Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis and Investigation of Photophysical, Electrochemical and Theoretical properties of Phenazine-Amine based Cyan blue-Red Fluorescent Materials for Organic Electronics

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Supporting Information

Sr. No.

1. Absorption spectra of compound **1–8** in various solvents.

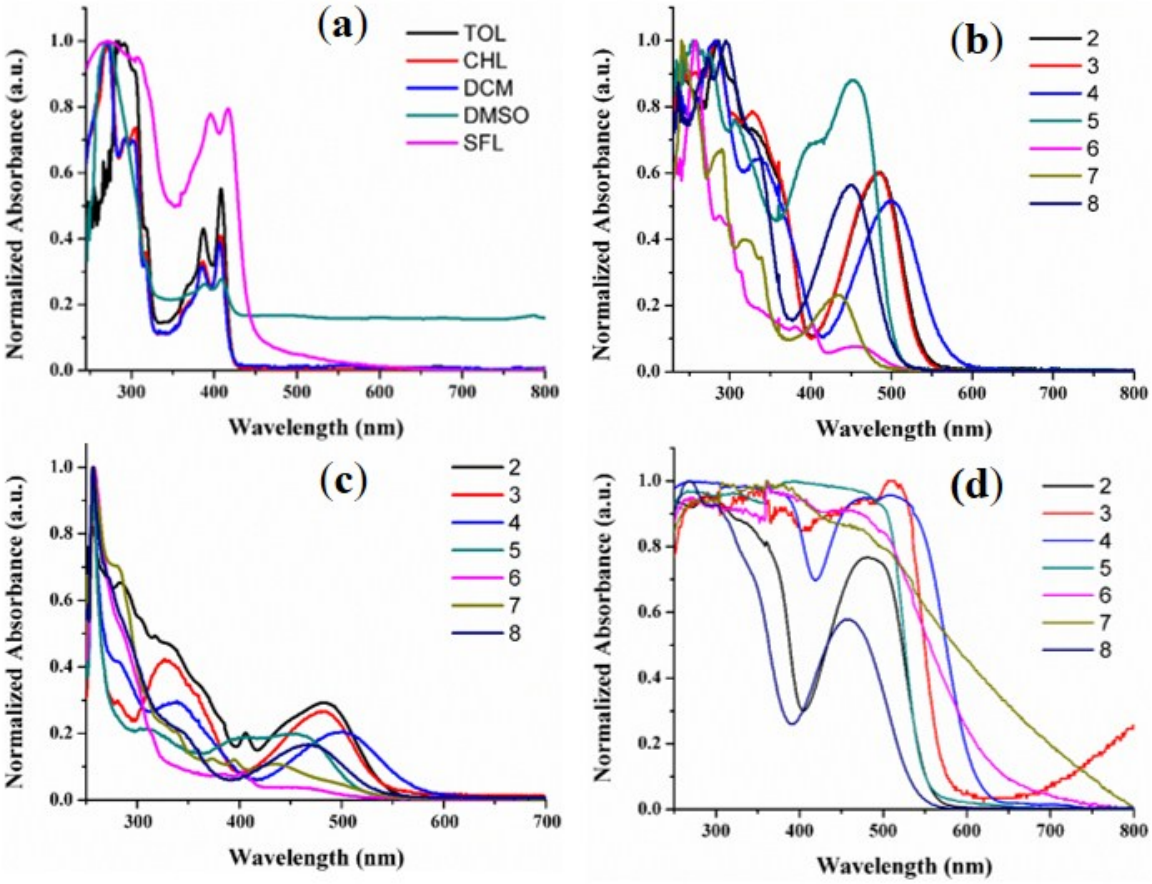

Figure S1: Absorption spectra of compound **1** in various solvent and neat solid flim (**a**); Absorption spectra of compounds **2–8** in chloroform (**b**), dimethyl sulphoxide (DMSO) (**c**) and in neat solid film (**d**).

2. Emission spectra of compound **2–8** in various solvents.

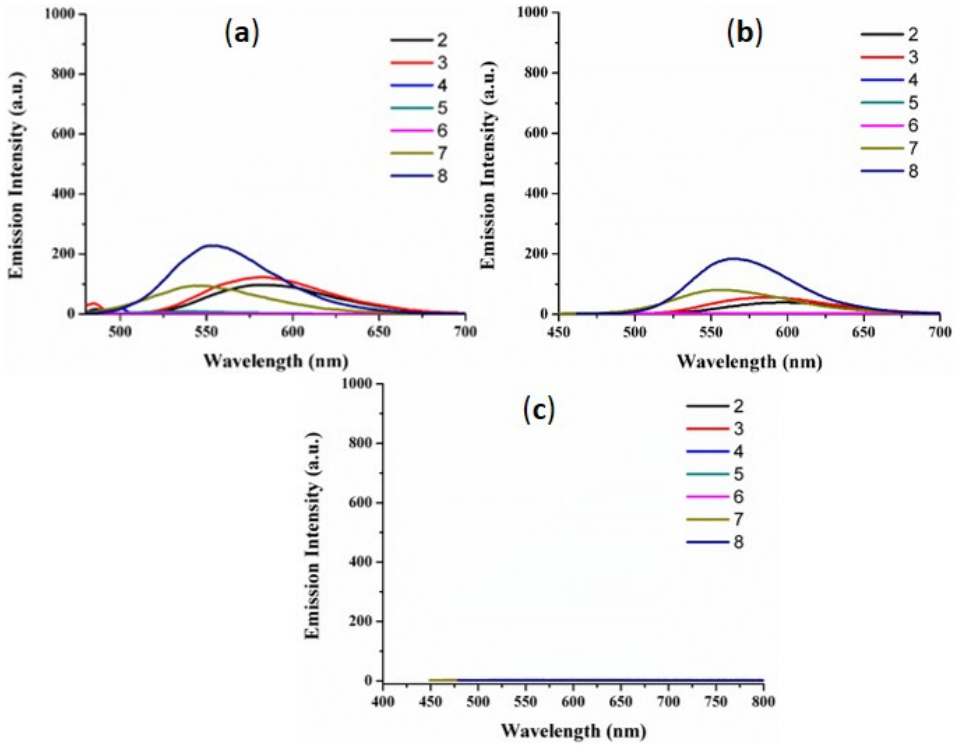

Figure S2: Emission spectra of **2–8** in chloroform (**a**); DCM (**b**) and in DMSO (**c**).

3. Solvatochromic fluorescence of **1–8.**

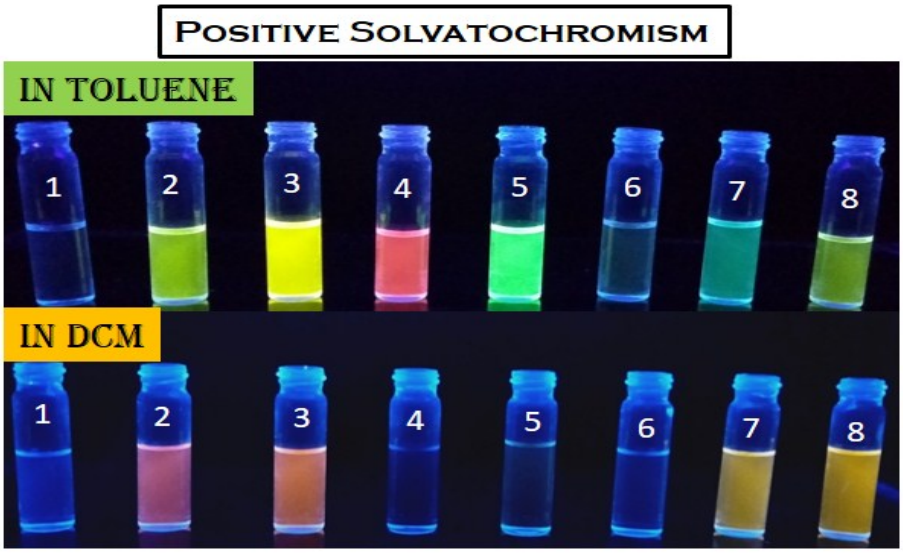

Figure S3. Fluorescence image of **1**−**8** in toluene and dichloromethane (10^{-6} M) under 365 nm UV illumination.

4. Aggregation Induced Emission studies of dye **5** and **7**

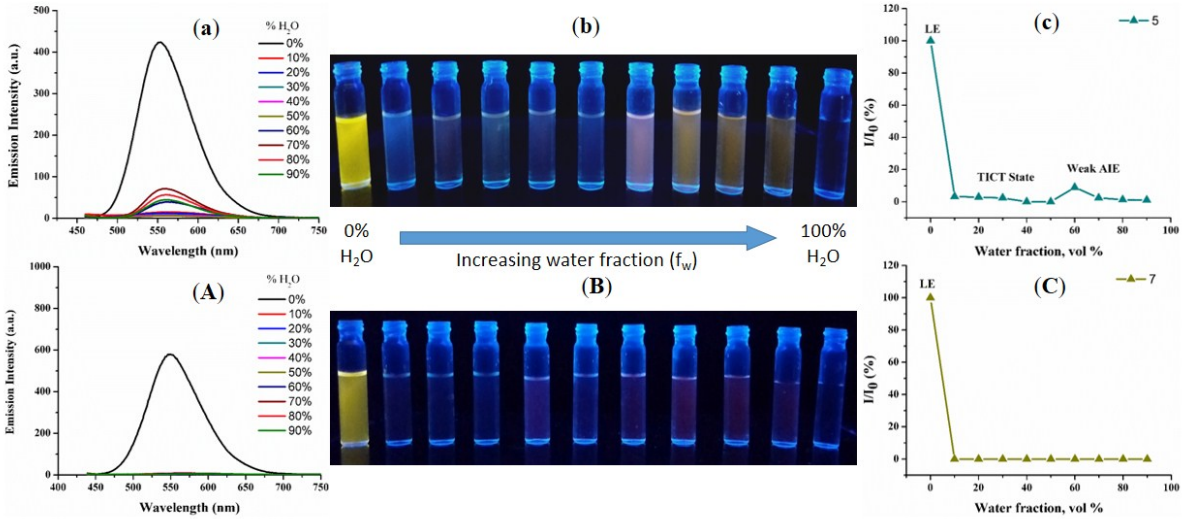

Figure S4: Fluorescence spectra of **5** (**a**) and **7** (**A**), photograph of **5** (**b**) and **7** (**B**) in THF–water mixture with increasing water fractions (f_w) and **5** (**c**) and **7** (**C**) plots of PL intensity (I/I_0) versus f_w .

5. Absorption Spectra of AIE studies in THF−water Mixture

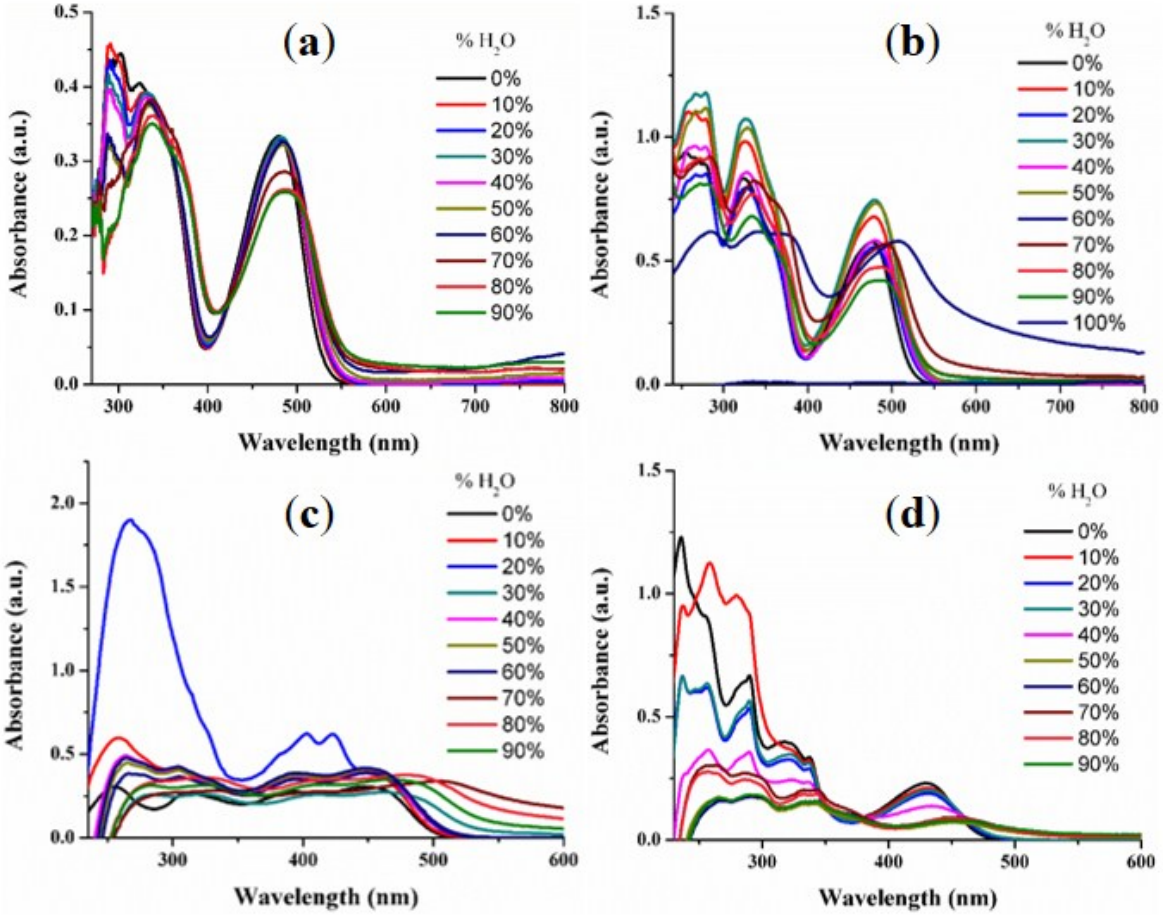

Figure S5: Absorption spectra in THF–water mixture in increase in water fraction by 10% (f_w) of compound **2** (**a**), **3** (**b**), **5** (**c**) and **7** (**d**).

6. Cyclic voltammetry (CV) of compounds **1–8** in anhydrous dichloromethane

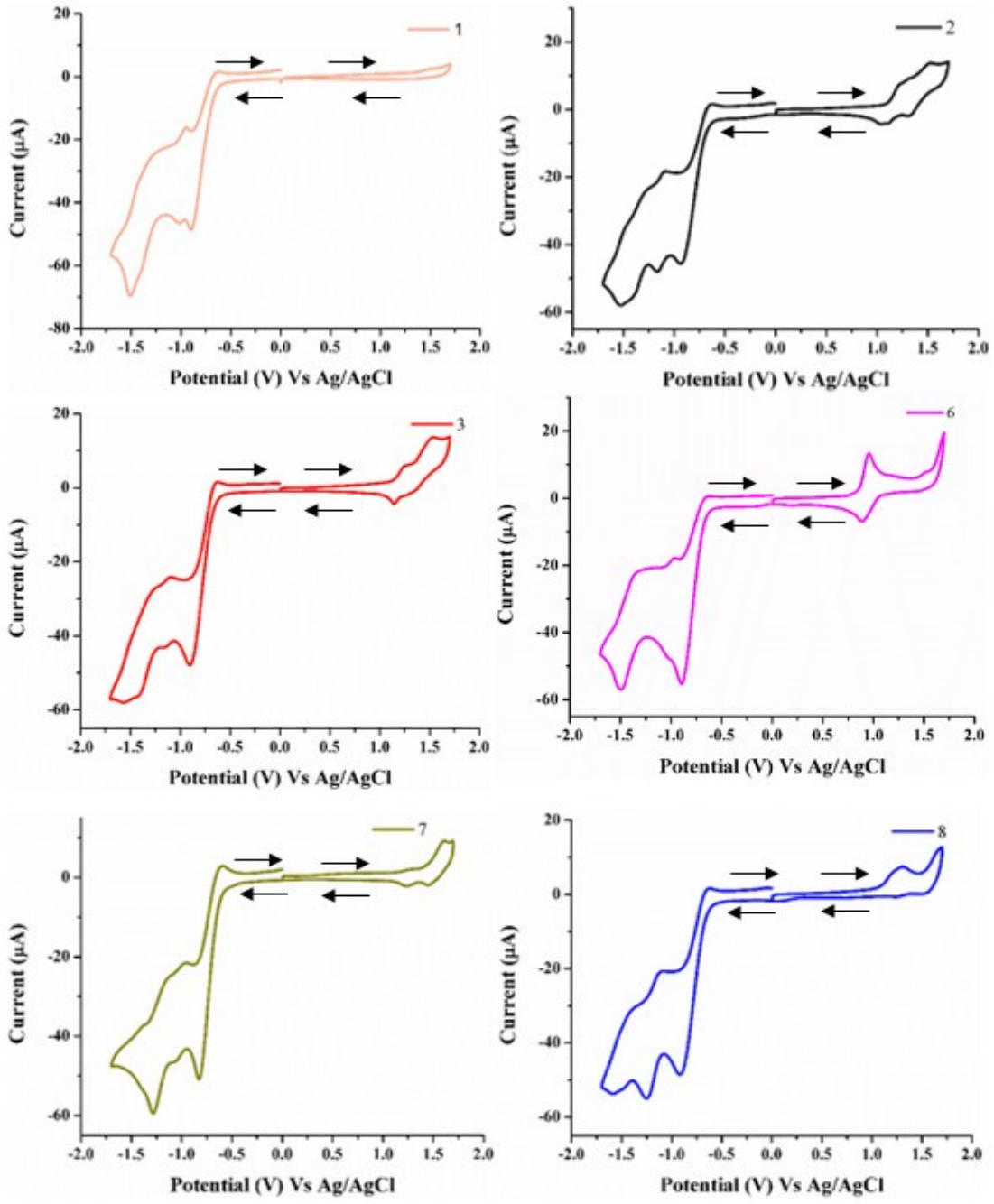

Figure S6: Cyclic voltammetry of compounds **1–3** and **6–8**.

7. MALDI-TOF spectra of compounds **1–8**

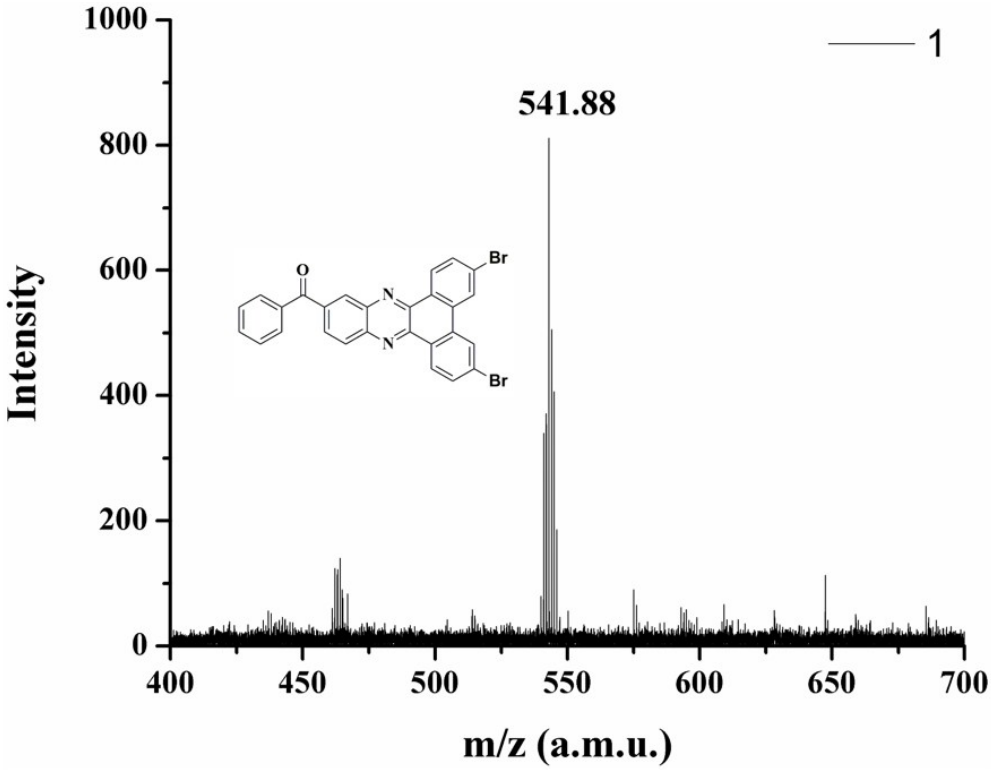

Figure S7: MALDI-TOF mass of **1**.

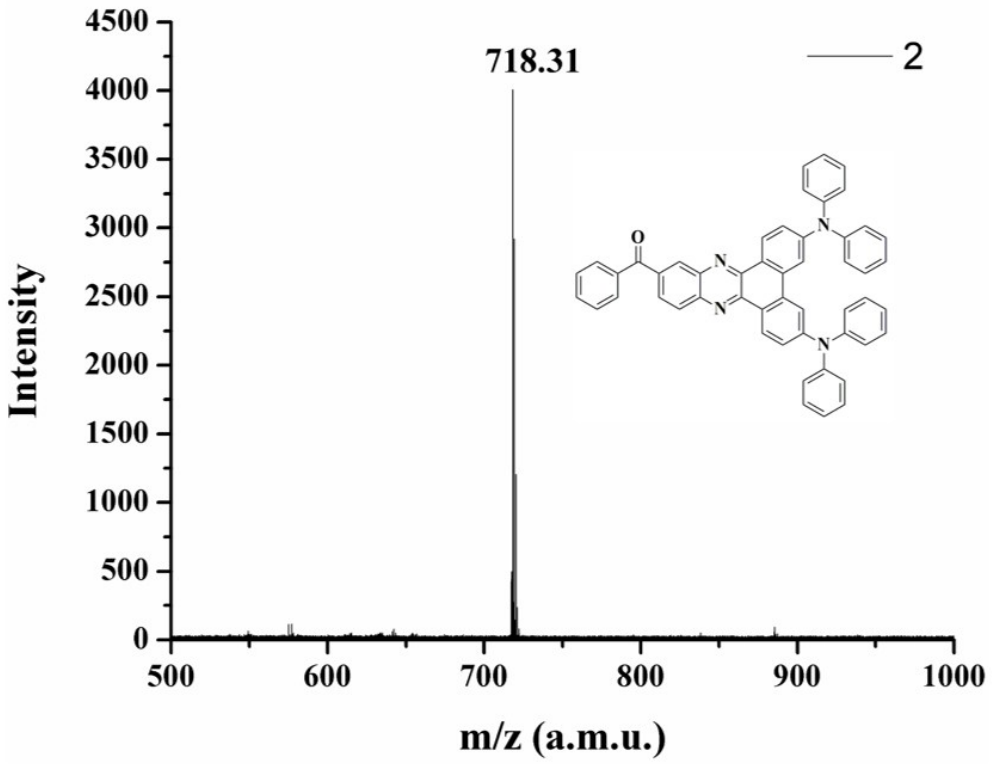

Figure S8: MALDI-TOF mass of **2**.

