Electronic Supplementary Information (ESI) for:

Assessment of Time-Dependent Density Functionals for the Electronic Excitation Energies of Organic Dyes Used in DSSCs

Qabas Alkhatib,[a] Wissam Helal,*[a] and Akef T. Afaneh[b]

[a] *Department of Chemistry, The University of Jordan, Amman 11942, Jordan.*
[b] *Department of Chemistry, Al-Balqa Applied University, 19117 Al-Salt, Jordan.*
* Corresponding author: wissam.helal@ju.edu.jo

List of Tables

List of Figures

Table S1: Vertical Excitation Energies (eV) Using GGA Functionals.

	OLYP	BLYP	BP86	XLYP	PBE	mPWPW	mPWLYP	B97-D3	Exp
N1	1.621	1.603	1.626	1.602	1.633	1.622	1.604	1.609	2.743
N2	1.529	1.507	1.497	1.511	1.489	1.496	1.507	1.537	2.666
N3	1.225	1.157	1.161	1.160	1.163	1.164	1.151	1.186	2.495
N4	1.139	1.102	1.124	1.101	1.134	1.126	1.102	1.115	2.331
N5	1.832	1.797	1.815	1.798	1.820	1.814	1.796	1.821	2.407
N6	1.978	1.954	1.976	1.951	1.975	1.976	1.953	1.963	2.422
N7	1.977	1.935	1.939	1.936	1.932	1.937	1.925	1.976	2.799
N8	1.352	1.321	1.346	1.321	1.342	1.342	1.317	1.373	2.530
N9	1.048	1.020	1.037	1.020	1.037	1.036	1.018	1.046	2.743
N10	1.611	1.578	1.609	1.576	1.615	1.607	1.577	1.603	2.755
N11	2.194	2.171	2.178	2.171	2.178	2.178	2.169	2.193	2.362
N12	2.116	2.090	2.106	2.083	2.107	2.112	2.090	2.123	2.300
N13	1.728	1.688	1.693	1.692	1.681	1.690	1.678	1.734	2.357
MAE	0.889	0.922	0.908	0.922	0.908	0.908	0.925	0.895	
Max	-0.168	-0.191	-0.184	-0.191	-0.184	-0.184	-0.193	-0.169	
Min	-1.695	-1.723	-1.706	-1.723	-1.706	-1.707	-1.725	-1.697	
SD	0.073	0.070	0.070	0.070	0.071	0.072	0.070	0.070	
R^2	0.073	0.070	0.070	0.069	0.071	0.073	0.071	0.070	

Table S2: Vertical Excitation Energies (eV) Using GH-GGA Functionals.

	O3LYP	B3LYP	B3P86	X3LYP	PBE0	mPW1PW	mPW1LYP	BH&HLYP	Exp
N1	0.901	1.262	1.273	1.346	1.511	1.514	1.499	2.483	2.743
N2	1.429	1.170	1.173	1.292	1.521	1.523	1.508	2.475	2.666
N3	1.024	1.375	1.376	1.452	1.593	1.596	1.596	2.594	2.495
N4	1.606	1.939	1.945	2.010	2.136	2.136	2.133	2.846	2.331
N5	2.736	1.066	1.075	1.140	1.289	1.290	1.275	2.340	2.407
N6	2.173	1.561	1.536	1.724	1.981	1.996	2.018	2.659	2.422
N7	1.698	1.377	1.380	1.472	1.652	1.653	1.658	2.903	2.799
N8	1.950	1.292	1.287	1.401	1.594	1.601	1.604	2.656	2.530
N9	1.471	0.843	0.837	0.958	1.160	1.172	1.184	2.590	2.743
N10	1.147	1.461	1.470	1.533	1.670	1.673	1.665	2.619	2.755
N11	1.024	0.837	0.842	0.956	1.182	1.187	1.186	2.513	2.362
N12	1.579	1.039	1.066	1.183	1.429	1.436	1.427	2.807	2.300
N13	0.981	1.296	1.289	1.361	1.475	1.481	1.487	2.533	2.357
MAE	1.065	1.261	1.259	1.160	0.978	0.973	0.975	0.209	
Max	0.329	-0.392	-0.386	-0.321	-0.195	-0.195	-0.198	0.515	
Min	-1.842	-1.900	-1.906	-1.785	-1.583	-1.571	-1.559	-0.260	
SD	0.043	0.007	0.008	0.010	0.013	0.013	0.014	0.000	
R^2	0.043	0.007	0.008	0.010	0.013	0.013	0.014	0.000	

Table S3: Vertical Excitation Energies (eV) Using mGGA and GH-mGGA Functionals.

	M06-L	TPSS	TPSSh	TPSS0	M060	M06-2X	Exp
N1	1.792	1.701	2.202	1.571	1.678	2.493	2.743
N2	1.046	1.555	1.434	1.581	1.729	2.526	2.666
N3	2.413	2.275	2.507	1.651	1.737	2.542	2.495
N4	1.280	1.165	1.585	2.183	2.233	2.727	2.331
N5	2.082	1.916	2.736	3.031	2.927	2.353	2.407
N6	2.086	2.016	2.201	2.092	2.208	2.641	2.422
N7	2.195	2.081	2.392	2.649	2.592	2.908	2.799
N8	1.602	1.470	1.990	1.663	1.818	2.722	2.530
N9	1.207	1.109	1.491	1.256	1.458	2.597	2.743
N10	1.844	1.701	1.189	1.748	1.753	2.551	2.755
N11	2.323	2.241	1.028	1.261	1.452	2.475	2.362
N12	0.997	1.964	1.568	1.512	1.659	2.741	2.300
N13	2.061	1.885	1.029	1.571	1.510	2.438	2.357
MAE	0.768	0.756	0.788	0.799	0.707	0.184	
Max	-0.039	-0.121	0.329	0.624	0.520	0.441	
Min	-1.620	-1.634	-1.566	-1.487	-1.285	-0.250	
SD	0.002	0.060	0.017	0.001	0.001	0.030	
R^2	0.002	0.060	0.017	0.001	0.001	0.029	

Table S4: Vertical Excitation Energies (eV) Using RSH-GGA Functionals.

	LC-BLYP	CAM-B3LYP	ωB97	ωB97X	ωB97X-D3	ωB97X-D3(BJ)	ωB97X-V	Exp
N1	2.853	2.559	2.961	2.889	2.828	2.908	2.908	2.743
N2	2.822	2.566	2.914	2.842	2.782	2.860	2.860	2.666
N3	2.957	2.633	3.089	3.007	2.931	3.033	3.033	2.495
N4	2.971	2.786	3.162	3.065	2.986	3.093	3.093	2.331
N5	3.115	2.471	3.294	3.189	3.064	3.217	3.217	2.407
N6	2.826	2.654	2.936	2.864	2.806	2.885	2.885	2.422
N7	3.079	2.910	3.180	3.112	3.058	3.133	3.133	2.799
N8	3.064	2.737	3.191	3.090	3.003	3.108	3.108	2.530
N9	2.928	2.657	3.034	2.955	2.885	2.976	2.976	2.743
N10	3.002	2.651	3.148	3.064	2.983	3.087	3.087	2.755
N11	2.693	2.535	2.793	2.737	2.688	2.761	2.761	2.362
N12	2.971	2.789	3.146	3.058	2.984	3.088	3.088	2.300
N13	3.140	2.587	3.379	3.228	3.086	3.253	3.253	2.357
MAE	0.424	0.198	0.563	0.476	0.398	0.499	0.499	
Max	0.783	0.489	1.022	0.871	0.729	0.896	0.896	
Min	0.110	-0.184	0.218	0.146	0.085	0.165	0.165	
SD	0.227	0.134	0.266	0.248	0.229	0.251	0.251	
R^2	0.000	0.016	0.029	0.016	0.004	0.021	0.021	

Table S5: Vertical Excitation Energies (eV) Using DH-GGA and RSDH-GGA Functionals.

