Electronic Supplementary Information (ESI) for:

Accurate Predictions of the Electronic Excited States of BODIPY Based Dye Sensitizers Using Spin-Component-Scaled Double-Hybrid Functionals: A TD-DFT Benchmark Study

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Table S1: Experimental Maximum Absorption Values (eV) Used as Reference in This Study, and the Corresponding Solvents Used in Experiment. References are Cited in the Main Article.

	Absorption	Solvent	Reference
B1	2.321	Chloroform	[93]
B2	2.238	Chloroform	[94]
B3	2.242	Chloroform	[95]
B4	2.274	Chloroform	[96]
B5	2.330	Chloroform	[97]
B6	2.119	Tetrahydrofuran	[98]
B7	2.291	Chloroform	[96]
B8	1.712	Chloroform	[99]
B9	1.923	Dichloromethane	[100]
B10	1.864	Dichloromethane	[101]
B11	2.388	Dichloromethane	[102]
B12	1.526	Dichloromethane	[103]
B13	1.916	Tetrahydrofuran	[104]

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

	OLYP	BLYP	BP86	XLYP	PBE	mPWPW	mPWLYP	B97-D3	Exp
B1	2.346	2.298	2.312	2.300	2.318	2.320	2.294	2.325	2.321
B2	1.727	1.629	1.682	1.640	1.714	1.708	1.631	1.672	2.238
B3	1.461	1.410	1.441	1.415	1.460	1.457	1.411	1.433	2.242
B4	2.290	2.253	2.188	2.275	2.200	2.228	2.264	2.288	2.274
B5	1.621	1.494	1.644	1.461	1.667	1.615	1.463	1.490	2.330
B6	2.020	1.993	2.007	1.990	2.006	2.004	1.989	2.021	2.119
B7	1.615	1.633	1.605	1.649	1.609	1.615	1.642	1.616	2.291
B8	2.127	2.108	2.118	2.107	2.119	2.118	2.106	2.123	1.712
B9	2.137	2.115	2.125	2.114	2.126	2.125	2.113	2.130	1.923
B10	1.982	2.000	2.005	1.998	2.005	1.999	2.001	1.986	1.864
B11	2.153	2.110	2.031	2.134	2.016	2.032	2.108	2.146	2.388
B12	1.536	1.527	1.528	1.528	1.525	1.525	1.527	1.545	1.526
B13	1.903	1.877	1.878	1.878	1.877	1.879	1.874	1.895	1.916
MAE	0.294	0.319	0.314	0.315	0.308	0.308	0.320	0.310	
Max	0.415	0.396	0.406	0.395	0.407	0.406	0.394	0.411	
Min	-0.781	-0.836	-0.801	-0.869	-0.782	-0.785	-0.867	-0.840	
SD	0.289	0.314	0.286	0.317	0.280	0.289	0.317	0.314	
R^2	0.010	0.001	0.002	0.002	0.003	0.003	0.001	0.002	

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

	O3LYP	B3LYP	B3P86	X3LYP	PBE0	mPW1PW	mPW1LYP	BH&HLYP	Exp
B1	2.617	2.723	2.742	2.761	2.809	2.809	2.800	2.795	2.321
B2	2.317	2.491	2.499	2.520	2.580	2.580	2.563	2.705	2.238
B3	2.192	2.498	2.512	2.475	2.601	2.601	2.585	2.792	2.242
B4	1.692	2.219	2.220	2.315	2.476	2.478	2.464	2.696	2.274
B5	2.331	1.960	2.264	2.603	2.705	2.705	2.690	2.620	2.330
B6	2.271	2.439	2.449	2.476	2.553	2.553	2.540	2.578	2.119
B7	2.258	2.515	2.523	2.549	2.618	2.617	2.602	2.750	2.291
B8	1.469	1.703	1.699	1.755	1.841	1.845	1.853	2.033	1.712
B9	1.691	1.957	1.955	1.994	2.052	2.053	2.050	2.273	1.923
B10	2.276	2.418	2.430	2.446	2.509	2.507	2.492	2.224	1.864
B11	2.616	2.846	2.859	2.868	2.928	2.926	2.904	2.977	2.388
B12	1.391	1.555	1.548	1.585	1.626	1.629	1.639	1.935	1.526
B13	1.814	2.130	2.147	2.164	2.213	2.213	2.199	2.343	1.916
MAE	0.196	0.244	0.228	0.259	0.336	0.336	0.326	0.429	
Max	0.412	0.554	0.566	0.582	0.645	0.643	0.628	0.589	
Min	-0.582	-0.370	-0.066	0.041	0.100	0.103	0.113	0.290	
SD	0.164	0.176	0.184	0.175	0.167	0.165	0.158	0.086	
R^2	0.612	0.594	0.721	0.820	0.857	0.858	0.859	0.946	

Table S4: Vertical Excitation Energies (eV) Using mGGA and GH-mGGA Functionals.

	M06-L	TPSS	TPSSh	TPSS0	M060	M06-2X	Exp
B1	2.530	2.433	2.661	2.852	2.777	2.704	2.321
B2	2.062	1.939	2.368	2.623	2.563	2.618	2.238
B3	1.725	2.088	2.294	2.650	2.589	2.704	2.242
B4	2.324	2.321	2.582	2.545	2.550	2.615	2.274
B5	1.985	2.521	2.363	2.749	2.692	2.611	2.330
B6	2.178	2.062	2.285	2.598	2.560	2.498	2.119
B7	1.810	2.603	2.296	2.657	2.600	2.665	2.291
B8	2.178	2.165	2.343	1.892	1.906	1.979	1.712
B9	2.241	2.172	2.281	2.087	2.051	2.232	1.923
B10	2.021	2.021	2.290	2.540	1.594	2.164	1.864
B11	2.492	2.264	2.722	2.595	2.834	2.888	2.388
B12	1.649	1.573	1.403	1.662	1.667	1.872	1.526
B13	2.025	1.950	1.792	2.244	2.172	2.293	1.916
MAE	0.240	0.172	0.233	0.350	0.304	0.361	
Max	0.466	0.453	0.631	0.676	0.446	0.500	
Min	-0.517	-0.299	-0.124	0.136	-0.270	0.267	
SD	0.167	0.126	0.183	0.159	0.109	0.067	
R^2	0.151	0.519	0.579	0.823	0.875	0.965	

Table S5: Vertical Excitation Energies (eV) Using RSH-GGA Functionals.

	LC-BLYP	CAM-B3LYP	ωB97	ωB97X	ωB97X-D3	ωB97X-D3(BJ)	ωB97X-V	Exp
B1	2.820	2.776	2.878	2.869	2.855	2.891	2.891	2.321
B2	2.719	2.672	2.777	2.766	2.752	2.789	2.789	2.238
B3	2.771	2.746	2.823	2.817	2.807	2.841	2.841	2.242
B4	2.755	2.693	2.808	2.801	2.788	2.822	2.822	2.274
B5	2.786	2.706	2.845	2.832	2.815	2.855	2.855	2.330
B6	2.660	2.565	2.727	2.711	2.690	2.734	2.734	2.119
B7	2.760	2.719	2.813	2.808	2.796	2.825	2.825	2.291
B8	2.139	2.030	2.194	2.170	2.144	2.191	2.191	1.712
B9	2.310	2.259	2.351	2.336	2.319	2.355	2.355	1.923
B10	2.365	2.233	2.419	2.399	2.375	2.424	2.424	1.864
B11	2.844	2.910	2.864	2.885	2.899	2.912	2.912	2.388
B12	2.014	1.923	2.052	2.041	2.023	2.058	2.058	1.526
B13	2.300	2.306	2.332	2.335	2.334	2.358	2.358	1.916
MAE	0.469	0.415	0.518	0.510	0.496	0.532	0.532	
Max	0.541	0.522	0.608	0.592	0.571	0.615	0.615	
Min	0.384	0.318	0.416	0.413	0.396	0.432	0.432	
SD	0.048	0.060	0.056	0.053	0.053	0.054	0.054	
R^2	0.975	0.979	0.966	0.972	0.976	0.972	0.972	

Table S6: Vertical Excitation Energies (eV) Using DH-GGA and RSDH-GGA Functionals.

	B2PLYP	B2GPPLYP	mPW2PLYP	DSDBLYP	DSDPBEP86	ωB2PLYP	ωB2GPPLYP	Exp
B1	2.472	2.615	2.552	2.220	2.170	2.786	2.763	2.321
B2	2.403	2.499	2.462	2.113	2.065	2.678	2.655	2.238
B3	2.520	2.587	2.568	2.216	2.176	2.733	2.711	2.242
B4	2.376	2.536	2.460	2.177	2.127	2.716	2.694	2.274
B5	2.294	2.537	2.407	2.155	2.096	2.748	2.724	2.330
B6	2.236	2.394	2.315	1.991	1.928	2.619	2.594	2.119
B7	2.466	2.564	2.525	2.219	2.176	2.721	2.701	2.291
B8	1.820	1.927	1.867	1.724	1.669	2.109	2.095	1.712
B9	2.124	2.176	2.153	1.994	1.965	2.281	2.268	1.923
B10	1.958	2.124	2.028	1.884	1.819	2.334	2.319	1.864
B11	2.811	2.797	2.830	2.502	2.496	2.804	2.787	2.388
B12	1.716	1.804	1.760	1.579	1.523	1.967	1.951	1.526
B13	2.198	2.221	2.220	1.998	1.982	2.281	2.268	1.916
MAE	0.179	0.280	0.231	0.083	0.106	0.433	0.414	
Max	0.423	0.409	0.442	0.114	0.108	0.500	0.475	
Min	-0.036	0.207	0.077	-0.175	-0.234	0.358	0.345	
SD	0.102	0.053	0.090	0.048	0.069	0.043	0.040	
R^2	0.865	0.972	0.917	0.886	0.848	0.979	0.980	

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	528.5	2.346	0.592	H-1→L (0.704)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	717.8	1.727	0.411	H-1→L (0.726)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	848.6	1.461	0.255	H-1→L (0.642)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	541.4	2.290	0.223	H-4→L (0.440)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	764.7	1.621	0.150	H-3→L (0.560)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	613.9	2.020	0.559	H-1→L (0.769)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	767.9	1.615	0.329	H-1→L (0.626)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	583.0	2.127	0.404	H-2→L (0.656)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	580.2	2.137	0.622	H-2→L (0.623)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	625.4	1.982	0.632	H-1→L (0.427)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	575.8	2.153	0.271	H-5→L+1 (0.576)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	807.0	1.536	0.251	H-1→L (0.907)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	651.5	1.903	0.625	H→L (0.665)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	539.6	2.298	0.564	H-1→L (0.697)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	761.0	1.629	0.369	H-1→L (0.716)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	879.6	1.410	0.234	H-1→L (0.640)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	550.3	2.253	0.201	H-4→L (0.474)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	829.7	1.494	0.111	H-3→L (0.621)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	622.1	1.993	0.542	H-1→L (0.775)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	759.4	1.633	0.345	H-1→L (0.635)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	588.0	2.108	0.385	H-2→L (0.694)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	586.1	2.115	0.604	H-2→L (0.619)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	619.9	2.000	0.661	H-1→L (0.503)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	587.6	2.110	0.255	H-5→L+1 (0.567)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	812.0	1.527	0.248	H-1→L (0.903)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	660.4	1.877	0.614	H→L (0.677)	$\pi \rightarrow \pi^*$

Table S9: Excited state properties calculated with the BP86 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	536.3	2.312	0.578	H-1→L (0.704)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	737.3	1.682	0.391	H-1→L (0.720)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	860.1	1.441	0.245	H-1→L (0.639)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	566.6	2.188	0.161	H-4→L (0.544)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	754.0	1.644	0.163	H-3→L (0.515)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	617.7	2.007	0.552	H-1→L (0.770)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	772.6	1.605	0.326	H-1→L (0.632)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	585.4	2.118	0.392	H-2→L (0.683)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	583.5	2.125	0.622	H-2→L (0.628)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	618.4	2.005	0.656	H-1→L (0.464)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	610.5	2.031	0.189	H-5→L+1 (0.634)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	811.2	1.528	0.252	H-1→L (0.905)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	660.4	1.878	0.594	H→L (0.682)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	539.0	2.300	0.564	H-1→L (0.697)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	756.0	1.640	0.375	H-1→L (0.718)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	876.0	1.415	0.236	H-1→L (0.639)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	545.1	2.275	0.226	H-4→L (0.417)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	848.5	1.461	0.102	H-3→L (0.643)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	623.0	1.990	0.540	H-1→L (0.776)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	751.8	1.649	0.354	H-1→L (0.637)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	588.3	2.107	0.385	H-2→L (0.694)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	586.5	2.114	0.601	H-2→L (0.617)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	620.5	1.998	0.660	H-1→L (0.503)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	581.1	2.134	0.272	H-5→L+1 (0.547)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	811.4	1.528	0.247	H-1→L (0.903)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	660.3	1.878	0.618	H→L (0.677)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	534.8	2.318	0.581	H-1→L (0.704)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	723.5	1.714	0.403	H-1→L (0.724)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	849.0	1.460	0.250	H-1→L (0.636)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	563.5	2.200	0.166	H-4→L (0.530)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	743.9	1.667	0.172	H-3→L (0.478)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	618.1	2.006	0.549	H-1→L (0.770)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	770.5	1.609	0.326	H-1→L (0.628)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	585.2	2.119	0.394	H-2→L (0.681)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	583.1	2.126	0.626	H-2→L (0.628)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	618.3	2.005	0.652	H-1→L (0.456)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	614.9	2.016	0.177	H-5→L+1 (0.663)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	813.0	1.525	0.251	H-1→L (0.905)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	660.4	1.877	0.586	H→L (0.680)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	534.4	2.320	0.581	H-1→L (0.703)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	725.9	1.708	0.401	H-1→L (0.724)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	850.8	1.457	0.249	H-1→L (0.635)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	556.4	2.228	0.180	H-4→L (0.507)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	767.9	1.615	0.150	H-3→L (0.534)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	618.7	2.004	0.547	H-1→L (0.770)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	767.8	1.615	0.330	H-1→L (0.629)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	585.5	2.118	0.395	H-2→L (0.679)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	583.3	2.125	0.626	H-2→L (0.627)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	620.2	1.999	0.651	H-1→L (0.459)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	610.1	2.032	0.189	H-5→L+1 (0.650)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	812.9	1.525	0.251	H-1→L (0.905)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	659.9	1.879	0.592	H→L (0.679)	$\pi \rightarrow \pi^*$

