-2→L+2(28%) H-4→L+0(6%) H-1→L+2(+6%)
	416.1	2.98	0.897	H-1→L+2(+32%) H-0→L+1(+14%) H-1→L+1(8%) H-2→L+0(8%) H-2→L+1(8%) H-0→L+2(+5%) H-3→L+0(5%)
OSTPP-βT	714.2	1.74	0.283	H-0→L+0(+87%)
	639.1	1.94	0.192	H-1→L+0(+49%) H-0→L+1(39%) H-0→L+0(8%)
	550.6	2.25	0.458	H-1→L+0(+38%) H-0→L+1(+28%) H-0→L+2(18%) H-1→L+2(8%)
	531.3	2.33	0.406	H-0→L+2(+49%) H-1→L+1(+29%) H-0→L+1(+7%) H-1→L+0(+6%)
	492.4	2.52	0.272	H-2→L+0(+76%) H-1→L+2(16%)
	455.4	2.72	0.208	H-5→L+0(+42%) H-1→L+1(24%) H-0→L+2(+9%) H-2→L+1(+8%)
	441.1	2.81	0.023	H-3→L+0(+60%) H-5→L+0(+20%)
	437.1	2.84	0.195	H-2→L+1(+31%) H-5→L+0(21%) H-3→L+0(+20%) H-1→L+1(13%) H-0→L+2(+6%)
	426.6	2.91	0.468	H-1→L+2(+23%) H-2→L+1(19%) H-4→L+0(+17%) H-5→L+1(+14%) H-1→L+1(5%)

	421.1	2.94	0.388	H-1→L+2(+30%) H-2→L+1(+13%) H-4→L+0(13%) H-0→L+1(+8%) H-1→L+1(+5%)
	417.9	2.97	0.113	H-4→L+0(+57%) H-5→L+1(9%) H-1→L+1(+8%) H-2→L+1(+6%) H-4→L+1(5%)
O ₂ TPP-βF	780.1	1.59	0.302	H-0→L+0(+94%)
	659.4	1.88	0.201	H-1→L+0(+58%) H-0→L+1(34%)
	565.3	2.19	0.510	H-1→L+0(+32%) H-0→L+1(+30%) H-0→L+2(23%) H-1→L+2(9%)
	541.6	2.29	0.271	H-0→L+2(+54%) H-1→L+1(+20%) H-0→L+1(+15%) H-1→L+0(+6%)
	480.5	2.58	0.542	H-2→L+0(+79%) H-1→L+2(15%)
	457.0	2.71	0.029	H-3→L+0(+61%) H-4→L+0(23%)
	438.5	2.83	0.030	H-4→L+0(+63%) H-3→L+0(+30%)
	433.0	2.86	0.619	H-1→L+1(+50%) H-0→L+2(17%) H-0→L+3(14%) H-1→L+2(6%)
	421.2	2.94	0.553	H-1→L+2(+45%) H-0→L+1(+10%) H-2→L+0(+9%) H-8→L+0(6%) H-5→L+0(6%) H-4→L+1(5%)
O ₂ TPP-βN	755.1	1.64	0.077	H-0→L+0(+93%)
	625.2	1.98	0.491	H-1→L+0(+87%) H-0→L+1(10%)
	574.7	2.16	0.018	H-0→L+2(+53%) H-0→L+1(+27%) H-1→L+1(8%)
	546.0	2.27	0.872	H-2→L+0(+31%) H-0→L+1(31%) H-0→L+2(+22%) H-1→L+0(8%) H-1→L+1(5%)
	506.6	2.45	0.124	H-2→L+0(+43%) H-1→L+2(+41%) H-0→L+1(+7%)
	455.9	2.72	0.257	H-1→L+1(+54%) H-3→L+0(+13%) H-2→L+1(12%) H-0→L+2(+5%) H-1→L+2(5%) H-2→L+2(+5%)
	439.3	2.82	0.023	H-3→L+0(+70%) H-2→L+1(+12%) H-1→L+1(6%)
	432.6	2.87	0.475	H-2→L+2(+41%) H-2→L+1(+26%) H-1→L+2(11%) H-2→L+0(+10%)
	415.9	2.98	0.455	H-2→L+2(+30%) H-0→L+3(24%) H-2→L+1(19%) H-0→L+2(7%) H-1→L+1(7%)
S ₂ TPP-βT	690.5	1.80	0.342	H-0→L+0(+87%)
	630.1	1.97	0.196	H-1→L+0(+52%) H-0→L+1(36%) H-0→L+0(8%)
	540.9	2.29	0.341	H-1→L+0(+33%) H-0→L+1(+29%) H-0→L+2(20%) H-1→L+2(9%)
	523.3	2.37	0.453	H-0→L+2(+45%) H-1→L+1(+31%) H-0→L+1(+9%) H-1→L+0(+8%)
	485.0	2.56	0.396	H-2→L+0(+78%) H-1→L+2(16%)
	439.4	2.82	0.296	H-1→L+1(+32%) H-3→L+0(+26%) H-0→L+2(16%) H-2→L+1(10%)
	436.1	2.84	0.292	H-3→L+0(+44%) H-1→L+1(13%) H-4→L+0(11%) H-2→L+1(+7%) H-1→L+2(+6%) H-0→L+2(+5%)
	423.8	2.93	0.057	H-4→L+0(+52%) H-3→L+0(+8%) H-1→L+2(+8%) H-6→L+0(7%) H-2→L+1(+7%) H-4→L+1(5%)

	420.7	2.95	0.253	H-6→L+0(+23%) H-4→L+0(+20%) H-1→L+2(20%) H-3→L+0(+9%) H-0→L+1(7%)
	418.1	2.97	0.190	H-6→L+0(+46%) H-1→L+2(+13%) H-5→L+0(+5%)
	415.8	2.98	0.411	H-2→L+1(+57%) H-1→L+2(11%) H-5→L+0(+6%)
S ₂ TPP-βN	693.2	1.79	0.080	H-0→L+0(+89%) H-1→L+1(7%)
	612.3	2.03	0.650	H-1→L+0(+90%) H-0→L+1(+8%)
	542.9	2.28	0.303	H-0→L+1(+43%) H-0→L+2(21%) H-2→L+0(+15%) H-1→L+1(6%)
	529.7	2.34	0.454	H-0→L+2(+45%) H-2→L+0(+31%) H-1→L+1(+11%) H-0→L+1(+7%)
	495.5	2.50	0.166	H-1→L+2(+37%) H-2→L+0(+34%) H-0→L+1(13%) H-1→L+1(9%)
	451.8	2.74	0.152	H-1→L+1(+45%) H-2→L+1(26%) H-0→L+2(9%) H-1→L+2(+7%) H-3→L+0(5%)
	434.5	2.85	0.027	H-3→L+0(+74%) H-2→L+1(14%)
	428.9	2.89	0.601	H-2→L+2(+32%) H-2→L+1(18%) H-1→L+2(15%) H-3→L+0(10%) H-2→L+0(+7%) H-0→L+1(6%)
	422.7	2.93	0.002	H-6→L+0(+44%) H-5→L+0(+16%) H-4→L+0(+15%) H-9→L+0(+7%)
	414.1	2.99	0.750	H-2→L+1(+30%) H-0→L+2(16%) H-1→L+1(+14%) H-1→L+2(11%) H-5→L+0(5%) H-2→L+0(+5%)

Table S3: The optimized coordinates of the fourteen core modified sensitizers at the B3LYP/6-31G* level.