	B2PLYP	B2GPPLYP	mPW2PLYP	DSDBLYP	DSDPBEP86	ωB2PLYP	ωB2GPPLYP	Exp
N1	2.192	2.463	2.285	2.329	2.227	2.852	2.844	2.743
N2	2.297	2.509	2.362	2.515	2.430	2.833	2.834	2.666
N3	2.205	2.524	2.319	2.291	2.152	2.968	2.956	2.495
N4	2.369	2.566	2.468	1.987	1.853	2.987	2.968	2.331
N5	1.739	2.416	1.910	2.502	2.198	3.207	3.209	2.407
N6	2.401	2.523	2.456	2.269	2.194	2.803	2.787	2.422
N7	2.743	2.874	2.787	2.811	2.749	3.107	3.108	2.799
N8	2.432	2.696	2.513	2.674	2.569	3.100	3.102	2.530
N9	2.362	2.627	2.446	2.595	2.490	2.970	2.975	2.743
N10	2.210	2.531	2.327	2.226	2.081	3.020	3.008	2.755
N11	2.240	2.417	2.313	2.153	2.070	2.695	2.682	2.362
N12	2.287	2.490	2.393	2.008	1.750	2.963	2.994	2.300
N13	1.906	2.355	2.067	1.798	1.544	3.158	3.133	2.357
MAE	0.277	0.126	0.215	0.250	0.360	0.443	0.438	
Max	0.038	0.235	0.137	0.144	0.039	0.801	0.802	
Min	-0.668	-0.280	-0.497	-0.559	-0.813	0.109	0.101	
SD	0.232	0.091	0.175	0.167	0.233	0.236	0.236	
R^2	0.163	0.293	0.158	0.452	0.506	0.000	0.000	

Table S6: Excited state properties calculated with the OLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	764.7	1.621	0.290	H-1→L (0.434)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	810.8	1.529	0.711	H-1→L (0.849)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1012.4	1.225	0.031	H→L (0.921)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1088.1	1.139	0.341	H→L (0.869)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	676.9	1.832	0.101	H-3→L (0.779)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	626.8	1.978	0.478	H-1→L (0.800)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	627.2	1.977	0.873	H-1→L (0.767)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	916.9	1.352	0.358	H-1→L (0.902)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1182.5	1.048	0.280	H-1→L (0.901)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	769.4	1.611	0.117	H-3→L (0.603)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	565.0	2.194	0.784	H-1→L+1 (0.551)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	585.8	2.116	0.195	H-2→L (0.441)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	717.3	1.728	0.128	H-1→L (0.870)	$\pi \rightarrow \pi^*$

Table S7: Excited state properties calculated with the BLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	773.6	1.603	0.290	H-1→L (0.429)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	822.8	1.507	0.708	H→L (0.844)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1071.2	1.157	0.026	H→L (0.937)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1125.5	1.102	0.323	H→L (0.866)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	690.1	1.797	0.095	H-3→L (0.785)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	634.6	1.954	0.460	H-1→L (0.768)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	640.8	1.935	0.845	H-1→L (0.757)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	938.6	1.321	0.351	H-1→L (0.903)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1215.2	1.020	0.270	H-1→L (0.897)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	785.7	1.578	0.119	H-3→L (0.593)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	571.0	2.171	0.769	H-1→L+1 (0.547)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	593.4	2.090	0.187	H-2→L (0.433)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	734.6	1.688	0.123	H-1→L (0.870)	$\pi \rightarrow \pi^*$

Table S8: Excited state properties calculated with the BP86 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	762.4	1.626	0.294	H-1→L (0.423)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	828.0	1.497	0.683	H→L (0.851)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1068.3	1.161	0.024	H→L (0.934)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1103.3	1.124	0.342	H→L (0.866)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	683.0	1.815	0.097	H-3→L (0.784)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	627.6	1.976	0.444	H-1→L (0.728)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	639.3	1.939	0.839	H-1→L (0.756)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	920.9	1.346	0.361	H-1→L (0.903)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1195.7	1.037	0.281	H-1→L (0.901)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	770.4	1.609	0.126	H-3→L (0.587)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	569.2	2.178	0.790	H-1→L+1 (0.564)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	588.9	2.106	0.147	H-2→L (0.392)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	732.4	1.693	0.124	H-1→L (0.864)	$\pi \rightarrow \pi^*$

Table S9: Excited state properties calculated with the XLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	773.9	1.602	0.291	H-1→L (0.430)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	820.3	1.511	0.715	H→L (0.843)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1069.0	1.160	0.026	H→L (0.937)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1126.5	1.101	0.320	H→L (0.866)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	689.7	1.798	0.096	H-3→L (0.784)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	635.5	1.951	0.462	H-1→L (0.775)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	640.5	1.936	0.846	H-1→L (0.757)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	938.8	1.321	0.351	H-1→L (0.903)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1216.0	1.020	0.269	H-1→L (0.896)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	786.7	1.576	0.118	H-3→L (0.597)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	571.0	2.171	0.769	H-1→L+1 (0.547)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	595.1	2.083	0.190	H-2→L (0.435)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	732.8	1.692	0.123	H-1→L (0.870)	$\pi \rightarrow \pi^*$

Table S10: Excited state properties calculated with the PBE functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	759.1	1.633	0.295	H-1→L (0.420)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	832.5	1.489	0.668	H→L (0.853)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1066.4	1.163	0.024	H→L (0.933)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1093.4	1.134	0.349	H→L (0.865)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	681.3	1.820	0.097	H-3→L (0.783)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	627.7	1.975	0.423	H-1→L (0.683)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	641.8	1.932	0.825	H-1→L (0.753)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	924.1	1.342	0.358	H-1→L (0.903)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1195.4	1.037	0.281	H-1→L (0.902)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	767.9	1.615	0.130	H-3→L (0.577)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	569.4	2.178	0.787	H-1→L (0.563)+1	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	588.4	2.107	0.149	H-2→L (0.394)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	737.5	1.681	0.121	H-1→L (0.866)	$\pi \rightarrow \pi^*$