Table S13: Excited state properties calculated with the mPWLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	540.6	2.294	0.561	H-1→L (0.696)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	760.1	1.631	0.370	H-1→L (0.716)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	878.6	1.411	0.233	H-1→L (0.638)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	547.7	2.264	0.213	H-4→L (0.444)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	847.5	1.463	0.102	H-3→L (0.641)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	623.2	1.989	0.539	H-1→L (0.776)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	755.1	1.642	0.349	H-1→L (0.636)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	588.6	2.106	0.383	H-2→L (0.696)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	586.8	2.113	0.600	H-2→L (0.617)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	619.7	2.001	0.662	H-1→L (0.503)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	588.2	2.108	0.253	H-5→L+1 (0.568)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	812.1	1.527	0.247	H-1→L (0.903)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	661.6	1.874	0.611	H→L (0.680)	$\pi \rightarrow \pi^*$

Table S14: Excited state properties calculated with the B97-D3 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	533.2	2.325	0.584	H-1→L (0.703)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	741.6	1.672	0.389	H-1→L (0.720)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	865.1	1.433	0.246	H-1→L (0.647)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	541.9	2.288	0.223	H-4→L (0.452)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	831.9	1.490	0.109	H-3→L (0.665)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	613.5	2.021	0.564	H-1→L (0.770)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	767.3	1.616	0.333	H-1→L (0.633)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	583.9	2.123	0.397	H-2→L (0.665)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	582.2	2.130	0.613	H-2→L (0.623)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	624.2	1.986	0.647	H-1→L (0.444)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	577.7	2.146	0.269	H-5→L+1 (0.535)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	802.7	1.545	0.252	H-1→L (0.905)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	654.2	1.895	0.630	H→L (0.677)	$\pi \rightarrow \pi^*$

Table S15: Excited state properties calculated with the M06-L functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	490.1	2.530	0.742	H-1→L (0.761)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	601.3	2.062	0.583	H-1→L (0.791)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	718.9	1.725	0.373	H-1→L (0.694)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	533.6	2.324	0.427	H-1→L+1 (0.446)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	624.5	1.985	0.319	H-3→L (0.410)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	569.4	2.178	0.649	H-1→L (0.782)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	685.0	1.810	0.422	H-1→L (0.655)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_3$	569.4	2.178	0.216	H-2→L (0.728)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	553.3	2.241	0.626	H-2→L (0.653)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	613.5	2.021	0.349	H-1→L (0.603)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_7$	497.6	2.492	0.289	H-4→L (0.587)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	752.0	1.649	0.274	H-1→L (0.917)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	612.3	2.025	0.730	H→L (0.703)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	509.5	2.433	0.656	H-1→L (0.729)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	639.4	1.939	0.518	H-1→L (0.771)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_5$	593.9	2.088	0.142	H-2→L (0.412)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_5$	534.3	2.321	0.323	H-1→L+1 (0.388)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_7$	491.9	2.521	0.781	H-4→L (0.337)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_3$	601.3	2.062	0.580	H-1→L (0.783)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_8$	476.3	2.603	0.246	H-4→L+1 (0.421)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_4$	572.7	2.165	0.409	H-2→L (0.648)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_5$	570.9	2.172	0.633	H-2→L (0.641)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_4$	613.5	2.021	0.633	H-1→L (0.422)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_9$	547.5	2.264	0.321	H-5→L+1 (0.491)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_2$	788.4	1.573	0.265	H-1→L (0.909)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_3$	635.7	1.950	0.662	H→L (0.681)	$\pi \rightarrow \pi^*$

Table S17: Excited state properties calculated with the O3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	473.8	2.617	0.854	H-1→L (0.867)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	535.2	2.317	0.842	H-1→L (0.926)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	565.6	2.192	0.710	H-1→L (0.896)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	732.7	1.692	0.401	H-1→L (0.881)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	531.8	2.331	0.595	H-2→L (0.540)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	545.9	2.271	0.704	H-1→L (0.862)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	549.2	2.258	0.861	H-1→L (0.902)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	844.0	1.469	0.327	H-1→L (0.955)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	733.4	1.691	0.695	H→L (0.868)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	544.6	2.276	0.521	H-1→L (0.841)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_5$	474.0	2.616	0.210	H-3→L (0.602)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	891.1	1.391	1.157	H→L (0.969)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	683.4	1.814	0.823	H→L+1 (0.557)	$\pi \rightarrow \pi^*$

Table S18: Excited state properties calculated with the B3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	455.2	2.723	0.890	H-1→L (0.846)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	497.7	2.491	1.011	H-1→L (0.968)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	496.3	2.498	0.999	H-1→L (0.947)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	558.7	2.219	0.819	H-1→L (0.964)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	632.6	1.960	0.211	H→L+1 (0.639)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	508.2	2.439	0.738	H-1→L (0.918)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	493.1	2.515	1.228	H-1→L (0.967)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	727.9	1.703	0.402	H-1→L (0.969)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	633.5	1.957	0.970	H→L (0.959)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	512.7	2.418	0.448	H-1→L (0.921)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	435.6	2.846	1.050	H-1→L+1 (0.714)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	797.3	1.555	1.348	H→L (0.986)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	582.0	2.130	1.629	H→L (0.850)	$\pi \rightarrow \pi^*$

Table S19: Excited state properties calculated with the B3P86 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	452.2	2.742	0.942	H-1→L (0.898)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	496.1	2.499	1.014	H-1→L (0.967)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	493.6	2.512	1.007	H-1→L (0.946)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	558.4	2.220	0.816	H-1→L (0.963)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	547.6	2.264	0.439	H-1→L (0.528)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	506.2	2.449	0.750	H-1→L (0.917)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	491.4	2.523	1.238	H-1→L (0.967)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	729.8	1.699	0.406	H-1→L (0.970)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	634.2	1.955	0.967	H→L (0.958)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	510.3	2.430	0.452	H-1→L (0.921)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	433.6	2.859	1.056	H-1→L+1 (0.701)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	800.9	1.548	1.355	H→L (0.987)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	577.5	2.147	1.652	H→L (0.871)	$\pi \rightarrow \pi^*$

Table S20: Excited state properties calculated with the X3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	449.0	2.761	0.965	H-1→L (0.936)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	492.1	2.520	1.011	H-1→L (0.960)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	500.9	2.475	0.812	H-1→L (0.774)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	535.5	2.315	0.913	H-1→L (0.970)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	476.3	2.603	0.962	H-1→L (0.887)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	500.7	2.476	0.735	H-1→L (0.925)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	486.4	2.549	1.266	H-1→L (0.964)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	706.5	1.755	0.422	H-1→L (0.971)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	621.9	1.994	1.008	H→L (0.966)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	506.9	2.446	0.420	H-1→L (0.931)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	432.2	2.868	1.062	H-1→L+1 (0.713)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	782.2	1.585	1.386	H→L (0.988)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	573.1	2.164	1.698	H→L (0.909)	$\pi \rightarrow \pi^*$

Table S21: Excited state properties calculated with the PBE0 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	441.4	2.809	0.973	H-1→L (0.949)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_2$	480.6	2.580	0.993	H-1→L (0.926)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_2$	476.7	2.601	1.084	H-1→L (0.942)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	500.7	2.476	1.075	H-1→L (0.968)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	458.3	2.705	1.120	H-1→L (0.920)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	485.6	2.553	0.730	H-1→L (0.929)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	473.5	2.618	1.307	H-1→L (0.938)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	673.4	1.841	0.462	H-1→L (0.974)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	604.3	2.052	1.063	H→L (0.974)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	494.1	2.509	0.368	H-1→L (0.946)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	423.5	2.928	1.080	H-1→L+1 (0.713)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	762.4	1.626	1.454	H→L (0.990)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	560.2	2.213	1.724	H→L (0.959)	$\pi \rightarrow \pi^*$

Table S22: Excited state properties calculated with the mPW1PW functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	441.3	2.809	0.973	H-1→L (0.949)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_2$	480.5	2.580	0.995	H-1→L (0.927)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_2$	476.6	2.601	1.085	H-1→L (0.942)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	500.3	2.478	1.079	H-1→L (0.968)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	458.3	2.705	1.121	H-1→L (0.919)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	485.6	2.553	0.728	H-1→L (0.929)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	473.7	2.617	1.301	H-1→L (0.935)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	672.2	1.845	0.462	H-1→L (0.974)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	604.0	2.053	1.065	H→L (0.974)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	494.6	2.507	0.367	H-1→L (0.947)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	423.7	2.926	1.078	H-1→L+1 (0.707)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	761.1	1.629	1.453	H→L (0.990)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	560.3	2.213	1.730	H→L (0.958)	$\pi \rightarrow \pi^*$

Table S23: Excited state properties calculated with the mPW1LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	442.9	2.800	0.966	H-1→L (0.949)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_2$	483.7	2.563	0.955	H-1→L (0.894)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_2$	479.7	2.585	1.065	H-1→L (0.939)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	503.1	2.464	1.066	H-1→L (0.968)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	460.9	2.690	1.107	H-1→L (0.917)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	488.1	2.540	0.711	H-1→L (0.930)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	476.5	2.602	1.258	H-1→L (0.924)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	669.2	1.853	0.459	H-1→L (0.973)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	604.9	2.050	1.065	H→L (0.974)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	497.6	2.492	0.363	H-1→L (0.946)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	426.9	2.904	1.049	H-1→L+1 (0.676)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	756.4	1.639	1.449	H→L (0.989)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	563.7	2.199	1.735	H→L (0.956)	$\pi \rightarrow \pi^*$

Table S24: Excited state properties calculated with the BH&HLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	443.6	2.795	1.132	H→L (0.513)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	458.3	2.705	1.617	H-1→L (0.451)	$\pi \rightarrow \pi^*$
					H→L (0.438)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	444.1	2.792	1.584	H-1→L (0.538)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	459.9	2.696	1.478	H-1→L (0.454)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	473.2	2.620	1.128	H→L (0.523)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	480.9	2.578	1.431	H→L (0.664)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	450.8	2.750	1.848	H-1→L (0.477)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	610.0	2.033	1.084	H→L (0.928)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	545.5	2.273	1.223	H→L (0.946)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	557.5	2.224	1.401	H→L (0.846)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	416.4	2.977	0.511	H→L (0.685)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	640.7	1.935	1.771	H→L (0.959)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	529.2	2.343	1.752	H→L (0.942)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_3$	466.0	2.661	0.887	H-1→L (0.868)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_3$	523.5	2.368	0.870	H-1→L (0.924)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_3$	540.5	2.294	0.769	H-1→L (0.895)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_4$	480.2	2.582	0.430	H-1→L+1 (0.615)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_4$	524.7	2.363	0.636	H-2→L (0.470)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	542.6	2.285	0.712	H-1→L (0.861)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	540.1	2.296	0.887	H-1→L (0.892)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_3$	529.2	2.343	0.252	H-2→L (0.876)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_3$	543.6	2.281	0.365	H-2→L (0.842)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	541.4	2.290	0.529	H-1→L (0.832)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_6$	455.5	2.722	0.472	H-3→L+1 (0.441)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	883.4	1.403	1.169	H→L (0.966)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	692.0	1.792	0.752	H→L+1 (0.571)	$\pi \rightarrow \pi^*$

Table S26: Excited state properties calculated with the TPSS0 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	434.7	2.852	0.992	H-1→L (0.953)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_2$	472.7	2.623	1.034	H-1→L (0.951)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_2$	467.8	2.650	1.111	H-1→L (0.954)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	487.2	2.545	1.143	H-1→L (0.967)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	451.1	2.749	1.159	H-1→L (0.919)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	477.2	2.598	0.739	H-1→L (0.932)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_3$	466.7	2.657	1.319	H-1→L (0.925)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	655.2	1.892	0.476	H-1→L (0.974)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	594.2	2.087	1.096	H→L (0.975)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_2$	488.1	2.540	0.362	H-1→L (0.950)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_4$	477.8	2.595	0.107	H-2→L (0.422)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	745.9	1.662	1.496	H→L (0.990)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	552.6	2.244	1.782	H→L (0.961)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_2$	446.4	2.777	0.930	H-1→L (0.955)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_2$	483.7	2.563	0.927	H-1→L (0.943)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_2$	478.9	2.589	1.093	H-1→L (0.950)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_3$	486.1	2.550	1.178	H-1→L (0.946)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_2$	460.5	2.692	1.152	H-1→L (0.910)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_2$	484.3	2.560	0.671	H-1→L (0.924)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_2$	476.9	2.600	1.221	H-1→L (0.898)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_2$	650.4	1.906	0.473	H-1→L (0.972)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	604.6	2.051	1.080	H→L (0.974)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	777.8	1.594	0.895	H→L (0.985)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_3$	437.5	2.834	0.282	H-1→L (0.602)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	743.7	1.667	1.456	H→L (0.989)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	571.0	2.172	1.625	H→L (0.968)	$\pi \rightarrow \pi^*$

Table S28: Excited state properties calculated with the M06-2X functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	458.6	2.704	1.099	H-1→L (0.492)	$\pi \rightarrow \pi^*$
					H→L (0.456)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	473.7	2.618	1.493	H-1→L (0.494)	$\pi \rightarrow \pi^*$
					H→L (0.403)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	458.5	2.704	1.453	H-1→L (0.626)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	474.1	2.615	1.383	H-1→L (0.493)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	474.8	2.611	1.174	H-1→L (0.520)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	496.4	2.498	1.349	H→L (0.609)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	465.3	2.665	1.681	H-1→L (0.518)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	626.5	1.979	1.027	H→L (0.914)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	555.5	2.232	1.159	H→L (0.937)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	572.9	2.164	1.332	H→L (0.826)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	429.3	2.888	0.475	H→L (0.936)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	662.1	1.872	1.692	H→L (0.954)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	540.6	2.293	1.633	H→L (0.948)	$\pi \rightarrow \pi^*$

Table S29: Excited state properties calculated with the LC-BLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	439.6	2.820	1.219	H-1→L (0.723)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	456.0	2.719	1.551	H-1→L (0.554)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	447.5	2.771	1.460	H-1→L (0.585)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	450.0	2.755	1.560	H-1→L (0.635)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	445.0	2.786	1.374	H-1→L (0.789)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	466.1	2.660	1.471	H-1→L (0.516)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	449.2	2.760	1.711	H-1→L (0.545)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	579.5	2.139	1.055	H→L (0.787)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	536.8	2.310	1.131	H→L (0.874)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	524.3	2.365	1.269	H→L (0.581)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	435.9	2.844	0.484	H→L (0.903)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	615.7	2.014	1.708	H→L (0.857)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	539.1	2.300	1.572	H→L (0.911)	$\pi \rightarrow \pi^*$