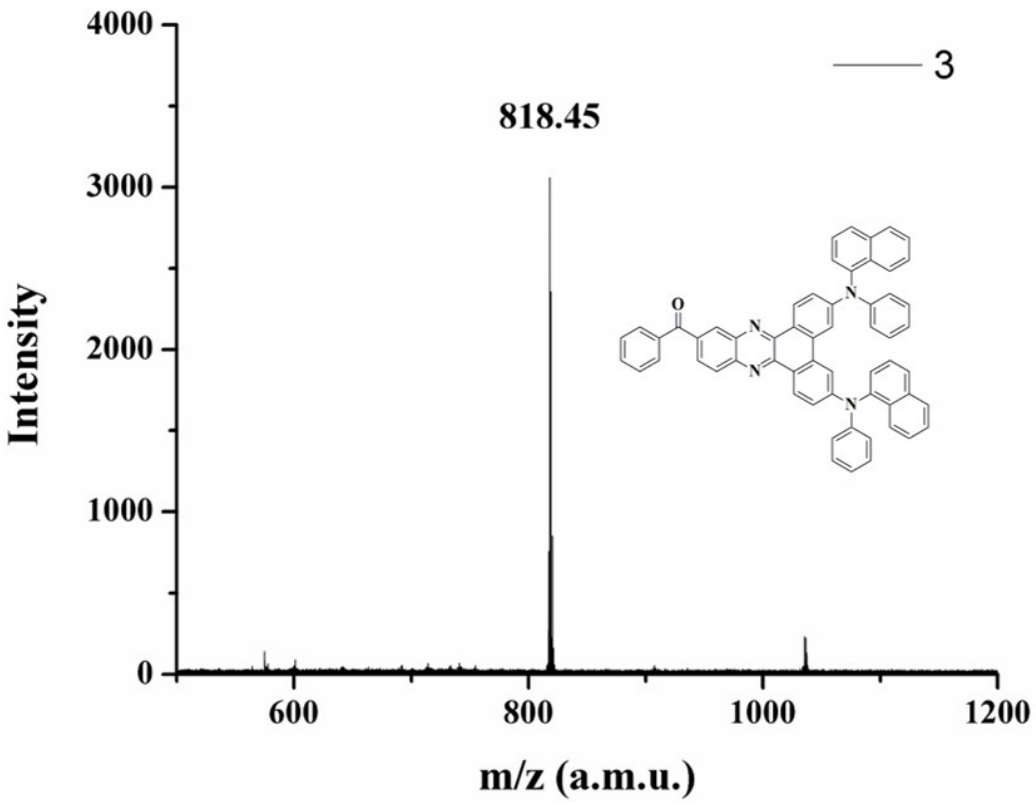

Figure S9: MALDI-TOF mass of **3**.

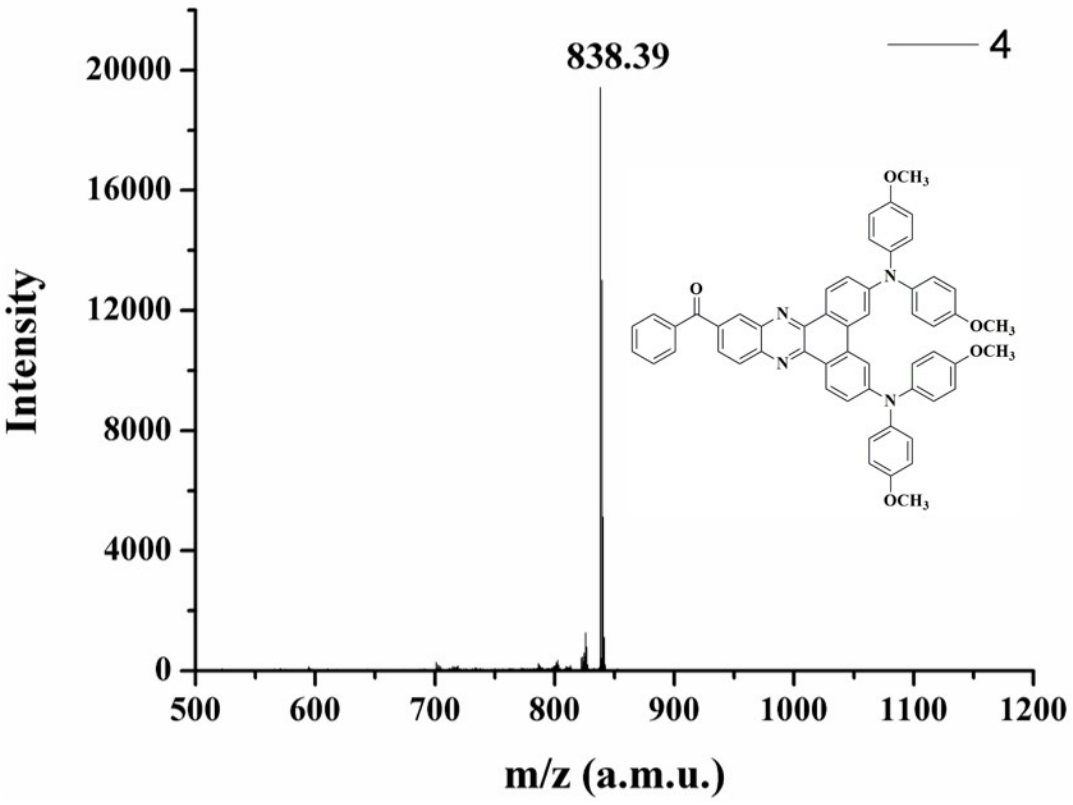

Figure S10: MALDI-TOF mass of **4**.

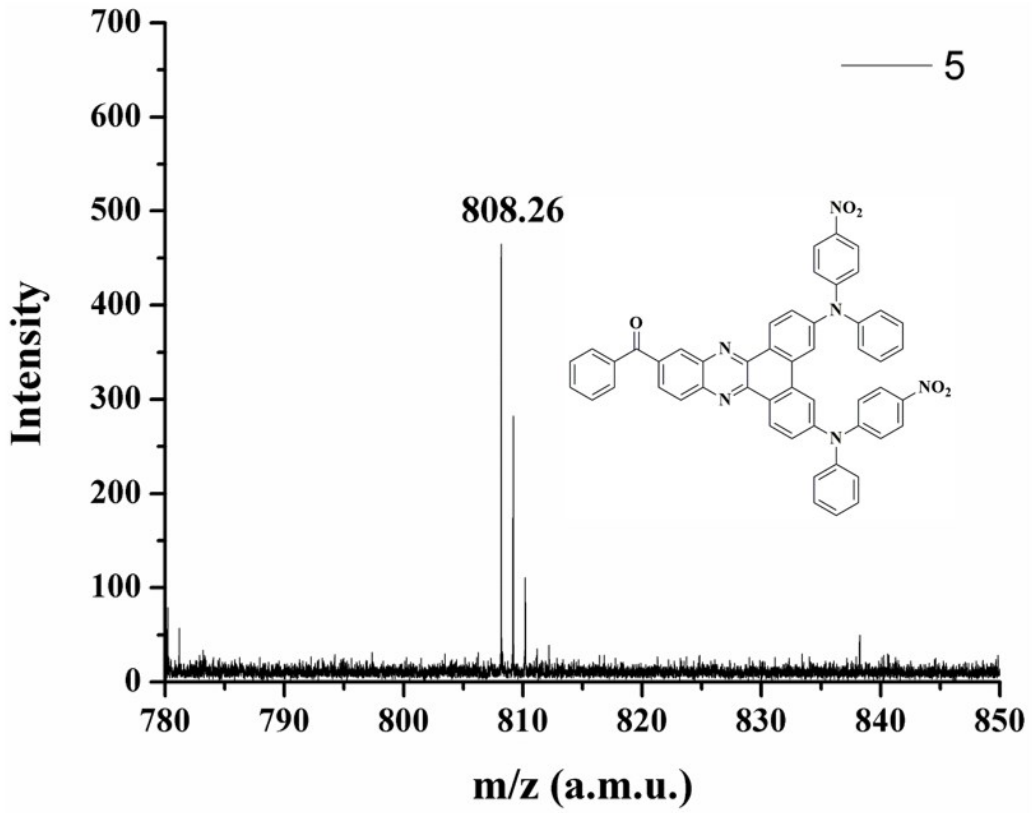

Figure S11: MALDI-TOF mass of **5**.

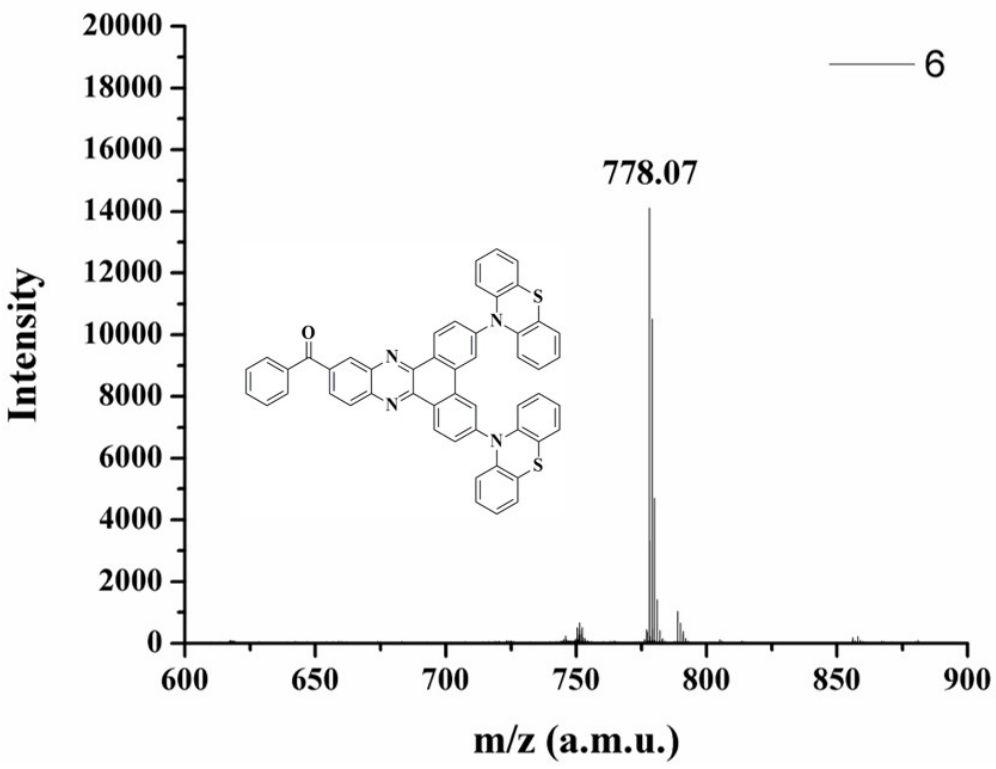

Figure S12: MALDI-TOF mass of **6**.

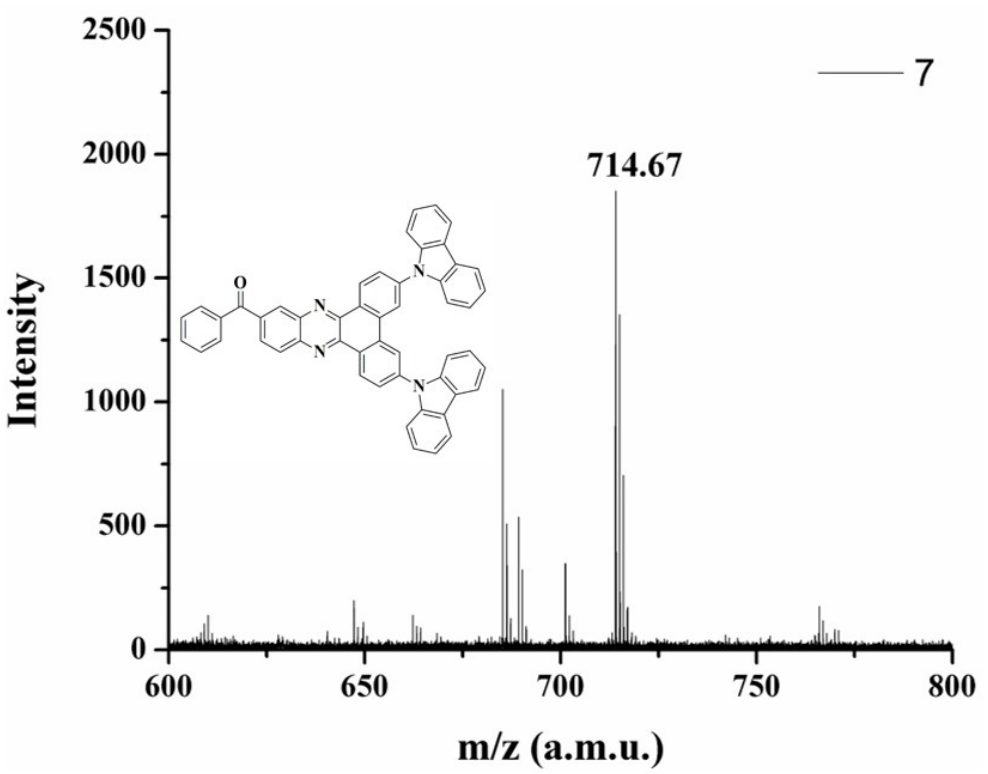

Figure S13: MALDI-TOF mass of **7**.

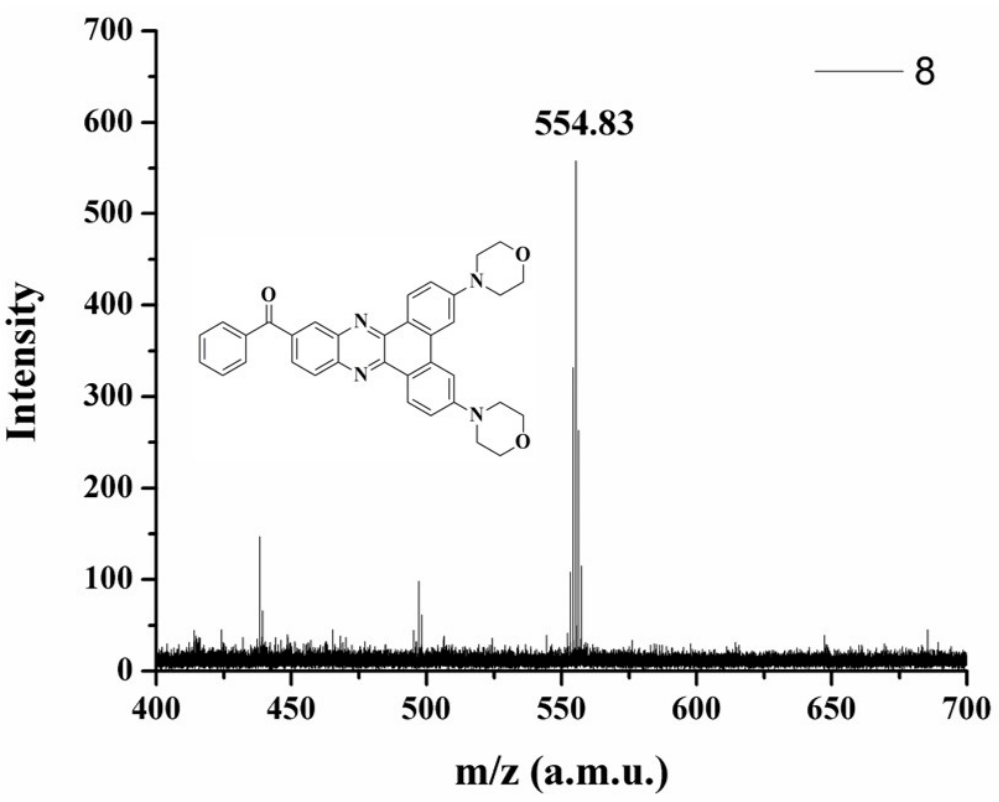

Figure S14: MALDI-TOF mass of **8**.

8. FTIR spectra of compounds **1**–**8**

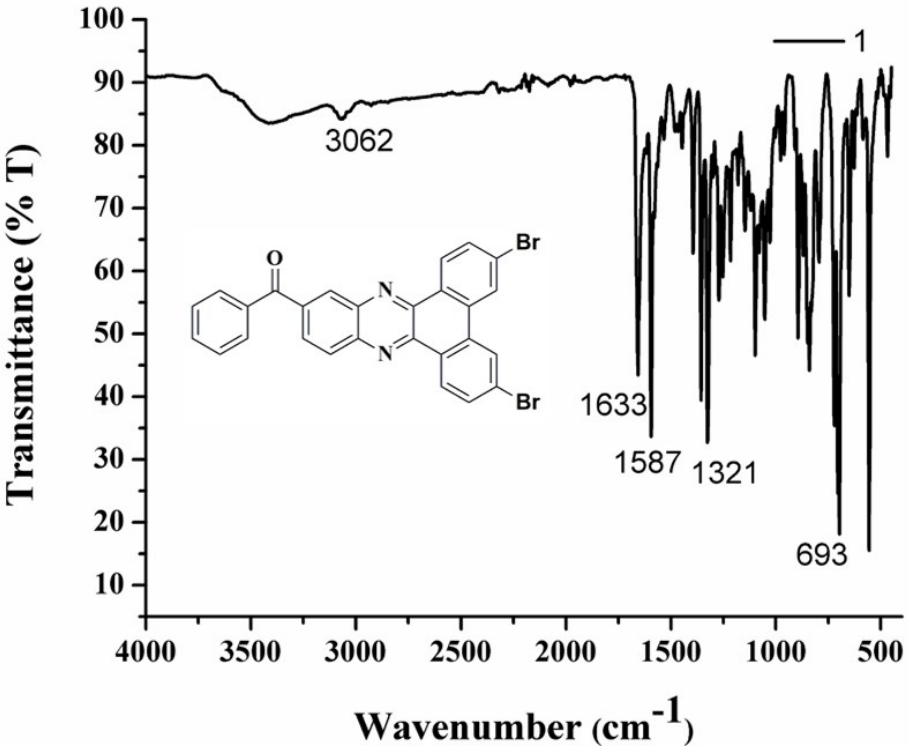

Figure S15: FTIR spectra of **1**.

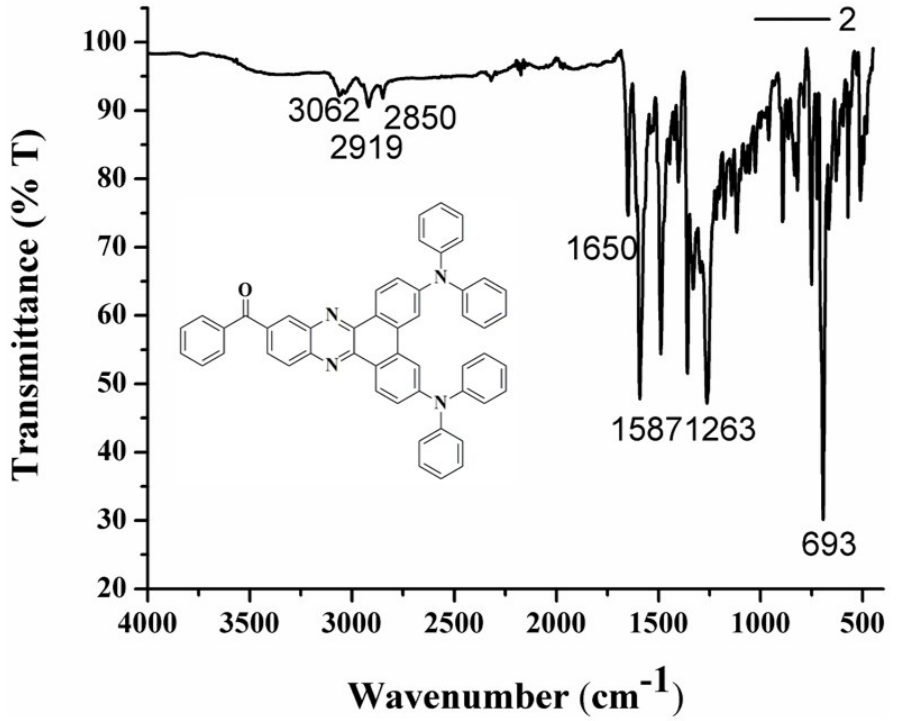

Figure S16: FTIR spectra of **2**.

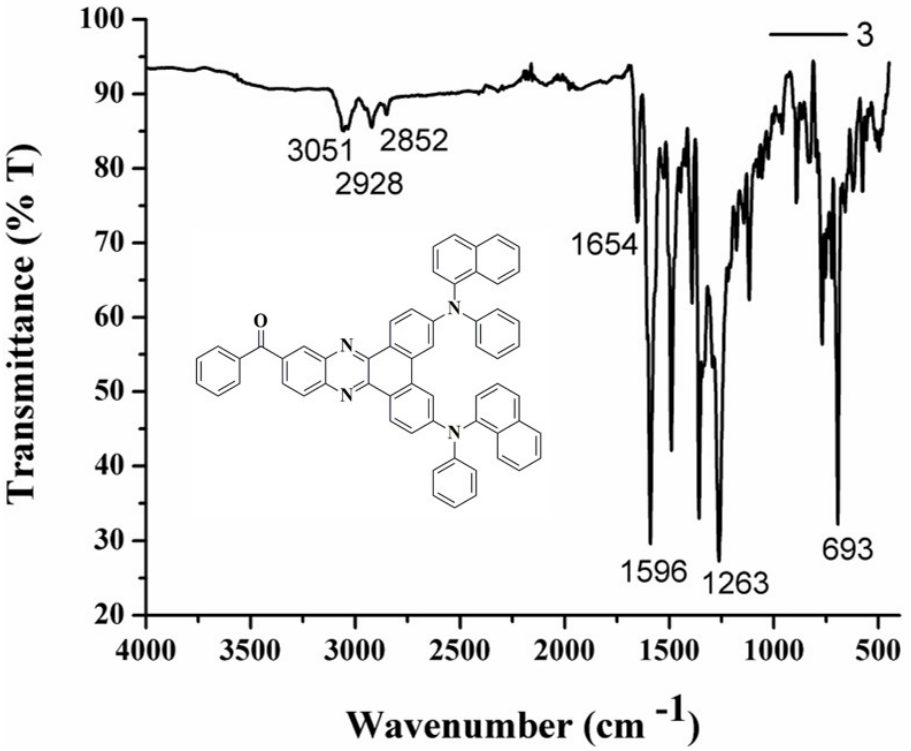

Figure S17: FTIR spectra of **3**.

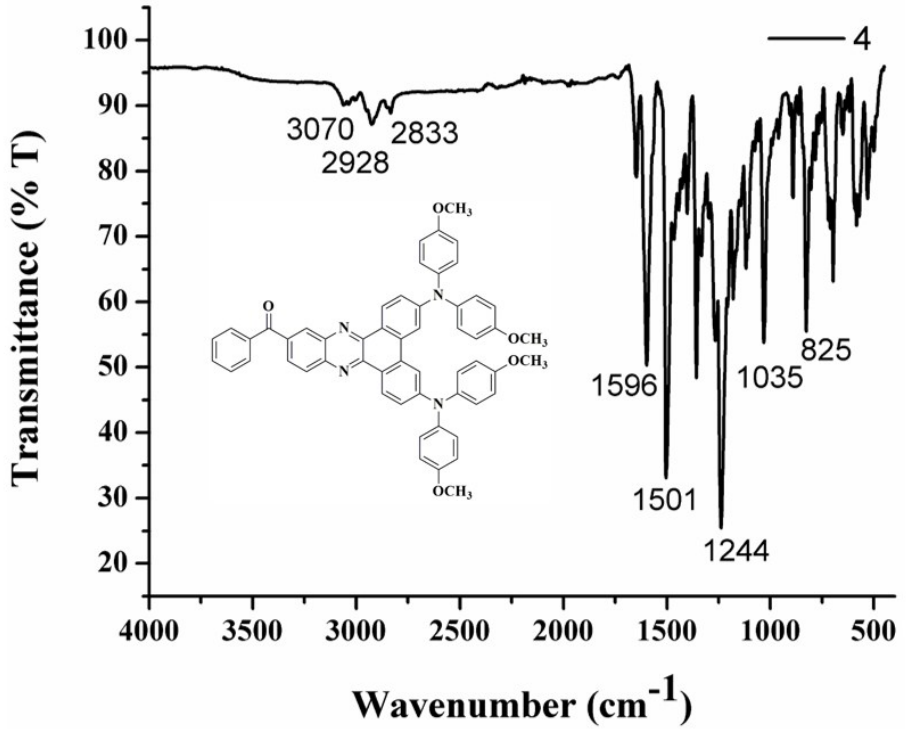

Figure S18: FTIR spectra of **4**.

