Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

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Signed error plots (TD-DFT/TDA)

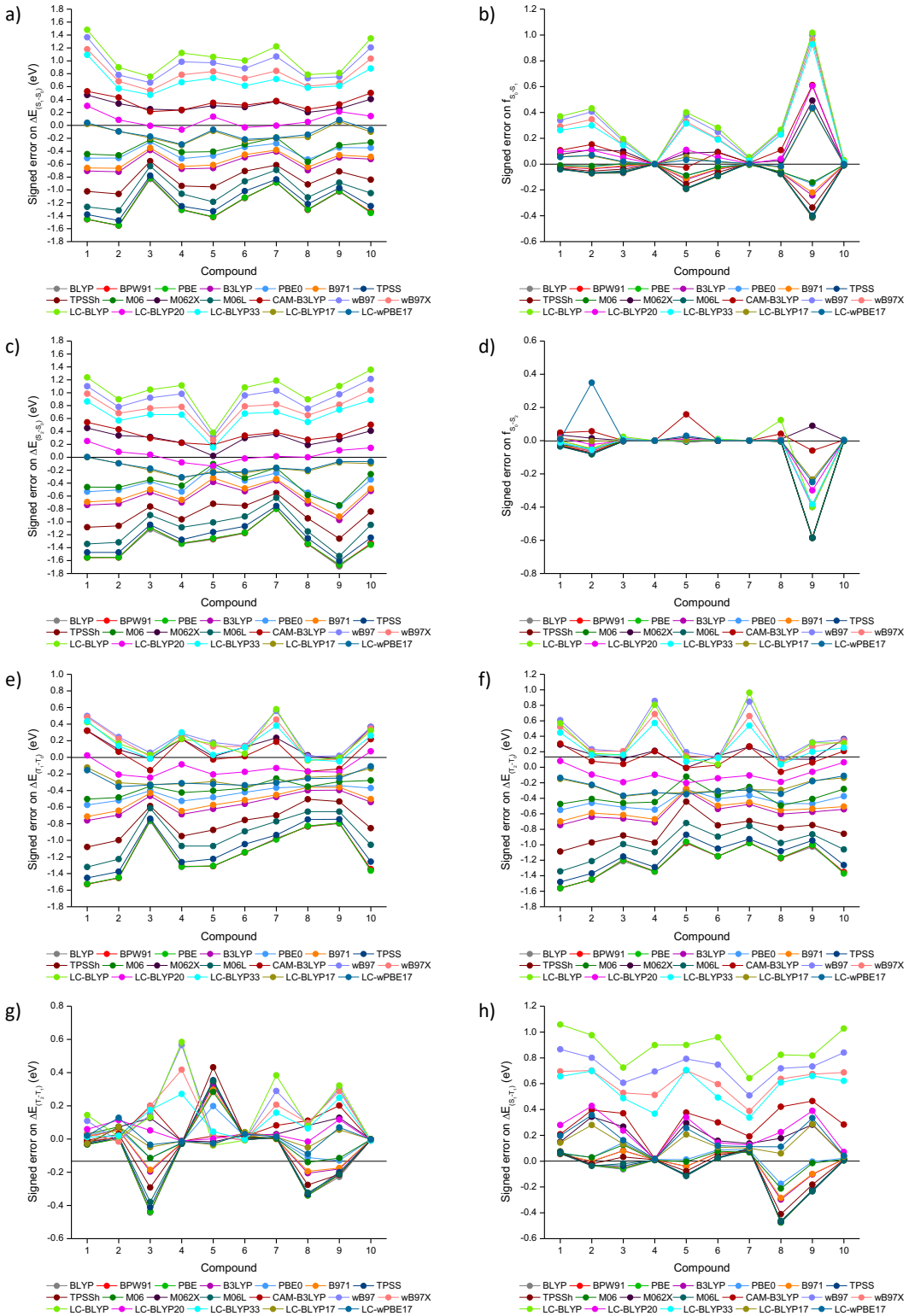


Figure S1. Signed errors on each property for each individual XC functional for all 10 compounds obtained using TD-DFT/TDA. a) First vertical singlet excitation energy, $\Delta E_{S_0-S_1}$. b) Oscillator strength for the first singlet excitation, $f_{S_0-S_1}$. c) Second vertical singlet excitation energy, $\Delta E_{S_2-S_0}$. d) Oscillator strength for the second vertical singlet excitation, $f_{S_0-S_2}$. e) First vertical triplet excitation energy, $\Delta E_{T_1-S_0}$. f) Second vertical triplet excitation energy, $\Delta E_{T_2-S_0}$. g) Triplet-triplet energy gap for the first two triplet excited states, $\Delta E_{T_2-T_1}$. h) Singlet-triplet gap for the first singlet and triplet excited states, $\Delta E_{S_1-T_1}$.

Mean signed errors tables

Table S1. Statistical analysis including mean signed errors (MSEs, eV) and standard deviations (eV) obtained from the comparison between TD-DFT calculations with different XCFs and riCC2 reference values.

	$\Delta E_{S_0-S_1}$ (eV)		$f_{S_0-S_1}$		$\Delta E_{S_0-S_2}$ (eV)		$f_{S_0-S_2}$		$\Delta E_{S_0-T_1}$ (eV)		$\Delta E_{S_0-T_2}$ (eV)		$\Delta E_{T_1-T_2}$ (eV)		$\Delta E_{S_1-T_1}$ (eV)	
	MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE	StdDev
BLYP	-1.242	0.213	-0.116	0.144	-1.329	0.231	-0.072	0.173	-1.153	0.265	-1.224	0.190	-0.070	0.201	-0.094	0.157
BPW91	-1.236	0.216	-0.113	0.143	-1.322	0.230	-0.072	0.173	-1.153	0.266	-1.220	0.193	-0.067	0.201	-0.090	0.157
PBE	-1.238	0.216	-0.113	0.143	-1.322	0.229	-0.072	0.173	-1.153	0.268	-1.225	0.195	-0.072	0.209	-0.090	0.157
M06L	-1.021	0.202	-0.109	0.138	-1.102	0.237	-0.072	0.173	-0.952	0.224	-1.005	0.178	-0.053	0.187	-0.069	0.148
TPSS	-1.166	0.204	-0.110	0.139	-1.244	0.223	-0.069	0.173	-1.090	0.251	-1.151	0.188	-0.062	0.198	-0.081	0.153
TPSSh	-0.850	0.149	-0.095	0.119	-0.904	0.191	-0.072	0.173	-0.820	0.158	-0.845	0.157	-0.025	0.177	-0.032	0.110
B3LYP	-0.596	0.110	-0.074	0.089	-0.628	0.172	-0.070	0.173	-0.610	0.086	-0.605	0.112	0.005	0.118	0.014	0.071
B971	-0.555	0.102	-0.068	0.083	-0.583	0.169	-0.070	0.173	-0.566	0.083	-0.563	0.105	0.003	0.111	0.012	0.069
PBE0	-0.430	0.089	-0.053	0.064	-0.445	0.164	-0.006	0.258	-0.526	0.068	-0.482	0.080	0.043	0.063	0.096	0.070
M06	-0.379	0.106	-0.050	0.057	-0.399	0.179	-0.068	0.173	-0.460	0.089	-0.430	0.091	0.030	0.041	0.081	0.068
M062X	0.283	0.102	0.084	0.107	0.246	0.132	-0.014	0.054	0.044	0.176	0.114	0.117	0.071	0.090	0.239	0.112
ωB97	0.882	0.239	0.254	0.233	0.850	0.238	-0.022	0.173	-0.381	0.208	-0.056	0.423	0.325	0.349	1.263	0.161
ωB97X	0.740	0.215	0.225	0.224	0.713	0.203	-0.047	0.141	-0.304	0.195	-0.006	0.373	0.299	0.321	1.044	0.142
CAM-B3LYP	0.311	0.124	0.100	0.145	0.316	0.118	-0.009	0.096	-0.332	0.177	-0.136	0.232	0.196	0.181	0.643	0.119
LC-ωPBE17	-0.136	0.109	0.045	0.104	-0.182	0.086	-0.039	0.120	-0.344	0.099	-0.302	0.086	0.042	0.063	0.209	0.127
LC-BLYP17	-0.157	0.106	0.044	0.100	-0.192	0.085	-0.039	0.116	-0.314	0.089	-0.287	0.079	0.027	0.051	0.156	0.102
LC-BLYP20	0.056	0.118	0.086	0.138	0.009	0.105	-0.042	0.132	-0.215	0.129	-0.147	0.094	0.068	0.076	0.270	0.136
LC-BLYP33	0.650	0.192	0.210	0.211	0.600	0.195	-0.053	0.139	-0.218	0.178	0.009	0.305	0.227	0.239	0.868	0.125
LC-BLYP	0.978	0.264	0.270	0.236	0.956	0.262	0.010	0.235	-0.623	0.239	-0.244	0.494	0.379	0.377	1.601	0.187
LC-BLYP20-M062X	/	/	/	/	/	/	/	/	/	/	/	/	/	/	0.012	0.179

Table S2. Statistical analysis including mean signed errors (MSEs, eV) and standard deviations (eV) obtained from the comparison between TD-DFT/TDA calculations with different XCFs and riCC2 reference values.

	$\Delta E_{S_0-S_1}$ (eV)		$f_{S_0-S_1}$		$\Delta E_{S_0-S_2}$ (eV)		$f_{S_0-S_2}$		$\Delta E_{S_0-T_1}$ (eV)		$\Delta E_{S_0-T_2}$ (eV)		$\Delta E_{T_1-T_2}$ (eV)		$\Delta E_{S_1-T_1}$ (eV)	
	MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE	StdDev		MSE	StdDev	MSE	StdDev	MSE	StdDev	MSE
BLYP	-1.220	0.226	-0.096	0.120	-1.318	0.242	-0.071	0.173	-1.148	0.269	-1.222	0.191	-0.074	0.205	-0.072	0.161
BPW91	-1.214	0.229	-0.093	0.119	-1.310	0.242	-0.071	0.173	-1.146	0.272	-1.217	0.194	-0.071	0.205	-0.067	0.162
PBE	-1.215	0.229	-0.093	0.119	-1.311	0.241	-0.071	0.173	-1.147	0.273	-1.218	0.196	-0.070	0.206	-0.068	0.162
M06L	-1.001	0.213	-0.093	0.118	-1.092	0.245	-0.072	0.173	-0.932	0.240	-0.992	0.184	-0.060	0.195	-0.069	0.157
TPSS	-1.144	0.216	-0.091	0.116	-1.236	0.236	-0.071	0.173	-1.079	0.259	-1.143	0.193	-0.064	0.202	-0.065	0.160
TPSSh	-0.828	0.160	-0.075	0.098	-0.894	0.198	-0.070	0.173	-0.784	0.190	-0.818	0.171	-0.034	0.196	-0.044	0.142
B3LYP	-0.574	0.120	-0.055	0.071	-0.618	0.177	-0.069	0.173	-0.560	0.122	-0.580	0.122	-0.020	0.148	-0.014	0.109
B971	-0.533	0.113	-0.050	0.065	-0.573	0.173	-0.068	0.173	-0.520	0.116	-0.540	0.115	-0.019	0.138	-0.013	0.105
PBE0	-0.407	0.099	-0.035	0.048	-0.435	0.168	-0.066	0.174	-0.436	0.079	-0.444	0.082	-0.008	0.093	0.028	0.080
M06	-0.356	0.113	-0.035	0.045	-0.389	0.182	-0.067	0.173	-0.372	0.079	-0.371	0.113	0.001	0.115	0.015	0.086
M062X	0.322	0.088	0.100	0.137	0.289	0.116	0.017	0.026	0.136	0.135	0.176	0.103	0.040	0.056	0.187	0.104
ωB97	0.966	0.208	0.287	0.274	0.903	0.234	-0.044	0.120	0.236	0.183	0.385	0.269	0.149	0.177	0.731	0.103
ωB97X	0.812	0.187	0.255	0.265	0.758	0.199	-0.041	0.117	0.199	0.179	0.322	0.213	0.123	0.141	0.612	0.100
CAM-B3LYP	0.356	0.105	0.113	0.175	0.351	0.109	0.025	0.054	0.053	0.168	0.113	0.118	0.060	0.080	0.303	0.127
LC-ωPBE17	-0.103	0.116	0.062	0.127	-0.153	0.091	0.014	0.136	-0.273	0.078	-0.264	0.089	0.010	0.056	0.171	0.109
LC-BLYP17	-0.125	0.113	0.061	0.125	-0.164	0.090	-0.022	0.071	-0.262	0.075	-0.261	0.079	0.001	0.042	0.137	0.090
LC-BLYP20	0.096	0.119	0.107	0.171	0.040	0.106	-0.029	0.091	-0.130	0.098	-0.094	0.095	0.036	0.047	0.226	0.130
LC-BLYP33	0.721	0.168	0.241	0.254	0.645	0.194	-0.043	0.115	0.157	0.168	0.255	0.184	0.098	0.101	0.563	0.127
LC-BLYP	1.073	0.230	0.305	0.280	1.030	0.254	-0.029	0.130	0.190	0.191	0.351	0.307	0.160	0.195	0.883	0.125
LC-BLYP20-M062X	/	/	/	/	/	/	/	/	/	/	/	/	/	/	-0.040	0.170

Excited state data tables

Table S3. Excited state data for compound **1** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	180->181	0.1704	2.969	179->181	0.0980	2.996	180->181	2.903	179->181	2.948	0.045	0.067
BLYP	180->181	0.1136	1.491	179->181	0.0602	1.437	180->181	1.376	179->181	1.391	0.015	0.061
BPW91	180->181	0.1164	1.492	179->181	0.0625	1.434	180->181	1.372	179->181	1.385	0.014	0.063
PBE	180->181	0.1164	1.493	179->181	0.0623	1.434	180->181	1.374	179->181	1.386	0.012	0.061
M06L	180->181	0.1148	1.688	179->181	0.0600	1.647	180->181	1.576	179->181	1.602	0.026	0.112
TPSS	180->181	0.1181	1.566	179->181	0.0632	1.514	180->181	1.447	179->181	1.465	0.018	0.067
TPSSh	180->181	0.1189	1.929	179->181	0.0596	1.906	180->181	1.816	179->181	1.857	0.041	0.090
B3LYP	180->181	0.1299	2.247	179->181	0.0618	2.249	180->181	2.133	179->181	2.197	0.063	0.114
B971	180->181	0.1335	2.294	179->181	0.0637	2.297	180->181	2.180	179->181	2.243	0.063	0.114
PBE0	180->181	0.1429	2.445	179->181	0.0683	2.454	180->181	2.315	179->181	2.387	0.072	0.130
M06	180->181	0.1427	2.509	179->181	0.0671	2.527	180->181	2.384	179->181	2.465	0.081	0.125
M06-2X	180->181	0.2333	3.417	179->181	0.1172	3.424	179->181	3.195	180->181	3.210	0.015	0.222
ωB97	180->181	0.4916	4.248	179->181	0.0744	4.042	169->181	2.629	180->183	3.042	0.412	1.619
ωB97X	180->181	0.4547	4.086	179->181	0.0853	3.935	169->181	2.739	180->183	3.121	0.382	1.347
CAM-B3LYP	180->181	0.2658	3.470	179->181	0.1356	3.519	167->181	2.754	180->183	3.054	0.300	0.716
LC-ωPBE17	180->181	0.2109	2.988	179->181	0.0949	2.984	177->181	2.720	180->181	2.789	0.069	0.268
LC-BLYP17	180->181	0.2136	2.968	179->181	0.1000	2.980	177->181	2.760	180->181	2.779	0.020	0.209
LC-BLYP20	180->181	0.2540	3.246	179->181	0.1023	3.225	179->181	2.897	180->181	2.999	0.102	0.349
LC-BLYP33	180->181	0.4245	4.001	179->181	0.0757	3.814	168->181	2.884	180->183	3.168	0.284	1.117
LC-BLYP	180->181	0.5119	4.347	179->181	0.0849	4.170	168->181	2.377	180->183	2.819	0.442	1.971
LC-BLYP20 - M06-2X												0.051

Table S4. Excited state data for compound **2** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	176->177	0.1571	3.468	175->177	0.1306	3.496	176->177	3.337	175->177	3.354	0.016	0.130
BLYP	176->177	0.0761	1.964	175->177	0.0458	1.937	176->177	1.881	175->177	1.903	0.023	0.084
BPW91	176->177	0.0786	1.968	175->177	0.0481	1.939	176->177	1.882	175->177	1.903	0.021	0.086
PBE	176->177	0.0786	1.971	175->177	0.0477	1.941	176->177	1.886	175->177	1.905	0.019	0.086
M06L	176->177	0.0817	2.194	175->177	0.0480	2.175	176->177	2.105	175->177	2.138	0.033	0.089
TPSS	176->177	0.0807	2.045	175->177	0.0807	2.045	176->177	1.956	175->177	1.981	0.024	0.089
TPSSh	176->177	0.0901	2.434	175->177	0.0522	2.427	176->177	2.330	175->177	2.377	0.047	0.104
B3LYP	176->177	0.1080	2.756	175->177	0.0620	2.771	176->177	2.629	175->177	2.702	0.074	0.127
B971	176->177	0.1125	2.810	175->177	0.0650	2.826	176->177	2.681	175->177	2.755	0.073	0.129
PBE0	176->177	0.1256	2.961	175->177	0.6988	2.981	176->177	2.791	175->177	2.864	0.072	0.169
M06	176->177	0.1309	2.998	175->177	0.0758	3.024	176->177	2.825	175->177	2.910	0.086	0.173
M06-2X	176->177	0.2676	3.865	175->177	0.1110	3.776	175->177	3.391	176->177	3.450	0.059	0.474
ωB97	176->177	0.5494	4.388	175->177	0.0653	4.215	173->177	2.868	176->179	3.052	0.184	1.520
ωB97X	176->177	0.5041	4.294	175->177	0.0713	4.125	172->177	2.967	176->179	3.134	0.167	1.327
CAM-B3LYP	176->177	0.3100	3.886	175->177	0.1717	3.893	170->177	2.958	176->179	3.085	0.127	0.928
LC-ωPBE17	176->177	0.2184	3.441	175->177	0.0944	3.375	174->177	2.950	176->177	3.075	0.125	0.492
LC-BLYP17	176->177	0.2123	3.412	175->177	0.1126	3.380	173->177	3.003	176->177	3.087	0.085	0.409
LC-BLYP20	176->177	0.2595	3.648	175->177	0.0928	3.549	173->177	3.097	176->177	3.198	0.101	0.551
LC-BLYP33	176->177	0.4595	4.210	175->177	0.0664	4.013	172->177	3.086	176->179	3.188	0.103	1.125
LC-BLYP	176->177	0.5666	4.467	175->177	0.0744	4.324	169->177	2.590	176->179	2.826	0.237	1.877
LC-BLYP20 - M06-2X												0.256

Table S5. Excited state data for compound **3** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	123->124	0.2307	2.474	122->124	0.0083	3.355	123->124	2.081	122->124	3.256	1.175	0.393
BLYP	123 ->124	0.1288	1.579	122->124	0.0048	2.209	123->124	1.289	122->124	2.038	0.749	0.290
BPW91	123 ->124	0.1355	1.602	122->124	0.0047	2.236	123->124	1.298	122->124	2.057	0.760	0.304
PBE	123 ->124	0.1360	1.598	122->124	0.0050	2.234	123->124	1.299	122->124	2.055	0.757	0.300
M06L	123 ->124	0.1494	1.781	122->124	0.0043	2.431	123->124	1.396	122->124	2.252	0.856	0.386
TPSS	123 ->124	0.1367	1.635	122->124	0.0047	2.280	123->124	1.298	122->124	2.096	0.798	0.337
TPSSh	123 ->124	0.1567	1.854	122->124	0.0045	2.561	123->124	1.399	122->124	2.360	0.961	0.454
B3LYP	123 ->124	0.1754	2.022	122->124	0.0047	2.783	123->124	1.504	122->124	2.577	1.073	0.518
B971	123 ->124	0.1814	2.054	122->124	0.0047	2.825	123->124	1.547	122->124	2.623	1.076	0.507
PBE0	123 ->124	0.1953	2.147	122->124	0.0049	2.950	123->124	1.508	122->124	2.711	1.203	0.640
M06	123 ->124	0.1983	2.182	122->124	0.0041	2.979	123->124	1.572	122->124	2.765	1.194	0.611
M06-2X	123 ->124	0.2814	2.632	122->124	0.0077	3.629	123->124	1.917	122->124	3.325	1.408	0.715
ωB97	123 ->124	0.3597	3.012	122->124	0.0254	4.216	123->124	1.591	123->126	3.191	1.600	1.422
ωB97X	123 ->124	0.3314	2.898	122->124	0.0168	4.063	123->124	1.651	123->126	3.280	1.629	1.247
CAM-B3LYP	123 ->124	0.2671	2.595	122->124	0.0076	3.614	123->124	1.594	122->124	3.194	1.601	1.001
LC-ωPBE17	123 ->124	0.2120	2.221	122->124	0.0060	3.142	123->124	1.639	122->124	2.866	1.227	0.582
LC-BLYP17	123 ->124	0.2070	2.200	122->124	0.0059	3.120	123->124	1.672	122->124	2.865	1.194	0.528
LC-BLYP20	123 ->124	0.2398	2.380	122->124	0.0071	3.355	123->124	1.687	122->124	3.029	1.342	0.693
LC-BLYP33	123 ->124	0.3288	2.834	122->124	0.0159	3.966	123->124	1.724	122->124	3.265	1.542	1.110
LC-BLYP	123 ->124	0.3753	3.094	122->124	0.0384	4.332	123->124	1.347	123->126	2.945	1.599	1.747
LC-BLYP20 - M06-2X												0.463

Table S6. Excited state data for compound **4** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	145->146	0.0000	2.456	144->146	0.0000	2.525	145->146	2.457	144->146	2.527	0.069	-0.002
BLYP	145->146	0.0000	1.144	144->146	0.0000	1.184	145->146	1.138	144->146	1.177	0.040	0.006
BPW91	145->146	0.0000	1.153	144->146	0.0000	1.194	145->146	1.145	144->146	1.185	0.041	0.008
PBE	145->146	0.0000	1.149	144->146	0.0000	1.191	145->146	1.141	144->146	1.182	0.041	0.008
M06L	145->146	0.0000	1.396	144->146	0.0000	1.439	145->146	1.389	144->146	1.431	0.042	0.007
TPSS	145->146	0.0000	1.203	144->146	0.0000	1.246	145->146	1.195	144->146	1.238	0.043	0.008
TPSSh	145->146	0.0000	1.518	144->146	0.0000	1.563	145->146	1.507	144->146	1.553	0.045	0.010
B3LYP	145->146	0.0000	1.779	144->146	0.0000	1.825	145->146	1.770	144->146	1.815	0.045	0.010
B971	145->146	0.0000	1.818	144->146	0.0000	1.865	145->146	1.808	144->146	1.855	0.047	0.010
PBE0	145->146	0.0000	1.941	144->146	0.0000	1.989	145->146	1.928	144->146	1.976	0.048	0.013
M06	145->146	0.0000	2.038	144->146	0.0000	2.082	145->146	2.032	144->146	2.075	0.044	0.006
M06-2X	145->146	0.0000	2.687	144->146	0.0000	2.745	145->146	2.676	144->146	2.735	0.058	0.011
ωB97	145->146	0.0000	3.430	144->146	0.0000	3.499	139->146	2.083	136->146	3.147	1.064	1.347
ωB97X	145->146	0.0000	3.232	144->146	0.0000	3.297	139->146	2.169	145->146	3.199	1.030	1.063
CAM-B3LYP	145->146	0.0000	2.690	144->146	0.0000	2.745	139->146	2.165	145->146	2.672	0.507	0.526
LC-ωPBE17	145->146	0.0001	2.159	144->146	0.0000	2.214	145->146	2.143	144->146	2.199	0.055	0.016
LC-BLYP17	145->146	0.0000	2.149	144->146	0.0000	2.204	145->146	2.136	144->146	2.191	0.055	0.014
LC-BLYP20	145->146	0.0000	2.385	144->146	0.0000	2.443	145->146	2.369	144->146	2.427	0.058	0.016
LC-BLYP33	145->146	0.0000	3.116	144->146	0.0000	3.177	139->146	2.327	145->146	3.088	0.761	0.789
LC-BLYP	145->146	0.0000	3.565	144->146	0.0000	3.626	139->146	1.813	145->150	2.933	1.121	1.752
LC-BLYP20 - M06-2X												-0.291

