Design and Synthesis of 2,3-dipheylquinoxaline Amine derivatives as Yellow-Blue Emissive materials for Optoelectrochemical study

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Supporting information

1. Absorption spectra of compounds 1 9 in various solvents.

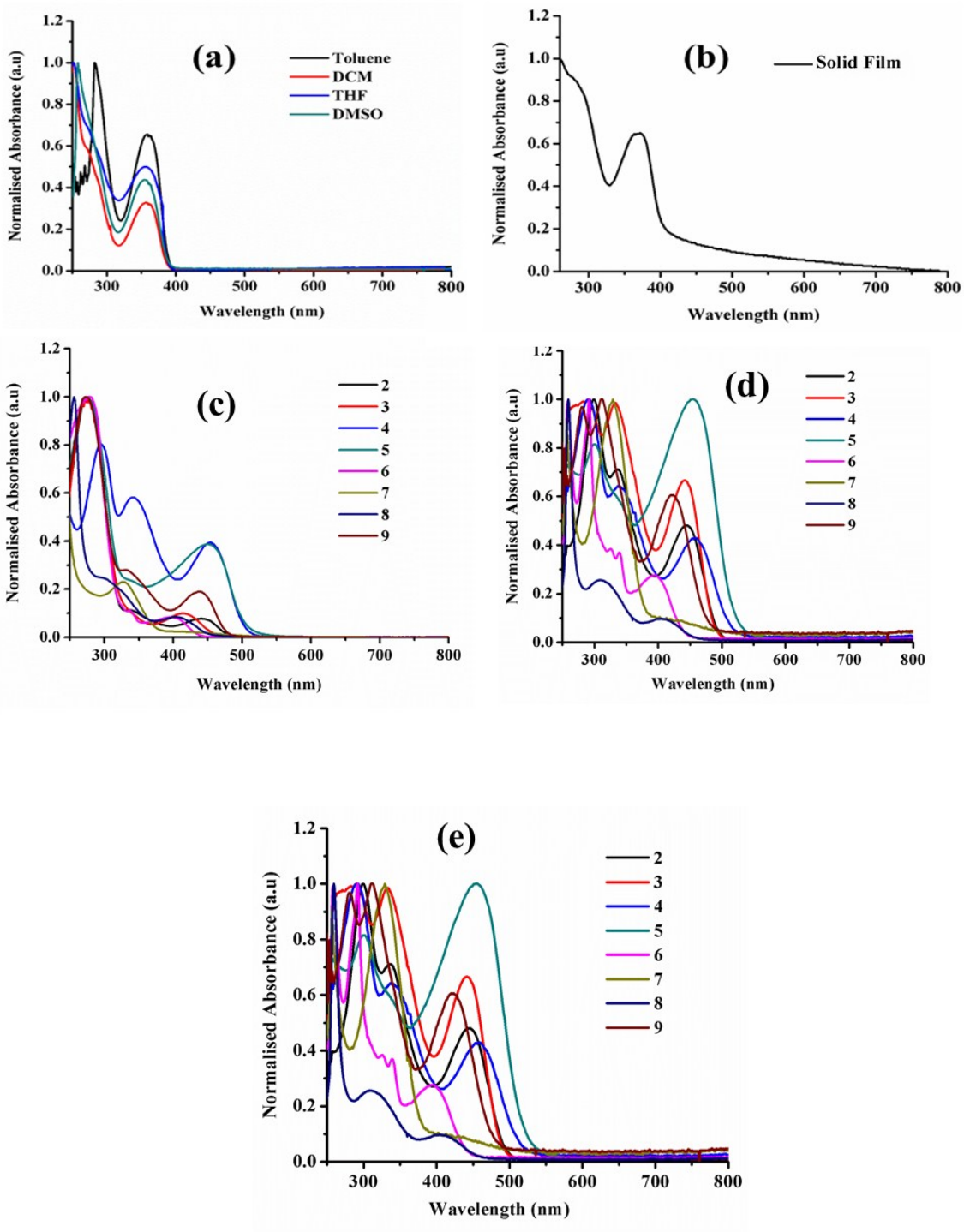

Fig. S1. UV−Vis absorption spectra of compounds **1** in various solvents (**a**), and neat solid film (**b**), UV−Vis absorption spectra of compounds **2−9** in dichloromethane (**c**) tetrahydrofuran (**d**) and dimethyl sulfoxide (**e**).

2. Emission images of 1−9 in various solvent and neat solid film.

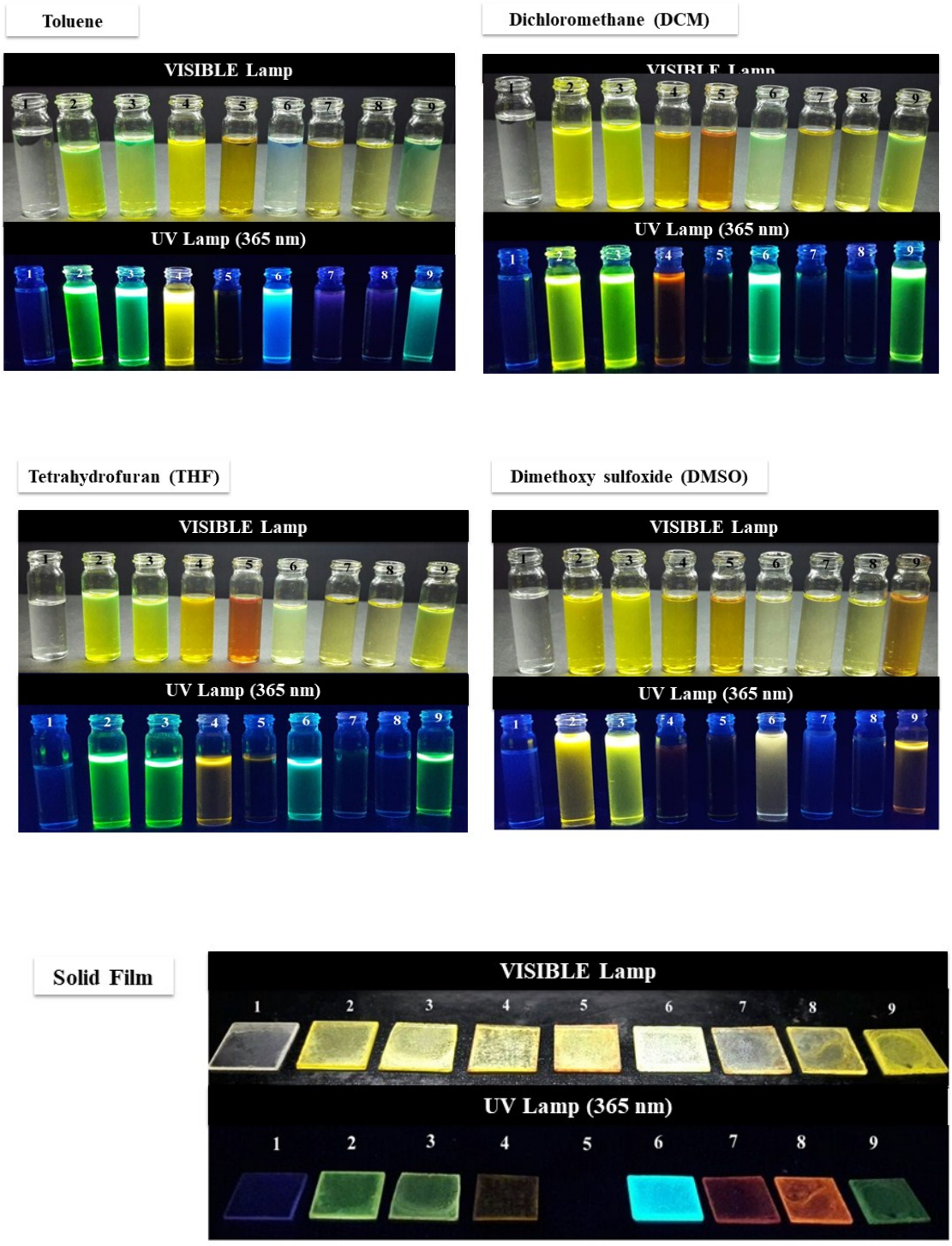

Fig. S2. Luminescence of **2−9** in various solvents and neat solid film under Visible (above) and 365nm UV lamp (below).

3. Emission of 1−9 in various solvents.

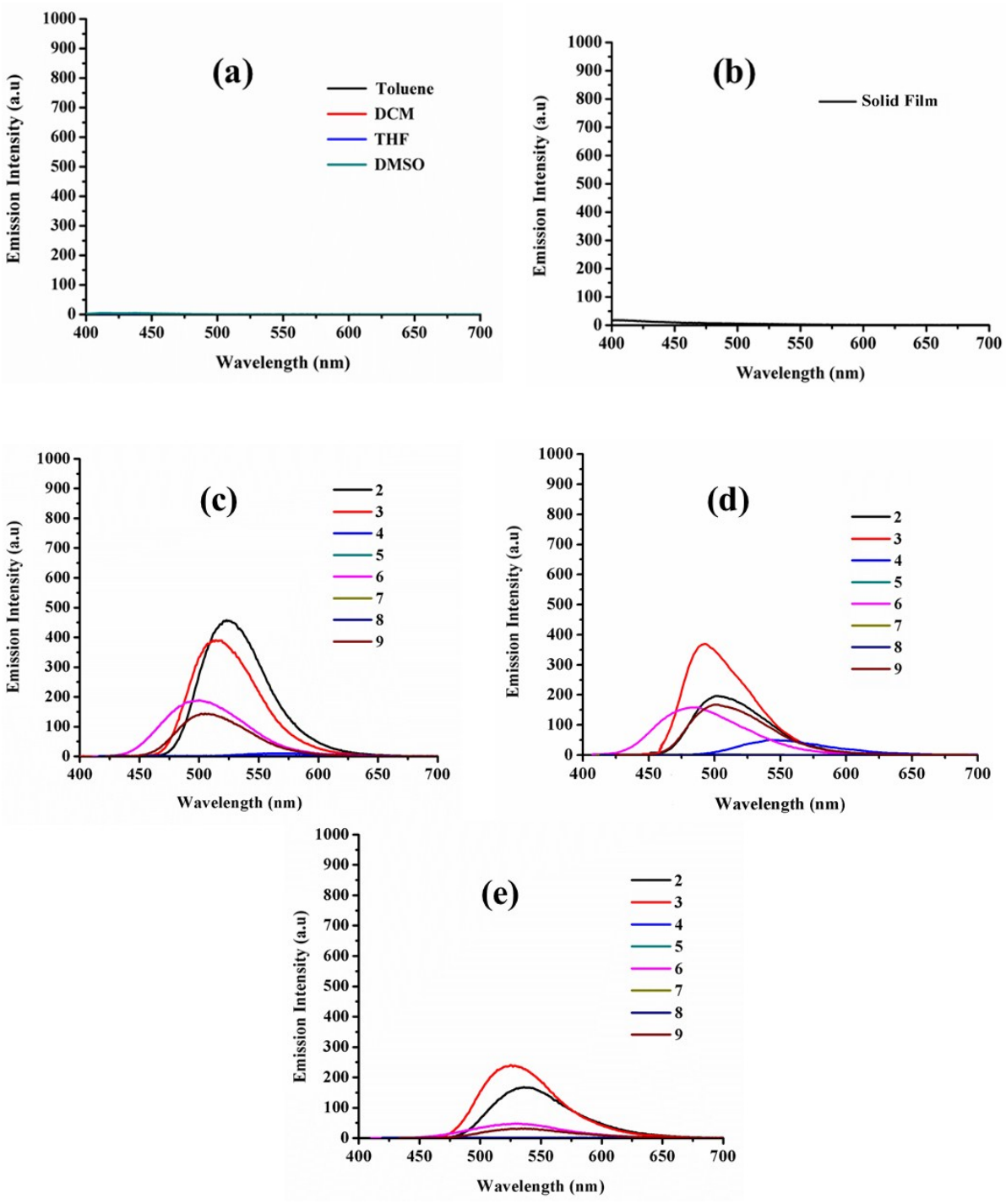

Fig. S3. Emission spectra (recorded in 10^{-5} M solution) of compounds **1** in various solvents (**a**) and neat solid film (**b**), Emission spectra **2**−**9** in DCM (**c**), THF (**d**) and DMSO (**e**).

Table S1. Stoke shift and quantum yield of **1**−**9** in DCM, THF and DMSO.

Compd	Stokes shift, cm^{-1} (ϕ_F)[a]		
	DCM	**THF**	**DMSO**
1	—	—	—
2	3503 (0.42)	2795 (0.70)	3866 (0.19)
3	3169 (0.44)	2910 (0.69)	3628 (0.32)
4	4290 (0.02)	3644 (0.18)	—
5	—	—	—
6	4938 (0.72)	4508 (0.66)	6168 (0.27)
7	—	—	—
8	—	—	—
9	4470 (0.52)	4136 (0.44)	4949 (0.20)

Recorded in 10^{-5}M solution. [a]Quantum yield (in parentheses) with reference to fluorescein (ϕ = 0.79 in 0.1 M NaOH).

4. AIE photophysical spectrum and luminescence photograph.

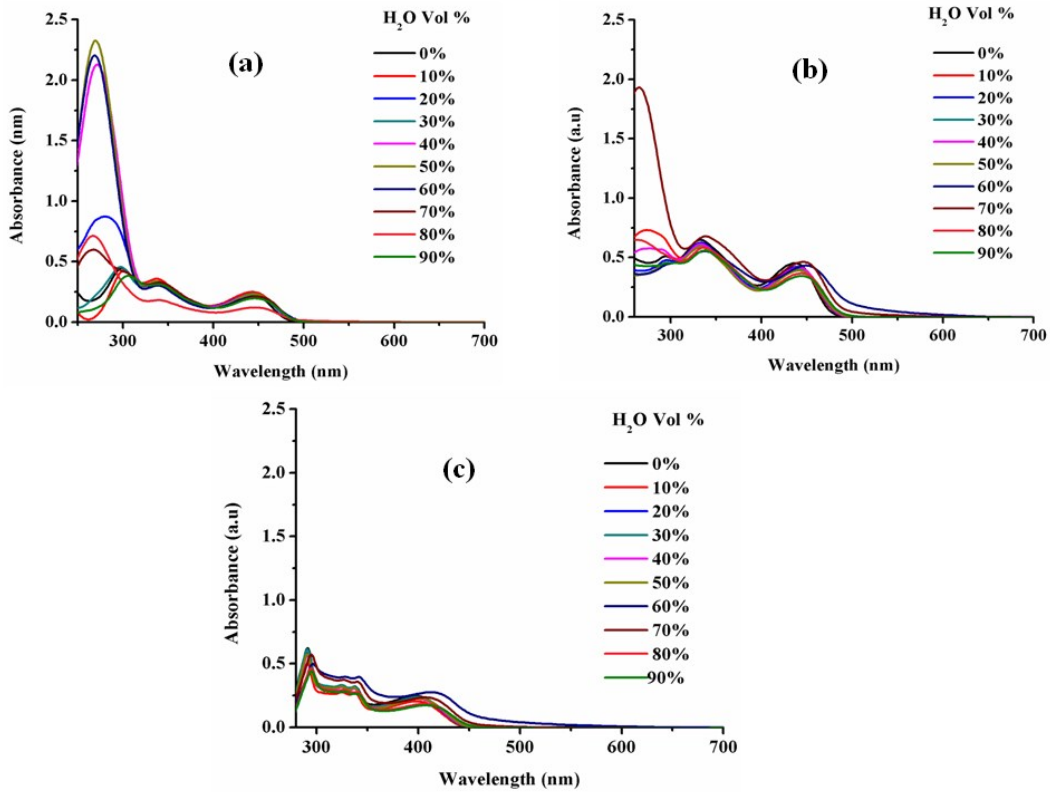

Fig. S4. Absorbance spectra of **2 (a)**, **3 (b)** and **6 (c)** in THF–water mixtures with different water fractions (10 μM).

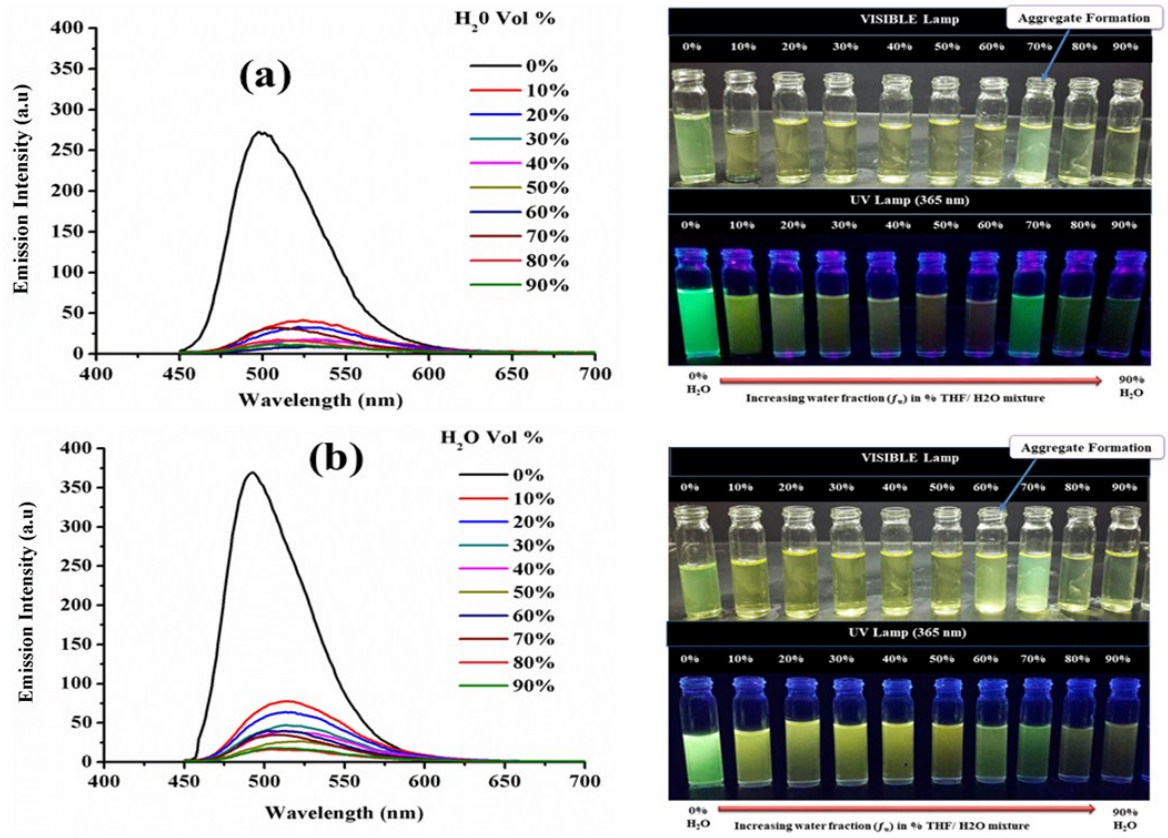

Fig. S5. Emission spectra (left) and images (right) of **2 (a)** and **3 (b)** in THF–water mixtures with different water fractions (10 μM) excited at 440 nm.

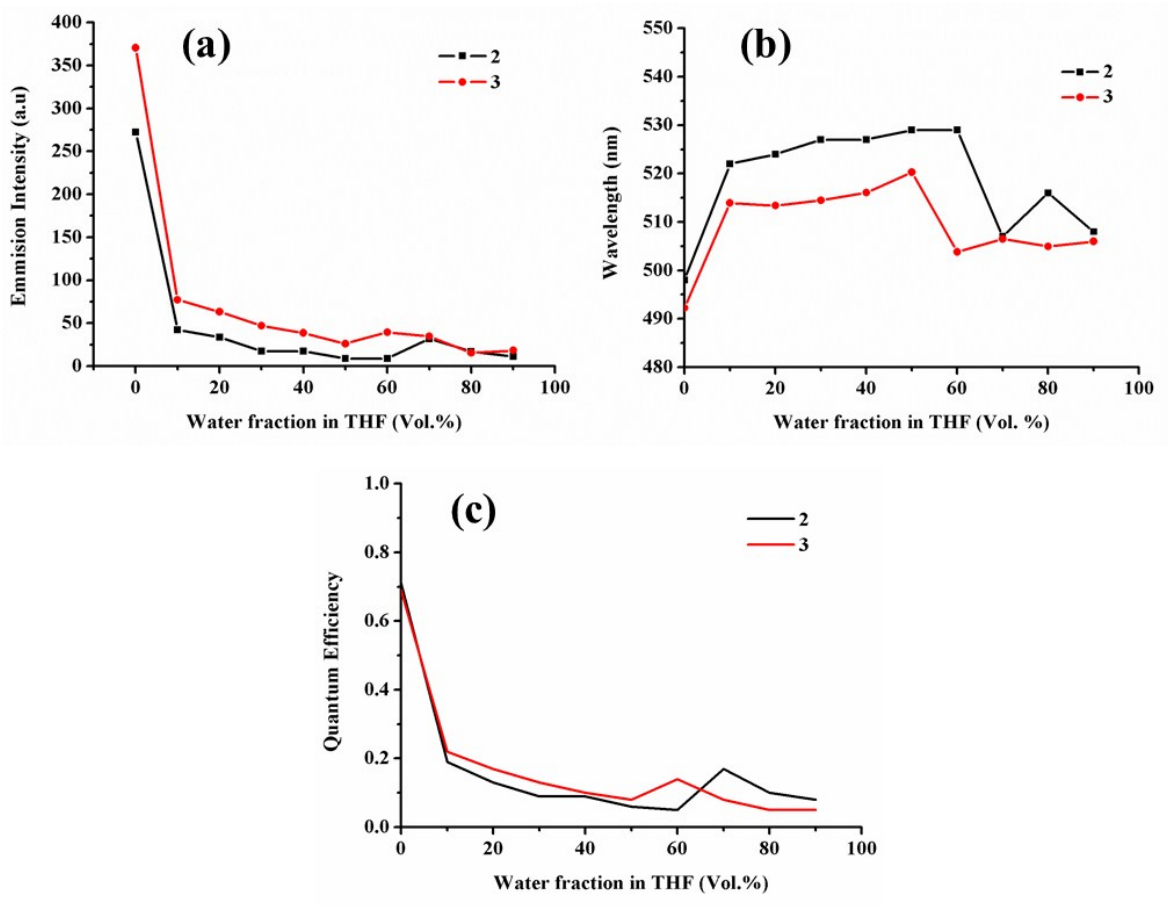

Fig. S6. Plot of emission intensity vs. % water fraction of **2** and **3. (a)** Plot of wavelength vs. % water fraction of **2** and **3. (b)** and plot of Quantum efficiency with reference to fluorescein (ϕ = 0.79 in 0.1 M NaOH) of **2** and **3** versus % of water fraction in THF/Water mixture.(**c**)