Table S30: Excited state properties calculated with the CAM-B3LYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	446.6	2.776	1.170	H-1→L (0.575)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	464.1	2.672	1.571	H-1→L (0.530)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	451.5	2.746	1.511	H-1→L (0.623)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	460.4	2.693	1.527	H-1→L (0.544)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	458.2	2.706	1.315	H-1→L (0.620)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	483.4	2.565	1.419	H-1→L (0.555)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	456.0	2.719	1.781	H-1→L (0.535)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	610.8	2.030	1.050	H→L (0.891)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	548.7	2.259	1.170	H→L (0.927)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	555.2	2.233	1.361	H→L (0.771)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	426.1	2.910	0.484	H→L (0.857)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	644.6	1.923	1.709	H→L (0.937)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	537.6	2.306	1.648	H→L (0.934)	$\pi \rightarrow \pi^*$

Table S31: Excited state properties calculated with the ωB97 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	430.8	2.878	1.245	H-1→L (0.714)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	446.4	2.777	1.577	H-1→L (0.512)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	439.1	2.823	1.482	H-1→L (0.485)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	441.6	2.808	1.579	H-1→L (0.652)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	435.8	2.845	1.403	H-1→L (0.804)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	454.7	2.727	1.509	H-1→L (0.511)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	440.8	2.813	1.732	H-1→L (0.535)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	565.2	2.194	1.086	H→L (0.780)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	527.4	2.351	1.159	H→L (0.869)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	512.5	2.419	1.262	H→L (0.564)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	432.9	2.864	0.509	H→L (0.917)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	604.3	2.052	1.751	H→L (0.848)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	531.6	2.332	1.616	H→L (0.906)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	432.1	2.869	1.252	H-1→L (0.711)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	448.2	2.766	1.611	H-1→L (0.528)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	440.2	2.817	1.515	H-1→L (0.530)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	442.7	2.801	1.612	H-1→L (0.640)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	437.8	2.832	1.426	H-1→L (0.791)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	457.4	2.711	1.526	H-1→L (0.500)	$\pi \rightarrow \pi^*$
					H→L (0.405)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	441.6	2.808	1.779	H-1→L (0.536)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	571.3	2.170	1.084	H→L (0.800)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	530.7	2.336	1.164	H→L (0.881)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	516.7	2.399	1.296	H→L (0.595)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	429.7	2.885	0.505	H→L (0.903)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	607.6	2.041	1.746	H→L (0.864)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	531.0	2.335	1.627	H→L (0.910)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	434.2	2.855	1.252	H-1→L (0.704)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	450.5	2.752	1.630	H-1→L (0.542)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	441.7	2.807	1.536	H-1→L (0.568)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	444.7	2.788	1.631	H-1→L (0.632)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	440.5	2.815	1.437	H-1→L (0.776)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	461.0	2.690	1.532	H-1→L (0.488)	$\pi \rightarrow \pi^*$
					H→L (0.425)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	443.4	2.796	1.814	H-1→L (0.542)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	578.2	2.144	1.081	H→L (0.817)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	534.6	2.319	1.168	H→L (0.890)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	521.9	2.375	1.323	H→L (0.624)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	427.7	2.899	0.500	H→L (0.885)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	612.8	2.023	1.741	H→L (0.877)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	531.2	2.334	1.638	H→L (0.913)	$\pi \rightarrow \pi^*$

Table S34: 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
B1	$S_0 \rightarrow S_1$	428.8	2.891	1.257	H-1→L (0.706)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	444.6	2.789	1.621	H-1→L (0.519)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	436.4	2.841	1.528	H-1→L (0.516)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	439.4	2.822	1.619	H-1→L (0.642)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	434.3	2.855	1.434	H-1→L (0.790)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	453.6	2.734	1.535	H-1→L (0.492)	$\pi \rightarrow \pi^*$
					H→L (0.415)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	438.9	2.825	1.786	H-1→L (0.535)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	566.0	2.191	1.088	H→L (0.805)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	526.5	2.355	1.169	H→L (0.884)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	511.6	2.424	1.304	H→L (0.601)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	425.7	2.912	0.507	H→L (0.906)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	602.3	2.058	1.754	H→L (0.867)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	525.8	2.358	1.643	H→L (0.910)	$\pi \rightarrow \pi^*$

Table S35: Excited state properties calculated with the ωB97X-V functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	428.8	2.891	1.257	H-1→L (0.706)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	444.6	2.789	1.621	H-1→L (0.519)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	436.4	2.841	1.528	H-1→L (0.516)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	439.4	2.822	1.619	H-1→L (0.642)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	434.3	2.855	1.434	H-1→L (0.790)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	453.6	2.734	1.535	H-1→L (0.492)	$\pi \rightarrow \pi^*$
					H→L (0.415)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	438.9	2.825	1.786	H-1→L (0.535)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	566.0	2.191	1.088	H→L (0.805)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	526.5	2.355	1.169	H→L (0.884)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	511.6	2.424	1.304	H→L (0.601)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	425.7	2.912	0.507	H→L (0.906)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	602.3	2.058	1.754	H→L (0.867)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	525.8	2.358	1.643	H→L (0.910)	$\pi \rightarrow \pi^*$

Table S36: Excited state properties calculated with the B2PLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	501.5	2.472	1.050	H-1→L (0.500)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	515.9	2.403	1.467	H-1→L (0.462)	$\pi \rightarrow \pi^*$
					H→L (0.420)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	492.1	2.520	1.447	H-1→L (0.512)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	521.8	2.376	1.378	H-1→L (0.508)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	540.5	2.294	1.088	H-1→L (0.507)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	554.6	2.236	1.276	H→L (0.631)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	502.8	2.466	1.693	H-1→L (0.490)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	681.4	1.820	0.972	H→L (0.918)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	583.7	2.124	1.143	H→L (0.941)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	633.2	1.958	1.227	H→L (0.819)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	441.0	2.811	0.490	H→L (0.675)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	722.6	1.716	1.570	H→L (0.953)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	564.2	2.198	1.645	H→L (0.937)	$\pi \rightarrow \pi^*$

Table S37: Excited state properties calculated with the B2GPPLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	474.1	2.615	1.176	H-1→L (0.608)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	496.2	2.499	1.573	H-1→L (0.449)	$\pi \rightarrow \pi^*$
					H→L (0.402)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	479.3	2.587	1.512	H→L (0.471)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	488.9	2.536	1.560	H-1→L (0.578)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	488.6	2.537	1.363	H-1→L (0.708)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	517.9	2.394	1.424	H→L (0.546)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	483.5	2.564	1.795	H-1→L (0.471)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	643.2	1.927	1.031	H→L (0.885)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	569.8	2.176	1.169	H→L (0.923)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	583.7	2.124	1.279	H→L (0.733)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	443.2	2.797	0.509	H→L (0.567)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	687.4	1.804	1.646	H→L (0.928)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	558.3	2.221	1.661	H→L (0.921)	$\pi \rightarrow \pi^*$

Table S38: Excited state properties calculated with the mPW2PLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	485.9	2.552	1.103	H-1→L (0.531)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	503.6	2.462	1.515	H-1→L (0.467)	$\pi \rightarrow \pi^*$
					H→L (0.411)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	482.8	2.568	1.482	H-1→L (0.497)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	504.0	2.460	1.456	H-1→L (0.531)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	515.1	2.407	1.188	H-1→L (0.557)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	535.7	2.315	1.335	H→L (0.612)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	491.1	2.525	1.744	H-1→L (0.493)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	663.9	1.867	0.998	H→L (0.913)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	576.0	2.153	1.157	H→L (0.938)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	611.4	2.028	1.264	H→L (0.803)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	438.2	2.830	0.496	H→L (0.665)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	704.3	1.760	1.610	H→L (0.949)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	558.4	2.220	1.659	H→L (0.934)	$\pi \rightarrow \pi^*$

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

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	558.6	2.220	1.004	H-1→L (0.620)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	586.7	2.113	1.337	H→L (0.422)	$\pi \rightarrow \pi^*$
					H-1→L (0.405)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	559.5	2.216	1.298	H→L (0.566)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	569.4	2.177	1.340	H-1→L (0.575)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	575.4	2.155	1.169	H-1→L (0.765)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	622.9	1.991	1.187	H→L (0.514)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	558.6	2.219	1.546	H-1→L (0.422)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	719.0	1.724	0.923	H→L (0.862)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	621.8	1.994	1.072	H→L (0.909)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	658.2	1.884	1.095	H→L (0.687)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	495.6	2.502	0.470	H→L (0.501)	$\pi \rightarrow \pi^*$
					H→L+1 (0.460)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	785.1	1.579	1.436	H→L (0.907)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	620.5	1.998	1.500	H→L (0.909)	$\pi \rightarrow \pi^*$

Table S40: Excited state properties calculated with the DSD-PBEP86 functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	571.4	2.170	0.983	H-1→L (0.621)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	600.4	2.065	1.306	H-1→L (0.420)	$\pi \rightarrow \pi^*$
					H→L (0.416)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	569.7	2.176	1.274	H→L (0.536)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	582.9	2.127	1.310	H-1→L (0.582)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	591.4	2.096	1.137	H-1→L (0.753)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	643.1	1.928	1.154	H→L (0.520)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	569.9	2.176	1.518	H-1→L (0.444)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	742.9	1.669	0.894	H→L (0.869)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	630.8	1.965	1.056	H→L (0.914)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	681.5	1.819	1.070	H→L (0.700)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	496.8	2.496	0.464	H→L (0.532)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	814.0	1.523	1.391	H→L (0.914)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	625.5	1.982	1.483	H→L (0.909)	$\pi \rightarrow \pi^*$

Table S41: Excited state properties calculated with the ωB2PLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	445.1	2.786	1.235	H-1→L (0.663)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	462.9	2.678	1.615	H-1→L (0.426)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	453.6	2.733	1.524	H→L (0.506)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	456.5	2.716	1.596	H-1→L (0.595)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	451.2	2.748	1.418	H-1→L (0.797)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	473.4	2.619	1.498	H-1→L (0.454)	$\pi \rightarrow \pi^*$
					H→L (0.443)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	455.6	2.721	1.778	H-1→L (0.439)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	587.9	2.109	1.087	H→L (0.812)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	543.6	2.281	1.180	H→L (0.882)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	531.1	2.334	1.266	H→L (0.605)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	442.1	2.804	0.521	H→L (0.786)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	630.4	1.967	1.729	H→L (0.866)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	543.7	2.281	1.644	H→L (0.900)	$\pi \rightarrow \pi^*$

Table S42: Excited state properties calculated with the ωB2GPPLYP functional.

Compound	Electronic transition	λ_{max} (nm)	Optical gap (eV)	Oscillator strength	MO designation (coefficient)	Nature
B1	$S_0 \rightarrow S_1$	448.7	2.763	1.232	H-1→L (0.645)	$\pi \rightarrow \pi^*$
B2	$S_0 \rightarrow S_1$	467.0	2.655	1.624	H→L (0.399)	$\pi \rightarrow \pi^*$
					H-1→L (0.395)	$\pi \rightarrow \pi^*$
B3	$S_0 \rightarrow S_1$	457.3	2.711	1.533	H→L (0.561)	$\pi \rightarrow \pi^*$
B4	$S_0 \rightarrow S_1$	460.2	2.694	1.599	H-1→L (0.580)	$\pi \rightarrow \pi^*$
B5	$S_0 \rightarrow S_1$	455.1	2.724	1.423	H-1→L (0.797)	$\pi \rightarrow \pi^*$
B6	$S_0 \rightarrow S_1$	477.9	2.594	1.497	H→L (0.458)	$\pi \rightarrow \pi^*$
					H-1→L (0.438)	$\pi \rightarrow \pi^*$
B7	$S_0 \rightarrow S_1$	459.0	2.701	1.791	H-1→L (0.408)	$\pi \rightarrow \pi^*$
B8	$S_0 \rightarrow S_1$	591.8	2.095	1.092	H→L (0.817)	$\pi \rightarrow \pi^*$
B9	$S_0 \rightarrow S_1$	546.7	2.268	1.188	H→L (0.883)	$\pi \rightarrow \pi^*$
B10	$S_0 \rightarrow S_1$	534.7	2.319	1.266	H→L (0.615)	$\pi \rightarrow \pi^*$
B11	$S_0 \rightarrow S_1$	444.9	2.787	0.526	H→L (0.673)	$\pi \rightarrow \pi^*$
B12	$S_0 \rightarrow S_1$	635.5	1.951	1.729	H→L (0.869)	$\pi \rightarrow \pi^*$
B13	$S_0 \rightarrow S_1$	546.6	2.268	1.657	H→L (0.897)	$\pi \rightarrow \pi^*$

Table S43: Calculated ground state optimized geometries (xyz coordinates in Å) for all dyes (**B1** – **B13)**, determined at the BPE0/def2-TZVP level in solvent with CPCM solvation model.