Table S7. Excited state data for compound **5** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscilator strength	Energy (eV)	Transition	oscilator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	123 ->124	0.3962	3.524	115->124	0.0037	3.718	123->124	3.227	115->124	3.411	0.185	0.297
BLYP	123 ->124	0.1815	2.075	122->124	0	2.443	123 ->124	1.913	122 ->124	2.429	0.162	0.516
BPW91	123 ->124	0.1841	2.077	122->124	0.0000	2.455	123 ->124	1.910	122 ->124	2.439	0.529	0.167
PBE	123 ->124	0.1844	2.080	122->124	0.0000	2.463	123 ->124	1.914	122 ->124	2.447	0.533	0.166
M06L	123 ->124	0.1886	2.314	122->124	0.0000	2.706	123 ->124	2.141	122 ->124	2.685	0.544	0.173
TPSS	123 ->124	0.1894	2.167	122->124	0.0000	2.556	123 ->124	1.993	122 ->124	2.538	0.545	0.174
TPSSh	123 ->124	0.2191	2.543	122->124	0.0000	2.994	123 ->124	2.323	120 ->124	2.920	0.597	0.220
B3LYP	123 ->124	0.2553	2.834	122->124	0.0000	3.331	123 ->124	2.560	120 ->124	3.056	0.496	0.274
B971	123 ->124	0.2629	2.882	122->124	0.0000	3.395	123 ->124	2.612	120 ->124	3.085	0.473	0.270
PBE0	123 ->124	0.2858	3.024	122->124	0.0000	3.572	123 ->124	2.654	120 ->124	3.058	0.404	0.371
M06	123 ->124	0.2883	3.086	122->124	0.0000	3.607	123 ->124	2.732	122 ->125	3.047	0.314	0.354
M06-2X	123 ->124	0.4545	3.782	115->124	0.0204	3.662	120 ->124	3.145	123 ->124	3.332	0.187	0.637
ωB97	123 ->124	0.7371	4.406	120->124	0.0051	3.995	122 ->125	2.961	120 ->124	2.980	0.019	1.446
ωB97X	123 ->124	0.6987	4.285	120->124	0.0064	3.948	120 ->124	3.034	122 ->125	3.069	0.035	1.251
CAM-B3LYP	123 ->124	0.3934	3.824	116->124	0.1124	3.880	120 ->124	2.943	122 ->125	3.062	0.119	0.881
LC-ωPBE17	123 ->124	0.3911	3.413	121->124	0.0447	3.457	121 ->124	2.841	123 ->124	3.008	0.167	0.572
LC-BLYP17	123 ->124	0.4161	3.395	121->124	0.0143	3.473	121 ->124	2.883	123 ->124	3.048	0.165	0.512
LC-BLYP20	123 ->124	0.4480	3.617	121->124	0.0442	3.552	121 ->124	2.960	123 ->124	3.148	0.188	0.657
LC-BLYP33	123 ->124	0.6833	4.187	120->124	0.0055	3.837	120 ->124	3.063	122 ->125	3.172	0.108	1.124
LC-BLYP	123 ->124	0.7493	4.484	117->124	0.0054	4.053	122 ->125	2.688	120 ->124	2.781	0.093	1.796
LC-BLYP20 - M06-2X												0.472

Table S8. Excited state data for compound **6** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	177 ->178	0.2074	3.565	176->178	0.0012	3.646	176->178	3.494	177->178	3.502	0.009	0.071
BLYP	177 -> 178	0.1103	2.427	176->178	0.0003	2.454	177 -> 178	2.343	176 ->178	2.349	0.005	0.083
BPW91	177 -> 178	0.1118	2.433	176->178	0.0003	2.460	177 -> 178	2.346	176 ->178	2.348	0.002	0.088
PBE	177 -> 178	0.1112	2.434	176->178	0.0003	2.460	177 -> 178	2.347	176 ->178	2.351	0.004	0.087
M06L	177 -> 178	0.1170	2.688	176->178	0.0003	2.713	176 -> 178	2.591	177 ->178	2.593	0.002	0.097
TPSS	177 -> 178	0.1157	2.535	176->178	0.0003	2.561	177 -> 178	2.443	176 ->178	2.443	0.001	0.092
TPSSh	177 -> 178	0.1364	2.842	176->178	0.0005	2.878	177 -> 178	2.727	176 ->178	2.729	0.002	0.115
B3LYP	177 -> 178	0.1586	3.053	176->178	0.0006	3.101	177 -> 178	2.921	176 ->178	2.924	0.003	0.132
B971	177 -> 178	0.1635	3.096	176->178	0.0007	3.144	177 -> 178	2.966	176 ->178	2.974	0.009	0.130
PBE0	177 -> 178	0.1774	3.213	176->178	0.0008	3.267	176 -> 178	2.986	177 ->178	3.042	0.055	0.227
M06	177 -> 178	0.1765	3.250	176->178	0.0007	3.307	176 -> 178	3.015	175 ->181	3.046	0.031	0.235
M06-2X	177 -> 178	0.2899	3.816	176->178	0.0025	3.915	176 -> 178	3.541	177 ->178	3.588	0.047	0.275
ωB97	177 -> 178	0.4592	4.383	176->178	0.0205	4.546	175 -> 180	2.962	174 ->180	2.963	0.001	1.421
ωB97X	177 -> 178	0.4027	4.241	176->178	0.0055	4.396	175 -> 180	3.070	174 ->180	3.072	0.001	1.171
CAM-B3LYP	177 -> 178	0.2886	3.846	176->178	0.0021	3.953	174 -> 181	3.063	175 ->181	3.065	0.002	0.783
LC-ωPBE17	177 -> 178	0.2193	3.327	176->178	0.0013	3.404	176 -> 178	3.125	177 ->178	3.140	0.016	0.202
LC-BLYP17	177 -> 178	0.2154	3.303	176->178	0.0013	3.381	177 -> 178	3.133	176 ->178	3.155	0.022	0.170
LC-BLYP20	177 -> 178	0.2507	3.508	176->178	0.0017	3.602	176 -> 178	3.277	177 ->180	3.299	0.022	0.231
LC-BLYP33	177 -> 178	0.3928	4.131	176->178	0.0059	4.284	174 -> 180	3.174	174 ->181	3.176	0.002	0.957
LC-BLYP	177 -> 178	0.4933	4.488	176->178	0.0198	4.623	175 -> 180	2.688	174 ->180	2.689	0.001	1.800
LC-BLYP20 - M06-2X												-0.033

Table S9. Excited state data for compound **7** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	153 ->154	0.0938	1.923	152->154	0.0017	1.882	153->154	1.853	152->154	1.852	0.000	0.071
BLYP	153 ->154	0.0862	1.012	152->154	0.0010	1.043	152 ->154	0.873	153 ->154	0.879	0.006	0.139
BPW91	153 ->154	0.0886	1.009	152->154	0.0010	1.040	152 ->154	0.862	153 ->154	0.871	0.008	0.146
PBE	153 ->154	0.0883	1.007	152->154	0.0009	1.037	152 ->154	0.859	153 ->154	0.868	0.009	0.148
M06L	152 ->154	0.0851	1.210	153->154	0.0013	1.222	153 ->154	1.071	152 ->154	1.080	0.009	0.138
TPSS	153 ->154	0.0892	1.058	152->154	0.0010	1.087	152 ->154	0.909	153 ->154	0.917	0.008	0.149
TPSSh	153 ->154	0.0850	1.286	152->154	0.0014	1.297	153 ->154	1.139	152 ->154	1.142	0.003	0.146
B3LYP	153 ->154	0.0823	1.497	152->154	0.0017	1.498	153 ->154	1.347	152 ->154	1.365	0.018	0.150
B971	153 ->154	0.0835	1.523	152->154	0.0017	1.520	153 ->154	1.376	152 ->154	1.390	0.015	0.147
PBE0	153 ->154	0.0854	1.624	152->154	0.0019	1.616	153 ->154	1.439	152 ->154	1.476	0.037	0.185
M06	153 ->154	0.0801	1.717	152->154	0.0019	1.698	153 ->154	1.548	152 ->154	1.587	0.039	0.169
M06-2X	153 ->154	0.0987	2.271	152->154	0.0022	2.215	153 ->154	2.002	152 ->154	2.098	0.096	0.268
ωB97	153 ->154	0.1425	2.957	152->154	0.0024	2.883	144 ->154	1.885	152 ->154	2.615	0.730	1.071
ωB97X	153 ->154	0.1264	2.739	152->154	0.0024	2.676	144 ->154	1.886	152 ->154	2.455	0.569	0.853
CAM-B3LYP	153 ->154	0.1000	2.280	152->154	0.0023	2.247	153 ->154	1.814	152 ->154	2.092	0.279	0.467
LC-ωPBE17	153 ->154	0.0892	1.709	153 ->154	0.0016	1.692	153 ->154	1.496	152 ->154	1.549	0.053	0.212
LC-BLYP17	153 ->154	0.0879	1.702	152->154	0.0017	1.687	153 ->154	1.514	152 ->154	1.555	0.041	0.188
LC-BLYP20	153 ->154	0.0924	1.899	152->154	0.0018	1.873	153 ->154	1.660	152 ->154	1.734	0.074	0.239
LC-BLYP33	153 ->154	0.1200	2.613	152->154	0.0022	2.554	144 ->154	1.916	152 ->154	2.345	0.429	0.697
LC-BLYP	153 ->154	0.1530	3.110	152->154	0.0027	3.036	144 ->154	1.763	152 ->154	2.687	0.924	1.347
LC-BLYP20 - M06-2X												-0.104

Table S10. Excited state data for compound **8** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	179 ->180	0.0833	3.076	178->180	0.0049	3.150	177 ->180	2.575	165 ->180	2.961	0.386	0.501
BLYP	179 ->180	0.0070	1.762	178->180	0.0009	1.801	179 ->180	1.736	178 ->180	1.785	0.050	0.027
BPW91	179 ->180	0.0076	1.768	178->180	0.0009	1.806	179 ->180	1.738	178 ->180	1.788	0.050	0.030
PBE	179 ->180	0.0074	1.773	178->180	0.0009	1.810	179 ->180	1.744	178 ->180	1.744	0.000	0.029
M06L	179 ->180	0.0094	1.958	178->180	0.0010	2.000	179 ->180	1.887	178 ->180	1.981	0.094	0.071
TPSS	179 ->180	0.0084	1.855	178->180	0.0010	1.895	179 ->180	1.814	178 ->180	1.876	0.062	0.042
TPSSh	179 ->180	0.0121	2.157	178->180	0.0014	2.203	177 ->180	1.958	179 ->180	2.141	0.184	0.200
B3LYP	179 ->180	0.0175	2.376	178->180	0.0021	2.428	177 ->180	2.027	179 ->180	2.329	0.302	0.349
B971	179 ->180	0.0194	2.426	178->180	0.0023	2.479	177 ->180	2.076	179 ->180	2.380	0.304	0.350
PBE0	179 ->180	0.0239	2.542	178->180	0.0028	2.597	177 ->180	1.989	179 ->180	2.417	0.428	0.552
M06	179 ->180	0.0251	2.504	178->180	0.0029	2.561	177 ->180	1.998	179 ->180	2.390	0.393	0.506
M06-2X	179 ->180	0.1645	3.236	178->180	0.0141	3.321	177 ->180	2.430	179 ->181	2.946	0.516	0.806
ωB97	179 ->180	0.2725	3.641	178->180	0.2985	3.835	177 ->180	1.921	179 ->181	2.459	0.537	1.720
ωB97X	179 ->180	0.2532	3.529	178->180	0.0540	3.748	177 ->180	2.003	179 ->181	2.526	0.523	1.526
CAM-B3LYP	179 ->180	0.2020	3.238	179 ->180	0.0002	3.375	177 ->180	1.991	179 ->181	2.507	0.516	1.247
LC-ωPBE17	179 ->180	0.0994	2.904	178->180	0.0052	2.940	177 ->180	2.173	173->180	2.580	0.407	0.731
LC-BLYP17	179 ->180	0.0879	2.870	178->180	0.0065	2.925	177 ->180	2.221	173->180	2.637	0.416	0.649
LC-BLYP20	179 ->180	0.1639	3.065	178->180	0.0075	3.129	177 ->180	2.252	179 ->181	2.703	0.452	0.814
LC-BLYP33	179 ->180	0.2493	3.508	178->180	0.0132	3.646	177 ->180	2.128	179 ->181	2.601	0.473	1.381
LC-BLYP	179 ->180	0.2836	3.684	178->180	0.5888	3.892	177 ->180	1.629	179 ->181	2.213	0.585	2.056
LC-BLYP20 - M06-2X												0.635

Table S11. Excited state data for compound **9** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	118->119	1.0105	2.692	116->119	0.5851	3.488	118->119	2.159	116->119	2.809	0.651	0.534
BLYP	118->119	0.5002	1.613	117->119	0.0000	1.796	118->119	1.352	117->119	1.782	0.431	0.262
BPW91	118->119	0.5062	1.624	117->119	0.0000	1.816	118->119	1.355	117->119	1.801	0.445	0.269
PBE	118->119	0.5063	1.625	117->119	0.0000	1.820	118->119	1.357	117->119	1.805	0.448	0.268
M06L	118->119	0.5225	1.761	117->119	0.0000	1.957	118->119	1.470	116->119	1.872	0.402	0.291
TPSS	118->119	0.5219	1.675	117->119	0.0000	1.879	118->119	1.393	116->119	1.818	0.425	0.282
TPSSh	118->119	0.5886	1.935	117->119	0.0000	2.226	118->119	1.544	116->119	1.949	0.406	0.391
B3LYP	118->119	0.6944	2.153	117->119	0.0000	2.513	118->119	1.640	116->119	2.149	0.509	0.512
B971	118->119	0.7180	2.189	117->119	0.0001	2.566	118->119	1.683	116->119	2.195	0.512	0.505
PBE0	118->119	0.7894	2.304	117->119	0.0001	2.729	116->119	1.603	116->119	2.247	0.644	0.701
M06	118->119	0.8144	2.339	117->119	0.0001	2.742	116->119	1.668	116->119	2.320	0.651	0.671
M06-2X	118->119	1.3958	2.870	116->119	0.4123	3.631	118->119	1.956	116->119	2.820	0.865	0.915
ωB97	118->119	1.8454	3.317	116->119	0.1245	4.327	116->119	1.522	115->119	2.772	1.250	1.795
ωB97X	118->119	1.8107	3.227	116->119	0.1233	4.176	116->119	1.592	115->119	2.782	1.190	1.635
CAM-B3LYP	118->119	1.5167	2.933	116->119	0.3071	3.696	116->119	1.609	114->119	2.666	1.057	1.324
LC-ωPBE17	118->119	1.3586	2.700	116->119	0.1894	3.303	116->119	1.698	116->119	2.547	0.849	1.002
LC-BLYP17	118->119	1.3483	2.678	116->119	0.1989	3.286	116->119	1.772	116->119	2.577	0.804	0.906
LC-BLYP20	118->119	1.4964	2.819	116->119	0.1507	3.477	116->119	1.778	115->119	2.662	0.884	1.041
LC-BLYP33	118->119	1.7685	3.185	116->119	0.1206	4.094	116->119	1.663	115->119	2.775	1.112	1.522
LC-BLYP	118->119	1.8646	3.368	116->119	0.1308	4.447	116->119	1.337	114->119	2.668	1.331	2.031
LC-BLYP20 - M06-2X												0.864

Table S12. Excited state data for compound **10** calculated using TD-DFT with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	151->152	0.0323	3.022	150->152	0.0104	3.031	151->152	3.010	150->152	3.019	0.009	0.012
BLYP	151->152	0.0222	1.681	150->152	0.0075	1.692	151->152	1.664	150->152	1.668	0.004	0.017
BPW91	151->152	0.0222	1.680	150->152	0.0074	1.691	151->152	1.661	150->152	1.665	0.004	0.019
PBE	151->152	0.0223	1.662	150->152	0.0071	1.673	151->152	1.643	150->152	1.647	0.004	0.019
M06L	151->152	0.0213	1.971	150->152	0.0072	1.980	151->152	1.954	150->152	1.957	0.004	0.018
TPSS	151->152	0.0227	1.771	150->152	0.0076	1.781	151->152	1.751	150->152	1.755	0.004	0.020
TPSSh	151->152	0.0226	2.178	150->152	0.0076	2.188	151->152	2.152	150->152	2.158	0.005	0.025
B3LYP	151->152	0.0244	2.496	150->152	0.0084	2.506	151->152	2.466	150->152	2.473	0.007	0.030
B971	151->152	0.0249	2.531	150->152	0.0086	2.541	151->152	2.502	150->152	2.509	0.007	0.029
PBE0	151->152	0.0262	2.670	150->152	0.0091	2.680	151->152	2.628	150->152	2.638	0.010	0.042
M06	151->152	0.0258	2.755	150->152	0.0088	2.765	151->152	2.719	150->152	2.731	0.012	0.036
M06-2X	151->152	0.0359	3.420	150->152	0.0118	3.431	150->156	3.279	151->156	3.279	0.000	0.141
ωB97	151->152	0.0677	4.206	150->152	0.0092	4.223	151->156	2.863	150->156	2.863	0.000	1.343
ωB97X	151->152	0.0546	4.039	150->152	0.0135	4.055	151->156	2.945	150->156	2.945	0.000	1.095
CAM-B3LYP	151->152	0.0377	3.515	150->152	0.0124	3.527	151->156	2.887	150->156	2.887	0.000	0.628
LC-ωPBE17	151->152	0.0314	2.951	150->152	0.0116	2.962	150->156	2.866	151->156	2.867	0.001	0.085
LC-BLYP17	151->152	0.0311	2.919	150->152	0.0112	2.930	151->152	2.868	150->152	2.875	0.008	0.051
LC-BLYP20	151->152	0.0341	3.159	150->152	0.0118	3.170	151->156	2.974	150->156	2.974	0.000	0.185
LC-BLYP33	151->152	0.0507	3.890	150->152	0.0135	3.904	151->156	2.952	150->156	2.952	0.000	0.938
LC-BLYP	151->152	0.0874	4.339	150->152	0.0035	4.348	151->156	2.638	150->156	2.638	0.000	1.701
LC-BLYP20 - M06-2X												-0.120

Table S13. Excited state data for compound **1** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	180->181	0.1704	2.969	179->181	0.0980	2.996	180->181	2.903	179->181	2.948	0.045	0.067
BLYP	180->181	0.1309	1.515	179->181	0.0645	1.446	180->181	1.378	179->181	1.393	0.014	0.137
BPW91	180->181	0.1345	1.516	179->181	0.0670	1.443	180->181	1.374	179->181	1.387	0.013	0.142
PBE	180->181	0.1344	1.517	179->181	0.0669	1.443	180->181	1.376	179->181	1.387	0.011	0.141
M06L	180->181	0.1293	1.707	179->181	0.0628	1.654	180->181	1.582	179->181	1.605	0.023	0.125
TPSS	180->181	0.1345	1.588	179->181	0.0668	1.522	180->181	1.450	179->181	1.467	0.016	0.138
TPSSh	180->181	0.1388	1.948	179->181	0.0669	1.913	180->181	1.823	179->181	1.860	0.037	0.125
B3LYP	180->181	0.1479	2.264	179->181	0.0692	2.256	180->181	2.142	179->181	2.201	0.059	0.121
B971	180->181	0.1518	2.311	179->181	0.0713	2.304	180->181	2.189	179->181	2.248	0.059	0.122
PBE0	180->181	0.1609	2.461	179->181	0.0761	2.462	180->181	2.330	179->181	2.396	0.067	0.132
M06	180->181	0.1595	2.525	179->181	0.0746	2.534	180->181	2.399	179->181	2.473	0.075	0.127
M06-2X	180->181	0.2461	3.440	179->181	0.1322	3.449	179->181	3.224	180->181	3.239	0.015	0.216
ωB97	180->181	0.5093	4.334	179->181	0.0849	4.096	169->181	3.401	166->181	3.555	0.154	0.933
ωB97X	180->181	0.4619	4.149	179->181	0.0987	3.981	169->181	3.387	166->181	3.468	0.081	0.762
CAM-B3LYP	180->181	0.2773	3.496	179->181	0.1467	3.538	180->181	3.222	179->181	3.251	0.030	0.275
LC-ωPBE17	180->181	0.2252	3.010	179->181	0.1064	2.999	177->181	2.747	180->181	2.812	0.065	0.263
LC-BLYP17	180->181	0.2289	2.990	179->181	0.1115	2.995	179->181	2.780	180->181	2.797	0.017	0.210
LC-BLYP20	180->181	0.2672	3.271	179->181	0.1163	3.246	179->181	2.925	180->181	3.029	0.104	0.346
LC-BLYP33	180->181	0.4327	4.060	179->181	0.0883	3.859	173->181	3.337	168->181	3.394	0.056	0.723
LC-BLYP	180->181	0.5403	4.450	179->181	0.0968	4.234	168->181	3.326	180->183	3.515	0.189	1.124
LC-BLYP20 - M06-2X												0.047

Table S14. Excited state data for compound **2** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	176->177	0.1571	3.468	175->177	0.1306	3.496	176->177	3.337	175->177	3.354	0.016	0.130
BLYP	176->177	0.0855	1.978	175->177	0.0485	1.942	176->177	1.883	175->177	1.905	0.022	0.095
BPW91	176->177	0.0875	1.983	175->177	0.0502	1.944	176->177	1.885	175->177	1.905	0.020	0.098
PBE	176->177	0.0873	1.986	175->177	0.0501	1.946	176->177	1.888	175->177	1.906	0.018	0.098
M06L	176->177	0.0893	2.206	175->177	0.0494	2.179	176->177	2.112	175->177	2.141	0.030	0.095
TPSS	176->177	0.0895	2.059	175->177	0.0510	2.023	176->177	1.960	175->177	1.983	0.023	0.099
TPSSh	176->177	0.1031	2.448	175->177	0.0582	2.433	176->177	2.339	175->177	2.383	0.045	0.109
B3LYP	176->177	0.1206	2.770	175->177	0.0686	2.777	176->177	2.642	175->177	2.712	0.070	0.128
B971	176->177	0.1251	2.825	175->177	0.0719	2.832	176->177	2.694	175->177	2.764	0.070	0.131
PBE0	176->177	0.1378	2.977	175->177	0.0809	2.989	176->177	2.818	175->177	2.893	0.075	0.159
M06	176->177	0.1419	3.014	175->177	0.0826	3.032	176->177	2.854	175->177	2.944	0.090	0.160
M06-2X	176->177	0.2686	3.904	175->177	0.1456	3.834	175->177	3.431	176->177	3.519	0.088	0.474
ωB97	176->177	0.5623	4.513	175->177	0.0732	4.275	173->177	3.582	176->179	3.585	0.003	0.931
ωB97X	176->177	0.5034	4.393	175->177	0.0813	4.179	176->179	3.561	172->177	3.561	0.000	0.832
CAM-B3LYP	176->177	0.3093	3.930	175->177	0.1876	3.927	176->177	3.404	175->177	3.431	0.027	0.526
LC-ωPBE17	176->177	0.2259	3.471	175->177	0.4800	3.400	174->177	2.984	176->177	3.128	0.144	0.488
LC-BLYP17	176->177	0.2210	3.442	175->177	0.1276	3.404	173->177	3.031	176->177	3.121	0.090	0.411
LC-BLYP20	176->177	0.2657	3.688	175->177	0.1072	3.581	173->177	3.130	176->177	3.260	0.130	0.558
LC-BLYP33	176->177	0.4560	4.303	175->177	0.0763	4.064	173->177	3.475	176->179	3.511	0.036	0.828
LC-BLYP	176->177	0.5890	4.609	175->177	0.0828	4.394	169->177	3.503	176->179	3.534	0.031	1.106
LC-BLYP20 - M06-2X												0.257