5. Cyclic voltammetry (CV) of compounds 1-9.

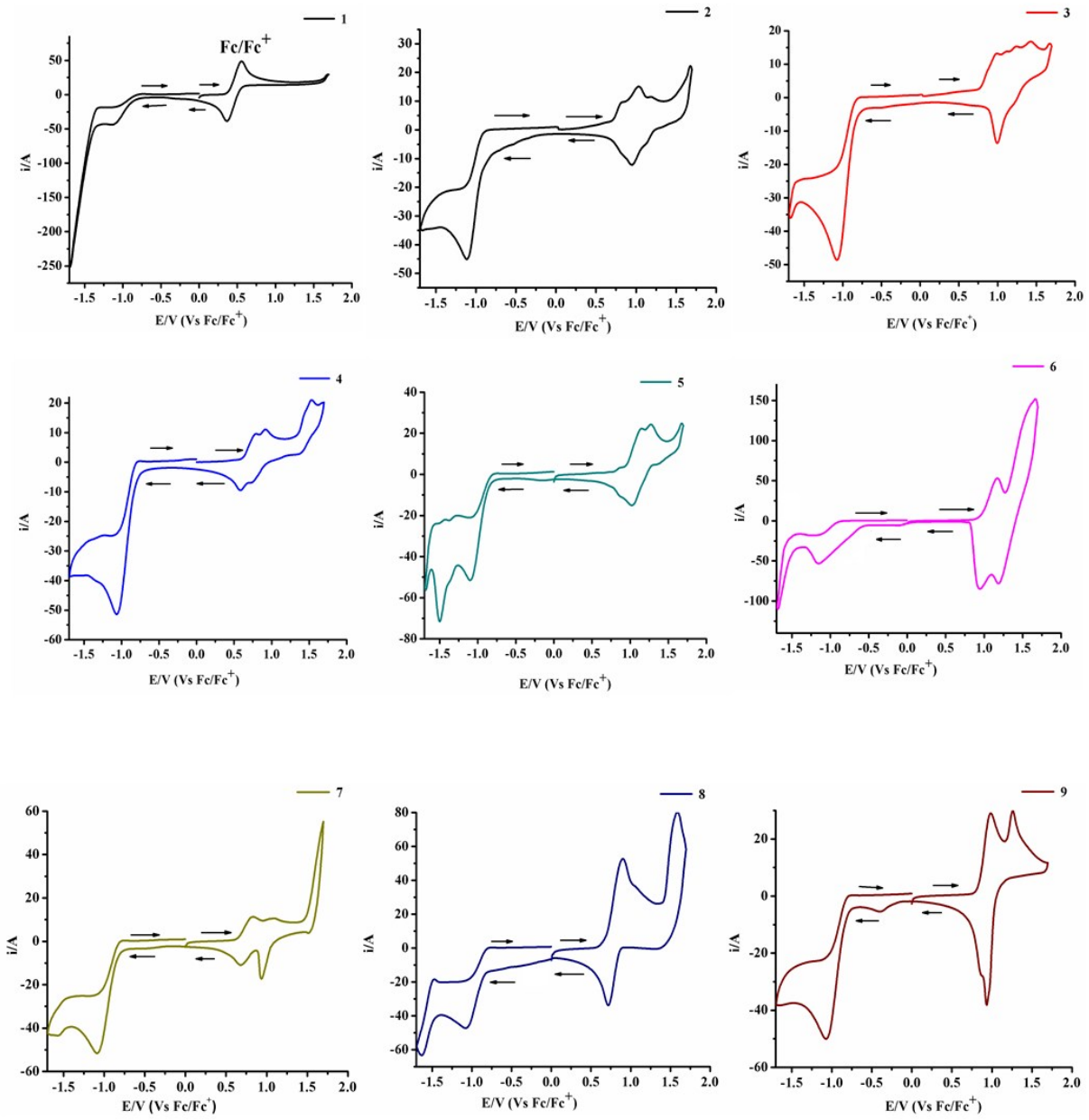

Fig. S7. Cyclic voltammogram (full scan) of compounds **1−9.**

Calculation of HOMO energy level of 1 from optical band gap

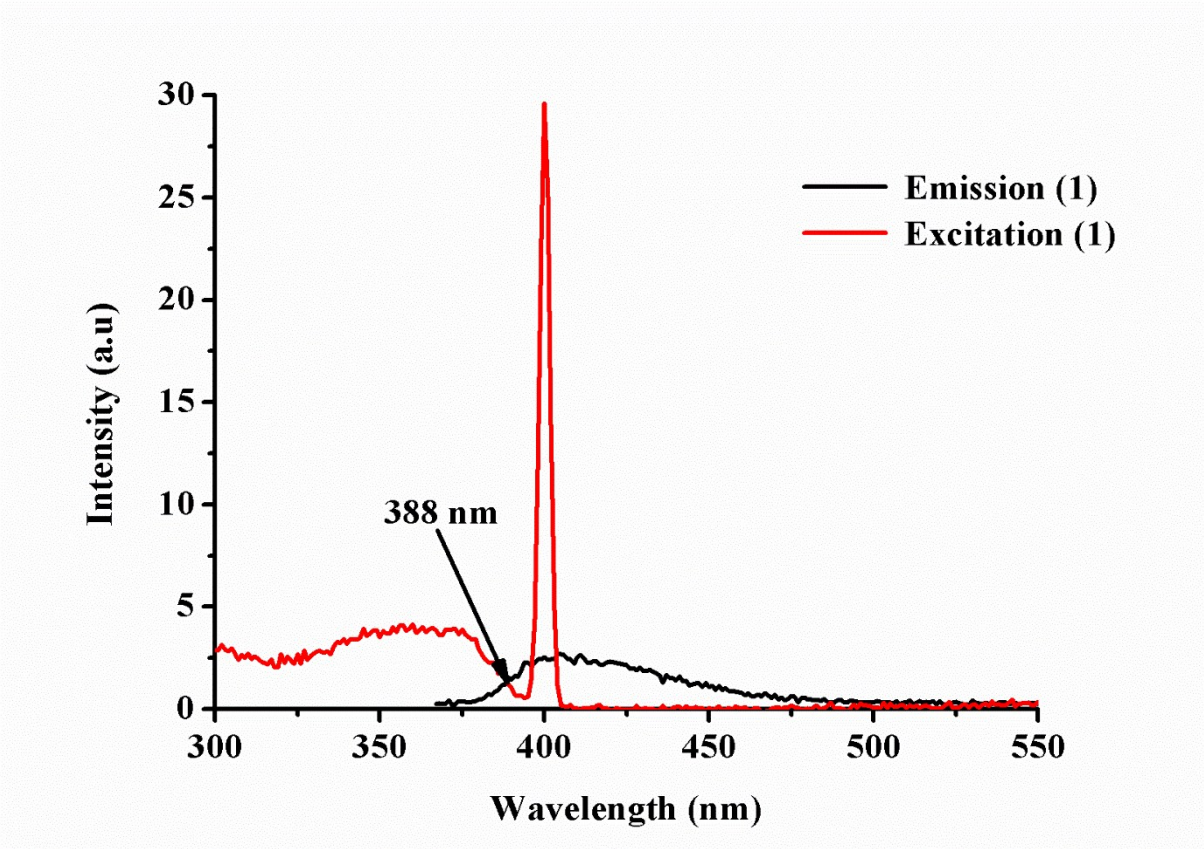

Fig. S8. Excitation and Emission spectra of 1.

Calculation:

$$E_g^{opt} = \frac{1240.8}{\lambda_{optedge}}\,eV = \frac{1240.8}{388\,nm}\,eV = 3.19 \text{ eV}$$

HOMO (eV) = − (E_g^{opt} − LUMO) eV = −[3.19 – (−3.60)] eV = −6.79 eV

6. DSC plot of compound 2-9.

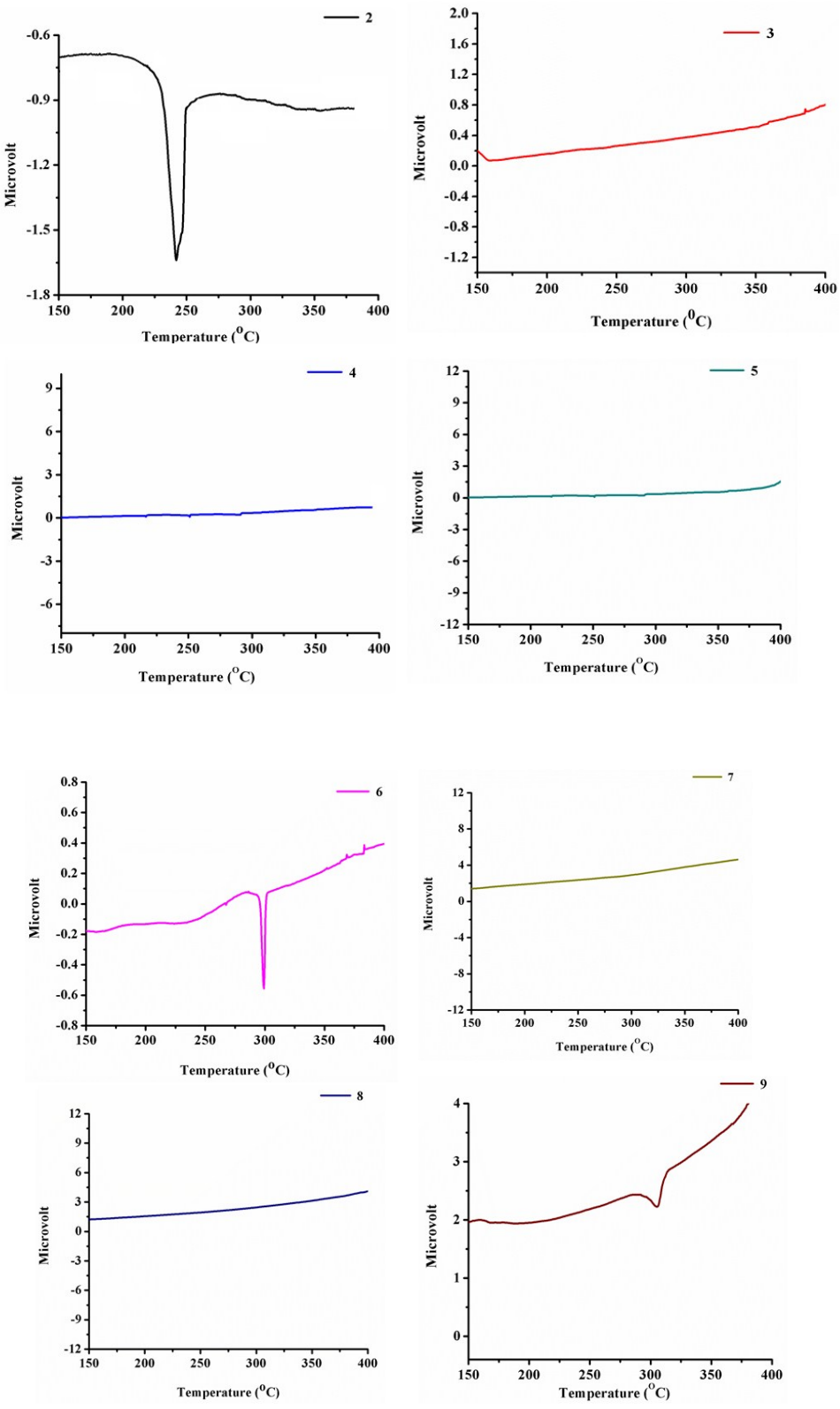

Fig. S9. DSC plot of compounds **2−9.**

7. MALDI-TOF Spectra of compounds 1−9.

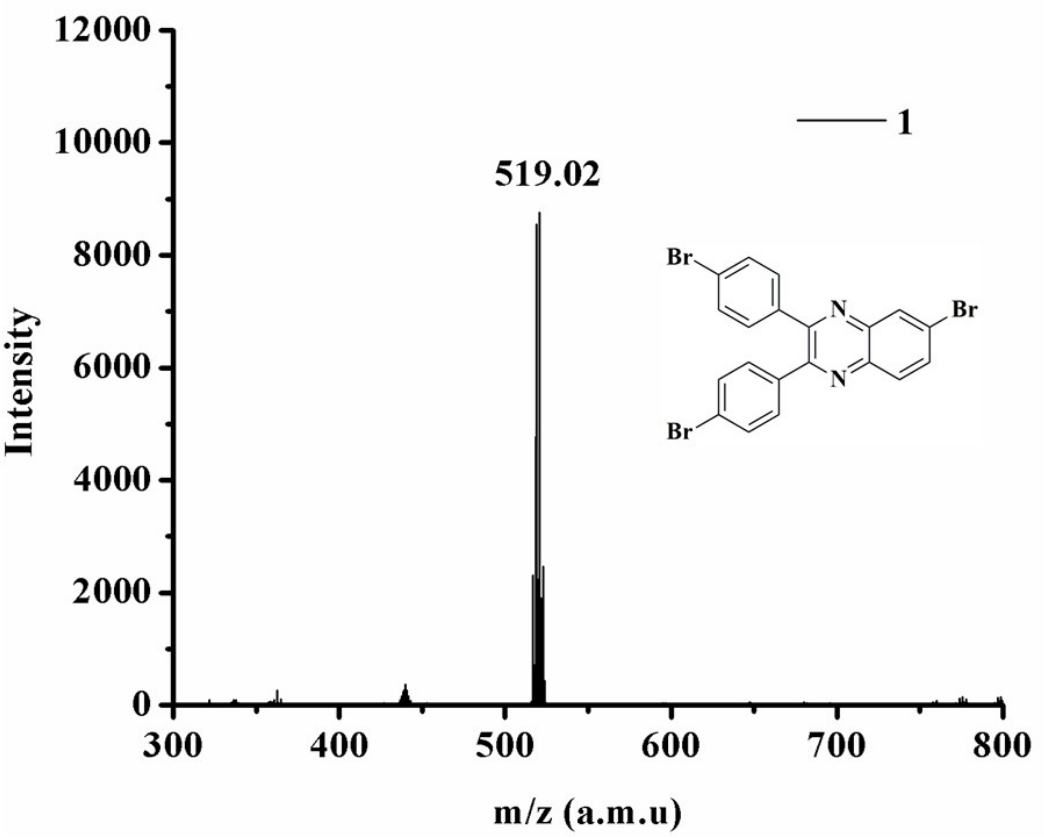

Fig. S10. MALDI-TOF spectrum of compound **1**.

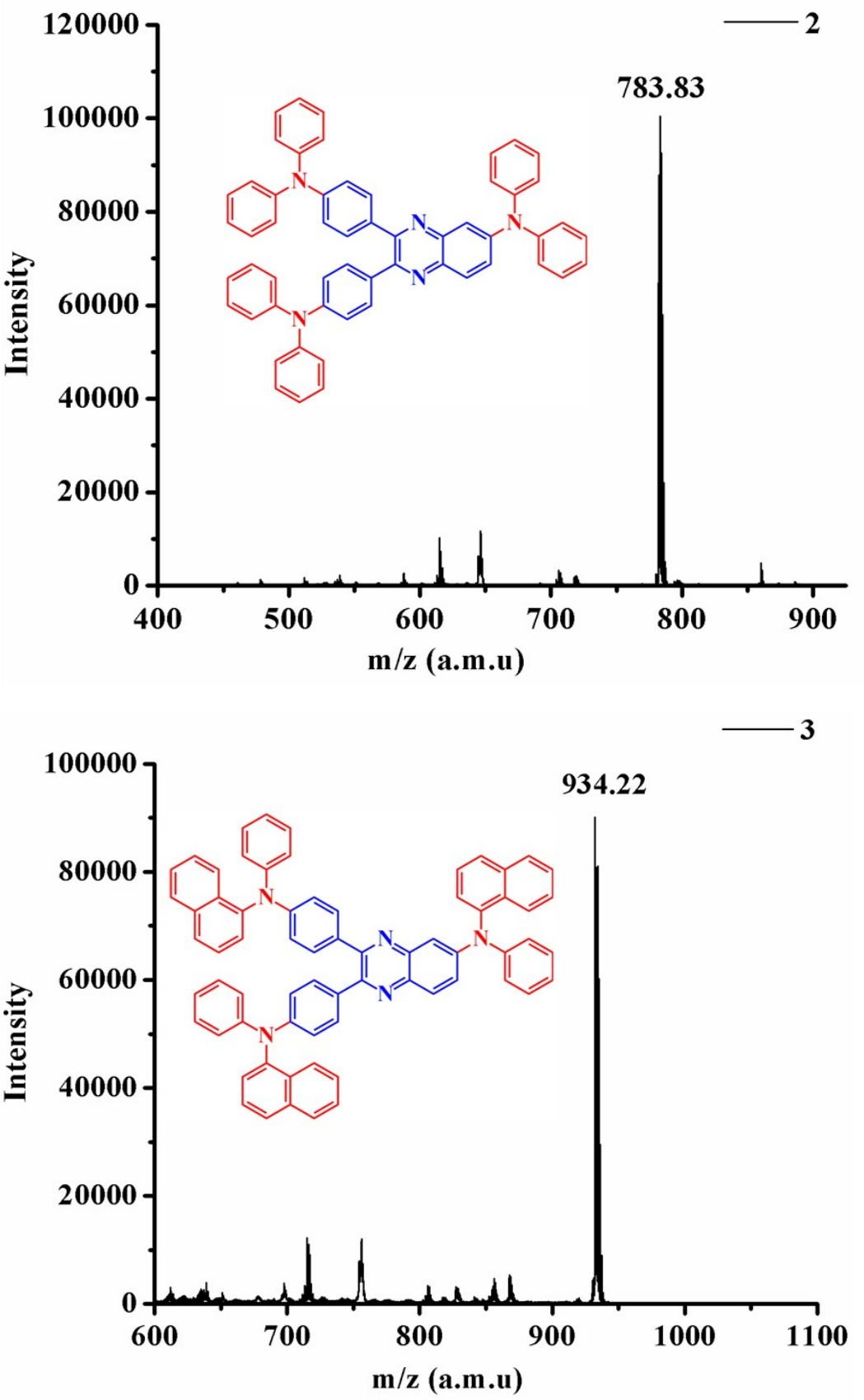

Fig. S11. MALDI-TOF spectrum of compound **2** and **3**.

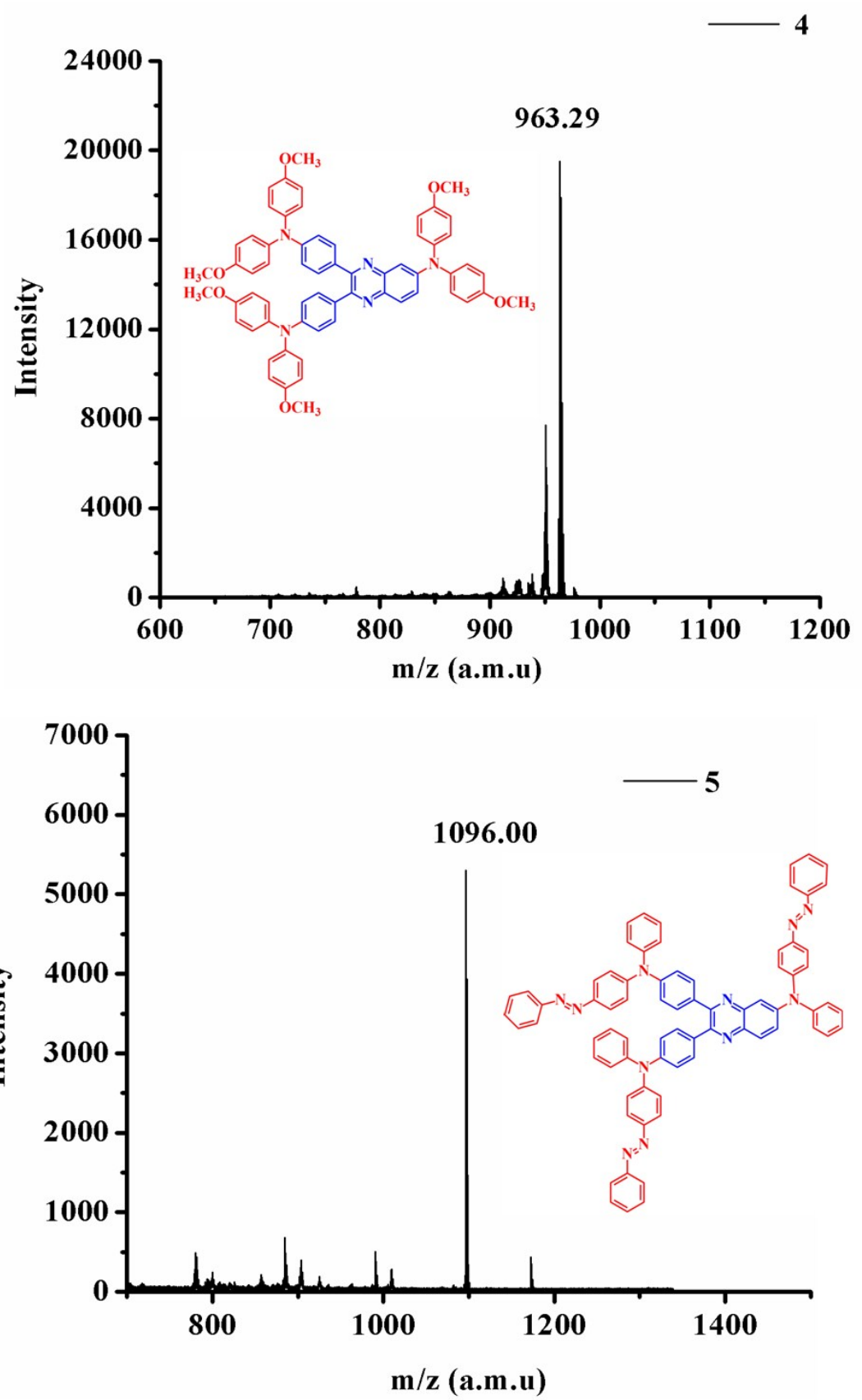

Fig. S12. MALDI-TOF spectrum of compound **4** and **5**.

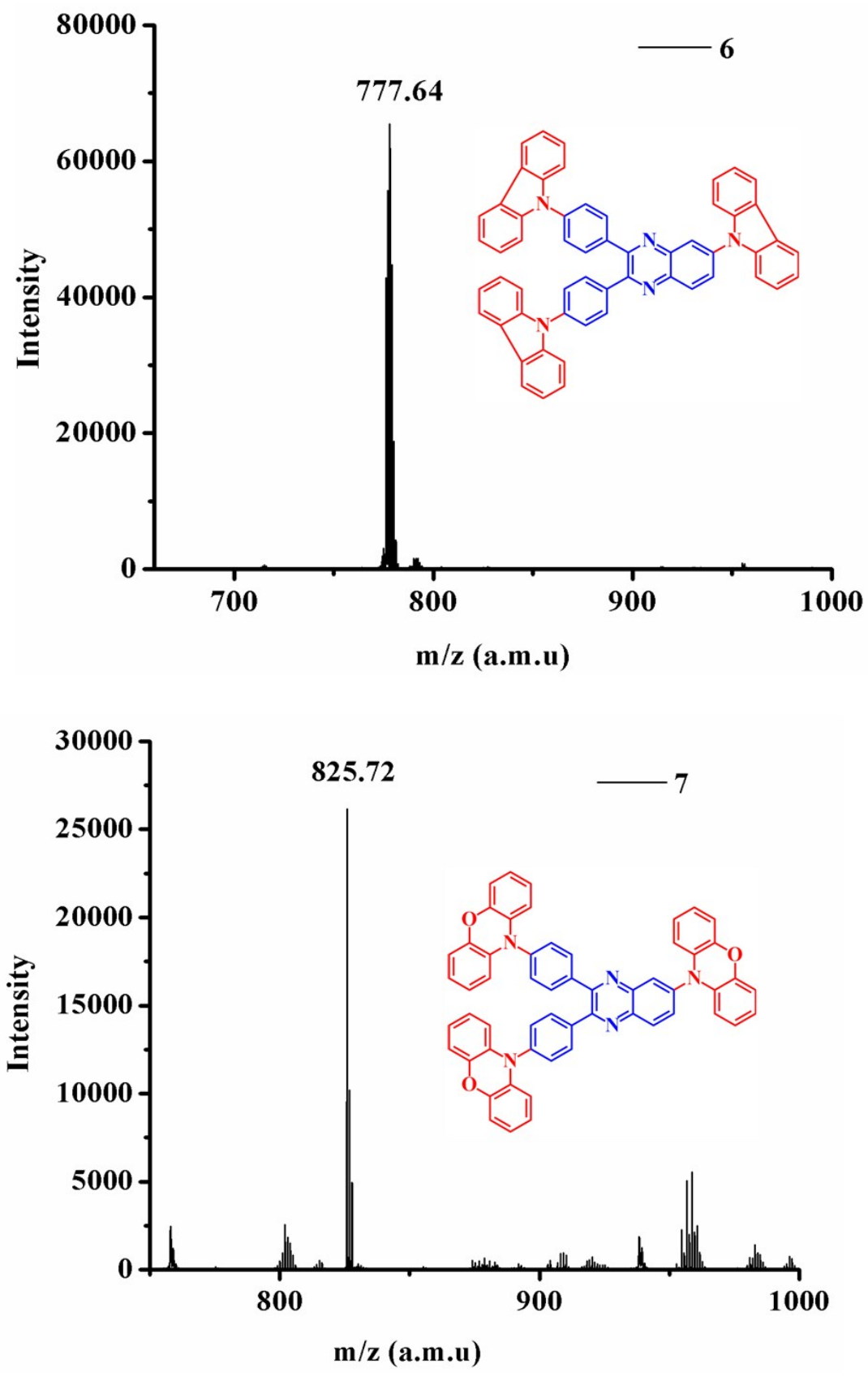

Fig. S13. MALDI-TOF spectrum of compound **6** and **7**.