TPP-βN				1	-9.716595	-1.497088	-2.933661
6	-2.283459	3.180370	0.293449	1	-9.777043	-2.981589	1.103659
6	-4.610220	2.367738	-0.141537	1	-10.923706	-2.629797	-1.076356
6	-2.838985	-2.953310	-0.041614	6	-4.128185	4.807852	0.064952
6	-3.841149	-3.974505	-0.161713	6	-4.521134	5.427482	-1.131220
6	-5.058157	-3.366795	-0.309210	6	-4.191767	5.546508	1.256433
6	-6.648026	1.440195	-0.396860	6	-4.965148	6.750430	-1.135870
6	-6.039566	2.642388	-0.276916	1	-4.472465	4.866213	-2.060226
6	-1.303013	4.194953	0.554591	6	-4.635957	6.869615	1.252220
6	-0.097620	3.582416	0.754911	1	-3.898239	5.074350	2.190013
6	1.595083	-1.230898	0.390885	6	-5.023599	7.475527	0.055745
6	0.925583	-2.423710	0.250996	1	-5.262233	7.215201	-2.072303
6	-0.481542	-2.132789	0.242401	1	-4.682899	7.424678	2.185422
6	-4.856334	-1.948054	-0.264509	1	-5.369505	8.505659	0.051983
6	0.524956	-0.204387	0.478890	6	2.087481	1.706326	1.022943
6	-0.278572	2.165821	0.591242	6	2.832659	2.480582	0.117997
6	-5.588045	0.436484	-0.337833	6	2.627943	1.445676	2.291768
6	0.726959	1.187087	0.668661	6	4.091743	2.972316	0.467355
6	-5.838885	-0.949370	-0.385290	1	2.426730	2.681570	-0.869879
6	-1.457079	-3.150931	0.093039	6	3.880099	1.949212	2.647198
6	-3.654034	3.384316	0.065175	1	2.057259	0.852031	3.000487
7	-3.506243	-1.748776	-0.097967	6	4.614829	2.709990	1.735974
7	-4.363541	1.025685	-0.183718	1	4.676455	3.534039	-0.254489
7	-1.616084	1.976826	0.321268	1	4.281688	1.742920	3.635782
7	-0.700955	-0.785843	0.369274	1	5.596108	3.090178	2.005258
1	-6.498265	3.620325	-0.256315	6	-0.978932	-4.570676	0.063390
1	-3.638618	-5.034251	-0.137022	6	-0.361066	-5.143631	1.186563
1	-1.512741	5.253276	0.588649	6	-1.126906	-5.354081	-1.093057
1	1.362901	-3.396897	0.096459	6	0.095918	-6.461204	1.154547
1	-6.017875	-3.844522	-0.436214	1	-0.237680	-4.550094	2.087593
1	-7.704602	1.236468	-0.494007	6	-0.672109	-6.672558	-1.123864
1	0.843018	4.056980	0.987576	1	-1.588741	-4.918327	-1.974672
1	-2.050468	1.070123	0.189795	6	-0.060018	-7.230179	0.000228
1	-3.078425	-0.831434	-0.028766	1	0.579093	-6.882213	2.031482
6	-7.250998	-1.414289	-0.574523	1	-0.788181	-7.260445	-2.030589
6	-7.910009	-1.218877	-1.798361	1	0.299119	-8.255380	-0.025426
6	-7.942113	-2.056514	0.464755	6	3.022814	-1.055775	0.301391
6	-9.223675	-1.653701	-1.977790	1	3.368881	-0.085622	-0.037580
1	-7.382885	-0.728226	-2.611861	6	4.002298	-1.983320	0.559579
6	-9.255986	-2.491236	0.285597	6	5.423292	-1.753240	0.320105
1	-7.445736	-2.205194	1.419785	6	6.457343	-2.651143	0.563012
6	-9.900566	-2.291464	-0.936530	16	6.032340	-0.260373	-0.350022

6	7.718599	-2.147211	0.214299
1	6.287300	-3.638013	0.976785
6	7.689579	-0.853251	-0.299877
1	8.645429	-2.699484	0.330780
6	8.846730	-0.137082	-0.710638
1	9.777424	-0.697120	-0.635007
6	9.004584	1.139887	-1.183502
6	3.698226	-3.267467	1.122874
7	3.511327	-4.316704	1.592283
6	7.931464	2.062912	-1.342681
7	7.049401	2.815301	-1.461832
6	10.383214	1.570827	-1.528389
8	11.373777	0.873688	-1.424422
8	10.425816	2.845213	-1.979675
1	11.362743	3.029477	-2.177448

STPP-βT

16	-1.089106	-0.533697	0.274168
7	-4.320220	0.994716	-0.125170
7	-3.413591	-1.882411	-0.182462
7	-1.565041	2.111956	0.288400
6	0.557587	0.080162	0.413202
6	1.500446	-1.019851	0.350399
6	0.861602	-2.251952	0.204322
6	-0.544025	-2.198455	0.158305
6	-1.426303	-3.289559	0.002516
6	-2.825413	-3.105752	-0.118050
6	-3.834181	-4.163431	-0.134997
6	-5.036103	-3.539988	-0.217941
6	-4.751654	-2.103932	-0.253493
6	-5.731374	-1.090778	-0.323638
6	-5.509458	0.303754	-0.284109
6	-6.537296	1.296053	-0.403237
6	-5.960349	2.531506	-0.298406
6	-4.548880	2.357879	-0.123031
6	-3.624822	3.416074	0.045082
6	-2.238877	3.294007	0.247604
6	-1.314359	4.416063	0.425920
6	-0.083529	3.870607	0.584077
6	-0.260421	2.419966	0.479577
6	0.786260	1.460283	0.552876
6	2.163765	1.994484	0.802313
6	2.756755	1.859048	2.067081
6	4.026148	2.384234	2.313695
6	4.722806	3.042827	1.298632
6	4.143265	3.183745	0.035597

6	2.868091	2.669965	-0.207495
6	-0.865920	-4.670143	-0.036665
6	-0.052239	-5.155394	1.001832
6	0.477773	-6.444334	0.949871
6	0.201909	-7.273855	-0.138132
6	-0.605501	-6.805260	-1.176860
6	-1.134039	-5.516146	-1.127877
6	-7.159937	-1.531795	-0.449964
6	-7.614092	-2.146561	-1.626973
6	-8.939261	-2.567743	-1.744719
6	-9.830574	-2.384916	-0.685898
6	-9.389203	-1.777950	0.491396
6	-8.065074	-1.353491	0.607838
6	-4.195550	4.804826	0.007288
6	-4.595408	5.382401	-1.207229
6	-5.117202	6.676274	-1.242184
6	-5.247521	7.412197	-0.062926
6	-4.851880	6.847677	1.150978
6	-4.329332	5.553905	1.185820
1	-3.405170	0.562845	-0.033337
1	1.397706	-3.180659	0.069510
1	-3.642439	-5.224546	-0.061761
1	-6.016957	-3.993327	-0.233031
1	-7.583339	1.076204	-0.551125
1	-6.456929	3.488905	-0.336322
1	-1.580177	5.463615	0.427123
1	0.852063	4.385955	0.748501
1	2.214633	1.346526	2.857056
1	4.470589	2.276257	3.299638
1	4.695555	3.672379	-0.760934
1	2.415198	2.780009	-1.189219
1	0.161234	-4.522253	1.857201
1	1.109712	-6.793381	1.761227
1	-0.817802	-7.440823	-2.032583
1	-1.745401	-5.148616	-1.946878
1	-6.922532	-2.287183	-2.452939
1	-9.274967	-3.036874	-2.665755
1	-10.862021	-2.714489	-0.776998
1	-10.074427	-1.637622	1.323181
1	-7.722075	-0.887673	1.527503
1	-4.488806	4.813568	-2.126874
1	-5.417745	7.110142	-2.192209
1	-5.653472	8.419821	-0.090061
1	-4.951223	7.413053	2.073802
1	-4.024301	5.114870	2.131705
1	0.616447	-8.277531	-0.179003