Table S15. Excited state data for compound **3** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	123->124	0.2307	2.474	122->124	0.0083	3.355	123->124	2.081	122->124	3.256	1.175	0.393
BLYP	123 ->124	0.1609	1.642	122->124	0.0056	2.238	123->124	1.312	122->124	2.043	0.731	0.330
BPW91	123 ->124	0.1670	1.665	122->124	0.0057	2.267	123->124	1.325	122->124	2.063	0.738	0.340
PBE	123 ->124	0.1674	1.662	122->124	0.0059	2.265	123->124	1.324	122->124	2.061	0.737	0.338
M06L	123 ->124	0.1791	1.842	122->124	0.0052	2.459	123->124	1.469	122->124	2.265	0.796	0.373
TPSS	123 ->124	0.1677	1.698	122->124	0.0056	2.310	123->124	1.342	122->124	2.105	0.763	0.356
TPSSh	123 ->124	0.1921	1.919	122->124	0.0056	2.591	123->124	1.494	122->124	2.377	0.883	0.425
B3LYP	123 ->124	0.2116	2.091	122->124	0.0056	2.812	123->124	1.617	122->124	2.595	0.979	0.474
B971	123 ->124	0.2185	2.123	122->124	0.0058	2.855	123->124	1.651	122->124	2.639	0.988	0.472
PBE0	123 ->124	0.2337	2.219	122->124	0.0060	2.980	123->124	1.681	122->124	2.740	1.060	0.538
M06	123 ->124	0.2335	2.254	122->124	0.0050	3.008	123->124	1.735	122->124	2.795	1.060	0.519
M06-2X	123 ->124	0.3314	2.725	122->124	0.0093	3.669	123->124	2.065	122->124	3.367	1.302	0.661
ωB97	123 ->124	0.4082	3.137	122->124	0.0233	4.277	123->124	2.137	114->124	3.460	1.323	0.999
ωB97X	123 ->124	0.3779	3.013	122->124	0.0171	4.114	123->124	2.091	114->124	3.464	1.373	0.922
CAM-B3LYP	123 ->124	0.3089	2.688	122->124	0.0089	3.651	123->124	1.925	122->124	3.299	1.374	0.763
LC-ωPBE17	123 ->124	0.2503	2.302	122->124	0.0072	3.180	123->124	1.748	122->124	2.889	1.141	0.554
LC-BLYP17	123 ->124	0.2446	2.280	122->124	0.0071	3.157	123->124	1.755	122->124	2.881	1.126	0.525
LC-BLYP20	123 ->124	0.2806	2.467	122->124	0.0085	3.395	123->124	1.837	122->124	3.064	1.227	0.630
LC-BLYP33	123 ->124	0.3771	2.947	122->124	0.0168	4.018	123->124	2.066	114->124	3.416	1.350	0.881
LC-BLYP	123 ->124	0.4245	3.229	122->124	0.0317	4.404	123->124	2.111	114->124	3.417	1.305	1.118
LC-BLYP20 - M06-2X												0.402

Table S16. Excited state data for compound **4** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	145->146	0.0000	2.456	144->146	0.0000	2.525	145->146	2.457	144->146	2.527	0.069	-0.002
BLYP	145->146	0.0000	1.144	144->146	0.0000	1.185	145->146	1.138	144->146	1.177	0.040	0.007
BPW91	145->146	0.0000	1.153	144->146	0.0000	1.194	145->146	1.145	144->146	1.186	0.041	0.008
PBE	145->146	0.0000	1.149	144->146	0.0000	1.191	145->146	1.141	144->146	1.183	0.041	0.008
M06L	145->146	0.0000	1.396	144->146	0.0000	1.439	145->146	1.389	144->146	1.431	0.042	0.007
TPSS	145->146	0.0000	1.203	144->146	0.0000	1.247	145->146	1.195	144->146	1.238	0.043	0.008
TPSSh	145->146	0.0000	1.518	144->146	0.0000	1.564	145->146	1.509	144->146	1.554	0.045	0.009
B3LYP	145->146	0.0000	1.780	144->146	0.0000	1.826	145->146	1.771	144->146	1.816	0.045	0.009
B971	145->146	0.0000	1.819	144->146	0.0000	1.866	145->146	1.810	144->146	1.857	0.047	0.009
PBE0	145->146	0.0000	1.942	144->146	0.0000	1.991	145->146	1.931	144->146	1.979	0.048	0.012
M06	145->146	0.0000	2.040	144->146	0.0000	2.084	145->146	2.033	144->146	2.077	0.044	0.006
M06-2X	145->146	0.0000	2.693	144->146	0.0000	2.750	145->146	2.682	144->146	2.740	0.058	0.011
ωB97	145->146	0.0000	3.440	144->146	0.0000	3.508	139->146	2.747	136->146	3.382	0.635	0.692
ωB97X	145->146	0.0000	3.239	144->146	0.0000	3.304	139->146	2.728	145->146	3.215	0.486	0.511
CAM-B3LYP	145->146	0.0000	2.694	144->146	0.0000	2.749	145->146	2.677	144->146	2.733	0.056	0.017
LC-ωPBE17	145->146	0.0000	2.161	144->146	0.0000	2.216	145->146	2.145	144->146	2.201	0.055	0.015
LC-BLYP17	145->146	0.0000	2.151	144->146	0.0000	2.206	145->146	2.137	144->146	2.193	0.055	0.013
LC-BLYP20	145->146	0.0000	2.388	144->146	0.0000	2.445	145->146	2.372	144->146	2.430	0.058	0.016
LC-BLYP33	145->146	0.0000	3.123	144->146	0.0000	3.184	139->146	2.757	145->146	3.098	0.341	0.366
LC-BLYP	145->146	0.0000	3.576	144->146	0.0000	3.637	139->146	2.679	136->146	3.333	0.654	0.897
LC-BLYP20 - M06-2X												-0.294

Table S17. Excited state data for compound **5** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	123 ->124	0.3962	3.524	115->124	0.0037	3.718	123->124	3.227	115->124	3.411	0.185	0.297
BLYP	123 ->124	0.2024	2.103	122 ->124	0.0000	2.445	123 ->124	1.918	122 ->124	2.430	0.513	0.185
BPW91	123 ->124	0.2052	2.105	122 ->124	0.0000	2.457	123 ->124	1.916	122 ->124	2.441	0.525	0.190
PBE	123 ->124	0.2057	2.109	122 ->124	0.0000	2.464	123 ->124	1.919	122 ->124	2.449	0.529	0.190
M06L	123 ->124	0.2059	2.339	122 ->124	0.0000	2.708	123 ->124	2.157	122 ->124	2.691	0.534	0.182
TPSS	123 ->124	0.2097	2.195	122 ->124	0.0000	2.558	123 ->124	2.003	122 ->124	2.541	0.538	0.192
TPSSh	123 ->124	0.2409	2.571	122 ->124	0.0000	2.996	123 ->124	2.351	122 ->124	2.968	0.617	0.219
B3LYP	123 ->124	0.2770	2.862	122 ->124	0.0000	3.334	123 ->124	2.605	120 ->124	3.113	0.508	0.257
B971	123 ->124	0.2847	2.911	122 ->124	0.0000	3.398	123 ->124	2.654	120 ->124	3.135	0.481	0.257
PBE0	123 ->124	0.3080	3.054	122 ->124	0.0000	3.576	123 ->124	2.745	120 ->124	3.128	0.383	0.309
M06	123 ->124	0.3075	3.116	122 ->124	0.0001	3.612	123 ->124	2.823	120 ->124	3.291	0.468	0.294
M06-2X	123 ->124	0.4807	3.830	115->124	0.0236	3.739	120 ->124	3.237	123 ->124	3.405	0.168	0.593
ωB97	123 ->124	0.7730	4.494	120 ->124	0.0037	4.033	120 ->124	3.405	118 ->124	3.607	0.202	1.090
ωB97X	123 ->124	0.7232	4.358	120 ->124	0.0045	3.985	120 ->124	3.358	123 ->124	3.561	0.202	0.999
CAM-B3LYP	123 ->124	0.3683	3.874	123 ->124	0.1620	3.911	120 ->124	3.201	116 ->124	3.404	0.202	0.673
LC-ωPBE17	123 ->124	0.4289	3.457	121->124	0.0333	3.479	121 ->124	2.904	123 ->124	3.063	0.159	0.553
LC-BLYP17	123 ->124	0.4517	3.437	121->124	0.0057	3.495	121 ->124	2.934	123 ->124	3.084	0.150	0.503
LC-BLYP20	123 ->124	0.5065	3.658	121 ->124	0.0126	3.581	121 ->124	3.021	123 ->124	3.207	0.187	0.638
LC-BLYP33	123 ->124	0.7096	4.258	120 ->124	0.0038	3.869	120 ->124	3.255	123 ->124	3.484	0.229	1.003
LC-BLYP	123 ->124	0.7978	4.585	117->124	0.0040	4.098	120 ->124	3.389	122 ->125	3.535	0.146	1.196
LC-BLYP20 - M06-2X												0.421

Table S18. Excited state data for compound **6** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	177 ->178	0.2074	3.565	176->178	0.0012	3.646	176->178	3.494	177->178	3.502	0.009	0.071
BLYP	177 -> 178	0.1131	2.437	176->178	0.0004	2.470	177 -> 178	2.346	176 ->178	2.352	0.007	0.092
BPW91	177 -> 178	0.1146	2.444	176->178	0.0004	2.477	177 -> 178	2.349	176 ->178	2.354	0.004	0.095
PBE	177 -> 178	0.1148	2.444	176->178	0.0004	2.477	177 -> 178	2.350	176 ->178	2.355	0.005	0.095
M06L	177 -> 178	0.1189	2.698	176->178	0.0003	2.729	177 -> 178	2.602	176 ->178	2.607	0.005	0.096
TPSS	177 -> 178	0.1191	2.546	176->178	0.0004	2.578	177 -> 178	2.448	176 ->178	2.452	0.004	0.098
TPSSh	177 -> 178	0.1440	2.856	176->178	0.0005	2.895	177 -> 178	2.737	176 ->178	2.753	0.016	0.118
B3LYP	177 -> 178	0.1668	3.069	176->178	0.0007	3.119	177 -> 178	2.934	176 ->178	2.963	0.029	0.136
B971	177 -> 178	0.1719	3.112	176->178	0.0007	3.162	177 -> 178	2.977	176 ->178	3.008	0.031	0.134
PBE0	177 -> 178	0.1862	3.230	176->178	0.0009	3.286	177 -> 178	3.072	176 ->178	3.096	0.024	0.159
M06	177 -> 178	0.1836	3.268	176->178	0.0008	3.326	177 -> 178	3.121	176 ->178	3.145	0.024	0.148
M06-2X	177 -> 178	0.3012	3.848	176->178	0.0031	3.943	177 -> 178	3.618	176 ->178	3.650	0.032	0.229
ωB97	177 -> 178	0.4563	4.449	176->178	0.0086	4.602	175 -> 178	3.631	174 ->180	3.632	0.001	0.818
ωB97X	177 -> 178	0.4044	4.292	176->178	0.0057	4.434	175 -> 178	3.624	174 ->180	3.626	0.002	0.668
CAM-B3LYP	177 -> 178	0.2963	3.877	176->178	0.0026	3.980	176 -> 178	3.507	174 ->180	3.531	0.024	0.371
LC-ωPBE17	177 -> 178	0.2280	3.348	176->178	0.0015	3.427	177 -> 178	3.157	176 ->178	3.195	0.038	0.191
LC-BLYP17	177 -> 178	0.2241	3.324	176->178	0.0014	3.403	177 -> 178	3.145	176 ->178	3.195	0.050	0.179
LC-BLYP20	177 -> 178	0.2594	3.532	176->178	0.0020	3.626	177 -> 178	3.319	176 ->180	3.360	0.041	0.214
LC-BLYP33	177 -> 178	0.3965	4.179	176->178	0.0063	4.322	174 -> 178	3.615	174 ->181	3.622	0.006	0.563
LC-BLYP	177 -> 178	0.4894	4.568	176->178	0.0110	4.726	175 -> 178	3.538	174 ->180	3.539	0.001	1.030
LC-BLYP20 - M06-2X												-0.086

Table S19. Excited state data for compound **7** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscilator strength	Energy (eV)	Transition	oscilator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	153 ->154	0.0938	1.923	152->154	0.0017	1.882	153->154	1.853	152->154	1.852	0.000	0.071
BLYP	153 ->154	0.1054	1.042	152->154	0.0015	1.086	152 ->154	0.878	153 ->154	0.884	0.006	0.164
BPW91	153 ->154	0.1087	1.040	152->154	0.0015	1.085	152 ->154	0.867	153 ->154	0.876	0.008	0.173
PBE	153 ->154	0.1092	1.038	152->154	0.0014	1.082	152 ->154	0.863	153 ->154	0.873	0.010	0.175
M06L	152 ->154	0.0982	1.233	152->154	0.0017	1.254	153 ->154	1.080	152 ->154	1.093	0.013	0.153
TPSS	153 ->154	0.1082	1.087	152->154	0.0015	1.128	152 ->154	0.916	153 ->154	0.925	0.009	0.172
TPSSh	153 ->154	0.1000	1.309	152->154	0.0019	1.328	152 ->154	1.153	153 ->154	1.159	0.006	0.156
B3LYP	153 ->154	0.0938	1.517	152->154	0.0022	1.522	153 ->154	1.373	152 ->154	1.375	0.002	0.144
B971	153 ->154	0.0950	1.542	152->154	0.0022	1.545	152 ->154	1.400	153 ->154	1.400	0.000	0.143
PBE0	153 ->154	0.0959	1.643	152->154	0.0023	1.639	153 ->154	1.486	152 ->154	1.490	0.004	0.157
M06	153 ->154	0.0885	1.735	152->154	0.0023	1.718	153 ->154	1.597	152 ->154	1.599	0.002	0.139
M06-2X	153 ->154	0.1055	2.295	152->154	0.0026	2.242	153 ->154	2.088	152 ->154	2.116	0.028	0.207
ωB97	153 ->154	0.1384	2.989	152->154	0.0026	2.912	153 ->154	2.410	152 ->154	2.699	0.289	0.579
ωB97X	153 ->154	0.1253	2.767	152->154	0.0026	2.702	153 ->154	2.308	152 ->154	2.514	0.206	0.459
CAM-B3LYP	153 ->154	0.1046	2.302	152->154	0.0026	2.269	153 ->154	2.039	152 ->154	2.121	0.082	0.263
LC-ωPBE17	153 ->154	0.0967	1.730	152 ->154	0.0019	1.716	153 ->154	1.546	152 ->154	1.560	0.014	0.183
LC-BLYP17	153 ->154	0.0953	1.722	152->154	0.0020	1.711	153 ->154	1.551	152 ->154	1.564	0.013	0.172
LC-BLYP20	153 ->154	0.0982	1.920	152->154	0.0021	1.896	153 ->154	1.723	152 ->154	1.747	0.024	0.197
LC-BLYP33	153 ->154	0.1201	2.641	152->154	0.0021	2.581	153 ->154	2.233	152 ->154	2.391	0.158	0.408
LC-BLYP	153 ->154	0.1470	3.147	152->154	0.0029	3.069	153 ->154	2.433	152 ->154	2.816	0.383	0.714
LC-BLYP20 - M06-2X												-0.168

Table S20. Excited state data for compound **8** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	179 ->180	0.0833	3.076	178->180	0.0049	3.150	177 ->180	2.575	165 ->180	2.961	0.386	0.501
BLYP	179 ->180	0.0071	1.765	178->180	0.0009	1.803	179 ->180	1.739	178 ->180	1.786	0.047	0.025
BPW91	179 ->180	0.0076	1.771	178->180	0.0010	1.808	179 ->180	1.743	178 ->180	1.790	0.047	0.027
PBE	179 ->180	0.0074	1.776	178->180	0.0009	1.812	179 ->180	1.749	178 ->180	1.794	0.046	0.027
M06L	179 ->180	0.0096	1.961	178->180	0.0011	2.002	179 ->180	1.922	178 ->180	1.984	0.062	0.039
TPSS	179 ->180	0.0084	1.858	178->180	0.0011	1.896	179 ->180	1.826	178 ->180	1.878	0.052	0.032
TPSSh	179 ->180	0.0130	2.161	178->180	0.0016	2.205	179 ->180	2.070	177 ->180	2.180	0.109	0.091
B3LYP	179 ->180	0.0179	2.381	178->180	0.0024	2.431	177 ->180	2.177	179 ->180	2.357	0.180	0.204
B971	179 ->180	0.0197	2.432	178->180	0.0026	2.482	177 ->180	2.215	179 ->180	2.406	0.191	0.217
PBE0	179 ->180	0.0236	2.548	178->180	0.0031	2.601	177 ->180	2.222	179 ->180	2.496	0.274	0.326
M06	179 ->180	0.0243	2.511	178->180	0.0031	2.565	177 ->180	2.221	179 ->180	2.468	0.246	0.289
M06-2X	179 ->180	0.1092	3.279	178->180	0.0137	3.341	177 ->180	2.600	179 ->180	3.067	0.467	0.679
ωB97	179 ->180	0.3357	3.806	178->180	0.0116	3.905	177 ->180	2.587	179 ->181	3.064	0.477	1.220
ωB97X	179 ->180	0.3135	3.681	178->180	0.0141	3.803	177 ->180	2.542	179 ->181	3.025	0.483	1.139
CAM-B3LYP	179 ->180	0.1916	3.326	177->180	0.0459	3.423	177 ->180	2.404	179 ->181	2.901	0.496	0.922
LC-ωPBE17	179 ->180	0.0663	2.932	178->180	0.0057	2.954	177 ->180	2.320	173 ->180	2.617	0.297	0.612
LC-BLYP17	179 ->180	0.0582	2.895	178->180	0.0067	2.935	177 ->180	2.334	173 ->181	2.668	0.335	0.561
LC-BLYP20	179 ->180	0.1229	3.130	178->180	0.0079	3.150	177 ->180	2.403	172 ->180	2.772	0.369	0.727
LC-BLYP33	179 ->180	0.3119	3.659	178->180	0.0068	3.696	177 ->180	2.548	179 ->181	2.998	0.449	1.110
LC-BLYP	179 ->180	0.3487	3.862	178->180	0.1288	4.046	177 ->180	2.537	179 ->181	3.002	0.465	1.325
LC-BLYP20 - M06-2X												0.530

Table S21. Excited state data for compound **9** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			2nd singlet state			1st triplet state		2nd triplet state		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	118->119	1.0105	2.692	116->119	0.5851	3.488	118->119	2.159	116->119	2.809	0.651	0.534
BLYP	118->119	0.5950	1.663	117->119	0.0000	1.798	118->119	1.361	117->119	1.784	0.422	0.302
BPW91	118->119	0.6011	1.674	117->119	0.0000	1.818	118->119	1.367	117->119	1.802	0.435	0.307
PBE	118->119	0.6031	1.675	117->119	0.0000	1.822	118->119	1.368	117->119	1.806	0.439	0.308
M06L	118->119	0.6037	1.805	117->119	0.0000	1.958	118->119	1.505	117->119	1.943	0.438	0.300
TPSS	118->119	0.6118	1.724	117->119	0.0000	1.881	118->119	1.413	117->119	1.865	0.452	0.310
TPSSh	118->119	0.6740	1.978	117->119	0.0000	2.228	118->119	1.626	116->119	2.063	0.437	0.352
B3LYP	118->119	0.7680	2.195	117->119	0.0001	2.515	118->119	1.764	116->119	2.234	0.470	0.431
B971	118->119	0.7912	2.232	117->119	0.0001	2.569	118->119	1.798	116->119	2.274	0.476	0.434
PBE0	118->119	0.8586	2.348	117->119	0.0001	2.732	118->119	1.818	116->119	2.339	0.521	0.530
M06	118->119	0.8692	2.384	117->119	0.0001	2.745	118->119	1.865	116->119	2.401	0.536	0.518
M06-2X	118->119	1.5024	2.950	116->119	0.6742	3.766	116->119	2.135	116->119	2.913	0.778	0.815
ωB97	118->119	2.0066	3.444	116->119	0.1851	4.462	116->119	2.177	115->119	3.131	0.954	1.267
ωB97X	118->119	1.9746	3.345	116->119	0.1980	4.301	116->119	2.137	115->119	3.076	0.939	1.208
CAM-B3LYP	118->119	1.6224	3.018	116->119	0.5250	3.817	116->119	2.019	114->119	2.872	0.852	0.999
LC-ωPBE17	118->119	1.4457	2.776	116->119	0.3349	3.423	116->119	1.908	116->119	2.628	0.720	0.867
LC-BLYP17	118->119	1.4380	2.752	116->119	0.3517	3.406	116->119	1.932	116->119	2.639	0.707	0.821
LC-BLYP20	118->119	1.6152	2.906	116->119	0.2859	3.596	116->119	1.983	115->119	2.750	0.768	0.923
LC-BLYP33	118->119	1.9375	3.303	116->119	0.2024	4.223	116->119	2.110	115->119	3.009	0.899	1.193
LC-BLYP	118->119	2.0285	3.504	116->119	0.1854	4.589	116->119	2.153	114->119	3.126	0.973	1.352
LC-BLYP20 - M06-2X												0.771

Table S22. Excited state data for compound **10** calculated using TD-DFT/TDA with the functionals mentioned in the table, 6-311G(d) as the basis set and cyclohexane for the PCM model.