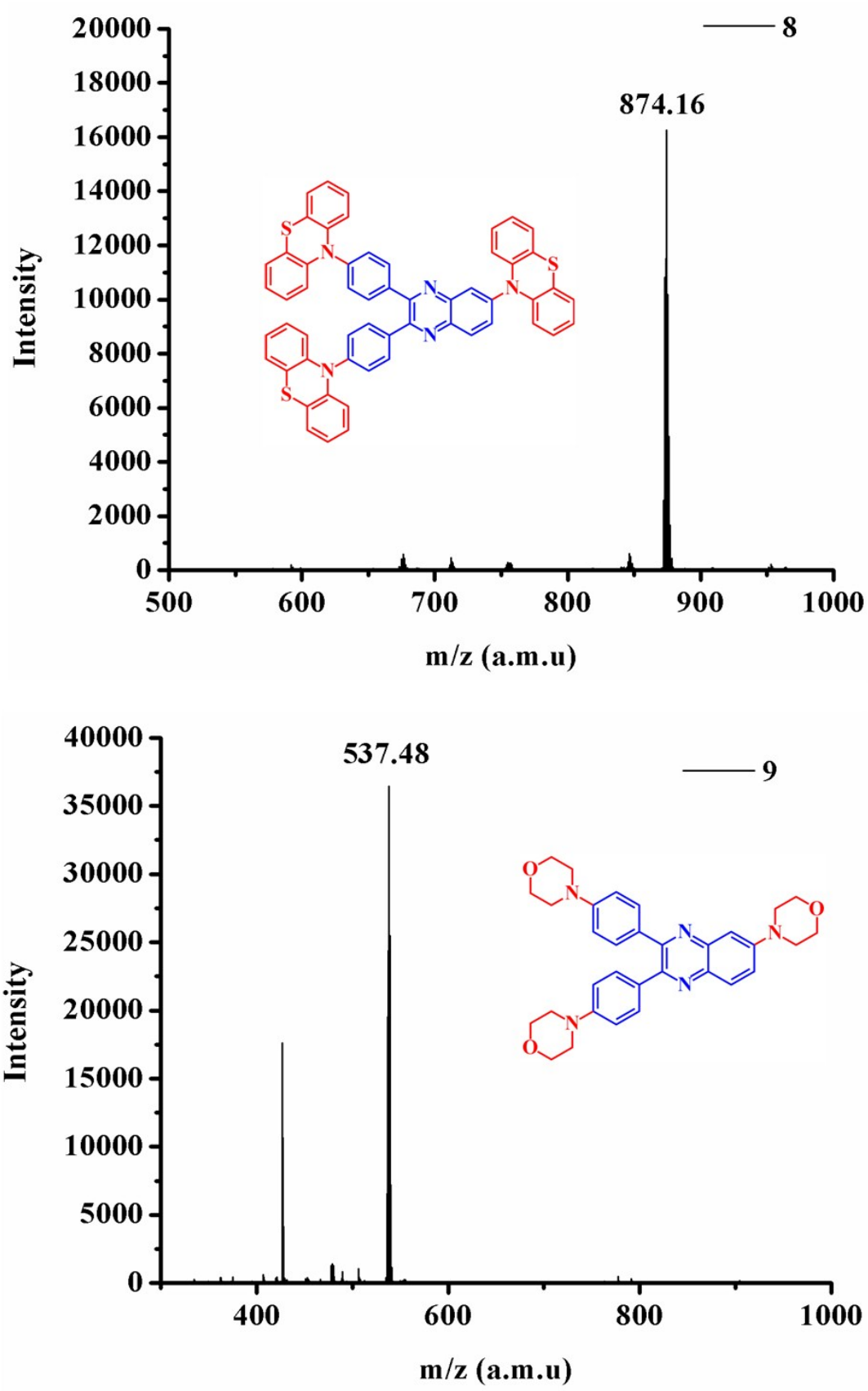

Fig. S14. MALDI-TOF spectrum of compound **8** and **9**.

8. FT-IR Spectra of compounds 1−9.

Fig. S15. FTIR spectrum of compound **1.**

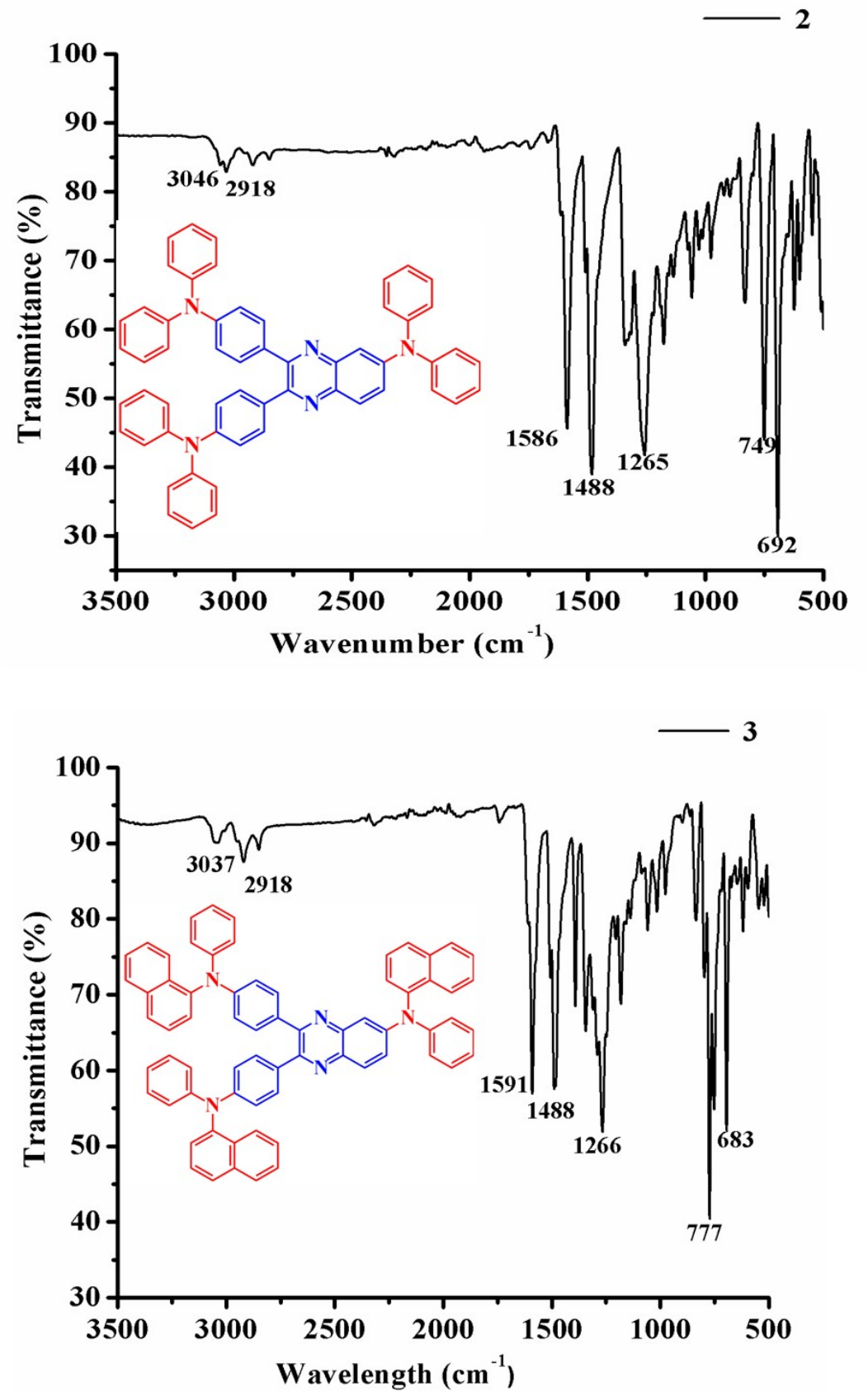

Fig. S16. FTIR spectrum of compound **2** and **3**.

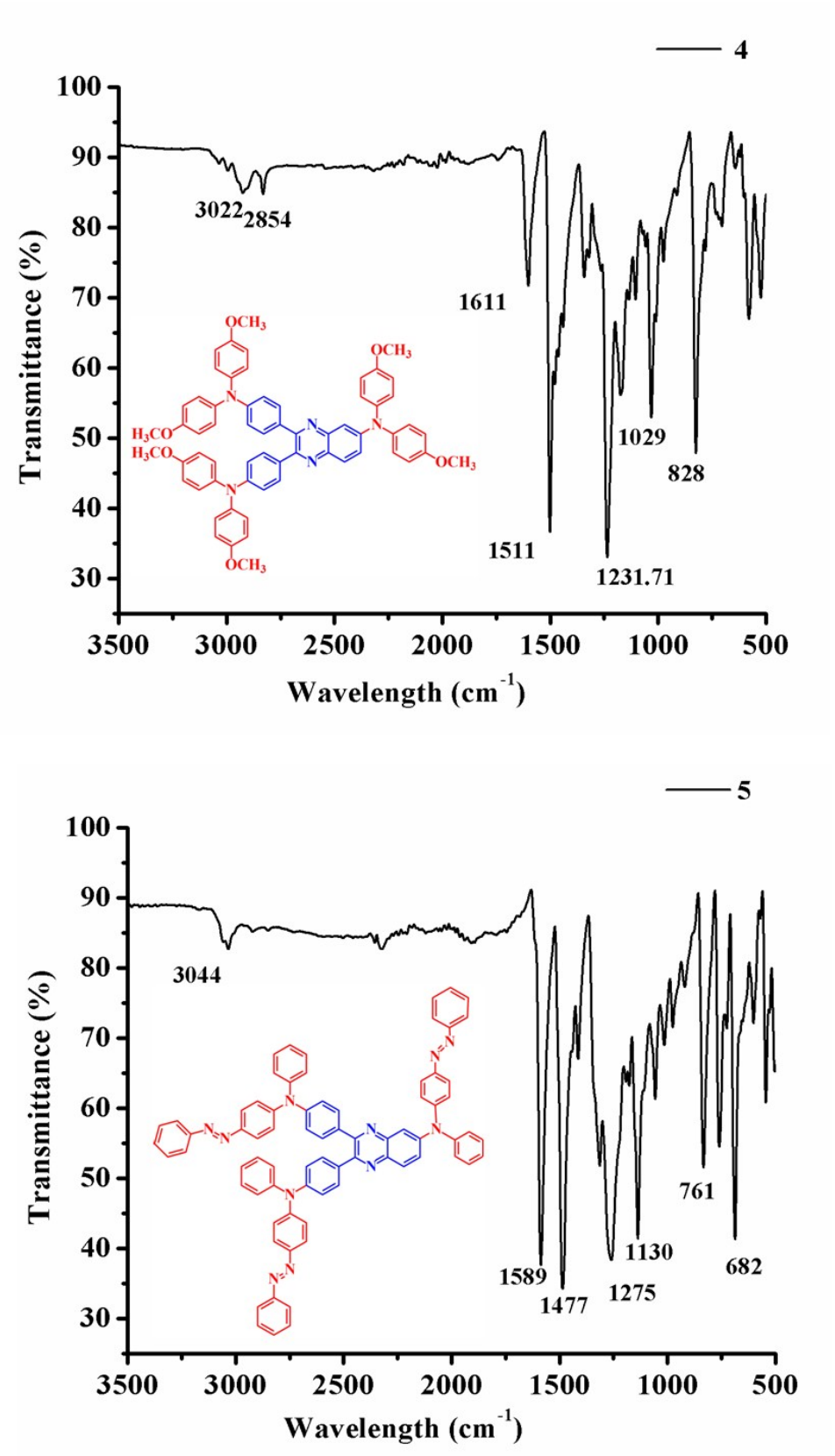

Fig. S17. FTIR spectrum of compound **4** and **5**.

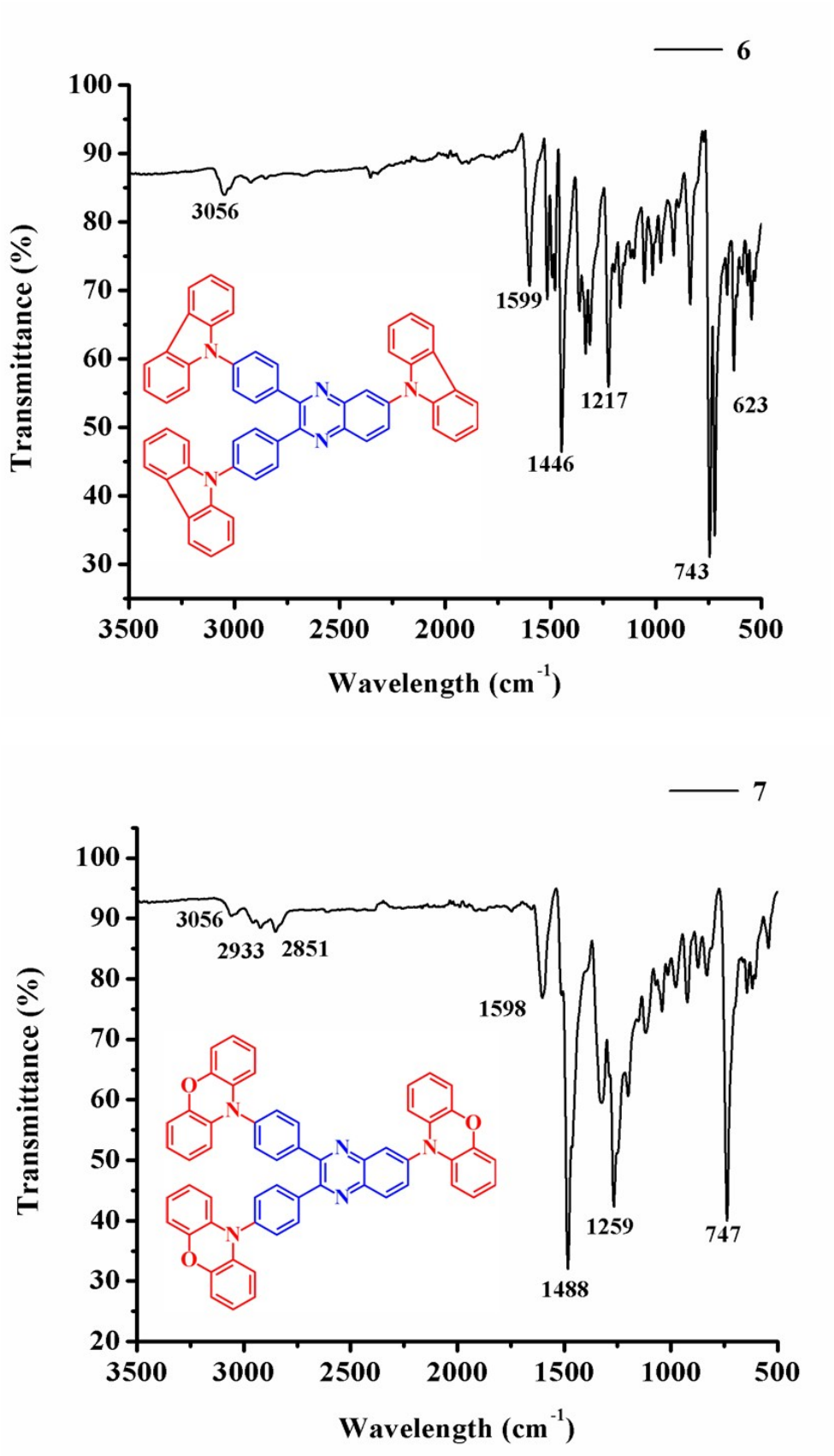

Fig. S18. FTIR spectrum of compound **6** and **7**.

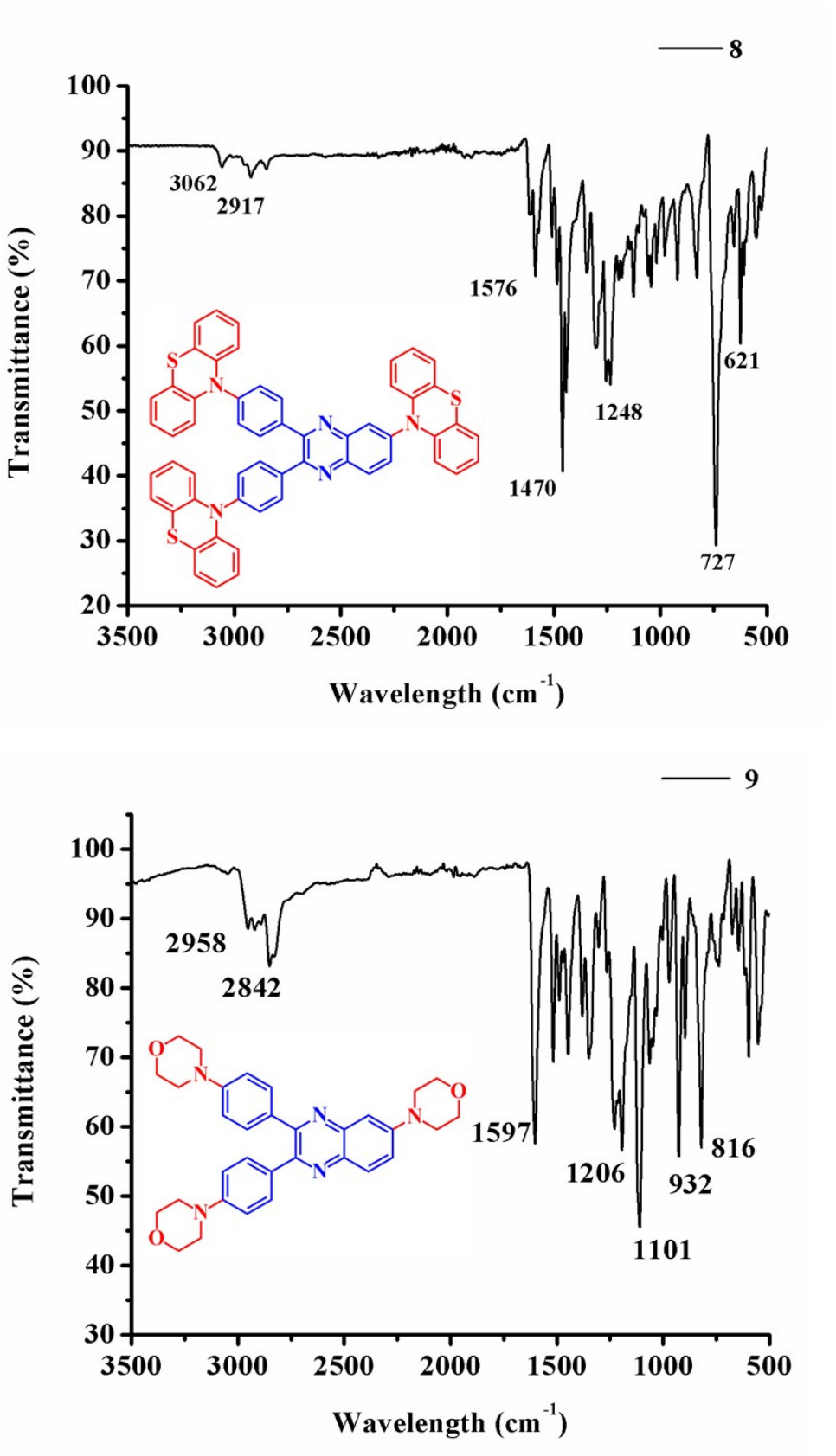

Fig. S19. FTIR spectrum of compound **8** and **9**.

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

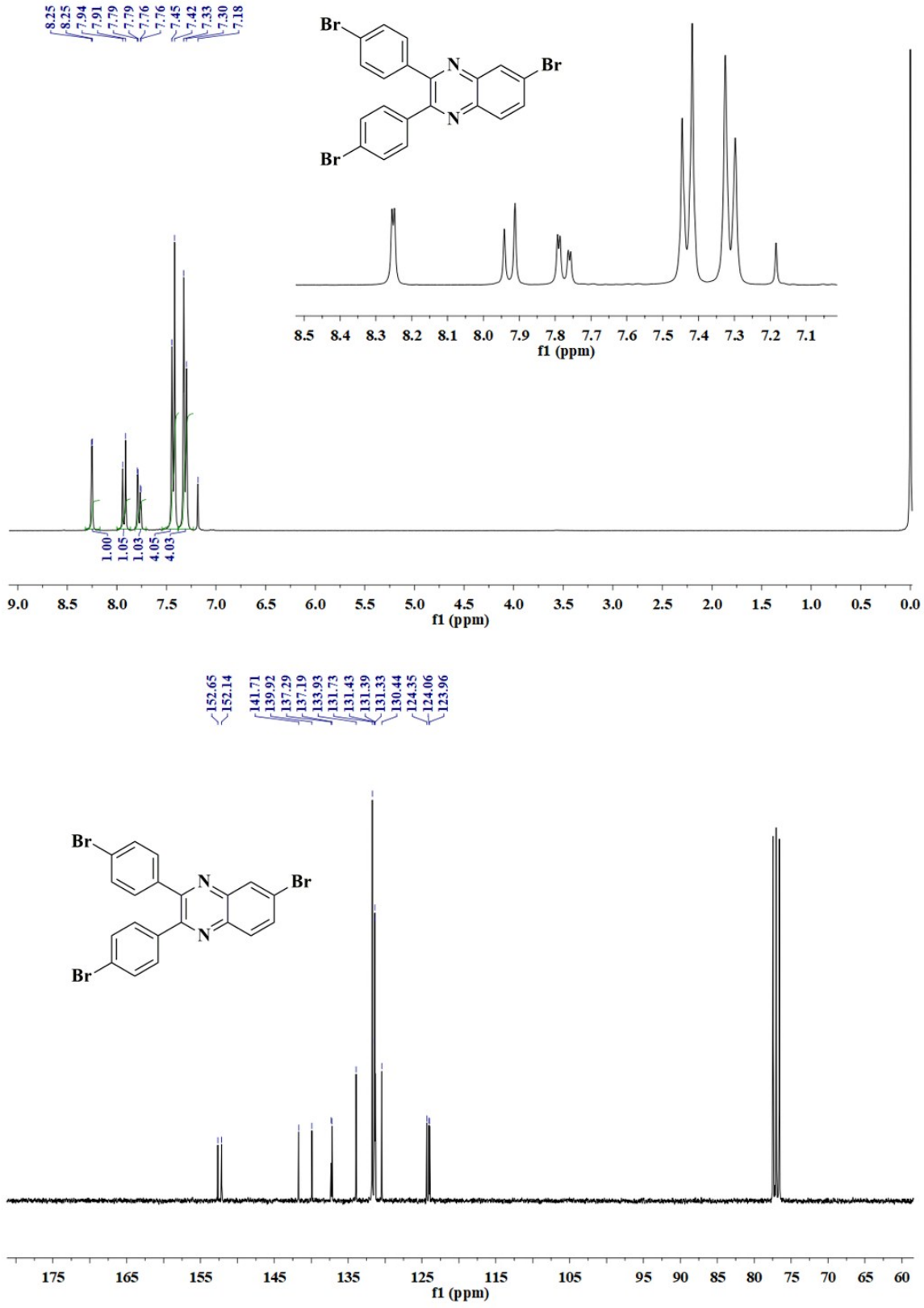

Fig. S20. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **1**.