Table S11: Excited state properties calculated with the mPWPW functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	764.4	1.622	0.290	H-1→L (0.422)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	828.7	1.496	0.679	H→L (0.851)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1065.3	1.164	0.024	H→L (0.933)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1101.4	1.126	0.343	H→L (0.866)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	683.3	1.814	0.096	H-3→L (0.784)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	627.6	1.976	0.447	H-1→L (0.733)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	640.2	1.937	0.834	H-1→L (0.755)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	923.6	1.342	0.358	H-1→L (0.903)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1196.9	1.036	0.279	H-1→L (0.901)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	771.4	1.607	0.126	H-3→L (0.583)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	569.3	2.178	0.785	H-1→L+1 (0.557)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	587.1	2.112	0.159	H-2→L (0.404)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	733.7	1.690	0.122	H-1→L (0.867)	$\pi \rightarrow \pi^*$

Table S12: Excited state properties calculated with the mPWLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	772.9	1.604	0.292	H-1→L (0.428)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	822.7	1.507	0.710	H→L (0.844)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1076.7	1.151	0.025	H→L (0.938)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1125.0	1.102	0.323	H→L (0.865)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	690.3	1.796	0.095	H-3→L (0.785)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	634.7	1.953	0.455	H-1→L (0.758)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	644.2	1.925	0.834	H-1→L (0.754)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	941.1	1.317	0.351	H-1→L (0.903)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1218.0	1.018	0.269	H-1→L (0.897)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	786.4	1.577	0.120	H-3→L (0.590)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	571.5	2.169	0.769	H-1→L+1 (0.547)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	593.2	2.090	0.182	H-2→L (0.425)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	738.7	1.678	0.121	H-1→L (0.870)	$\pi \rightarrow \pi^*$

Table S13: Excited state properties calculated with the B97-D3 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	770.4	1.609	0.288	H-1→L (0.438)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	806.7	1.537	0.732	H→L (0.845)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_2$	1045.2	1.186	0.025	H→L (0.934)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1111.7	1.115	0.323	H→L (0.870)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	680.8	1.821	0.099	H-3→L (0.782)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	631.6	1.963	0.479	H-1→L (0.812)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	627.5	1.976	0.883	H-1→L (0.767)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	903.3	1.373	0.367	H-1→L (0.904)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1185.5	1.046	0.275	H-1→L (0.896)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	773.2	1.603	0.113	H-3→L (0.623)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	565.4	2.193	0.793	H-1→L+1 (0.555)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_7$	584.1	2.123	0.165	H-2→L (0.404)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	715.1	1.734	0.133	H-1→L (0.861)	$\pi \rightarrow \pi^*$

Table S14: Excited state properties calculated with the M06-L functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	691.8	1.792	0.338	H-1→L (0.442)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_2$	1185.5	1.046	0.332	H-1→L (0.821)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_5$	513.9	2.413	0.213	H-2→L (0.425)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	968.3	1.280	0.381	H→L (0.893)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	595.4	2.082	0.195	H-3→L (0.690)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	594.5	2.086	0.545	H-1→L (0.839)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	564.8	2.195	1.057	H-1→L (0.823)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	773.9	1.602	0.431	H-1→L (0.915)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1027.4	1.207	0.309	H-1→L (0.896)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	672.5	1.844	0.125	H-3→L (0.712)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	533.7	2.323	0.857	H-1→L+1 (0.620)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_3$	1243.9	0.997	0.138	H-1→L (0.849)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	601.6	2.061	0.179	H-1→L (0.876)	$\pi \rightarrow \pi^*$

Table S15: Excited state properties calculated with the TPSS functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_3$	728.7	1.701	0.322	H-1→L (0.433)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_3$	797.2	1.555	0.703	H→L (0.861)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_5$	544.9	2.275	0.161	H-2→L (0.389)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	1064.0	1.165	0.345	H→L (0.880)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	647.0	1.916	0.122	H-3→L (0.758)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	615.0	2.016	0.504	H-1→L (0.835)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	595.7	2.081	0.971	H-1→L (0.794)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	843.2	1.470	0.402	H-1→L (0.910)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_3$	1118.3	1.109	0.297	H-1→L (0.901)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_3$	729.1	1.701	0.120	H-3→L (0.642)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_5$	553.3	2.241	0.821	H-1→L+1 (0.590)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_4$	631.4	1.964	0.024	H-1→L+1 (0.847)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_4$	657.7	1.885	0.150	H-1→L (0.863)	$\pi \rightarrow \pi^*$

Table S16: Excited state properties calculated with the O3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	1376.7	0.901	0.311	H→L (0.978)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_2$	867.5	1.429	0.565	H-1→L (0.942)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	1210.5	1.024	0.324	H→L (0.989)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	771.9	1.606	0.616	H→L (0.967)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	453.1	2.736	1.084	H-1→L (0.704)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	570.6	2.173	0.516	H-1→L (0.906)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_3$	730.2	1.698	0.171	H-2→L (0.751)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	635.9	1.950	0.531	H-1→L (0.979)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_2$	842.6	1.471	0.486	H-1→L (0.943)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_2$	1081.3	1.147	0.166	H-1→L (0.575)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_2$	1211.0	1.024	0.179	H→L+1 (0.979)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_3$	785.2	1.579	0.272	H-1→L (0.952)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	1263.3	0.981	0.200	H→L (0.986)	$\pi \rightarrow \pi^*$

Table S17: Excited state properties calculated with the B3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	982.2	1.262	0.498	H→L (0.993)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	1060.0	1.170	0.580	H→L (0.987)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	901.8	1.375	0.457	H→L (0.984)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	639.3	1.939	0.842	H→L (0.986)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	1162.9	1.066	0.017	H→L (0.984)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	794.3	1.561	0.304	H→L (0.972)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	900.2	1.377	0.020	H→L (0.928)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	959.5	1.292	0.269	H→L (0.982)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	1471.4	0.843	0.112	H→L (0.984)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	848.4	1.461	0.366	H→L (0.966)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	1480.6	0.837	0.253	H→L (0.990)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	1193.1	1.039	0.048	H→L (0.825)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	956.8	1.296	0.255	H→L (0.987)	$\pi \rightarrow \pi^*$

Table S18: Excited state properties calculated with the B3P86 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	974.1	1.273	0.501	H→L (0.993)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	1056.8	1.173	0.572	H→L (0.987)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	901.1	1.376	0.458	H→L (0.985)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	637.5	1.945	0.859	H→L (0.986)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	1153.1	1.075	0.017	H→L (0.984)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	807.3	1.536	0.288	H→L (0.974)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	898.3	1.380	0.019	H→L (0.929)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	963.6	1.287	0.263	H→L (0.983)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	1480.6	0.837	0.110	H→L (0.984)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	843.3	1.470	0.370	H→L (0.964)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	1472.8	0.842	0.258	H→L (0.990)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	1162.8	1.066	0.050	H→L (0.804)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	961.9	1.289	0.260	H→L (0.987)	$\pi \rightarrow \pi^*$