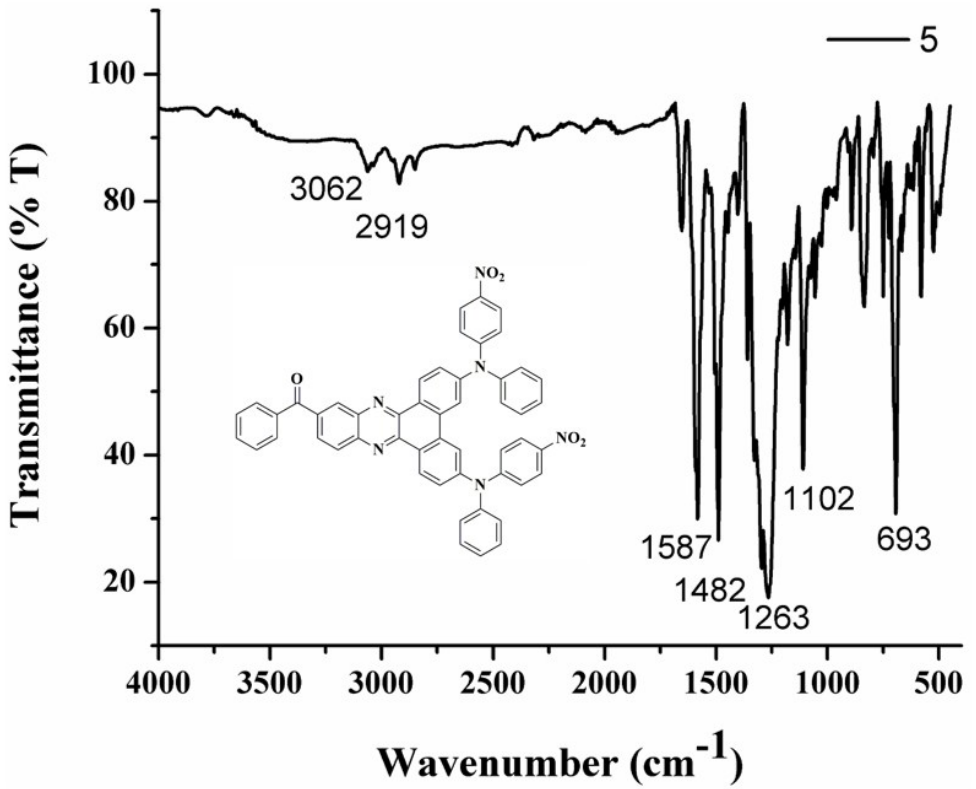

Figure S19: FTIR spectra of **5**.

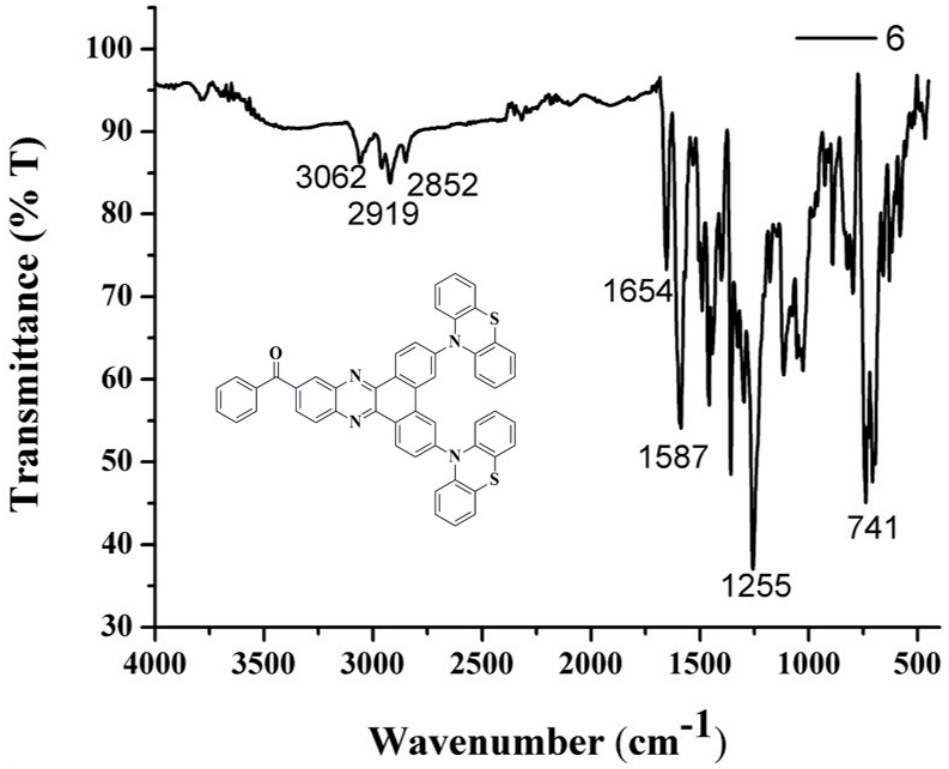

Figure S20: FTIR spectra of **6**.

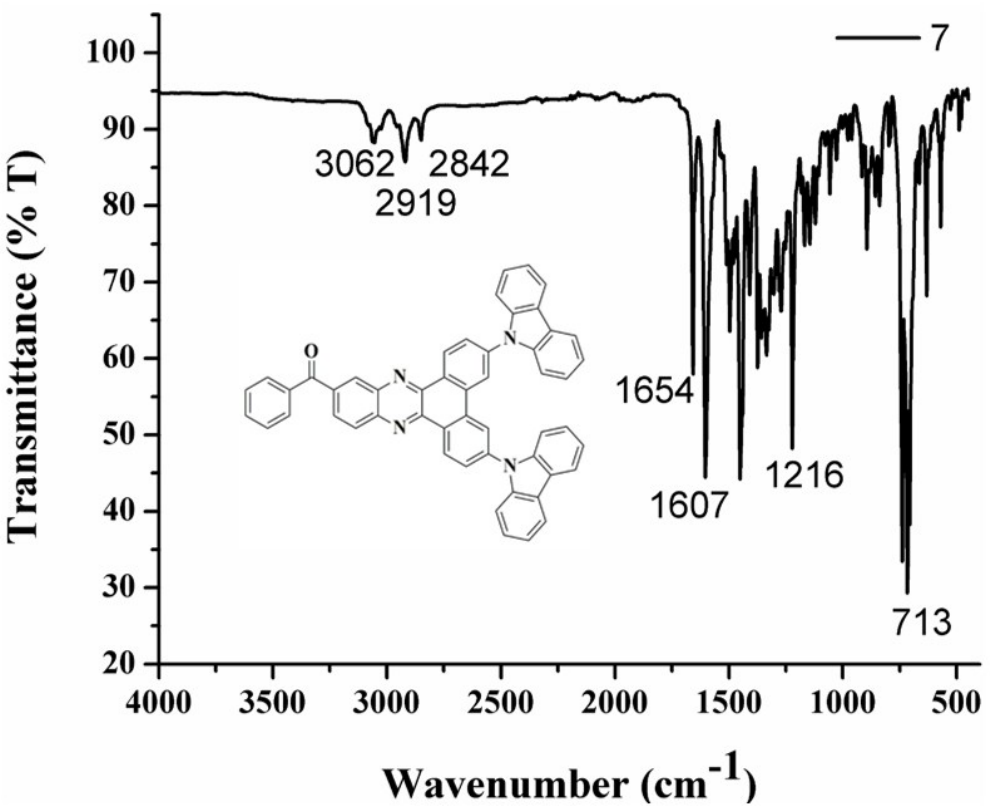

Figure S21: FTIR spectra of **7**.

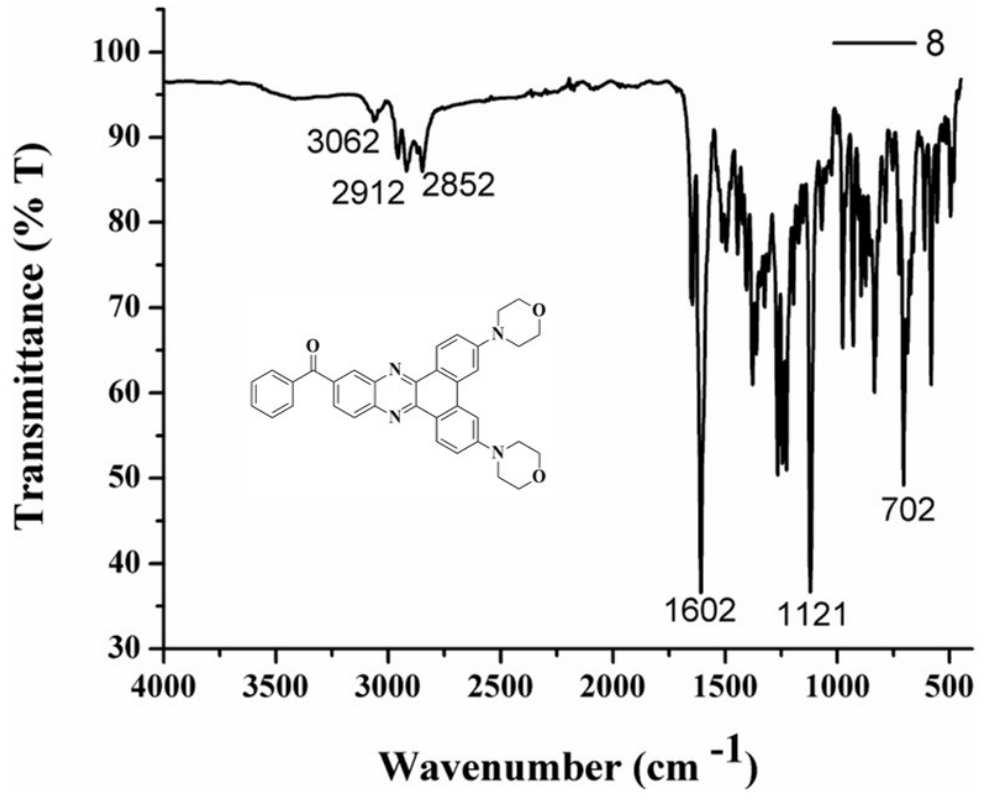

Figure S22: FTIR spectra of **8**.

9. ^{1}H and ^{13}C NMR spectra of compounds **1–8**

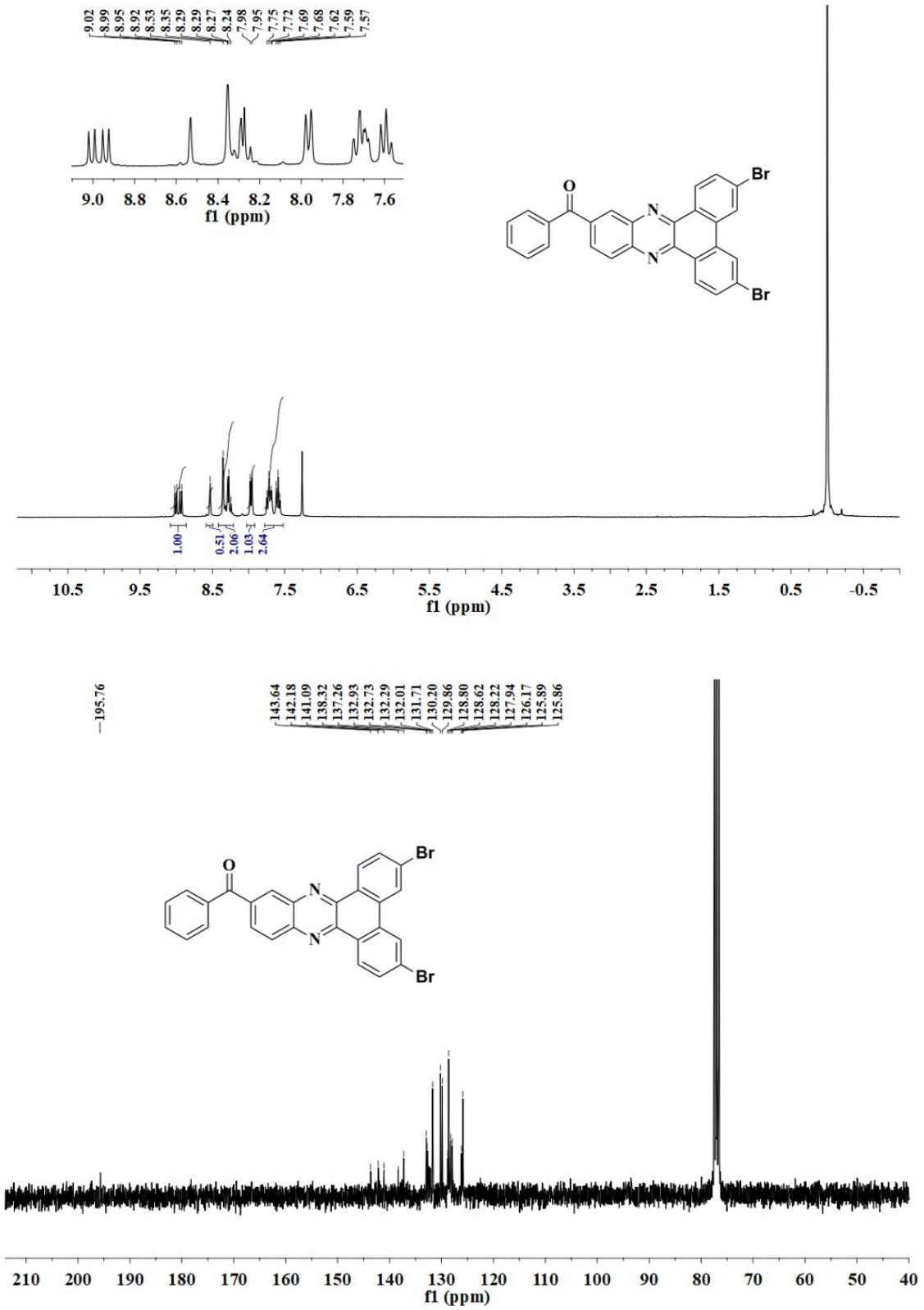

Figure S23: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **1**.

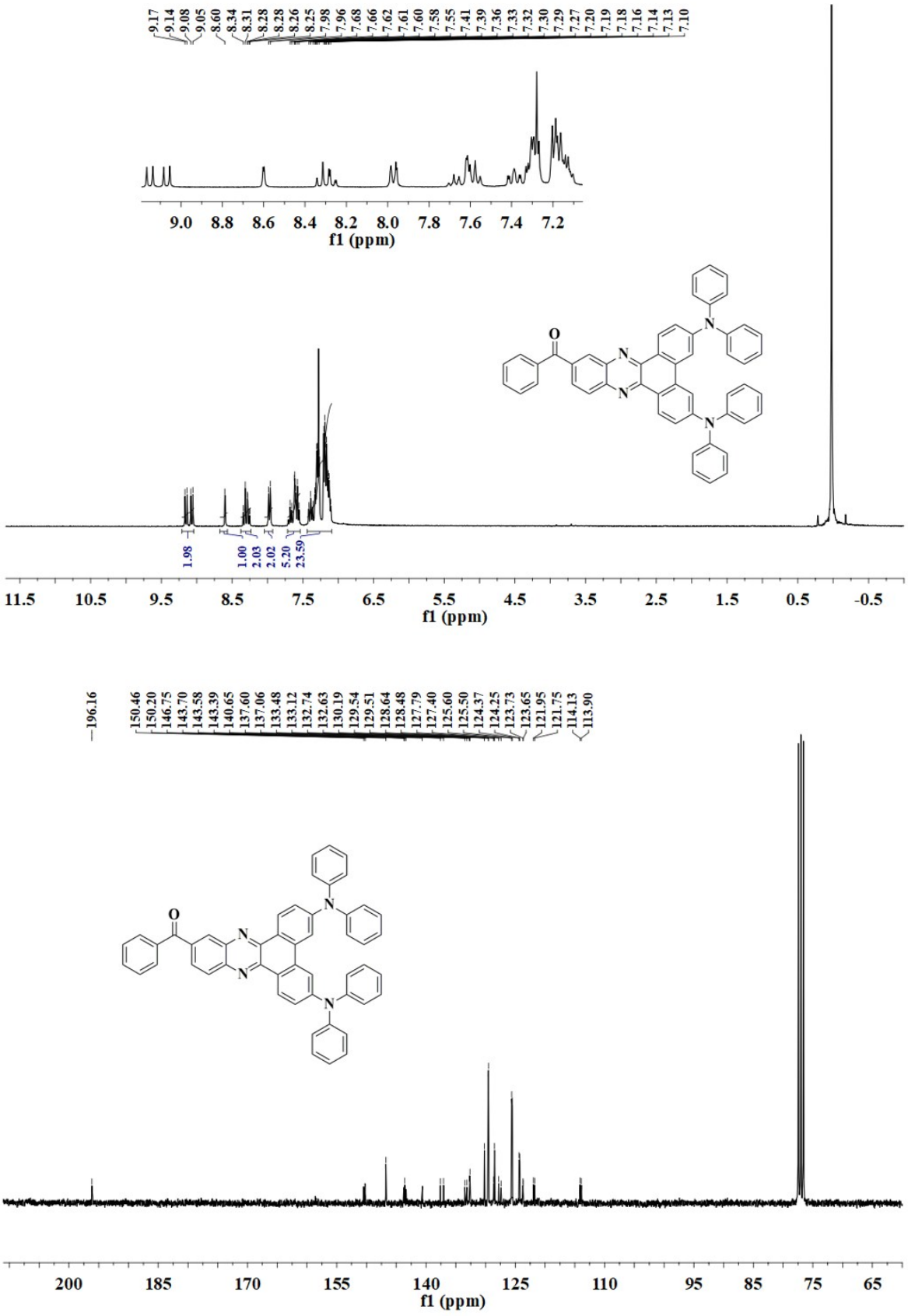

Figure S24: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **2**.

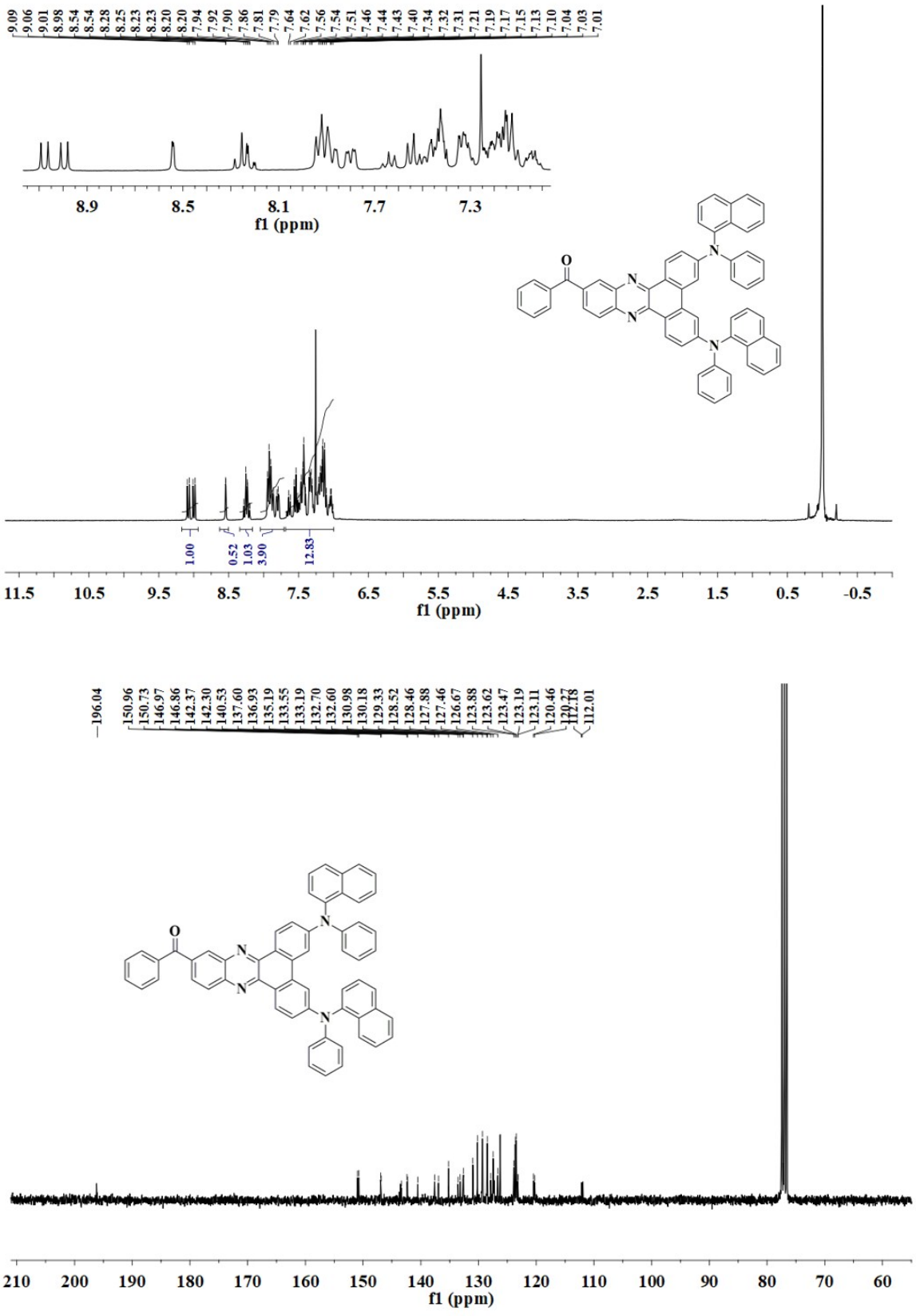

Figure S25: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **3**.

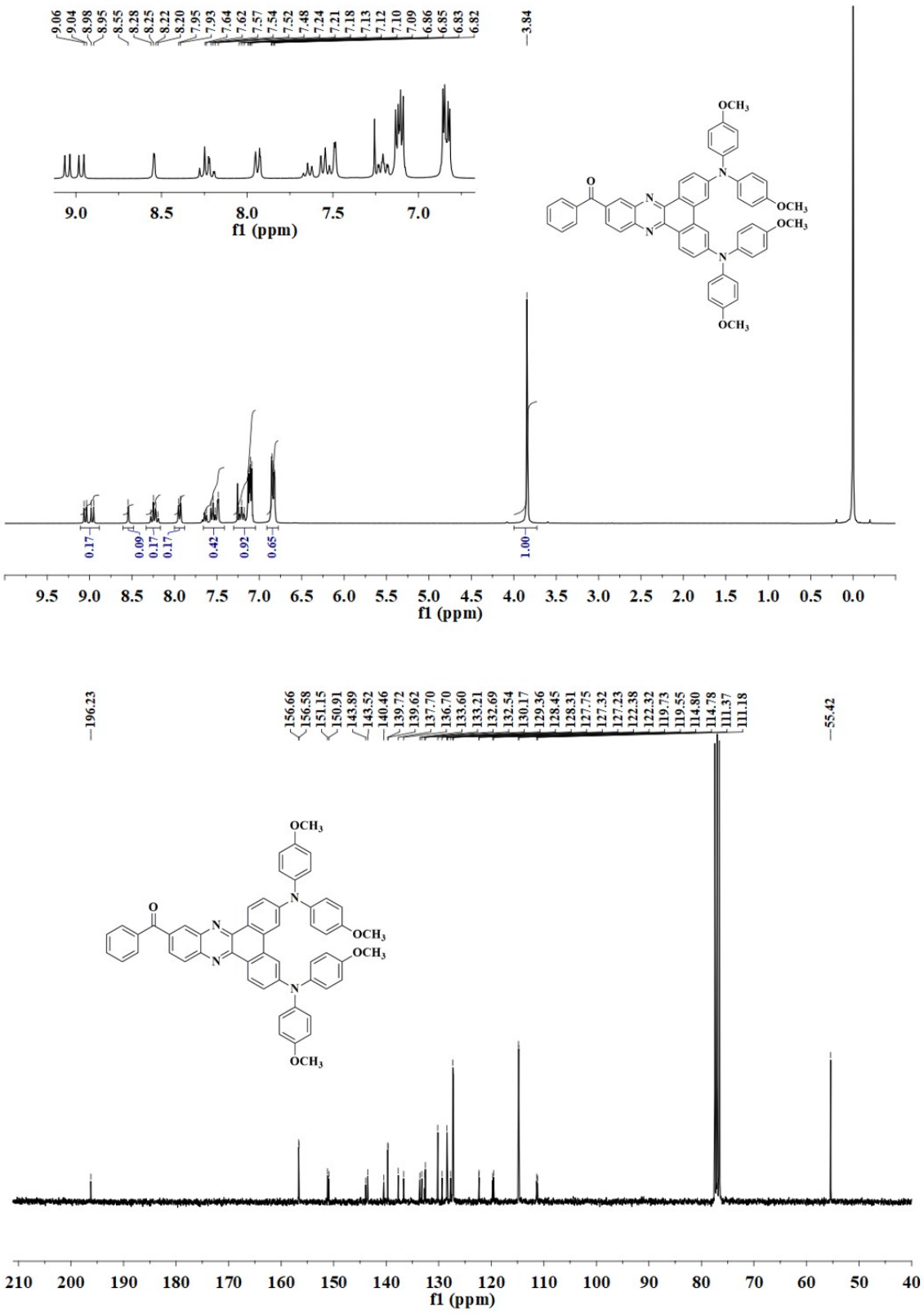

Figure S26: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **4**.