	1st singlet state			**2nd singlet state**			**1st triplet state**		**2nd triplet state**		$\Delta E_{T_1-T_2}$	$\Delta E_{S_1-T_1}$
	Transition	oscillator strength	Energy (eV)	Transition	oscillator strength	Energy (eV)	Transition	Energy (eV)	Transition	Energy (eV)	Energy (eV)	Energy (eV)
RI-CC2	151->152	0.0323	3.022	150->152	0.0104	3.031	151->152	3.010	150->152	3.019	0.009	0.012
BLYP	151->152	0.0227	1.683	150->152	0.0079	1.696	151->152	1.665	150->152	1.668	0.003	0.019
BPW91	151->152	0.0231	1.682	150->152	0.0081	1.694	151->152	1.662	150->152	1.666	0.004	0.020
PBE	151->152	0.0233	1.664	150->152	0.0081	1.677	151->152	1.644	150->152	1.647	0.003	0.020
M06L	151->152	0.0216	1.973	150->152	0.0077	1.983	151->152	1.956	150->152	1.959	0.003	0.017
TPSS	151->152	0.0231	1.773	150->152	0.0081	1.785	151->152	1.753	150->152	1.756	0.004	0.020
TPSSh	151->152	0.0245	2.180	150->152	0.0092	2.191	151->152	2.156	150->152	2.160	0.004	0.024
B3LYP	151->152	0.0260	2.499	150->152	0.0100	2.510	151->152	2.472	150->152	2.477	0.005	0.027
B971	151->152	0.0265	2.534	150->152	0.0101	2.545	151->152	2.507	150->152	2.513	0.005	0.027
PBE0	151->152	0.0277	2.674	150->152	0.0106	2.685	151->152	2.639	150->152	2.646	0.006	0.034
M06	151->152	0.0269	2.759	150->152	0.0102	2.769	151->152	2.732	150->152	2.739	0.007	0.027
M06-2X	151->152	0.0365	3.429	150->152	0.0133	3.441	151->152	3.375	150->152	3.384	0.008	0.054
ωB97	151->152	0.0571	4.226	150->152	0.0151	4.243	151->156	3.374	150->156	3.374	0.000	0.852
ωB97X	151->152	0.0502	4.054	150->152	0.0153	4.069	151->156	3.355	150->156	3.355	0.000	0.699
CAM-B3LYP	151->152	0.0374	3.523	150->152	0.0138	3.535	151->156	3.228	150->156	3.228	0.000	0.295
LC-ωPBE17	151->152	0.0321	2.955	150->152	0.0132	2.967	151->152	2.902	150->152	2.908	0.007	0.054
LC-BLYP17	151->152	0.0318	2.923	150->152	0.0127	2.935	151->152	2.876	150->152	2.882	0.006	0.047
LC-BLYP20	151->152	0.0344	3.164	150->152	0.0133	3.176	150->156	3.082	151->156	3.083	0.001	0.083
LC-BLYP33	151->152	0.0473	3.903	150->152	0.0152	3.917	151->156	3.270	150->156	3.270	0.000	0.633
LC-BLYP	151->152	0.0631	4.369	150->152	0.0144	4.387	151->156	3.330	150->156	3.330	0.000	1.039
LC-BLYP20 - M06-2X												-0.211

Optimized geometries and HOMO/LUMO topologies

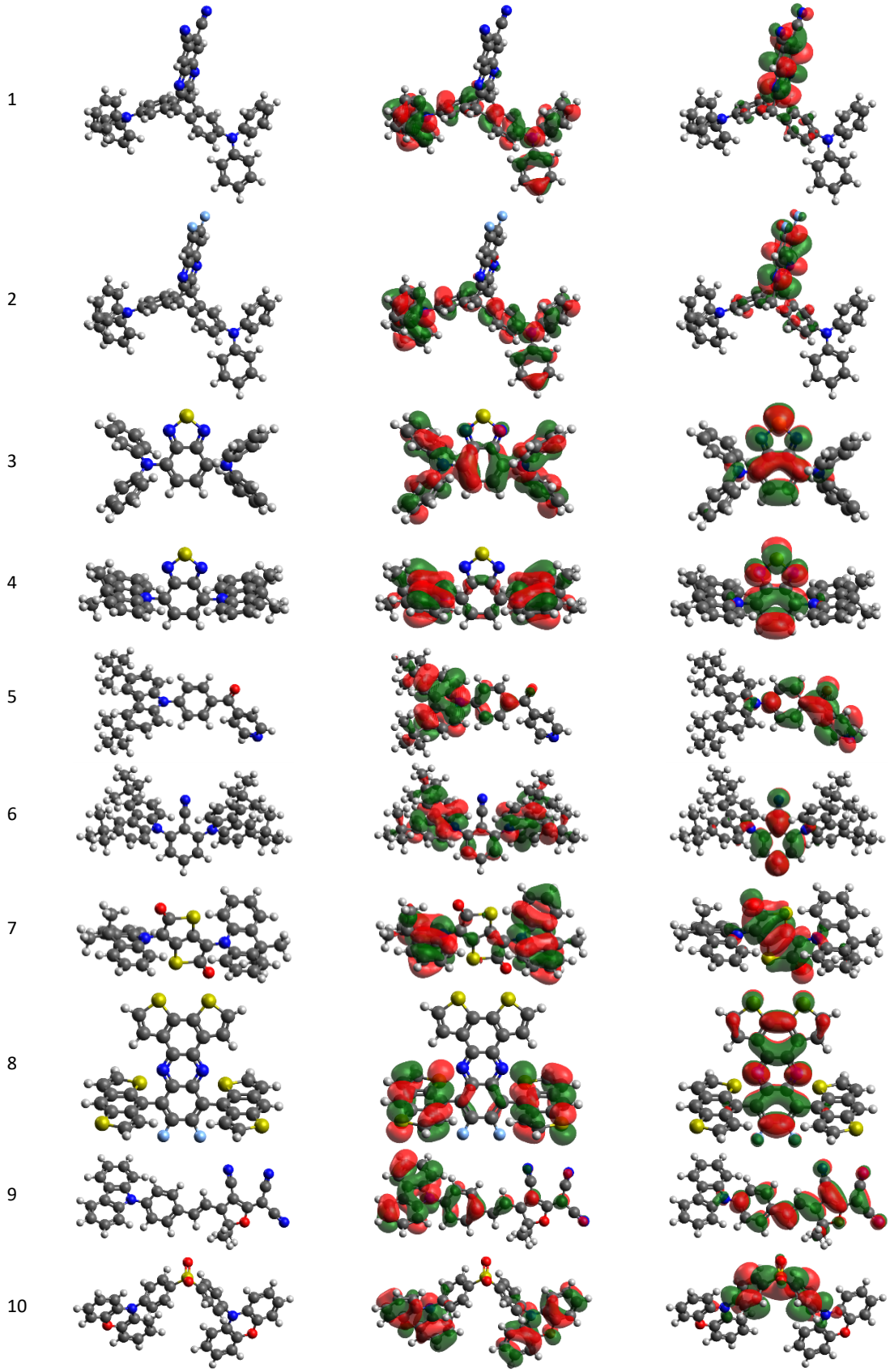
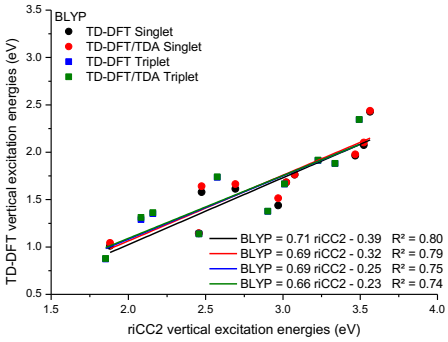
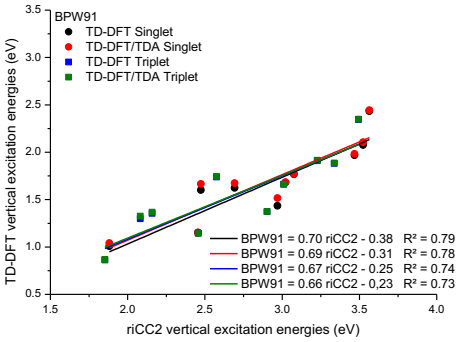
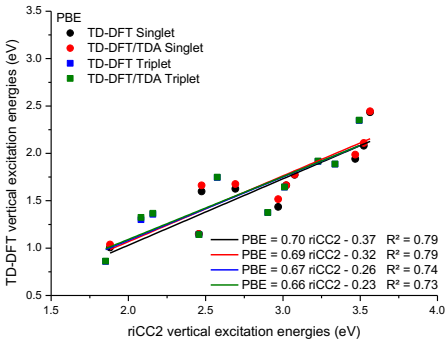


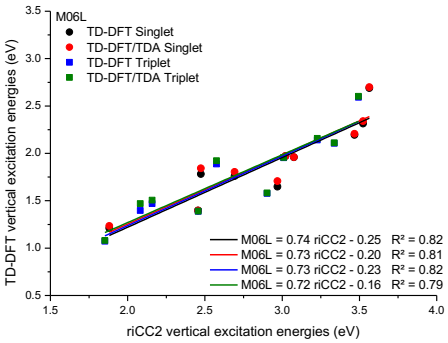
Figure S2. Optimized geometries and HOMO and LUMO topologies for all compounds (calculated using M06 and 6-311G(d)). Isocontour value = 0.02 a.u. for all orbitals.

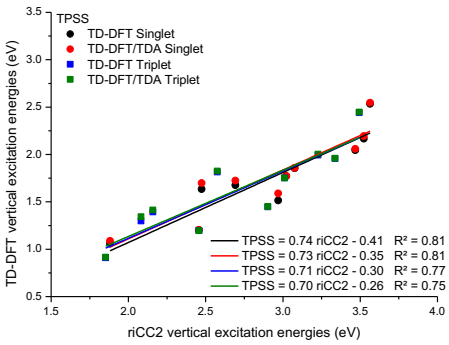
TDDFT versus riCC2 correlation plots

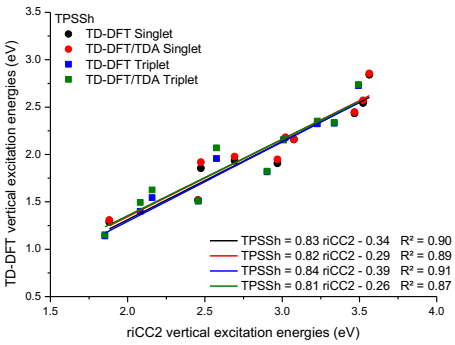


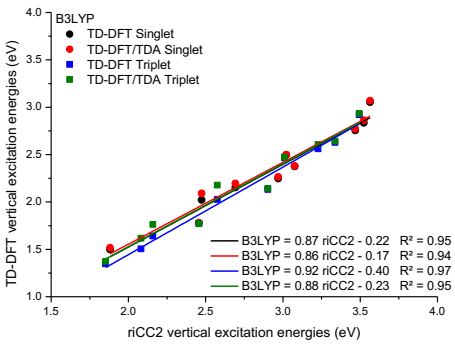


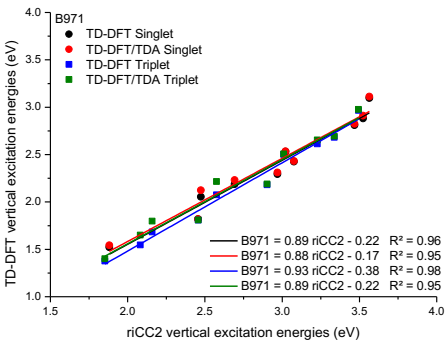


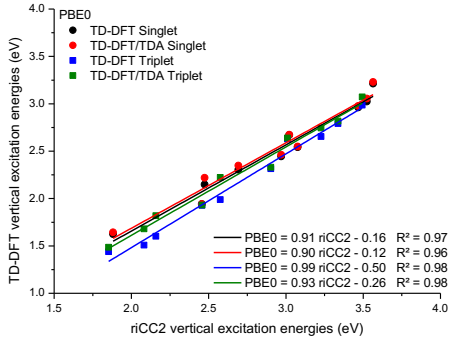


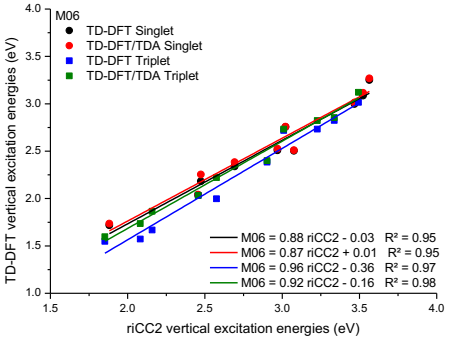


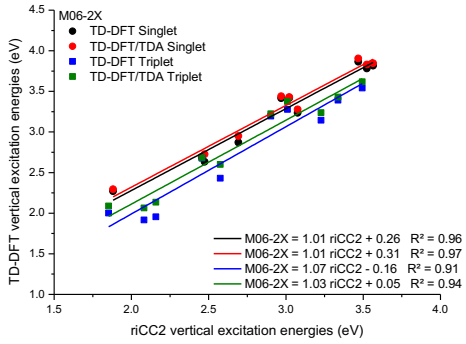


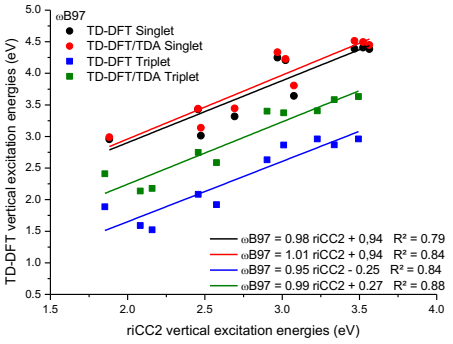


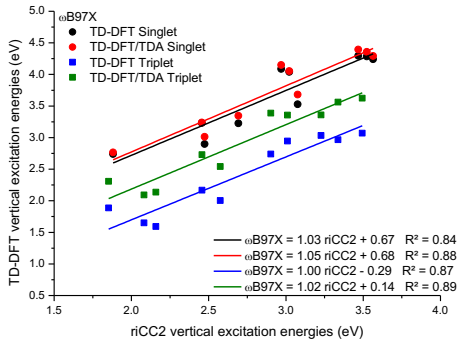


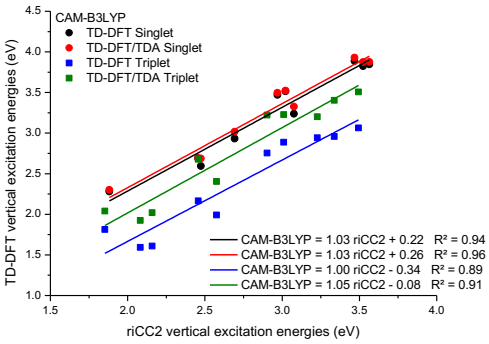

PBE0
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
PBE0 = 0.91 riCC2 - 0.16 R² = 0.97
PBE0 = 0.90 riCC2 - 0.12 R² = 0.96
PBE0 = 0.99 riCC2 - 0.50 R² = 0.98
PBE0 = 0.93 riCC2 - 0.26 R² = 0.98
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)

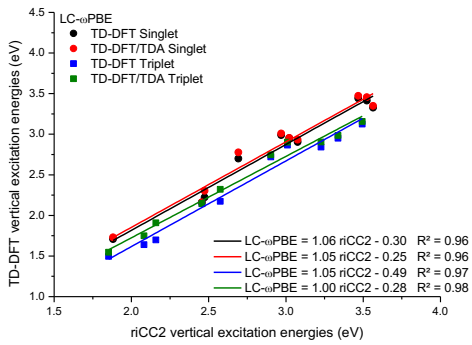

M06
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
M06 = 0.88 riCC2 - 0.03 R² = 0.95
M06 = 0.87 riCC2 + 0.01 R² = 0.95
M06 = 0.96 riCC2 - 0.36 R² = 0.97
M06 = 0.92 riCC2 - 0.16 R² = 0.98
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)

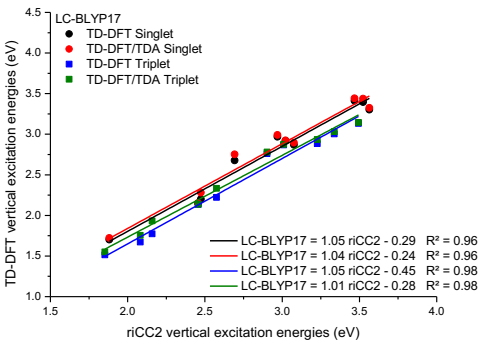

M06-2X
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
M06-2X = 1.01 riCC2 + 0.26 R² = 0.96
M06-2X = 1.01 riCC2 + 0.31 R² = 0.97
M06-2X = 1.07 riCC2 - 0.16 R² = 0.91
M06-2X = 1.03 riCC2 + 0.05 R² = 0.94
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)


ωB97
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
ωB97 = 0.98 riCC2 + 0.94 R² = 0.79
ωB97 = 1.01 riCC2 + 0.94 R² = 0.84
ωB97 = 0.95 riCC2 - 0.25 R² = 0.84
ωB97 = 0.99 riCC2 + 0.27 R² = 0.88
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)


ωB97X
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
ωB97X = 1.03 riCC2 + 0.67 R² = 0.84
ωB97X = 1.05 riCC2 + 0.68 R² = 0.88
ωB97X = 1.00 riCC2 - 0.29 R² = 0.87
ωB97X = 1.02 riCC2 + 0.14 R² = 0.89
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)


CAM-B3LYP
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
CAM-B3LYP = 1.03 riCC2 + 0.22 R² = 0.94
CAM-B3LYP = 1.03 riCC2 + 0.26 R² = 0.96
CAM-B3LYP = 1.00 riCC2 - 0.34 R² = 0.89
CAM-B3LYP = 1.05 riCC2 - 0.08 R² = 0.91
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)


LC-ωPBE
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
LC-ωPBE = 1.06 riCC2 - 0.30 R² = 0.96
LC-ωPBE = 1.05 riCC2 - 0.25 R² = 0.96
LC-ωPBE = 1.05 riCC2 - 0.49 R² = 0.97
LC-ωPBE = 1.00 riCC2 - 0.28 R² = 0.98
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)


LC-BLYP17
TD-DFT Singlet
TD-DFT/TDA Singlet
TD-DFT Triplet
TD-DFT/TDA Triplet
LC-BLYP17 = 1.05 riCC2 - 0.29 R² = 0.96
LC-BLYP17 = 1.04 riCC2 - 0.24 R² = 0.96
LC-BLYP17 = 1.05 riCC2 - 0.45 R² = 0.98
LC-BLYP17 = 1.01 riCC2 - 0.28 R² = 0.98
TD-DFT vertical excitation energies (eV)
riCC2 vertical excitation energies (eV)

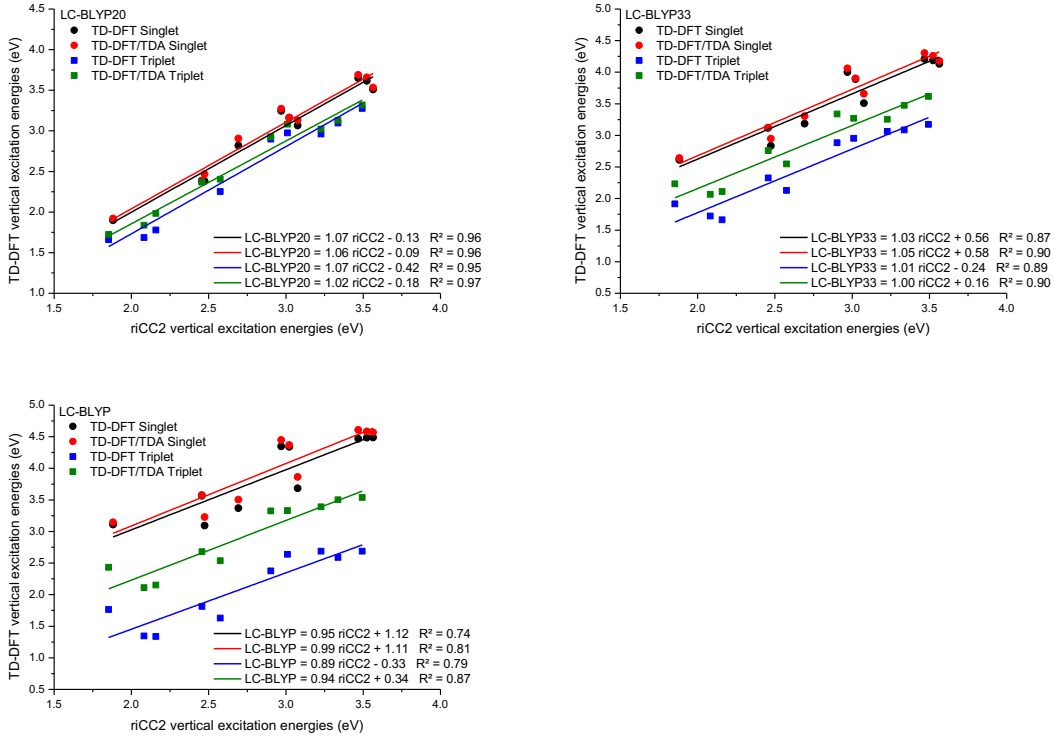


Figure S3. TDDFT versus riCC2 excitation energies as determined with different exchange-correlation functionals.

Experimental section

Materials and methods

Unless stated otherwise, all reagents and chemicals were obtained from commercial sources and used without further purification. Compounds **1**[1], **3**-**6**,[2-4] and **9**[5] were synthesized according to their respective literature procedures. Compound **10** was obtained from Lumtech Inc (LT-N545).

Preparative (recycling) size exclusion chromatography (prep-SEC) was performed on a JAI LC-9110 NEXT system equipped with JAIGEL 1H and 2H columns (eluent $CHCl_3$, flow rate 3.5 mL min^{-1}). It was used to purify all synthesized compounds before performing any further analysis. NMR measurements were performed in $CDCl_3$ on 400 MHz instruments (Varian or Jeol). The chemical shifts (δ, in ppm) were determined relative to the residual $CHCl_3$ (7.26 ppm) proton signals. MALDI-ToF mass spectra were recorded on a Bruker Daltonics Ultraflex II Tof/Tof. 1 µL of the matrix solution (16 mg mL^{-1} *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile in $CHCl_3$) was spotted onto an MTP Anchorchip 600/384 MALDI plate. The spot was allowed to dry and 1 µL of the analyte solution (0.5 mg mL^{-1} in $CHCl_3$) was spotted on top of the matrix.

Synthesis procedures

Synthesis of TPA-QNX(F)2 (2)

(9*R*,10*R*)-2,6-bis(diphenylamino)-9,10-dihydro-9,10-ethanoanthracene-11,12-dione (TPA-DK) was synthesised according to literature.[1] TPA-DK (68.3 mg, 0.12 mmol) and 4,5-difluoro-1,2-benzenediamine (20.6 mg, 0.14 mmol) were heated to reflux for 1 h in ethanol/acetic acid (10 mL, 19/1). Orange crystals were formed at an early stage of the reaction. After the reaction, the mixture was cooled down to room temperature. The crystals were collected by filtration, washed with ethanol and dried under reduced pressure to obtain TPA-QNX(F)2 (19.7 mg, 24%). ^{1}H NMR (400 MHz, $CDCl_3$): 7.67 (t, *J* = 9.3 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.25-7.18 (m, 10H), 7.06-6.98 (m, 12H), 6.82 (dd, *J* = 8.1, 2.2 Hz, 2H), 5.34 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): 158.12, 152.90/152.73/150.36/150.19 (dd, *J* = 255.5, 17.3 Hz), 147.56, 146.85, 142.97, 136.29/136.23/136.17 (t, *J* = 5.9 Hz), 134.90, 129.39, 125.64, 124.74, 123.24, 121.19, 119.76, 114.81/114.74/114.68/114.62 (dd, *J* = 12.6, 6.8 Hz), 54.48. MS (ESI+) Calcd. for $C_{46}H_{30}F_2N_4$ [M]+: *m/z* 676.244, found: 676.240.