1	5.717479	3.438175	1.483297	6	-5.751600	0.570763	-0.364592
6	2.944361	-0.890220	0.316262	6	-5.967099	-0.828190	-0.434242
1	3.332268	0.037214	-0.090021	6	-7.357419	-1.339258	-0.621855
6	3.877261	-1.812989	0.714693	6	-8.087944	-1.009474	-1.775485
6	5.316607	-1.651566	0.526032	6	-9.388738	-1.480537	-1.954604
6	6.304634	-2.542770	0.928518	6	-9.983771	-2.287565	-0.983207
16	6.008265	-0.265151	-0.278087	6	-9.269565	-2.620056	0.169444
6	7.598994	-2.117141	0.595361	6	-7.968153	-2.151001	0.348535
1	6.080922	-3.469101	1.444155	6	-0.912330	-4.666906	0.104095
6	7.638917	-0.891859	-0.064488	6	-1.177642	-5.473263	-1.016172
1	8.499562	-2.676288	0.827224	6	-0.782032	-6.810322	-1.041129
6	8.841607	-0.259449	-0.486926	6	-0.113860	-7.365820	0.051836
1	9.746705	-0.834544	-0.298450	6	0.158915	-6.574973	1.169148
6	9.067903	0.951281	-1.086044	6	-0.236876	-5.237945	1.195897
6	10.478043	1.301729	-1.398199	6	2.124861	1.722377	0.802927
8	11.435729	0.591091	-1.163491	6	2.722555	1.619453	2.067736
8	10.587904	2.516439	-1.981401	6	3.975821	2.186397	2.307099
1	11.539485	2.652247	-2.145890	6	4.651878	2.851483	1.282877
6	3.507388	-3.016797	1.405259	6	4.068452	2.957554	0.017790
7	3.271282	-3.997402	1.987090	6	2.808669	2.404131	-0.216855
6	8.037409	1.881941	-1.404099	6	-4.070931	4.838133	0.191969
7	7.189871	2.641935	-1.653358	6	-4.059961	5.525570	1.415331

STPP-βN

16	-3.243792	-1.239415	-0.059580	6	-4.442529	6.865907	1.482376
7	-1.640103	1.892233	0.289501	6	-4.841215	7.540387	0.326723
7	-0.551165	-0.903732	0.385168	6	-4.857816	6.866102	-0.895429
7	-4.520480	1.119743	-0.225595	6	-4.477211	5.524940	-0.962009
6	-4.908030	-1.745277	-0.312659	1	-2.090559	0.990180	0.169796
6	-4.983497	-3.166345	-0.363325	1	-5.918189	-3.689684	-0.522984
6	-3.773865	-3.797706	-0.188568	1	-3.652109	-4.873737	-0.178558
6	-2.676553	-2.904504	-0.024953	1	1.557139	-3.472361	0.173383
6	-1.322445	-3.231839	0.130773	1	0.865065	3.959630	0.825981
6	-0.311919	-2.240329	0.289338	1	-1.488590	5.171098	0.539917
6	1.100620	-2.502823	0.296002	1	-6.562893	3.774597	-0.100725
6	1.747242	-1.288057	0.387847	1	-7.850216	1.442632	-0.416774
6	0.649172	-0.279997	0.445596	1	-7.624153	-0.389967	-2.537836
6	0.768741	1.126298	0.561080	1	-9.935662	-1.219499	-2.856755
6	-0.281973	2.072856	0.499556	1	-9.727719	-3.240425	0.935188
6	-0.087370	3.488497	0.641706	1	-7.421679	-2.399077	1.254069
6	-1.294806	4.110443	0.500277	1	-1.677945	-5.039392	-1.877272
6	-2.298433	3.110085	0.286014	1	-0.987572	-7.415306	-1.920310
6	-3.674753	3.391825	0.115436	1	0.684751	-6.994827	2.021836
6	-4.706120	2.459541	-0.105548	1	-0.025188	-4.629223	2.069900
6	-6.133351	2.786292	-0.183340	1	2.197847	1.097861	2.863451
6	-6.784120	1.607246	-0.345007	1	4.424519	2.102624	3.293385
				1	5.635638	3.276652	1.458204
				1	4.609640	3.450087	-0.783767

1	2.352313	2.486374	-1.199812	6	-1.589986	-1.137802	0.403910
1	-3.755780	5.000947	2.316925	6	-0.921049	-2.346708	0.276983
1	-4.432486	7.381349	2.439092	6	0.475393	-2.121134	0.263674
1	-5.138222	8.584368	0.378660	6	1.432640	-3.169893	0.151260
1	-5.164843	7.383975	-1.800216	6	2.821950	-3.038722	-0.020875
1	-4.487606	5.002440	-1.914507	6	3.782399	-4.146652	-0.011394
1	0.197662	-8.406574	0.030251	6	5.004589	-3.591863	-0.209663
1	-10.997359	-2.653553	-1.122694	6	4.783535	-2.152225	-0.332819
6	3.171575	-1.087582	0.305943	6	5.787585	-1.158220	-0.492933
1	3.503010	-0.119220	-0.052221	6	7.202805	-1.587537	-0.693504
6	4.165691	-1.989728	0.600152	6	7.557419	-2.369872	-1.805307
6	5.586331	-1.742285	0.377417	6	8.877405	-2.776575	-1.999287
6	6.627101	-2.625309	0.646463	6	9.866546	-2.412694	-1.083658
16	6.189118	-0.249847	-0.300523	6	9.526620	-1.639281	0.027831
6	7.887395	-2.111778	0.310062	6	8.207330	-1.229239	0.220945
1	6.462119	-3.609105	1.069390	6	4.031483	4.924841	0.087180
6	7.851947	-0.824350	-0.219933	6	4.545885	5.494072	-1.088963
1	8.818312	-2.652511	0.446344	6	5.046427	6.796385	-1.090702
6	9.008712	-0.102807	-0.622018	6	5.043692	7.551594	0.083416
1	9.942432	-0.654559	-0.525385	6	4.536542	6.996231	1.259628
6	9.165323	1.169411	-1.107957	6	4.034774	5.694409	1.261822
6	3.877201	-3.267106	1.186669	6	-2.156655	1.766808	1.024703
7	3.702529	-4.310122	1.674306	6	-2.708392	1.498542	2.286776
6	8.089836	2.084223	-1.294714	6	-3.976925	1.973910	2.622438
7	7.207662	2.832509	-1.436831	6	-4.716225	2.713648	1.697555
6	10.546578	1.605017	-1.436719	6	-4.180616	2.984420	0.435897
8	11.539607	0.915482	-1.308695	6	-2.905454	2.521162	0.106392
8	10.588253	2.873929	-1.903105	6	0.883458	-4.562614	0.211176
1	11.526986	3.061907	-2.088493	6	0.211733	-5.031298	1.352275
STPP-βP				6	-0.292224	-6.330879	1.400047
16	3.843480	0.792310	-0.170764	6	-0.131782	-7.185783	0.308414
7	0.643013	-0.747712	0.375030	6	0.533245	-6.732714	-0.832637
7	1.530997	2.095961	0.359980	6	1.036665	-5.432886	-0.881251
7	3.469203	-1.856832	-0.208532	1	1.535912	-0.260647	0.370230
6	5.481335	0.209938	-0.442739	1	7.435229	1.176425	-0.763412
6	6.378032	1.310455	-0.569087	1	6.313918	3.479671	-0.441045
6	5.779509	2.538066	-0.404588	1	1.333659	5.423931	0.703131
6	4.376412	2.466287	-0.165920	1	-0.998263	4.172869	1.090810
6	3.495523	3.529282	0.089107	1	-1.376241	-3.311967	0.133686
6	2.118675	3.319190	0.360521	1	3.548709	-5.188772	0.152150
6	1.136844	4.362306	0.652312	1	5.962289	-4.092562	-0.241191
6	-0.045853	3.728383	0.842168	1	6.791837	-2.647042	-2.524350
6	0.214315	2.298943	0.633578	1	9.133171	-3.375518	-2.869344
6	-0.773243	1.292683	0.689429	1	10.288040	-1.358965	0.750895
6	-0.573280	-0.098287	0.489047	1	7.944122	-0.641326	1.095664
				1	4.538178	4.913640	-2.007338