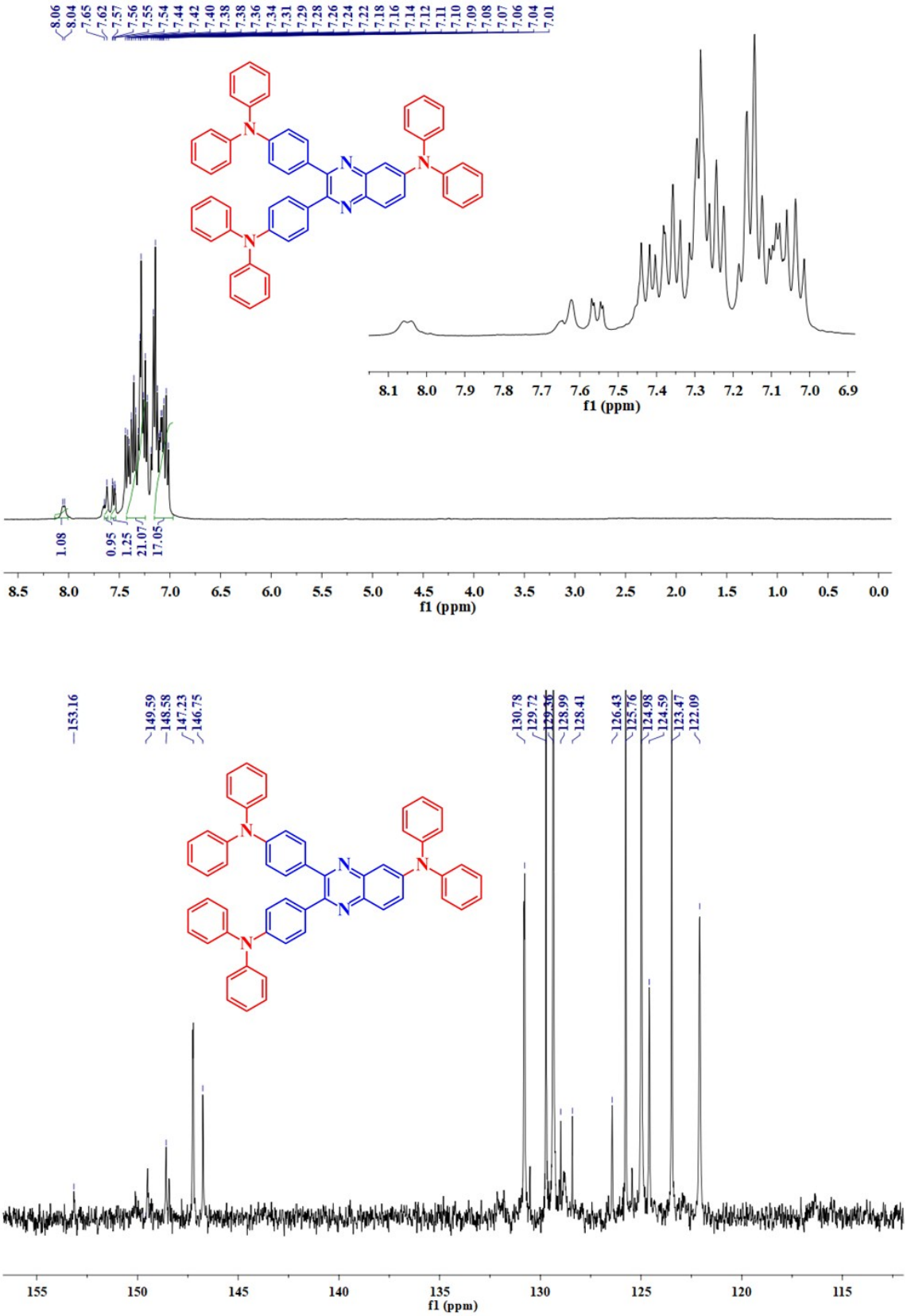

Fig. S21. ^{1}H and (above) and ^{13}C (below) NMR spectrum of compound **2**.

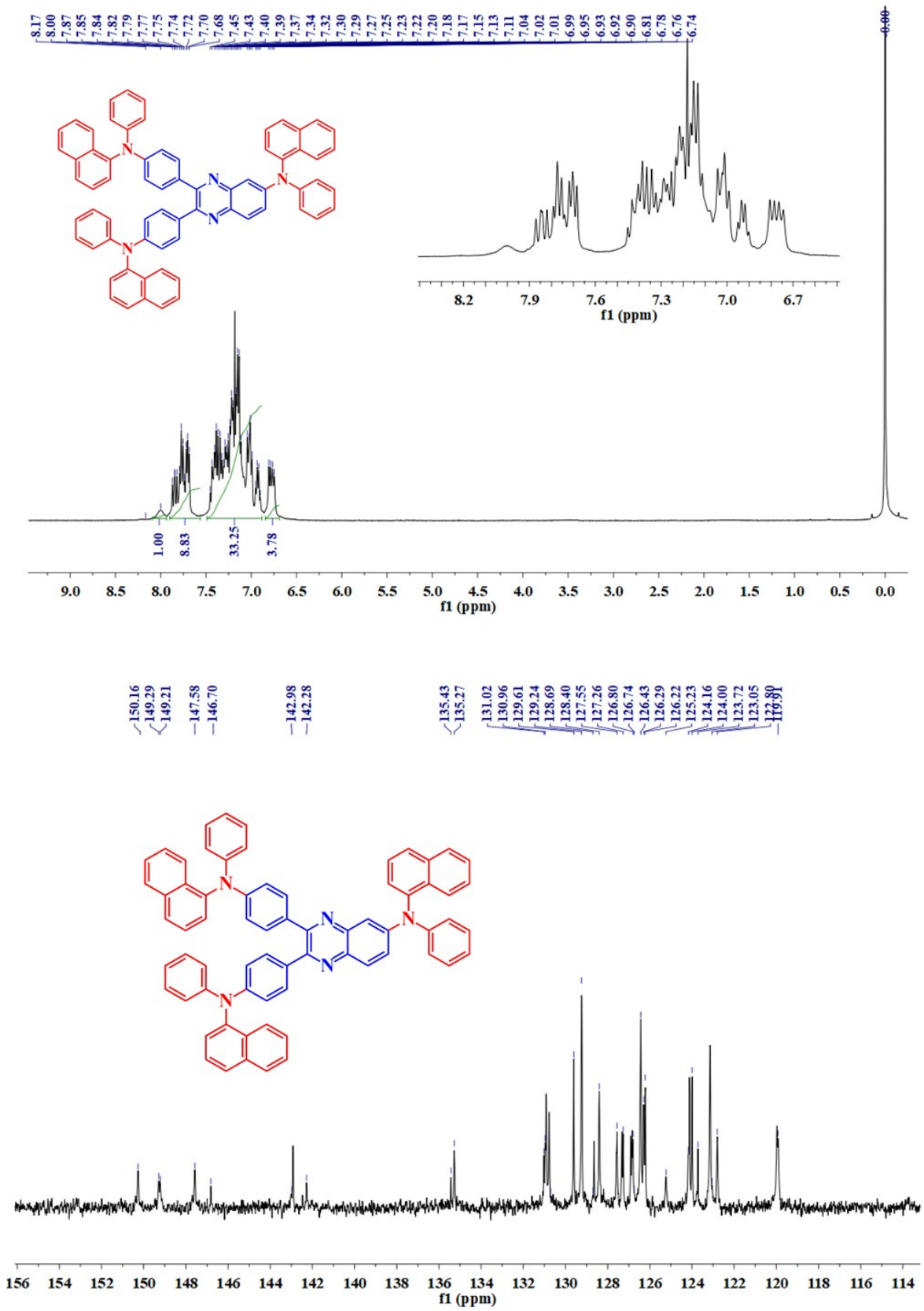

Fig. S22. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **3**.

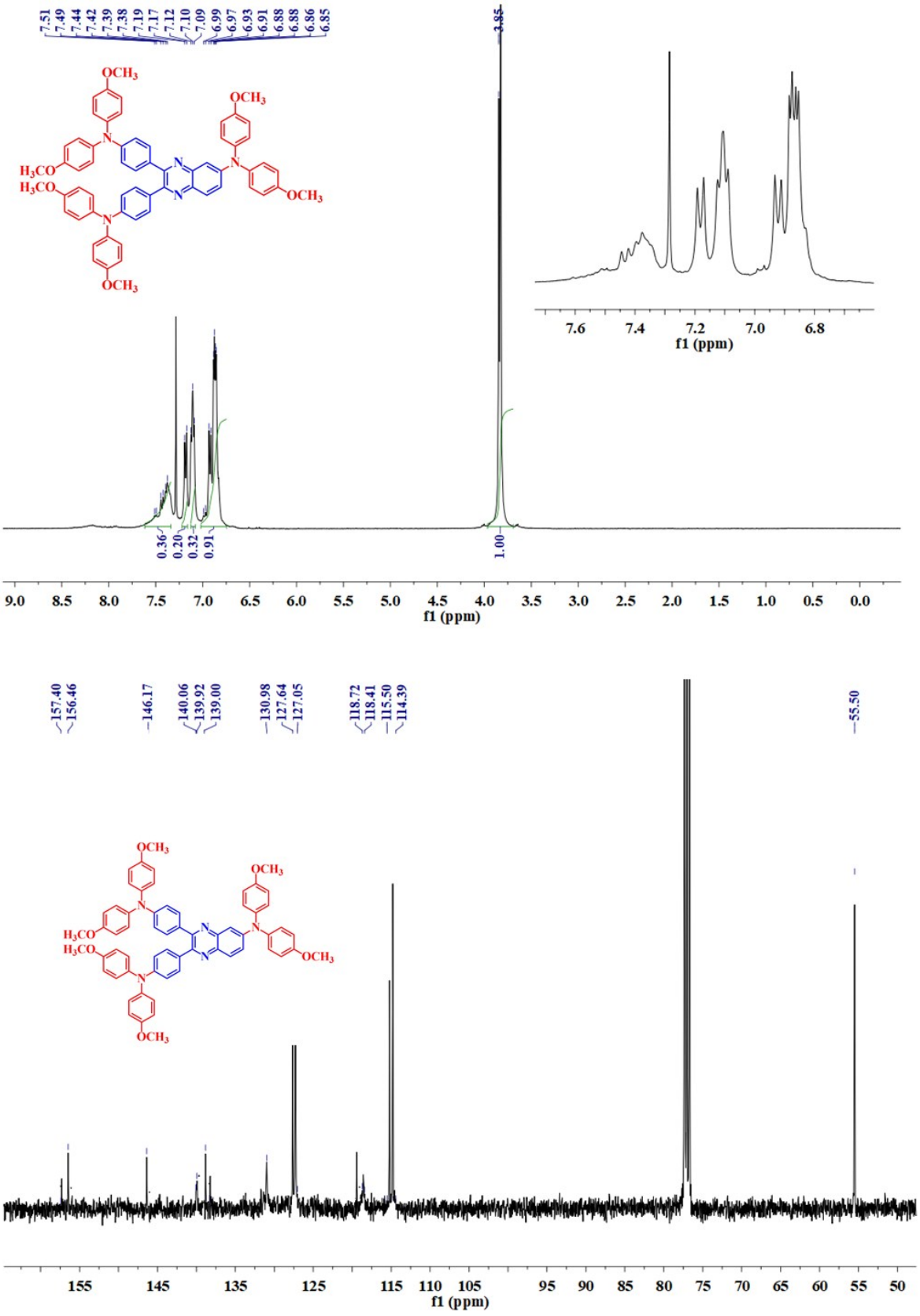

Fig. S23. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **4**.

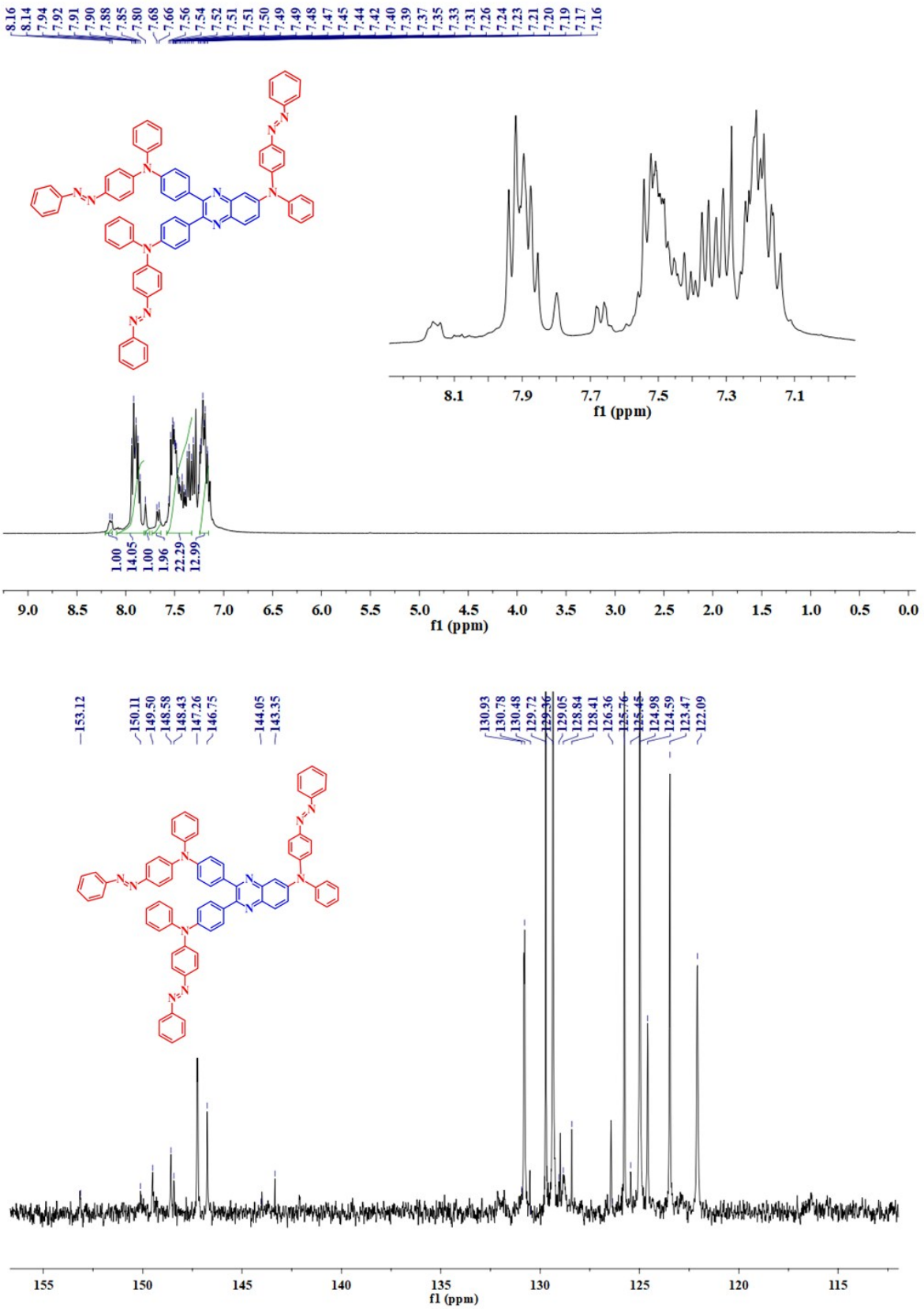

Fig. S24. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **5**.

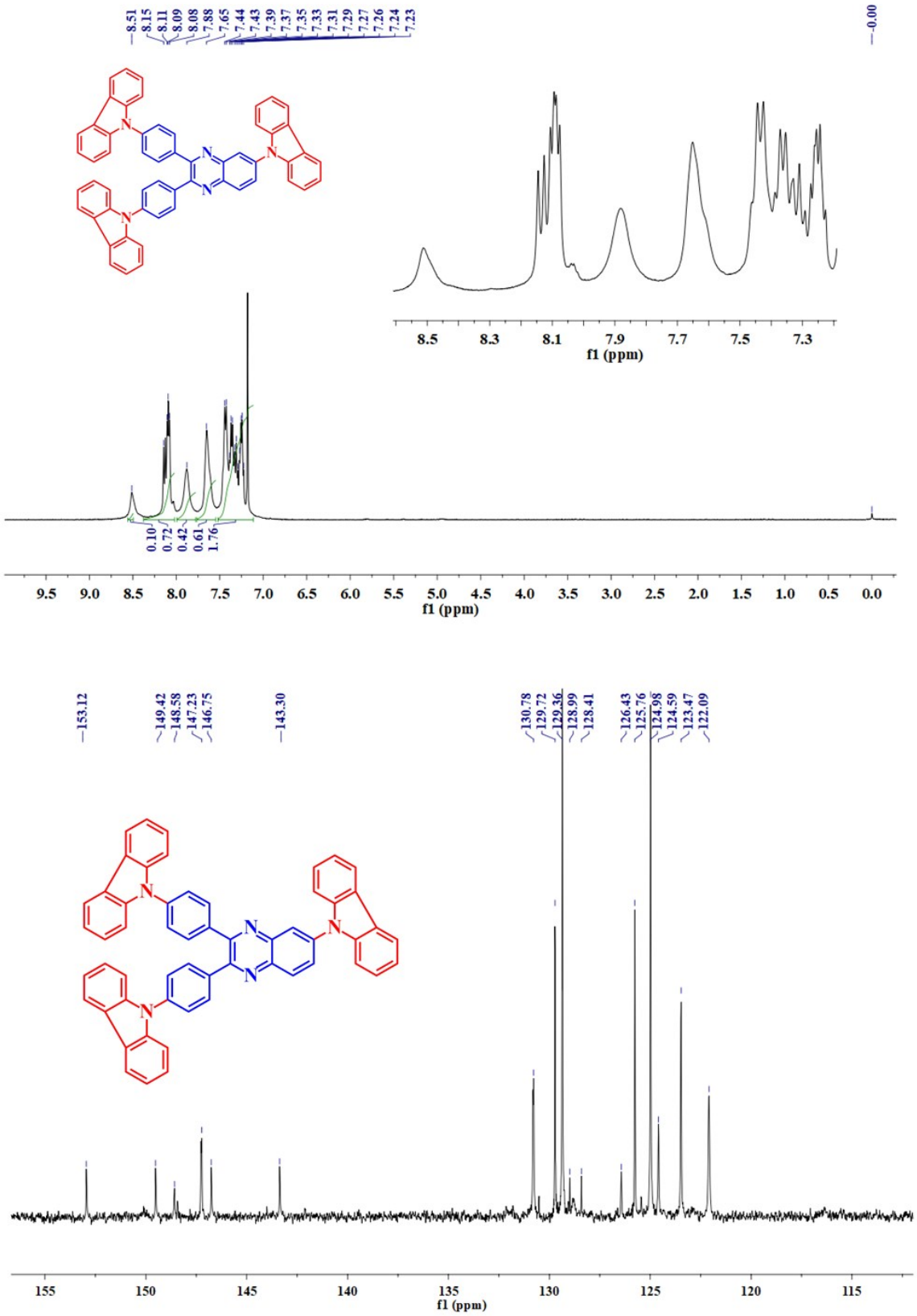

Fig. S25. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **6**.

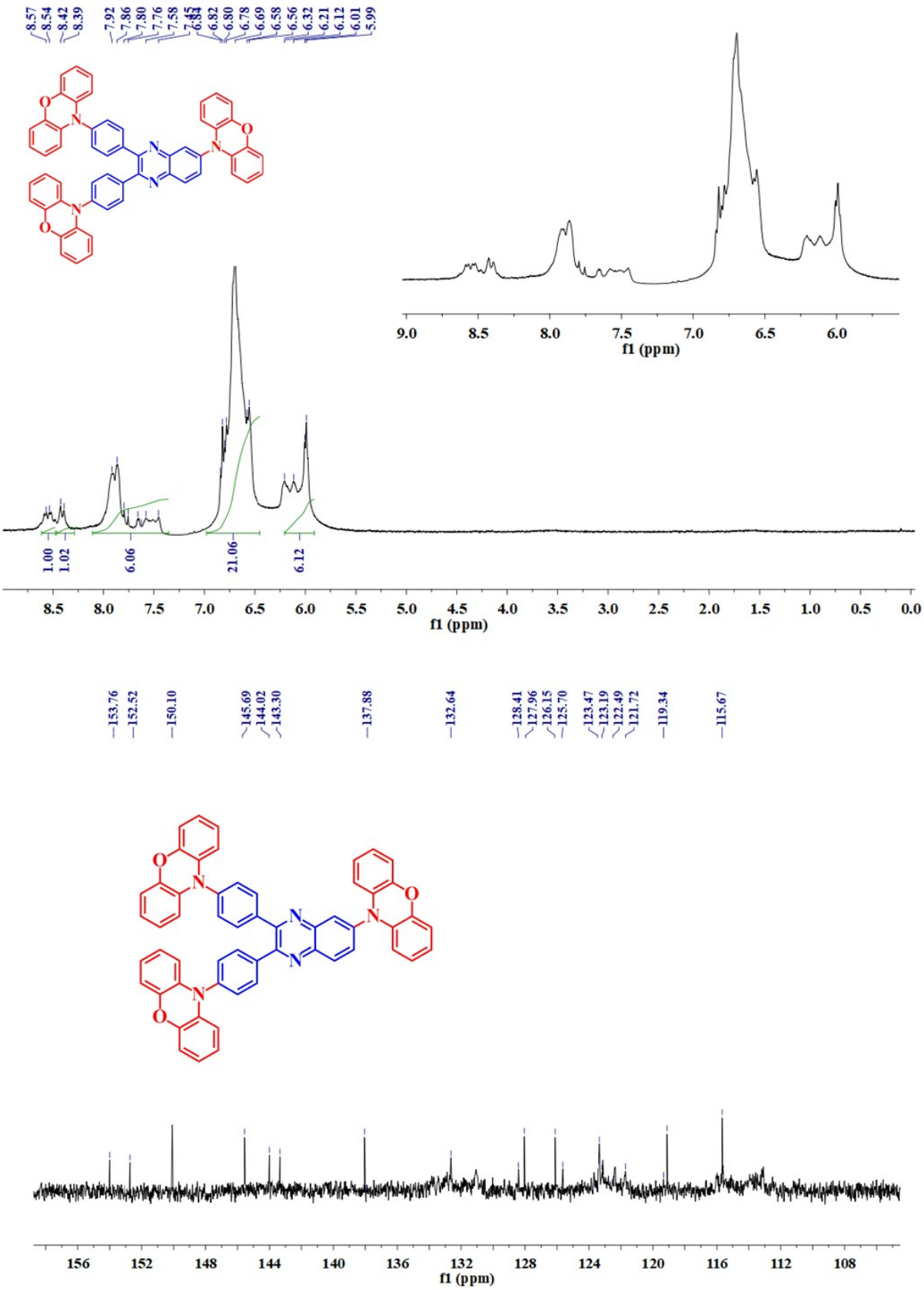

Fig. S26. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **7**.

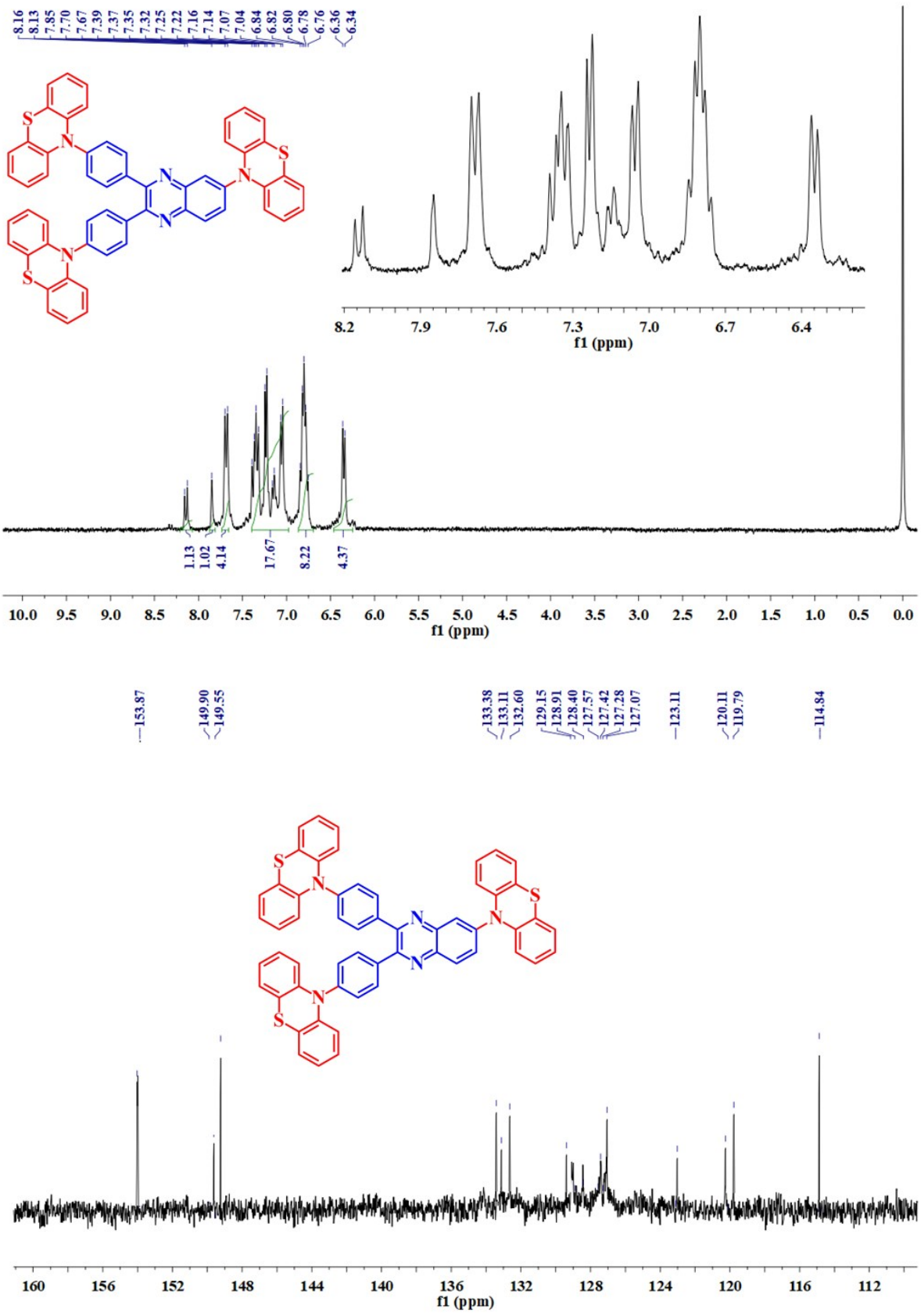

Fig. S27. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **8**.