Synthesis of TTD-DMAC (7)

3,6-bis(9,9-dimethylacridin-10(9H)-yl)thieno[3,2-b]thiophene (DMAC-TT)

3,6-Dibromothieno[3,2-*b*]thiophene (504.8 mg, 1.69 mmol), 9,9-dimethyl-9,10-dihydroacridine (737.1 mg, 3.52 mmol), palladium(II) acetate (22.9 mg, 0.10 mmol), XPhos (84.2 mg, 0.18 mmol) and sodium *tert*-butoxide (339.2 mg, 3.53 mmol) were dissolved in dry toluene under argon atmosphere (12 mL) in a flame-dried Schlenk tube. The mixture was stirred at 110 °C for 24 h and then cooled down to room temperature. The reaction mixture was poured into water and extracted with CH_2Cl_2. The organic phase was dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by silica gel column chromatography with CH_2Cl_2/petroleum ether (v/v = 20/80) as the eluent. The obtained solid was further purified by trituration in isopropanol, filtered and washed with CH_2Cl_2. The product was obtained as a white solid (456.7 mg, 49%). ^{1}H NMR (400 MHz, $CDCl_3$): 7.52 (dd, *J* = 7.7, 1.6 Hz, 4H), 7.51 (s, 2H), 7.11 (ddd, *J* = 8.3, 7.3, 1.6 Hz, 4H), 7.03 (td, *J* = 7.5, 1.3 Hz, 4H), 6.64 (dd, *J* = 8.2, 1.3 Hz, 4H), 1.74 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): 139.78, 137.41, 132.43, 131.10, 127.70, 126.80, 125.17, 121.58, 114.02, 36.15, 30.51.

10,10'-(2,5-bis(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thieno[3,2-b]thiophene-3,6-diyl)bis(9,9-dimethyl-9,10-dihydroacridine) (DMAC-TT-pinacol)[6]

DMAC-TT (199.0 mg, 0.36 mmol), bis(pinacolato)diboron (276.7 mg, 1.09 mmol), 4,4'-di-*tert*-butyl-2,2'-bipyridine (22.5 mg, 0.08 mmol), and $[Ir(OMe)(COD)]_2$ (28.1 mg, 0.04 mmol) were added to a flame-dried Schlenk under argon atmosphere and subsequently dry cyclohexane (10 mL) was added. The resulting mixture was stirred at 80 °C for 15 h in the dark. After cooling down to room temperature, the reaction mixture was poured in water and the organic material was extracted using CH_2Cl_2. The organic layer was washed with brine and dried over $MgSO_4$. After removing the solvent under reduced pressure, the residue was purified by silica gel column chromatography with CH_2Cl_2 to afford the product as a beige solid (156.4 mg, 54%). ^{1}H NMR (400 MHz, $CDCl_3$): 7.48 (dd, *J* = 7.7, 1.6 Hz, 4H), 7.02 (ddd, *J* = 8.2, 7.2, 1.6 Hz, 4H), 6.94 (td, *J* = 7.4, 1.3 Hz, 4H), 6.39 (dd, *J* = 8.1, 1.3 Hz, 4H), 1.86 (s, br, 6H), 1.66 (s, br, 6H), 0.99 (s, 24H). ^{13}C NMR (100 MHz, $CDCl_3$): 144.08, 139.98, 134.43 (br), 130.37, 126.52, 125.13, 120.67, 113.75, 84.10, 53.48, 36.05, 33.92 (br), 29.29 (br), 24.39.

3,6-bis(9,9-dimethylacridin-10(9H)-yl)thieno[3,2-b]thiophene-2,5-dione (TTD-DMAC)[6]

To a solution of DMAC-TT-pinacol (152.0 mg, 0.19 mmol) in THF (10 mL) and H_2O (1 mL) was added Oxone (372.8 mg, 0.61 mmol) in one portion at room temperature. The mixture was stirred at room temperature for 3 h in the dark, and then quenched with $Na_2S_2O_3$ (aq.). The organic layer was extracted with hexanes, washed with water and dried over $MgSO_4$. After evaporation of the solvent, the residue was purified by silica gel column chromatography with CH_2Cl_2/petroleum ether (v/v= 20/80) to give TTD-DMAC (18.9 mg, 17%) as a dark green/black solid. ^{1}H NMR (400 MHz, $CDCl_3$): 7.52 (dd, *J* = 7.8, 1.5 Hz, 4H), 7.23 (ddd, *J* = 8.1, 7.3, 1.5 Hz, 4H), 7.11 (td, *J* = 7.5, 1.2 Hz, 4H), 6.76 (dd, *J* = 8.1, 1.2 Hz, 4H), 1.69 (s, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): 183.17, 155.48, 137.69, 133.24, 132.17, 127.12, 125.89, 123.08, 114.18, 36.19, 30.63. MS (MALDI-TOF) Calcd. for $C_{36}H_{28}N_2O_2S_2$ [M]+: *m/z* 584.159, found: 584.165.

Synthesis of DTBQx-BDT-TIPS (8)

2,6-bis(triisopropylsilyl)benzo[1,2-b:4,5-b']dithiophene (BDT-TIPS)[7]

To a solution of benzo[1,2-*b*:4,5-*b*']dithiophene (1.26 g, 6.63 mmol) in THF (10.0 mL), *n*-BuLi (2.5 M in hexane; 8.0 mL, 19.89 mmol) was added dropwise at 0 °C and the mixture was stirred for 1 h at room temperature. Afterwards, triisopropylsilyl chloride (4.2 mL, 19.6 mmol) was slowly added. After the mixture was heated to reflux for 16 h, it was poured out in a beaker containing water

(100 mL) and hydrochloric acid (1 M, 100 mL). The resulting precipitate was collected by vacuum filtration and washed with water, methanol and *n*-hexane. The filtrate was then evaporated under reduced pressure and the remaining solid was triturated in *n*-hexane, followed by filtration and subsequent washing with *n*-hexane. BDT-TIPS was obtained as a white solid (2.49 g, 75%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.30 (s, 2H), 7.50 (s, 2H), 1.48-1.37 (m, 6H), 1.16 (d, *J* = 7.4 Hz, 36H). ^{13}C NMR (100 MHz, $CDCl_3$): 140.62, 138.95, 138.31, 131.55, 115.63, 18.66, 11.85.

(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzo[1,2-b:4,5-b'] dithiophene-2,6-diyl)bis(triisopropylsilane) (BDT-TIPS-pinacol)[7]
A mixture of BDT-TIPS (1.635 g 3.25 mmol), bis(pinacolato)diboron (1.48 g, 5.81 mmol), $[Ir(OMe)(COD)]_2$ (107.2 mg, 0.16 mmol), and 4,4'-di-*tert*-butyl-2,2'-bipyridine (94.8 mg, 0.35 mmol) in dry cyclohexane was stirred in the dark at 80 °C for 16 h under nitrogen atmosphere. After cooling down to room temperature, evaporation of the solvent under reduced pressure gave a residue, which was purified by silica gel column chromatography with CH_2Cl_2/petroleum ether (v/v= 20/80) to yield BDT-TIPS-pinacol as a white solid (555.3 mg, 27%). The reaction also yields unreacted BDT-TIPS as well as disubstituted BDT-TIPS-pinacol as the main side products. ^{1}H NMR (400 MHz, $CDCl_3$): 8.39 (s, 1H), 8.35 (s, 1H), 7.52 (s, 1H), 1.47 (s, 12H), 1.50-1.39 (m, 6H), 1.19 (d, *J* = 7.4 Hz, 36H). ^{13}C NMR (100 MHz, $CDCl_3$): 148.3, 144.0, 140.0, 138.7, 138.0, 137.7, 134.1, 130.8, 118.1, 116.0, 83.7, 24.8, 18.4, 11.6.

1,2-di(thiophen-3-yl)ethane-1,2-dione
3-Bromothiophene (2.34 mL, 24.69 mmol) was added dropwise to a solution of *n*-BuLi (2.5 M in *n*-hexane; 11.0 mL, 27.50 mmol) in THF (50 mL) and the resulting mixture was stirred at −78 °C for 1 h. The reaction mixture was subsequently added to a homogeneously stirred suspension of CuBr (3.59 g, 25.03 mmol) and LiBr (4.34 g, 49.98 mmol) in THF (50 mL) at 0 °C and the mixture was stirred for 1 h at this temperature. After dropwise addition of oxalyl chloride (1.1 mL, 12.57 mmol), the reaction mixture was again stirred for 1 h at 0 °C. The reaction was quenched with a saturated aqueous NH_4Cl solution (40 mL). After partial removal of the reaction solvent under reduced pressure, the product was extracted with hexanes and the organic phase was washed with a saturated aqueous NH_4Cl solution, water and brine. The organic phase was dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography with CH_2Cl_2/petroleum ether (v/v= 50/50) to give a yellow crystalline product (2.11 g, 76%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.36 (dd, *J* = 2.9, 1.2 Hz, 2H), 7.70 (dd, *J* = 5.1, 1.2 Hz, 2H), 7.40 (dd, *J* = 5.1, 2.9 Hz, 2H).

benzo[2,1-b:3,4-b']dithiophene-4,5-dione
To a stirring solution of 1,2-di(thiophen-3-yl)ethane-1,2-dione (1.00 g, 4.50 mmol) in CH_2Cl_2 (200 mL), a solution of $FeCl_3$ (2.92 g, 18.00 mmol) in nitromethane (25 mL) was added dropwise. The reaction mixture was stirred for at room temperature for 3 h after which the reaction was quenched with a 1 M aqueous HCl solution (50 mL). The product was extracted with chloroform and washed with a 1 M aqueous HCl solution, water and brine. The organic phase dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The residue was purified by silica gel column chromatography using chloroform as the eluent and after evaporation of the solvent under reduced pressure, a black crystalline product was obtained (0.60 g, 61%). ^{1}H NMR (400 MHz, $CDCl_3$): 7.50 (d, *J* = 5.2 Hz, 2H), 7.21 (d, *J* = 5.2 Hz, 2H).

3,6-dibromo-4,5-difluorobenzene-1,2-diamine
1,4-Dibromo-2,3-difluoro-5,6-dinitrobenzene[8] (1.00 g, 2.76 mmol) and iron powder (2.25 g, 40.29 mmol) were stirred in acetic acid (40 mL) at 45 °C for 6 h. The solution was cooled down to room temperature and then poured into a cold NaOH solution (5%, 100 mL). The product was extracted with ethyl acetate and washed with a saturated aqueous $NaHCO_3$ solution. The organic phase was collected, dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure to obtain the product in a quantitative yield (0.82 g). ^{1}H NMR (400 MHz, $CDCl_3$): 5.16 (s, 4H).

8,11-dibromo-9,10-difluorodithieno[3,2-a:2',3'-c]phenazine (DTPz)
Benzo[2,1-*b*:3,4-*b'*]dithiophene-4,5-dione (0.50 g, 2.27 mmol) and 3,6-dibromo-4,5-difluorobenzene-1,2-diamine (0.69 g, 2.27 mmol) were dissolved in acetic acid (20 mL) and the resulting solution was stirred at 75 °C for 16 h. The reaction was quenched with a saturated aqueous $NaHCO_3$ solution. The product was extracted with chloroform and washed with a saturated aqueous $NaHCO_3$ solution, water and brine. The organic phase dried over $MgSO_4$, filtered and the solvent was removed under reduced pressure. The product was purified by recrystallization from CH_2Cl_2/MeOH to acquire a yellow crystalline product (0.94 g, 85%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.53 (d, *J* = 5.3 Hz, 2H), 7.65 (d, *J* = 5.3 Hz, 2H).

8,11-bis(2,6-bis(triisopropylsilyl)benzo[1,2-b:4,5-b']dithiophen-4-yl)-9,10-difluorodithieno[3,2-a:2',3'-c]phenazine (DTPz-BDT-TIPS)
DTPz (90.2 mg, 186.5 µmol), BDT-TIPS-pinacol (245.0 mg, 389.6 µmol) and tetrakis(triphenylphosphine)palladium(0) (10.7 mg, 9.3 µmol) were added to a flame-dried Schlenk flask. The flask was evacuated and backfilled with nitrogen three times and pre-degassed anhydrous DMF (16 mL) and a K_2CO_3 solution (2 M, 4 mL) were added. The reaction mixture was heated at 130 °C and stirred for 24 h under a nitrogen atmosphere. The reaction mixture was poured into water, then extracted with dichloromethane and dried over $MgSO_4$, filtered and washed. After evaporation of the solvent under reduced pressure, the product was purified by silica gel column chromatography with CH_2Cl_2/petroleum ether (v/v= 20/80) as the eluent. DTPz-BDT-TIPS was further purified using preparative (recycling) GPC and was obtained as a yellow solid (60.0 mg, 24%). ^{1}H NMR (400 MHz, $CDCl_3$): 8.57 (d, *J* = 2.0 Hz, 2H), 7.70 (d, *J* = 1.9 Hz, 2H), 7.47 (dd, *J* = 5.3, 1.7 Hz, 2H), 7.23 (s, 1H), 7.16 (dd, *J* = 5.3, 2.1 Hz, 2H), 7.12 (s, 1H), 1.45-1.18 (m, 12H), 1.17-0.90 (m, 72H). ^{13}C NMR (100 MHz, $CDCl_3$): 151.72, 151.55, 149.16, 148.97, 142.74, 142.64, 140.86, 140.80, 139.19, 139.16, 138.94, 138.54, 138.48, 138.24, 138.18, 137.07, 137.03, 136.06, 134.61, 131.90, 131.76, 131.62, 131.54, 124.41, 124.34, 124.33, 124.27, 119.24, 119.18, 116.53, 77.38, 18.69, 18.66, 18.60, 18.55, 18.50, 18.46, 18.38, 11.85, 11.82, 11.76, 11.71. MS (ESI+) Calcd. for $C_{72}H_{94}F_2N_2S_6Si_4$ [M]+: *m/z* 1328.479, found: 1328.475.

UV-VIS absorption and emission (fluorescence) spectra

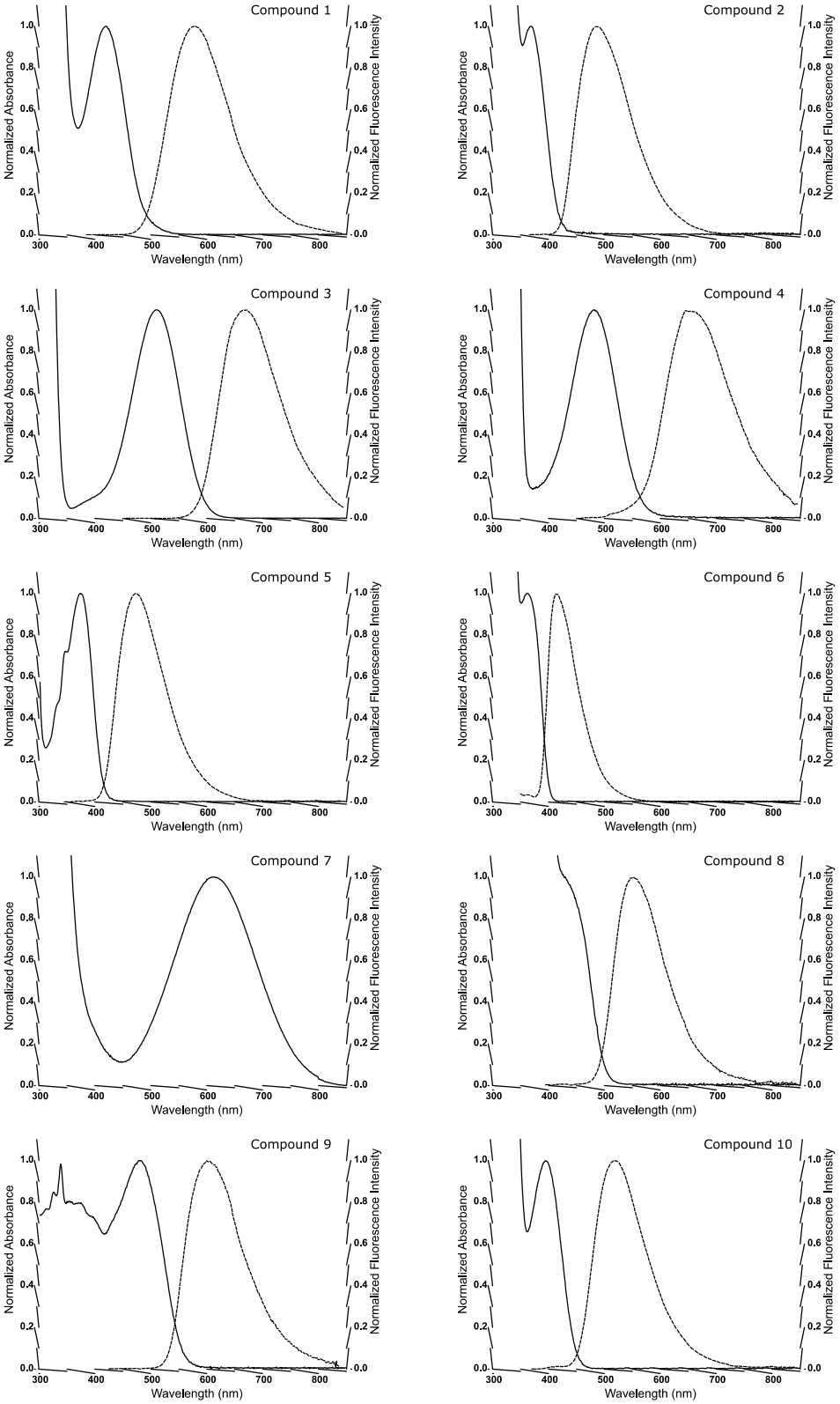


Figure S4. Normalized absorption spectra (solid lines) of all compounds and their corresponding normalized fluorescence spectra (dashed lines) in toluene. Spectra are normalized to their charge transfer bands.

Table S23. Spectroscopic data for all compounds in toluene.[a]

Compound	λ_{abs} (nm)[b]	λ_{em} (nm)[c]	$\Delta\bar{\nu}$ (cm^{-1})[d]
1	421	578	6452
2	368	486	6598
3	510	668	4638
4	481	645	5286
5	375	473	5525
6	362	414	3470
7	613	-[e]	-[e]
8	430	553	5173
9	480	602	4222
10	395	519	6049

[a] Only data on the charge transfer bands are given.
[b] Charge transfer absorption maximum.
[c] Charge transfer fluorescence emission maximum.
[d] Stokes shift.
[e] No fluorescence observed.