1	5.433470	7.222548	-2.012539	6	5.759982	-1.038280	-0.607770
1	4.534629	7.574782	2.179648	6	4.810819	-2.066624	-0.367118
1	3.649545	5.261461	2.180717	6	5.088640	-3.487782	-0.154897
1	-2.133643	0.923163	3.007337	6	3.893271	-4.063190	0.127450
1	-4.386835	1.763758	3.606785	6	2.893858	-2.984984	0.073495
1	-5.709327	3.072797	1.952084	6	1.510885	-3.166162	0.278585
1	-4.765552	3.533651	-0.295488	6	0.489635	-2.187138	0.374815
1	-2.486950	2.732851	-0.873796	6	-0.881556	-2.455828	0.311822
1	0.085574	-4.372243	2.205994	6	-1.578297	-1.257769	0.445060
1	-0.815385	-6.669842	2.289314	6	-0.581054	-0.232569	0.627026
1	-0.527471	-8.197148	0.344515	6	-0.766389	1.137944	0.904472
1	0.654659	-7.388638	-1.690654	6	0.192949	2.181325	0.857940
1	1.543336	-5.078771	-1.774347	6	-0.108809	3.585044	1.197621
1	5.433531	8.565895	0.081699	6	1.018166	4.290540	0.939064
1	10.894518	-2.731101	-1.234187	6	2.008736	3.313264	0.483804
6	-3.023965	-0.982699	0.305940	6	3.347350	3.570683	0.106853
1	-3.381285	-0.037771	-0.086729	6	3.846772	4.978883	0.091910
6	-3.983821	-1.912875	0.609663	6	3.924415	5.726036	1.278415
6	-5.409312	-1.726015	0.350342	6	4.390341	7.041059	1.263124
6	-6.423151	-2.636609	0.623464	6	4.786154	7.632242	0.062001
16	-6.045586	-0.277120	-0.385676	6	4.713968	6.899483	-1.124146
6	-7.693206	-2.177514	0.242623	6	4.249731	5.583984	-1.109640
1	-6.234673	-3.600906	1.080296	6	7.178990	-1.415917	-0.866246
6	-7.687923	-0.906217	-0.324489	6	8.218363	-0.962111	-0.036395
1	-8.608016	-2.745989	0.374468	6	9.540554	-1.331051	-0.283425
6	-8.857948	-0.232256	-0.773750	6	9.849337	-2.157643	-1.365457
1	-9.776213	-0.811193	-0.689363	6	8.825937	-2.617512	-2.196307
6	-9.037490	1.023229	-1.291041	6	7.502866	-2.253336	-1.947382
6	-3.659456	-3.155173	1.252302	6	1.020209	-4.579858	0.371453
7	-3.458390	-4.168021	1.790224	6	1.216961	-5.472104	-0.696176
6	-7.982282	1.964467	-1.465137	6	0.765728	-6.789226	-0.615449
7	-7.113548	2.730449	-1.594220	6	0.112197	-7.238293	0.533846
6	-10.421485	1.411799	-1.668151	6	-0.090293	-6.362026	1.601327
8	-11.396579	0.695440	-1.553218	6	0.358735	-5.044316	1.520428
8	-10.484867	2.668657	-2.161904	6	-2.150180	1.557521	1.311200
1	-11.422383	2.827324	-2.378532	6	-2.926103	2.395515	0.492499
				6	-4.199591	2.804252	0.892450
				6	-4.707443	2.392684	2.127413
				6	-3.941813	1.568592	2.954526
				6	-2.675038	1.148652	2.547094
				1	6.102866	3.611941	-0.646285
				1	7.282750	1.347391	-1.038437
				1	6.061822	-3.958347	-0.181172
				1	3.701336	-5.097137	0.376037
				1	-1.303919	-3.426841	0.115273
				1	-1.047634	3.963862	1.573894
OSTPP-βF							
16	3.745294	0.833875	-0.190150				
7	3.493990	-1.806051	-0.219310				
7	1.476452	2.067315	0.452261				
6	4.230639	2.525003	-0.230413				
6	5.607271	2.651523	-0.570863				
6	6.237538	1.444766	-0.770843				
6	5.389148	0.318848	-0.568875				

1	1.174060	5.354396	1.051438	7	-0.542810	-0.858488	0.510320
1	3.628348	5.264914	2.216422	7	-4.496886	1.149235	-0.084530
1	4.447971	7.601842	2.192311	6	-2.445823	3.109963	0.307554
1	5.014479	7.353337	-2.064840	6	-1.394269	4.001210	0.663202
1	4.183763	5.020468	-2.036162	6	-0.186818	3.375601	0.868002
1	7.980710	-0.333793	0.817087	6	-0.233125	1.965091	0.670241
1	10.329357	-0.977164	0.375133	6	0.858094	1.079333	0.758455
1	9.056998	-3.259027	-3.042590	6	0.690489	-0.320931	0.565385
1	6.709638	-2.605698	-2.600420	6	1.721743	-1.373419	0.367025
1	1.716247	-5.121664	-1.594702	6	0.998767	-2.538624	0.207435
1	0.919006	-7.462503	-1.454654	6	-0.401702	-2.191897	0.301990
1	-0.242242	-8.263595	0.595069	6	-1.455649	-3.138214	0.203166
1	-0.602201	-6.700752	2.497327	6	-2.841418	-2.911245	0.132926
1	0.202825	-4.367634	2.355405	6	-3.849655	-3.902645	0.230923
1	-2.529584	2.716194	-0.466940	6	-5.062017	-3.281970	0.066777
1	-4.802577	3.421351	0.233241	6	-4.813875	-1.901566	-0.132288
1	-5.698394	2.710695	2.439203	6	-5.790898	-0.915356	-0.373363
1	-4.329594	1.250988	3.918845	6	-5.630390	0.487713	-0.405470
1	-2.079180	0.509226	3.192584	6	-6.689516	1.439895	-0.777625
1	10.879886	-2.443325	-1.558222	6	-6.148405	2.676774	-0.651513
1	5.148155	8.656755	0.050276	6	-4.766994	2.468758	-0.209237
8	0.659476	-0.827179	0.546276	6	-3.784382	3.459375	0.029889
6	-3.002434	-1.091042	0.263836	6	-4.176429	4.896995	-0.017833
1	-3.329711	-0.108713	-0.055572	6	-5.194832	5.386948	0.817659
6	-3.981775	-2.038430	0.408803	6	-5.571482	6.729072	0.771706
6	-5.388377	-1.811675	0.086317	6	-4.940617	7.605925	-0.112639
6	-6.413729	-2.745665	0.174439	6	-3.929367	7.131746	-0.950575
16	-5.982178	-0.276462	-0.493713	6	-3.549346	5.790746	-0.902819
6	-7.658488	-2.236205	-0.225622	6	2.198676	1.646936	1.087070
1	-6.251497	-3.761721	0.514178	6	2.823905	1.313570	2.300237
6	-7.621608	-0.902536	-0.622247	6	4.071532	1.847187	2.624709
1	-8.577282	-2.813382	-0.228497	6	4.719652	2.707319	1.736014
6	-8.763443	-0.171293	-1.056200	6	4.110806	3.043064	0.524526
1	-9.683388	-0.751565	-1.105107	6	2.854623	2.524829	0.207445
6	-8.912648	1.140318	-1.419865	6	-1.054652	-4.583752	0.186944
6	-10.270990	1.582285	-1.831951	6	-1.328193	-5.394213	-0.927599
8	-11.249456	0.862746	-1.871192	6	-0.932822	-6.731482	-0.950023
8	-10.304563	2.891864	-2.164383	6	-0.259427	-7.282212	0.142215
1	-11.226343	3.083742	-2.418533	6	0.018517	-6.487640	1.255612
6	-3.700808	-3.346845	0.928295	6	-0.374969	-5.149734	1.277812
7	-3.530139	-4.415074	1.358621	6	-7.177931	-1.444902	-0.596873
6	-7.850103	2.089201	-1.406820	6	-7.482444	-2.213592	-1.731501
7	-6.975341	2.858706	-1.383722	6	-8.776442	-2.690044	-1.943744
				6	-9.787085	-2.410029	-1.021903
				6	-9.496331	-1.648586	0.111603
				6	-8.203210	-1.168110	0.321256
OSTPP-βP							
16	-1.874056	1.443412	0.291350				