Table S19: Excited state properties calculated with the X3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	921.3	1.346	0.549	H→L (0.993)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	959.9	1.292	0.706	H→L (0.977)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	854.0	1.452	0.491	H→L (0.981)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	616.9	2.010	0.897	H→L (0.984)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	1087.3	1.140	0.018	H→L (0.980)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	719.0	1.724	0.389	H→L (0.981)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	842.3	1.472	0.031	H→L (0.916)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	884.8	1.401	0.311	H→L (0.973)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	1294.7	0.958	0.138	H→L (0.980)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	809.0	1.533	0.394	H→L (0.963)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	1297.6	0.956	0.307	H→L (0.983)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	1048.5	1.183	0.056	H→L (0.761)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	911.2	1.361	0.270	H→L (0.985)	$\pi \rightarrow \pi^*$

Table S20: Excited state properties calculated with the PBE0 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	820.5	1.511	0.652	H→L (0.989)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	814.9	1.521	0.958	H→L (0.946)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	778.5	1.593	0.555	H→L (0.974)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	580.5	2.136	1.017	H→L (0.975)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	962.1	1.289	0.023	H→L (0.973)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	625.9	1.981	0.539	H→L (0.979)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	750.6	1.652	0.010	H→L (0.893)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	777.8	1.594	0.387	H→L (0.954)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	1068.5	1.160	0.189	H→L (0.968)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	742.2	1.670	0.452	H→L (0.958)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	1049.2	1.182	0.434	H→L (0.963)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	867.6	1.429	0.068	H→L (0.633)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	840.6	1.475	0.307	H→L (0.982)	$\pi \rightarrow \pi^*$

Table S21: Excited state properties calculated with the mPW1PW functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	819.1	1.514	0.655	H→L (0.989)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	814.1	1.523	0.966	H→L (0.946)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	776.6	1.596	0.556	H→L (0.973)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	580.4	2.136	1.011	H→L (0.974)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	961.1	1.290	0.023	H→L (0.973)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	621.3	1.996	0.551	H→L (0.979)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	750.1	1.653	0.011	H→L (0.893)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	774.4	1.601	0.392	H→L (0.953)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	1057.9	1.172	0.194	H→L (0.968)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	741.1	1.673	0.453	H→L (0.958)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	1044.3	1.187	0.436	H→L (0.963)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	863.7	1.436	0.069	H→L (0.637)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	837.3	1.481	0.307	H→L (0.982)	$\pi \rightarrow \pi^*$

Table S22: Excited state properties calculated with the mPW1LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	826.8	1.499	0.653	H→L (0.989)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	822.0	1.508	0.976	H→L (0.946)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	777.0	1.596	0.558	H→L (0.973)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	581.4	2.133	0.993	H→L (0.973)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	972.5	1.275	0.022	H→L (0.972)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	614.3	2.018	0.581	H→L (0.978)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	747.9	1.658	0.017	H→L (0.888)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	772.8	1.604	0.403	H→L (0.949)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	1047.0	1.184	0.205	H→L (0.968)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	744.6	1.665	0.450	H→L (0.959)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	1045.7	1.186	0.436	H→L (0.961)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	868.7	1.427	0.070	H→L (0.640)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	833.6	1.487	0.300	H→L (0.982)	$\pi \rightarrow \pi^*$

Table S23: Excited state properties calculated with the BH&HLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	499.2	2.483	1.569	H→L (0.758)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	500.9	2.475	2.618	H→L (0.572)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	478.0	2.594	1.256	H→L (0.784)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	435.6	2.846	1.568	H→L (0.773)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	529.9	2.340	0.129	H→L (0.841)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	466.2	2.659	1.037	H→L (0.861)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	427.0	2.903	1.816	H-1→L (0.901)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	466.7	2.656	1.135	H→L (0.565)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	478.8	2.590	1.257	H→L (0.517)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	473.5	2.619	1.035	H→L (0.843)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	493.4	2.513	1.822	H-1→L (0.422)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	441.6	2.807	0.208	H→L+1 (0.313)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	489.5	2.533	0.741	H→L (0.877)	$\pi \rightarrow \pi^*$

Table S24: Excited state properties calculated with the TPSSh functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_2$	563.2	2.202	0.637	H-1→L (0.788)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_2$	864.5	1.434	0.588	H-1→L (0.933)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_4$	494.6	2.507	0.266	H-2→L (0.759)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	782.3	1.585	0.577	H→L (0.964)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_4$	453.2	2.736	1.026	H-1→L (0.686)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_2$	563.4	2.201	0.534	H-1→L (0.899)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_4$	518.3	2.392	1.234	H-1→L (0.828)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_3$	623.0	1.990	0.554	H-1→L (0.977)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_2$	831.7	1.491	0.497	H-1→L (0.936)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_2$	1042.4	1.189	0.259	H→L (0.655)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_2$	1206.2	1.028	0.177	H→L (0.978)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_3$	790.5	1.568	0.268	H-1→L+1 (0.948)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	1204.8	1.029	0.201	H→L (0.986)	$\pi \rightarrow \pi^*$

Table S25: Excited state properties calculated with the TPSS0 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	789.4	1.571	0.697	H→L (0.988)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	784.0	1.581	1.039	H→L (0.940)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	750.9	1.651	0.582	H→L (0.973)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	567.8	2.183	1.023	H→L (0.972)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_3$	409.1	3.031	1.526	H-1→L (0.960)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	592.7	2.092	0.612	H→L (0.974)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_2$	468.0	2.649	1.605	H-1→L (0.962)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	745.6	1.663	0.415	H→L (0.949)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	987.2	1.256	0.220	H→L (0.966)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	709.4	1.748	0.491	H→L (0.952)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	983.3	1.261	0.476	H→L (0.959)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	820.3	1.512	0.074	H→L (0.635)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	789.4	1.571	0.324	H→L (0.982)	$\pi \rightarrow \pi^*$

Table S26: Excited state properties calculated with the M06 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	738.9	1.678	0.761	H→L (0.974)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	716.9	1.729	1.270	H→L (0.884)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	713.8	1.737	0.610	H→L (0.959)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	555.4	2.233	1.102	H→L (0.954)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_2$	423.6	2.927	1.294	H-1→L (0.829)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	561.5	2.208	0.746	H→L (0.939)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	478.4	2.592	1.541	H-1→L (0.934)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	682.1	1.818	0.519	H→L (0.904)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	850.2	1.458	0.319	H→L (0.935)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	707.2	1.753	0.462	H→L (0.958)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	854.0	1.452	0.631	H→L (0.917)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	747.4	1.659	0.075	H→L (0.502)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	820.8	1.510	0.338	H→L (0.978)	$\pi \rightarrow \pi^*$

Table S27: Excited state properties calculated with the M06-2X functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	497.3	2.493	1.528	H→L (0.739)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	490.7	2.526	2.548	H→L (0.517)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	487.7	2.542	1.192	H→L (0.776)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	454.6	2.727	1.517	H→L (0.792)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	527.0	2.353	0.137	H→L (0.812)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	469.5	2.641	1.002	H→L (0.790)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	426.3	2.908	1.773	H-1→L (0.908)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	455.5	2.722	1.197	H→L (0.515)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	477.4	2.597	1.217	H→L (0.469)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	486.1	2.551	0.965	H→L (0.840)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	501.0	2.475	1.617	H-1→L (0.465)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	452.4	2.741	0.153	H-1→L+1 (0.314)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	508.5	2.438	0.669	H→L (0.867)	$\pi \rightarrow \pi^*$