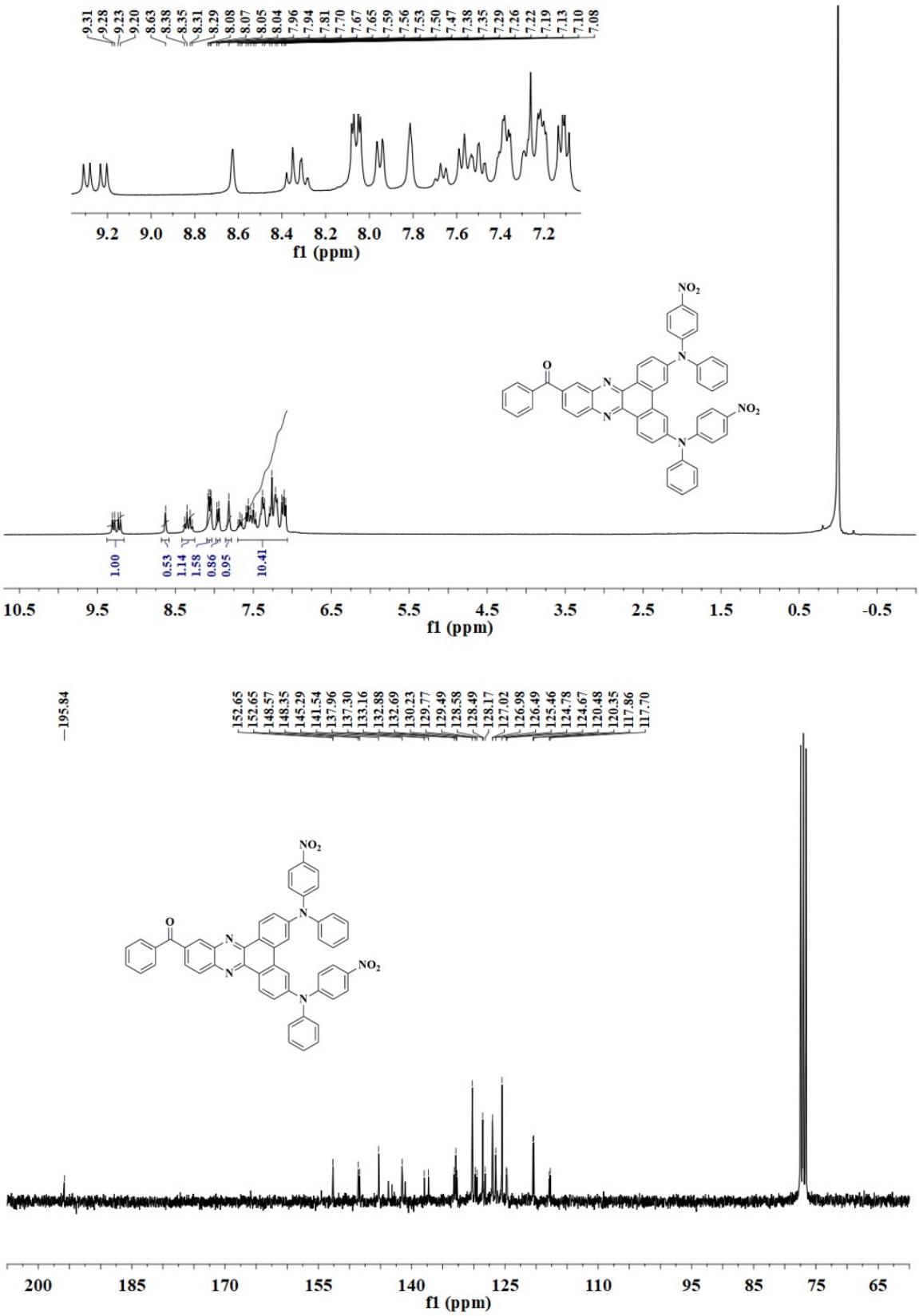

Figure S27: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **5**.

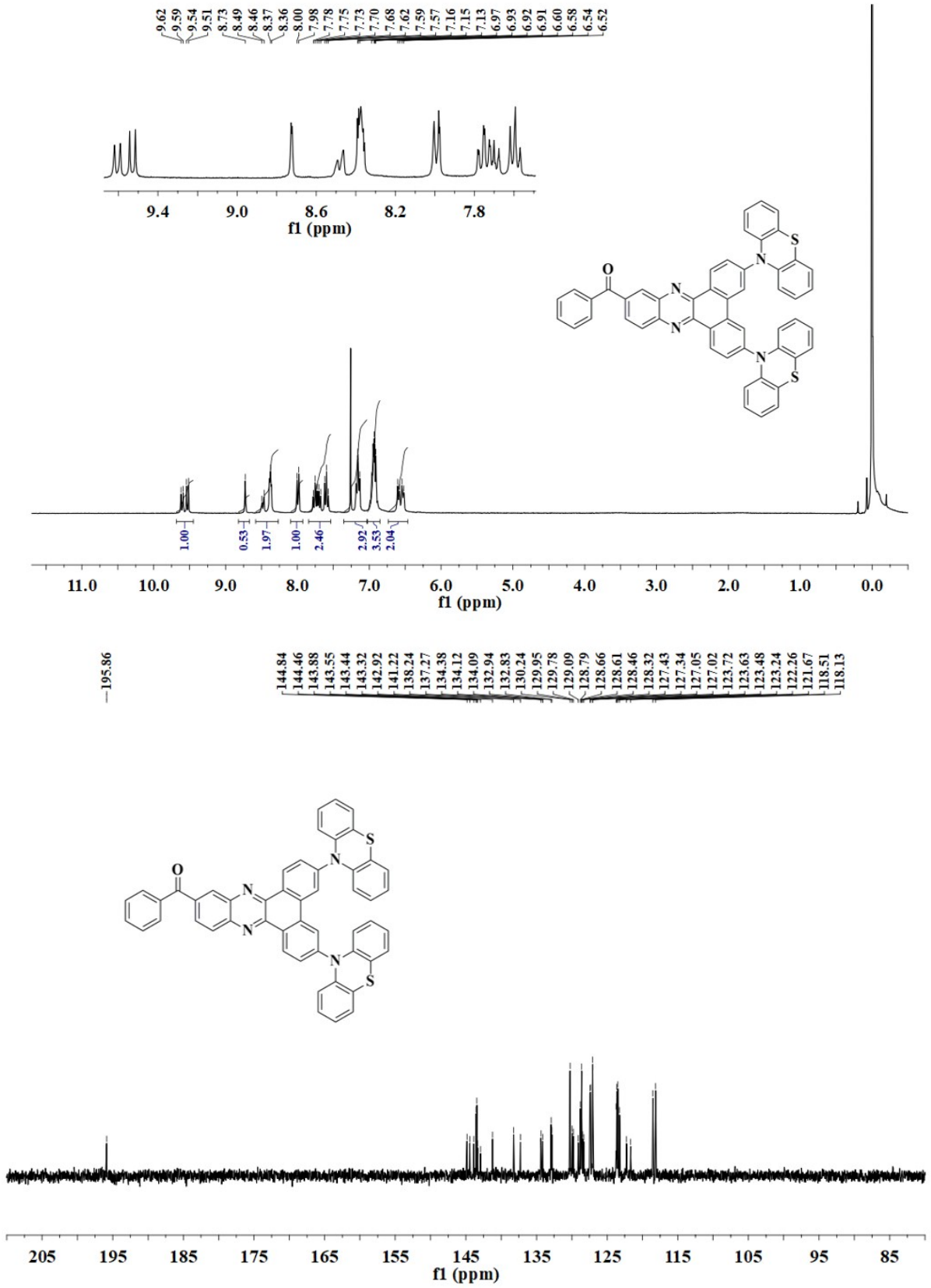

Figure S28: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **6**.

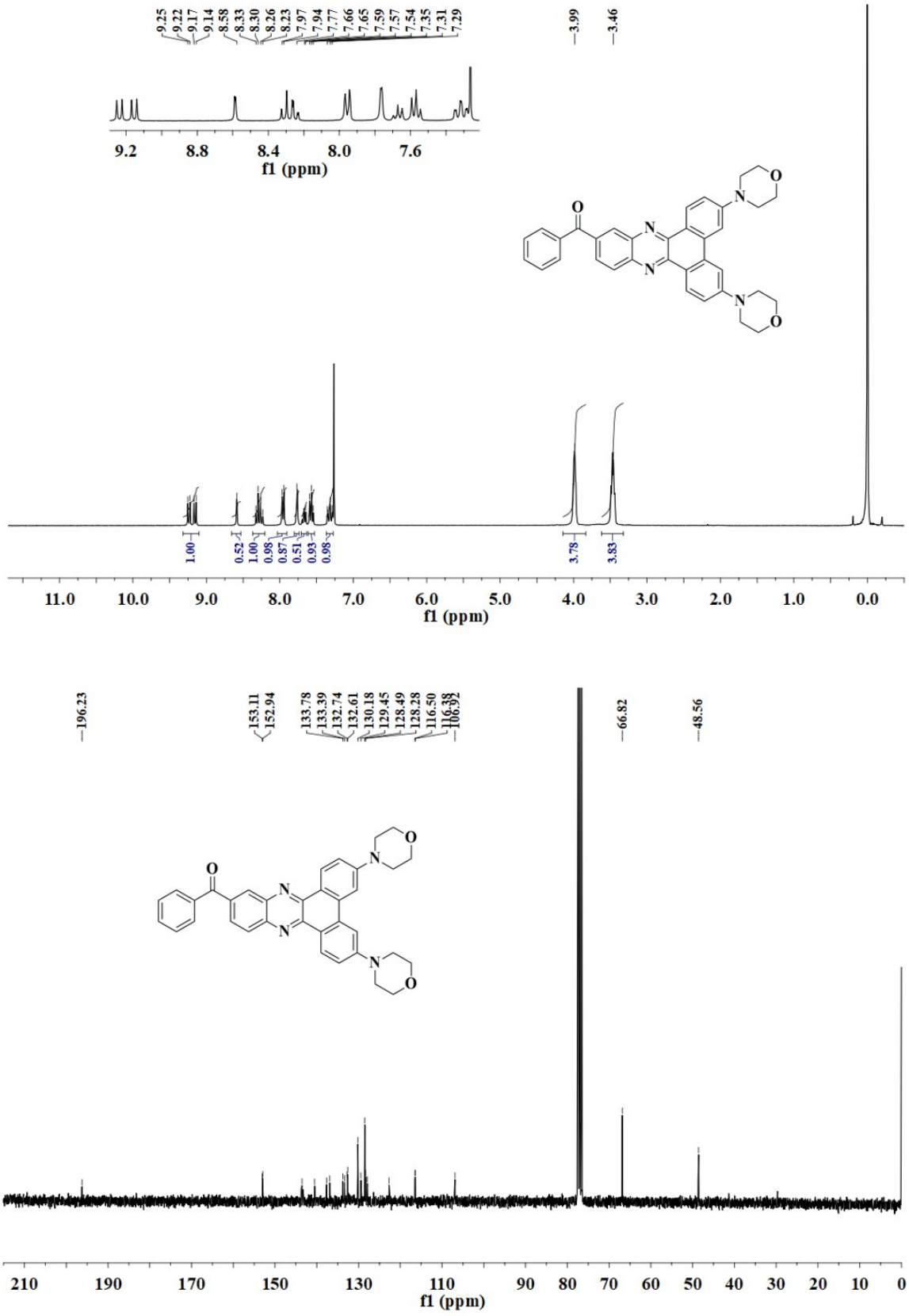

Figure S29: ^{1}H-NMR (above) and ^{13}C-NMR (below) spectra in $CDCl_3$ of compound **8**.

10. Optimized structures of compounds 1–8

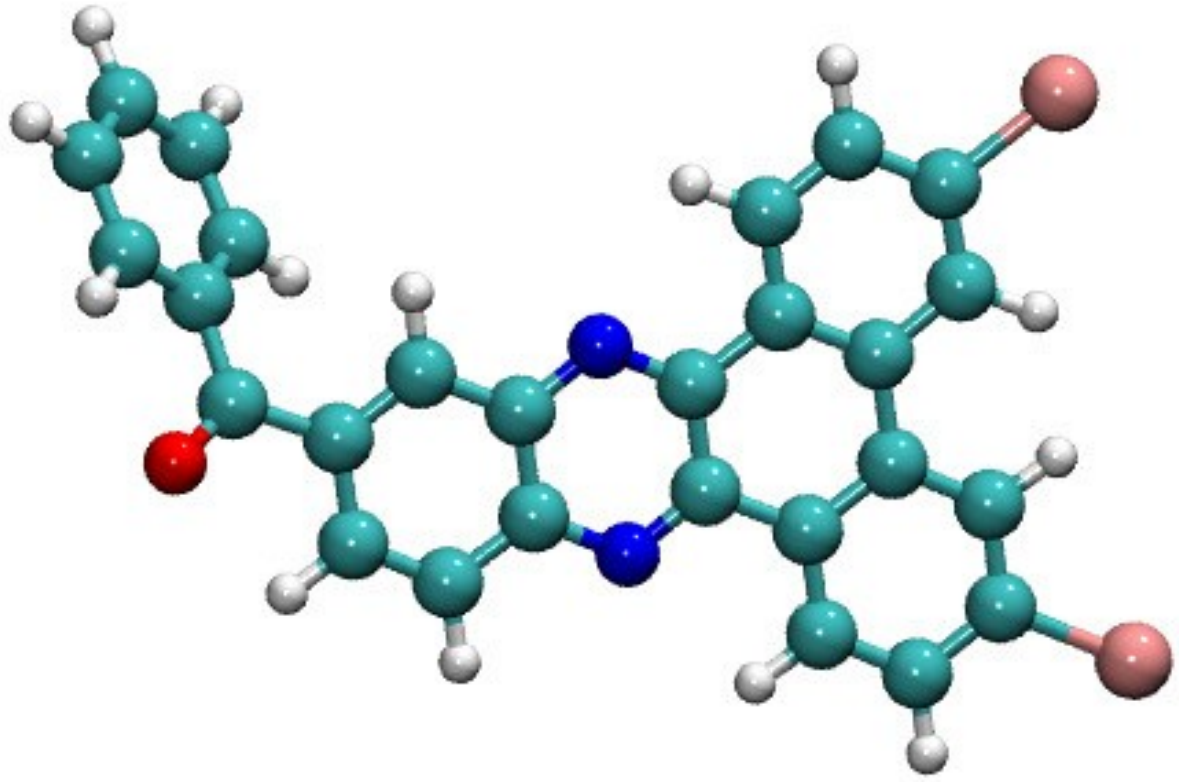

Figure S30: Optimized structures of compound **1**.

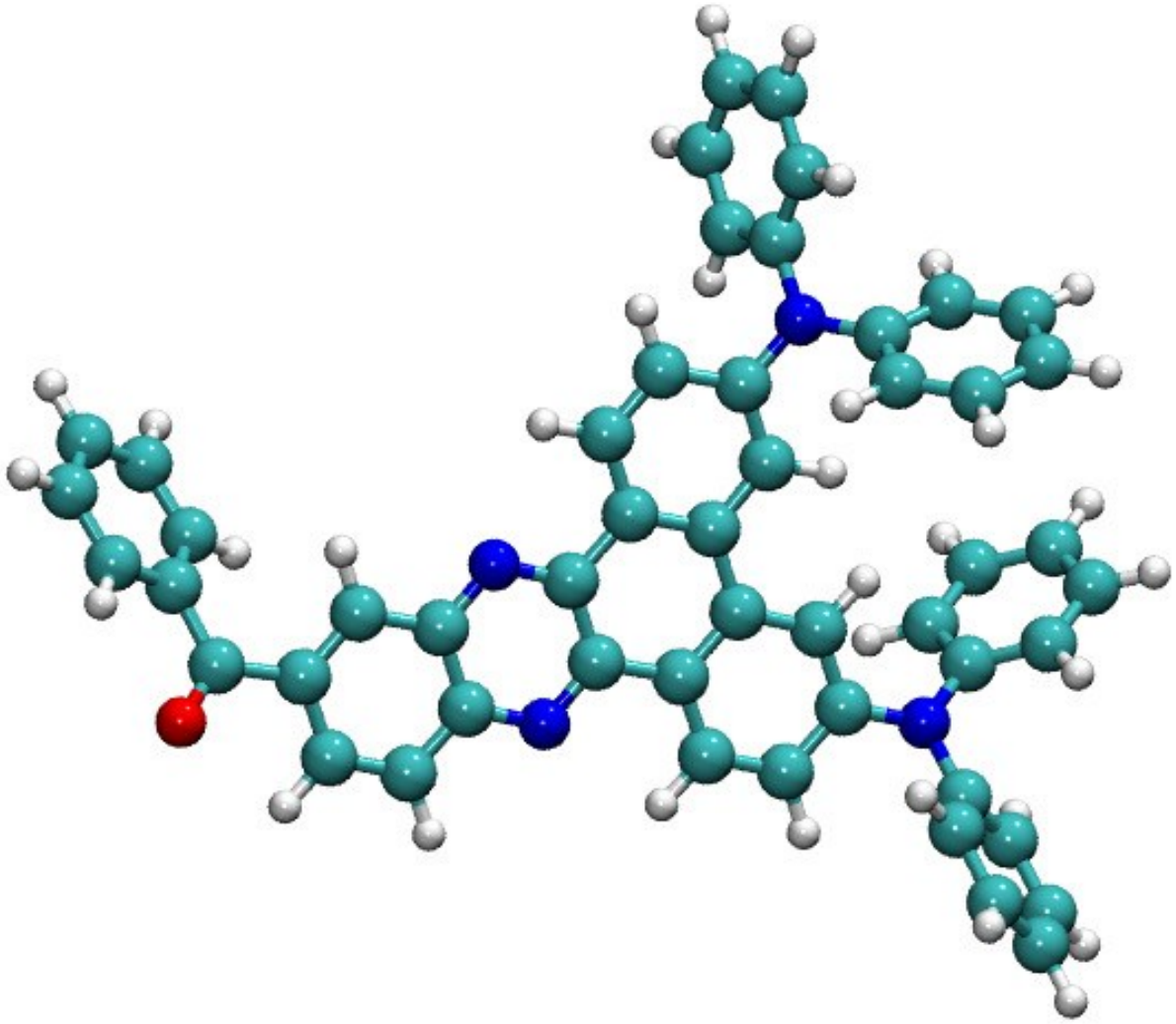

Figure S31: Optimized structures of compound **2**.

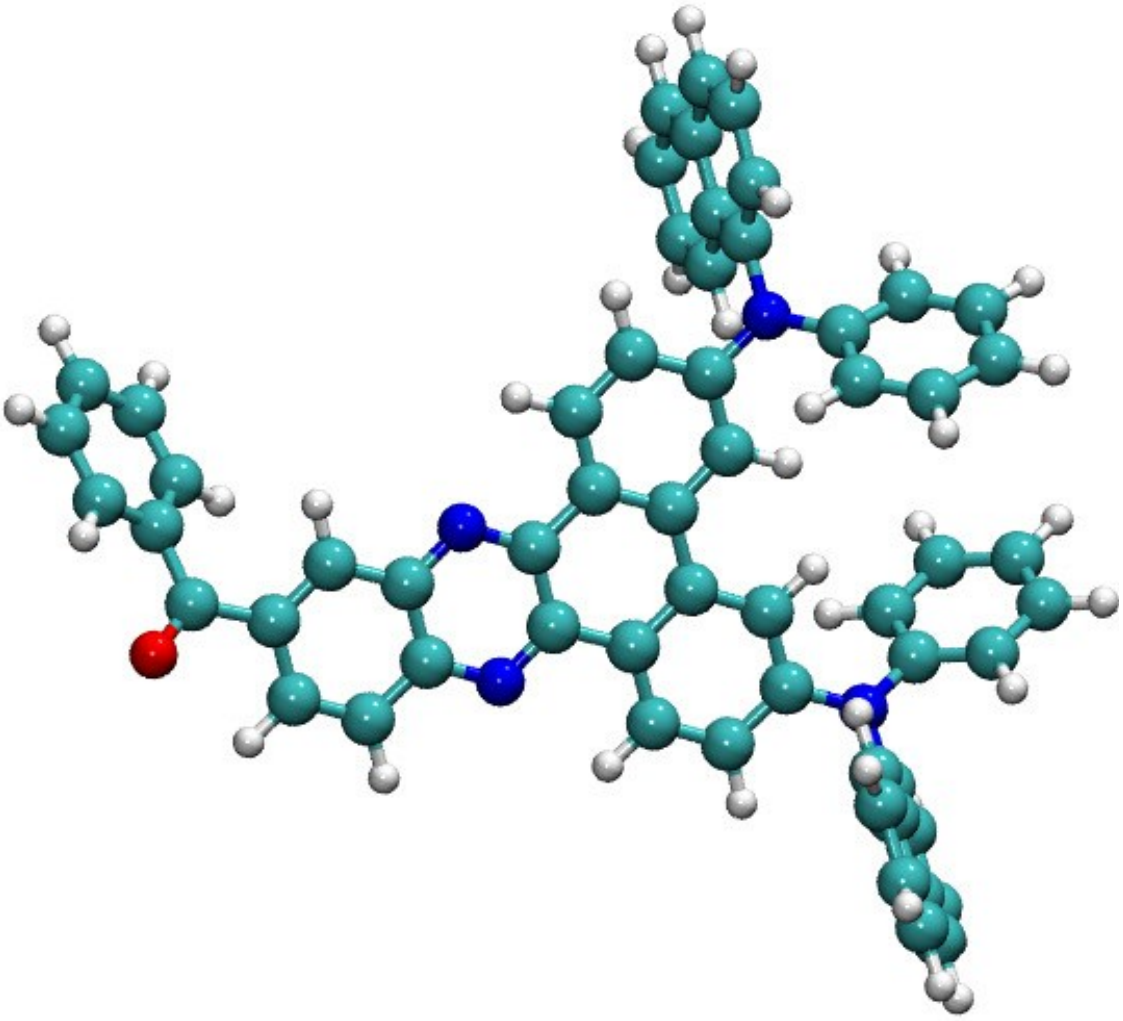

Figure S32: Optimized structures of compound **3**.