1	-1.547122	5.068061	0.772315
1	0.719981	3.894116	1.154158
1	1.390067	-3.518202	-0.017324
1	-3.670227	-4.948699	0.424793
1	-6.040468	-3.735369	0.102059
1	-7.687509	1.185742	-1.105796
1	-6.614851	3.629251	-0.862162
1	-5.679462	4.709995	1.515241
1	-6.355863	7.090383	1.431504
1	-3.438421	7.805179	-1.648109
1	-2.773496	5.422423	-1.567790
1	2.320774	0.641474	2.989736
1	4.539075	1.584525	3.569961
1	4.631308	3.684603	-0.178949
1	2.383645	2.779955	-0.737971
1	-1.839684	-4.964538	-1.784408
1	-1.143278	-7.340326	-1.825301
1	0.052646	-8.322790	0.123095
1	0.547587	-6.905777	2.107058
1	-0.157324	-4.534805	2.146038
1	-6.699757	-2.426249	-2.454463
1	-8.995357	-3.276232	-2.832307
1	-10.794670	-2.782240	-1.186280
1	-10.275898	-1.429304	0.836331
1	-7.977833	-0.578683	1.205436
8	-3.453953	-1.690181	-0.064864
1	-5.235188	8.651242	-0.149193
1	5.701449	3.106045	1.973177
6	3.141569	-1.196464	0.220241
1	3.470482	-0.184657	0.007163
6	4.133942	-2.144125	0.296519
6	5.545059	-1.871836	0.046805
6	6.578835	-2.802110	0.080069
16	6.145608	-0.280140	-0.352538
6	7.831164	-2.246276	-0.215261
1	6.414251	-3.848300	0.308852
6	7.797502	-0.879002	-0.478079
1	8.755687	-2.813954	-0.239469
6	8.950163	-0.109066	-0.792911
1	9.874365	-0.682242	-0.846800
6	9.115698	1.229234	-1.038640
6	3.851292	-3.502593	0.659391
7	3.676361	-4.614106	0.959700
6	8.056421	2.180539	-1.006727
7	7.191100	2.960531	-0.974410
6	10.492524	1.696728	-1.342111

8	11.472981	0.979555	-1.391056
8	10.546243	3.030055	-1.562833
1	11.480981	3.233905	-1.751530

OSTPP-βT

16	-1.108081	-0.555329	0.306033
7	-1.460250	2.078450	0.283732
7	-3.407184	-1.857711	-0.154934
6	-0.588241	-2.234286	0.220176
6	0.815154	-2.325799	0.247934
6	1.480245	-1.105405	0.382757
6	0.556046	0.004672	0.476170
6	0.831636	1.371572	0.699481
6	-0.183679	2.358636	0.632820
6	-0.034092	3.780143	0.959694
6	-1.258668	4.333742	0.785969
6	-2.146312	3.241683	0.356646
6	-3.519039	3.403434	0.063857
6	-4.474038	2.410542	-0.226475
6	-5.802098	2.635807	-0.664980
6	-6.409710	1.412075	-0.793852
6	-5.460392	0.422073	-0.438075
6	-5.685190	-0.965818	-0.412243
6	-4.747181	-2.010431	-0.231485
6	-5.108126	-3.431464	-0.119388
6	-3.941740	-4.111396	0.006216
6	-2.882113	-3.102054	-0.026203
6	-1.491907	-3.319667	0.100775
6	-0.967185	-4.712608	0.110702
6	-1.293149	-5.601586	-0.929983
6	-0.801989	-6.906143	-0.933048
6	0.024320	-7.348559	0.102237
6	0.356870	-6.477325	1.140744
6	-0.135087	-5.172682	1.146549
6	2.200060	1.835928	1.084147
6	2.943936	2.674487	0.237502
6	4.209983	3.126277	0.614858
6	4.739974	2.761451	1.854352
6	4.004443	1.938324	2.709951
6	2.746864	1.472821	2.325976
6	-4.045288	4.809657	0.037154
6	-4.981221	5.248721	0.986924
6	-5.455158	6.560861	0.966822
6	-5.004291	7.454577	-0.006648
6	-4.074751	7.029268	-0.957572
6	-3.597319	5.718394	-0.934515

6	-7.114283	-1.371844	-0.633424
6	-8.101600	-1.076275	0.319515
6	-9.425900	-1.467081	0.118481
6	-9.785546	-2.154963	-1.042052
6	-8.812690	-2.452663	-1.998307
6	-7.487388	-2.066808	-1.794557
1	1.328058	-3.267067	0.109361
1	0.871567	4.266179	1.294382
1	-1.547545	5.362237	0.949527
1	-6.228401	3.604967	-0.872623
1	-7.416892	1.211957	-1.125205
1	-6.110698	-3.835015	-0.116204
1	-3.805886	-5.175495	0.139884
1	-1.918030	-5.254614	-1.747584
1	-1.057930	-7.574718	-1.750826
1	1.004268	-6.806519	1.948112
1	0.120165	-4.506761	1.964731
1	2.531462	2.957763	-0.726946
1	4.790921	3.740095	-0.066451
1	4.409675	1.656014	3.678080
1	2.174390	0.834144	2.992806
1	-5.327195	4.557404	1.750439
1	-6.172950	6.885672	1.715403
1	-5.374025	8.476259	-0.023152
1	-3.721055	7.717434	-1.720672
1	-2.875960	5.388297	-1.676576
1	-7.822248	-0.547405	1.226560
1	-10.175345	-1.237220	0.871184
1	-10.817073	-2.458083	-1.199728
1	-9.084766	-2.984631	-2.906056
1	-6.732031	-2.297721	-2.540304
8	-4.278144	1.052006	-0.112922
6	2.920460	-0.979078	0.286774
1	3.284125	-0.033154	-0.099554
6	3.879076	-1.911604	0.590046
6	5.304503	-1.720950	0.335763
6	6.320236	-2.629812	0.608678
16	5.939589	-0.265042	-0.388145
6	7.590300	-2.163987	0.237310
1	6.132801	-3.597281	1.059207
6	7.583793	-0.888982	-0.321966
1	8.506468	-2.730057	0.370139
6	8.754595	-0.210162	-0.761099
1	9.673425	-0.787764	-0.673822
6	8.935504	1.048049	-1.271567
1	0.410106	-8.364430	0.096789

6	10.321401	1.439644	-1.637776
8	11.296891	0.724169	-1.519593
8	10.387168	2.698863	-2.125721
1	11.326109	2.858587	-2.335157
6	7.880928	1.989252	-1.449083
7	7.013852	2.756505	-1.581921
6	3.555560	-3.152712	1.234789
7	3.354226	-4.163789	1.776263
1	5.725440	3.112682	2.147121