Table S28: Excited state properties calculated with the LC-BLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	434.6	2.853	1.762	H→L (0.456)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	439.4	2.822	2.699	H→L (0.305)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	419.3	2.957	1.481	H→L (0.494)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	417.3	2.971	1.635	H→L (0.626)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	398.0	3.115	0.885	H-1→L (0.400)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	438.7	2.826	1.063	H→L (0.764)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	402.7	3.079	1.796	H-1→L (0.774)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	404.6	3.064	1.349	H-1→L (0.441)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	423.5	2.928	1.357	H-1→L (0.399)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	413.0	3.002	1.302	H→L (0.625)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	460.4	2.693	1.435	H→L (0.542)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	417.3	2.971	0.140	H-1→L+1 (0.422)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	394.8	3.140	1.098	H→L (0.561)	$\pi \rightarrow \pi^*$

Table S29: Excited state properties calculated with the CAM-B3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	484.6	2.559	1.621	H→L (0.667)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	483.2	2.566	2.655	H→L (0.451)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	470.9	2.633	1.268	H→L (0.708)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	445.0	2.786	1.551	H→L (0.745)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	501.8	2.471	0.182	H→L (0.746)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	467.2	2.654	1.010	H→L (0.788)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	426.1	2.910	1.786	H-1→L (0.886)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	453.0	2.737	1.172	H→L (0.437)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	466.6	2.657	1.288	H-1→L (0.401)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	467.6	2.651	1.056	H→L (0.798)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	489.1	2.535	1.654	H-1→L (0.497)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	444.6	2.789	0.148	H-1→L+1 (0.390)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	479.2	2.587	0.783	H→L (0.818)	$\pi \rightarrow \pi^*$

Table S30: Excited state properties calculated with the ωB97 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	418.7	2.961	1.796	H→L (0.437)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	425.4	2.914	2.741	H→L (0.307)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	401.3	3.089	1.567	H→L (0.460)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	392.1	3.162	1.735	H→L (0.588)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	376.4	3.294	1.252	H-1→L (0.604)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	422.3	2.936	1.111	H→L (0.798)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	389.9	3.180	1.820	H-1→L (0.725)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	388.6	3.191	1.414	H-1→L (0.455)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	408.6	3.034	1.378	H-1→L (0.366)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	393.8	3.148	1.409	H→L (0.593)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	443.9	2.793	1.507	H-1→L (0.529)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	394.1	3.146	0.208	H-1→L+1 (0.313)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	366.9	3.379	1.341	H→L (0.519)	$\pi \rightarrow \pi^*$

Table S31: Excited state properties calculated with the ωB97X functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	429.1	2.889	1.792	H→L (0.465)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	436.2	2.842	2.758	H→L (0.324)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	412.3	3.007	1.526	H→L (0.493)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	404.6	3.065	1.690	H→L (0.612)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	388.7	3.189	1.056	H-1→L (0.489)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	432.9	2.864	1.083	H→L (0.793)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	398.4	3.112	1.825	H-1→L (0.749)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	401.2	3.090	1.356	H-1→L (0.441)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	419.6	2.955	1.357	H-1→L (0.377)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	404.7	3.064	1.356	H→L (0.625)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	453.0	2.737	1.520	H-1→L (0.530)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	405.4	3.058	0.174	H-1→L+1 (0.378)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	384.1	3.228	1.211	H→L (0.566)	$\pi \rightarrow \pi^*$

Table S32: Excited state properties calculated with the ωB97X-D3 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	438.4	2.828	1.790	H→L (0.493)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	445.6	2.782	2.776	H→L (0.339)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	423.0	2.931	1.480	H→L (0.526)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	415.2	2.986	1.655	H→L (0.635)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	404.6	3.064	0.806	H→L (0.412)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	441.8	2.806	1.058	H→L (0.781)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	405.5	3.058	1.830	H-1→L (0.794)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	412.9	3.003	1.305	H-1→L (0.432)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	429.7	2.885	1.340	H-1→L (0.396)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	415.6	2.983	1.302	H→L (0.656)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	461.3	2.688	1.532	H-1→L (0.534)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	415.5	2.984	0.155	H-1→L+1 (0.413)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	401.8	3.086	1.107	H→L (0.613)	$\pi \rightarrow \pi^*$

Table S33: Excited state properties calculated with the ωB97X-D3(BJ) functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	426.4	2.908	1.803	H→L (0.470)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	433.5	2.860	2.782	H→L (0.332)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	408.8	3.033	1.542	H→L (0.497)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	400.8	3.093	1.699	H→L (0.615)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	385.4	3.217	1.076	H-1→L (0.494)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	429.7	2.885	1.089	H→L (0.803)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	395.7	3.133	1.837	H-1→L (0.693)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	398.9	3.108	1.360	H-1→L (0.434)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	416.6	2.976	1.362	H-1→L (0.370)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	401.6	3.087	1.370	H→L (0.630)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	449.0	2.761	1.545	H-1→L (0.524)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	401.5	3.088	0.178	H-1→L+1 (0.381)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	381.2	3.253	1.226	H→L (0.573)	$\pi \rightarrow \pi^*$

Table S34: Excited state properties calculated with the ωB97X-V functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	426.3	2.908	1.803	H→L (0.470)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	433.5	2.860	2.782	H→L (0.332)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	408.8	3.033	1.542	H→L (0.497)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	400.8	3.093	1.699	H→L (0.615)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	385.4	3.217	1.076	H-1→L (0.494)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	429.7	2.885	1.089	H→L (0.803)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	395.7	3.133	1.837	H-1→L (0.693)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	398.9	3.108	1.360	H-1→L (0.434)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	416.6	2.976	1.362	H→L (0.370)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	401.6	3.087	1.370	H→L (0.630)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	449.0	2.761	1.545	H-1→L (0.524)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	401.5	3.088	0.178	H-1→L+1 (0.381)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	381.2	3.253	1.226	H→L (0.573)	$\pi \rightarrow \pi^*$

Table S35: Excited state properties calculated with the B2PLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	565.7	2.192	1.404	H→L (0.722)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	539.7	2.297	2.449	H→L (0.545)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	562.3	2.205	1.099	H→L (0.749)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	523.4	2.369	1.314	H→L (0.746)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	713.0	1.739	0.126	H→L (0.808)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	516.3	2.401	0.941	H→L (0.866)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	452.0	2.743	1.710	H-1→L (0.879)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	509.8	2.432	1.054	H→L (0.537)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	525.0	2.362	1.157	H→L (0.491)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	560.9	2.210	0.906	H→L (0.819)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	553.4	2.240	1.626	H-1→L (0.441)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	542.1	2.287	0.184	H→L+1 (0.283)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	650.5	1.906	0.594	H→L (0.850)	$\pi \rightarrow \pi^*$