NMR spectra

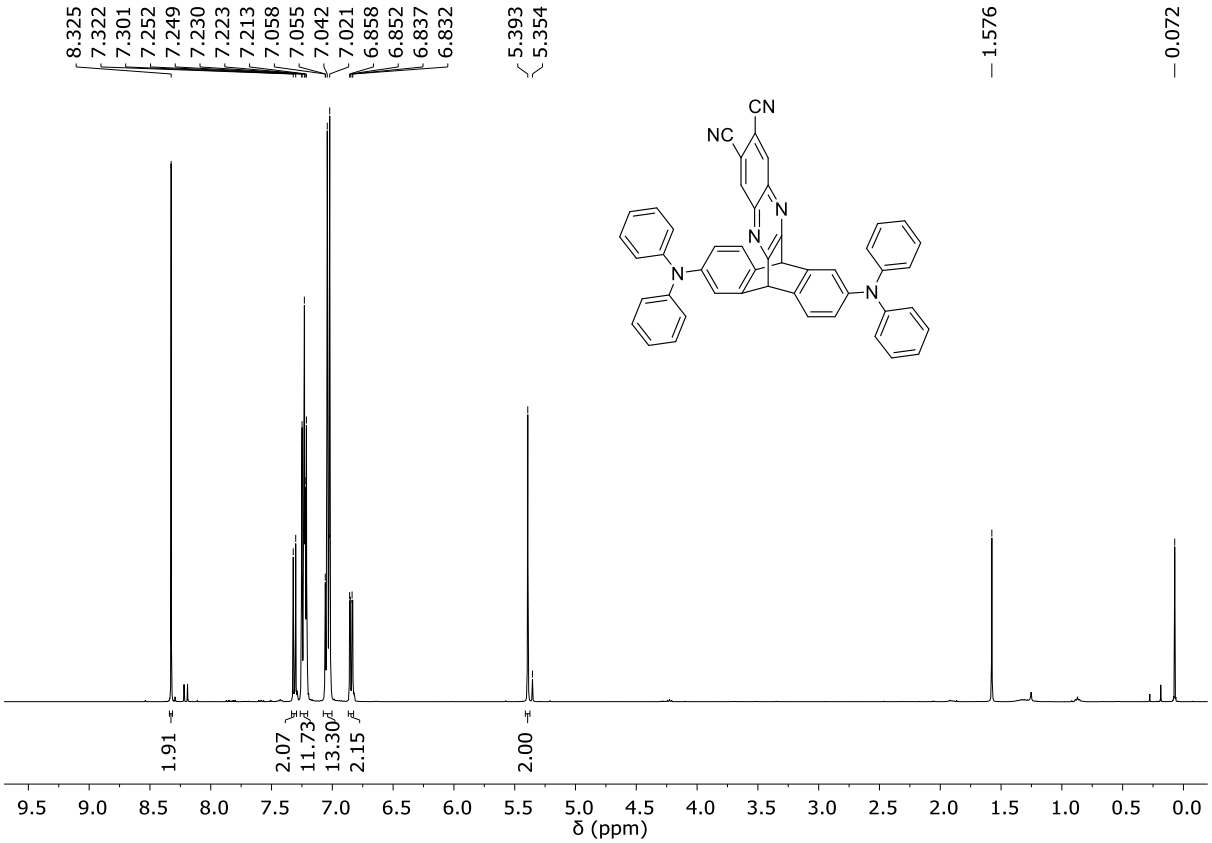


Figure S5. ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

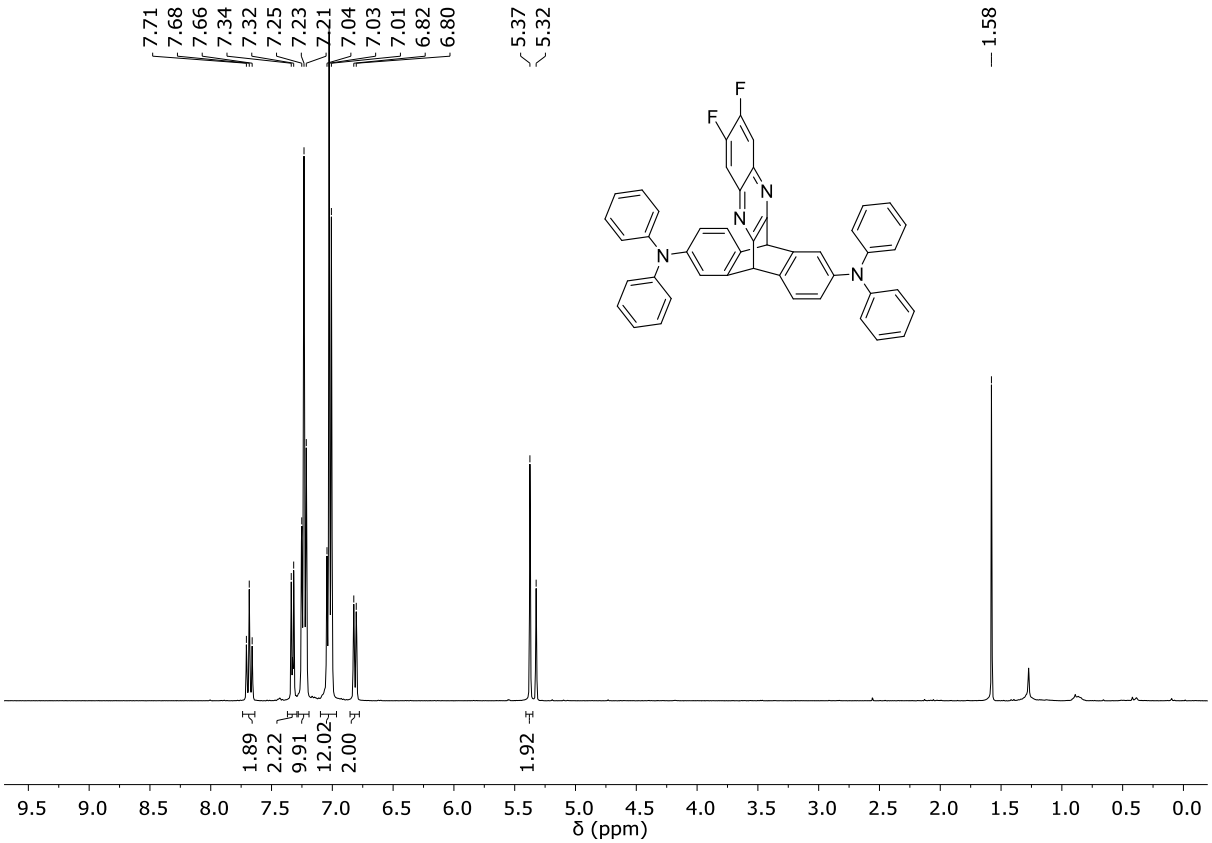


Figure S6. ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

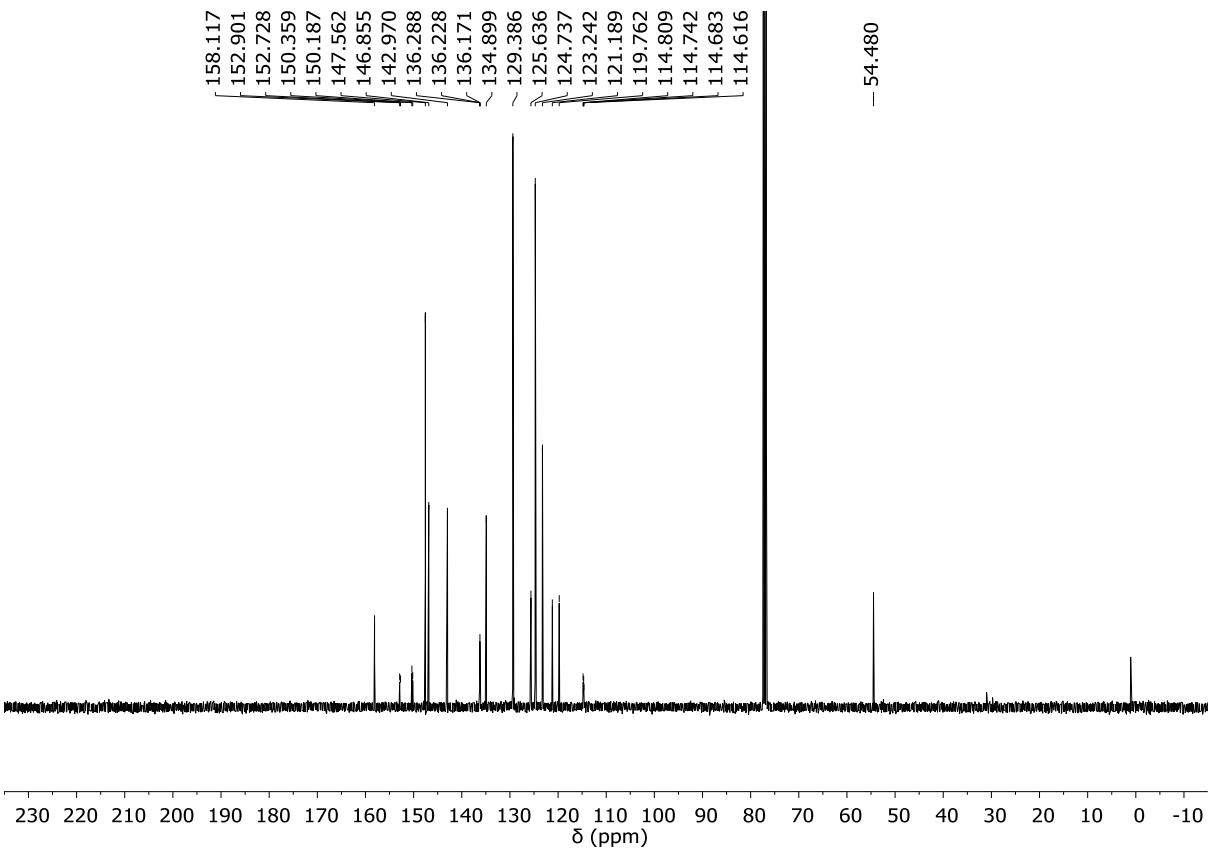


Figure S7. ^{13}C NMR spectrum of compound **2** in $CDCl_{3z}$.

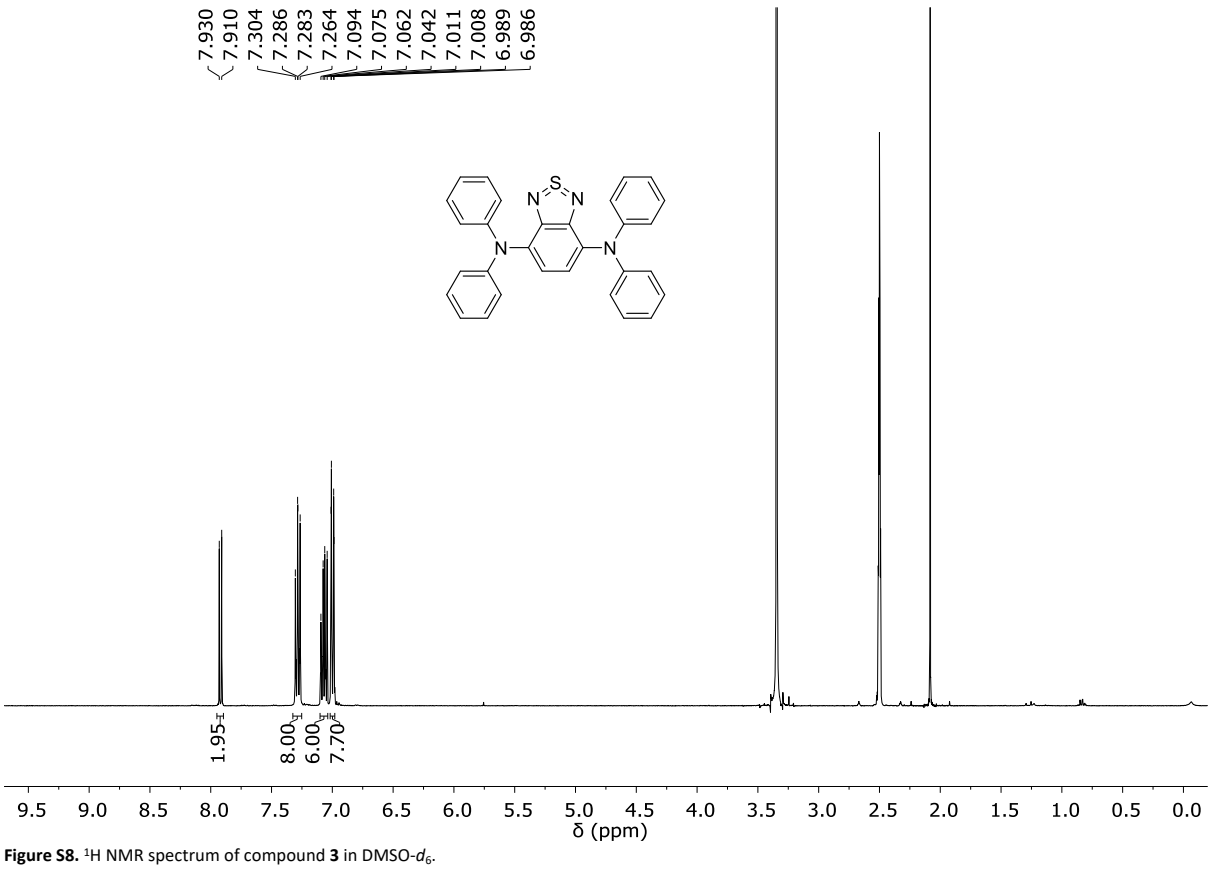


Figure S8. ^{1}H NMR spectrum of compound **3** in DMSO-d_6.

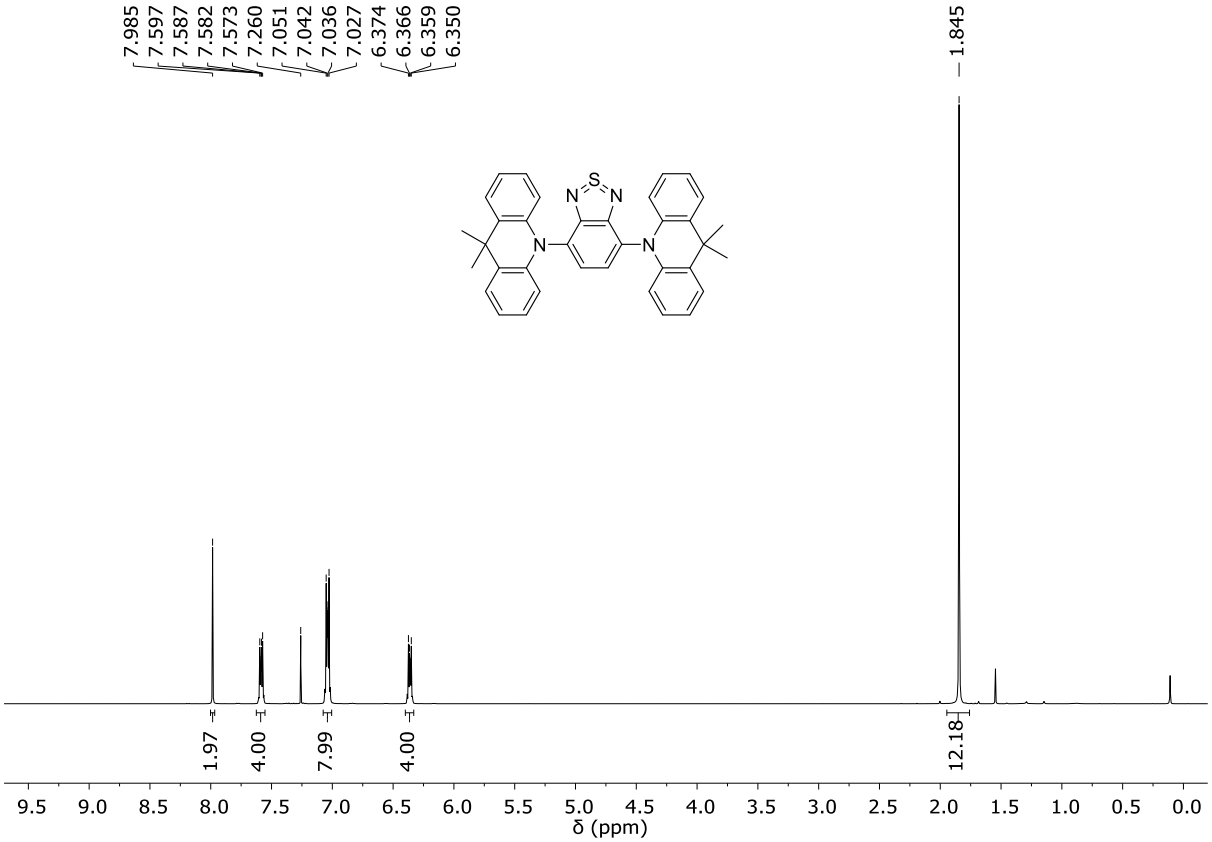


Figure S9. ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

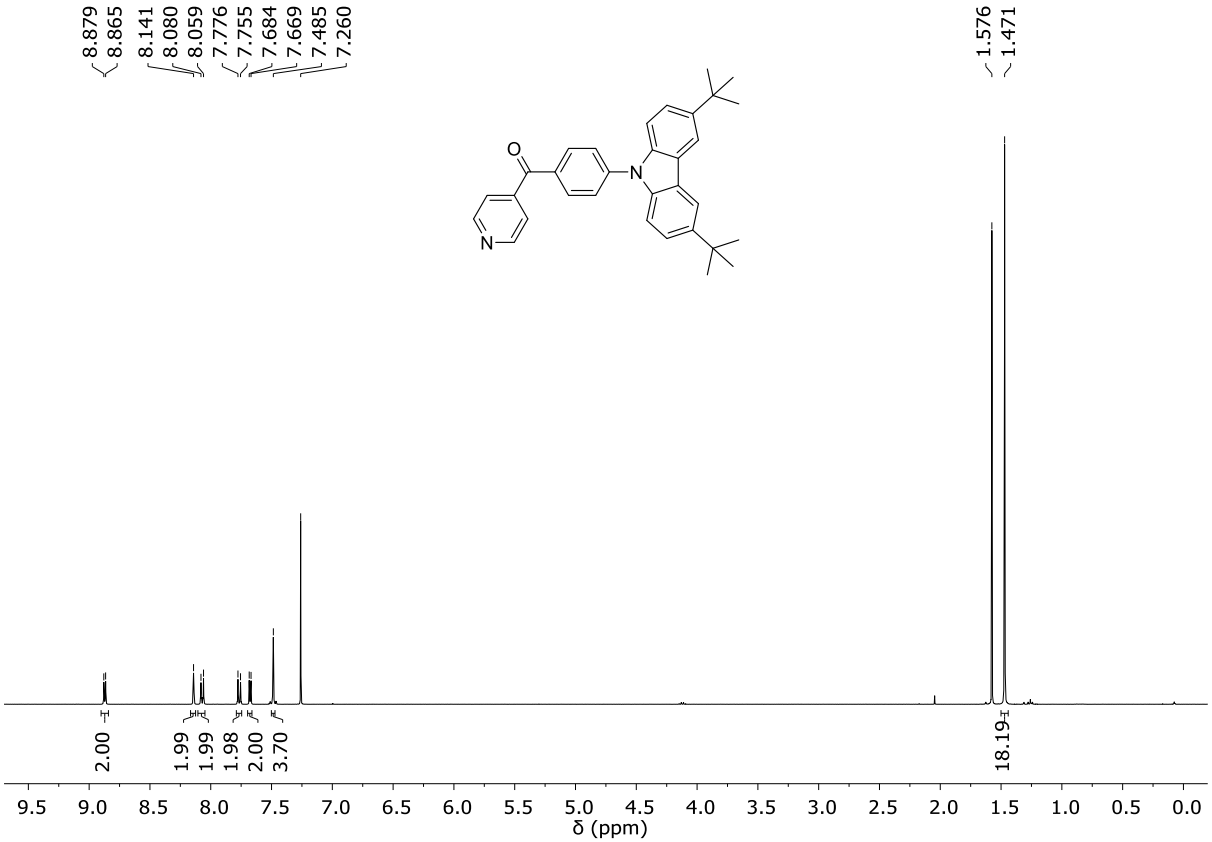


Figure S10. ^{1}H NMR spectrum of compound **5** in $CDCl_3$.

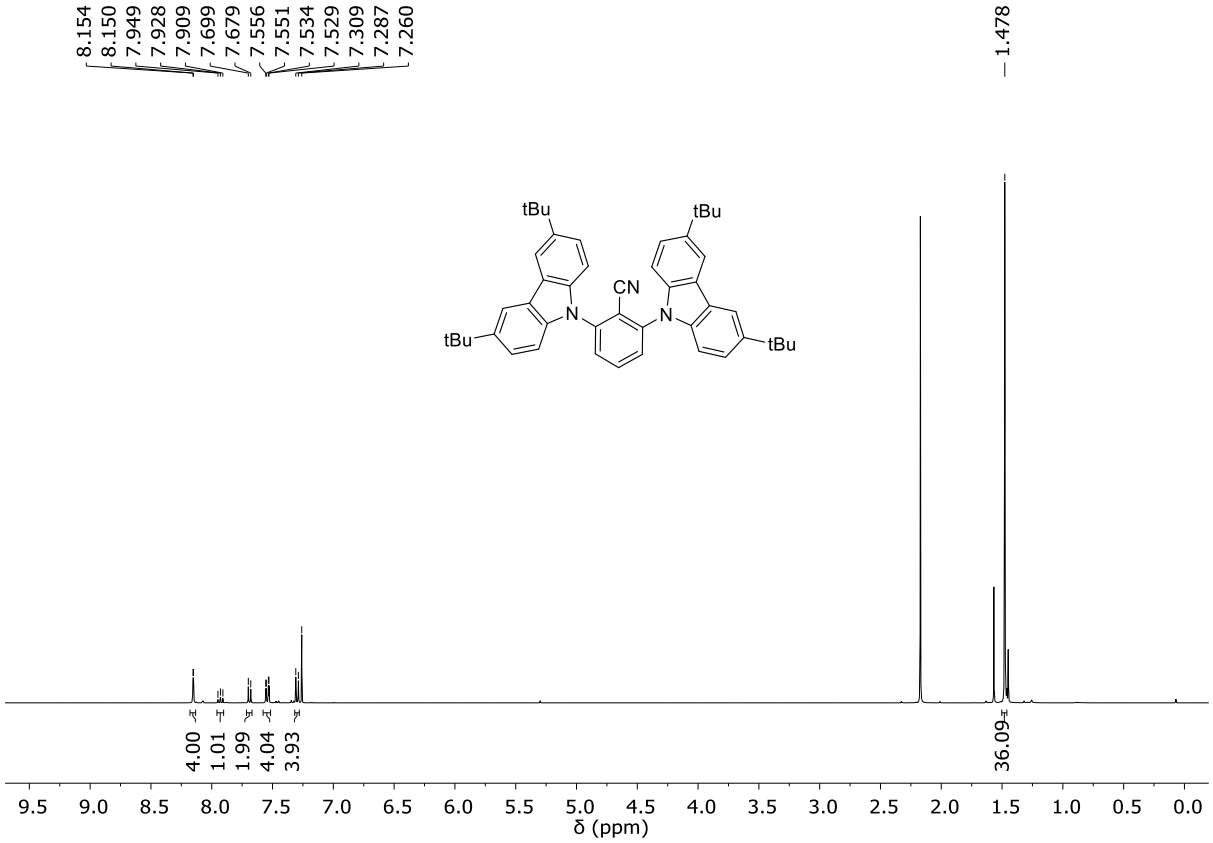


Figure S11. ^{1}H NMR spectrum of compound **6** in $CDCl_3$.

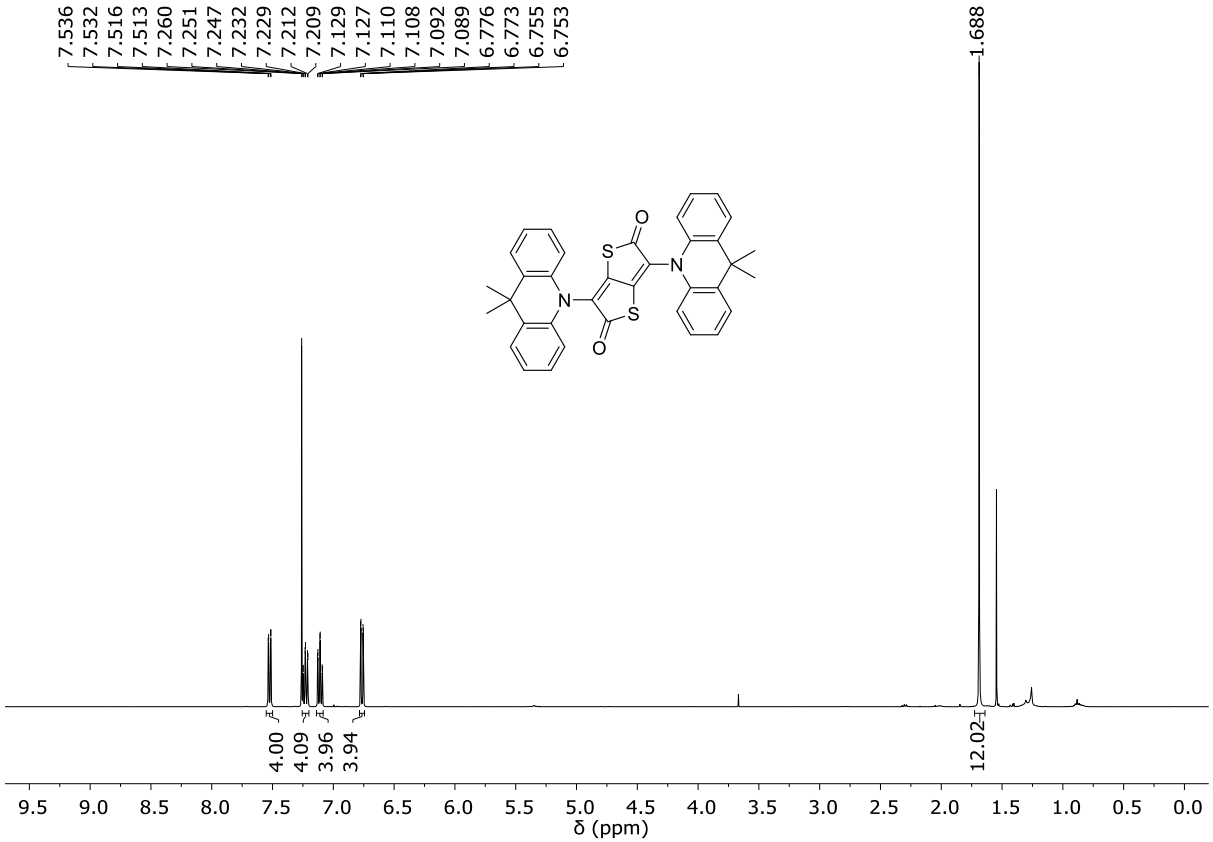


Figure S12. ^{1}H NMR spectrum of compound **7** in $CDCl_3$.

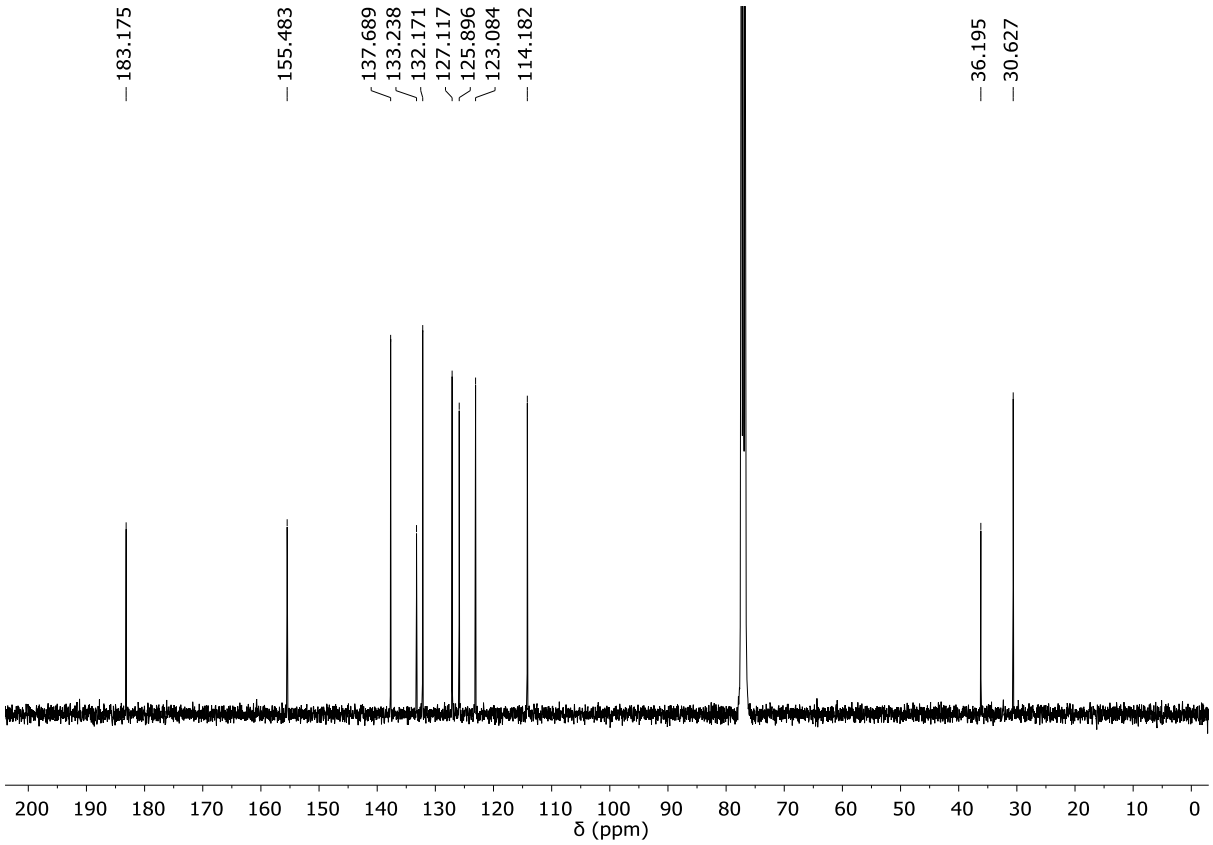


Figure S13. ^{13}C NMR spectrum of compound **7** in $CDCl_3$.