O₂TPP-βF

8	0.718190	-0.975778	0.714834
8	4.212492	1.294717	-0.161786
7	1.419967	1.844202	0.504580
7	3.518603	-1.533001	-0.046451
6	0.633149	-2.317822	0.446497
6	1.754831	-3.178676	0.418751
6	3.100489	-2.777071	0.312271
6	4.240421	-3.682850	0.516746
1	4.187438	-4.706547	0.859663
6	5.345560	-2.955868	0.235986
1	6.379314	-3.265492	0.301494
6	4.863774	-1.615975	-0.132397
6	5.722851	-0.569894	-0.561352
6	5.369545	0.779173	-0.681733
6	6.101966	1.833885	-1.284215
1	7.037858	1.717246	-1.809676
6	5.383972	2.990474	-1.095119
1	5.630587	3.983938	-1.438204
6	4.211392	2.645280	-0.376111
6	3.207671	3.491704	0.114976
6	1.966223	3.072520	0.653729
6	1.091809	3.959241	1.439160
1	1.317879	4.972631	1.740171
6	-0.001202	3.225820	1.742698
1	-0.852048	3.518918	2.341027
6	0.213988	1.905899	1.124067
6	-0.761645	0.882232	1.133056
6	-0.542812	-0.453370	0.743022
6	-1.475106	-1.497459	0.411114
6	-0.707984	-2.657222	0.252737
1	-1.056586	-3.636211	-0.032310
6	1.446399	-4.637726	0.471232
6	0.654450	-5.178999	1.499475
1	0.273794	-4.524934	2.278188
6	0.370512	-6.543136	1.539998

1	-0.241221	-6.940843	2.344800
6	0.868985	-7.393309	0.551333
1	0.642805	-8.455680	0.580280
6	1.654642	-6.870425	-0.477711
1	2.038182	-7.523436	-1.257131
6	1.941614	-5.506909	-0.517621
1	2.539496	-5.100606	-1.327676
6	7.126379	-0.918005	-0.936883
6	7.381263	-1.883354	-1.926487
1	6.544289	-2.363510	-2.424646
6	8.688662	-2.214255	-2.280872
1	8.864689	-2.956944	-3.054485
6	9.767146	-1.591208	-1.649394
1	10.785822	-1.851305	-1.924186
6	9.529306	-0.634054	-0.661227
1	10.362455	-0.151591	-0.157021
6	8.221696	-0.299206	-0.309896
1	8.040926	0.434103	0.470755
6	3.490836	4.957331	0.049899
6	4.629751	5.508424	0.662224
1	5.309338	4.856167	1.203307
6	4.880427	6.879166	0.603480
1	5.761273	7.286668	1.092608
6	3.998867	7.725584	-0.071782
1	4.194449	8.793497	-0.118244
6	2.863239	7.192314	-0.684632
1	2.173735	7.842928	-1.215943
6	2.610085	5.822362	-0.622412
1	1.730250	5.409263	-1.106731
6	-2.129305	1.243017	1.618567
6	-2.884604	2.241219	0.978735
1	-2.473820	2.738276	0.104670
6	-4.158021	2.579255	1.439262
1	-4.746547	3.321180	0.908838
6	-4.687501	1.935481	2.560186
1	-5.679373	2.197645	2.917685
6	-3.942974	0.950366	3.213229
1	-4.347283	0.451753	4.090212
6	-2.677650	0.601450	2.742600
1	-2.098561	-0.163134	3.252902
6	-2.880344	-1.321590	0.143424
1	-3.204377	-0.293750	0.026497
6	-3.849509	-2.279009	-0.011284
6	-5.234646	-1.982920	-0.365377
6	-6.244446	-2.913524	-0.580625
16	-5.822789	-0.352865	-0.583285

6	-7.471276	-2.325784	-0.922599
1	-6.083207	-3.981533	-0.494086
6	-7.437410	-0.935053	-0.973564
1	-8.375877	-2.887882	-1.130175
6	-8.565811	-0.128359	-1.292087
1	-9.469539	-0.687612	-1.528699
6	-8.723031	1.230733	-1.351673
6	-3.577215	-3.673585	0.185536
7	-3.405896	-4.814256	0.344073
6	-7.684061	2.162218	-1.065329
7	-6.832041	2.919544	-0.823759
6	-10.067172	1.742747	-1.727056
8	-11.026517	1.042665	-1.985064
8	-10.112976	3.093507	-1.751889
1	-11.024520	3.328673	-2.006484

O₂TPP-βP

8	-3.576118	-1.592491	-0.023902
8	-1.277724	1.897356	0.582176
7	-0.801172	-0.977446	0.801538
7	-4.045885	1.280188	-0.131902
6	-4.938298	-1.607920	-0.138015
6	-5.682498	-0.497350	-0.575463
6	-5.199642	0.825390	-0.680522
6	-5.925342	1.904348	-1.370608
1	-6.842625	1.796721	-1.932543
6	-5.183914	3.020642	-1.193231
1	-5.371635	4.012676	-1.579688
6	-4.018632	2.607195	-0.393845
6	-3.039045	3.509328	0.086210
6	-1.817277	3.150496	0.675637
6	-0.940077	3.966892	1.433059
1	-1.126288	4.996825	1.697660
6	0.135771	3.190790	1.788439
1	0.981632	3.477298	2.394375
6	-0.068953	1.901972	1.229271
6	0.801118	0.806069	1.236452
6	0.459051	-0.512007	0.809338
6	1.426385	-1.572420	0.400822
6	0.644917	-2.694330	0.218031
1	0.961419	-3.662668	-0.137723
6	-0.718397	-2.300100	0.476265
6	-1.809233	-3.206419	0.423916
6	-3.162615	-2.850991	0.327069
6	-4.304108	-3.671694	0.488679
1	-4.286264	-4.703938	0.804444

6	-5.406862	-2.899957	0.199155
1	-6.445142	-3.193192	0.236610
6	-7.108284	-0.765893	-0.933069
6	-7.446080	-1.715878	-1.912458
1	-6.653928	-2.253586	-2.425598
6	-8.778828	-1.955353	-2.246228
1	-9.018424	-2.686232	-3.014025
6	-9.800477	-1.253189	-1.603576
1	-10.839001	-1.440934	-1.862522
6	-9.479991	-0.307570	-0.627627
1	-10.268910	0.239642	-0.118493
6	-8.147159	-0.064527	-0.296907
1	-7.900780	0.664778	0.468994
6	-3.321122	4.974775	0.012874
6	-4.479330	5.513177	0.599988
1	-5.164230	4.851734	1.122241
6	-4.744391	6.880632	0.532081
1	-5.641267	7.278460	0.999458
6	-3.859286	7.736215	-0.127010
1	-4.067193	8.801428	-0.181076
6	-2.706036	7.215292	-0.716949
1	-2.015741	7.872193	-1.239437
6	-2.438301	5.848456	-0.645367
1	-1.547142	5.445422	-1.118019
6	2.155905	1.059139	1.808788
6	3.001111	2.062093	1.299718
1	2.674963	2.652094	0.447834
6	4.264949	2.280148	1.849050
1	4.920369	3.026420	1.411065
6	4.697388	1.507402	2.929662
1	5.682288	1.675132	3.356728
6	3.867245	0.512174	3.449956
1	4.198290	-0.089773	4.292036
6	2.611207	0.283196	2.890071
1	1.965300	-0.489199	3.297015
6	-1.510093	-4.666482	0.474285
6	-0.705784	-5.195757	1.499508
1	-0.322732	-4.532005	2.268480
6	-0.411199	-6.557366	1.544813
1	0.211197	-6.945965	2.345868
6	-0.911179	-7.417104	0.565264
1	-0.675699	-8.477290	0.597744
6	-1.707910	-6.906209	-0.461336
1	-2.088730	-7.565956	-1.236380
6	-2.005595	-5.545227	-0.506179
1	-2.605788	-5.149149	-1.320020

6	2.814960	-1.390656	0.090430
1	3.149263	-0.359323	0.048263
6	3.778771	-2.332198	-0.187328
6	5.147187	-2.000634	-0.563184
6	6.149515	-2.901457	-0.910141
16	5.729427	-0.354702	-0.640108
6	7.361147	-2.278959	-1.239638
1	5.990109	-3.973121	-0.924243
6	7.328879	-0.889072	-1.150380
1	8.256319	-2.814937	-1.538082
6	8.441989	-0.051955	-1.429240
1	9.335257	-0.580746	-1.757915
6	8.599446	1.308581	-1.355823
6	9.925920	1.859386	-1.730099
8	10.874713	1.194174	-2.098619
8	9.974617	3.206847	-1.616896
1	10.876228	3.465858	-1.883018
6	3.506433	-3.736825	-0.115234
7	3.332105	-4.887280	-0.062524
6	7.574790	2.202271	-0.932316
7	6.734278	2.928270	-0.578927