Table S36: Excited state properties calculated with the B2GPPLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	503.4	2.463	1.596	H→L (0.605)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	494.2	2.509	2.660	H→L (0.468)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	491.2	2.524	1.324	H→L (0.626)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	483.2	2.566	1.441	H→L (0.651)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	513.1	2.416	0.576	H→L (0.534)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	491.4	2.523	0.998	H→L (0.873)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	431.5	2.874	1.758	H→L (0.540)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	459.9	2.696	1.202	H→L (0.464)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	472.0	2.627	1.274	H→L (0.464)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	489.8	2.531	1.132	H→L (0.722)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	513.0	2.417	1.732	H-1→L (0.463)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	497.9	2.490	0.338	H-1→L (0.334)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	526.5	2.355	0.908	H→L (0.726)	$\pi \rightarrow \pi^*$

Table S37: Excited state properties calculated with the mPW2PLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	542.5	2.285	1.472	H→L (0.701)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	524.9	2.362	2.520	H→L (0.529)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	534.7	2.319	1.170	H→L (0.727)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	502.4	2.468	1.373	H→L (0.730)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	649.0	1.910	0.164	H→L (0.781)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	504.8	2.456	0.964	H→L (0.868)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	444.9	2.787	1.732	H-1→L (0.858)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	493.4	2.513	1.097	H→L (0.521)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	506.9	2.446	1.200	H→L (0.483)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	532.9	2.327	0.971	H→L (0.803)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	536.0	2.313	1.676	H-1→L (0.449)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	518.0	2.393	0.204	H→L+1 (0.264)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	599.8	2.067	0.667	H→L (0.832)	$\pi \rightarrow \pi^*$

Table S38: Excited state properties calculated with the DSD-BLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	532.3	2.329	1.485	H→L (0.537)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	493.0	2.515	2.613	H→L (0.428)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	541.2	2.291	1.204	H→L (0.551)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	624.0	1.987	1.115	H→L (0.585)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	495.6	2.502	1.001	H-1→L (0.624)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	546.5	2.269	0.902	H→L (0.871)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	441.1	2.811	1.685	H→L (0.805)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	463.6	2.674	1.202	H→L (0.433)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	477.7	2.595	1.227	H→L (0.470)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	556.9	2.226	1.025	H→L (0.648)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	575.9	2.153	1.531	H-1→L (0.453)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	617.3	2.008	0.567	H-1→L (0.478)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	689.7	1.798	0.791	H→L (0.617)	$\pi \rightarrow \pi^*$

Table S39: Excited state properties calculated with the DSD-PBEP86 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	556.8	2.227	1.431	H→L (0.558)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	510.3	2.430	2.546	H→L (0.439)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	576.1	2.152	1.134	H→L (0.575)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	669.0	1.853	1.045	H→L (0.612)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	564.0	2.198	0.788	H-1→L (0.530)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	565.1	2.194	0.871	H→L (0.870)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	451.1	2.749	1.661	H→L (0.773)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	482.6	2.569	1.161	H→L (0.437)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	497.9	2.490	1.187	H→L (0.458)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	595.7	2.081	0.952	H→L (0.674)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	598.8	2.070	1.468	H-1→L (0.461)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	708.5	1.750	0.345	H-1→L (0.424)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	803.2	1.544	0.652	H→L (0.656)	$\pi \rightarrow \pi^*$

Table S40: Excited state properties calculated with the ωB2PLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	434.7	2.852	1.747	H→L (0.455)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	437.7	2.833	2.762	H→L (0.354)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	417.8	2.968	1.525	H→L (0.466)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	415.0	2.987	1.658	H→L (0.553)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	386.6	3.207	1.384	H-1→L (0.715)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	442.3	2.803	1.093	H→L (0.842)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	399.0	3.107	1.804	H-1→L (0.767)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	399.9	3.100	1.383	H→L (0.400)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	417.4	2.970	1.353	H→L (0.401)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	410.6	3.020	1.385	H→L (0.581)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	460.0	2.695	1.694	H-1→L (0.475)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	418.4	2.963	0.618	H→L+1 (0.418)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	392.6	3.158	1.386	H→L (0.505)	$\pi \rightarrow \pi^*$

Table S41: Excited state properties calculated with the ωB2GPPLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
N1	$S_0 \rightarrow S_1$	436.0	2.844	1.741	H→L (0.457)	$\pi \rightarrow \pi^*$
N2	$S_0 \rightarrow S_1$	437.5	2.834	2.783	H→L (0.363)	$\pi \rightarrow \pi^*$
N3	$S_0 \rightarrow S_1$	419.4	2.956	1.517	H→L (0.467)	$\pi \rightarrow \pi^*$
N4	$S_0 \rightarrow S_1$	417.8	2.968	1.648	H→L (0.537)	$\pi \rightarrow \pi^*$
N5	$S_0 \rightarrow S_1$	386.3	3.209	1.412	H-1→L (0.736)	$\pi \rightarrow \pi^*$
N6	$S_0 \rightarrow S_1$	444.9	2.787	1.094	H→L (0.848)	$\pi \rightarrow \pi^*$
N7	$S_0 \rightarrow S_1$	398.9	3.108	1.804	H→L (0.777)	$\pi \rightarrow \pi^*$
N8	$S_0 \rightarrow S_1$	399.7	3.102	1.385	H-1→L (0.388)	$\pi \rightarrow \pi^*$
N9	$S_0 \rightarrow S_1$	416.8	2.975	1.350	H→L (0.429)	$\pi \rightarrow \pi^*$
N10	$S_0 \rightarrow S_1$	412.2	3.008	1.384	H→L (0.573)	$\pi \rightarrow \pi^*$
N11	$S_0 \rightarrow S_1$	462.2	2.682	1.749	H-1→L (0.459)	$\pi \rightarrow \pi^*$
N12	$S_0 \rightarrow S_1$	414.2	2.994	0.985	H-1→L (0.483)	$\pi \rightarrow \pi^*$
N13	$S_0 \rightarrow S_1$	395.7	3.133	1.432	H→L (0.497)	$\pi \rightarrow \pi^*$