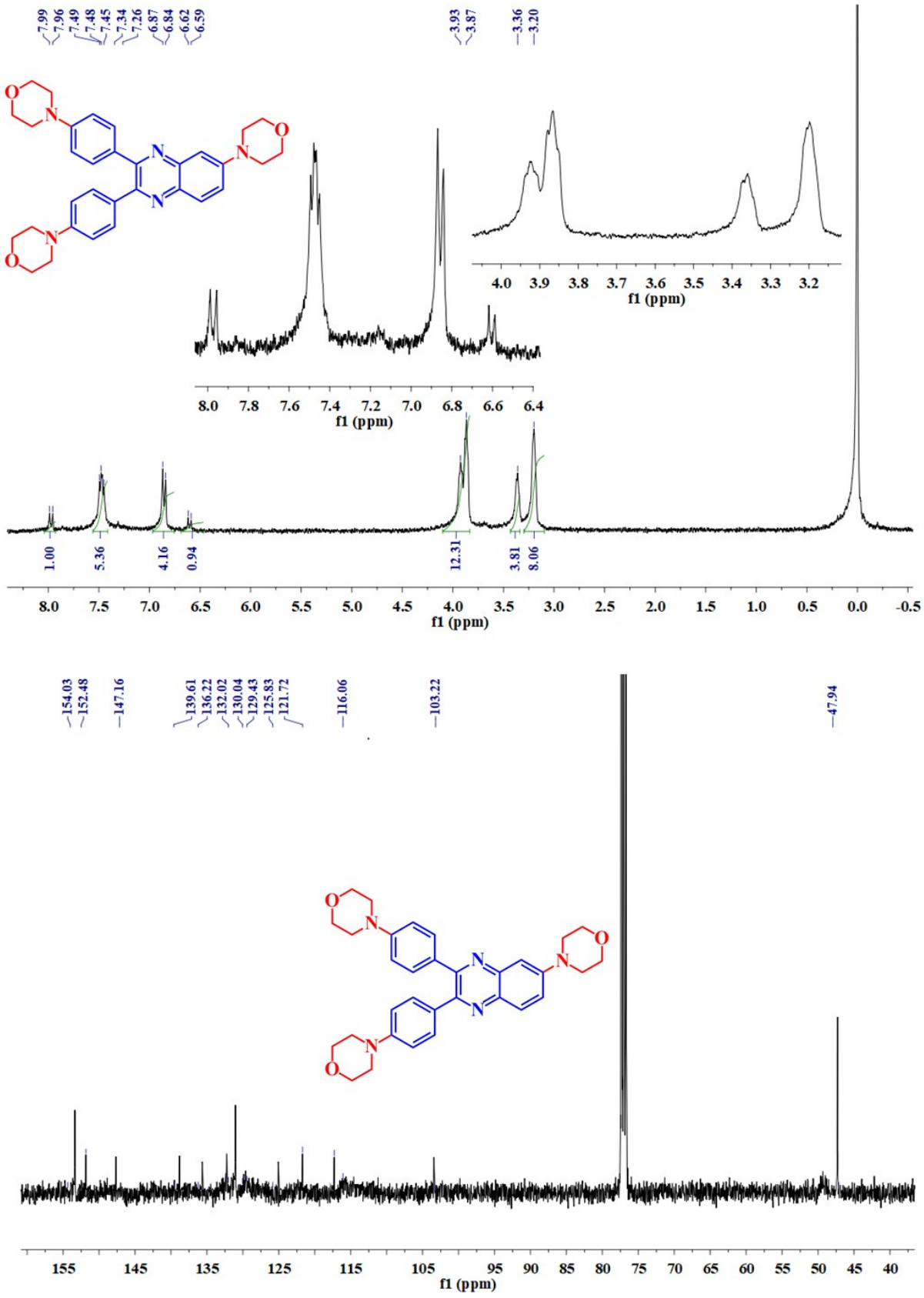

Fig. S28. ^{1}H (above) and ^{13}C (below) NMR spectrum of compound **9.**

10. Optimized structures of compounds 1 9.

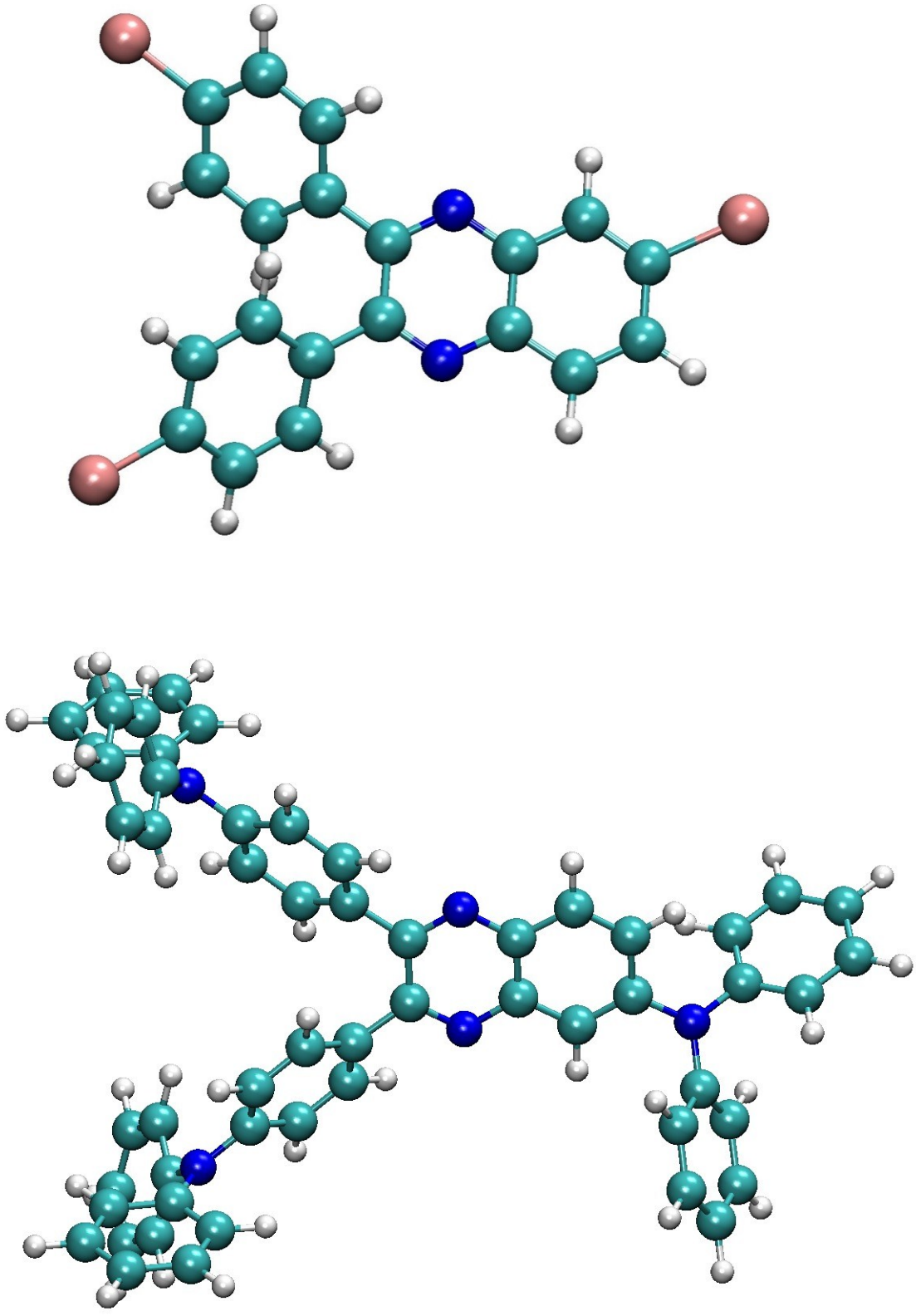

Fig. S29. Optimized structure of **1** (above) and **2** (below).

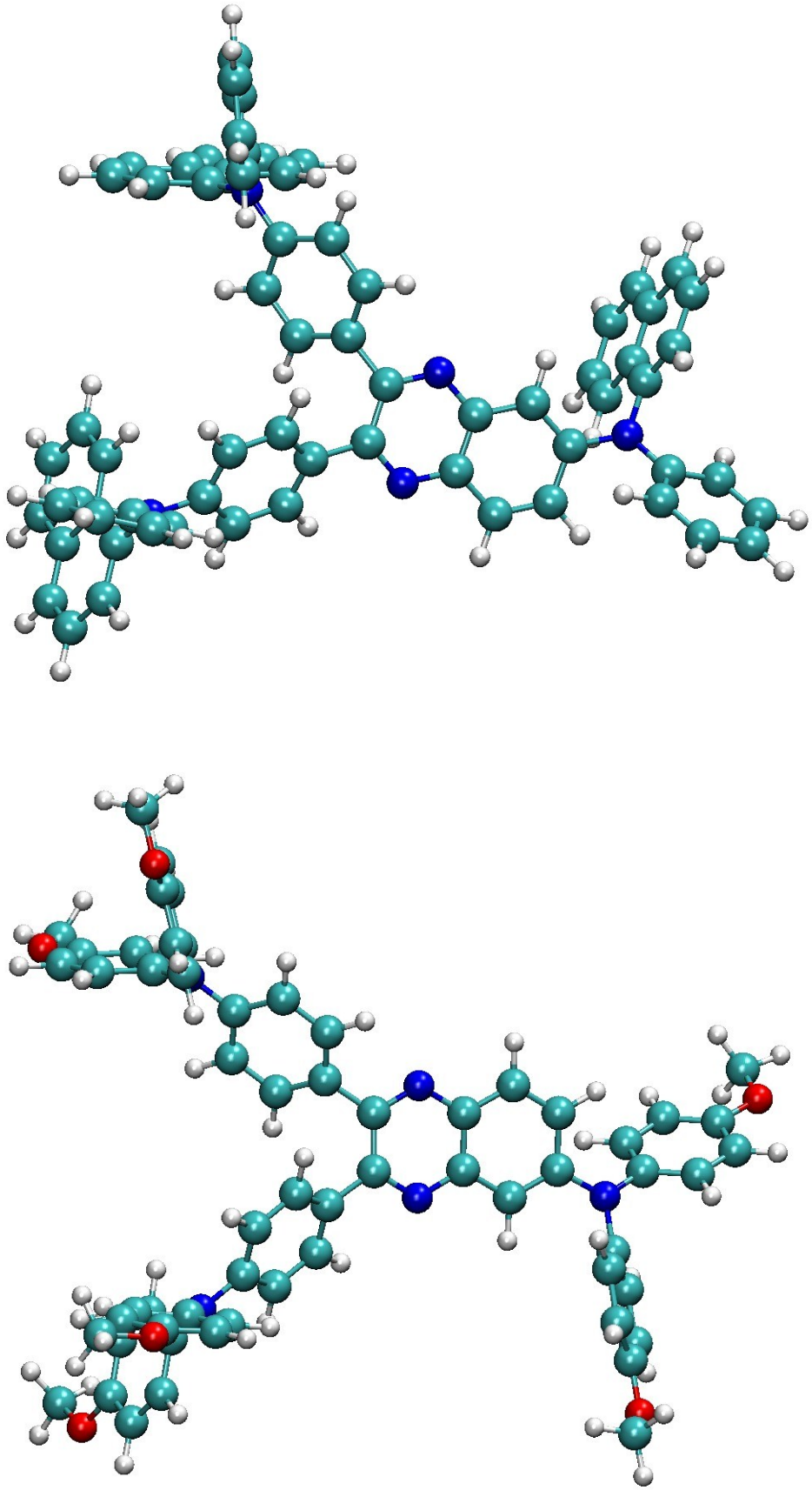

Fig. S30. Optimized structure of **3** (above) and **4** (below).

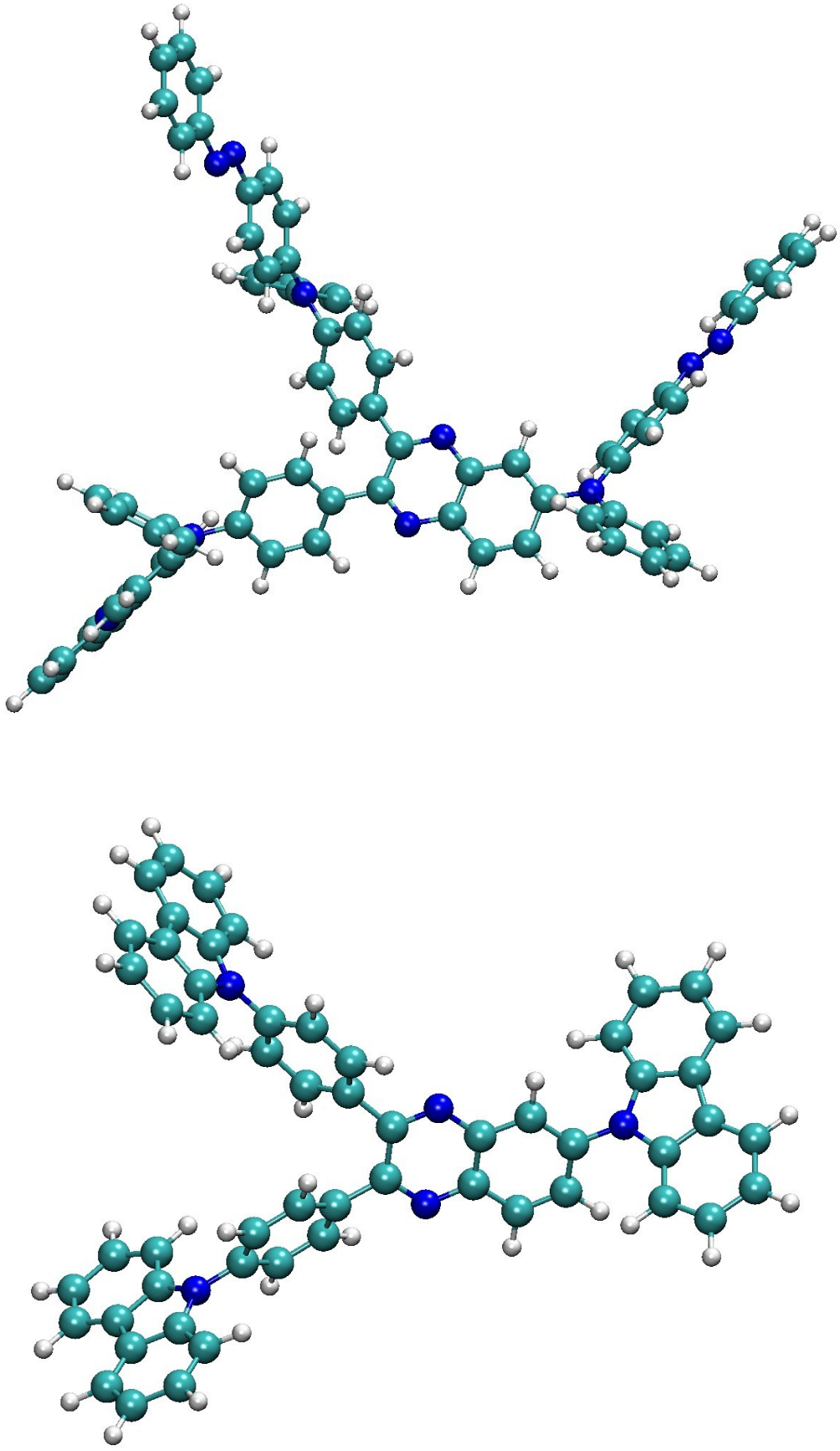

Fig. S31. Optimized structure of **5** (above) and **6** (below).

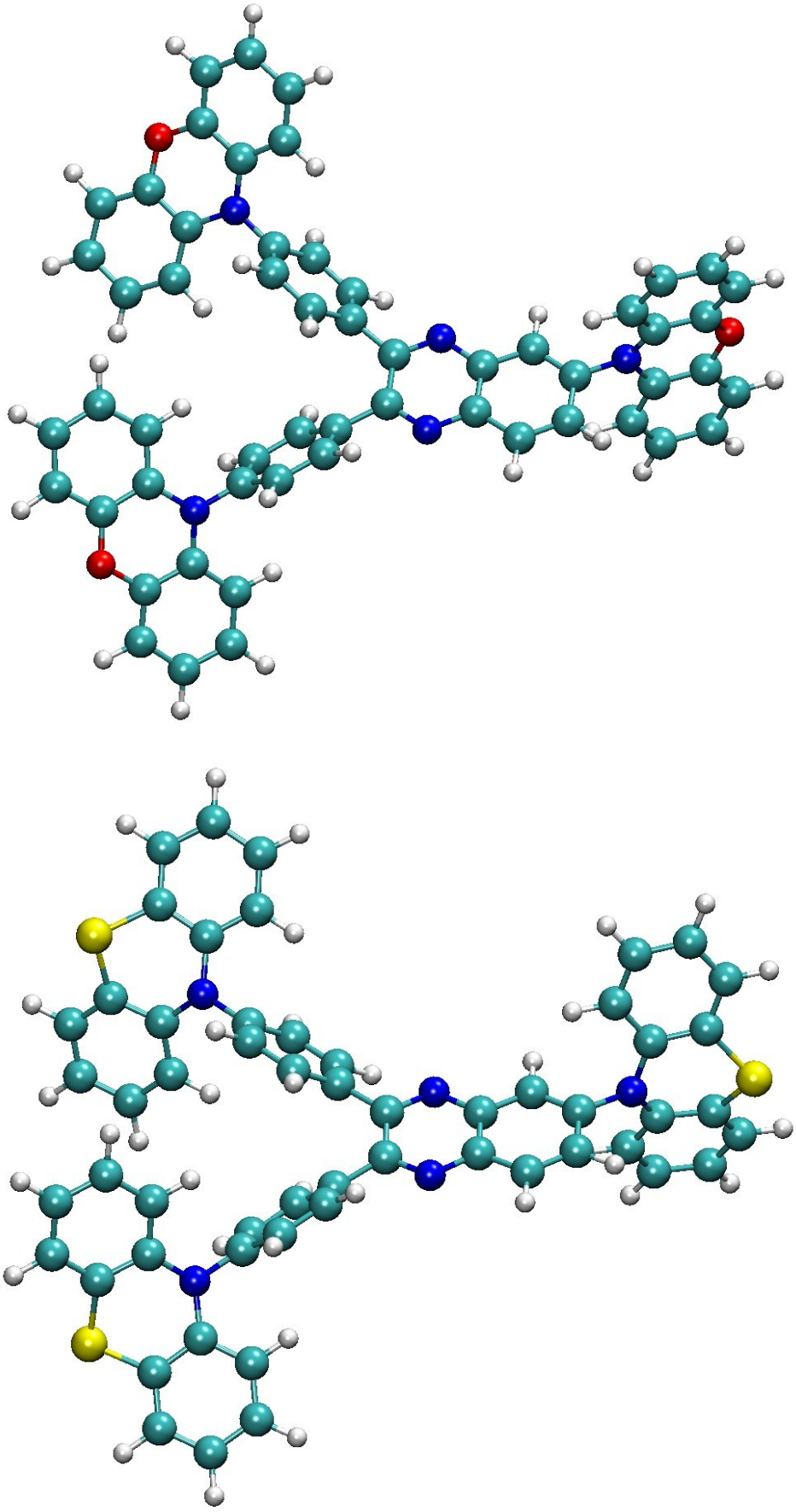

Fig. S32. Optimized structure of **7** (above) and **8** (below).