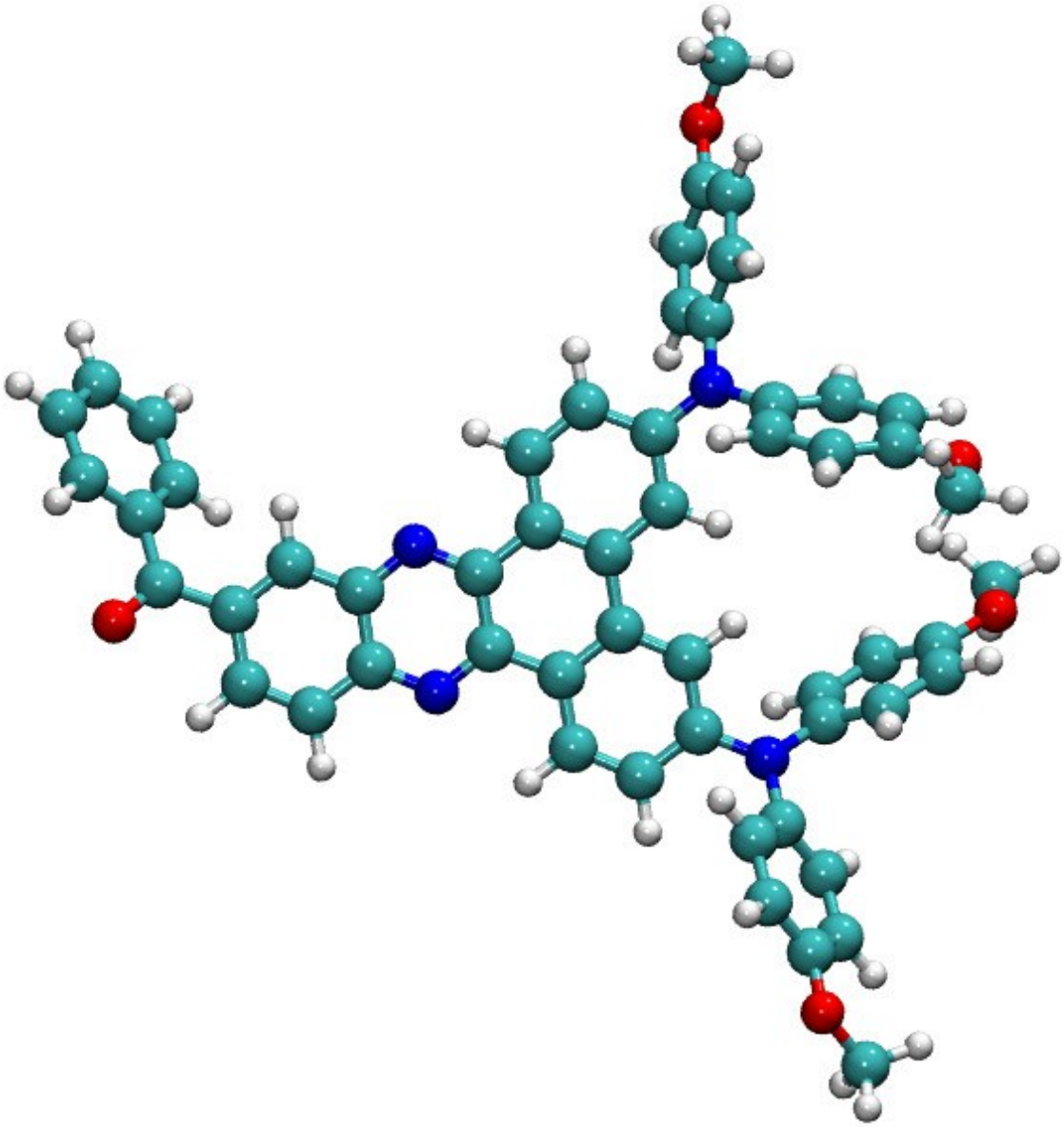

Figure S33: Optimized structures of compound **4**.

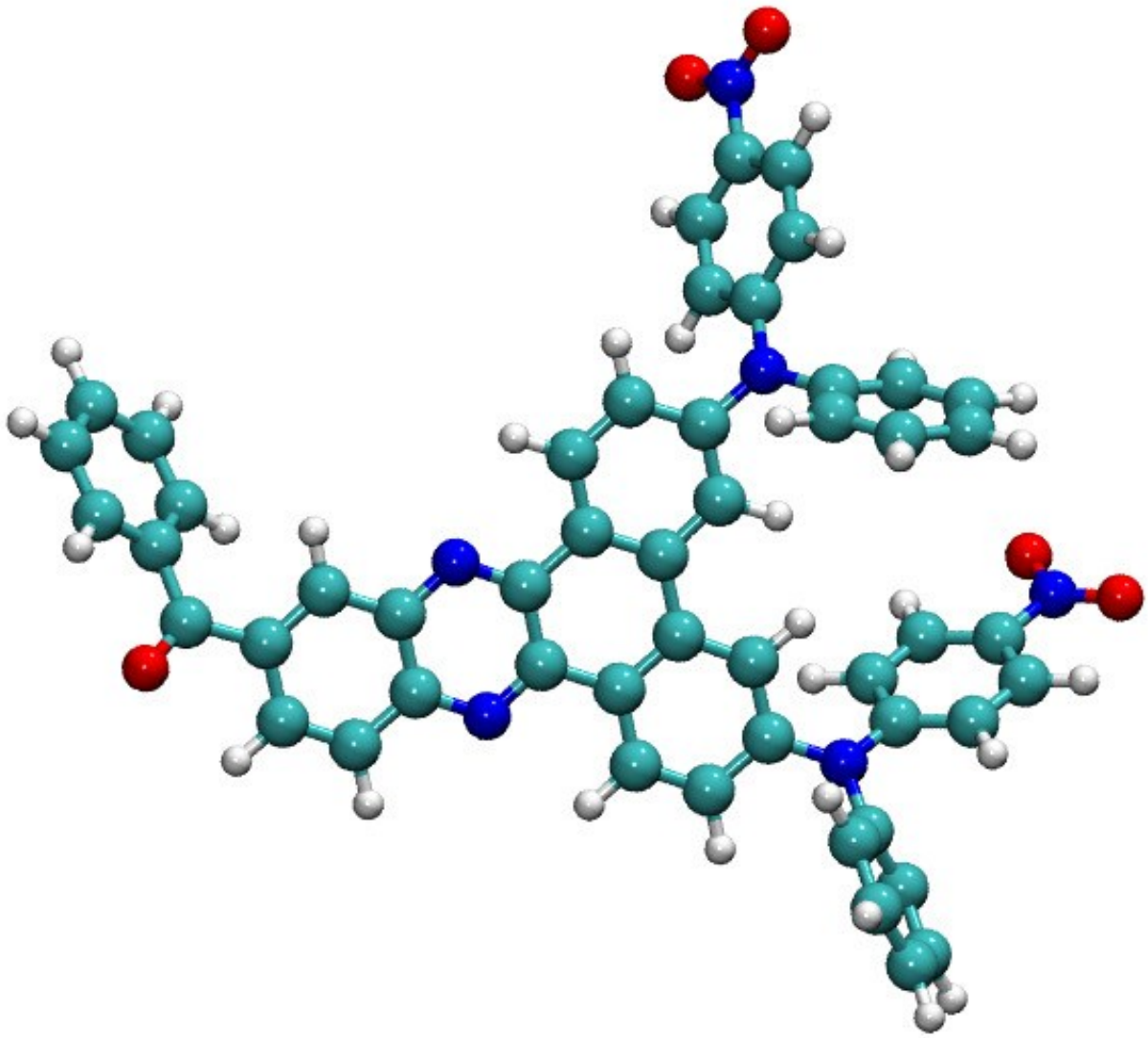

Figure S34: Optimized structures of compound **5**.

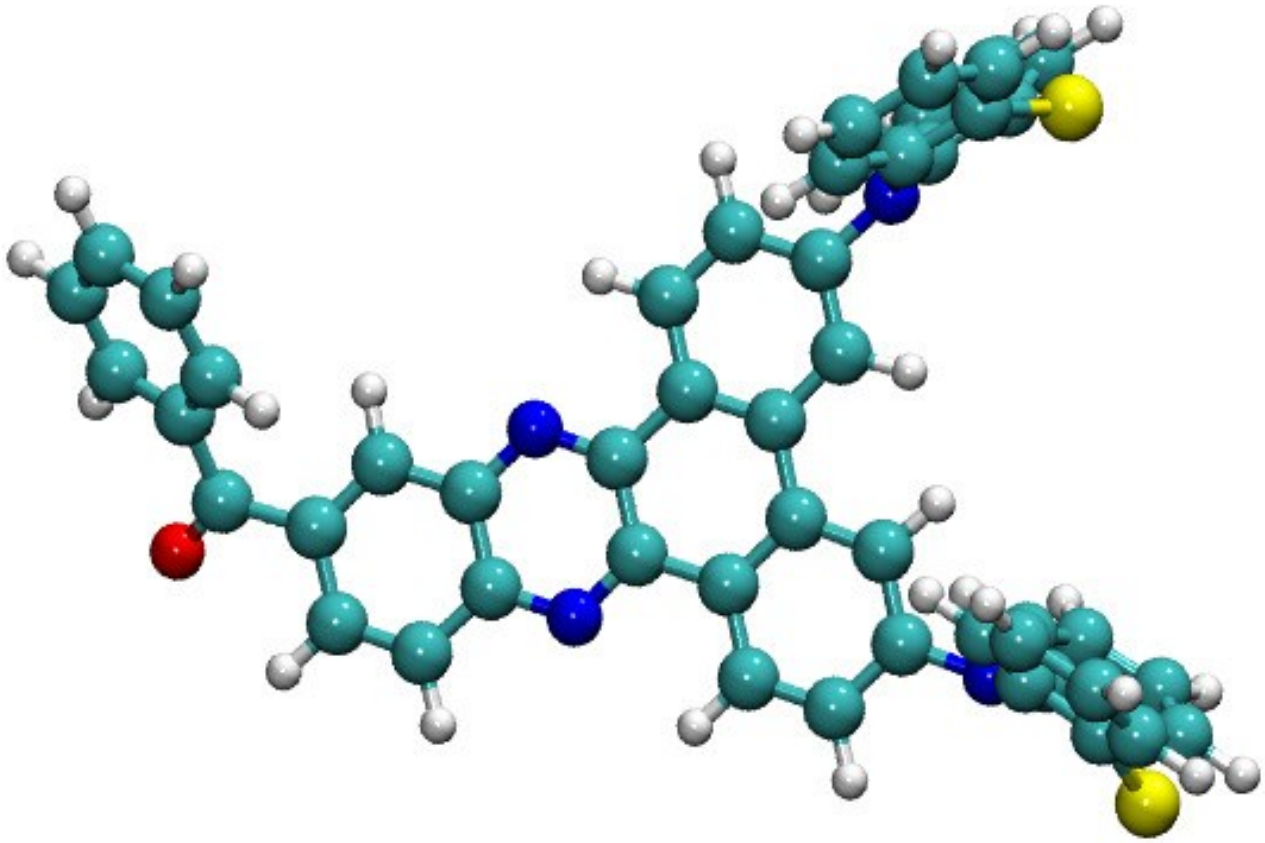

Figure S35: Optimized structures of compound **6**.

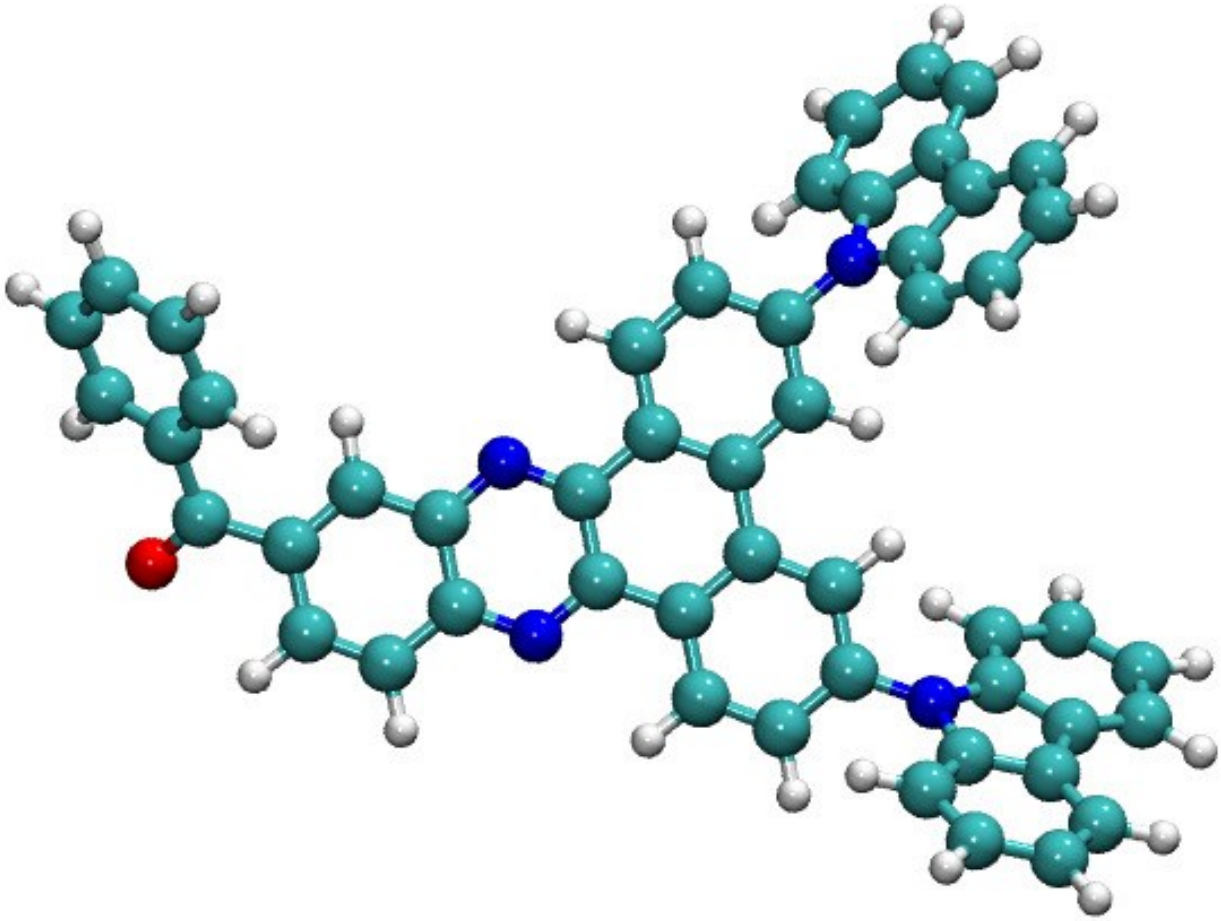

Figure S36: Optimized structures of compound **7**.

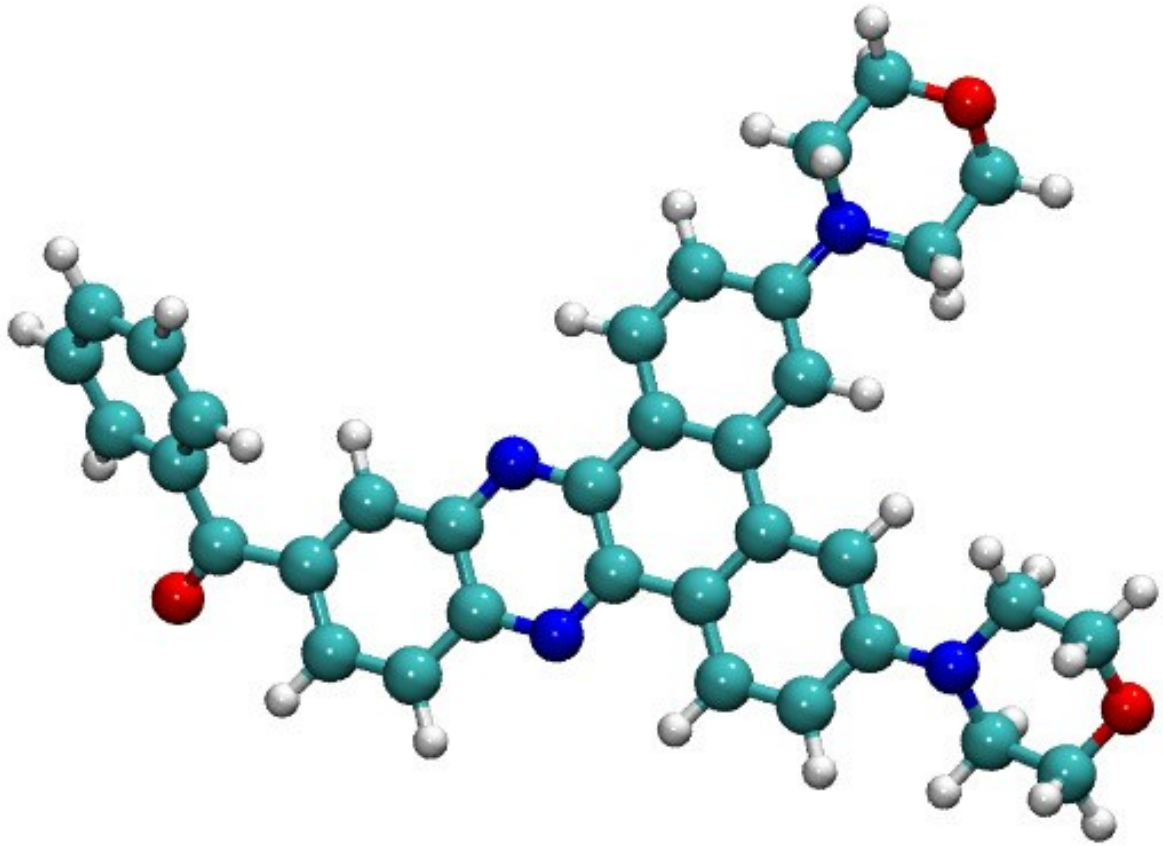

Figure S37: Optimized structures of compound **8**.

11. Frontier molecular orbitals of compounds **1–8**.

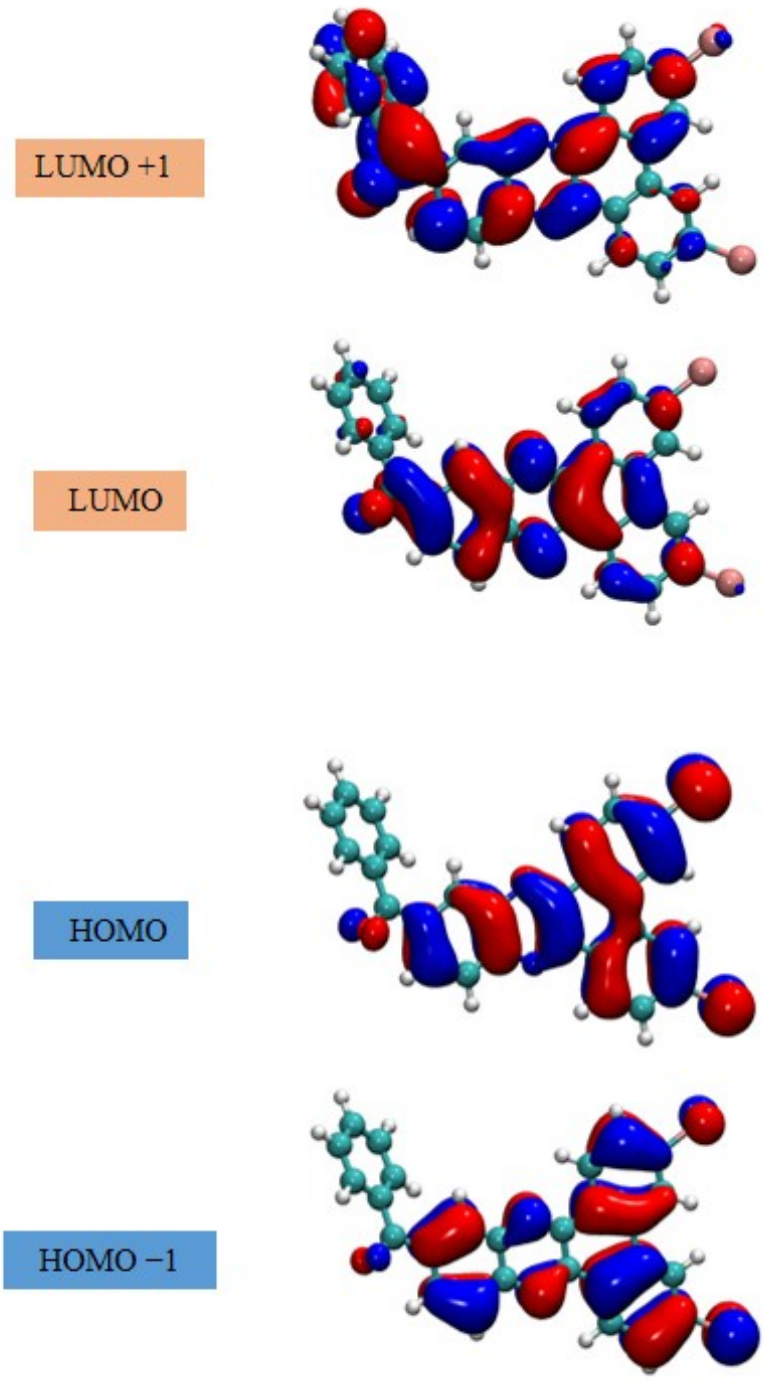

Figure S38: Frontier molecular orbital of compound 1.

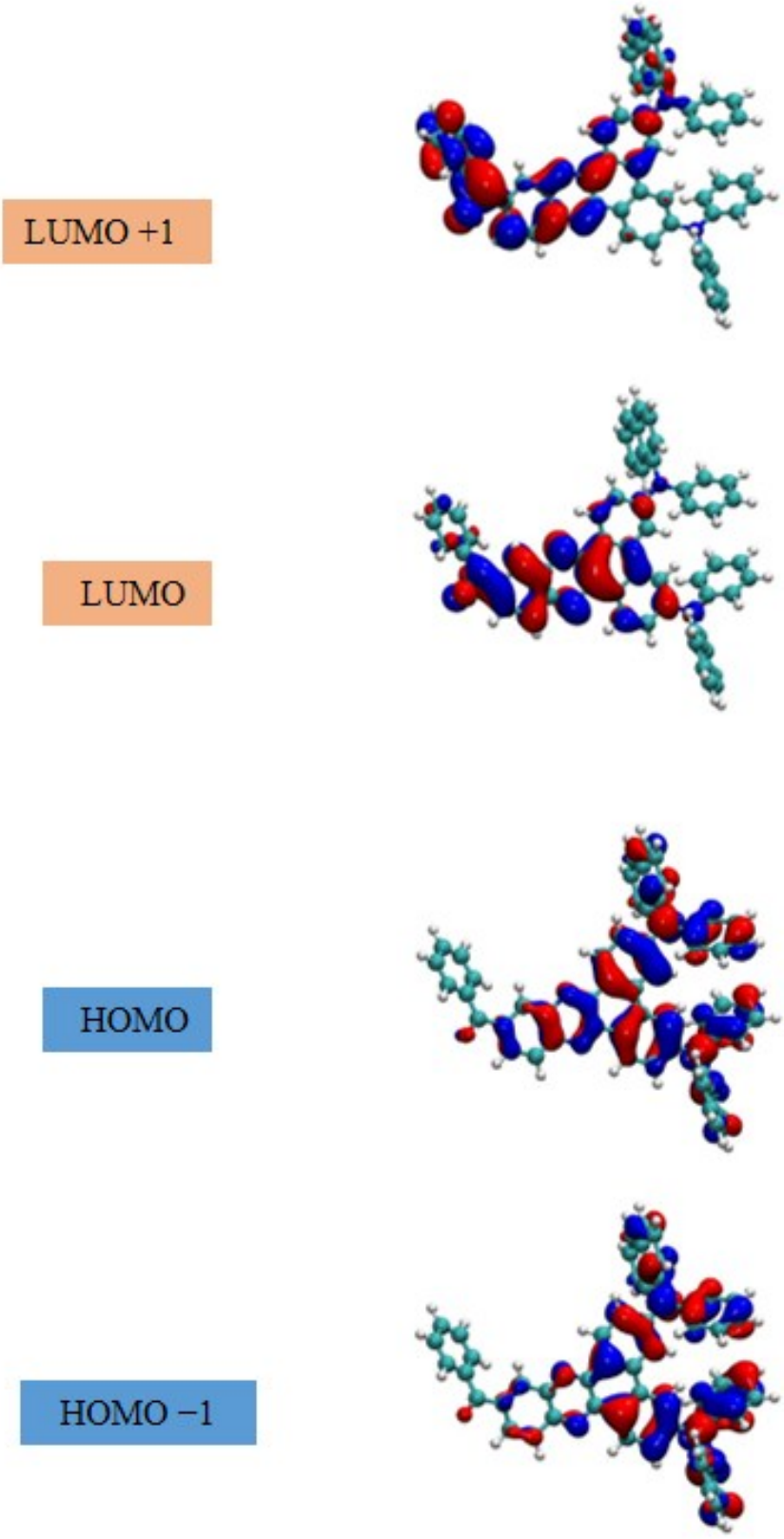

Figure S39: Frontier molecular orbital of compound 3.