S₂TPP-βT

16	-3.808446	0.771734	-0.078992
7	-3.409496	-1.975836	-0.192100
6	-5.431919	0.151082	-0.336705
6	-5.726289	-1.226597	-0.393080
6	-4.734828	-2.238888	-0.290369
6	-2.776862	-3.172605	-0.080329
6	-1.374662	-3.300407	0.067217
6	-4.367310	2.434559	-0.118876
6	-5.774406	2.473894	-0.337879
6	-6.352023	1.231063	-0.468661
6	-4.973309	-3.681527	-0.225195
6	-3.753215	-4.263735	-0.094169
6	-7.150836	-1.645666	-0.559463
6	-8.117345	-1.320359	0.406523
6	-9.444048	-1.721893	0.250097
6	-9.829086	-2.451047	-0.876571
6	-8.878119	-2.779114	-1.844591
6	-7.550115	-2.382521	-1.686717
6	-0.779571	-4.668513	0.065265
6	-1.002120	-5.538928	-1.016722
6	-0.445592	-6.817169	-1.028486
6	0.343738	-7.249826	0.039279
6	0.574440	-6.395410	1.118541

6	0.017363	-5.117028	1.132662
1	-6.326995	3.403701	-0.394900
1	-5.938378	-4.168100	-0.249378
1	-3.531823	-5.316213	0.012902
1	-7.818487	-0.764316	1.290581
1	-10.175917	-1.468796	1.012580
1	-10.862975	-2.762326	-0.998764
1	-9.169744	-3.342606	-2.726922
1	-6.813821	-2.632609	-2.445146
1	-1.600577	-5.199155	-1.856906
1	-0.622368	-7.472273	-1.877477
1	0.779914	-8.245046	0.027552
1	1.193025	-6.716148	1.951466
1	0.196556	-4.463163	1.980271
6	-0.504043	-2.189548	0.212754
6	-3.507357	3.537896	0.071321
16	-1.042531	-0.522720	0.323707
6	0.902700	-2.242281	0.252997
6	-2.115755	3.406525	0.298768
6	-4.096948	4.912444	0.032635
6	0.601759	0.090958	0.460104
6	1.543294	-1.009820	0.390222
1	1.439275	-3.170450	0.116935
7	-1.475205	2.209912	0.334350
6	-1.160845	4.498474	0.496810
6	-4.112957	5.716135	1.183723
6	-4.641417	5.427529	-1.154657
6	0.849201	1.474018	0.612643
6	-0.162239	2.469824	0.541819
6	0.053430	3.915891	0.664326
1	-1.393998	5.554075	0.502616
6	-4.659444	6.999466	1.148101
1	-3.701632	5.324929	2.109971
6	-5.185430	6.711753	-1.189864
1	-4.623398	4.819939	-2.055161
6	2.236970	1.970103	0.886095
1	1.000112	4.405314	0.843540
6	-5.196954	7.501334	-0.038527
1	-4.667418	7.605707	2.050048
1	-5.595451	7.096903	-2.119739
6	2.960690	2.665855	-0.095968
6	2.818329	1.781036	2.149396
1	-5.621051	8.501409	-0.066167
6	4.242612	3.148947	0.173167
1	2.517705	2.816321	-1.076758
6	4.093997	2.276607	2.422745

1	2.261489	1.252132	2.917983
6	4.809251	2.957200	1.435456
1	4.808657	3.652932	-0.604059
1	4.528547	2.128631	3.407860
1	5.808022	3.330916	1.642212
6	2.987797	-0.885612	0.329695
1	3.371583	0.032785	-0.100317
6	3.924193	-1.805802	0.723933
6	5.360047	-1.653399	0.501893
6	6.353234	-2.544828	0.890193
16	6.038383	-0.277897	-0.331023
6	7.641463	-2.128130	0.522494
1	6.137785	-3.465109	1.420025
6	7.670778	-0.909308	-0.149547
1	8.544863	-2.688975	0.738689
6	8.865172	-0.283824	-0.605225
6	9.079726	0.923439	-1.215314
6	10.482538	1.268424	-1.564919
8	11.443614	0.555585	-1.352023
8	10.580822	2.480563	-2.155237
1	11.528200	2.613193	-2.344757
6	8.043873	1.856178	-1.509528
7	7.191260	2.617087	-1.737824
1	-7.407718	1.074971	-0.653608
1	9.772785	-0.861085	-0.436546
6	3.563544	-2.995659	1.442958
7	3.336110	-3.964264	2.047794

S₂TPP-βN

16	1.842295	1.459070	0.083322
7	4.616596	1.151636	-0.029674
6	2.433750	3.109299	0.182435
6	3.798508	3.451088	0.059113
6	4.832426	2.488812	-0.077905
6	5.814187	0.548727	-0.232325
6	5.974992	-0.858687	-0.289060
6	0.181747	1.962405	0.349597
6	0.127655	3.377207	0.530545
6	1.350367	3.999917	0.437359
6	6.249417	2.763726	-0.330063
6	6.860794	1.554771	-0.427355
6	4.172194	4.897318	0.076438
6	3.675512	5.781574	-0.895774
6	4.031776	7.129987	-0.881547
6	4.887110	7.620092	0.107133
6	5.386231	6.752124	1.080085

6	5.034059	5.402448	1.064147	1	-4.468596	2.139299	3.244940
6	7.353205	-1.409411	-0.465225	6	1.240450	-5.529553	1.086426
6	8.340736	-1.180878	0.506919	6	0.212830	-5.224367	-1.078094
6	9.630117	-1.688626	0.345924	1	-5.686371	3.363851	1.446269
6	9.956104	-2.430138	-0.791042	6	0.893557	-6.880492	1.059627
6	8.984103	-2.661323	-1.766280	1	1.764076	-5.118924	1.945245
6	7.693548	-2.157145	-1.604477	6	-0.130663	-6.576168	-1.104786
1	-0.798394	3.899518	0.735616	1	-0.045719	-4.580601	-1.914255
1	1.493125	5.065762	0.565834	6	0.207883	-7.407655	-0.036033
1	6.696783	3.741420	-0.443044	1	1.153259	-7.519178	1.899561
1	7.903530	1.356051	-0.632535	1	-0.663351	-6.978879	-1.962000
1	3.019725	5.401447	-1.673919	1	-0.064504	-8.459288	-0.055100
1	3.644175	7.796653	-1.647287	6	-3.283561	-1.181319	0.265614
1	5.163017	8.671030	0.119031	1	-3.615948	-0.189009	-0.018197
1	6.048188	7.125868	1.856748	6	-4.282341	-2.091449	0.517914
1	5.416143	4.731602	1.828221	6	-5.705001	-1.809670	0.358409
1	8.087420	-0.611316	1.396541	6	-6.748833	-2.692063	0.618580
1	10.379121	-1.506833	1.112103	16	-6.309999	-0.275040	-0.218476
1	10.960882	-2.824234	-0.916944	6	-8.012337	-2.144467	0.358880
1	9.231040	-3.230527	-2.658537	1	-6.583649	-3.698978	0.982801
1	6.943804	-2.327649	-2.371949	6	-7.977468	-0.831620	-0.104662
6	4.893997	-1.763126	-0.196156	1	-8.945740	-2.679001	0.502271
6	-0.913809	1.076355	0.416411	6	-9.140597	-0.080639	-0.426614
16	3.226096	-1.245481	-0.032648	1	-10.075606	-0.626336	-0.309913
6	4.961746	-3.186935	-0.221619	6	-9.305535	1.210402	-0.856480
6	-0.789801	-0.337173	0.289134	6	-8.231778	2.122237	-1.064666
6	-2.245846	1.702191	0.695055	7	-7.353906	2.871093	-1.228402
6	2.638850	-2.901135	-0.031637	6	-10.696528	1.669771	-1.102717
6	3.735319	-3.806066	-0.145292	8	-11.689406	0.984394	-0.953068
1	5.900740	-3.720955	-0.299995	8	-10.747453	2.955567	-1.519159
7	0.419866	-0.927384	0.177941	1	-11.691990	3.158012	-1.652388
6	-1.857799	-1.376932	0.298925	6	-3.999853	-3.418031	0.983343
6	-2.928970	2.416455	-0.302079	7	-3.829943	-4.504899	1.365295
6	-2.814059	1.610304	1.974998				
6	1.274060	-3.233738	0.043816				
1	3.600568	-4.880436	-0.168210				
6	0.225961	-2.274048	0.136897				
6	-1.178095	-2.578742	0.226368				
6	-4.164061	3.008183	-0.031895				
1	-2.493665	2.492062	-1.295039				
6	-4.041587	2.215865	2.248477				
1	-2.286980	1.066458	2.754076				
6	0.902826	-4.683595	0.018294				
1	-1.606429	-3.568534	0.201450				
6	-4.720581	2.910093	1.245400				
1	-4.707836	3.525108	-0.815761				
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OTPP-βN