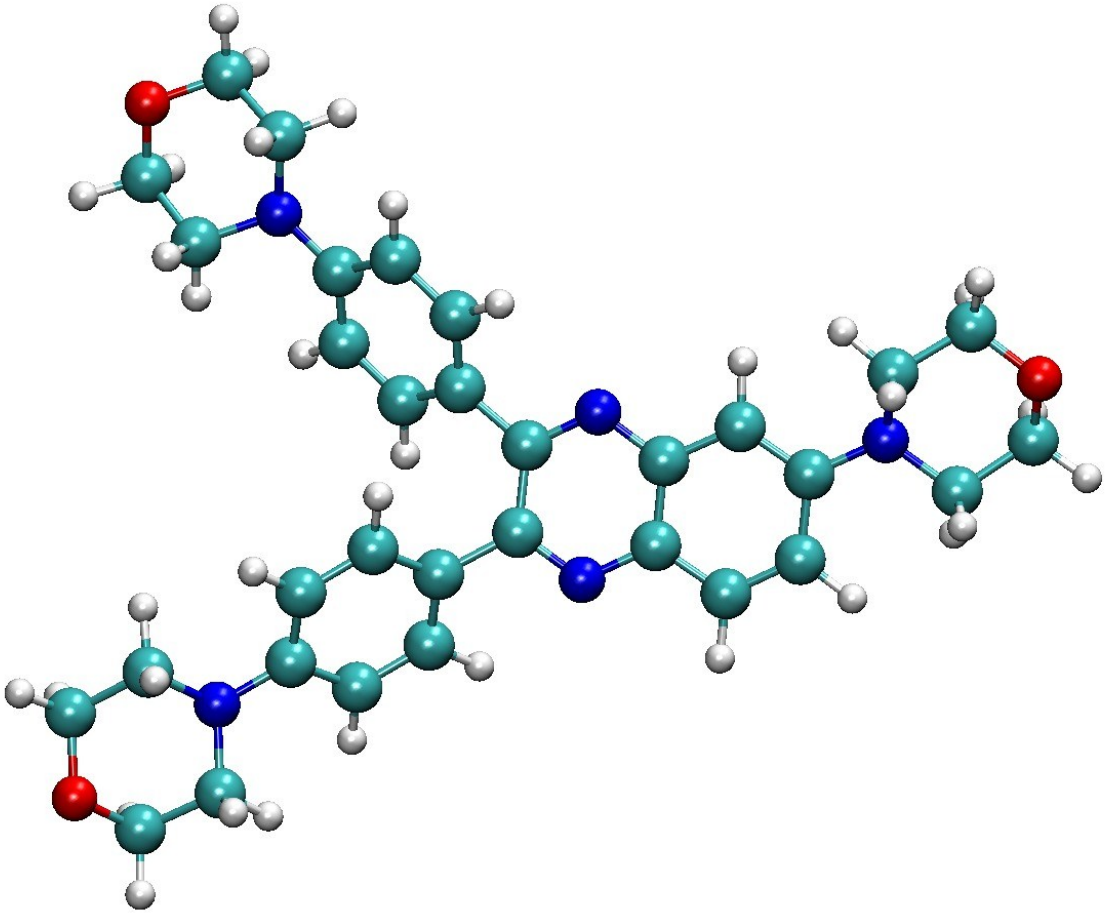

Fig. S33. Optimized structure of **9**

11. Frontier molecular orbital of compounds 1 9.

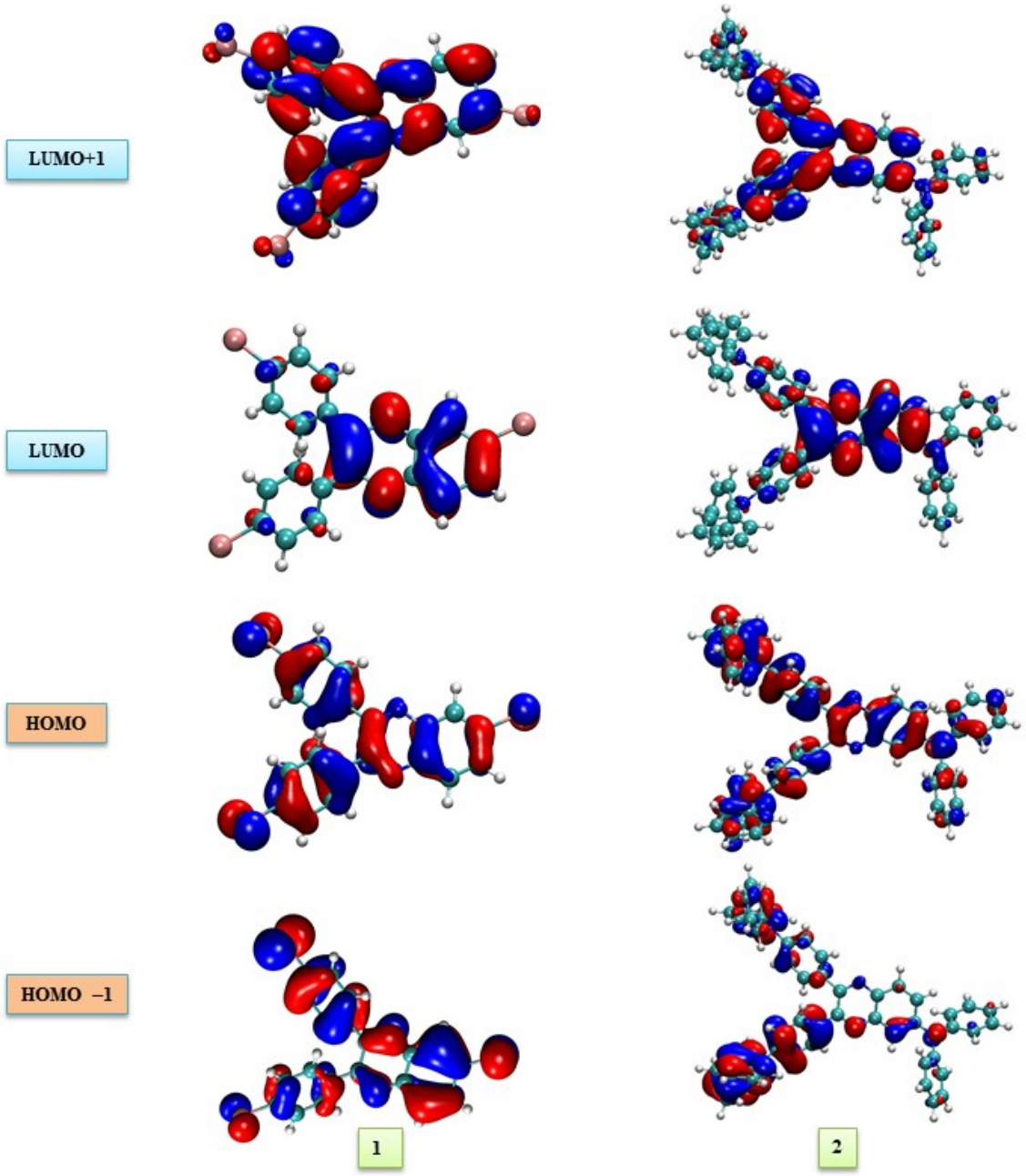

Fig. S34. Frontier molecular orbitals of compound **1** and **2**.

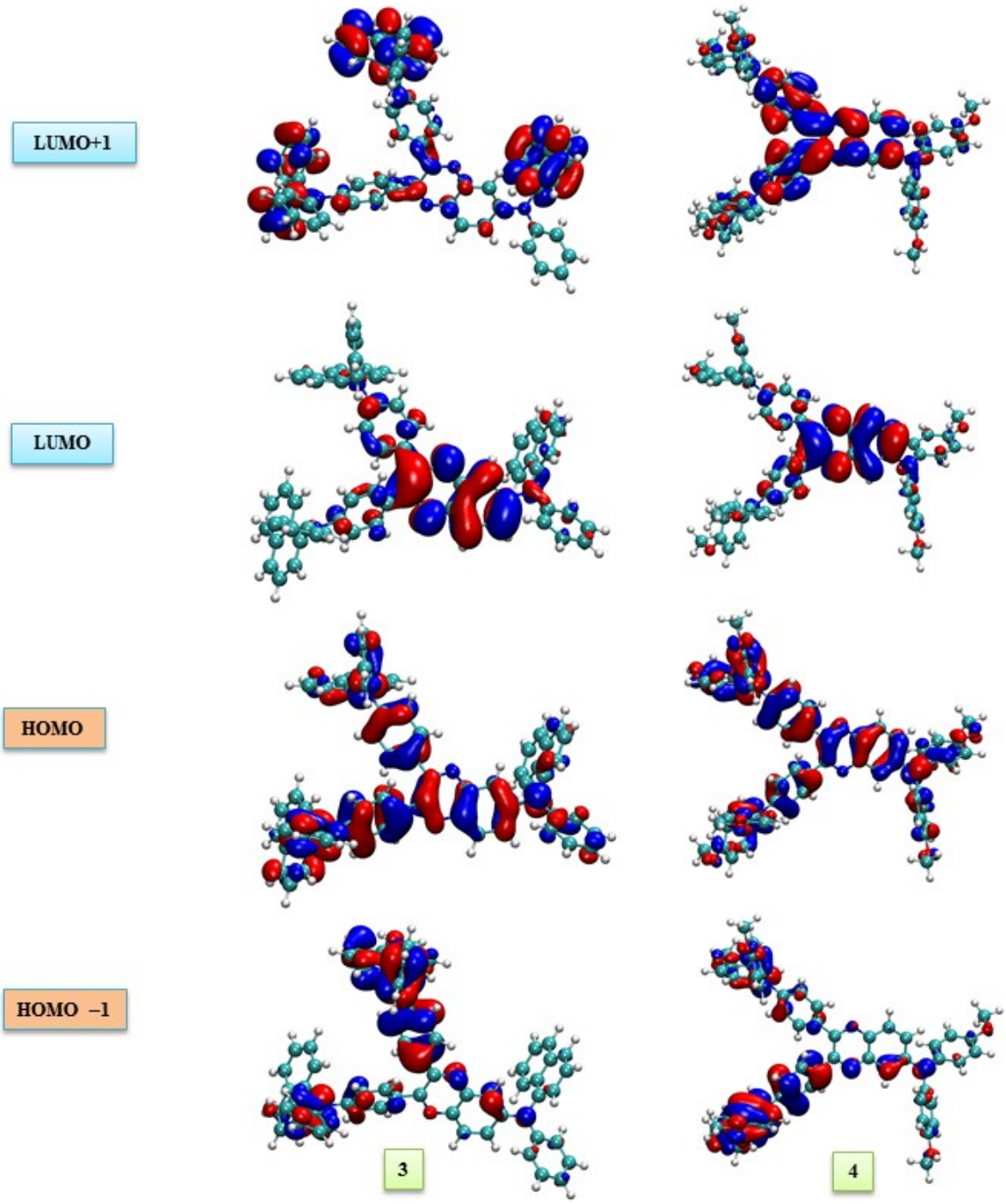

Fig. S35. Frontier molecular orbitals of compound **3** and **4**.

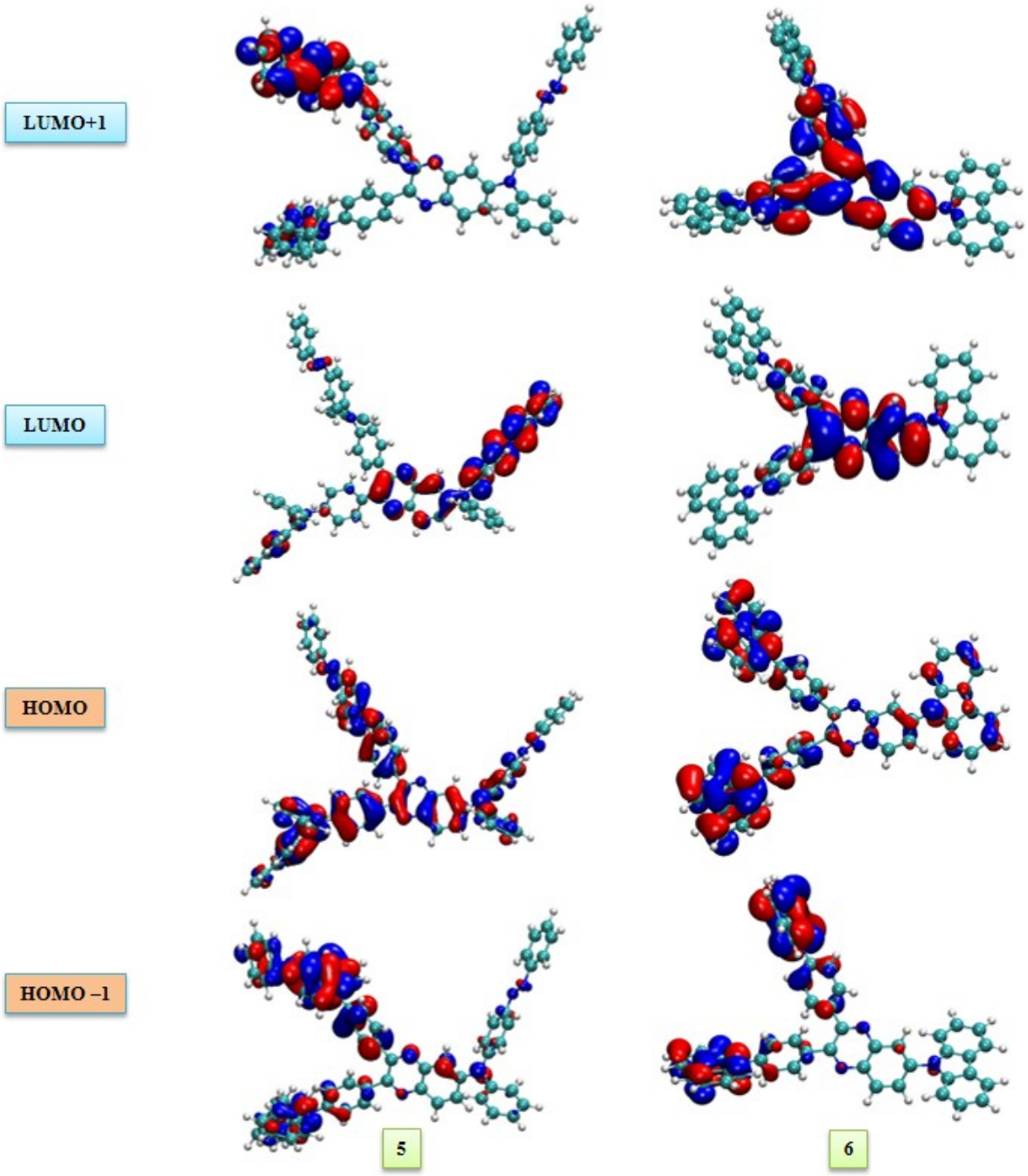

Fig. S36. Frontier molecular orbitals of compound **5** and **6**.

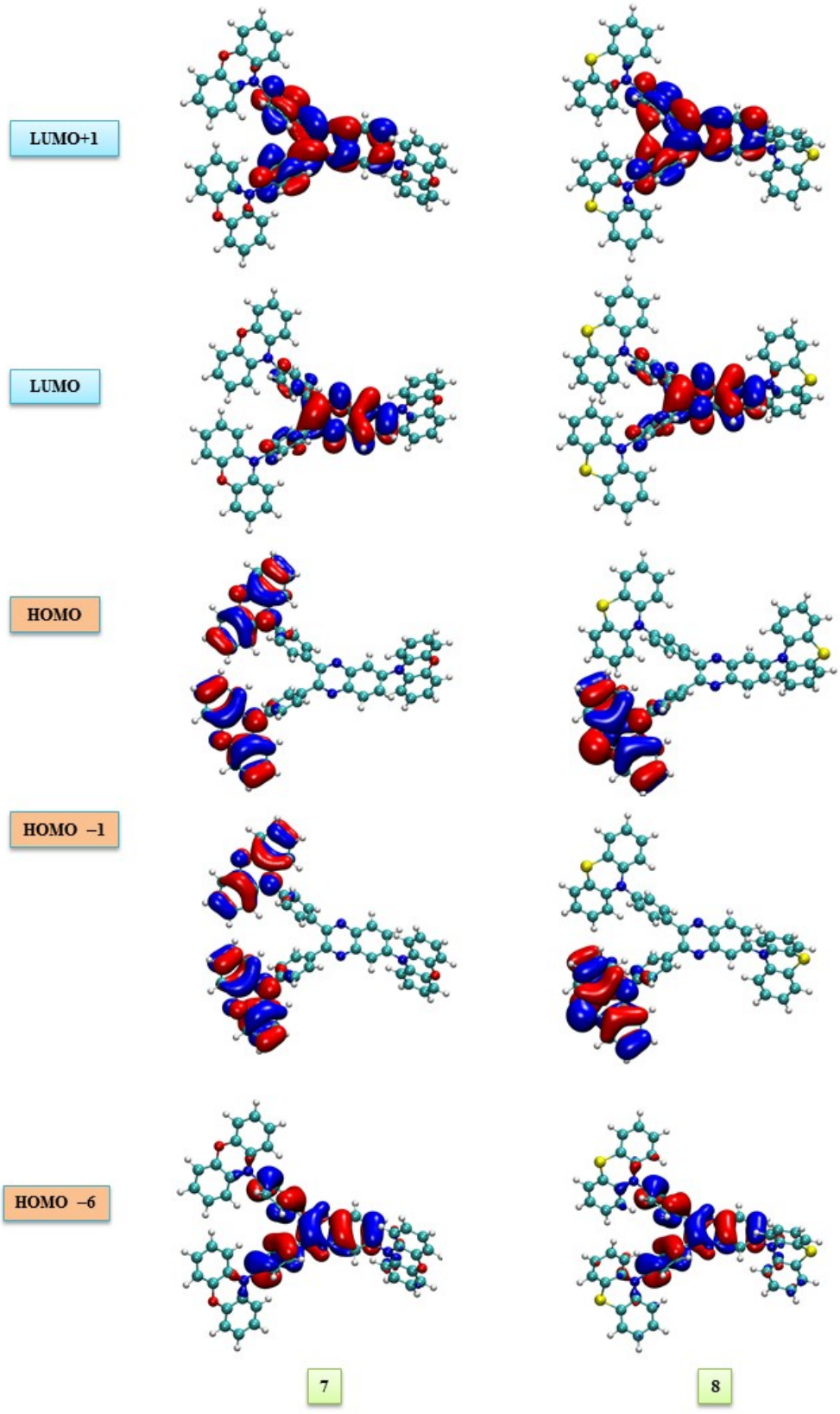

Fig. S37. Frontier molecular orbitals of compound **7** and **8**.

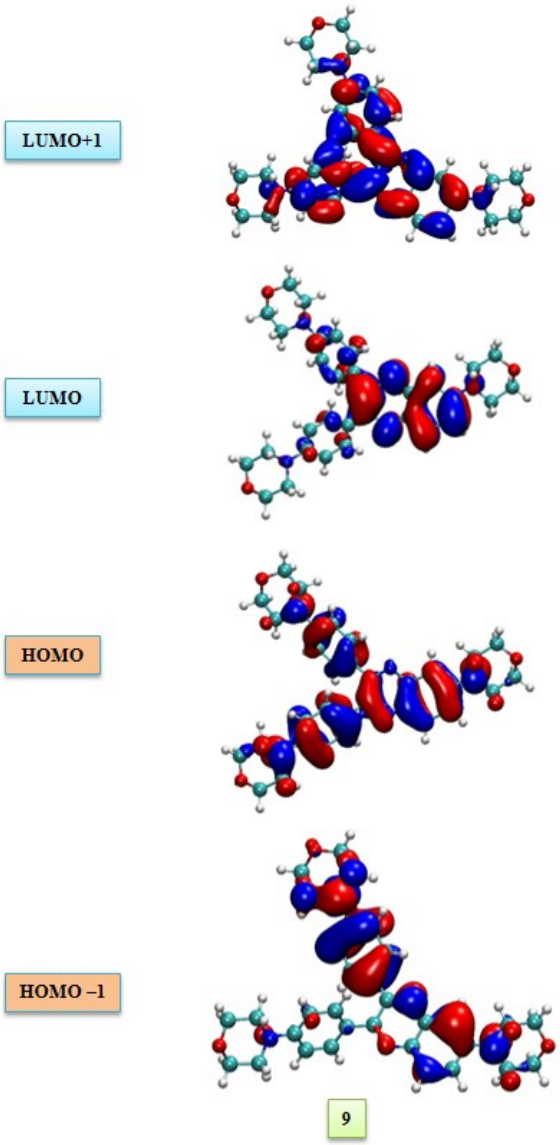

Fig. S38. Frontier molecular orbitals of compound **9**.

12. Cartesian coordinates and Charges (Mulliken and Lowdin) of compounds 1 9

Table S2. Cartesian coordinates of optimized structure of molecule **1**.

Total energy: –8600.91787235Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	0.695509	0.42127	-0.31617	-0.31408	-0.03408
C	-0.261322	-0.27734	-1.15264	-0.42261	-0.03722
N	-0.179456	-0.20535	-2.46677	0.21884	-0.03062
C	0.860613	0.46274	-3.02209	-0.06992	-0.05503
C	1.87045	1.03372	-2.19908	0.21858	-0.04901
N	1.744829	1.01592	-0.84868	0.22122	-0.03222
C	0.975529	0.55875	-4.43071	-0.27809	-0.00547
C	2.061772	1.18259	-4.99449	-0.12542	-0.06601
C	3.068221	1.72813	-4.16086	0.05625	-0.23386
C	2.991532	1.66591	-2.79211	-0.40039	-0.05521
C	0.558222	0.55899	1.15988	0.50988	-0.08296
C	-1.353616	-1.13833	-0.62146	0.54543	-0.08284
Br	4.567974	2.58226	-4.9892	-0.16949	0.27823
C	-0.668097	0.86892	1.76058	-0.18899	-0.01235
C	-0.763666	1.05918	3.13575	-0.37142	-0.07355
C	0.377792	0.92531	3.92042	0.062	-0.23711
C	1.611276	0.6252	3.34911	-0.2049	-0.07492
C	1.695507	0.45588	1.97085	-0.34141	-0.00679
C	-1.138422	-2.04189	0.4264	-0.16081	-0.01263
C	-2.154265	-2.88665	0.86379	-0.39126	-0.07349
C	-3.403363	-2.81809	0.2541	0.06432	-0.23751
C	-3.64348	-1.93385	-0.79394	-0.19388	-0.07528
C	-2.613636	-1.10794	-1.2324	-0.37814	-0.00742
Br	0.248841	1.16379	5.81679	-0.16953	0.2701
Br	-4.812843	-3.96384	0.86255	-0.17045	0.2698
H	0.197068	0.12017	-5.04341	0.18784	0.07213
H	2.160042	1.25666	-6.06963	0.23308	0.06262
H	3.749901	2.0936	-2.14995	0.24084	0.07472
H	-1.559458	0.97779	1.15523	0.20831	0.07546
H	-1.71415	1.30971	3.58832	0.24016	0.06297
H	2.493795	0.52995	3.96846	0.23859	0.0619
H	2.653519	0.24344	1.51274	0.21031	0.07391
H	-0.167538	-2.10261	0.90236	0.206	0.07539
H	-1.973486	-3.58901	1.66705	0.2395	0.063
H	-4.617252	-1.89334	-1.26462	0.23889	0.06172
H	-2.782911	-0.43142	-2.06088	0.21074	0.07364

Table S3. Cartesian coordinates of optimized structure of molecule **2**.