B1	X	Y	Z
C	5.31907	-0.69498	0.65022
C	5.20320	0.56226	-1.24807
C	6.09638	-0.09625	-0.36642
C	0.23354	-0.55967	0.96406
C	-0.61519	0.03426	0.03734
C	0.19981	0.67099	-0.93215
N	3.96104	0.41683	-0.79346
N	1.48454	0.47290	-0.63303
C	1.56565	-0.27526	0.53770
C	3.98635	-0.34169	0.37598
F	2.57928	0.63303	-2.76552
F	2.73281	2.41628	-1.35799
B	2.68512	1.02414	-1.43108
C	-2.08184	0.01512	0.03789
C	-2.80705	-0.32785	-1.10584
C	-2.80718	0.33268	1.18896
C	-4.19007	-0.35004	-1.10398
H	-2.28026	-0.58886	-2.01692
C	-4.18955	0.29850	1.20435
H	-2.27885	0.61654	2.09219
C	-4.90420	-0.04129	0.05484
H	-4.72489	-0.61452	-2.00842
H	-4.72358	0.54275	2.11487
C	2.79487	-0.64327	1.06940
C	2.87013	-1.31845	2.39870
H	2.86067	-2.40791	2.28949
H	3.78399	-1.04703	2.92027
H	2.02999	-1.03960	3.02696
N	-6.30980	-0.06987	0.06373
C	-6.99815	-1.09637	-0.61453
C	-7.03005	0.92095	0.76097
C	-8.15461	-0.81372	-1.34222
C	-6.53445	-2.41155	-0.56658
C	-6.61679	2.25331	0.72406
C	-8.16637	0.58664	1.49872
C	-8.83351	-1.82812	-1.99869
H	-8.51991	0.20537	-1.38969
C	-7.21042	-3.41768	-1.23862
H	-5.64147	-2.64264	0.00220
C	-7.32022	3.22467	1.41826
H	-5.74030	2.52500	0.14762
C	-8.87367	1.56680	2.17702
H	-8.49345	-0.44568	1.53827
C	-8.36567	-3.13508	-1.95569
H	-9.73036	-1.59011	-2.55980
H	-6.83614	-4.43421	-1.18870
C	-8.45482	2.89053	2.14624
H	-6.98389	4.25476	1.37702
H	-9.75356	1.28808	2.74621
H	-8.89608	-3.92484	-2.47482

H	-9.00680	3.65316	2.68305
C	5.81985	-1.67769	1.64796
H	6.79158	-2.06403	1.33892
H	5.95311	-1.23593	2.63944
H	5.14047	-2.52397	1.74382
C	-0.20962	-1.41424	2.09877
H	-0.10979	-0.90466	3.06242
H	-1.26052	-1.67644	1.97637
H	0.36734	-2.33799	2.15747
C	5.56457	1.36619	-2.43831
H	6.36474	0.87804	-2.99873
H	4.71364	1.51427	-3.09796
H	5.93797	2.34732	-2.12982
C	-0.24059	1.46514	-2.10188
H	-0.24107	0.84814	-3.00568
H	-1.25273	1.83659	-1.94545
H	0.43027	2.30489	-2.28123
C	7.50188	-0.12981	-0.59756
C	8.52257	-0.17454	0.30049
H	7.81310	-0.08734	-1.63713
C	8.34002	0.01281	1.69633
N	8.20464	0.22155	2.82204
C	9.93382	-0.29406	-0.11486
O	10.85807	-0.30169	0.66314
O	10.09053	-0.39979	-1.43590
H	11.04059	-0.46318	-1.61307

B2	X	Y	Z
C	4.21040	0.50804	0.45462
C	3.94342	-1.36470	-0.81192
C	4.89326	-0.58125	-0.11901
C	-0.88445	1.06764	0.46308
C	-1.78071	0.17422	-0.11635
C	-1.01887	-0.80366	-0.80009
N	2.73913	-0.81435	-0.65531
N	0.27918	-0.54778	-0.63590
C	0.42732	0.60619	0.12841
C	2.84933	0.34087	0.11025
F	1.28479	-2.70080	-1.01034
F	1.44108	-1.14206	-2.66751
B	1.43008	-1.34219	-1.28249
C	-3.24680	0.19057	-0.04351
C	-3.95994	-0.95803	0.30896
C	-3.98594	1.34104	-0.32893
C	-5.34163	-0.96468	0.36480
H	-3.42308	-1.86972	0.54633
C	-5.36732	1.35022	-0.25454
H	-3.47124	2.24971	-0.62045
C	-6.07012	0.19331	0.08725
H	-5.86331	-1.87626	0.63038
H	-5.90958	2.26205	-0.47379
C	1.69723	1.08482	0.45139
C	1.85106	2.43550	1.07255
H	2.67326	2.44149	1.78369
H	0.96042	2.70218	1.63131
N	-7.47383	0.19132	0.14884

C	-8.13591	-0.55123	1.14950
C	-8.22714	0.93886	-0.77897
C	-9.28079	-1.28696	0.84280
C	-7.65848	-0.55868	2.46022
C	-7.85169	0.98998	-2.12209
C	-9.36278	1.63852	-0.36882
C	-9.93603	-2.00580	1.83022
H	-9.65633	-1.29092	-0.17368
C	-8.31012	-1.29264	3.43882
H	-6.77376	0.01533	2.70955
C	-8.58965	1.73541	-3.02760
H	-6.97705	0.44322	-2.45414
C	-10.10508	2.36796	-1.28414
H	-9.66205	1.60781	0.67219
C	-9.45445	-2.01764	3.13275
H	-10.82427	-2.57248	1.57390
H	-7.92557	-1.28577	4.45268
C	-9.72250	2.42661	-2.61785
H	-8.28190	1.76355	-4.06703
H	-10.98361	2.90621	-0.94594
H	-9.96596	-2.58557	3.90113
H	-10.30095	3.00338	-3.33000
C	6.28271	-0.93598	-0.01236
O	7.19780	0.02946	0.17898
C	6.91579	-2.16435	-0.05423
C	8.43292	-0.56136	0.27230
C	8.27973	-1.92493	0.12478
H	6.43910	-3.12384	-0.16368
C	9.50835	0.31077	0.50720
H	9.06812	-2.65924	0.16121
H	9.23748	1.35604	0.61044
C	10.83697	0.01396	0.62273
C	11.33326	-1.30663	0.49643
C	11.85275	1.04111	0.88621
N	11.71369	-2.39081	0.39168
O	13.03749	0.80857	0.96554
O	11.34103	2.26701	1.03492
H	12.07968	2.87230	1.19467
C	4.83235	1.55412	1.31556
H	5.89464	1.36744	1.44085
H	4.72272	2.55261	0.88552
H	4.38089	1.57230	2.31039
C	-1.29161	2.20369	1.33700
H	-1.05431	3.17550	0.89567
H	-2.36752	2.17289	1.50467
H	-0.80666	2.15590	2.31467
C	4.17518	-2.57671	-1.63348
H	5.16594	-2.54355	-2.08676
H	4.11512	-3.48107	-1.02009
H	3.42929	-2.66349	-2.42114
C	-1.52061	-1.93315	-1.61729
H	-1.51596	-2.86194	-1.03907
H	-2.54335	-1.73895	-1.93823
H	-0.89130	-2.09270	-2.49264
C	2.09823	3.50094	-0.00443

H	3.00001	3.24427	-0.57097
H	1.27070	3.47834	-0.72230
C	2.23415	4.89939	0.57486
H	3.05694	4.91724	1.30050
H	1.32618	5.15180	1.13658
C	2.47821	5.95682	-0.49162
H	3.38839	5.70269	-1.04702
H	1.65952	5.92779	-1.21990
C	2.60243	7.35989	0.07872
H	3.43120	7.42399	0.78980
H	2.78103	8.09609	-0.70869
H	1.69018	7.65206	0.60690

B3	X	Y	Z
C	3.63308	-0.32565	-0.61930
C	3.42732	1.79857	0.17052
C	4.35718	0.79958	-0.18988
C	-1.48276	-0.61377	-0.81993
C	-2.35419	0.41548	-0.48069
C	-1.57246	1.51454	-0.06221
N	2.19473	1.32236	-0.01456
N	-0.27849	1.18894	-0.13307
C	-0.16169	-0.11861	-0.59532
C	2.26680	0.01888	-0.49496
F	0.85369	3.31818	-0.24703
F	0.82037	2.22239	1.74810
B	0.89062	2.06441	0.35911
C	1.08977	-0.71071	-0.76202
C	1.18175	-2.15032	-1.15342
H	2.07288	-2.32247	-1.75067
H	0.33939	-2.41952	-1.78459
C	5.78516	0.95178	-0.09242
O	6.51852	-0.13032	0.22025
C	6.61915	2.04101	-0.24725
C	7.83713	0.24015	0.25991
C	7.92389	1.58760	-0.02433
H	6.31848	3.03855	-0.52241
C	8.73665	-0.79513	0.56892
H	8.83059	2.16905	-0.07207
H	8.27284	-1.75750	0.75688
C	10.09744	-0.75138	0.66129
C	10.83614	0.43283	0.42002
C	10.89942	-1.93475	1.00295
N	11.41820	1.40784	0.21659
O	12.10728	-1.93055	1.06634
O	10.16156	-3.02436	1.23889
H	10.76963	-3.74716	1.45197
C	4.24323	-1.56999	-1.16871
H	5.32628	-1.48774	-1.19179
H	3.99425	-2.45019	-0.57135
H	3.90656	-1.75652	-2.19124
C	-1.92786	-1.92899	-1.35900
H	-1.59991	-2.76692	-0.73985
H	-3.01598	-1.95814	-1.40621
H	-1.55133	-2.09685	-2.37164
C	3.70420	3.15640	0.69548

H	4.63999	3.16257	1.25439
H	3.79926	3.87362	-0.12578
H	2.90082	3.50112	1.34344
C	-2.05397	2.83371	0.40919
H	-1.86729	3.60347	-0.34474
H	-3.12492	2.79450	0.60305
H	-1.53353	3.13934	1.31819
C	-3.82450	0.36493	-0.52610
C	-4.56729	1.18868	-1.36779
C	-4.52111	-0.53981	0.27555
C	-5.94963	1.09261	-1.43437
H	-4.06055	1.91775	-1.99045
C	-5.89781	-0.66270	0.18907
H	-3.97857	-1.17413	0.96828
C	-6.64118	0.13926	-0.68579
H	-6.48927	1.76523	-2.08848
S	-6.72830	-1.89798	1.12329
N	-8.02712	-0.03989	-0.78070
C	-8.22969	-1.03228	1.42058
C	-8.75154	-0.21996	0.40638
C	-8.91424	-1.21139	2.61376
C	-9.98713	0.39041	0.62282
C	-10.15428	-0.61817	2.80488
H	-8.47756	-1.83462	3.38624
H	-10.41506	1.03086	-0.13734
C	-10.68581	0.17914	1.80307
H	-10.69568	-0.77867	3.72947
H	-11.65055	0.65472	1.93798
C	-8.72603	0.41241	-1.97267
H	-9.19262	1.39544	-1.82171
H	-7.97817	0.54299	-2.75401
C	-9.75135	-0.59724	-2.46934
H	-10.48095	-0.81616	-1.68558
H	-9.23239	-1.53656	-2.68361
C	-10.46707	-0.09763	-3.71264
H	-11.18797	-0.83475	-4.07182
H	-11.01207	0.82889	-3.51052
H	-9.76131	0.10190	-4.52404
C	1.20791	-3.07107	0.07252
H	2.05249	-2.79860	0.71481
H	0.30654	-2.89885	0.67111
C	1.30107	-4.53963	-0.30807
H	0.45628	-4.80175	-0.95733
H	2.20599	-4.70499	-0.90604
C	1.31661	-5.46723	0.89749
H	2.15894	-5.20012	1.54594
H	0.41059	-5.29923	1.49109
C	1.41213	-6.93520	0.51530
H	2.32530	-7.13527	-0.05269
H	1.42156	-7.57818	1.39860
H	0.56409	-7.23579	-0.10688

B4	X	Y	Z
C	4.06984	0.72063	0.61646
C	3.92407	-1.20952	-0.57240
C	4.82369	-0.33644	0.07868

C	-1.02276	1.08569	0.48886
C	-1.88225	0.12698	-0.03922
C	-1.07869	-0.87618	-0.63143
N	2.68397	-0.72771	-0.44326
N	0.21067	-0.56817	-0.46819
C	0.30421	0.64151	0.21162
C	2.72583	0.46388	0.26795
F	1.31548	-2.70101	-0.66032
F	1.42357	-1.27782	-2.43349
B	1.40492	-1.36254	-1.03670
C	-3.35034	0.12756	0.00270
C	-4.06616	-0.96620	0.49528
C	-4.08930	1.22536	-0.44452
C	-5.44872	-0.96829	0.54071
H	-3.52986	-1.83692	0.85714
C	-5.47152	1.23747	-0.39802
H	-3.57072	2.09079	-0.84271
C	-6.18026	0.13760	0.09575
H	-5.97042	-1.83607	0.92599
H	-6.01178	2.10779	-0.75069
C	1.54474	1.18137	0.54232
N	-7.57812	0.14501	0.13811
C	-8.27342	-0.52581	1.16953
C	-8.31950	0.81100	-0.86541
C	-9.39134	-1.30179	0.88689
C	-7.87093	-0.40548	2.50178
C	-8.00654	0.64130	-2.21577
C	-9.39155	1.63075	-0.53433
C	-10.10298	-1.93614	1.89740
H	-9.72211	-1.40768	-0.13985
C	-8.55911	-1.04968	3.51033
H	-7.00695	0.20132	2.74722
C	-8.73742	1.27965	-3.19737
H	-7.17870	0.00026	-2.49645
C	-10.14631	2.26086	-1.51593
H	-9.65160	1.77505	0.50811
C	-9.68619	-1.81887	3.21928
H	-10.97154	-2.52638	1.63743
H	-8.24285	-0.95240	4.54270
C	-9.81922	2.09279	-2.85772
H	-8.49133	1.14421	-4.24441
H	-10.97684	2.88748	-1.21930
C	6.25581	-0.54057	0.15512
C	6.93755	-1.73284	0.35161
C	8.74268	-0.28359	0.17567
C	8.32413	-1.59320	0.36678
H	6.43024	-2.67432	0.51171
C	10.02915	0.31113	0.14432
H	9.00374	-2.41771	0.52868
H	10.04575	1.38398	-0.01921
C	11.25726	-0.26239	0.29302
C	11.44418	-1.64853	0.52394
C	12.50103	0.52477	0.23756
N	11.58677	-2.77712	0.71375
O	13.60203	0.04597	0.38000

O	12.29640	1.82542	0.01397
H	13.16241	2.25845	-0.00184
C	4.60855	1.80383	1.48569
H	5.58743	1.52405	1.87565
H	4.73274	2.74736	0.94456
H	3.95631	1.99707	2.33687
C	-1.46157	2.27128	1.27490
H	-1.33583	3.20528	0.71838
H	-2.51970	2.17943	1.52046
H	-0.90269	2.36920	2.20691
C	4.23129	-2.45088	-1.32155
H	5.25818	-2.43035	-1.68556
H	4.11717	-3.32948	-0.67940
H	3.55556	-2.57377	-2.16714
C	-1.53240	-2.08617	-1.35549
H	-1.45330	-2.97080	-0.71681
H	-2.57319	-1.97512	-1.65678
H	-0.91734	-2.26738	-2.23745
C	1.63200	2.53455	1.16750
H	1.64283	2.46350	2.26022
H	2.54017	3.04634	0.86068
H	0.78658	3.15308	0.88333
O	-10.30415	-2.40382	4.27338
O	-10.48507	2.66743	-3.88768
C	-11.58365	3.50168	-3.58030
H	-11.27556	4.35718	-2.97137
H	-11.96959	3.85822	-4.53346
H	-12.36878	2.94843	-3.05553
C	-11.44481	-3.19651	4.01272
H	-11.20228	-4.03991	3.35894
H	-11.77933	-3.57308	4.97754
H	-12.24496	-2.60473	3.55728
S	7.36898	0.74459	-0.03514