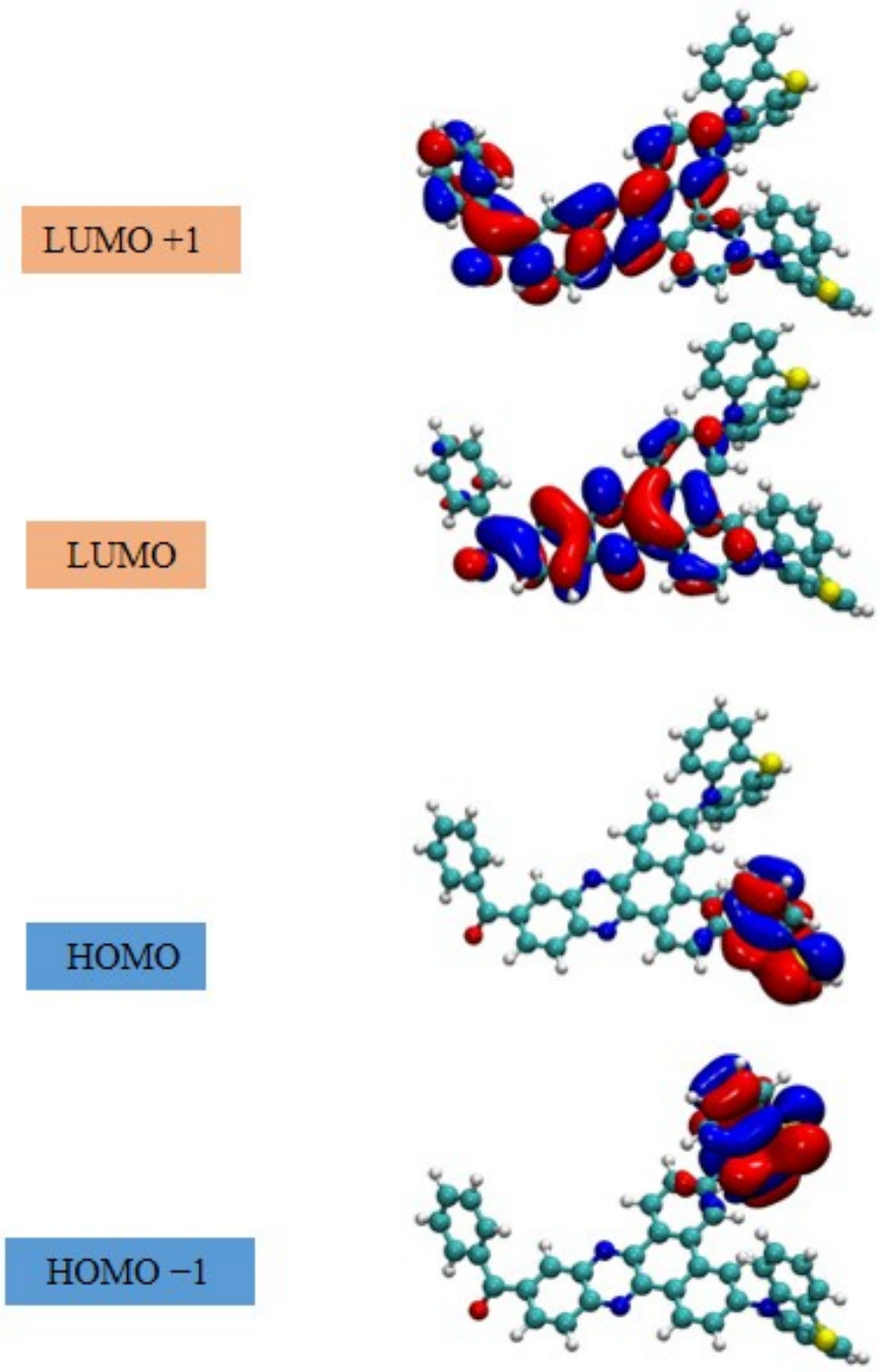

Figure S40: Frontier molecular orbital of compound 6.

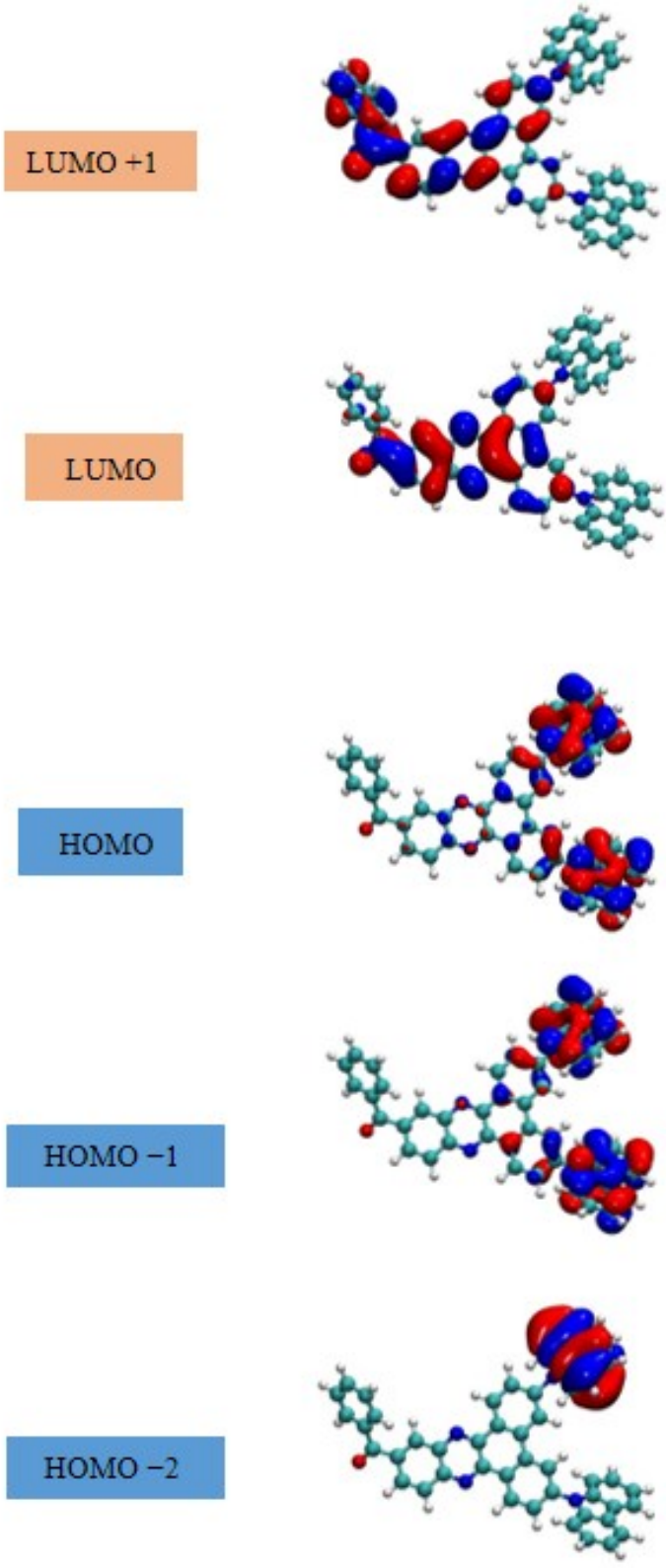

Figure S41: Frontier molecular orbital of compound 7.

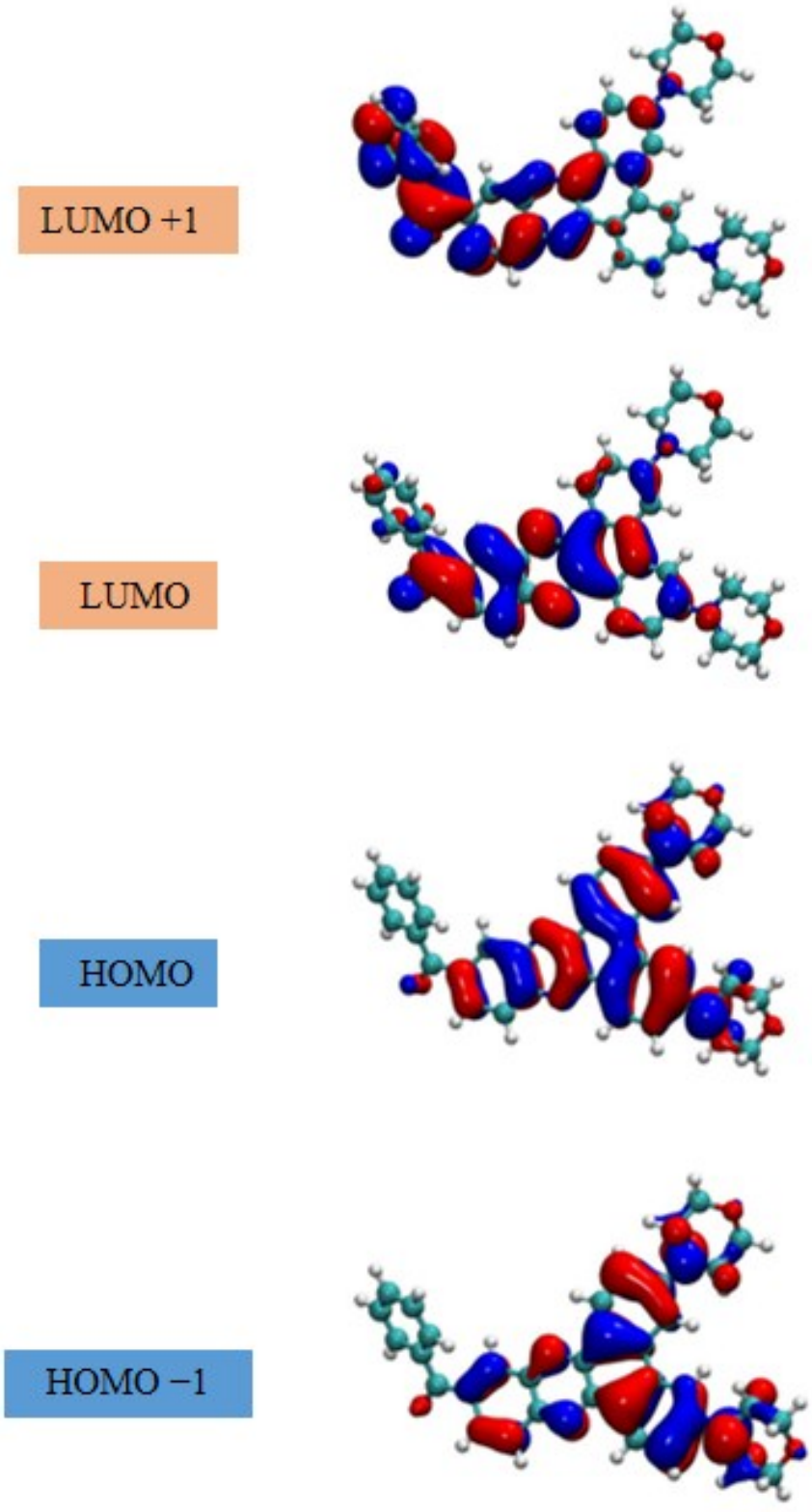

Figure S42: Frontier molecular orbital of compound 8.

12. Cartesian coordinates and charges (Mulliken and Lowdin) of compounds **1–8**.

A. Table S1: Cartesian coordinates of optimized structure of compound **1.**
Total Energy: – 6370.67 Hartrees

Atom	X	Y	Z	Mulliken Charges	Lowdin Charges
C	6.909965	9.741661	6.843187	-0.29744	-0.02758
C	8.009613	10.19348	6.116429	-0.25972	-0.04206
C	9.295776	9.796801	6.476712	-0.89809	-0.02603
C	9.489642	8.927235	7.558166	1.252826	-0.09421
C	8.374969	8.459055	8.268386	0.406206	0.001555
C	10.8394	8.403564	7.942559	-0.95445	0.024908
C	12.06862	9.241798	7.732019	0.727969	-0.07567
C	13.30783	8.55935	7.537871	0.23655	0.010206
C	14.48161	9.249197	7.405577	-0.34281	-0.00883
C	14.48858	10.66858	7.49086	0.070138	-0.03945
C	13.25507	11.35881	7.711502	0.186201	-0.04603
C	12.04966	10.61681	7.820163	-0.93283	0.006104
N	15.64584	11.34956	7.371147	0.165383	-0.04076
C	15.60493	12.6703	7.469982	-0.20357	-0.02107
C	14.36627	13.36325	7.698279	-0.23479	-0.02551
N	13.22375	12.70393	7.813392	0.185698	-0.03669
O	10.95261	7.293764	8.436978	-0.18438	-0.15856
C	16.84762	13.4302	7.344658	0.413713	-0.04931
C	16.83437	14.84103	7.449469	0.593089	-0.02888
C	15.56598	15.55062	7.685208	0.566473	-0.02997
C	14.35969	14.82195	7.806335	0.493173	-0.04866
C	15.5117	16.95365	7.796667	-0.64862	-0.06616
C	14.30681	17.5934	8.018438	-0.10031	-0.2269
C	13.11097	16.87986	8.139368	-0.40092	-0.06833
C	13.15106	15.50288	8.032094	-0.27221	0.008059
C	18.0609	12.7566	7.12016	-0.27975	0.00954
C	19.2528	13.44439	6.997897	-0.35969	-0.06814
C	19.23227	14.83813	7.102914	-0.13962	-0.22602
C	18.05613	15.5301	7.32311	-0.74364	-0.06644
Br	14.27268	19.5027	8.164448	-0.14907	0.277264
Br	20.87405	15.80999	6.938147	-0.14805	0.278185
H	6.24023	8.519243	8.485676	0.178279	0.056844
H	5.9105	10.05912	6.567623	0.163875	0.056017
H	7.867285	10.85319	5.268127	0.1834	0.056779
H	10.14387	10.14325	5.899121	0.18209	0.068216
H	8.533097	7.768962	9.088189	0.21778	0.073486
H	13.29079	7.477237	7.502629	0.229287	0.076466
H	15.42575	8.743006	7.243427	0.187361	0.070924

H	11.13449	11.16676	7.998881	0.220091	0.08265
H	16.40713	17.55097	7.71114	0.076315	0.061288
H	12.17656	17.39694	8.31355	0.244858	0.062704
H	12.24388	14.92005	8.121713	0.178672	0.077377
H	18.0409	11.67746	7.045119	0.194163	0.077874
H	20.18263	12.91881	6.825195	0.244159	0.062877
H	18.09457	16.60668	7.395744	0.070204	0.061281

B. Table S2: Cartesian coordinates of optimized structure of compound **2.** Total Energy: –2258.74 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	-11.8869	4.510302	8.058431	-0.31929	-0.03094
C	-11.9193	3.470675	8.989779	-0.27238	-0.04153
C	-11.4556	2.208326	8.639467	0.343712	-0.00038
C	-10.9265	1.975303	7.362309	1.286811	-0.09217
C	-10.8983	3.02318	6.433036	-0.90119	-0.02646
C	-10.4905	0.580343	7.024149	-0.78267	0.024548
C	-9.37887	0.350079	6.044488	0.585589	-0.08266
C	-9.36252	-0.89071	5.339677	0.166743	0.003747
C	-8.34769	-1.19734	4.473841	-0.26125	-0.01256
C	-7.27004	-0.28982	4.282702	0.025558	-0.043
C	-7.26419	0.942719	5.006397	0.131592	-0.05081
C	-8.34115	1.244309	5.878508	-0.93399	0.004055
N	-6.26765	-0.59522	3.432651	0.161072	-0.04908
C	-5.27843	0.277034	3.295994	-0.19563	-0.02011
C	-5.26542	1.51398	4.037621	-0.33051	-0.02507
N	-6.24913	1.823805	4.86809	0.184166	-0.04445
O	-11.038	-0.37515	7.551759	-0.18971	-0.16437
C	-4.18682	-0.02176	2.37772	0.160322	-0.06151
C	-3.11319	0.886606	2.212738	-0.10006	-0.02263
C	-3.08621	2.138844	2.991281	-0.13871	-0.02426
C	-4.14965	2.439834	3.875322	0.193535	-0.06031
C	-2.03332	3.060324	2.873895	-0.3012	-0.02413
C	-1.9994	4.241829	3.613726	-0.3183	-0.03481
C	-3.06729	4.52809	4.488212	-0.13664	-0.02631
C	-4.11621	3.642207	4.605303	-0.29175	0.01036
C	-4.19191	-1.21981	1.639103	-0.26997	0.012124
C	-3.18278	-1.52475	0.752509	-0.10753	-0.02693
C	-2.10778	-0.62965	0.574982	-0.24694	-0.03297
C	-2.08776	0.553297	1.314058	-0.31474	-0.02499
N	-0.90753	5.132775	3.499346	0.741517	-0.0945

N	-1.07617	-0.92321	-0.34425	0.736184	-0.09391
C	-1.12182	6.539255	3.54213	-0.15753	-0.05757
C	0.415948	4.631694	3.333581	-0.30509	-0.0578
C	-0.62736	-2.26359	-0.51728	-0.08301	-0.05801
C	-0.47179	0.117133	-1.10806	-0.29253	-0.05819
C	-0.26595	7.364685	4.283669	0.17399	-0.03573
C	-0.47208	8.740629	4.316052	-0.37325	-0.03718
C	-1.53958	9.314118	3.625726	-0.3809	-0.057
C	-2.39629	8.494312	2.892276	-0.36075	-0.03785
C	-2.18726	7.119141	2.840535	0.258464	-0.0389
C	1.276874	5.201305	2.387044	0.160195	-0.03538
C	2.574914	4.720055	2.239955	-0.32592	-0.03697
C	3.028855	3.657228	3.019693	-0.37841	-0.05611
C	2.171262	3.084142	3.958486	-0.24865	-0.03758
C	0.877738	3.57	4.123166	0.074531	-0.03523
C	0.920498	0.1765	-1.24683	0.05148	-0.03439
C	1.507041	1.181664	-2.01094	-0.29697	-0.03667
C	0.719093	2.148632	-2.63346	-0.41828	-0.05549
C	-0.66734	2.095862	-2.49046	-0.1795	-0.03764
C	-1.26235	1.084984	-1.7417	0.063346	-0.03514
C	-0.39594	-2.77214	-1.80209	0.171995	-0.03507
C	0.05109	-4.07952	-1.96897	-0.37903	-0.03699
C	0.259947	-4.90334	-0.86329	-0.38138	-0.05598
C	0.025455	-4.40095	0.416106	-0.35971	-0.03739
C	-0.40612	-3.08943	0.592652	0.196544	-0.03823
H	-11.3738	5.083101	6.04813	0.180542	0.055932
H	-12.2564	5.493224	8.328871	0.161234	0.054926
H	-12.3122	3.645336	9.985021	0.176412	0.055826
H	-11.4958	1.385757	9.343154	0.215138	0.072823
H	-10.5197	2.850833	5.433148	0.185762	0.068471
H	-10.1763	-1.58372	5.512764	0.224359	0.074652
H	-8.33242	-2.12967	3.921702	0.176939	0.069101
H	-8.29949	2.180429	6.420738	0.20433	0.081212
H	-1.21242	2.865666	2.199295	-0.0682	0.074109
H	-3.05459	5.439015	5.073225	0.180785	0.076187
H	-4.93327	3.849417	5.283929	0.2321	0.075975
H	-5.02602	-1.89616	1.772228	0.246338	0.076449
H	-3.21669	-2.44497	0.18327	0.179987	0.07626
H	-1.24922	1.219718	1.174648	-0.07789	0.073943
H	0.558579	6.923656	4.830713	0.166663	0.074665
H	0.198515	9.365251	4.895742	0.186012	0.055416
H	-1.70087	10.38526	3.658343	0.158871	0.053022
H	-3.22568	8.927069	2.343872	0.190962	0.055431
H	-2.84875	6.489251	2.258078	0.151752	0.074427

H	0.925917	6.022137	1.773384	0.170621	0.074713
H	3.229141	5.171377	1.502318	0.188707	0.055363
H	4.038015	3.281117	2.898654	0.162287	0.05314
H	2.514126	2.262835	4.577973	0.191927	0.055777
H	0.219872	3.12928	4.862484	0.177106	0.07547
H	1.536908	-0.56787	-0.75737	0.16991	0.074877
H	2.586478	1.214724	-2.10838	0.190513	0.055471
H	1.178793	2.932995	-3.22336	0.159149	0.05324
H	-1.29258	2.836607	-2.97652	0.192753	0.055742
H	-2.34043	1.040419	-1.64465	0.173058	0.07545
H	-0.56649	-2.1391	-2.66451	0.167233	0.074707
H	0.22388	-4.45907	-2.96993	0.186369	0.055481
H	0.601865	-5.92299	-0.99685	0.159132	0.053236
H	0.19179	-5.02786	1.285102	0.192035	0.055759
H	-0.57529	-2.70053	1.589547	0.15284	0.074695

C. Table S3: Cartesian coordinates of optimized structure of compound **3.**
Total Energy: –2566.08 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	11.33942	8.799746	10.12792	-0.3112	-0.0314
C	10.40604	8.96996	9.107528	-0.25081	-0.04362
C	9.283237	8.147245	9.043148	-0.88996	-0.02628
C	9.075575	7.157509	10.01247	1.271575	-0.09201
C	10.00805	7.010034	11.0489	0.344795	-0.00067
C	7.846874	6.297285	10.04076	-0.76371	0.024454
C	7.172993	5.895863	8.763166	0.516933	-0.08364
C	5.780095	5.59104	8.816553	0.146243	0.002832
C	5.109123	5.158767	7.704468	-0.25756	-0.01298
C	5.800493	4.977254	6.475694	0.058371	-0.04335
C	7.201014	5.255952	6.419756	0.112867	-0.05131
C	7.865342	5.724902	7.581534	-0.92552	0.00381
N	5.139696	4.540529	5.382967	0.164124	-0.04981
C	5.828879	4.37287	4.263082	-0.16356	-0.01958
C	7.244468	4.646572	4.208907	-0.36831	-0.02464
N	7.898274	5.080395	5.275228	0.187508	-0.04516
O	7.393307	5.916774	11.10888	-0.1901	-0.16521
C	5.142266	3.900225	3.067596	0.134087	-0.0645
C	5.850105	3.701951	1.856635	-0.06801	-0.02281
C	7.300335	3.971319	1.803927	-0.13189	-0.02459
C	7.970201	4.44051	2.960081	0.147118	-0.06311
C	8.042595	3.7883	0.628074	-0.29575	-0.03485