Total energy: –2433.01652920Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	-0.87719	-0.33918	0.26784	-0.45826	-0.03601
C	-0.1034	-1.50953	-0.09653	-0.49489	-0.04418
N	-0.65546	-2.71039	-0.06057	0.26294	-0.03749
C	-1.97046	-2.81733	0.23557	-0.21868	-0.06156
C	-2.76164	-1.65566	0.45929	0.2523	-0.04551
N	-2.17515	-0.43136	0.49267	0.30743	-0.04057
C	-2.59699	-4.0887	0.28308	-0.14616	-0.0068
C	-3.94247	-4.18934	0.52227	0.21531	-0.02076
C	-4.74795	-3.02534	0.71354	-1.03198	-0.04305
C	-4.15241	-1.77655	0.67644	-0.29191	-0.02275
C	-0.28819	1.01185	0.46612	0.14665	-0.09059
C	1.30592	-1.46148	-0.56597	0.12686	-0.09024
N	-6.13018	-3.17869	0.96831	0.78748	-0.09627
C	0.9087	1.20545	1.16835	-0.40316	-0.00985
C	1.39882	2.48086	1.4154	-0.00891	-0.03284
C	0.70549	3.61316	0.96267	-0.7519	-0.04707
C	-0.49612	3.42553	0.26345	0.16407	-0.03299
C	-0.98346	2.14729	0.02863	-0.1488	-0.00474
C	2.20179	-2.47014	-0.18412	-0.16789	-0.00527
C	3.50495	-2.49622	-0.66021	0.14888	-0.03352
C	3.95927	-1.51177	-1.55082	-0.92083	-0.04735
C	3.06455	-0.50655	-1.94674	0.04862	-0.03332
C	1.76348	-0.4856	-1.46189	-0.35628	-0.01054
N	1.20313	4.91616	1.21365	0.79433	-0.09772
N	5.28762	-1.53685	-2.04365	0.78235	-0.0977
C	1.09734	5.92624	0.21768	-0.43559	-0.05711
C	1.80494	5.22254	2.46547	-0.3348	-0.05684
C	-6.88282	-4.16261	0.26832	-0.2694	-0.0592
C	-6.8084	-2.26795	1.83102	-0.31325	-0.0576
C	5.55682	-1.19494	-3.39784	-0.3257	-0.0569
C	6.36013	-1.91209	-1.18748	-0.36882	-0.05724
C	6.65401	-0.3846	-3.72052	0.061	-0.03784
C	6.9236	-0.06196	-5.0473	-0.28245	-0.03887
C	6.09833	-0.52509	-6.07139	-0.43242	-0.05966
C	5.00144	-1.32528	-5.75276	-0.15256	-0.03877
C	4.7343	-1.66667	-4.43023	0.11841	-0.03847

C	7.35939	-2.78411	-1.6405	0.12101	-0.03719
C	8.41293	-3.14093	-0.80384	-0.30691	-0.03858
C	8.48108	-2.64961	0.49938	-0.39215	-0.05899
C	7.48429	-1.78756	0.9555	-0.2537	-0.03896
C	6.43613	-1.41301	0.11999	0.21534	-0.0383
C	-7.85885	-4.91229	0.93971	-0.02671	-0.03539
C	-8.60094	-5.86982	0.25599	-0.34526	-0.03765
C	-8.37477	-6.10771	-1.09999	-0.37258	-0.05754
C	-7.40131	-5.36774	-1.76892	-0.21269	-0.03767
C	-6.66558	-4.39541	-1.0963	0.22363	-0.0408
C	-8.01523	-1.67899	1.4354	0.33154	-0.0351
C	-8.68189	-0.80423	2.28963	-0.43698	-0.03769
C	-8.14968	-0.49363	3.53973	-0.34667	-0.05524
C	-6.94358	-1.07428	3.9329	-0.35224	-0.03749
C	-6.27937	-1.9608	3.09133	0.22334	-0.03294
C	2.97679	5.98946	2.52226	0.12262	-0.03792
C	3.55805	6.2945	3.74956	-0.27376	-0.03883
C	2.99347	5.82969	4.93689	-0.43779	-0.05964
C	1.83079	5.06147	4.8831	-0.17676	-0.03874
C	1.23389	4.76552	3.66129	0.06436	-0.03846
C	0.69657	7.22455	0.56136	0.10421	-0.03742
C	0.60351	8.21254	-0.41451	-0.24572	-0.03848
C	0.89189	7.92218	-1.7476	-0.41877	-0.05908
C	1.28465	6.62962	-2.09363	-0.18787	-0.03871
C	1.39574	5.63989	-1.12151	0.13005	-0.03845
H	-1.98467	-4.9698	0.13092	0.1915	0.06957
H	-4.41315	-5.16322	0.57151	0.19028	0.07645
H	-4.72585	-0.87166	0.8304	0.20675	0.08621
H	1.46649	0.35109	1.53207	0.24312	0.07406
H	2.32317	2.60439	1.96599	0.16364	0.07532
H	-1.05094	4.28736	-0.08667	0.17998	0.07517
H	-1.92841	2.01844	-0.48488	0.22186	0.07238
H	1.85746	-3.25254	0.48096	0.22995	0.0721
H	4.17693	-3.28645	-0.34853	0.17917	0.075
H	3.39188	0.25822	-2.6401	0.16343	0.07509
H	1.0968	0.30279	-1.78916	0.24419	0.07377
H	7.29313	-0.01288	-2.92879	0.15743	0.07408
H	7.77659	0.56645	-5.2788	0.18501	0.05476
H	6.30714	-0.26684	-7.103	0.1538	0.05233
H	4.35558	-1.70015	-6.53915	0.18699	0.055
H	3.88747	-2.29844	-4.19093	0.17873	0.0749
H	7.30643	-3.17761	-2.64841	0.16132	0.07427

H	9.17707	-3.81773	-1.17	0.18541	0.05488
H	9.29933	-2.9343	1.15046	0.15336	0.05244
H	7.52812	-1.39149	1.96409	0.1845	0.05487
H	5.67061	-0.7343	0.47607	0.15428	0.07329
H	-8.03138	-4.73852	1.99498	0.1642	0.07449
H	-9.35125	-6.44244	0.78992	0.18494	0.05523
H	-8.95065	-6.85911	-1.62747	0.15517	0.05288
H	-7.22057	-5.53551	-2.82489	0.18518	0.05549
H	-5.9217	-3.81237	-1.62574	0.18113	0.0749
H	-8.42819	-1.91202	0.46147	0.17347	0.0746
H	-9.61531	-0.3549	1.96917	0.18401	0.05516
H	-8.66728	0.19238	4.20005	0.16103	0.05294
H	-6.52216	-0.84609	4.90556	0.18761	0.05547
H	-5.34702	-2.41595	3.40311	0.17375	0.07449
H	3.42642	6.34513	1.60309	0.15603	0.07408
H	4.46505	6.88844	3.77518	0.18543	0.05478
H	3.45233	6.06356	5.89044	0.1534	0.05234
H	1.37511	4.70034	5.79852	0.18691	0.05499
H	0.32487	4.17736	3.62729	0.18008	0.07495
H	0.46133	7.45414	1.59361	0.15853	0.07424
H	0.29043	9.2115	-0.13146	0.18588	0.05488
H	0.81232	8.69233	-2.5059	0.14992	0.05246
H	1.52069	6.3911	-3.12486	0.18566	0.05492
H	1.71261	4.6406	-1.3945	0.14147	0.07319

Table S4. Cartesian coordinates of optimized structure of molecule **3**.

Total energy: –2894.04179310Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	1.148631	-0.25352	-0.03158	-0.523	-0.03416
C	1.292608	0.92455	0.80083	-0.44609	-0.04379
N	2.26328	0.9927	1.696	0.26727	-0.03754
C	3.169906	-0.00847	1.75511	-0.19961	-0.06286
C	3.114398	-1.09363	0.83693	0.18623	-0.04272
N	2.072073	-1.19864	-0.02543	0.32309	-0.04269
C	4.224179	0.02791	2.70366	-0.141	-0.00717
C	5.182283	-0.95089	2.71354	0.06873	-0.02861
C	5.157572	-2.01921	1.76386	-0.39225	-0.04597
C	4.127697	-2.07968	0.84192	-0.37336	-0.02288
C	-0.031222	-0.51708	-0.89634	0.10353	-0.09329
C	0.426846	2.12794	0.69706	0.16828	-0.09365

N	6.150414	-3.02225	1.82942	0.75976	-0.10486
C	-1.340094	-0.23929	-0.48455	-0.28788	-0.00474
C	-2.432101	-0.56709	-1.27906	-0.33401	-0.03592
C	-2.251952	-1.18782	-2.52358	-0.36672	-0.0465
C	-0.940762	-1.48216	-2.936	0.08459	-0.04385
C	0.141392	-1.1563	-2.13338	-0.07142	-0.00339
C	0.045742	2.81587	1.85528	-0.1544	-0.00142
C	-0.71094	3.97891	1.79123	-0.10979	-0.03455
C	-1.105521	4.50716	0.55345	-0.49571	-0.04786
C	-0.715909	3.82832	-0.61343	-0.0681	-0.0433
C	0.035039	2.66427	-0.53818	-0.4286	-0.01112
N	-3.359322	-1.54884	-3.32506	0.70136	-0.10508
N	-1.901916	5.67463	0.48146	0.74887	-0.10611
C	-4.636808	-1.76531	-2.71643	-0.42498	-0.04887
C	-3.302823	-1.45988	-4.7449	0.06258	-0.05287
C	7.506822	-2.69697	2.11273	0.11055	-0.05435
C	5.869905	-4.32518	1.30124	-0.51388	-0.04884
C	-1.703419	6.64513	-0.53946	0.05903	-0.05203
C	-2.742043	6.02217	1.58775	-0.47567	-0.04913
C	-0.424105	6.93724	-1.03248	-0.04472	-0.04461
C	-0.257167	7.89728	-2.02702	-0.20228	-0.03889
C	-1.353282	8.59302	-2.53491	-0.42105	-0.0613
C	-2.625911	8.31273	-2.03775	-0.40826	-0.03776
C	-2.804141	7.34434	-1.05501	0.11569	-0.03431
C	-2.46718	7.15367	2.32776	0.09799	-0.02377
C	-3.275887	7.51962	3.42432	-0.33907	-0.03645
C	-4.348437	6.74138	3.78563	-0.2674	-0.03022
C	-4.673836	5.57458	3.04662	0.42372	-0.06205
C	-3.873575	5.20824	1.91592	0.04607	-0.05583
C	8.079824	-1.49704	1.67015	-0.06571	-0.04579
C	9.410353	-1.20486	1.96126	-0.23184	-0.038
C	10.194896	-2.1069	2.67714	-0.41841	-0.05924
C	9.630788	-3.30883	3.10601	-0.38888	-0.03666
C	8.298713	-3.60158	2.83465	0.04924	-0.03245
C	4.936721	-5.18215	1.96748	0.06538	-0.05388
C	4.671165	-6.47114	1.40145	0.36151	-0.06128
C	5.352832	-6.87205	0.22307	-0.33123	-0.02776
C	6.262592	-6.03605	-0.37623	-0.40011	-0.03582
C	6.515651	-4.75628	0.16183	0.15582	-0.0219
C	-2.623886	-0.41395	-5.38453	0.01848	-0.0439
C	-2.589219	-0.34557	-6.77471	-0.25895	-0.03896
C	-3.24155	-1.30365	-7.54922	-0.44848	-0.05984

C	-3.928478	-2.33878	-6.91507	-0.38884	-0.03738
C	-3.955339	-2.42323	-5.52668	0.06696	-0.03288
C	-4.834934	-2.8693	-1.82545	0.09391	-0.05677
C	-6.125089	-3.03883	-1.22512	0.25384	-0.06243
C	-7.17269	-2.13817	-1.5491	-0.2969	-0.03096
C	-6.958318	-1.10734	-2.43106	-0.39416	-0.03765
C	-5.685338	-0.91726	-3.00873	0.09815	-0.02444
C	4.278541	-4.81954	3.17162	-0.16848	-0.01289
C	3.390664	-5.67761	3.77602	-0.33103	-0.03499
C	3.113255	-6.94208	3.20787	-0.44375	-0.04226
C	3.742894	-7.32814	2.05003	0.04266	-0.02884
C	-5.793507	4.76927	3.38592	0.00433	-0.02972
C	-6.122604	3.66412	2.63994	-0.54247	-0.04263
C	-5.34708	3.31746	1.50984	-0.28234	-0.03649
C	-4.250663	4.06858	1.15766	-0.13683	-0.01322
C	-3.81797	-3.81425	-1.52729	-0.16476	-0.01209
C	-4.056284	-4.85956	-0.66668	-0.41311	-0.03467
C	-5.322284	-5.01474	-0.05714	-0.39773	-0.0423
C	-6.331739	-4.12602	-0.33489	0.09565	-0.0303
H	4.247381	0.84472	3.41561	0.19046	0.0693
H	5.97545	-0.92462	3.45012	0.18753	0.07615
H	4.059731	-2.88426	0.12158	0.25898	0.0873
H	-1.518001	0.23612	0.47206	0.27862	0.07498
H	-3.432441	-0.34573	-0.92944	0.18942	0.07562
H	-0.775792	-1.978	-3.88453	0.1785	0.07458
H	1.143342	-1.415	-2.45296	0.20578	0.07246
H	0.361384	2.43529	2.81899	0.23039	0.07223
H	-0.994735	4.48465	2.70552	0.19892	0.0763
H	-1.005483	4.21645	-1.58199	0.15136	0.07492
H	0.318757	2.16679	-1.45766	0.25148	0.07372
H	0.435962	6.41293	-0.63474	0.18524	0.07441
H	0.740249	8.11137	-2.39523	0.18814	0.05474
H	-1.217935	9.34318	-3.30524	0.15729	0.05198
H	-3.489532	8.84238	-2.42465	0.18386	0.05461
H	-3.796468	7.12536	-0.67921	0.15919	0.07439
H	-1.613093	7.76432	2.05912	0.15224	0.07677
H	-3.032989	8.41308	3.98833	0.1813	0.05624
H	-4.965026	7.01245	4.63598	0.14477	0.05937
H	7.484602	-0.79703	1.09678	0.18042	0.07439
H	9.837313	-0.27143	1.61128	0.18743	0.05524
H	11.231396	-1.87874	2.89628	0.15559	0.05255
H	10.22775	-4.01982	3.66642	0.18561	0.05509

H	7.863945	-4.53282	3.17772	0.15847	0.07481
H	5.14633	-7.85214	-0.19352	0.14722	0.05971
H	6.78328	-6.34676	-1.27486	0.18215	0.0564
H	7.225292	-4.09642	-0.32334	0.1544	0.07685
H	-2.125639	0.34298	-4.79151	0.15209	0.07304
H	-2.060314	0.47157	-7.25298	0.1894	0.05482
H	-3.216556	-1.24397	-8.63102	0.15581	0.05222
H	-4.437661	-3.09386	-7.5038	0.18651	0.0548
H	-4.4828	-3.2345	-5.03923	0.16286	0.07462
H	-8.147175	-2.28244	-1.09479	0.14928	0.05939
H	-7.761759	-0.42341	-2.68042	0.18103	0.05619
H	-5.521327	-0.09361	-3.69368	0.147	0.07651
H	4.485584	-3.85405	3.61387	0.17821	0.07564
H	2.89889	-5.38409	4.69662	0.17923	0.05572
H	2.406716	-7.60656	3.69235	0.16347	0.05432
H	3.541973	-8.30088	1.61329	0.15676	0.05941
H	-6.391173	5.04803	4.24759	0.14988	0.05928
H	-6.980743	3.05912	2.91033	0.16886	0.05431
H	-5.621778	2.45291	0.91601	0.13332	0.05495
H	-3.664683	3.79499	0.2902	0.18936	0.07609
H	-2.844217	-3.70464	-1.98554	0.18576	0.0775
H	-3.266997	-5.57138	-0.45279	0.18168	0.05635
H	-5.494406	-5.84073	0.62379	0.16301	0.05427
H	-7.309628	-4.24535	0.12001	0.16173	0.05914

Table S5. Cartesian coordinates of optimized structure of molecule **4**.

Total energy: –3120.34811675Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	0.412084	0.44298	1.063481	-0.3893	-0.03566
C	1.062406	-0.85208	1.016303	-0.40358	-0.04673
N	1.67308	-1.32887	2.088503	0.26453	-0.03999
C	1.603099	-0.63357	3.245393	-0.28801	-0.06546
C	0.845255	0.56845	3.327522	0.31092	-0.0452
N	0.284148	1.0925	2.207183	0.30028	-0.04603
C	2.24382	-1.1136	4.416012	-0.1977	-0.00883
C	2.116528	-0.44202	5.603157	0.15909	-0.02522
C	1.327767	0.74658	5.701697	-0.65086	-0.03965
C	0.70186	1.23389	4.565062	-0.30431	-0.03157

C	-0.106092	1.15219	-0.13551	0.11262	-0.09636
C	1.060901	-1.74243	-0.17333	0.04385	-0.09504
N	1.236958	1.4103	6.941	0.83236	-0.09899
C	-1.295274	1.89035	-0.0509	-0.12142	-0.00497
C	-1.772534	2.62005	-1.12974	0.16352	-0.04017
C	-1.062718	2.65426	-2.34239	-0.58342	-0.04227
C	0.138281	1.93042	-2.42699	-0.10927	-0.0403
C	0.601195	1.19441	-1.34457	-0.34078	-0.0092
C	-0.079344	-1.93428	-0.96622	-0.34006	-0.01132
C	-0.081195	-2.83282	-2.02417	-0.03523	-0.03896
C	1.066572	-3.58128	-2.33372	-0.68247	-0.04441
C	2.209596	-3.39812	-1.53813	0.14815	-0.04078
C	2.198884	-2.50159	-0.47874	-0.10021	-0.00588
N	-1.538986	3.4028	-3.43934	0.83261	-0.10107
N	1.067065	-4.49397	-3.41119	0.83098	-0.10106
C	-2.939148	3.54449	-3.66719	-0.55772	-0.07536
C	1.017602	2.82076	6.995714	-0.63363	-0.07571
C	1.200515	0.67149	8.159588	-0.48408	-0.077
C	2.256958	-4.73395	-4.15712	-0.67241	-0.07436
C	-0.104671	-5.24117	-3.72667	-0.58772	-0.07503
C	3.028054	-3.66498	-4.64064	0.22282	-0.02183
C	4.183593	-3.89549	-5.3691	-0.21494	-0.02753
C	4.592066	-5.20415	-5.65608	-0.72059	-0.03017
C	3.825668	-6.27576	-5.19434	0.27249	-0.06988
C	2.674722	-6.03443	-4.44196	0.06346	-0.0212
C	-0.539257	-5.35741	-5.05605	0.11402	-0.01866
C	-1.669005	-6.09521	-5.37241	-0.13253	-0.02798
C	-2.410009	-6.72419	-4.36446	-0.73435	-0.03027
C	-1.992651	-6.60934	-3.03669	0.15607	-0.07103
C	-0.841308	-5.88252	-2.72967	0.16089	-0.02293
C	-0.035104	3.35434	7.752186	0.08513	-0.01765
C	-0.236106	4.72448	7.820664	-0.06185	-0.02642
C	0.601406	5.5986	7.118534	-0.78864	-0.0273
C	1.65072	5.0774	6.356621	0.10851	-0.06871
C	1.857367	3.69905	6.310077	0.24762	-0.01704
C	1.954847	1.09482	9.265086	0.11479	-0.01706
C	1.916741	0.39533	10.46001	-0.16467	-0.02559
C	1.135683	-0.76136	10.58001	-0.69971	-0.02916
C	0.385196	-1.1959	9.485857	0.07002	-0.07041
C	0.41217	-0.47226	8.292009	0.12596	-0.02571
C	-3.49654	4.80714	-3.91994	0.11447	-0.01786
C	-4.854668	4.94937	-4.15587	-0.03755	-0.02714

C	-5.699576	3.83314	-4.12778	-0.79737	-0.02951
C	-5.158135	2.57182	-3.87003	0.0697	-0.07108
C	-3.785818	2.43532	-3.65472	0.20742	-0.02251
C	-0.630756	4.0217	-4.34652	-0.69894	-0.07482
C	0.451875	4.78029	-3.87372	0.16005	-0.0218
C	1.330165	5.3893	-4.75519	-0.07695	-0.02742
C	1.139948	5.27604	-6.13817	-0.76622	-0.02983
C	0.058885	4.53618	-6.62084	0.13561	-0.06993
C	-0.809204	3.90828	-5.72571	0.12062	-0.02006
O	2.054779	5.9222	-6.92203	-0.15833	-0.17838
O	1.175948	-1.38583	11.79477	-0.16022	-0.17753
O	-7.023548	4.07953	-4.36225	-0.15967	-0.17833
O	5.739617	-5.32489	-6.38959	-0.15865	-0.17853
O	0.3149	6.92872	7.239852	-0.15893	-0.17718
O	-3.513728	-7.41835	-4.77684	-0.16003	-0.17892
C	1.919282	5.83365	-8.33283	-0.32674	0.05527
H	2.743027	6.41185	-8.74846	0.17744	0.05326
H	1.994743	4.79658	-8.67825	0.15082	0.04483
H	0.969497	6.26186	-8.6723	0.15023	0.04451
C	0.402254	-2.56303	11.97683	-0.3243	0.05572
H	0.58692	-2.8858	13.00017	0.17622	0.05353
H	-0.667291	-2.3634	11.8478	0.15094	0.04487
H	0.71061	-3.35556	11.28592	0.15183	0.04496
C	1.121523	7.8628	6.536272	-0.32734	0.05599
H	0.710686	8.84435	6.767206	0.17531	0.05347
H	2.16506	7.82072	6.867466	0.15026	0.04464
H	1.075439	7.69621	5.454474	0.15565	0.04582
C	-4.299708	-8.0813	-3.79759	-0.32316	0.055
H	-5.112433	-8.56032	-4.3414	0.17548	0.05313
H	-3.719488	-8.8449	-3.2676	0.15079	0.04467
H	-4.717165	-7.37385	-3.0723	0.15176	0.04462
C	6.209772	-6.6285	-6.69966	-0.32071	0.05514
H	7.124135	-6.48713	-7.27383	0.17655	0.05322
H	6.436774	-7.19879	-5.79201	0.15039	0.04478
H	5.48429	-7.18287	-7.3056	0.15008	0.04445
C	-7.928186	2.98489	-4.35103	-0.32519	0.05523
H	-8.910392	3.40766	-4.55646	0.17585	0.05331
H	-7.680355	2.25214	-5.12702	0.15018	0.04463
H	-7.945286	2.48867	-3.37422	0.15209	0.04485
H	2.836718	-2.01792	4.343071	0.18738	0.06828
H	2.621371	-0.8078	6.488229	0.1927	0.07479
H	0.108624	2.13849	4.591019	0.23987	0.08449

H	-1.838345	1.90157	0.886365	0.22035	0.07168
H	-2.695594	3.17831	-1.03474	0.18646	0.07326
H	0.709602	1.94742	-3.34648	0.18689	0.07372
H	1.53076	0.64769	-1.44586	0.24725	0.07382
H	-0.983087	-1.37524	-0.75611	0.24846	0.0732
H	-0.978503	-2.96089	-2.61657	0.17712	0.07324
H	3.105442	-3.96877	-1.74886	0.19074	0.07336
H	3.080722	-2.39526	0.141143	0.22687	0.07136
H	2.71562	-2.64799	-4.43594	0.17414	0.07527
H	4.78039	-3.07151	-5.7418	0.20612	0.06892
H	4.113786	-7.29849	-5.39743	0.20172	0.05934
H	2.0916	-6.87269	-4.07981	0.16933	0.07489
H	0.020818	-4.86711	-5.84347	0.1698	0.07545
H	-2.005084	-6.18635	-6.39846	0.20515	0.06848
H	-2.539061	-7.08774	-2.23485	0.20497	0.0596
H	-0.519679	-5.80761	-1.69773	0.1803	0.07644
H	-0.694524	2.68676	8.293955	0.17847	0.07567
H	-1.048433	5.13958	8.405122	0.20621	0.06888
H	2.319015	5.72635	5.806749	0.21011	0.06018
H	2.677773	3.30338	5.723045	0.16721	0.07597
H	2.569782	1.98291	9.179822	0.17679	0.0757
H	2.498136	0.72066	11.31442	0.20465	0.06911
H	-0.234019	-2.08072	9.548106	0.2032	0.0599
H	-0.185979	-0.80915	7.453679	0.18279	0.07624
H	-2.853356	5.67903	-3.93424	0.1727	0.07565
H	-5.287073	5.92338	-4.35126	0.20749	0.06873
H	-5.782258	1.68852	-3.84759	0.20835	0.05955
H	-3.372133	1.45162	-3.46656	0.16455	0.07497
H	0.602855	4.88529	-2.80596	0.18827	0.07665
H	2.166753	5.97425	-4.39196	0.20721	0.06898
H	-0.115826	4.4282	-7.68298	0.20206	0.0594
H	-1.641872	3.3307	-6.10943	0.16372	0.07487

Table S6. Cartesian coordinates of optimized structure of molecule **5**.