B5	X	Y	Z
C	12.45700	20.46984	3.08905
C	14.07450	21.15317	4.54284
C	13.25399	21.57262	3.46520
C	12.52579	15.87744	5.29227
C	13.31318	15.51786	6.38400
C	14.15265	16.62066	6.68430
N	13.83728	19.86785	4.79208
N	13.88845	17.61665	5.83889
C	12.90083	17.20750	4.94819
C	12.85677	19.40385	3.91679
F	14.43653	19.57339	7.11458
F	15.92135	18.89783	5.52497
B	14.56964	19.00296	5.84933
C	12.42109	18.06499	3.96268
C	11.48230	17.55865	2.91853
H	11.63643	16.49956	2.73663
H	10.43947	17.69860	3.22141
C	11.29012	20.52843	2.16830
H	10.98652	21.56426	2.01375
H	11.51186	20.11054	1.18244
H	10.43691	19.98891	2.57846

C	11.43556	15.04987	4.70968
H	11.72792	14.59735	3.75677
H	11.17844	14.23695	5.38821
H	10.53569	15.63891	4.53131
C	15.10377	21.95232	5.24619
H	14.81553	23.00374	5.28232
H	15.26172	21.59318	6.26060
H	16.05684	21.89290	4.71160
C	15.18513	16.70724	7.74184
H	14.77778	17.18240	8.63941
H	15.52607	15.70904	8.01520
H	16.03434	17.30484	7.41234
C	13.28702	22.90600	2.95999
H	13.53325	23.68225	3.67798
C	13.09709	23.34743	1.68811
C	13.11669	24.78308	1.34114
O	13.02385	25.19756	0.21029
O	13.24585	25.58063	2.40309
H	13.26713	26.49414	2.08181
C	13.00362	22.47357	0.57224
N	12.97523	21.76596	-0.33736
C	13.27833	14.27631	7.13942
C	13.24019	14.11949	8.50325
S	13.26004	12.73841	6.36428
C	13.16893	12.77378	8.91182
H	13.21905	14.95479	9.19103
C	13.16364	11.89000	7.85757
H	13.06793	12.47844	9.94660
C	12.85204	8.34844	8.43268
C	12.42802	8.51798	7.12747
C	11.98479	7.41410	6.33428
C	12.78301	7.08908	9.10777
N	12.50738	9.82623	6.76110
C	12.98738	10.45619	7.81693
N	13.24078	9.60106	8.85655
C	12.33064	5.97473	8.34162
C	11.95939	6.13255	6.93421
C	11.55869	5.04766	6.14769
H	11.52788	4.04264	6.54764
C	11.60376	7.56019	4.99756
H	11.62909	8.54917	4.55512
C	11.19083	5.20749	4.82324
C	11.20858	6.47995	4.23925
H	10.92215	6.62444	3.20619
C	13.06715	6.89433	10.46653
H	13.37265	7.72858	11.08089
C	12.21585	4.73743	8.97875
H	11.86474	3.86698	8.44048
C	12.51514	4.56858	10.31888
C	12.94241	5.66366	11.07375
H	13.16576	5.56638	12.12753
C	13.99807	9.91670	10.04756
H	14.54883	10.83900	9.88074
H	13.35180	10.03747	10.91952
O	12.35247	3.32170	10.81824

O	10.82707	4.07985	4.16583
C	12.59883	3.12236	12.19644
H	11.93474	3.73702	12.81170
H	12.39775	2.07047	12.38950
H	13.63931	3.34468	12.45174
C	10.47851	4.18923	2.80024
H	10.24137	3.18033	2.46811
H	9.60345	4.83121	2.66087
H	11.31122	4.57897	2.20682
H	14.71950	9.12371	10.23816
H	11.62641	18.08463	1.97900

B6	X	Y	Z
C	-0.33706	0.01070	-0.18784
C	-0.40944	-0.04429	1.20311
N	0.74869	0.03121	1.97611
B	2.17335	0.27983	1.43198
C	0.89529	0.12800	-0.84034
C	1.22415	0.12698	-2.21683
C	2.62027	0.21972	-2.27590
C	3.11044	0.27583	-0.94989
N	2.07858	0.21967	-0.10910
C	0.42173	-0.06529	3.26295
C	-1.51683	-0.18686	2.07980
C	-0.98421	-0.20955	3.37066
F	2.62651	1.53891	1.83524
F	3.04700	-0.69603	1.90329
C	-2.96556	-0.30109	1.77525
H	-3.28790	0.43121	1.03437
H	-3.21248	-1.28939	1.37817
H	-3.54262	-0.15530	2.68946
C	0.34647	0.03766	-3.41146
H	-0.37111	-0.77984	-3.33112
H	-0.22981	0.95530	-3.55346
H	0.95609	-0.11927	-4.30213
C	1.39840	-0.03549	4.37212
H	1.89142	-1.00752	4.46888
H	2.17450	0.71005	4.19868
H	0.88762	0.18135	5.30968
C	4.52394	0.36684	-0.52563
H	4.64833	1.08773	0.28327
H	4.87471	-0.60180	-0.15827
H	5.14646	0.65982	-1.37023
C	-1.58028	-0.06895	-0.99249
C	-2.15977	-1.30271	-1.26482
C	-2.16864	1.08643	-1.49348
C	-3.31740	-1.39447	-2.02373
H	-1.71053	-2.21937	-0.89879
C	-3.33824	1.00324	-2.23188
H	-1.72189	2.05356	-1.29411
C	-3.92844	-0.22492	-2.49636
H	-3.81874	1.89749	-2.61245
C	3.42592	0.23912	-3.42756
C	-1.68255	-0.35155	4.58429
C	-2.26010	-0.48106	5.64129
C	4.14080	0.25090	-4.40506

O	-3.85490	-2.62764	-2.24489
O	-5.06267	-0.26039	-3.25053
C	-3.80867	-3.07615	-3.59761
H	-2.77142	-3.15138	-3.93702
H	-4.36340	-2.40617	-4.25766
C	-6.23796	-0.68052	-2.56051
H	-7.04507	-0.66589	-3.29122
H	-6.46880	0.01503	-1.74818
C	-2.90305	-0.63446	6.89443
C	-2.14872	-0.80689	8.06284
C	-4.29916	-0.61551	7.00869
C	-2.76267	-0.95206	9.28909
H	-1.06745	-0.83938	7.99849
C	-4.91385	-0.75088	8.23732
H	-4.90462	-0.47445	6.12102
C	-4.15660	-0.91933	9.40124
H	-2.15727	-1.09421	10.17587
H	-5.99463	-0.71662	8.30038
N	-4.77019	-1.04247	10.65301
C	-4.15203	-0.48345	11.79506
C	-6.00624	-1.70663	10.79127
C	-4.05598	-1.21734	12.97636
C	-3.63364	0.81012	11.75238
C	-6.26022	-2.88914	10.09563
C	-6.98990	-1.19286	11.63676
C	-3.45036	-0.66310	14.09350
H	-4.45492	-2.22447	13.01437
C	-3.01868	1.35315	12.86927
H	-3.71452	1.38786	10.83887
C	-7.47754	-3.53569	10.23818
H	-5.49815	-3.30158	9.44482
C	-8.19921	-1.85349	11.78489
H	-6.80262	-0.27305	12.17827
C	-2.92451	0.62160	14.04635
H	-3.37733	-1.24731	15.00405
H	-2.62171	2.36102	12.82126
C	-8.45397	-3.02504	11.08408
H	-7.65761	-4.45499	9.69196
H	-8.95316	-1.43914	12.44498
H	-9.40271	-3.53630	11.19783
H	-2.44544	1.04938	14.91940
C	4.99942	0.25400	-5.53157
C	4.49188	0.46169	-6.82143
C	6.37640	0.04310	-5.36706
C	5.33798	0.45837	-7.91294
H	3.42988	0.62578	-6.95656
C	7.21522	0.03932	-6.46158
H	6.77475	-0.12029	-4.37332
C	6.70566	0.24617	-7.74248
H	4.93516	0.62030	-8.90439
H	8.27832	-0.12586	-6.33704
C	7.64591	0.22955	-8.88286
O	8.83685	0.03820	-8.78334
O	7.05238	0.44734	-10.05952
H	7.73620	0.41941	-10.74499

H	-6.12398	-1.68912	-2.15844
H	-4.26577	-4.06423	-3.60899

B7	X	Y	Z
C	17.41350	18.97528	-2.17130
C	18.24243	20.44003	-3.69456
C	18.60124	19.48508	-2.71800
C	12.68493	20.33266	-3.56961
C	12.37779	21.19841	-4.61503
C	13.60091	21.66985	-5.14521
N	16.90933	20.52027	-3.75245
N	14.61608	21.12273	-4.47214
C	14.10775	20.29020	-3.48174
C	16.35624	19.65271	-2.81999
F	16.46105	21.22387	-6.01615
F	16.35304	22.79185	-4.36684
B	16.10607	21.45208	-4.68717
C	11.04797	21.58976	-5.09876
C	10.69758	21.45964	-6.44388
C	10.09353	22.13169	-4.23494
C	9.45930	21.86219	-6.91122
H	11.41003	21.03620	-7.14359
C	8.84937	22.52849	-4.68985
H	10.33260	22.25303	-3.18398
C	8.51338	22.40732	-6.04045
H	9.22082	21.75401	-7.96248
H	8.13041	22.94378	-3.99391
C	14.96196	19.57756	-2.64204
C	14.40358	18.75800	-1.52596
H	14.22610	17.72651	-1.84817
H	13.45879	19.16197	-1.17647
N	7.25540	22.81206	-6.50942
C	6.62839	22.08268	-7.54809
C	6.62362	23.95206	-5.98221
C	6.09607	22.73403	-8.65282
C	6.53074	20.69204	-7.48236
C	7.36767	25.09000	-5.65019
C	5.24570	23.96461	-5.80182
C	5.46703	22.02755	-9.66991
H	6.16483	23.81365	-8.72101
C	5.92878	19.97865	-8.49913
H	6.93577	20.16668	-6.62504
C	6.72345	26.20294	-5.14674
H	8.44037	25.09572	-5.79531
C	4.60892	25.09843	-5.30502
H	4.64794	23.09510	-6.04686
C	5.38712	20.64044	-9.60098
H	5.05933	22.57069	-10.51223
H	5.85463	18.89850	-8.44763
C	5.34406	26.23077	-4.96910
H	7.30354	27.08468	-4.89800
H	4.86788	27.12110	-4.58251
C	19.96447	19.14831	-2.35425
C	21.04451	18.96509	-3.18505
C	22.04083	18.67843	-1.07865
C	22.22343	18.69929	-2.46131

H	20.97442	18.99885	-4.26315
C	17.33258	17.85244	-1.19460
H	18.27428	17.30392	-1.17351
H	17.13714	18.19814	-0.17462
H	16.54361	17.14844	-1.45886
C	11.67780	19.56087	-2.79031
H	11.57272	19.93607	-1.76745
H	10.70106	19.64092	-3.26809
H	11.93737	18.50320	-2.72433
C	19.13665	21.26989	-4.53600
H	20.10650	21.38856	-4.05318
H	19.29961	20.79837	-5.50997
H	18.70259	22.25255	-4.71590
C	13.79457	22.63469	-6.25293
H	14.06757	22.11380	-7.17543
H	12.87427	23.18800	-6.43492
H	14.59913	23.33436	-6.02549
H	15.08714	18.72869	-0.68233
O	3.26314	24.99998	-5.17189
O	4.80830	19.85807	-10.54312
C	4.22355	20.49360	-11.65607
H	4.96634	21.04930	-12.23767
H	3.80448	19.70074	-12.27301
H	3.42366	21.17679	-11.35198
C	2.57193	26.10706	-4.63835
H	1.52156	25.82270	-4.60811
H	2.91251	26.34050	-3.62459
H	2.68771	26.99396	-5.26931
S	20.40571	19.00934	-0.67437
C	23.20767	18.39413	-0.37382
C	24.30408	18.20442	-1.20776
S	23.84944	18.37665	-2.88698
H	23.28737	18.32677	0.70313
C	25.57022	17.91966	-0.62445
C	26.85187	17.70102	-1.04217
H	25.47569	17.87502	0.45822
C	27.42017	17.68567	-2.39873
O	28.58928	17.53485	-2.63699
O	26.50220	17.85592	-3.36180
H	26.97514	17.83824	-4.20543
C	27.81025	17.46171	-0.01248
N	28.54728	17.27135	0.85257

B8	X	Y	Z
C	-5.46993	-0.03866	0.01317
C	-4.76932	1.14148	-0.24285
N	-3.39229	1.18911	-0.19931
B	-2.47495	-0.03990	0.00068
C	-4.76899	-1.22088	0.25853
C	-5.23798	-2.50988	0.60275
C	-4.13982	-3.32425	0.73078
C	-2.99197	-2.53599	0.47053
N	-3.39229	-1.26920	0.20141
C	-2.99393	2.45489	-0.47523
C	-5.24084	2.42947	-0.58792
C	-4.14372	3.24262	-0.72882

F	-1.66577	-0.21163	-1.12670
F	-1.66488	0.13225	1.12741
C	-6.94419	-0.03118	0.02547
C	-7.63875	0.85408	0.85227
C	-7.66799	-0.90337	-0.79133
C	-9.02192	0.86896	0.86398
H	-7.08711	1.52058	1.50422
C	-9.05006	-0.88260	-0.78699
H	-7.13953	-1.58265	-1.44931
C	-9.73641	0.00247	0.04021
H	-9.54784	1.55333	1.51691
H	-9.61202	-1.54872	-1.43008
C	-1.62008	2.85130	-0.43649
H	-0.91378	2.09463	-0.11701
C	-1.61709	-2.92850	0.42421
H	-0.91569	-2.16673	0.10628
C	-1.17064	-4.16872	0.71676
H	-1.88151	-4.90950	1.07480
C	-1.18356	4.09351	-0.73569
H	-1.90204	4.82615	-1.09525
C	0.17212	4.57782	-0.60758
C	0.49825	5.85406	-1.08559
C	1.19579	3.84980	0.01763
C	1.76739	6.38003	-0.95403
H	-0.26649	6.44163	-1.58345
C	2.46081	4.37073	0.16756
H	0.99044	2.86879	0.43014
C	2.77499	5.65127	-0.31225
H	1.98321	7.36641	-1.34552
H	3.21817	3.79172	0.68105
C	0.19105	-4.63685	0.58670
C	0.53563	-5.90799	1.06535
C	1.20479	-3.89377	-0.03707
C	1.81393	-6.41342	0.93904
H	-0.22117	-6.50745	1.56119
C	2.47882	-4.39393	-0.18105
H	0.98498	-2.91714	-0.45241
C	2.81258	-5.66774	0.30298
H	2.04449	-7.39584	1.33230
H	3.22880	-3.80330	-0.69220
H	-4.14364	4.29379	-0.97180
H	-4.13795	-4.37633	0.96995
C	-11.21764	-0.00852	0.00960
O	-11.87868	-0.73239	-0.69780
O	-11.76874	0.87435	0.84737
H	-12.73066	0.80108	0.76120
N	4.10325	-6.17322	0.14108
N	4.05391	6.18120	-0.13999
H	-6.27286	-2.78419	0.73592
H	-6.27661	2.70377	-0.71340
C	4.25215	7.57021	0.02507
C	5.31894	8.20240	-0.61261
C	3.40548	8.32198	0.83934
C	5.53522	9.55955	-0.43350
H	5.98045	7.62417	-1.24713