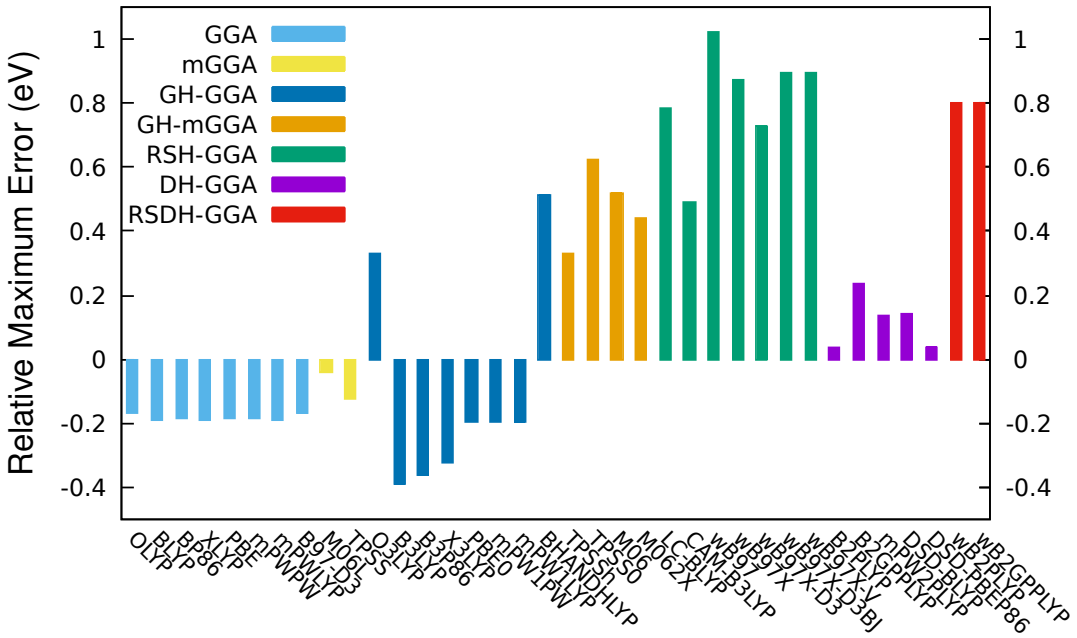

Figure S1: Relative maximum errors (Max) of TD-DFT excitation energies.

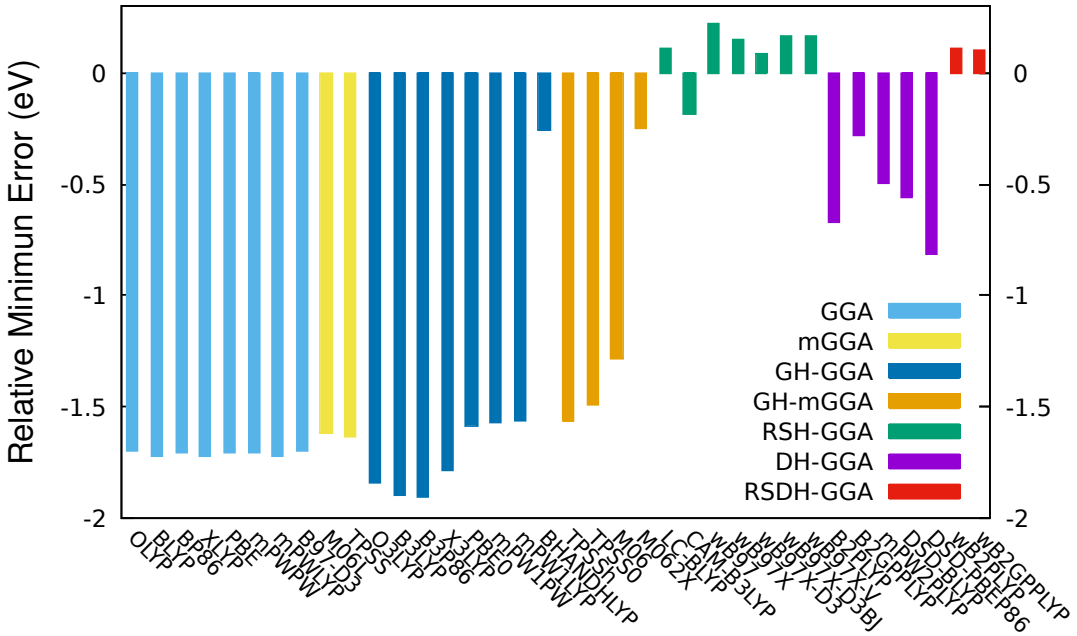

Figure S2: Relative minimum errors (Min) of TD-DFT excitation energies.

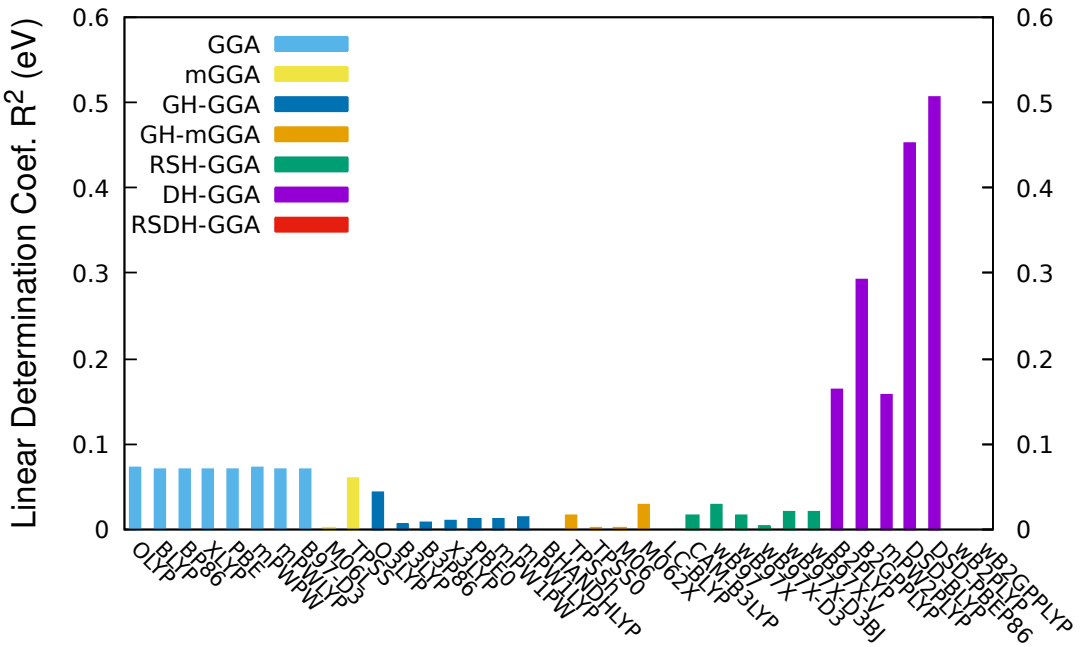

Figure S3: Linear determination coefficients (R^2) of TD-DFT excitation energies.