7	4.180524	1.186032	-0.158896	1	-0.280767	-6.979959	2.291244
6	1.954361	3.160418	0.535986	6	0.612744	-5.222548	1.434212
6	1.043839	4.039472	1.177364	1	0.328937	-4.583017	2.264564
1	1.238473	5.077932	1.398060	6	7.202212	-0.977127	-0.841740
6	-0.075694	3.313504	1.490580	6	8.256220	-0.465295	-0.066855
1	-0.955686	3.656889	2.011847	1	8.027688	0.174051	0.780934
6	0.129301	1.987917	1.020963	6	9.581535	-0.780891	-0.366942
6	-0.773087	0.922379	1.051318	1	10.382484	-0.380641	0.249002
6	-0.485229	-0.430599	0.701410	6	8.840273	-2.123301	-2.230617
6	-1.504441	-1.486250	0.440128	1	9.061898	-2.763104	-3.080723
6	-0.773865	-2.646763	0.297253	6	9.878023	-1.610519	-1.449886
1	-1.145581	-3.626592	0.042215	1	10.910504	-1.854967	-1.684545
6	0.611660	-2.288871	0.432726	6	7.514804	-1.811258	-1.928242
6	1.672924	-3.219694	0.341177	1	6.711037	-2.202319	-2.545547
6	3.031298	-2.874686	0.212573	6	3.575964	4.917101	0.017702
6	4.137393	-3.786266	0.201339	6	2.851678	5.802692	-0.797127
1	4.056447	-4.849298	0.369515	1	2.043261	5.416784	-1.411801
6	5.278171	-3.070269	-0.044396	6	3.170345	7.160412	-0.836443
1	6.286661	-3.449012	-0.112700	1	2.603459	7.828035	-1.479835
6	4.914901	-1.692591	-0.189596	6	4.216971	7.657820	-0.057856
6	5.784857	-0.629258	-0.519034	6	4.943318	6.788917	0.759029
6	5.394536	0.719836	-0.571245	1	5.755595	7.168801	1.373032
6	6.235955	1.806791	-1.073801	6	4.626479	5.431029	0.795956
1	7.224659	1.701472	-1.497376	1	5.188171	4.758628	1.437888
6	5.506685	2.937157	-0.930094	1	-5.635371	2.154904	3.039852
1	5.781705	3.943478	-1.211762	1	4.465040	8.715376	-0.087343
6	4.229011	2.528466	-0.332620	6	-2.908527	-1.303376	0.196159
6	3.233472	3.458944	0.057469	1	-3.224034	-0.280254	0.022750
6	-2.128029	1.266528	1.586276	6	-3.904314	-2.248275	0.117684
6	-2.596028	0.647216	2.757611	6	-5.285405	-1.940959	-0.234983
1	-1.967105	-0.082518	3.259289	6	-6.324396	-2.855443	-0.376766
6	-3.846528	0.973018	3.282201	16	-5.835540	-0.313079	-0.550264
1	-4.189031	0.490815	4.193915	6	-7.539615	-2.258208	-0.739445
6	-4.655545	1.911689	2.638348	1	-6.189081	-3.919537	-0.223603
6	-4.208370	2.529698	1.467940	6	-7.472485	-0.873980	-0.880079
1	-4.847593	3.230314	0.939601	1	-8.461520	-2.808249	-0.898212
6	-2.950658	2.214236	0.952009	6	-8.581216	-0.058717	-1.232879
1	-2.609422	2.686959	0.035069	1	-9.501716	-0.605869	-1.429998
6	1.329173	-4.672378	0.357491	6	-8.705027	1.300470	-1.367039
6	1.690946	-5.517486	-0.706361	6	-3.659366	-3.632247	0.398426
1	2.224157	-5.102764	-1.556862	7	-3.512486	-4.764965	0.626296
6	1.350021	-6.869383	-0.690793	6	-7.641333	2.218471	-1.134539
1	1.628611	-7.503819	-1.528031	7	-6.768284	2.964050	-0.933780
6	0.642499	-7.402909	0.388268	6	-10.036377	1.825274	-1.761697
1	0.373426	-8.455552	0.398137	8	-11.016721	1.138889	-1.976491
6	0.274465	-6.575080	1.449973	8	-10.049099	3.174518	-1.860575

1 -10.956683 3.415974 -2.122933

OTPP-βP

8 -4.505988 1.012482 -0.106116
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7 -0.649169 -0.727539 0.051917
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6 -4.756461 2.350752 0.042438
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1 -7.796266 1.066151 0.158826
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6 0.556030 -0.070804 0.167956
6 0.694652 1.333510 0.194666
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6 -0.176337 3.701691 0.114975
1 0.774300 4.214317 0.131574
6 -1.412234 4.244513 0.068917
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1 2.103746 1.848993 2.460827
6 3.901153 2.749560 1.676318
1 4.338024 2.908780 2.658704
6 4.024798 2.932993 -0.729803
1 4.574852 3.219978 -1.620505
6 4.595267 3.137198 0.528887
1 5.581586 3.584500 0.603921
6 2.763576 2.343765 -0.837838
1 2.315535 2.189328 -1.816023
6 -4.259092 4.738612 0.157070
6 -4.869447 5.346337 -0.950454
1 -4.967291 4.786234 -1.876476
6 -5.336839 6.659478 -0.875370
1 -5.800744 7.116683 -1.745379
6 -5.203999 7.384079 0.310383
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1 -4.496341 7.344692 2.347936
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1 -3.664569 5.013961 2.208675
1 -5.567585 8.406415 0.369404
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6 3.015937 -0.943805 0.334470
1 3.419610 -0.021821 -0.065801
6 3.932817 -1.839841 0.822574
6 5.379485 -1.653112 0.743489
6 6.346287 -2.496479 1.279700
16 6.112811 -0.304511 -0.088808
6 7.656101 -2.062794 1.029562
1 6.095984 -3.394581 1.831605
6 7.730827 -0.880177 0.298465
1 8.543433 -2.586083 1.370525
6 8.954805 -0.252445 -0.064010
1 9.848674 -0.792196 0.244537
6 9.215838 0.915577 -0.730766

6	10.642782	1.272233	-0.942195	6	3.539455	-3.046994	1.492832
8	11.586161	0.601658	-0.571048	7	3.288798	-4.034687	2.055849
8	10.786863	2.443060	-1.602941	6	8.205266	1.796614	-1.211334
1	11.747322	2.586686	-1.691606	7	7.374676	2.517832	-1.596284