C	3.61989	9.68142	1.00218
H	2.58073	7.83622	1.34740
C	4.68660	10.30859	0.37103
H	6.36933	10.03590	-0.93648
H	2.95398	10.25124	1.64062
H	4.85562	11.37042	0.50619
C	5.17729	5.32369	-0.07160
C	6.12113	5.48192	0.94172
C	5.35333	4.31523	-1.01758
C	7.22070	4.64042	1.00695
H	5.98784	6.26481	1.67930
C	6.44818	3.46912	-0.93839
H	4.62684	4.19653	-1.81315
C	7.38792	3.62689	0.07235
H	7.94554	4.77213	1.80247
H	6.57350	2.68895	-1.68080
H	8.24561	2.96689	0.12994
C	5.20988	-5.29298	0.09063
C	6.16883	-5.42589	-0.91209
C	5.35411	-4.28671	1.04428
C	7.25149	-4.56160	-0.95938
H	6.06068	-6.20720	-1.65542
C	6.43205	-3.41781	0.98300
H	4.61608	-4.18773	1.83188
C	7.38692	-3.55049	-0.01706
H	7.98807	-4.67340	-1.74713
H	6.53209	-2.63931	1.73100
H	8.23156	-2.87282	-0.06033
C	4.33001	-7.55663	-0.03142
C	5.40691	-8.17125	0.60672
C	3.50235	-8.32049	-0.85406
C	5.65239	-9.52219	0.41897
H	6.05347	-7.58405	1.24834
C	3.74616	-9.67389	-1.02573
H	2.66977	-7.84874	-1.36247
C	4.82323	-10.28312	-0.39469
H	6.49431	-9.98442	0.92212
H	3.09539	-10.25282	-1.67153
H	5.01561	-11.34002	-0.53730

B9	X	Y	Z
C	3.02195	3.44941	-9.27242
C	3.01953	4.33099	-8.19137
N	3.57543	3.96455	-6.97675
B	4.27191	2.61667	-6.69219
C	3.58028	2.17555	-9.15888
C	3.69769	1.11241	-10.10631
C	4.35596	0.09272	-9.45696
C	4.64295	0.51102	-8.14079
N	4.16540	1.76383	-7.97437
C	3.43139	4.99003	-6.10908
C	2.50026	5.65680	-8.06087
C	2.76554	6.04523	-6.76836
F	5.61710	2.82624	-6.36482
F	3.64488	1.96351	-5.62419
C	2.44230	3.88485	-10.56667

C	1.11417	3.61030	-10.87762
C	3.23162	4.58481	-11.47640
C	0.57725	4.03373	-12.08149
H	0.49829	3.06526	-10.17149
C	2.69601	5.01283	-12.67692
H	4.26721	4.79653	-11.23649
C	1.36580	4.74136	-12.98534
H	-0.45729	3.81926	-12.31621
H	3.30272	5.56224	-13.38624
C	3.89370	4.94788	-4.75094
H	4.34867	4.02434	-4.41310
C	5.33462	-0.20449	-7.10762
H	5.45115	0.30343	-6.15803
C	5.83700	-1.44143	-7.28615
H	5.70189	-1.92059	-8.25205
C	3.76786	5.99941	-3.91750
H	3.31503	6.90827	-4.30431
C	4.16320	6.07740	-2.52543
C	3.96477	7.28659	-1.84849
C	4.72002	5.01057	-1.80722
C	4.30466	7.43338	-0.51789
H	3.54550	8.13056	-2.38587
C	5.04558	5.14448	-0.47204
H	4.88229	4.05386	-2.28965
C	4.84063	6.35858	0.18531
H	4.16426	8.38604	-0.02224
H	5.44391	4.29836	0.07469
C	6.57600	-2.23176	-6.32080
C	7.03673	-3.49520	-6.70898
C	6.87075	-1.79737	-5.02126
C	7.76424	-4.29419	-5.84705
H	6.81015	-3.85670	-7.70638
C	7.60623	-2.58518	-4.15912
H	6.53876	-0.82342	-4.68165
C	8.06088	-3.83969	-4.56654
H	8.09739	-5.27580	-6.16179
H	7.84948	-2.22369	-3.16704
H	2.49951	6.99546	-6.33095
H	4.61128	-0.86443	-9.88580
C	0.83235	5.22946	-14.27796
O	1.46421	5.89814	-15.06317
O	-0.43024	4.86029	-14.50220
H	-0.69885	5.22432	-15.35899
N	8.82646	-4.63603	-3.69277
N	5.16696	6.50231	1.54629
C	4.34989	7.06855	2.51640
C	5.05389	7.12507	3.73615
C	3.02880	7.49417	2.42181
C	4.43453	7.64767	4.86895
C	2.43328	8.00560	3.56296
H	2.47603	7.42712	1.49332
C	3.12719	8.09162	4.77428
H	4.96790	7.70336	5.81162
H	1.40489	8.34521	3.51254
H	2.63204	8.50416	5.64574

C	6.38875	6.19110	2.12915
C	6.35707	6.56321	3.48885
C	7.53064	5.64371	1.55385
C	7.48012	6.36306	4.28749
C	8.63474	5.45450	2.36907
H	7.56713	5.37610	0.50551
C	8.61328	5.80400	3.72291
H	7.46730	6.64417	5.33491
H	9.53505	5.02591	1.94341
H	9.49490	5.63959	4.33144
C	8.46615	-5.01491	-2.40840
C	9.49904	-5.79812	-1.85295
C	7.29186	-4.75796	-1.70915
C	9.35718	-6.31638	-0.56808
C	7.17436	-5.28694	-0.43411
H	6.49131	-4.17100	-2.14238
C	8.19535	-6.05391	0.13680
H	10.14348	-6.92029	-0.12849
H	6.26820	-5.10117	0.13145
H	8.07033	-6.45016	1.13779
C	10.07780	-5.16540	-3.97307
C	10.53216	-5.89113	-2.85284
C	10.85845	-5.02775	-5.11563
C	11.78416	-6.50090	-2.88715
C	12.09982	-5.64248	-5.12449
H	10.51556	-4.45752	-5.96993
C	12.56062	-6.37564	-4.02615
H	12.14706	-7.06104	-2.03225
H	12.72696	-5.54952	-6.00400
H	13.53673	-6.84469	-4.06874
C	3.22256	1.04482	-11.51540
H	2.13382	1.10395	-11.57726
H	3.62107	1.85984	-12.12257
H	3.53690	0.10043	-11.96107
C	1.79890	6.50490	-9.06323
H	2.43173	6.72226	-9.92603
H	0.89511	6.02483	-9.44349
H	1.51484	7.45196	-8.60305

B10	X	Y	Z
C	-0.09855	0.08707	-0.15271
C	0.23195	1.15039	0.68324
N	1.25973	1.06034	1.60003
B	2.14263	-0.19407	1.82077
C	0.62439	-1.11290	-0.08097
C	0.46517	-2.32607	-0.77480
C	1.43172	-3.19386	-0.29780
H	-0.28254	-2.53146	-1.52430
C	2.16110	-2.51312	0.68695
N	1.67024	-1.26325	0.81201
H	1.60693	-4.21406	-0.60431
C	1.38448	2.25424	2.22495
C	-0.29772	2.46331	0.74600
C	0.40648	3.14293	1.70307
H	0.26731	4.17002	2.00192
H	-1.09627	2.84496	0.12964

C	2.38527	2.50528	3.21140
H	3.04770	1.68153	3.44594
C	2.54523	3.70080	3.82215
H	1.86369	4.50817	3.56638
C	3.55809	4.04804	4.78673
C	3.58491	5.34853	5.30939
C	4.55190	3.15990	5.22895
C	4.54367	5.75022	6.21430
H	2.82452	6.05701	4.99659
C	5.51488	3.54979	6.12995
H	4.58674	2.14720	4.84450
C	5.53564	4.85778	6.64250
H	4.52935	6.76215	6.59922
H	6.27836	2.84457	6.43311
N	6.51910	5.26627	7.53444
C	3.28712	-3.03167	1.49850
H	4.18037	-2.41565	1.37154
H	3.04011	-3.02344	2.56309
H	3.51794	-4.05358	1.20089
C	-1.19450	0.24484	-1.10570
C	-2.47072	0.69537	-0.84987
S	-0.98098	-0.09714	-2.77168
C	-3.27035	0.74936	-2.00282
H	-2.81590	0.94849	0.14345
C	-2.59175	0.35450	-3.12908
H	-4.30554	1.06232	-2.01550
C	-3.05625	0.28311	-4.51162
O	-2.36608	-0.07864	-5.43876
O	-4.32774	0.66310	-4.64893
H	-4.56114	0.58879	-5.58662
F	3.48804	0.11503	1.60061
F	1.99215	-0.65787	3.13184
C	6.92440	6.62511	7.56657
C	6.93847	7.31611	8.77855
C	7.31785	7.26356	6.38921
C	7.33711	8.64276	8.83063
H	6.62755	6.80354	9.68163
C	7.71053	8.58520	6.44052
H	7.31379	6.71133	5.45531
C	7.72156	9.27935	7.65676
H	7.33475	9.16950	9.77867
C	8.18748	9.46844	5.30459
C	8.18387	10.64112	7.40526
C	8.46311	10.76600	6.03824
C	8.36453	11.71606	8.26744
C	8.92939	11.96404	5.52775
C	8.82841	12.91775	7.74799
H	8.14979	11.62413	9.32683
C	9.11019	13.04179	6.39045
H	9.15284	12.07157	4.47110
H	8.97395	13.76752	8.40561
H	9.47370	13.98662	6.00201
C	7.17567	4.34942	8.38562
C	8.56432	4.41242	8.52776
C	6.44533	3.39383	9.09838

C	9.23247	3.53598	9.36739
H	9.11924	5.15720	7.96956
C	7.11375	2.51429	9.92571
H	5.36583	3.36035	8.99687
C	8.50577	2.58007	10.06576
H	10.31118	3.59886	9.46132
C	6.53362	1.41251	10.79156
C	8.92604	1.54704	11.00697
C	7.78580	0.86147	11.44501
C	10.18723	1.19741	11.47530
C	7.90001	-0.17249	12.35653
C	10.29584	0.15662	12.38904
H	11.07352	1.72388	11.13733
C	9.16273	-0.52287	12.82731
H	7.02321	-0.70937	12.70440
H	11.27168	-0.12990	12.76537
H	9.26519	-1.33270	13.54104
C	5.83587	0.34298	9.94575
H	4.96824	0.76611	9.43361
H	6.51281	-0.06965	9.19464
H	5.48800	-0.47402	10.58260
C	5.55741	1.97045	11.83153
H	5.20305	1.17019	12.48581
H	6.03377	2.73497	12.44892
H	4.68837	2.41463	11.34003
C	9.46094	8.90926	4.66177
H	10.24775	8.76751	5.40583
H	9.25683	7.94632	4.18704
H	9.83056	9.59304	3.89378
C	7.10163	9.64546	4.23886
H	6.87099	8.68689	3.76742
H	6.18352	10.04625	4.67385
H	7.44393	10.33179	3.46048

B11	X	Y	Z
C	-3.77057	1.28227	-3.41586
C	-5.00054	-0.34604	-2.44227
C	-3.69853	0.06901	-2.75407
C	-8.12412	3.69403	-4.64627
C	-9.39449	3.22949	-4.35533
C	-9.27631	2.03268	-3.63437
N	-5.87063	0.56778	-2.89750
N	-7.97615	1.74172	-3.48060
C	-7.22342	2.74150	-4.08553
C	-5.15845	1.59626	-3.50297
F	-7.71547	0.63905	-1.34438
F	-7.92941	-0.65285	-3.20667
B	-7.40027	0.53807	-2.70646
C	-5.82945	2.67846	-4.07566
C	-2.59470	2.03782	-3.92532
H	-1.67746	1.51624	-3.64978
H	-2.61786	2.13429	-5.01288
H	-2.54922	3.04927	-3.51566
C	-7.83274	4.93240	-5.41750
H	-7.34840	4.70810	-6.37050
H	-8.76395	5.46002	-5.62698

H	-7.17029	5.60917	-4.87365
C	-5.40607	-1.58114	-1.73136
H	-4.52588	-2.09592	-1.34876
H	-6.07721	-1.35534	-0.90005
H	-5.94243	-2.25692	-2.40265
C	-10.37242	1.18722	-3.10654
H	-10.19267	0.91111	-2.06602
H	-11.31996	1.71983	-3.17698
H	-10.45392	0.25829	-3.67776
H	-10.32758	3.69933	-4.63056
H	-2.79842	-0.47744	-2.51275
C	-5.04775	3.79838	-4.63205
C	-4.60424	3.97756	-5.91124
S	-4.58938	5.08052	-3.55344
C	-3.87363	5.18065	-6.02099
H	-4.79770	3.27686	-6.71202
C	-3.77621	5.89511	-4.82116
C	-3.04418	7.05850	-5.09795
C	-2.71388	7.00525	-6.46701
N	-3.22220	5.85403	-7.02643
C	-1.98123	8.09243	-6.92281
C	-1.74780	9.00345	-5.89762
S	-2.44145	8.47403	-4.37624
H	-1.63936	8.22926	-7.93795
C	-3.14408	5.50387	-8.39693
C	-2.43354	4.39380	-8.81110
C	-3.76960	6.32503	-9.35372
C	-2.30726	4.07425	-10.15698
H	-1.95124	3.77310	-8.06416
C	-3.63592	6.02366	-10.69862
C	-2.89411	4.91117	-11.10100
H	-1.74409	3.20003	-10.45172
H	-4.08677	6.64392	-11.46128
C	-1.08798	10.25026	-5.89474
C	-0.45421	10.90706	-6.91487
H	-1.08337	10.77524	-4.94457
C	0.16634	12.22544	-6.73281
O	0.74392	12.82067	-7.61576
O	0.03123	12.71275	-5.49716
H	0.47261	13.57441	-5.47013
C	-0.34384	10.37654	-8.22288
N	-0.26362	9.93167	-9.28486
O	-4.45154	7.37849	-8.87942
O	-2.79864	4.73923	-12.43347
C	-4.96623	8.33732	-9.79855
H	-4.16062	8.67440	-10.46096
H	-5.74628	7.87617	-10.41536
C	-1.86174	3.79282	-12.94098
H	-2.22289	2.77508	-12.75270
H	-0.90362	3.91666	-12.42415
C	-1.70163	4.05684	-14.41881
H	-2.67027	3.93458	-14.91496
H	-1.40696	5.10349	-14.55081
C	-0.66525	3.15162	-15.06685
H	-0.97726	2.10436	-14.97544