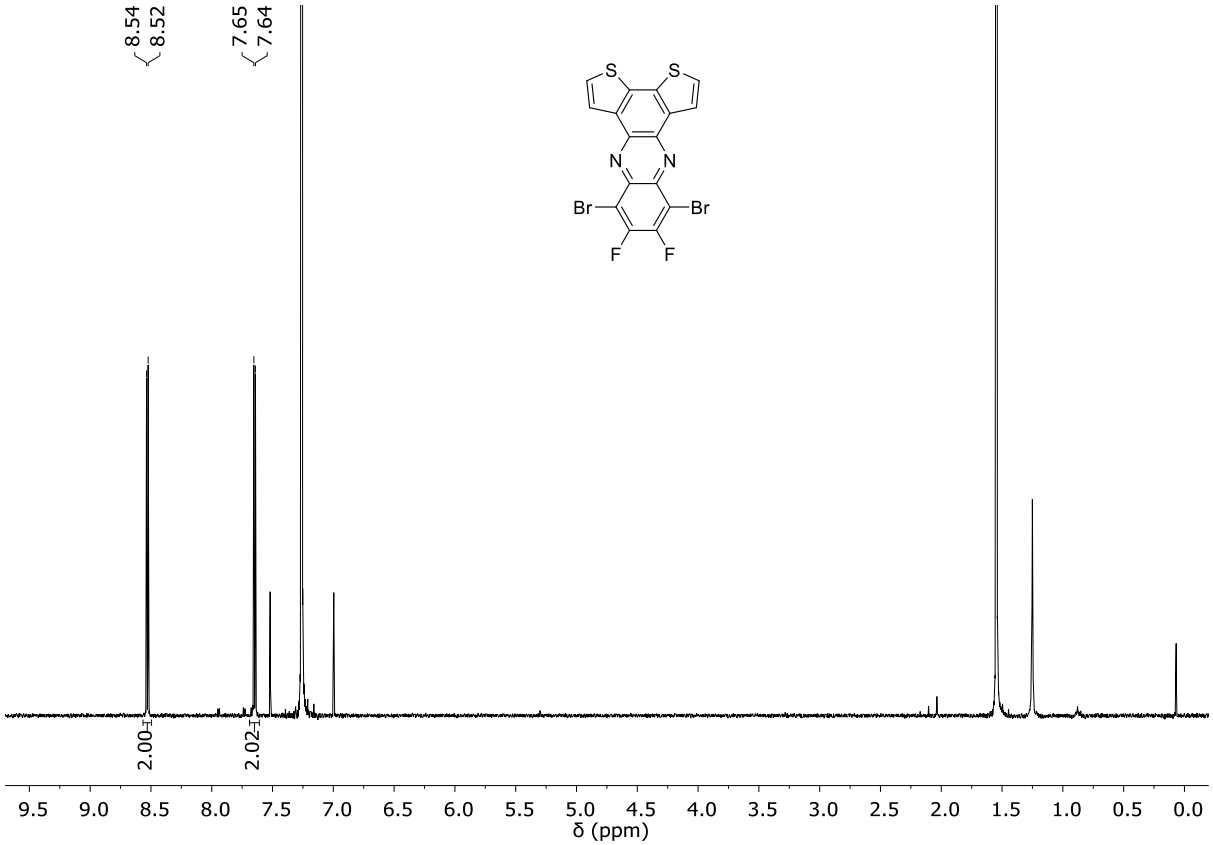


Figure S14. ^{1}H NMR spectrum of 8,11-dibromo-9,10-difluorodithieno[3,2-*a*:2',3'-*c*]phenazine (DTPz) in $CDCl_3$.

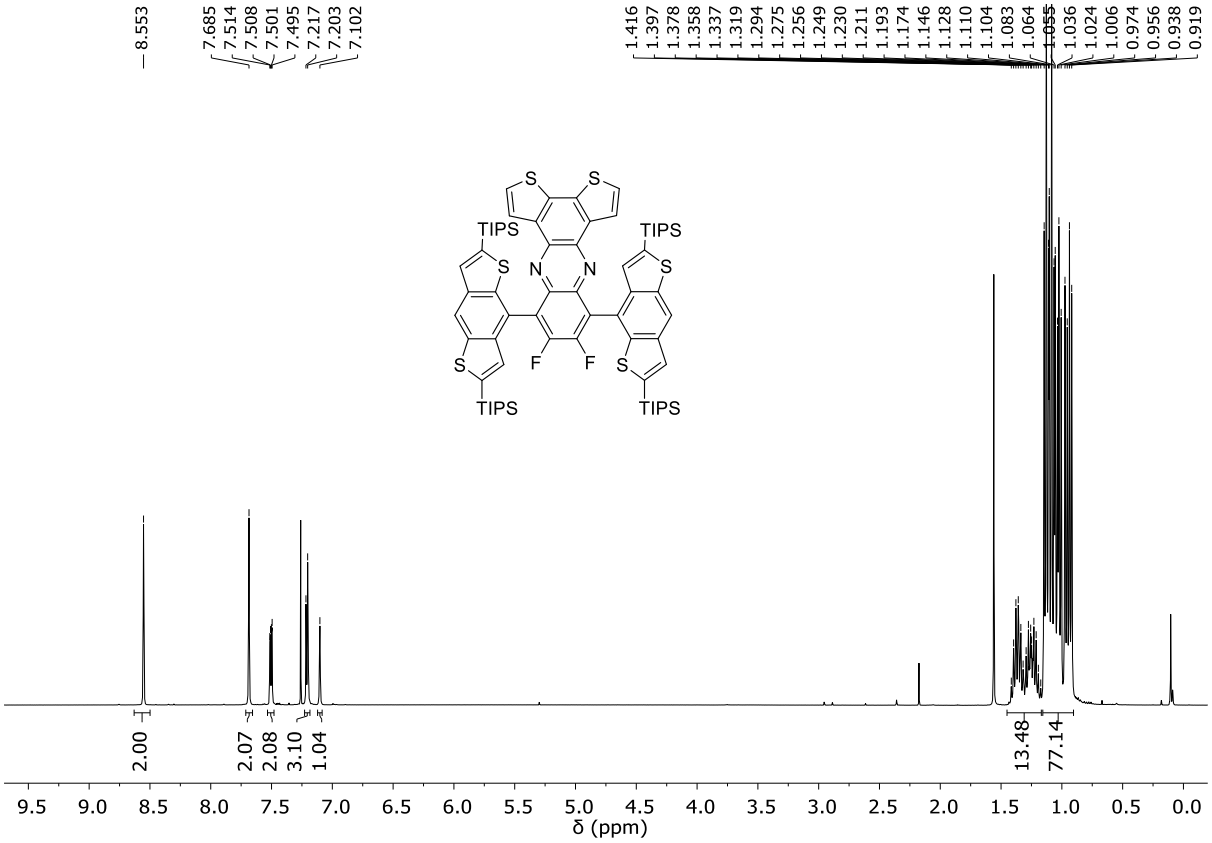


Figure S15. ^{1}H NMR spectrum of compound **8** in $CDCl_3$.

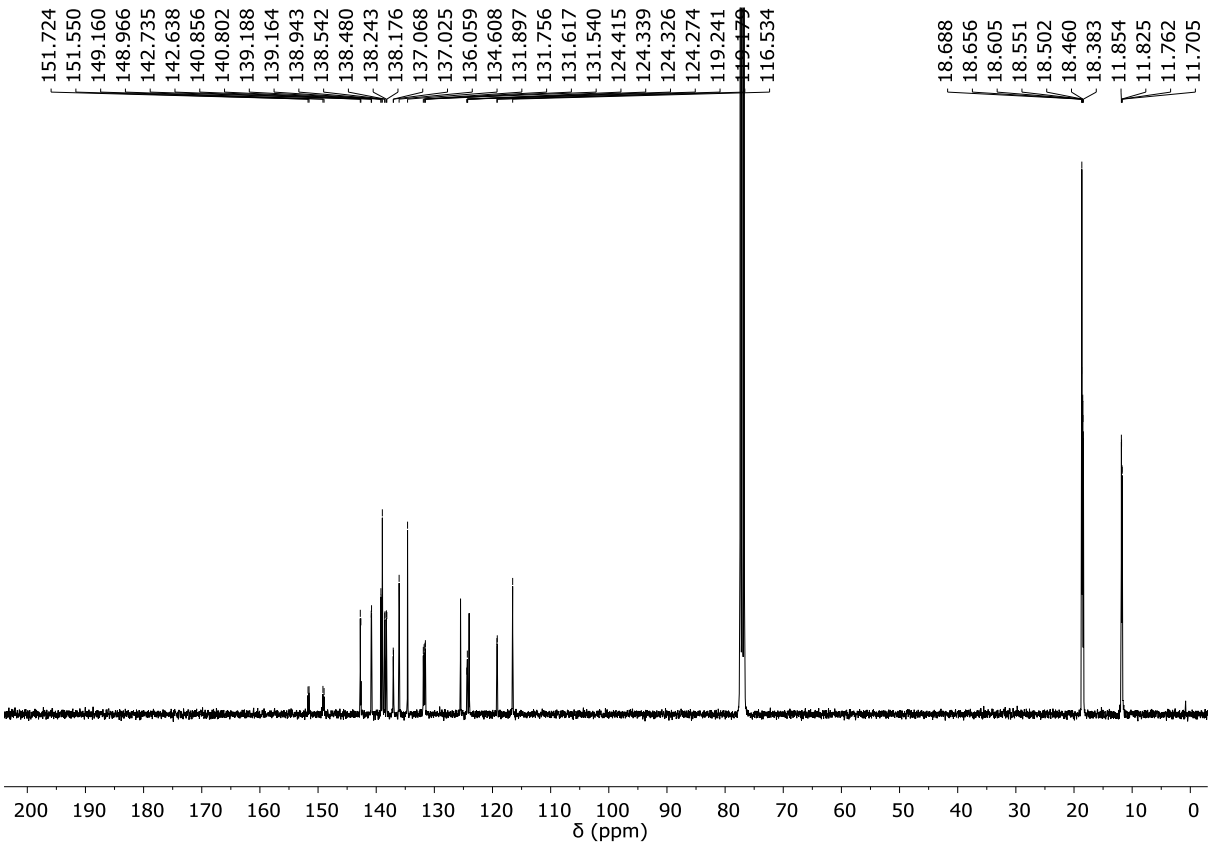


Figure S16. ^{13}C NMR spectrum of compound **8** in $CDCl_3$.

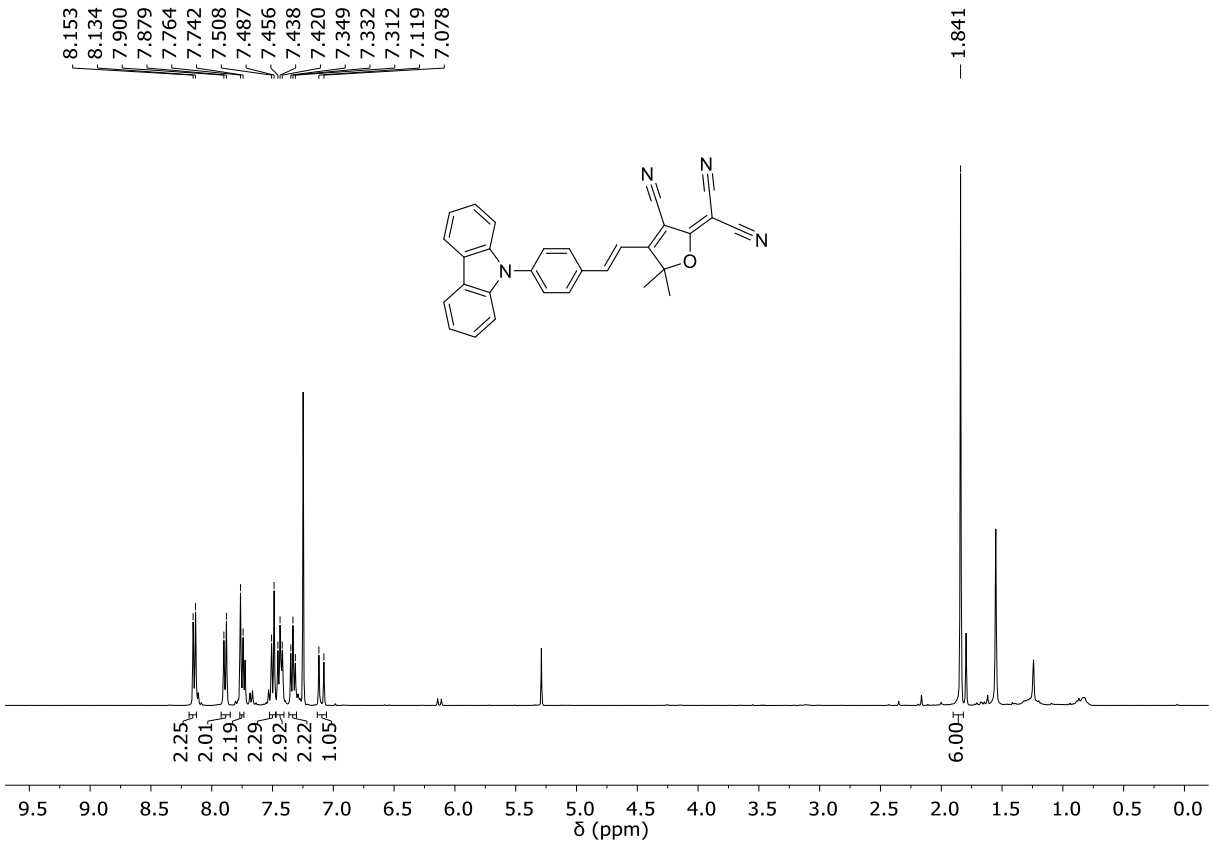


Figure S17. ^{1}H NMR spectrum of compound **9** in $CDCl_3$.

Coordinates of optimized geometries

Compound **1**:

C	-0.49299	0.54175	1.20389
C	-0.27555	1.93432	0.66634
C	-1.39464	-0.13318	0.18650
C	-0.86233	-0.13217	-1.10567
C	0.49299	0.54175	-1.20389
C	0.86233	-0.13217	1.10567
C	1.39464	-0.13318	-0.18650
C	0.27555	1.93432	-0.66634
C	2.61935	-0.70832	-0.45063
C	3.34802	-1.29575	0.59216
C	2.81679	-1.28150	1.88410
C	1.57927	-0.70714	2.13843
C	-2.61935	-0.70832	0.45063
C	-3.34802	-1.29575	-0.59216
C	-2.81679	-1.28150	-1.88410
C	-1.57927	-0.70714	-2.13843
N	0.54616	3.01952	-1.31894
C	0.27070	4.18433	-0.65388
C	-0.27070	4.18433	0.65388
N	-0.54616	3.01952	1.31894
C	0.53490	5.40617	-1.29109
C	0.27246	6.60045	-0.65724
C	-0.27247	6.60045	0.65724
C	-0.53490	5.40617	1.29109
C	-0.55007	7.82927	1.32612
N	-0.78038	8.81420	1.88015
C	0.55007	7.82927	-1.32612
N	0.78038	8.81420	-1.88015
N	-4.59677	-1.88989	-0.33837
N	4.59677	-1.88989	0.33837
C	5.47313	-1.32916	-0.62242
C	4.98965	-3.05894	1.03366
C	-5.47313	-1.32916	0.62242
C	-4.98965	-3.05894	-1.03366
C	-6.12687	-2.15052	1.53993
C	-6.99270	-1.60259	2.47263
C	-7.20642	-0.23155	2.51462
C	-6.55242	0.58860	1.60517
C	-5.69862	0.04642	0.65810
C	-6.28475	-3.17365	-1.53707
C	-6.67429	-4.32392	-2.20423
C	-5.77762	-5.36674	-2.39241
C	-4.48595	-5.25231	-1.89628
C	-4.09383	-4.11245	-1.21321
C	6.12687	-2.15052	-1.53993
C	6.99270	-1.60259	-2.47263
C	7.20642	-0.23155	-2.51462
C	6.55242	0.58860	-1.60517
C	5.69862	0.04642	-0.65809
C	6.28475	-3.17365	1.53707
C	6.67429	-4.32392	2.20423
C	5.77762	-5.36674	2.39241
C	4.48595	-5.25231	1.89628
C	4.09383	-4.11245	1.21321
H	-0.90602	0.56452	2.21684
H	0.90602	0.56452	-2.21684
H	3.02037	-0.71370	-1.46258
H	3.38756	-1.72566	2.69596
H	1.18252	-0.70093	3.15236
H	-3.02037	-0.71370	1.46258
H	-3.38756	-1.72566	-2.69596
H	-1.18251	-0.70093	-3.15236
H	0.95048	5.38455	-2.29496
H	-0.95048	5.38455	2.29496
H	-5.95017	-3.22377	1.51296
H	-7.49633	-2.25474	3.18270
H	-7.88120	0.19612	3.25192
H	-6.71915	1.66329	1.62209
H	-5.19856	0.68760	-0.06480
H	-6.98389	-2.35161	-1.39862
H	-7.68766	-4.39958	-2.59213
H	-6.08431	-6.26525	-2.92203
H	-3.77690	-6.06649	-2.02902
H	-3.08606	-4.02962	-0.81170
H	5.95017	-3.22377	-1.51296
H	7.49633	-2.25474	-3.18270
H	7.88120	0.19612	-3.25191

H	6.71915	1.66329	-1.62209
H	5.19856	0.68760	0.06480
H	6.98389	-2.35161	1.39862
H	7.68766	-4.39958	2.59213
H	6.08431	-6.26525	2.92203
H	3.77690	-6.06649	2.02902
H	3.08606	-4.02962	0.81170

Compound **2**:

C	1.39153	0.08556	-0.19235
C	0.48796	0.76594	-1.20430
C	-0.86328	0.08428	-1.10217
C	0.86327	0.08428	1.10217
C	-1.39153	0.08556	0.19235
C	-0.48796	0.76594	1.20430
C	0.27115	2.16048	-0.66381
C	-0.27115	2.16048	0.66381
C	1.57776	-0.49992	2.13065
C	2.81384	-1.07826	1.87206
C	3.34025	-1.08762	0.58018
C	2.61258	-0.49563	-0.45979
C	-1.57776	-0.49992	-2.13065
C	-2.81384	-1.07826	-1.87206
C	-3.34025	-1.08762	-0.58018
C	-2.61258	-0.49563	0.45979
N	0.53939	3.24656	-1.31855
N	-0.53939	3.24656	1.31855
C	0.26849	4.41178	-0.65629
C	-0.26849	4.41178	0.65629
C	0.53078	5.63634	-1.29736
C	-0.53078	5.63634	1.29736
C	-0.26629	6.80751	0.65097
C	0.26629	6.80751	-0.65098
F	0.50302	7.97865	-1.23025
F	-0.50302	7.97865	1.23025
N	4.59100	-1.68347	0.31918
C	5.49301	-1.06850	-0.58030
C	6.19338	-1.83491	-1.51172
C	7.08160	-1.23012	-2.38626
C	7.27251	0.14476	-2.35829
C	6.57071	0.91051	-1.43719
C	5.69396	0.31133	-0.54740
C	4.95368	-2.88966	0.96136
C	6.24422	-3.06237	1.46167
C	6.60044	-4.25007	2.07973
C	5.67546	-5.27511	2.22402
C	4.38810	-5.10272	1.73358
C	4.02865	-3.92493	1.09902
N	-4.59100	-1.68347	-0.31918
C	-5.49301	-1.06850	0.58030
C	-6.19338	-1.83491	1.51172
C	-7.08160	-1.23012	2.38626
C	-7.27251	0.14476	2.35829
C	-6.57071	0.91051	1.43719
C	-5.69396	0.31133	0.54740
C	-4.95368	-2.88966	-0.96136
C	-6.24422	-3.06237	-1.46167
C	-6.60044	-4.25007	-2.07973
C	-5.67546	-5.27511	-2.22402
C	-4.38810	-5.10272	-1.73358
C	-4.02865	-3.92493	-1.09902
H	0.89790	0.78912	-2.21868
H	-0.89790	0.78912	2.21868
H	1.18148	-0.49669	3.14486
H	3.38530	-1.52953	2.67980
H	3.01414	-0.49969	-1.47182
H	-1.18148	-0.49669	-3.14486
H	-3.38530	-1.52953	-2.67980
H	-3.01414	-0.49969	1.47182
H	0.94162	5.63691	-2.30276
H	-0.94162	5.63692	2.30276
H	6.03430	-2.91074	-1.54271
H	7.62060	-1.84073	-3.10736
H	7.96485	0.61709	-3.05077
H	6.71616	1.98786	-1.40001
H	5.15426	0.91074	0.18276
H	6.96663	-2.25525	1.36052
H	7.61075	-4.36928	2.46498
H	5.95631	-6.20334	2.71541
H	3.65558	-5.90086	1.83276
H	3.02346	-3.79700	0.70304

H	-6.03430	-2.91074	1.54271
H	-7.62060	-1.84073	3.10736
H	-7.96485	0.61709	3.05077
H	-6.71616	1.98786	1.40001
H	-5.15426	0.91074	-0.18276
H	-6.96663	-2.25525	-1.36052
H	-7.61075	-4.36928	-2.46498
H	-5.95631	-6.20334	-2.71541
H	-3.65558	-5.90086	-1.83275
H	-3.02346	-3.79700	-0.70304

Compound **3**:

C	-1.45073	-0.24520	0.05712
C	-0.70724	-1.39693	0.01635
C	0.70724	-1.39693	-0.01636
C	1.45073	-0.24519	-0.05713
C	0.72061	0.98567	-0.04173
C	-0.72062	0.98567	0.04172
N	1.24465	2.20604	-0.08403
S	-0.00001	3.24974	-0.00000
N	-1.24466	2.20603	0.08403
N	-2.85048	-0.23919	0.13601
N	2.85048	-0.23918	-0.13601
C	-3.59569	0.55696	-0.76921
C	-3.51291	-1.20649	0.92766
C	3.59569	0.55697	0.76920
C	3.51291	-1.20648	-0.92766
C	-4.61103	-1.90665	0.42994
C	-5.25937	-2.84206	1.22181
C	-4.81549	-3.10571	2.50937
C	-3.71617	-2.41502	3.00389
C	-3.07271	-1.46812	2.22583
C	-4.74486	1.21419	-0.33458
C	-5.47484	1.99233	-1.21557
C	-5.06276	2.13886	-2.53466
C	-3.91602	1.48908	-2.96616
C	-3.19006	0.69266	-2.09348
C	4.61103	-1.90664	-0.42994
C	5.25938	-2.84205	-1.22180
C	4.81551	-3.10571	-2.50935
C	3.71619	-2.41503	-3.00388
C	3.07272	-1.46812	-2.22583
C	4.74485	1.21420	0.33459
C	5.47483	1.99234	1.21558
C	5.06275	2.13887	2.53467
C	3.91601	1.48909	2.96617
C	3.19006	0.69267	2.09348
H	-1.22606	-2.35314	0.03364
H	1.22607	-2.35314	-0.03365
H	-4.95513	-1.71026	-0.58297
H	-6.11529	-3.37956	0.81943
H	-5.32340	-3.84324	3.12581
H	-3.36302	-2.60499	4.01514
H	-2.22212	-0.91530	2.61890
H	-5.05157	1.11503	0.70438
H	-6.36808	2.50413	-0.86407
H	-5.63347	2.75889	-3.22173
H	-3.58656	1.59140	-3.99790
H	-2.29874	0.16936	-2.43508
H	4.95513	-1.71024	0.58297
H	6.11530	-3.37955	-0.81942
H	5.32343	-3.84323	-3.12579
H	3.36304	-2.60500	-4.01514
H	2.22213	-0.91531	-2.61891
H	5.05157	1.11504	-0.70438
H	6.36807	2.50414	0.86408
H	5.63346	2.75890	3.22173
H	3.58654	1.59140	3.99790
H	2.29873	0.16936	2.43507

Compound **4**:

C	-1.43304	-0.00000	-0.56141
C	-0.71173	0.00000	-1.71751
C	0.71170	0.00000	-1.71752
C	1.43304	0.00000	-0.56145
C	0.71853	0.00000	0.67158
C	-0.71850	-0.00000	0.67160
N	1.25089	0.00000	1.89022
S	0.00004	0.00000	2.92995
N	-1.25084	0.00000	1.89025

C	-3.43872	3.64341	-0.40146
C	-4.80524	3.69387	-0.17643
C	-5.50731	2.50664	-0.06756
C	-4.89669	1.25885	-0.17585
C	-3.51775	1.22412	-0.41135
C	-2.80269	2.42319	-0.51883
C	-5.73757	0.00000	-0.01924
C	-4.89669	-1.25885	-0.17585
C	-3.51775	-1.22412	-0.41135
N	-2.84823	-0.00000	-0.55506
C	-5.50731	-2.50664	-0.06756
C	-4.80524	-3.69387	-0.17643
C	-3.43872	-3.64341	-0.40146
C	-2.80269	-2.42319	-0.51883
C	-6.84476	0.00000	-1.08201
C	-6.36352	0.00000	1.38302
C	3.43872	-3.64341	-0.40154
C	4.80523	-3.69387	-0.17647
C	5.50730	-2.50664	-0.06756
C	4.89668	-1.25885	-0.17587
C	3.51775	-1.22412	-0.41140
C	2.80269	-2.42319	-0.51891
C	5.73755	0.00000	-0.01920
C	4.89668	1.25885	-0.17587
C	3.51775	1.22412	-0.41140
N	2.84823	-0.00000	-0.55512
C	5.50730	2.50664	-0.06756
C	4.80523	3.69387	-0.17647
C	3.43872	3.64341	-0.40154
C	2.80269	2.42319	-0.51891
C	6.84481	0.00000	-1.08190
C	6.36341	0.00000	1.38309
H	-1.25154	0.00000	-2.66203
H	1.25149	0.00000	-2.66206
H	-2.85792	4.55892	-0.48811
H	-5.32025	4.64655	-0.08372
H	-6.57914	2.55236	0.11597
H	-1.73154	2.39900	-0.70055
H	-6.57914	-2.55236	0.11597
H	-5.32025	-4.64655	-0.08372
H	-2.85792	-4.55892	-0.48812
H	-1.73154	-2.39900	-0.70055
H	-6.41516	0.00000	-2.09011
H	-7.48831	-0.88170	-0.99148
H	-7.48831	0.88170	-0.99148
H	-6.99259	0.88286	1.54141
H	-6.99259	-0.88286	1.54141
H	-5.58255	0.00000	2.15172
H	2.85793	-4.55892	-0.48822
H	5.32024	-4.64655	-0.08374
H	6.57912	-2.55236	0.11600
H	1.73155	-2.39900	-0.70066
H	6.57912	2.55236	0.11600
H	5.32024	4.64655	-0.08374
H	2.85793	4.55892	-0.48821
H	1.73155	2.39900	-0.70066
H	6.41527	-0.00000	-2.09003
H	7.48835	0.88170	-0.99134
H	7.48835	-0.88170	-0.99134
H	6.99248	-0.88287	1.54152
H	6.99248	0.88286	1.54152
H	5.58240	0.00000	2.15175

Compound **5**:

C	5.28677	-0.52589	-1.09942
O	5.68719	-0.90143	-2.17940
C	8.43949	0.65143	0.56291
C	7.49784	0.37506	-0.41462
C	6.27768	-0.17166	-0.03247
C	6.08041	-0.44706	1.31655
C	7.10175	-0.15384	2.21031
N	8.25763	0.39643	1.85676
C	3.83173	-0.41367	-0.81822
C	3.30434	0.44216	0.14923
C	1.93603	0.55350	0.32307
C	1.06769	-0.19366	-0.47055
C	1.58797	-1.04187	-1.45028
C	2.95312	-1.14080	-1.62351
N	-0.32089	-0.08976	-0.29238
C	-1.21250	-1.15848	-0.17105
C	-0.97492	-2.52312	-0.14802

C	-2.05987	-3.37149	0.02260
C	-3.37201	-2.90456	0.17698
C	-3.57813	-1.52701	0.16925
C	-2.51368	-0.65282	0.00100
C	-2.41128	0.78661	-0.02169
C	-3.34716	1.80685	0.07098
C	-2.95561	3.14063	-0.01826
C	-1.59520	3.41223	-0.21596
C	-0.63538	2.41449	-0.31217
C	-1.05108	1.09770	-0.20038
C	-4.00624	4.24307	0.08939
C	-3.40271	5.63782	-0.03166
C	-5.03787	4.07926	-1.02879
C	-4.70788	4.15081	1.44602
C	-4.56197	-3.84364	0.35810
C	-4.15320	-5.31231	0.34577
C	-5.24281	-3.55706	1.69819
C	-5.56357	-3.62509	-0.77782
H	9.39705	1.09704	0.29172
H	7.69646	0.57118	-1.46483
H	5.16158	-0.90901	1.66967
H	6.97787	-0.37445	3.27127
H	3.96756	1.04144	0.76856
H	1.52939	1.20509	1.09224
H	0.90680	-1.59485	-2.09212
H	3.37078	-1.77370	-2.40242
H	0.02854	-2.92950	-0.24721
H	-1.86363	-4.43975	0.03708
H	-4.57993	-1.11962	0.30195
H	-4.39705	1.54937	0.20746
H	-1.25927	4.44146	-0.30396
H	0.40657	2.67113	-0.48599
H	-2.91177	5.79281	-0.99999
H	-4.19350	6.39226	0.05524
H	-2.67149	5.84130	0.75999
H	-5.79764	4.86941	-0.97103
H	-4.56142	4.14046	-2.01470
H	-5.55999	3.11773	-0.97345
H	-5.21617	3.19022	1.58465
H	-5.46427	4.94028	1.54371
H	-3.99093	4.26691	2.26782
H	-3.45827	-5.55438	1.15893
H	-5.03934	-5.94433	0.47750
H	-3.68559	-5.60273	-0.60278
H	-6.09685	-4.23006	1.84851
H	-4.54613	-3.70455	2.53225
H	-5.61981	-2.53030	1.76046
H	-5.94785	-2.59933	-0.79912
H	-6.42474	-4.29674	-0.66747
H	-5.10214	-3.82541	-1.75239

Compound **6**:

C	-1.21252	0.07414	-1.52168
C	-1.20052	0.06858	-2.91081
C	0.00001	-0.00002	-3.59844
C	1.20053	-0.06860	-2.91080
C	1.21252	-0.07414	-1.52167
C	-0.00000	0.00001	-0.81534
C	-4.62408	-0.21476	-0.31062
C	-4.21138	1.02268	0.30834
C	-2.86584	1.22930	-0.04168
N	-2.43587	0.16066	-0.83617
C	-3.51326	-0.70851	-1.01708
C	-3.58406	-1.90068	-1.71650
C	-4.78982	-2.58869	-1.70806
C	-5.92020	-2.12696	-1.02059
C	-5.81411	-0.92818	-0.31817
C	-4.86971	1.95944	1.09246
C	-4.21201	3.10696	1.52831
C	-2.87633	3.28538	1.14331
C	-2.19012	2.36653	0.36274
C	4.62408	0.21476	-0.31062
C	4.21138	-1.02268	0.30834
C	2.86584	-1.22929	-0.04167
N	2.43586	-0.16065	-0.83615
C	3.51325	0.70851	-1.01706
C	3.58406	1.90068	-1.71649
C	4.78982	2.58869	-1.70805
C	5.92020	2.12696	-1.02059
C	5.81411	0.92818	-0.31816
C	4.86971	-1.95944	1.09246

C	4.21200	-3.10695	1.52831
C	2.87633	-3.28538	1.14332
C	2.19012	-2.36652	0.36276
C	-0.00000	0.00001	0.60971
N	-0.00000	0.00002	1.76319
C	4.95627	-4.11672	2.39862
C	4.08925	-5.31290	2.77521
C	6.17992	-4.64260	1.64548
C	5.40879	-3.43809	3.69324
C	7.24372	2.88818	-1.01263
C	7.18272	4.17369	-1.82994
C	7.61058	3.26283	0.42488
C	8.34538	2.00703	-1.60535
C	-4.95627	4.11672	2.39862
C	-4.08925	5.31289	2.77521
C	-6.17992	4.64260	1.64548
C	-5.40878	3.43808	3.69324
C	-7.24372	-2.88818	-1.01262
C	-7.18272	-4.17369	-1.82994
C	-7.61056	-3.26284	0.42489
C	-8.34538	-2.00704	-1.60533
H	-2.14724	0.13715	-3.44049
H	0.00001	-0.00003	-4.68543
H	2.14726	-0.13718	-3.44047
H	-2.72439	-2.29867	-2.25135
H	-4.83929	-3.52342	-2.25914
H	-6.66693	-0.53813	0.23649
H	-5.91196	1.78668	1.35905
H	-2.33749	4.17193	1.46458
H	-1.15272	2.54448	0.08951
H	2.72438	2.29867	-2.25133
H	4.83929	3.52342	-2.25914
H	6.66694	0.53813	0.23649
H	5.91196	-1.78669	1.35905
H	2.33748	-4.17192	1.46459
H	1.15272	-2.54447	0.08953
H	4.66650	-6.00720	3.39723
H	3.20584	-5.01650	3.35327
H	3.75077	-5.87093	1.89374
H	6.72265	-5.37578	2.25614
H	6.88457	-3.84352	1.39009
H	5.88472	-5.13455	0.71066
H	4.54993	-3.05010	4.25383
H	5.93970	-4.15099	4.33749
H	6.08612	-2.59780	3.50451
H	8.15394	4.68125	-1.79458
H	6.95512	3.98156	-2.88552
H	6.43562	4.87563	-1.44031
H	8.55712	3.81822	0.44913
H	7.73056	2.38184	1.06485
H	6.83626	3.89516	0.87571
H	8.10878	1.72379	-2.63820
H	9.30437	2.54111	-1.61294
H	8.48900	1.08315	-1.03435
H	-4.66650	6.00720	3.39723
H	-3.20584	5.01650	3.35327
H	-3.75077	5.87093	1.89374
H	-6.72265	5.37577	2.25616
H	-6.88458	3.84352	1.39010
H	-5.88473	5.13455	0.71067
H	-4.54992	3.05009	4.25382
H	-5.93969	4.15098	4.33750
H	-6.08611	2.59780	3.50452
H	-8.15393	-4.68125	-1.79458
H	-6.95512	-3.98156	-2.88552
H	-6.43561	-4.87563	-1.44031
H	-8.55711	-3.81823	0.44915
H	-7.73055	-2.38185	1.06486
H	-6.83624	-3.89517	0.87571
H	-8.10880	-1.72379	-2.63819
H	-9.30437	-2.54112	-1.61292
H	-8.48900	-1.08316	-1.03433

Compound **7**:

S	0.45660	-0.11355	-2.08518
C	0.63355	-0.16894	-0.35971
C	-0.63355	-0.16894	0.35971
C	-1.72405	-0.12961	-0.42772
C	-1.39455	-0.08653	-1.87457
C	1.72405	-0.12961	0.42772
C	1.39455	-0.08653	1.87457

S	-0.45660	-0.11355	2.08518
O	-2.14042	-0.03733	-2.79653
O	2.14042	-0.03733	2.79653
N	3.06606	-0.05520	0.05521
C	3.70403	1.20128	0.11778
C	5.10200	1.25300	0.16276
C	5.86460	-0.04595	0.35697
C	5.16517	-1.15110	-0.42009
C	3.76384	-1.17430	-0.44801
C	5.84462	-2.21672	-0.99963
C	5.17569	-3.30185	-1.54651
C	3.79236	-3.33662	-1.50848
C	3.08686	-2.27470	-0.96827
C	2.95082	2.37341	0.08693
C	3.58076	3.60602	0.08793
C	4.96364	3.67485	0.09556
C	5.70734	2.50349	0.12953
C	5.79144	-0.40833	1.85266
C	7.33207	0.08655	-0.02472
N	-3.06606	-0.05520	-0.05521
C	-3.70403	1.20128	-0.11778
C	-5.10200	1.25300	-0.16277
C	-5.86460	-0.04595	-0.35698
C	-5.16518	-1.15110	0.42009
C	-3.76384	-1.17430	0.44801
C	-5.84462	-2.21672	0.99963
C	-5.17569	-3.30185	1.54652
C	-3.79236	-3.33662	1.50849
C	-3.08686	-2.27470	0.96828
C	-2.95082	2.37341	-0.08693
C	-3.58077	3.60602	-0.08793
C	-4.96364	3.67485	-0.09555
C	-5.70734	2.50349	-0.12953
C	-5.79143	-0.40833	-1.85267
C	-7.33207	0.08655	0.02470
H	6.93103	-2.21690	-1.00935
H	5.73745	-4.12248	-1.98533
H	3.24960	-4.18735	-1.91342
H	2.00142	-2.30674	-0.95779
H	1.86528	2.32276	0.03703
H	2.98297	4.51394	0.06410
H	5.46796	4.63773	0.08143
H	6.79134	2.57546	0.14661
H	4.75768	-0.49406	2.20279
H	6.29593	-1.36517	2.03645
H	6.28427	0.36644	2.45323
H	7.82423	0.85608	0.57775
H	7.87496	-0.84173	0.17771
H	7.46350	0.34010	-1.08320
H	-6.93103	-2.21690	1.00934
H	-5.73745	-4.12248	1.98534
H	-3.24960	-4.18734	1.91342
H	-2.00142	-2.30674	0.95779
H	-1.86528	2.32276	-0.03702
H	-2.98297	4.51394	-0.06410
H	-5.46796	4.63773	-0.08143
H	-6.79135	2.57545	-0.14661
H	-4.75767	-0.49406	-2.20279
H	-6.29592	-1.36517	-2.03646
H	-6.28426	0.36643	-2.45324
H	-7.87495	-0.84173	-0.17772
H	-7.46351	0.34009	1.08319
H	-7.82422	0.85608	-0.57776

Compound **8**:

C	0.70998	4.35036	-0.85725
C	0.71865	1.94533	-0.41095
C	-0.71864	1.94533	-0.41096
C	1.41993	3.17893	-0.63476
C	2.82795	3.37948	-0.64417
C	3.16089	4.67124	-0.87514
S	1.77312	5.69721	-1.08747
S	-1.77310	5.69722	-1.08748
C	-3.16087	4.67125	-0.87515
C	-2.82793	3.37948	-0.64420
C	-1.41990	3.17893	-0.63478
C	-0.70996	4.35036	-0.85726
C	0.70801	-2.61692	0.55487
C	-0.70802	-2.61691	0.55487
C	-1.43813	-1.49172	0.30463
C	-0.71414	-0.28724	0.04310

C	0.71415	-0.28724	0.04311
C	1.43812	-1.49172	0.30464
F	1.30144	-3.77320	0.81641
F	-1.30146	-3.77319	0.81643
N	1.40079	0.83356	-0.20456
N	-1.40078	0.83356	-0.20459
C	-2.91573	-1.51508	0.29868
C	2.91573	-1.51510	0.29869
C	-3.61570	-2.21883	-0.68997
C	-5.03285	-2.23105	-0.68022
C	-5.77208	-1.56854	0.28039
C	3.61568	-2.21876	-0.69004
C	5.03284	-2.23098	-0.68029
C	5.77207	-1.56856	0.28038
C	-5.08464	-0.86508	1.26536
C	-3.66746	-0.84693	1.25821
C	-3.09143	-2.96785	-1.79391
C	-4.05350	-3.51530	-2.56378
C	-5.62175	-0.11565	2.36230
C	-4.66648	0.43164	3.14008
C	5.08464	-0.86520	1.26542
C	3.66746	-0.84705	1.25828
C	3.09141	-2.96768	-1.79403
C	4.05347	-3.51507	-2.56396
C	5.62175	-0.11587	2.36244
C	4.66648	0.43134	3.14027
S	3.04586	0.08901	2.60014
S	5.66887	-3.16769	-2.01550
S	-5.66889	-3.16787	-2.01535
S	-3.04586	0.08926	2.59997
H	3.53970	2.57692	-0.47687
H	4.14871	5.10990	-0.93763
H	-4.14869	5.10990	-0.93765
H	-3.53968	2.57692	-0.47690
H	-6.86022	-1.59159	0.27624
H	6.86021	-1.59161	0.27622
H	-2.03085	-3.07934	-1.99785
H	-3.92244	-4.12234	-3.45134
H	-6.68665	-0.00626	2.54619
H	-4.80165	1.03962	4.02650
H	2.03083	-3.07915	-1.99797
H	3.92241	-4.12204	-3.45156
H	6.68665	-0.00650	2.54633
H	4.80166	1.03923	4.02675

Compound **9**:

C	0.95725	-1.51166	0.79312
C	0.06878	-0.55890	0.27909
C	0.61205	0.58352	-0.32707
C	1.97526	0.76077	-0.41308
C	2.84884	-0.19606	0.11326
C	2.32458	-1.33667	0.72009
C	-1.35259	-0.79640	0.39437
C	-2.34390	0.02150	-0.02048
C	-6.00488	0.03977	-0.05433
O	-5.82954	-1.13675	0.53770
C	-4.41496	-1.43279	0.69740
C	-3.74276	-0.22475	0.09495
C	-4.71843	0.62736	-0.33960
C	-4.18094	-1.57560	2.18884
C	-4.16351	-2.71397	-0.07377
C	-4.45561	1.87088	-0.96194
N	-4.14288	2.86476	-1.45828
C	-7.26633	0.50605	-0.29833
C	-8.38634	-0.27754	0.08590
N	-9.29551	-0.91636	0.39909
C	-7.49646	1.75575	-0.92741
N	-7.70744	2.76988	-1.43796
C	6.29963	0.95217	0.14432
C	6.45137	-0.39375	-0.34764
C	5.16467	-0.95971	-0.40604
N	4.23467	-0.00968	0.02814
C	4.92569	1.15921	0.36401
C	4.44715	2.35206	0.89209
C	5.36832	3.34971	1.16768
C	6.73301	3.16734	0.93378
C	7.20523	1.96884	0.42924
C	7.55251	-1.13914	-0.75597
C	7.35706	-2.42698	-1.22213
C	6.07114	-2.96674	-1.29568
C	4.95902	-2.24411	-0.89442

H	0.55901	-2.40194	1.27767
H	-0.04063	1.33914	-0.75761
H	2.38361	1.63270	-0.91727
H	2.99901	-2.06841	1.15688
H	-1.61445	-1.74185	0.87122
H	-2.08667	0.97023	-0.49320
H	-3.14834	-1.85882	2.41059
H	-4.39875	-0.63570	2.70555
H	-4.84497	-2.34966	2.58544
H	-3.13021	-3.05482	0.03500
H	-4.82794	-3.49762	0.30280
H	-4.36825	-2.56990	-1.13922
H	3.39077	2.50164	1.09936
H	5.01766	4.29321	1.57908
H	7.42779	3.97235	1.15927
H	8.27021	1.81799	0.26274
H	8.55169	-0.70945	-0.71533
H	8.20776	-3.02245	-1.54360
H	5.93559	-3.97465	-1.68082
H	3.96234	-2.66923	-0.97869

Compound **10**:

S	0.00000	3.71085	-0.00000
C	1.37898	2.57473	0.08411
C	-1.37898	2.57473	-0.08411
O	0.07230	4.40991	-1.27028
O	-0.07230	4.40992	1.27026
C	-1.87018	2.20090	-1.32577
C	-2.88856	1.26231	-1.38790
C	-3.38868	0.70216	-0.21878
C	-2.89373	1.09638	1.02100
C	-1.88449	2.04099	1.09371
C	1.87018	2.20091	1.32578
C	2.88857	1.26233	1.38792
C	3.38868	0.70217	0.21880
C	2.89374	1.09637	-1.02098
C	1.88449	2.04099	-1.09370
N	4.39342	-0.29744	0.29585
N	-4.39341	-0.29745	-0.29582
C	4.01893	-1.63719	0.49205
C	5.01161	-2.62302	0.47710
O	6.33218	-2.31834	0.27840
C	6.65936	-1.03607	-0.07804
C	5.71652	-0.00303	-0.07153
C	-4.01893	-1.63720	-0.49203
C	-5.01162	-2.62303	-0.47709
O	-6.33218	-2.31834	-0.27838
C	-6.65937	-1.03606	0.07804
C	-5.71651	-0.00303	0.07154
C	-2.70146	-2.03183	-0.69851
C	-2.38384	-3.37003	-0.90477
C	-3.37647	-4.33260	-0.89572
C	-4.69441	-3.95084	-0.67423
C	-7.97263	-0.79390	0.42322
C	-8.38406	0.49036	0.75964
C	-7.46487	1.52344	0.74485
C	-6.13957	1.27887	0.40328
C	2.70146	-2.03181	0.69853
C	2.38383	-3.37001	0.90478
C	3.37645	-4.33259	0.89571
C	4.69440	-3.95083	0.67422
C	7.97262	-0.79392	-0.42325
C	8.38405	0.49033	-0.75969
C	7.46487	1.52342	-0.74489
C	6.13957	1.27887	-0.40330
H	-1.46841	2.65918	-2.22598
H	-3.30207	0.94356	-2.34194
H	-3.31066	0.65114	1.92192
H	-1.49235	2.37116	2.05262
H	1.46842	2.65920	2.22598
H	3.30208	0.94359	2.34196
H	3.31066	0.65113	-1.92190
H	1.49236	2.37114	-2.05262
H	-1.91217	-1.28419	-0.70278
H	-1.34702	-3.64907	-1.07478
H	-3.13585	-5.37974	-1.05718
H	-5.50562	-4.67424	-0.65332
H	-8.66295	-1.63366	0.41357
H	-9.42105	0.67403	1.02681
H	-7.76969	2.53574	0.99702
H	-5.42646	2.09900	0.38411

H	1.91217	-1.28417	0.70280
H	1.34701	-3.64906	1.07479
H	3.13583	-5.37974	1.05716
H	5.50560	-4.67424	0.65331
H	8.66293	-1.63368	-0.41361
H	9.42103	0.67400	-1.02688
H	7.76968	2.53572	-0.99707
H	5.42647	2.09900	-0.38412

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