C	9.416298	4.035025	0.572339	-0.03639	-0.03456
C	10.06615	4.508562	1.729451	-0.27812	-0.02646
C	9.348621	4.706119	2.890248	-0.24255	0.015101
C	3.763286	3.627814	3.105072	-0.22737	0.016887
C	3.083122	3.182327	1.992261	-0.28459	-0.02718
C	3.772077	2.980637	0.779023	-0.02021	-0.03267
C	5.145556	3.23503	0.737625	-0.29468	-0.03606
N	10.13541	3.838598	-0.6254	0.736991	-0.10322
N	3.091142	2.50232	-0.3582	0.724478	-0.10234
C	11.3412	4.576354	-0.86008	-0.33874	-0.05036
C	9.815955	2.778427	-1.52196	-0.01201	-0.05213
C	3.468322	2.893022	-1.67589	-0.02092	-0.05284
C	1.881375	1.749664	-0.20142	-0.3067	-0.05034
C	11.29234	5.994084	-1.0539	0.123123	-0.05629
C	12.52306	6.695956	-1.26951	0.368586	-0.06175
C	13.74256	5.972152	-1.3148	-0.12566	-0.02782
C	13.75143	4.607959	-1.15494	-0.3969	-0.03563
C	12.54781	3.910688	-0.91965	0.092306	-0.02153
C	9.917614	2.983651	-2.90442	0.026458	-0.03222
C	9.637526	1.948698	-3.79141	-0.43868	-0.03543
C	9.240046	0.698516	-3.3192	-0.44629	-0.05728
C	9.136055	0.491916	-1.94423	-0.10769	-0.03759
C	9.428178	1.517179	-1.04912	0.134588	-0.04148
C	1.91175	0.453685	0.406372	0.120596	-0.05668
C	0.676351	-0.25673	0.558368	0.349058	-0.06174
C	-0.52722	0.322068	0.079398	-0.1287	-0.02721
C	-0.51699	1.55409	-0.52765	-0.41553	-0.03569
C	0.690376	2.271678	-0.66117	0.091863	-0.02104
C	3.435199	1.954046	-2.71495	0.037081	-0.03091
C	3.774561	2.328468	-4.01159	-0.45719	-0.035
C	4.162984	3.637781	-4.29184	-0.44476	-0.05604
C	4.197244	4.57439	-3.25946	-0.11825	-0.03783
C	3.845839	4.211925	-1.96225	0.138677	-0.04075
C	10.07908	6.731736	-1.06379	-0.31819	-0.01422
C	10.08262	8.092995	-1.25651	-0.26689	-0.03501
C	11.29817	8.789083	-1.44734	-0.28966	-0.04155
C	12.48806	8.10345	-1.45672	-0.15843	-0.02871
C	3.110894	-0.16791	0.84465	-0.32264	-0.0147
C	3.088747	-1.41556	1.42164	-0.26661	-0.03415
C	1.867654	-2.10694	1.592983	-0.2925	-0.04086
C	0.691723	-1.54001	1.166817	-0.14664	-0.02833
H	11.8623	7.684263	11.89517	0.175969	0.055641
H	12.21786	9.434023	10.17117	0.161057	0.054758
H	10.55036	9.743223	8.361521	0.179762	0.0559

H	8.557231	8.293355	8.252934	0.187547	0.0686
H	9.826784	6.258733	11.80794	0.214744	0.07271
H	5.270044	5.708793	9.764455	0.224811	0.074364
H	4.048545	4.937556	7.729332	0.172566	0.068881
H	8.929105	5.91273	7.508826	0.199748	0.081018
H	7.554155	3.449149	-0.27355	-0.19018	0.073113
H	11.12942	4.710048	1.707258	0.204388	0.077511
H	9.84539	5.060514	3.783923	0.263906	0.07604
H	3.23745	3.78854	4.037072	0.271088	0.076587
H	2.01945	2.989862	2.046412	0.205249	0.077755
H	5.664762	3.054032	-0.19188	-0.14979	0.072863
H	14.66711	6.51359	-1.48438	0.15253	0.060028
H	14.6848	4.057978	-1.19399	0.18358	0.056793
H	12.56397	2.836013	-0.78083	0.152113	0.076953
H	10.21981	3.954852	-3.27758	0.167939	0.07495
H	9.719906	2.125927	-4.85802	0.190915	0.05531
H	9.016149	-0.10377	-4.01244	0.163808	0.052891
H	8.839506	-0.47848	-1.56153	0.194032	0.055406
H	9.35871	1.342467	0.017513	0.18874	0.074844
H	-1.45497	-0.22805	0.194735	0.152958	0.060163
H	-1.43811	1.991062	-0.89602	0.18288	0.056798
H	0.689471	3.249556	-1.12836	0.152628	0.076709
H	3.140325	0.933769	-2.50085	0.16919	0.075205
H	3.745484	1.588553	-4.8037	0.191042	0.055475
H	4.433742	3.925167	-5.30105	0.164785	0.053069
H	4.485938	5.599287	-3.46513	0.193648	0.055424
H	3.861347	4.948944	-1.16868	0.189478	0.074848
H	9.143019	6.209268	-0.91776	0.07862	0.075903
H	9.145759	8.638651	-1.26284	0.180485	0.055824
H	11.28638	9.863467	-1.59212	0.166034	0.054751
H	13.42413	8.62938	-1.61306	0.14409	0.05977
H	4.0516	0.351773	0.719887	0.083579	0.076064
H	4.014992	-1.87442	1.748586	0.180703	0.056101
H	1.864436	-3.08757	2.055247	0.166772	0.054988
H	-0.2479	-2.06957	1.284816	0.14496	0.059906

D. Table S4: Cartesian coordinates of optimized structure of compound **4.**
Total Energy: –2716.96 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	-8.7372	10.37594	-8.01076	-0.30151	-0.03226
C	-7.87606	10.93591	-8.9563	-0.28422	-0.04245
C	-6.55539	11.20799	-8.61965	0.338308	-0.00116
C	-6.06962	10.89764	-7.34183	1.296671	-0.09137
C	-6.93997	10.33683	-6.39838	-0.84921	-0.02661
C	-4.65025	11.26376	-7.01964	-0.81026	0.02433
C	-3.85887	10.44689	-6.04426	0.603774	-0.0851
C	-2.77806	11.08718	-5.36783	0.155637	0.001467
C	-1.97134	10.39018	-4.50917	-0.27928	-0.01399
C	-2.18089	9.000254	-4.29663	0.064596	-0.04405
C	-3.2473	8.345968	-4.98719	0.107488	-0.05232
C	-4.0805	9.097433	-5.85397	-0.93828	0.003343
N	-1.37614	8.312865	-3.45913	0.157493	-0.05231
C	-1.60299	7.016041	-3.30033	-0.16563	-0.01976
C	-2.67812	6.354073	-4.0013	-0.36038	-0.02476
N	-3.47278	7.02314	-4.82241	0.181522	-0.04761
O	-4.13439	12.23036	-7.55967	-0.19204	-0.16687
C	-0.75036	6.247552	-2.40455	0.120413	-0.0669
C	-0.96503	4.860879	-2.21258	-0.13502	-0.02113
C	-2.05782	4.18224	-2.93572	-0.17907	-0.02297
C	-2.89301	4.925748	-3.80378	0.142058	-0.06593
C	-2.30526	2.810221	-2.77851	-0.29652	-0.03054
C	-3.3361	2.158363	-3.45964	-0.15278	-0.03057
C	-4.15893	2.914665	-4.32192	-0.10653	-0.03259
C	-3.93537	4.264811	-4.47989	-0.24126	0.010398
C	0.303852	6.877084	-1.71548	-0.23676	0.012004
C	1.12749	6.18003	-0.86008	-0.08598	-0.03291
C	0.929149	4.796334	-0.65916	-0.109	-0.02908
C	-0.1121	4.164275	-1.3439	-0.31768	-0.0312
N	-3.54456	0.775697	-3.29887	0.824606	-0.09685
N	1.758108	4.074366	0.217692	0.820743	-0.09626
C	-4.85453	0.219906	-3.38921	-0.31526	-0.0751
C	-2.44735	-0.0986	-3.0335	-0.68204	-0.07709
C	3.127883	4.432459	0.389822	-0.38142	-0.07515
C	1.256336	2.938929	0.924443	-0.65861	-0.07778
C	-1.30104	-0.06965	-3.82808	0.1256	-0.01916
C	-0.22418	-0.91858	-3.57094	0.362557	-0.06947

C	-0.29499	-1.83211	-2.51622	-0.9474	-0.02829
C	-1.44845	-1.87726	-1.72375	-0.06117	-0.02467
C	-2.50521	-1.01637	-1.97471	0.074873	-0.0175
C	-5.93286	0.804926	-2.70724	0.160229	-0.02323
C	-7.20374	0.259337	-2.78921	-0.19529	-0.02672
C	-7.43025	-0.90203	-3.53835	-0.72828	-0.02893
C	-6.36218	-1.50185	-4.20894	0.16223	-0.06837
C	-5.08951	-0.93325	-4.13861	0.100331	-0.01834
C	3.947315	4.698212	-0.71832	0.158629	-0.0231
C	5.280503	5.035641	-0.5498	-0.20669	-0.02618
C	5.839908	5.095876	0.732693	-0.72907	-0.02856
C	5.037804	4.819581	1.842083	0.155285	-0.06831
C	3.690764	4.500753	1.664539	0.147962	-0.01787
C	0.091944	3.029699	1.687125	0.113174	-0.01835
C	-0.4037	1.924221	2.379232	0.366487	-0.06964
C	0.283074	0.708325	2.3303	-0.95834	-0.02762
C	1.459983	0.613721	1.577602	-0.08612	-0.02432
C	1.934082	1.712224	0.878223	0.089884	-0.01668
O	0.694707	-2.71226	-2.18307	-0.1033	-0.17399
C	1.890971	-2.70803	-2.94951	-0.31382	0.05548
O	-8.71498	-1.36628	-3.54624	-0.15654	-0.17715
C	-9.00791	-2.53673	-4.29606	-0.32475	0.056104
O	7.16413	5.425352	0.791845	-0.15613	-0.17668
C	7.786367	5.504484	2.066552	-0.32563	0.056277
O	-0.10572	-0.43011	2.976005	-0.10227	-0.17352
C	-1.28842	-0.39327	3.762487	-0.31251	0.055687
H	2.529766	-3.47172	-2.50877	0.169486	0.053799
H	1.696139	-2.96028	-3.9977	0.153049	0.04497
H	2.396586	-1.73755	-2.89631	0.148625	0.044898
H	-10.0729	-2.7184	-4.16086	0.178382	0.05379
H	-8.79772	-2.39261	-5.3616	0.151567	0.045265
H	-8.4438	-3.40053	-3.92709	0.150673	0.044833
H	-1.40295	-1.39433	4.175089	0.16998	0.053891
H	-1.20147	0.328338	4.582226	0.153361	0.045083
H	-2.16631	-0.14952	3.154041	0.149067	0.045011
H	8.824023	5.773085	1.875308	0.179053	0.053909
H	7.322198	6.275451	2.691368	0.151688	0.045282
H	7.751794	4.542115	2.589081	0.150557	0.044847
H	-8.94007	9.666189	-5.98887	0.179884	0.055692
H	-9.76987	10.1712	-8.27074	0.160237	0.054509
H	-8.23853	11.16545	-9.95201	0.174775	0.055395
H	-5.88167	11.66438	-9.33464	0.215147	0.072541
H	-6.58704	10.11815	-5.39816	0.187096	0.068587
H	-2.61288	12.14051	-5.55682	0.222121	0.074007

H	-1.15579	10.86851	-3.97948	0.17418	0.068442
H	-4.86928	8.568302	-6.37355	0.201101	0.080597
H	-1.68915	2.221191	-2.11558	-0.05296	0.072193
H	-4.95784	2.428303	-4.86688	0.190495	0.074643
H	-4.55665	4.845195	-5.14954	0.23454	0.075283
H	0.445928	7.939544	-1.86442	0.24573	0.0758
H	1.922264	6.691548	-0.33247	0.190985	0.074718
H	-0.24565	3.104137	-1.18835	-0.07663	0.072111
H	-1.24174	0.629656	-4.65372	0.174024	0.076928
H	0.649737	-0.86339	-4.20616	0.215709	0.06077
H	-1.48837	-2.58502	-0.90452	0.210701	0.069727
H	-3.3899	-1.05297	-1.35006	0.180016	0.07544
H	-5.76867	1.696119	-2.11322	0.162592	0.076126
H	-8.03785	0.710365	-2.26509	0.210578	0.069431
H	-6.50354	-2.39869	-4.79709	0.203403	0.059977
H	-4.26811	-1.40112	-4.66811	0.17556	0.075361
H	3.530019	4.641943	-1.71667	0.163276	0.076381
H	5.914349	5.243005	-1.40365	0.211099	0.069729
H	5.438885	4.858807	2.845959	0.20313	0.059971
H	3.074337	4.293608	2.531205	0.176976	0.075209
H	-0.43987	3.972616	1.737344	0.172916	0.076834
H	-1.31194	2.030931	2.957225	0.216039	0.060725
H	1.979043	-0.33654	1.54274	0.211557	0.069863
H	2.842121	1.62777	0.292892	0.180319	0.075615

E. **Table S5**: Cartesian coordinates of optimized structure of compound **5.**
Total Energy: –2667.86 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	14.02263	5.17257	5.825564	-0.30325	-0.0276
C	15.12085	4.332942	5.629634	-0.2753	-0.03955
C	14.94848	2.954263	5.61552	0.358782	0.001089
C	13.67094	2.397171	5.769063	1.271584	-0.09413
C	12.57395	3.24624	5.966554	-0.865	-0.02623
C	13.55316	0.903913	5.796021	-0.82272	0.024803
C	12.29514	0.232219	5.323971	0.58119	-0.07713
C	11.97997	-1.04476	5.878948	0.135381	0.008645
C	10.88652	-1.74939	5.454777	-0.28974	-0.01041
C	10.05698	-1.22891	4.423965	0.033276	-0.04078
C	10.38133	0.037625	3.843253	0.117275	-0.0473
C	11.50773	0.756536	4.321337	-0.87068	0.005271
N	8.984224	-1.92695	3.998767	0.172277	-0.04376

C	8.247535	-1.40673	3.027441	-0.16937	-0.02198
C	8.579081	-0.13656	2.437238	-0.24588	-0.0263
N	9.627918	0.557994	2.851241	0.185461	-0.03945
O	14.48175	0.219579	6.194635	-0.18553	-0.16
C	7.744513	0.403627	1.367267	0.153952	-0.05226
C	7.082753	-2.14342	2.546138	0.040725	-0.05248
C	6.615067	-0.31288	0.907054	-0.20616	-0.02467
C	5.827608	0.260944	-0.10542	-0.27524	-0.01485
C	6.145768	1.490492	-0.67396	-0.27466	-0.03804
C	7.285472	2.182301	-0.22223	-0.07307	-0.02325
C	8.058551	1.645108	0.78475	-0.27283	0.012706
C	6.751574	-3.38848	3.110838	-0.15388	0.015707
C	5.660441	-4.10888	2.673322	-0.00289	-0.01744
C	4.862397	-3.60365	1.630433	-0.26037	-0.0375
C	5.188879	-2.37857	1.055828	-0.34436	-0.02223
C	6.281525	-1.61836	1.504079	-0.14694	-0.02408
N	5.34454	2.021214	-1.721	0.802871	-0.08537
C	4.863614	1.133062	-2.7376	-0.45975	-0.06556
C	5.016837	3.385923	-1.76979	0.076124	-0.026
N	3.749751	-4.3535	1.160382	0.774212	-0.08407
C	2.538897	-3.73281	0.812921	-0.35631	-0.02587
C	3.899073	-5.76921	1.00004	-0.26747	-0.06525
C	3.498388	1.074175	-3.03538	0.040371	-0.03067
C	3.03779	0.209084	-4.02486	-0.25363	-0.03191
C	3.929867	-0.61259	-4.71277	-0.44926	-0.04415
C	5.290068	-0.55981	-4.40933	-0.19239	-0.03439
C	5.759178	0.312537	-3.4308	0.14493	-0.02763
C	4.824158	4.030168	-3.00758	0.033862	-0.02923
C	4.501192	5.375464	-3.062	-0.09213	0.014787
C	4.370003	6.097017	-1.87695	-0.63471	-0.07402
C	4.549509	5.482954	-0.63899	-0.17045	0.013721
C	4.865899	4.135981	-0.58686	0.040962	-0.03337
C	1.736436	-4.25808	-0.21865	0.002326	-0.03011
C	0.540143	-3.65139	-0.56298	-0.0455	0.013873
C	0.131541	-2.50638	0.11757	-0.46709	-0.07538
C	0.902371	-1.97043	1.148436	-0.02276	0.012156
C	2.094789	-2.58198	1.494645	-0.09243	-0.03132
C	2.969552	-6.64385	1.572476	0.145626	-0.03114
C	3.118517	-8.01897	1.415684	-0.3519	-0.03343
C	4.200795	-8.53389	0.702568	-0.35046	-0.0434
C	5.132517	-7.66214	0.140786	-0.3987	-0.03254
C	4.98225	-6.28485	0.281701	0.233857	-0.0285
N	4.037753	7.523018	-1.9331	-0.19566	0.155376
N	-1.12656	-1.8561	-0.25567	-0.21783	0.154901
O	3.859942	8.02742	-3.03843	-0.0078	-0.18976
O	-1.79495	-2.36933	-1.1493	0.000981	-0.19094
O	3.957214	8.135126	-0.87156	-0.00947	-0.19027
O	-1.44196	-0.83092	0.342653	0.000785	-0.19011

H	11.90115	5.276545	6.172972	0.183997	0.056849
H	14.1584	6.248136	5.844754	0.16429	0.056122
H	16.11005	4.755529	5.495019	0.178596	0.056761
H	15.79359	2.288894	5.487472	0.216911	0.073301
H	11.5854	2.830551	6.117689	0.184891	0.068151
H	12.63512	-1.441	6.64466	0.229434	0.076091
H	10.62916	-2.71248	5.879362	0.179519	0.070214
H	11.73326	1.706834	3.854372	0.20716	0.082329
H	4.946301	-0.24786	-0.46803	-0.05187	0.07482
H	7.555264	3.12989	-0.67137	0.184103	0.077692
H	8.938421	2.166412	1.138035	0.240262	0.077969
H	7.371934	-3.7658	3.913008	0.252013	0.078159
H	5.414879	-5.06115	3.126403	0.200337	0.078142
H	4.578136	-2.02223	0.239161	-0.01421	0.074447
H	2.803927	1.705001	-2.49305	0.174361	0.07767
H	1.977849	0.169741	-4.24851	0.205402	0.059863
H	3.567938	-1.28766	-5.47941	0.166682	0.056341
H	5.991631	-1.18972	-4.94445	0.19977	0.057501
H	6.81684	0.36183	-3.20015	0.170293	0.076627
H	4.938444	3.470643	-3.92652	0.193675	0.078538
H	4.364037	5.878267	-4.00952	0.26219	0.081676
H	4.423412	6.061687	0.265754	0.264406	0.081625
H	4.988123	3.653797	0.373935	0.176406	0.077774
H	2.06236	-5.13976	-0.75421	0.197171	0.078688
H	-0.07362	-4.04317	-1.36249	0.26216	0.08155
H	0.551246	-1.09364	1.675237	0.263451	0.081806
H	2.686424	-2.17748	2.305113	0.205211	0.07885
H	2.135706	-6.24387	2.137319	0.166062	0.076403
H	2.393929	-8.68923	1.8639	0.196609	0.058209
H	4.317901	-9.60509	0.587767	0.167653	0.056251
H	5.975368	-8.05299	-0.41778	0.197493	0.057902
H	5.702716	-5.60655	-0.15992	0.155906	0.076417

F. Table S6: Cartesian coordinates of optimized structure of compound **6.**
Total Energy: –3052.74 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	12.58624	8.268526	0.96658	-0.29511	-0.02727
C	12.23878	9.311842	0.106195	-0.31454	-0.03916
C	10.9052	9.668556	-0.05145	0.434563	0.001823
C	9.898345	8.968597	0.628657	1.215028	-0.09438
C	10.25495	7.923273	1.490882	-0.95131	-0.02602
C	8.48373	9.43189	0.46193	-0.80367	0.024983
C	7.344556	8.461295	0.599313	0.628487	-0.07532
C	6.08528	8.978287	1.031044	0.271386	0.010616

C	4.983332	8.172798	1.120376	-0.23679	-0.00809
C	5.069849	6.802103	0.751743	-0.05813	-0.03921
C	6.321156	6.282563	0.292254	0.216573	-0.04592
C	7.453239	7.13731	0.233856	-0.97546	0.005742
N	3.982703	6.009017	0.829338	0.167557	-0.03856
C	4.107781	4.741636	0.463298	-0.22536	-0.02012
C	5.364007	4.221221	-0.00365	-0.23533	-0.02505
N	6.43863	4.991272	-0.08047	0.205731	-0.03578
C	5.466692	2.815989	-0.40024	0.022045	-0.04341
C	2.939417	3.863723	0.534773	-0.09402	-0.04396
C	4.333317	1.973211	-0.32741	-0.29292	-0.02833
C	4.484604	0.627709	-0.71435	-0.53223	0.00998
C	5.699333	0.13158	-1.15581	-0.74567	-0.04959
C	6.816692	0.977532	-1.22745	-0.06761	-0.02565
C	6.694652	2.301554	-0.85297	-0.18685	0.005084
C	1.708568	4.368287	0.98853	-0.29529	0.012948
C	0.590237	3.559377	1.056578	0.181577	0.004827
C	0.681152	2.217352	0.666997	-0.06412	-0.04557
C	1.891111	1.706148	0.220437	-0.3295	-0.01884
C	3.045429	2.507459	0.143907	-0.24868	-0.03299
N	5.779164	-1.25522	-1.52906	1.126621	-0.09664
N	-0.49654	1.396271	0.737131	1.06136	-0.09766
O	8.242695	10.60059	0.207411	-0.18183	-0.15815
C	5.723475	-1.58227	-2.91058	-0.19971	-0.0447
C	5.500799	-2.91126	-3.3138	-0.0991	-0.25845
S	5.119709	-4.15588	-2.09966	-0.43624	0.561539
C	6.132319	-3.557	-0.76417	-0.08899	-0.25839
C	6.304764	-2.17331	-0.58043	-0.19828	-0.04481
C	-0.66463	0.548757	1.864532	-0.36771	-0.04435
C	-1.92698	0.000222	2.154347	-0.1168	-0.25818
S	-3.35061	0.499892	1.210022	-0.49845	0.55998
C	-2.5705	0.712787	-0.37561	-0.1169	-0.25825
C	-1.25336	1.200594	-0.44925	-0.36898	-0.0443
C	6.666843	-4.46776	0.144637	0.405838	-0.06308
C	7.335218	-4.02458	1.28362	-0.25953	-0.05687
C	7.482058	-2.65755	1.492176	-0.22965	-0.03687
C	6.986308	-1.74187	0.565941	-0.0566	-0.04746
C	5.865096	-0.60736	-3.90775	-0.0584	-0.04764
C	5.796583	-0.94791	-5.25739	-0.24221	-0.03632
C	5.613524	-2.27074	-5.64509	-0.25467	-0.05679
C	5.476046	-3.25078	-4.66474	0.417176	-0.06304
C	-3.31072	0.4848	-1.53368	0.330288	-0.0633
C	-2.78133	0.790049	-2.78556	-0.19304	-0.05639
C	-1.49286	1.306522	-2.86732	-0.24494	-0.03558