H	0.28424	3.23737	-14.52429
C	-0.43439	3.48823	-16.53232
H	-1.38042	3.39548	-17.08033
H	-0.13854	4.54162	-16.61560
C	0.62119	2.62062	-17.19996
H	0.32412	1.56798	-17.12628
H	1.56302	2.70983	-16.64590
C	0.85105	2.98646	-18.65752
H	1.60990	2.34862	-19.11746
H	-0.06979	2.88217	-19.23887
H	1.18503	4.02385	-18.75396
C	-5.51460	9.49025	-8.99463
H	-6.31357	9.12382	-8.34152
H	-4.72020	9.86917	-8.34286
C	-6.03500	10.61577	-9.87412
H	-5.23760	10.94884	-10.54964
H	-6.84407	10.24180	-10.51314
C	-6.53378	11.80458	-9.06727
H	-5.72486	12.16313	-8.41824
H	-7.33888	11.47703	-8.39752
C	-7.03048	12.95592	-9.92709
H	-6.22751	13.26975	-10.60436
H	-7.84747	12.60207	-10.56678
C	-7.50047	14.14818	-9.10968
H	-6.69220	14.53825	-8.48395
H	-8.32538	13.87031	-8.44689
H	-7.84706	14.96223	-9.75108

B12	X	Y	Z
C	-0.03577	3.04635	0.03467
C	-1.24772	2.34826	0.09397
N	-1.26641	0.96477	0.17960
B	-0.03481	0.05154	0.28034
C	1.17267	2.33877	0.00541
C	2.50273	2.82607	-0.06488
C	3.30855	1.70914	-0.08543
C	2.47969	0.56479	-0.00446
N	1.18813	0.95259	0.04579
C	-2.55695	0.57586	0.12457
C	-2.57716	2.83317	-0.02109
C	-3.38440	1.71772	0.00057
F	-0.09951	-0.95887	-0.68280
F	0.03631	-0.54370	1.54748
H	2.79211	3.86374	-0.09248
H	-2.86356	3.86606	-0.13499
C	-3.25325	-0.64053	0.13020
H	-2.79401	-1.61626	0.19357
C	3.17904	-0.65074	0.00209
H	2.72226	-1.62911	0.04278
C	-4.61336	-0.44353	0.00352
C	4.54085	-0.44835	-0.08782
S	-5.03948	1.25822	-0.10910
S	4.96614	1.25496	-0.16454
C	-5.64998	-1.44517	-0.04731
C	-5.37557	-2.79240	0.23695
C	-6.97322	-1.13384	-0.39028

C	-6.34826	-3.76167	0.18142
H	-4.37087	-3.09042	0.51354
C	-7.95876	-2.09122	-0.45264
H	-7.24419	-0.10907	-0.62422
C	-7.68285	-3.44796	-0.16781
H	-6.06743	-4.78272	0.40005
H	-8.96070	-1.77988	-0.71360
C	5.58348	-1.44544	-0.12196
C	6.90303	-1.13211	-0.47456
C	5.32154	-2.78519	0.20265
C	7.89510	-2.08419	-0.51865
H	7.16486	-0.11160	-0.73586
C	6.30264	-3.74793	0.17101
H	4.32382	-3.07909	0.50782
C	7.62910	-3.43757	-0.21045
H	8.89171	-1.77090	-0.79570
H	6.03592	-4.75755	0.45060
N	8.59476	-4.39327	-0.28894
N	-8.64824	-4.40121	-0.22611
C	-9.99150	-4.10359	-0.68667
H	-10.38973	-5.01887	-1.13179
H	-9.94443	-3.37101	-1.49531
C	-10.92223	-3.62313	0.41538
H	-11.01331	-4.37481	1.20322
H	-10.55679	-2.69887	0.86814
H	-11.91892	-3.43457	0.00917
C	-8.40160	-5.77103	0.18462
H	-9.34646	-6.16897	0.56329
H	-7.71080	-5.77890	1.03039
C	-7.88514	-6.66037	-0.93508
H	-8.59379	-6.68988	-1.76629
H	-6.92707	-6.30149	-1.31738
H	-7.74760	-7.68106	-0.57011
C	9.94896	-4.05603	-0.69002
H	10.40077	-4.96701	-1.08724
H	9.90711	-3.34968	-1.52348
C	10.82375	-3.49637	0.42283
H	10.38287	-2.60022	0.86476
H	10.96970	-4.23081	1.21720
H	11.80541	-3.22967	0.02321
C	8.32633	-5.76536	0.10476
H	7.36278	-6.07631	-0.30844
H	9.07947	-6.38863	-0.38035
C	8.35208	-6.01236	1.60686
H	8.12137	-7.06033	1.81353
H	9.33599	-5.79343	2.02573
H	7.61635	-5.39471	2.12615
C	-0.01220	4.50578	-0.02168
C	0.65600	5.30143	-0.92593
S	-0.83352	5.45463	1.14721
C	0.49083	6.67201	-0.67278
H	1.22052	4.89926	-1.75616
C	-0.29302	6.91124	0.42906
H	0.92319	7.46104	-1.27303
C	-0.68621	8.18773	1.01722

O	-1.38362	8.29637	2.00196
O	-0.18863	9.23305	0.35372
H	-0.48705	10.03991	0.79989

B13	X	Y	Z
C	12.76592	13.17435	3.05568
C	11.53222	13.78987	3.09573
N	11.39615	15.14965	2.84778
B	12.61181	16.10786	2.57631
C	13.93183	13.86662	2.80146
C	15.26405	13.41069	2.61929
C	16.03591	14.55252	2.30680
C	15.15856	15.67284	2.32693
N	13.92414	15.24289	2.61532
C	10.11295	15.51106	2.97117
C	10.24271	13.26833	3.38021
C	9.34648	14.35773	3.30229
F	12.63183	17.07676	3.56290
F	12.51109	16.67095	1.31540
H	12.81998	12.10532	3.22309
C	9.58720	16.86273	2.75384
C	8.93157	17.53500	3.80186
C	9.65848	17.46956	1.50351
C	8.36868	18.78747	3.57588
C	9.09671	18.71691	1.27846
H	10.15408	16.94460	0.69749
C	8.45440	19.36937	2.31854
H	7.86957	19.31576	4.37688
H	9.15873	19.17009	0.29662
H	8.01088	20.34583	2.15896
C	15.53350	17.07464	2.11356
C	15.42800	18.00398	3.14384
C	16.06870	17.48268	0.87828
C	15.83739	19.31722	2.96998
H	15.02633	17.68184	4.09592
C	16.47171	18.80290	0.70109
C	16.35458	19.70963	1.74583
H	15.75289	20.02435	3.78614
H	16.87218	19.12977	-0.24896
H	16.67432	20.73426	1.59252
O	8.91392	16.91087	4.99598
O	16.13606	16.54271	-0.08486
C	8.23130	17.53480	6.06823
H	7.17509	17.68726	5.82887
H	8.31751	16.85507	6.91335
H	8.68983	18.49412	6.32395
C	16.66759	16.90860	-1.34493
H	17.70053	17.25647	-1.25345
H	16.64085	16.00733	-1.95379
H	16.06174	17.68626	-1.81845
C	9.76191	11.98972	3.68297
H	10.42646	11.13551	3.74211
C	17.40140	14.45248	2.04660
H	17.98408	15.34052	1.82922
C	15.87343	12.15181	2.66731
H	15.30510	11.25774	2.89662

C	17.21648	12.06153	2.39111
H	17.68381	11.08578	2.38597
C	17.99991	13.20194	2.06967
C	7.97729	14.18212	3.50145
H	7.29894	15.02579	3.44280
C	8.41304	11.82951	3.88925
H	8.02566	10.83951	4.09380
C	7.50280	12.91501	3.79872
C	6.07010	12.68595	3.97882
C	5.41400	11.87871	4.90439
S	4.96427	13.47303	2.94473
C	4.02248	11.93811	4.75270
C	3.59882	12.76303	3.72318
H	3.34304	11.39255	5.39331
C	19.40635	13.05749	1.69979
C	20.37348	12.17158	2.17180
S	20.04400	14.08240	0.49135
C	21.61017	12.36656	1.54233
C	21.61315	13.37506	0.59188
H	22.48845	11.78773	1.79420
C	2.31238	13.07269	3.21576
C	1.08620	12.64858	3.63403
H	2.29527	13.73752	2.35800
C	22.62156	13.88468	-0.26362
C	23.91571	13.48671	-0.42535
H	22.32141	14.71587	-0.89364
C	24.81897	14.14618	-1.38407
O	25.97590	13.82829	-1.53929
O	24.23608	15.13235	-2.06873
H	24.89834	15.50546	-2.66903
C	-0.15334	13.04609	2.94583
O	-1.25442	12.69232	3.30034
O	0.05547	13.82922	1.88607
H	-0.80795	14.04304	1.50255
C	0.89718	11.79923	4.75314
N	0.75180	11.10936	5.66609
C	24.49674	12.41660	0.30056
N	24.96268	11.54369	0.89345
C	20.17211	11.15122	3.24582
H	19.46376	11.49393	4.00123
H	19.79284	10.21035	2.83629
C	6.07637	11.06772	5.97060
H	6.30302	10.05757	5.61712
H	7.01135	11.52202	6.30077
H	5.41515	10.97085	6.83289
H	21.12152	10.93373	3.73669

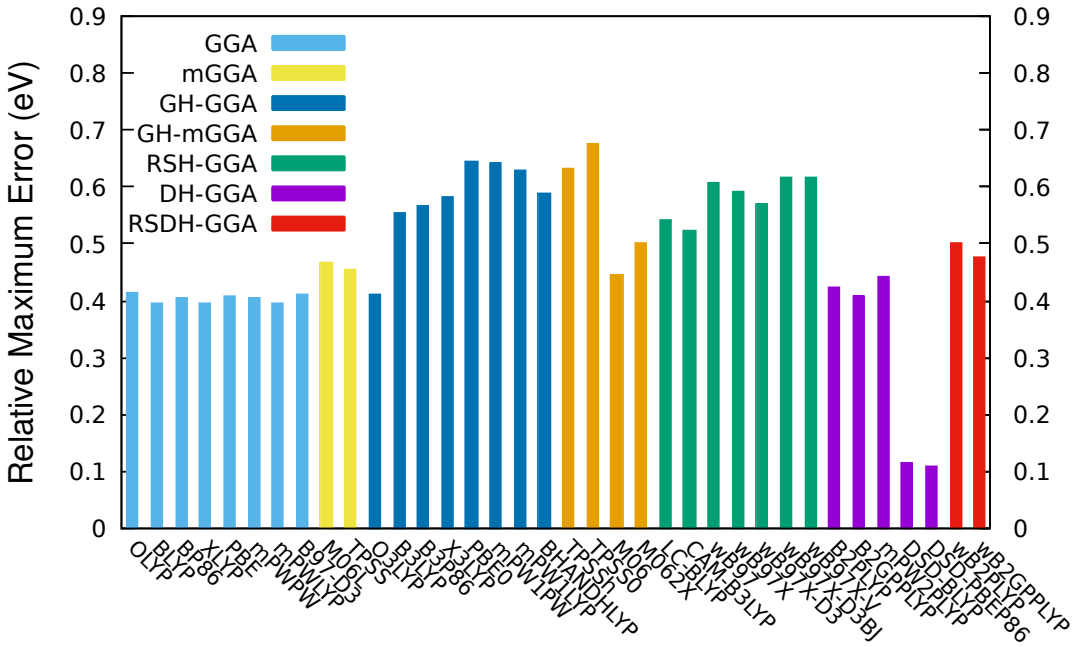


Figure S1: Relative maximum errors (Max) of TD-DFT excitation energies.

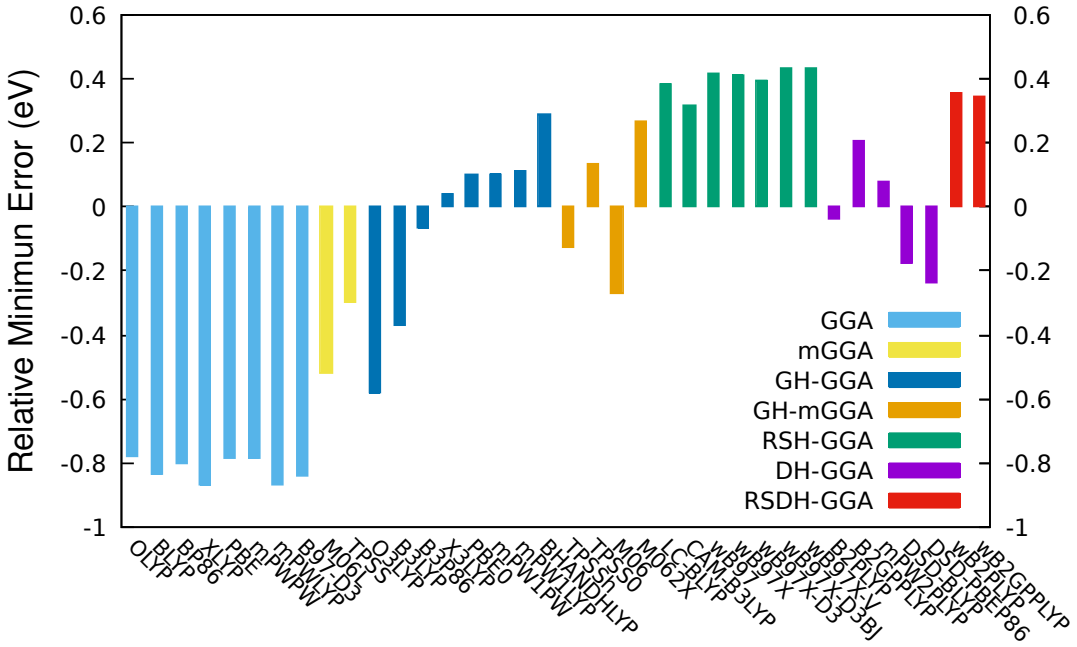


Figure S2: Relative minimum errors (Min) of TD-DFT excitation energies.