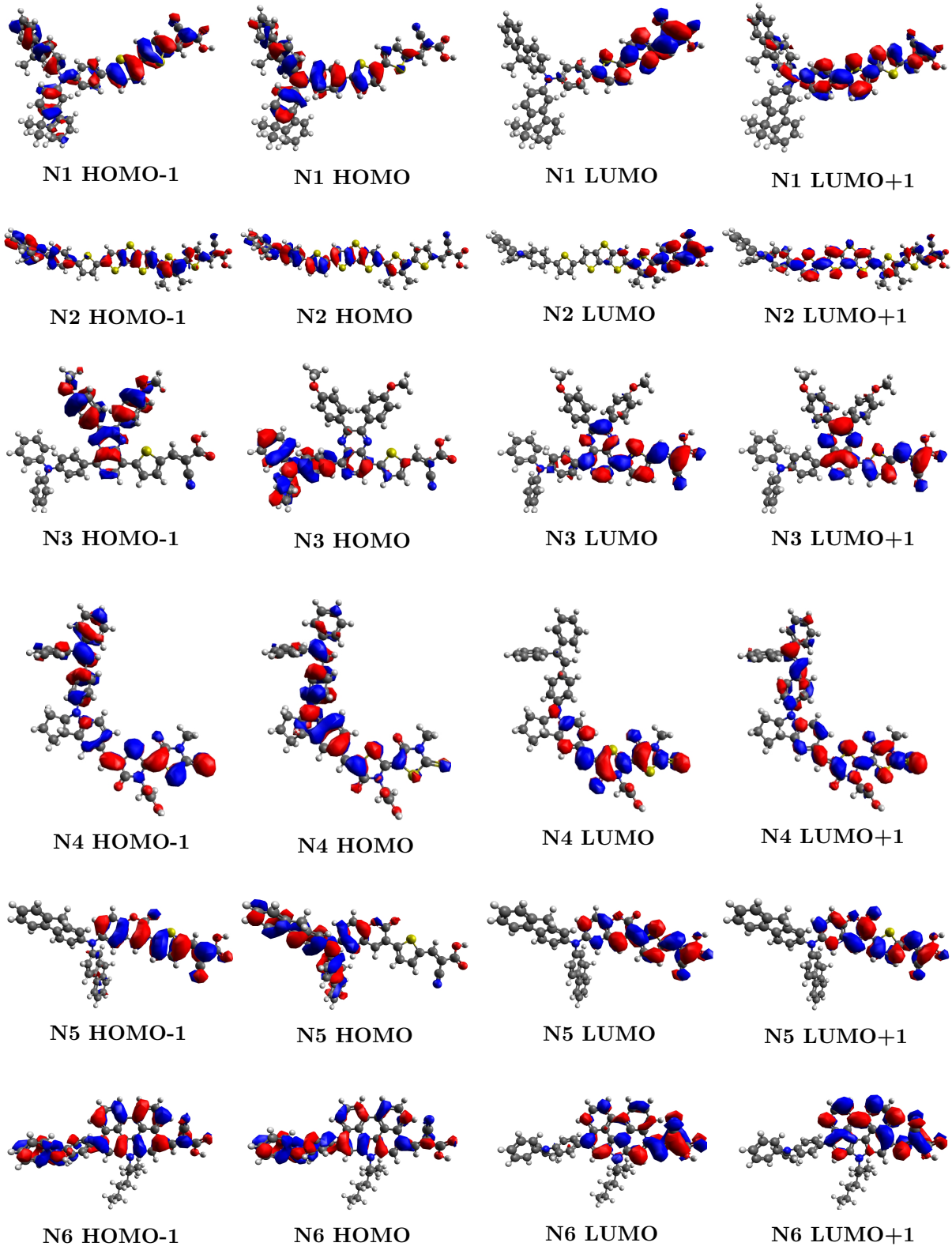

Figure S4: Molecular orbitals (HOMO-1, HOMO, LUOM and LUMO+1) involved in the main transitions of the dye sensitizers (**N1**–**N13**). Isosurface value = 0.02.

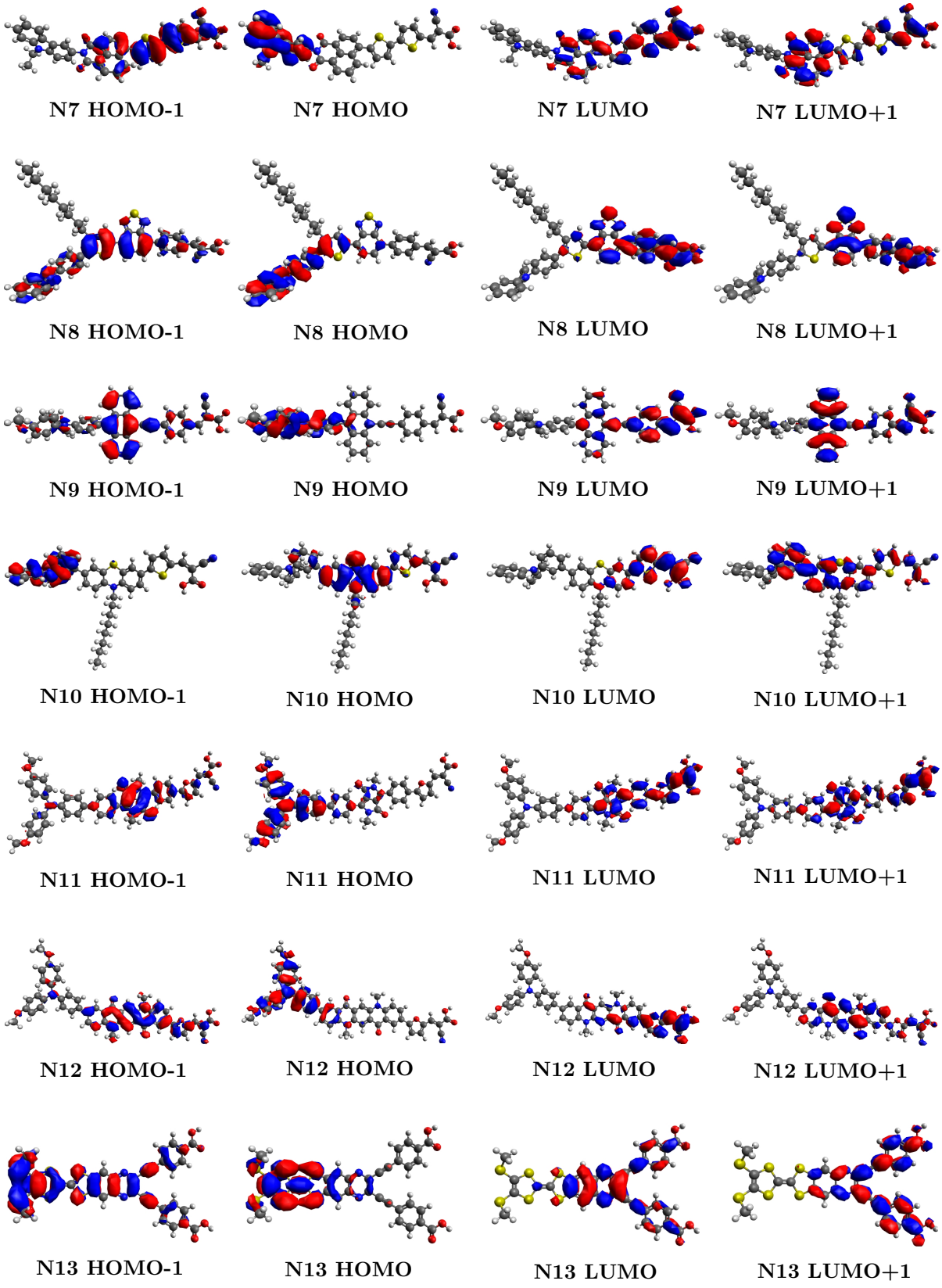

Figure S4: (*Cont.*) Molecular orbitals (HOMO-1, HOMO, LUOM and LUMO+1) involved in the main transitions of the dye sensitizers (**N1**–**N13**). Isosurface value = 0.02.