C	-0.73117	1.496435	-1.71593	-0.26848	-0.04553
C	0.398038	0.244848	2.72663	-0.25173	-0.04592
C	0.209352	-0.58116	3.83301	-0.26977	-0.03578
C	-1.03474	-1.14682	4.089687	-0.18437	-0.05659
C	-2.09841	-0.8589	3.237518	0.323938	-0.06335
H	11.86305	6.783144	2.346173	0.18437	0.056739
H	13.62767	7.995824	1.095823	0.163922	0.056095
H	13.00962	9.849136	-0.43446	0.178743	0.056931
H	10.62145	10.49032	-0.69758	0.218122	0.073597
H	9.491264	7.393182	2.046409	0.180739	0.068118
H	6.028088	10.02992	1.282704	0.231597	0.076596
H	4.02647	8.550618	1.460322	0.182375	0.071282
H	8.38314	6.717134	-0.12786	0.201515	0.082608
H	3.653175	-0.06238	-0.67628	-0.06589	0.080027
H	7.765972	0.586062	-1.57384	0.171886	0.08193
H	7.543561	2.970687	-0.8995	0.283341	0.077335
H	1.658466	5.408311	1.282084	0.252328	0.077645
H	-0.36021	3.945473	1.404633	0.171265	0.079321
H	1.921986	0.665664	-0.07245	0.267501	0.081
H	6.536428	-5.52861	-0.03679	0.176472	0.061092
H	7.730147	-4.73991	1.994966	0.156059	0.054177
H	7.994124	-2.29039	2.374189	0.178956	0.055331
H	7.12091	-0.68462	0.746206	0.183333	0.070175
H	6.016766	0.427024	-3.63308	0.184167	0.070199
H	5.898751	-0.16818	-6.00341	0.178972	0.055605
H	5.573231	-2.54098	-6.69342	0.15623	0.054247
H	5.325823	-4.28777	-4.94286	0.176122	0.061088
H	-4.31501	0.086096	-1.44531	0.171523	0.06091
H	-3.37158	0.627859	-3.67942	0.158977	0.054184
H	-1.06307	1.555791	-3.83064	0.175371	0.055737
H	0.271349	1.890186	-1.80644	0.173583	0.069866
H	1.376993	0.664935	2.543692	0.173265	0.06961
H	1.049479	-0.7873	4.486139	0.174723	0.055624
H	-1.18166	-1.80052	4.941009	0.159091	0.054142
H	-3.07874	-1.28405	3.420605	0.171444	0.060914

G. Table S7: Cartesian coordinates of optimized structure of compound **7.**

Total Energy: –2256.37 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	-9.85283	4.6339	8.466412	-0.26459	-0.0279

C	-9.06455	4.752736	7.323602	-0.28863	-0.04219
C	-7.67538	4.739694	7.428974	-0.80114	-0.02588
C	-7.0633	4.62581	8.684158	1.274956	-0.09405
C	-7.86515	4.530982	9.830516	0.368426	0.001292
C	-5.5775	4.68616	8.867363	-0.87809	0.024745
C	-4.6587	4.169763	7.796877	0.63808	-0.07679
C	-3.35822	4.751739	7.704418	0.178364	0.009111
C	-2.44184	4.293855	6.797536	-0.2864	-0.00941
C	-2.76361	3.200567	5.947309	-0.02045	-0.04007
C	-4.05439	2.593235	6.053369	0.130057	-0.04677
C	-4.99306	3.106647	6.986001	-0.83057	0.005611
N	-1.85865	2.742537	5.058935	0.172365	-0.04171
C	-2.19881	1.712797	4.297073	-0.18485	-0.02076
C	-3.49414	1.097235	4.409501	-0.27476	-0.02531
N	-4.39095	1.542572	5.276085	0.192585	-0.03751
C	-3.83395	-0.03934	3.554474	0.171482	-0.04713
C	-1.23453	1.197801	3.327176	0.13281	-0.04814
C	-2.89655	-0.5305	2.615521	-0.12213	-0.02679
C	-3.26579	-1.63163	1.822574	-0.30724	-0.00783
C	-4.51917	-2.21847	1.933991	-0.11424	-0.02924
C	-5.44451	-1.71954	2.864564	-0.06646	-0.01226
C	-5.09606	-0.64941	3.663545	-0.2633	0.011642
C	0.034141	1.793693	3.212405	-0.20854	0.013279
C	0.96642	1.323017	2.310348	-0.01262	-0.01275
C	0.640163	0.238481	1.480079	-0.10844	-0.02762
C	-0.61273	-0.35281	1.576091	-0.31472	-0.00884
C	-1.57024	0.099034	2.501222	-0.07938	-0.02562
N	-4.86457	-3.31765	1.106598	0.733396	-0.02954
N	1.588643	-0.25643	0.549718	0.732523	-0.02872
O	-5.10078	5.150264	9.890273	-0.18622	-0.1592
C	-5.29594	-4.57238	1.552961	0.287114	-0.02219
C	-5.5549	-5.39481	0.429419	0.211764	-0.06376
C	-5.26973	-4.60158	-0.7476	0.226338	-0.064
C	-4.84534	-3.32894	-0.29385	0.143268	-0.02118
C	2.048888	-1.5775	0.47091	0.122803	-0.02098
C	2.999321	-1.66968	-0.57472	0.228133	-0.06379
C	3.117734	-0.34851	-1.15442	0.215269	-0.06346
C	2.237302	0.496933	-0.43653	0.28472	-0.02198
C	1.728017	-2.67931	1.265161	-0.40508	-0.05002
C	2.359531	-3.88711	0.983869	-0.35534	-0.03596
C	3.292497	-3.99943	-0.05841	-0.35276	-0.05946
C	3.619207	-2.89502	-0.83655	-0.28385	-0.02174
C	3.866697	0.175261	-2.21215	-0.20852	-0.02196
C	3.727818	1.518908	-2.54026	-0.32672	-0.06022

C	2.840258	2.33955	-1.82729	-0.51182	-0.03758
C	2.081934	1.842927	-0.77134	-0.41033	-0.05149
C	-5.43647	-5.05009	2.856821	-0.40623	-0.05139
C	-5.86177	-6.36481	3.022346	-0.51455	-0.03761
C	-6.13598	-7.18929	1.920176	-0.32465	-0.06057
C	-5.98064	-6.71206	0.623894	-0.20531	-0.0221
C	-5.35165	-4.85084	-2.12076	-0.28095	-0.02184
C	-5.01861	-3.83935	-3.01403	-0.36152	-0.05996
C	-4.61308	-2.57951	-2.54713	-0.35055	-0.03635
C	-4.52294	-2.30518	-1.18583	-0.4251	-0.05022
H	-9.86238	4.432375	10.61117	0.177603	0.056698
H	-10.93383	4.634685	8.381873	0.163513	0.055906
H	-9.53004	4.857486	6.350227	0.184645	0.056706
H	-7.06998	4.844871	6.537262	0.182172	0.068261
H	-7.38299	4.467172	10.79842	0.218838	0.073412
H	-3.11768	5.565884	8.376655	0.229541	0.07614
H	-1.45754	4.737787	6.707686	0.181837	0.070635
H	-5.95741	2.618614	7.049258	0.206102	0.082486
H	-2.57199	-2.05887	1.11247	0.119442	0.076342
H	-6.42711	-2.16899	2.938315	0.199456	0.077798
H	-5.79708	-0.24822	4.383355	0.231592	0.077337
H	0.268473	2.625028	3.863857	0.243223	0.077826
H	1.950265	1.771129	2.247293	0.20186	0.077797
H	-0.8364	-1.16912	0.904121	0.132204	0.076135
H	1.019284	-2.60226	2.079972	0.174833	0.067653
H	2.125222	-4.75751	1.586164	0.171367	0.054863
H	3.764412	-4.95545	-0.25258	0.165405	0.053033
H	4.34895	-2.98205	-1.63391	0.131666	0.060614
H	4.54424	-0.4594	-2.77249	0.13268	0.060635
H	4.304105	1.937668	-3.35693	0.162158	0.052855
H	2.738217	3.382473	-2.1052	0.170521	0.054326
H	1.391706	2.483008	-0.23658	0.1544	0.067361
H	-5.2173	-4.42641	3.71438	0.155039	0.06754
H	-5.97935	-6.75894	4.025435	0.170233	0.054331
H	-6.46593	-8.20844	2.084196	0.162214	0.052795
H	-6.18237	-7.35535	-0.22543	0.132676	0.060573
H	-5.67491	-5.81976	-2.48485	0.131929	0.060566
H	-5.07597	-4.02079	-4.08087	0.164878	0.052935
H	-4.36583	-1.80083	-3.2597	0.171958	0.054683
H	-4.21854	-1.32653	-0.83694	0.173193	0.06754

H. Table S8: Cartesian coordinates of optimized structure of compound **8.**
Total Energy: –1796.94 Hartrees

Atom	X	y	Z	Mulliken Charges	Lowdin Charges
C	-5.67797	-5.61998	5.862785	-0.28451	-0.03113
C	-5.24845	-6.21558	4.678661	-0.27803	-0.04376
C	-6.17835	-6.62742	3.726076	-0.83016	-0.02624
C	-7.54978	-6.46209	3.959386	1.302108	-0.09204
C	-7.9728	-5.88388	5.164489	0.345044	-0.00029
C	-8.59882	-6.95767	3.008222	-0.84237	0.024559
C	-8.33447	-6.97941	1.532433	0.631691	-0.08311
C	-9.0467	-7.93381	0.746045	0.177108	0.002962
C	-8.89911	-7.97842	-0.6139	-0.26326	-0.01294
C	-8.04993	-7.04838	-1.27386	0.002303	-0.04351
C	-7.35592	-6.06976	-0.49656	-0.08337	-0.05138
C	-7.50942	-6.06291	0.913503	-0.8407	0.003606
N	-7.90845	-7.09149	-2.61507	0.160322	-0.04995
C	-7.11426	-6.19657	-3.18656	-0.14596	-0.01992
C	-6.42518	-5.20058	-2.40355	-0.32051	-0.02478
N	-6.554	-5.156	-1.08628	0.17728	-0.04539
O	-9.67573	-7.34433	3.434714	-0.19031	-0.16475
C	-6.9359	-6.21942	-4.63148	0.007888	-0.0664
C	-6.10159	-5.27748	-5.27402	0.075983	-0.01787
C	-5.40725	-4.25025	-4.47463	0.055117	-0.01958
C	-5.57146	-4.22678	-3.07229	0.048037	-0.06535
C	-7.59521	-7.18942	-5.41132	-0.23965	0.012717
C	-7.44483	-7.24329	-6.77677	-0.15891	-0.03845
C	-6.61839	-6.30905	-7.44622	-0.14573	-0.03073
C	-5.97055	-5.34103	-6.67357	-0.28707	-0.05463
C	-4.56651	-3.29026	-5.06897	-0.33392	-0.0541
C	-3.90672	-2.30764	-4.32658	-0.15019	-0.03245
C	-4.09187	-2.3042	-2.92362	-0.19882	-0.03777
C	-4.89913	-3.24185	-2.32369	-0.17821	0.011025
N	-3.11825	-1.31347	-4.93004	0.271163	-0.15911
N	-6.43666	-6.40379	-8.8351	0.270366	-0.15743
C	-3.07934	-1.23486	-6.38822	-0.04248	-0.03114
C	-2.50605	0.111847	-6.82457	-0.53087	0.025973
O	-1.22252	0.347211	-6.26351	-0.11042	-0.22911
C	-1.28639	0.324196	-4.84312	-0.38063	0.024146
C	-1.80885	-1.01328	-4.33351	-0.12838	-0.0148
C	-5.46463	-5.52534	-9.48139	-0.05099	-0.0306
C	-5.1356	-6.04566	-10.8789	-0.52611	0.025967
O	-6.30127	-6.19684	-11.6764	-0.10933	-0.22896
C	-7.2133	-7.09887	-11.0627	-0.38597	0.024328
C	-7.62288	-6.61623	-9.67688	-0.118	-0.01436
H	-7.37966	-4.99377	7.025952	0.175639	0.055771

H	-4.95278	-5.29158	6.599062	0.161015	0.054847
H	-4.18986	-6.36151	4.495871	0.181323	0.05586
H	-5.83672	-7.10015	2.813694	0.184021	0.06854
H	-9.03575	-5.78307	5.347204	0.216315	0.072863
H	-9.70898	-8.62093	1.257713	0.222511	0.07445
H	-9.42216	-8.70899	-1.21971	0.178146	0.068789
H	-6.97911	-5.30187	1.471824	0.206423	0.080926
H	-8.21971	-7.91183	-4.90221	0.225095	0.075756
H	-7.93977	-8.02981	-7.33136	0.168863	0.060588
H	-5.35958	-4.60677	-7.17285	0.027753	0.055548
H	-4.41323	-3.32016	-6.13566	0.034841	0.055743
H	-3.62656	-1.54022	-2.31428	0.170309	0.060779
H	-5.04807	-3.22792	-1.25188	0.204595	0.075252
H	-4.09554	-1.31968	-6.77944	0.14233	0.060957
H	-2.47305	-2.04772	-6.82319	0.174493	0.061504
H	-3.19454	0.917288	-6.5299	0.155406	0.057526
H	-2.38146	0.134932	-7.90858	0.187155	0.05601
H	-1.9335	1.138917	-4.48629	0.139907	0.056639
H	-0.27067	0.496192	-4.48302	0.185291	0.056421
H	-1.89137	-0.97365	-3.24836	0.117599	0.055123
H	-1.08588	-1.80607	-4.5863	0.178531	0.066489
H	-4.54372	-5.51409	-8.89451	0.142477	0.060755
H	-5.84005	-4.49053	-9.55475	0.177209	0.06204
H	-4.61227	-7.00962	-10.7979	0.155385	0.057549
H	-4.48981	-5.33807	-11.4017	0.187111	0.056145
H	-6.75829	-8.09776	-10.9916	0.140176	0.056711
H	-8.08478	-7.15378	-11.7173	0.185629	0.056661
H	-8.27859	-7.35698	-9.22198	0.11652	0.055214
H	-8.19248	-5.67743	-9.77204	0.181223	0.066953

13. Main vertical electronic transition in implicit water

Compound **1**

1	406.7nm	0.7856,	(HOMO -> LUMO)	-96%
2	400.6nm	0.1436,	(HOMO-1 -> LUMO)	-96%
3	386.6nm	0.0041,	(HOMO-3 -> LUMO)	(54%),
4	353.9nm	0.0925,	(HOMO-2 -> LUMO)	(93%),
5	349.7nm	0.0041,	(HOMO-7 -> LUMO)	(24%),
6	323.1nm	0.7805,	(HOMO-1 -> LUMO+1)	-69%
7	321.5nm	0.0912,	(HOMO-4 -> LUMO)	(39%),
8	318.2nm	0.2402,	(HOMO -> LUMO+1)	(58%),
9	314.8nm	0.0620,	(HOMO-6 -> LUMO)	(70%),
10	313.1nm	0.0735,	(HOMO -> LUMO+1)	(24%),

Compound **2**

1	572.9nm	0.7155,	(HOMO -> LUMO)	-99%
2	554.8nm	0.1515,	(HOMO-1 -> LUMO)	-99%
3	427.0nm	0.2613,	(HOMO -> LUMO+1)	-94%
4	412.9nm	0.3610,	(HOMO-1 -> LUMO+1)	-92%
5	396.1nm	0.0887,	(HOMO-2 -> LUMO)	-91%
6	384.2nm	0.0021,	(HOMO-5 -> LUMO)	-81%
7	381.7nm	0.0090,	(HOMO -> LUMO+2)	-94%
8	371.9nm	0.1685,	(HOMO-1 -> LUMO+2)	-83%
9	360.7nm	0.2682,	(HOMO-3 -> LUMO)	-79%
10	359.8nm	0.1907,	(HOMO -> LUMO+3)	(77%),

Compound **3**

1	557.4nm	0.7601,	(HOMO -> LUMO)	-99%
2	533.8nm	0.1433,	(HOMO-1 -> LUMO)	-98%
3	421.1nm	0.2602,	(HOMO -> LUMO+1)	-90%
4	405.4nm	0.2549,	(HOMO-1 -> LUMO+1)	(51%),
5	402.7nm	0.0813,	(HOMO-1 -> LUMO+1)	(35%),
6	393.0nm	0.2404,	(HOMO-3 -> LUMO)	(60%),
7	385.2nm	0.2777,	(HOMO -> LUMO+2)	(59%),
8	383.1nm	0.0569,	(HOMO -> LUMO+3)	(40%),
9	382.9nm	0.0382,	(HOMO-9 -> LUMO)	(52%),
10	374.4nm	0.0049,	(HOMO -> LUMO+4)	(63%),

Compound **4**

1	622.3nm	0.6358,	(HOMO -> LUMO)	-98%
2	603.5nm	0.2311,	(HOMO-1 -> LUMO)	-98%
3	456.8nm	0.2484,	(HOMO -> LUMO+1)	-96%
4	441.2nm	0.2858,	(HOMO-1 -> LUMO+1)	-96%
5	404.5nm	0.0028,	(HOMO -> LUMO+2)	-86%
6	402.5nm	0.0226,	(HOMO-2 -> LUMO)	(62%),
7	392.5nm	0.1639,	(HOMO-1 -> LUMO+2)	(67%),
8	383.2nm	0.0064,	(HOMO-7 -> LUMO)	-89%
9	377.8nm	0.4053,	(HOMO-3 -> LUMO)	(52%),
10	376.0nm	0.1466,	(HOMO -> LUMO+3)	-85%

Compound **5**

1	534.4nm	1.0575,	(HOMO -> LUMO)	-95%
2	518.5nm	0.2170,	(HOMO-1 -> LUMO)	(82%),
3	491.5nm	0.1814,	(HOMO -> LUMO+1)	(72%),
4	475.8nm	0.4704,	(HOMO -> LUMO+2)	(47%),
5	465.6nm	0.1212,	(HOMO -> LUMO+2)	(45%),
6	452.6nm	0.0020,	(HOMO-1 -> LUMO+2)	(75%),
7	394.4nm	0.0304,	(HOMO-2 -> LUMO)	-83%
8	386.6nm	0.0027,	(HOMO-5 -> LUMO)	(63%),
9	384.7nm	0.2152,	(HOMO -> LUMO+3)	-87%
10	376.8nm	0.2462,	(HOMO-1 -> LUMO+3)	-81%

Compound **6**

1	605.2nm	0.0001,	(HOMO -> LUMO)	-96%
2	599.9nm	0.0001,	(HOMO-1 -> LUMO)	-96%
3	436.2nm	0.0001,	(HOMO-1 -> LUMO+1)	(81%),
4	429.8nm	0.0001,	(HOMO -> LUMO+1)	(80%),
5	403.8nm	0.0419,	(HOMO-4 -> LUMO)	(97%),
6	398.7nm	0.0002,	(HOMO-2 -> LUMO)	(95%),
7	397.1nm	0.0016,	(HOMO-3 -> LUMO)	(95%),
8	393.4nm	0.8393,	(HOMO-5 -> LUMO)	(94%),
9	392.5nm	0.0016,	(HOMO -> LUMO+2)	-86%
10	391.8nm	0.0006,	(HOMO-1 -> LUMO+2)	-83%

Compound **7**

1	510.1nm	0.4202,	(HOMO -> LUMO)	-96%
2	503.2nm	0.0336,	(HOMO-1 -> LUMO)	-96%
3	425.8nm	0.0003,	(HOMO-3 -> LUMO)	-98%
4	425.3nm	0.0002,	(HOMO-2 -> LUMO)	-97%
5	394.8nm	0.0381,	(HOMO-4 -> LUMO)	-93%
6	386.8nm	0.0053,	(HOMO-7 -> LUMO)	(60%),
7	385.7nm	0.1848,	(HOMO -> LUMO+1)	(64%),
8	380.6nm	0.0492,	(HOMO-1 -> LUMO+1)	(39%),
9	374.6nm	0.8018,	(HOMO-5 -> LUMO)	(60%),
10	351.2nm	0.0563,	(HOMO-6 -> LUMO)	(79%),

Compound **8**

1	501.6nm	0.8005,	(HOMO -> LUMO)	-98%
2	485.0nm	0.1170,	(HOMO-1 -> LUMO)	-97%
3	385.6nm	0.0578,	(HOMO -> LUMO+1)	(71%),
4	382.3nm	0.0225,	(HOMO-4 -> LUMO)	(56%),
5	380.4nm	0.2018,	(HOMO-2 -> LUMO)	(71%),
6	373.8nm	0.5124,	(HOMO-1 -> LUMO+1)	(94%),
7	344.3nm	0.0237,	(HOMO-6 -> LUMO)	(28%),
8	338.8nm	0.0101,	(HOMO -> LUMO+2)	(92%),
9	332.7nm	0.0642,	(HOMO-3 -> LUMO)	-70%
10	326.4nm	0.1775,	(HOMO-1 -> LUMO+2)	-88%

14. Thermogram (TGA) curve of **1.**

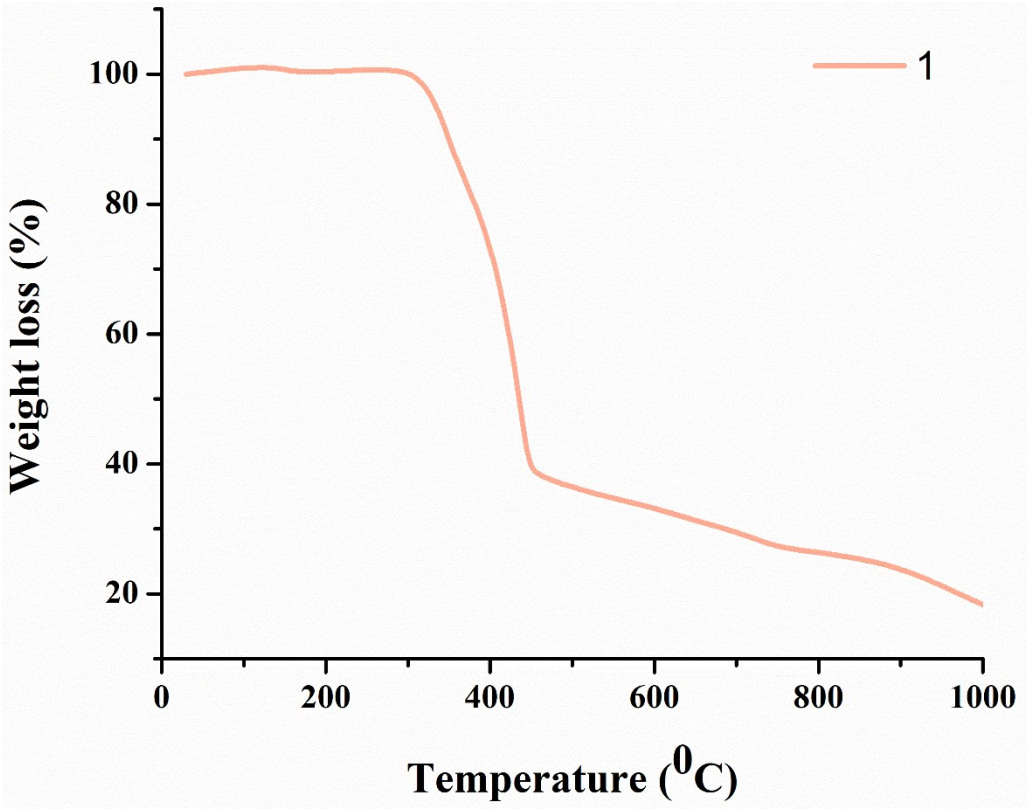

Figure S43: Thermogram (TGA) curve of **1.**