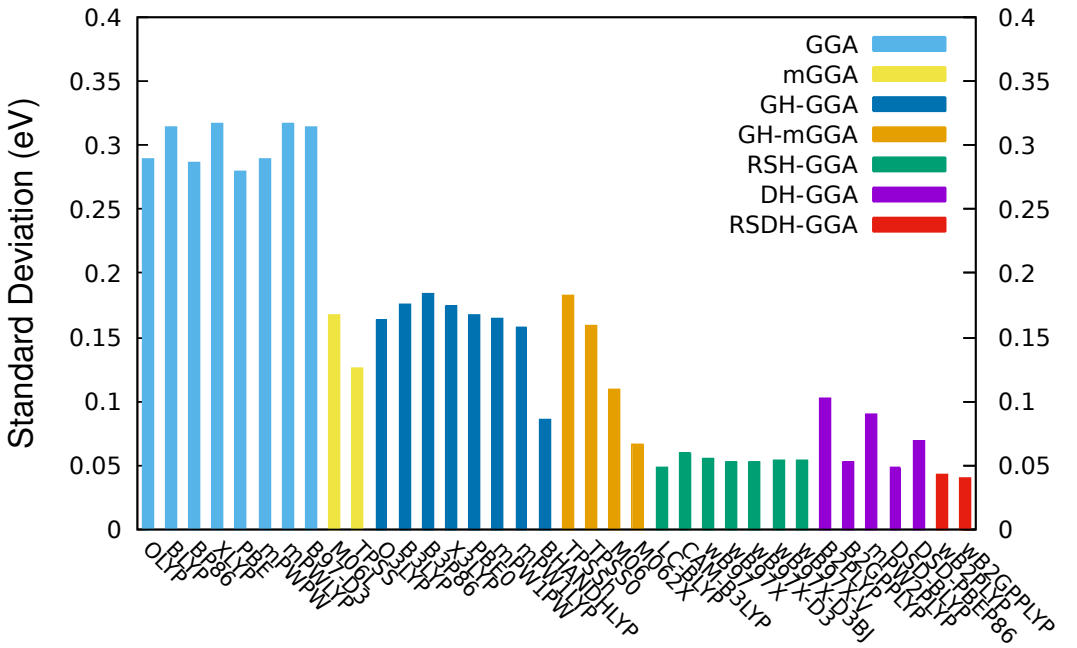


Figure S3: Standard deviations (SD) of TD-DFT excitation energies.

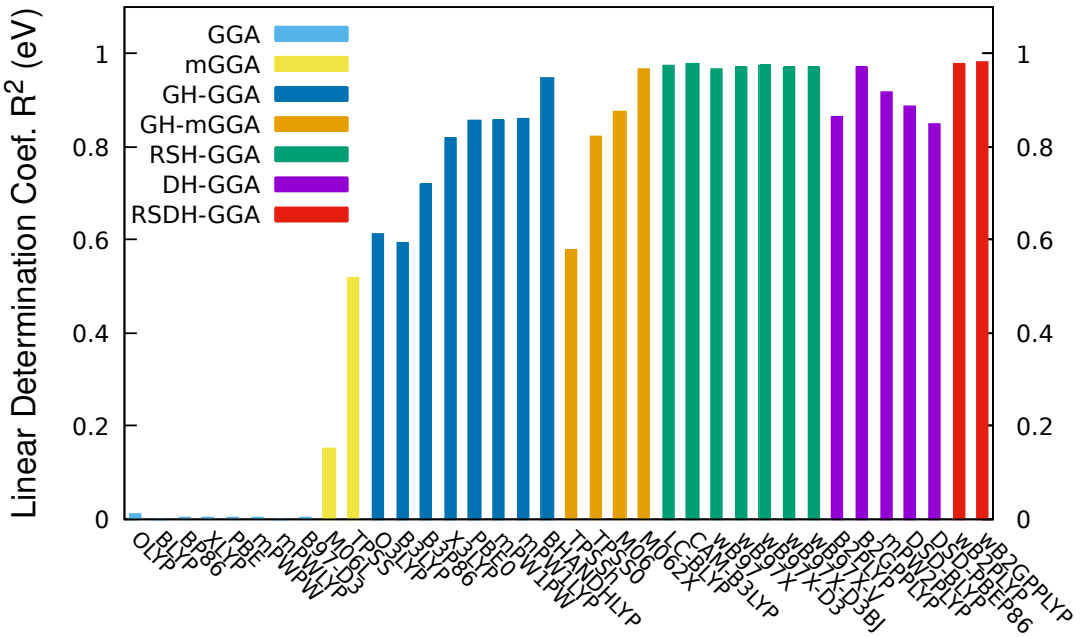


Figure S4: Linear determination coefficients (R^2) of TD-DFT excitation energies.

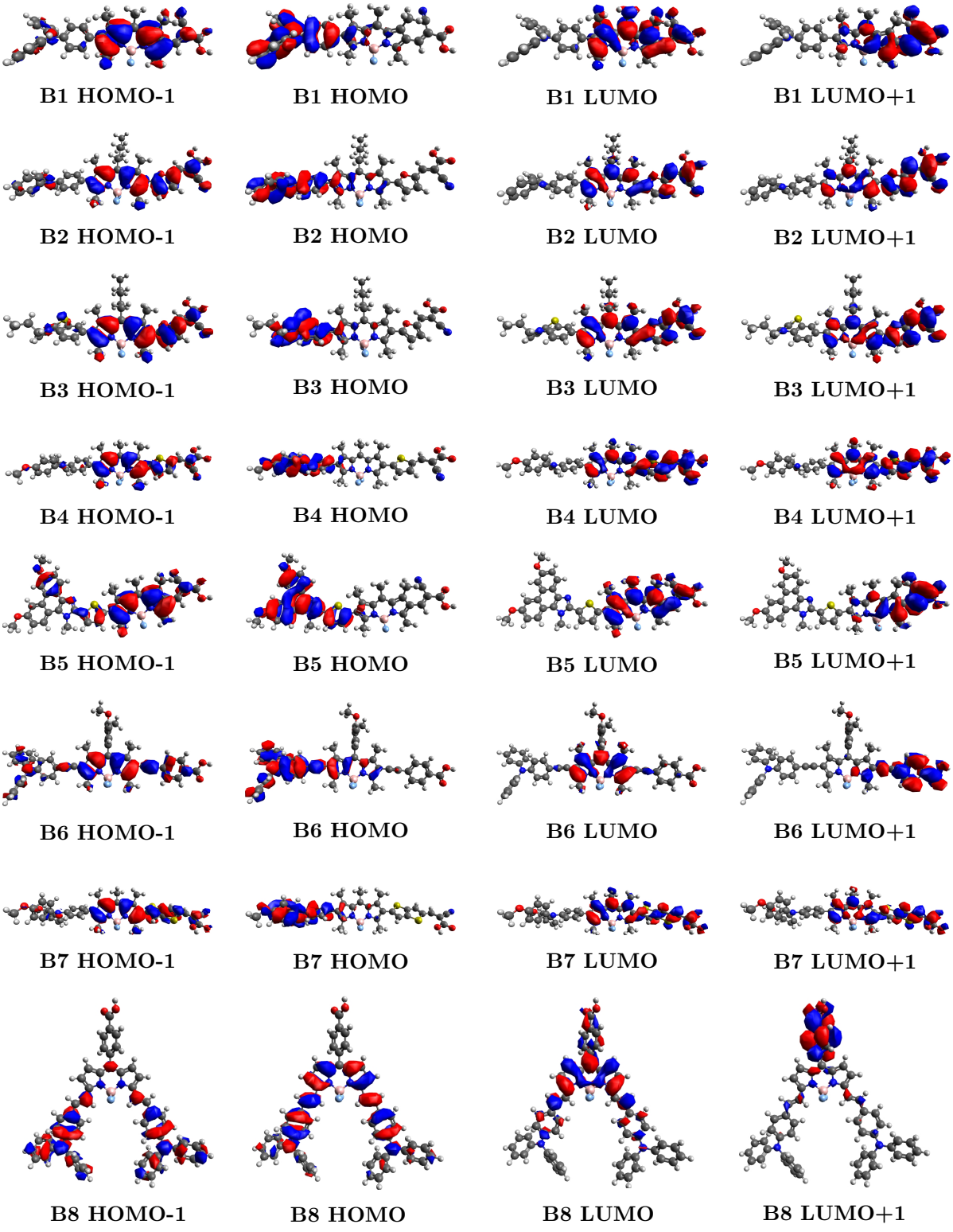
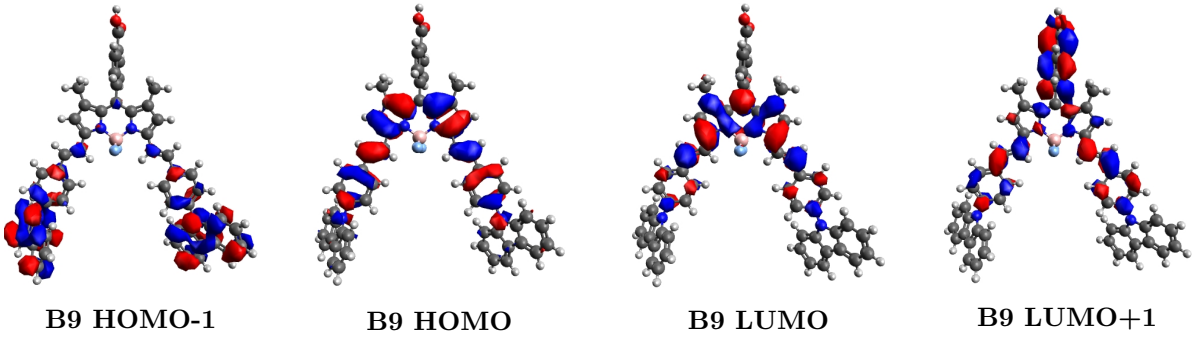
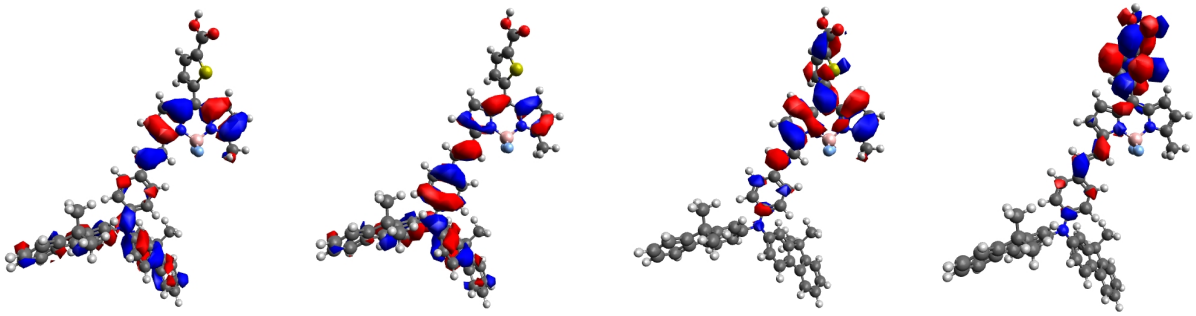


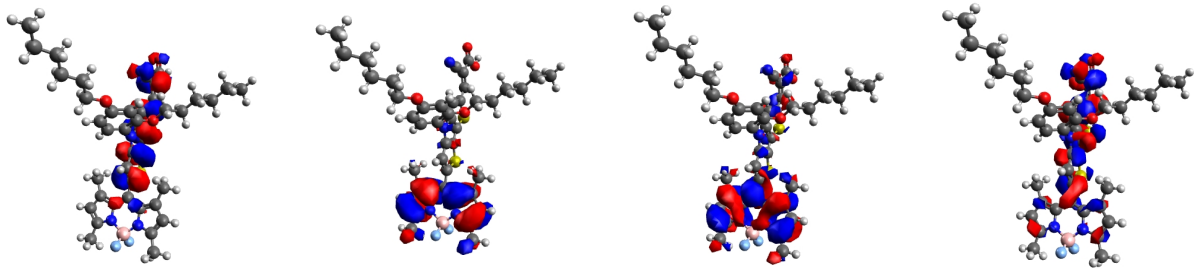
Figure S5: Frontier MOs (HOMO-1, HOMO, LUOM and LUMO+1) involved in the main transitions of BODIPY based dye sensitizers (**B1**–**B13**). Isosurface value 0.02.



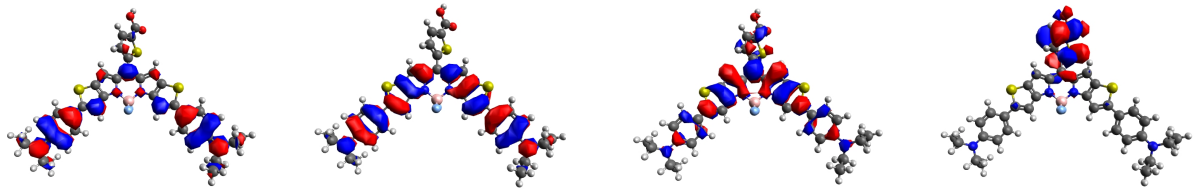
B9 HOMO-1 **B9 HOMO** **B9 LUMO** **B9 LUMO+1**



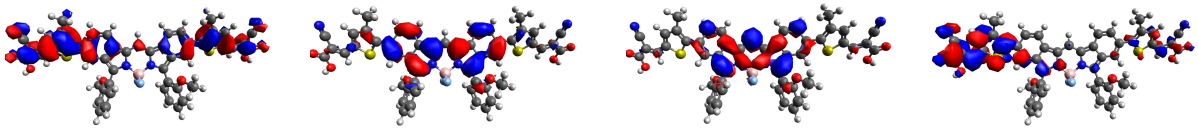
B10 HOMO-1 **B10 HOMO** **B10 LUMO** **B10 LUMO+1**



B11 HOMO-1 **B11 HOMO** **B11 LUMO** **B11 LUMO+1**



B12 HOMO-1 **B12 HOMO** **B12 LUMO** **B12 LUMO+1**



B13 HOMO-1 **B13 HOMO** **B13 LUMO** **B13 LUMO+1**

Continued Frontier MOs (HOMO-1, HOMO, LUOM and LUMO+1) involved in the main transitions of BODIPY based dye sensitizers (**B1**–**B13**). Isosurface value 0.02.