Total energy: –3454.81269468Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	-1.615837	0.11755	-0.149846	-0.4262	-0.03504
C	-1.895879	0.66638	-1.462371	-0.44001	-0.0424

N	-3.128858	0.66354	-1.93768	0.27038	-0.0352
C	-4.133243	0.21939	-1.147729	-0.20733	-0.05909
C	-3.874966	-0.19702	0.188436	0.27881	-0.04573
N	-2.598606	-0.25744	0.647507	0.31501	-0.03825
C	-5.469455	0.20487	-1.621887	-0.20116	-0.00449
C	-6.491484	-0.19034	-0.798372	0.08982	-0.01691
C	-6.240672	-0.58179	0.550751	-0.68041	-0.04444
C	-4.943781	-0.57498	1.031136	-0.2801	-0.01785
C	-0.243149	-0.10657	0.377124	0.15347	-0.08733
C	-0.869782	1.29404	-2.336266	0.13248	-0.08644
C	0.777239	-0.65371	-0.411842	-0.31093	-0.00868
C	2.031405	-0.92078	0.121126	-0.06541	-0.02739
C	2.30696	-0.64405	1.467326	-0.86288	-0.04869
C	1.285701	-0.11048	2.266411	0.17845	-0.03036
C	0.032762	0.14675	1.727786	-0.09411	-0.0033
C	0.103893	2.16794	-1.834258	-0.30389	-0.00942
C	1.009975	2.79493	-2.67944	-0.0456	-0.02665
C	0.971717	2.56492	-4.061277	-0.87434	-0.05016
C	-0.009024	1.70347	-4.572705	0.16527	-0.03049
C	-0.914912	1.08538	-3.721908	-0.11499	-0.00474
N	1.896749	3.21106	-4.924665	0.8472	-0.08898
N	3.589454	-0.9172	2.012292	0.8509	-0.08849
N	-7.328234	-0.98609	1.36477	0.84251	-0.08831
C	4.201339	-0.01575	2.909213	-0.4898	-0.03943
C	4.256978	-2.12541	1.648489	-0.42041	-0.06088
C	-8.55414	-0.25962	1.302734	-0.39044	-0.06232
C	-7.187827	-2.04659	2.292144	-0.55209	-0.04093
C	2.200486	4.58872	-4.707171	-0.40327	-0.06097
C	2.502124	2.51272	-5.98997	-0.4708	-0.03886
C	2.790528	3.16018	-7.202251	0.23561	-0.03972
C	3.399667	2.46779	-8.23803	0.08903	-0.0029
C	3.72817	1.11322	-8.104606	-0.87728	-0.1071
C	3.439466	0.46122	-6.892957	-0.07724	-0.00297
C	2.842087	1.15044	-5.854593	-0.04085	-0.03283
C	1.170806	5.51509	-4.503993	0.08499	-0.03213
C	1.470227	6.85583	-4.278127	-0.21231	-0.03656
C	2.794567	7.29191	-4.265654	-0.44931	-0.05206
C	3.821031	6.37093	-4.473774	-0.20488	-0.03711
C	3.530342	5.02635	-4.685563	0.07465	-0.03387
C	4.993377	-0.48426	3.969639	0.23976	-0.03877
C	5.600958	0.41067	4.837734	0.09921	-0.00281
C	5.431255	1.79198	4.683915	-0.89444	-0.10655

C	4.63971	2.26475	3.622651	-0.07522	-0.00313
C	4.040475	1.37631	2.749799	-0.03496	-0.03249
C	5.599664	-2.10024	1.252103	0.09329	-0.03384
C	6.247324	-3.28082	0.900151	-0.2166	-0.03705
C	5.563489	-4.49607	0.923179	-0.44349	-0.05205
C	4.223769	-4.52119	1.308869	-0.21582	-0.03642
C	3.573202	-3.34662	1.676843	0.08475	-0.03225
C	-6.466672	-3.20256	1.957359	0.21874	-0.03465
C	-6.337569	-4.235	2.873862	0.14448	-0.00291
C	-6.932445	-4.15208	4.13912	-1.05109	-0.10332
C	-7.658341	-2.99752	4.475691	0.00598	-0.00199
C	-7.778938	-1.96095	3.567501	0.0199	-0.02835
C	-9.776448	-0.94181	1.251254	0.04061	-0.03326
C	-10.97171	-0.23186	1.195423	-0.27134	-0.03587
C	-10.96601	1.16297	1.173149	-0.3527	-0.0517
C	-9.750086	1.84321	1.215405	-0.36854	-0.03571
C	-8.550124	1.14046	1.28814	0.26925	-0.03567
N	-6.73816	-5.26207	4.987589	0.09469	-0.04806
N	-7.30858	-5.19701	6.103987	0.10221	-0.05566
C	-7.101158	-6.31069	6.956457	-0.3833	-0.0934
C	-6.304014	-7.42225	6.639572	0.1036	-0.01986
C	-6.172156	-8.45551	7.557118	-0.19148	-0.04219
C	-6.8267	-8.39667	8.791997	-0.31642	-0.04006
C	-7.61796	-7.29373	9.107386	-0.20515	-0.04708
C	-7.75433	-6.25299	8.192895	0.033	-0.02029
N	4.340882	0.51068	-9.221208	0.10649	-0.04829
N	4.605397	-0.71136	-9.101871	0.08315	-0.05878
C	5.228062	-1.30905	-10.22642	-0.33157	-0.09324
C	5.55794	-0.63252	-11.4118	0.19698	-0.02077
C	6.168366	-1.32375	-12.44941	-0.24231	-0.04264
C	6.456514	-2.68667	-12.32263	-0.32188	-0.04143
C	6.129525	-3.35906	-11.14654	-0.20094	-0.04765
C	5.517439	-2.67274	-10.10144	-0.05743	-0.02149
N	6.090499	2.60654	5.626106	0.10723	-0.04821
N	5.911967	3.84273	5.494211	0.08338	-0.05846
C	6.580769	4.65603	6.443356	-0.32873	-0.09322
C	7.38945	4.17082	7.483622	0.19323	-0.02057
C	7.99496	5.06482	8.356086	-0.24212	-0.04255
C	7.805658	6.44263	8.206243	-0.32122	-0.04129
C	7.002985	6.92523	7.174257	-0.20388	-0.04765
C	6.391949	6.03496	6.295578	-0.0537	-0.02142
H	-5.655995	0.50852	-2.64521	0.19503	0.07052

H	-7.50939	-0.21123	-1.167242	0.19526	0.07755
H	-4.714697	-0.87292	2.046186	0.22598	0.08748
H	0.593699	-0.87802	-1.455427	0.2509	0.07454
H	2.803593	-1.34838	-0.506426	0.18217	0.07653
H	1.47562	0.0933	3.31313	0.18758	0.07666
H	-0.756317	0.53227	2.361552	0.2221	0.07351
H	0.157145	2.36565	-0.770768	0.24879	0.0744
H	1.750515	3.47108	-2.270196	0.18196	0.07657
H	-0.063221	1.52701	-5.640089	0.18637	0.07646
H	-1.684874	0.44286	-4.130963	0.23061	0.07312
H	2.53261	4.20414	-7.326817	0.17882	0.07515
H	3.619116	2.96153	-9.17759	0.19393	0.06816
H	3.708622	-0.58094	-6.780388	0.25263	0.07289
H	2.63903	0.64415	-4.919119	0.17399	0.07366
H	0.140629	5.17996	-4.521455	0.17281	0.07581
H	0.66326	7.56327	-4.123214	0.19093	0.05604
H	3.024444	8.33712	-4.094786	0.15618	0.05389
H	4.85513	6.69662	-4.458251	0.19309	0.05623
H	4.329917	4.31087	-4.836109	0.15748	0.07551
H	5.126025	-1.5495	4.109619	0.17937	0.07537
H	6.207253	0.05422	5.662382	0.19499	0.06825
H	4.522364	3.33237	3.490096	0.25318	0.07288
H	3.445791	1.74982	1.92541	0.17493	0.07373
H	6.12989	-1.1559	1.223507	0.15746	0.07548
H	7.286888	-3.24761	0.593783	0.19267	0.05623
H	6.06887	-5.41284	0.64274	0.15664	0.0539
H	3.683492	-5.46085	1.336553	0.19179	0.05617
H	2.534776	-3.36955	1.98503	0.17342	0.07598
H	-6.010066	-3.28603	0.979273	0.19568	0.0754
H	-5.785539	-5.13258	2.620735	0.20196	0.0686
H	-8.104753	-2.92479	5.458824	0.23033	0.07323
H	-8.32843	-1.06786	3.838493	0.18381	0.07593
H	-9.783353	-2.02516	1.256564	0.16353	0.07573
H	-11.91083	-0.77226	1.155324	0.19112	0.05651
H	-11.89864	1.7126	1.122948	0.15936	0.05414
H	-9.732654	2.92727	1.205444	0.18583	0.05639
H	-7.607657	1.67283	1.334895	0.18527	0.07566
H	-5.802589	-7.45415	5.681306	0.17691	0.06986
H	-5.555901	-9.31433	7.314467	0.18778	0.05409
H	-6.717054	-9.20837	9.502427	0.14755	0.05352
H	-8.126544	-7.24391	10.06344	0.1821	0.05434
H	-8.36279	-5.38406	8.414618	0.15866	0.06512

H	5.329724	0.42174	-11.49654	0.18207	0.06963
H	6.423932	-0.80213	-13.36533	0.18475	0.05389
H	6.933791	-3.21796	-13.13843	0.14727	0.05325
H	6.351102	-4.41527	-11.04355	0.18278	0.05406
H	5.25339	-3.17291	-9.176996	0.14856	0.06478
H	7.527196	3.10276	7.588289	0.18189	0.06969
H	8.619432	4.6913	9.160327	0.18506	0.05393
H	8.282901	7.13304	8.892659	0.14734	0.05327
H	6.853192	7.99221	7.054304	0.18275	0.05406
H	5.76286	6.385	5.4855	0.1485	0.06477

Table S7. Cartesian coordinates of optimized structure of molecule **6**.

Total energy: –2429.46419270Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	-0.804173	0.61527	0.25974	-0.37493	-0.03337
C	-0.574437	-0.19561	1.43977	-0.47705	-0.03695
N	-1.317533	-0.03315	2.51781	0.27193	-0.03187
C	-2.350828	0.84181	2.47534	-0.2012	-0.05236
C	-2.65513	1.53999	1.27371	0.19874	-0.04495
N	-1.845565	1.42145	0.19108	0.30598	-0.03331
C	-3.168626	1.03937	3.61561	-0.1458	-0.0023
C	-4.249947	1.88132	3.54855	0.21759	-0.01034
C	-4.575424	2.55234	2.33662	-0.71155	-0.03479
C	-3.790735	2.38114	1.21597	-0.14552	0.00092
C	0.107964	0.64489	-0.91678	0.25783	-0.07938
C	0.451335	-1.27121	1.52285	0.25814	-0.07944
N	-5.701615	3.41229	2.30548	0.78148	-0.02988
C	1.500386	0.69051	-0.77226	-0.37355	-0.0089
C	2.329374	0.78787	-1.88384	-0.07036	-0.01701
C	1.780234	0.84364	-3.16803	-0.68338	-0.03895
C	0.391125	0.80934	-3.32242	0.1659	-0.01769
C	-0.432534	0.71548	-2.2075	-0.09133	-0.00317
C	0.661369	-2.17789	0.47594	-0.32764	-0.00925
C	1.578795	-3.21426	0.60349	-0.05318	-0.01681
C	2.30462	-3.3697	1.78786	-0.69391	-0.03952
C	2.094197	-2.47697	2.84318	0.14411	-0.0179
C	1.175277	-1.44358	2.71011	-0.13065	-0.00419
N	2.625413	0.94089	-4.3044	0.75884	-0.02971

N	3.240815	-4.42842	1.92018	0.75835	-0.02988
C	2.650011	0.05283	-5.38577	0.22592	-0.02175
C	-7.007637	3.05787	2.66556	0.25947	-0.02317
C	-5.700253	4.759	1.91648	0.31385	-0.02033
C	2.963058	-5.79078	1.75899	0.1843	-0.02188
C	4.597437	-4.28838	2.23353	0.22139	-0.02186
C	1.749967	-6.42263	1.48069	-0.34979	-0.05139
C	1.746984	-7.81167	1.39739	-0.44775	-0.03816
C	2.919337	-8.55893	1.59053	-0.33752	-0.06152
C	4.121705	-7.92506	1.88129	-0.21021	-0.02252
C	4.152395	-6.53021	1.97107	0.13385	-0.06434
C	5.194782	-5.57224	2.27217	0.21644	-0.06409
C	6.559387	-5.68893	2.55247	-0.22175	-0.02236
C	7.30468	-4.53854	2.78335	-0.34968	-0.06145
C	6.699861	-3.27321	2.72805	-0.51051	-0.03838
C	5.343761	-3.12909	2.45093	-0.28134	-0.05231
C	-7.511935	1.82198	3.07378	-0.33099	-0.05217
C	-8.873122	1.73694	3.35149	-0.45011	-0.0374
C	-9.717366	2.84994	3.21919	-0.34932	-0.05997
C	-9.212649	4.0736	2.79431	-0.2732	-0.02183
C	-7.84865	4.18648	2.51051	0.13405	-0.06321
C	-7.015254	5.27052	2.03521	0.16949	-0.064
C	-7.265698	6.60938	1.72045	-0.27198	-0.02223
C	-6.213317	7.41438	1.30065	-0.36497	-0.05994
C	-4.913461	6.89478	1.2013	-0.38912	-0.03649
C	-4.63742	5.56569	1.50783	-0.31771	-0.04912
C	3.630199	0.48525	-6.31253	0.23732	-0.06407
C	3.852759	-0.25603	-7.47657	-0.22462	-0.02235
C	3.108334	-1.4087	-7.69862	-0.35185	-0.06134
C	2.15029	-1.8305	-6.76364	-0.50766	-0.03828
C	1.909118	-1.11112	-5.59709	-0.30202	-0.0522
C	3.580134	1.93905	-4.53045	0.16741	-0.02195
C	3.895839	3.05728	-3.75711	-0.35588	-0.05141
C	4.883073	3.91554	-4.23166	-0.44448	-0.03821
C	5.539957	3.6739	-5.4483	-0.33694	-0.06145
C	5.211129	2.56638	-6.22119	-0.2063	-0.02252
C	4.222268	1.68841	-5.76774	0.13795	-0.06421
H	-2.914653	0.515	4.52904	0.20004	0.07183
H	-4.866473	2.0545	4.42197	0.20188	0.07838
H	-4.022418	2.8789	0.28292	0.21118	0.08832
H	1.945251	0.65022	0.21433	0.25115	0.07483
H	3.405321	0.81172	-1.76117	0.20283	0.07793

H	-0.037675	0.87483	-4.3151	0.20171	0.07725
H	-1.508655	0.7149	-2.32834	0.2187	0.07399
H	0.106098	-2.07784	-0.44843	0.24937	0.07481
H	1.741461	-3.90233	-0.21703	0.20335	0.07792
H	2.639153	-2.60767	3.77031	0.20129	0.07712
H	0.996808	-0.76872	3.53796	0.22202	0.07359
H	0.83757	-5.85687	1.34066	0.16989	0.06728
H	0.816806	-8.32528	1.182	0.16982	0.05398
H	2.882548	-9.63958	1.5177	0.16046	0.05251
H	5.023374	-8.50591	2.04102	0.13163	0.06033
H	7.032039	-6.66435	2.58574	0.13259	0.06039
H	8.363081	-4.61598	3.003	0.16129	0.05256
H	7.300232	-2.38734	2.90184	0.17034	0.05387
H	4.888988	-2.1478	2.40202	0.15503	0.0659
H	-6.874185	0.95184	3.16469	0.16981	0.06737
H	-9.287845	0.7878	3.67152	0.16984	0.05445
H	-10.772879	2.74985	3.44341	0.16144	0.05295
H	-9.870156	4.92823	2.67969	0.13184	0.06069
H	-8.26738	7.01566	1.80641	0.13274	0.06056
H	-6.394212	8.45338	1.05129	0.16204	0.05292
H	-4.104223	7.54035	0.87937	0.16958	0.05462
H	-3.629434	5.17844	1.43215	0.18224	0.06767
H	4.599484	0.0616	-8.19589	0.1327	0.0604
H	3.270494	-1.9915	-8.59777	0.16132	0.05259
H	1.586211	-2.73733	-6.95053	0.17034	0.05391
H	1.173902	-1.4504	-4.87842	0.15525	0.0659
H	3.387718	3.25892	-2.8226	0.16984	0.06719
H	5.146124	4.79087	-3.64852	0.16984	0.05396
H	6.305433	4.36161	-5.78828	0.16062	0.05253
H	5.712693	2.38844	-7.166	0.13141	0.06035

Table S8. Cartesian coordinates of optimized structure of molecule **7**.

Total energy: –2655.11089400Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	-0.44389	0.68438	-0.66389	-0.3942	-0.0355
C	-0.71183	-0.66027	-1.13431	-0.41447	-0.03514
N	-1.38739	-0.85954	-2.24843	0.28616	-0.02794
C	-1.90276	0.2123	-2.90107	-0.07394	-0.04991

C	-1.75718	1.51994	-2.36008	-0.00767	-0.04882
N	-0.99917	1.72401	-1.25394	0.31511	-0.0259
C	-2.63267	0.03249	-4.10253	-0.1727	-0.00411
C	-3.21047	1.11479	-4.71931	-0.02176	-0.00619
C	-3.08702	2.41764	-4.16421	-0.70233	-0.05735
C	-2.37222	2.61985	-3.00765	-0.18719	0.01569
C	0.48837	1.00149	0.45399	0.19876	-0.0744
C	-0.30639	-1.88985	-0.39755	0.22733	-0.07484
N	-3.71109	3.52893	-4.81912	0.796	-0.07999
C	1.73863	0.37905	0.56565	-0.4834	-0.01324
C	2.6306	0.75683	1.56387	-0.05826	-0.01325
C	2.28035	1.75125	2.47913	-0.60927	-0.05948
C	1.03579	2.37331	2.37808	0.02665	-0.00719
C	0.15321	2.00997	1.36613	-0.07059	-0.0047
C	0.19176	-2.98941	-1.1074	-0.10664	-0.00603
C	0.52017	-4.16945	-0.44789	-0.05457	-0.00868
C	0.32772	-4.27912	0.92963	-0.6108	-0.05965
C	-0.18918	-3.19561	1.6423	-0.02183	-0.01205
C	-0.4934	-2.00786	0.98591	-0.45361	-0.01289
N	3.19445	2.1499	3.5077	0.72557	-0.08055
N	0.64495	-5.50453	1.59997	0.72453	-0.08069
C	4.15678	3.14708	3.24321	0.29247	-0.02348
C	-5.09217	3.75767	-4.63253	0.36905	-0.02463
C	-3.06936	4.13842	-5.91994	0.32012	-0.02458
C	1.85077	-5.62819	2.32068	0.30253	-0.02366
C	-0.34041	-6.50417	1.73978	0.30488	-0.02328
C	2.81407	-4.61702	2.37167	-0.23023	-0.0509
C	4.00085	-4.79359	3.08606	-0.27443	-0.04523
C	4.24158	-5.98153	3.76465	-0.2641	-0.05434
C	3.28703	-6.99964	3.72206	-0.32129	-0.02681
C	2.11416	-6.82585	3.00635	0.00289	-0.00086
C	-0.02232	-7.68094	2.43799	0.0048	-0.00083
C	-0.95293	-8.6941	2.59752	-0.31198	-0.02721
C	-2.23207	-8.56472	2.05286	-0.23349	-0.05495
C	-2.56255	-7.4084	1.35757	-0.31965	-0.04621
C	-1.62622	-6.38365	1.20558	-0.29849	-0.04909
C	-5.86871	3.02995	-3.72701	-0.12698	-0.04899
C	-7.22643	3.31135	-3.56264	-0.30638	-0.04554
C	-7.83001	4.31844	-4.30513	-0.23907	-0.05331
C	-7.06573	5.05003	-5.21616	-0.20279	-0.02589
C	-5.71686	4.77625	-5.37038	-0.20404	-0.00106
C	-3.74464	5.14879	-6.62391	-0.20182	-0.00105

C	-3.15446	5.78989	-7.70039	-0.22703	-0.0259
C	-1.86155	5.44534	-8.09891	-0.24	-0.05325
C	-1.17814	4.45034	-7.41115	-0.30495	-0.04544
C	-1.77833	3.79849	-6.33207	-0.0998	-0.04865
C	5.0561	3.50887	4.25972	-0.0087	-0.00111
C	6.01637	4.48535	4.05459	-0.31755	-0.0272
C	6.09776	5.14155	2.82472	-0.24123	-0.05487
C	5.21293	4.79932	1.80996	-0.28336	-0.04588
C	4.25262	3.80638	2.01471	-0.31365	-0.04883
C	3.31317	1.3861	4.68739	0.31384	-0.0237
C	2.54224	0.24835	4.94023	-0.23219	-0.05081
C	2.68582	-0.46253	6.13356	-0.28133	-0.04535
C	3.60662	-0.05187	7.08922	-0.251	-0.05455
C	4.3852	1.08177	6.8474	-0.30897	-0.02684
C	4.23411	1.7914	5.66792	-0.03019	-0.00115
O	5.00038	2.93029	5.51296	-0.15096	-0.09743
O	-5.00663	5.56851	-6.25113	-0.12885	-0.09611
O	1.23391	-7.88972	2.97278	-0.15371	-0.09746
H	-2.72891	-0.97002	-4.5019	0.2138	0.07233
H	-3.77683	0.99234	-5.63508	0.18744	0.08243
H	-2.26043	3.61094	-2.58556	0.18408	0.0909
H	2.02833	-0.38824	-0.14176	0.24462	0.07466
H	3.60498	0.28759	1.63472	0.18658	0.08093
H	0.77158	3.14694	3.08943	0.18163	0.07908
H	-0.80162	2.51178	1.27077	0.2273	0.074
H	0.3159	-2.91277	-2.18046	0.22398	0.07368
H	0.91812	-5.01566	-0.99562	0.18241	0.07913
H	-0.355	-3.29119	2.70902	0.19018	0.08093
H	-0.89858	-1.17764	1.55145	0.24024	0.07483
H	2.6361	-3.68834	1.84613	0.12188	0.06874
H	4.72997	-3.99236	3.10764	0.16409	0.05485
H	5.15884	-6.12439	4.32264	0.1684	0.05431
H	3.43963	-7.94221	4.234	0.18427	0.06987
H	-0.65647	-9.58034	3.14567	0.18354	0.06983
H	-2.95417	-9.3627	2.17543	0.15688	0.05391
H	-3.55045	-7.28966	0.9284	0.17363	0.0547
H	-1.89448	-5.48669	0.66324	0.1786	0.0717
H	-5.40875	2.24591	-3.14027	0.18409	0.07079
H	-7.80331	2.73498	-2.8491	0.1728	0.05498
H	-8.88295	4.54098	-4.18273	0.15848	0.05434
H	-7.49887	5.84523	-5.81092	0.18741	0.07014
H	-3.71843	6.56228	-8.20938	0.18721	0.07013

H	-1.40154	5.95482	-8.93678	0.15804	0.05434
H	-0.17319	4.17147	-7.7051	0.17345	0.05498
H	-1.23532	3.02777	-5.8012	0.18416	0.07081
H	6.68624	4.72544	4.87153	0.18403	0.06976
H	6.84558	5.90999	2.67132	0.15658	0.05391
H	5.26016	5.29878	0.84947	0.17505	0.05481
H	3.56847	3.54784	1.21741	0.18646	0.07176
H	1.82252	-0.0793	4.20199	0.12237	0.06875
H	2.0731	-1.33983	6.30389	0.16467	0.05481
H	3.7243	-0.60014	8.0159	0.16789	0.05423
H	5.11066	1.43648	7.56968	0.18451	0.06982

Table S9. Cartesian coordinates of optimized structure of molecule **8**.

Total energy: –3624.03272267Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	-0.25133	1.004801	0.11701	-0.39229	-0.03418
C	0.90844	0.881153	0.97982	-0.45958	-0.03404
N	1.33027	1.909907	1.68758	0.26874	-0.02917
C	0.71557	3.109196	1.53215	-0.03982	-0.04951
C	-0.33332	3.259376	0.58309	0.10504	-0.05154
N	-0.80969	2.181046	-0.08877	0.35087	-0.02918
C	1.14367	4.233943	2.27844	-0.29275	-0.0016
C	0.55881	5.458642	2.06542	0.29243	0.00671
C	-0.47146	5.616169	1.1014	-0.84962	-0.05065
C	-0.91106	4.534598	0.37115	-0.37067	-0.00879
C	-0.91924	-0.14717	-0.55094	0.05875	-0.07504
C	1.72346	-0.35983	1.10196	0.09437	-0.07548
N	-1.02573	6.929233	0.92175	1.06758	-0.10043
C	-1.14554	-1.35831	0.11399	-0.65809	-0.00948
C	-1.84254	-2.38975	-0.50805	0.02081	0.00052
C	-2.3184	-2.2342	-1.80911	-0.94279	-0.05693
C	-2.10079	-1.02719	-2.47927	0.15949	-0.03033
C	-1.41619	0.007552	-1.85229	-0.08245	-0.00902
C	2.20733	-0.74514	2.35937	-0.06955	-0.00971
C	3.01889	-1.86593	2.49454	0.10095	-0.03032
C	3.38024	-2.61206	1.36938	-0.97243	-0.05713
C	2.91859	-2.22351	0.1125	0.01367	0.0006
C	2.09276	-1.11143	-0.01991	-0.63921	-0.00973

N	-3.0355	-3.32088	-2.41954	1.07317	-0.09709
N	4.2269	-3.77021	1.46855	1.07909	-0.09702
C	-4.45523	-3.29029	-2.38448	-0.2272	-0.04511
C	-2.2547	7.248399	1.55881	-0.12564	-0.04488
C	-0.50216	7.746307	-0.11549	-0.06003	-0.0456
C	5.63171	-3.57209	1.53851	-0.20669	-0.04489
C	3.64054	-5.00417	1.85583	-0.09173	-0.04448
C	6.18712	-2.31624	1.8201	-0.14173	-0.04667
C	7.56838	-2.13942	1.87304	-0.33862	-0.03675
C	8.42766	-3.21487	1.67521	-0.22236	-0.05761
C	7.88946	-4.47016	1.40109	0.25716	-0.06421
C	6.51067	-4.64507	1.30453	-0.01579	-0.25859
C	4.33199	-6.21184	1.65151	-0.13194	-0.25815
C	3.78087	-7.42587	2.05565	0.34222	-0.06336
C	2.50827	-7.47453	2.61991	-0.19017	-0.05664
C	1.80132	-6.28988	2.79509	-0.35314	-0.03693
C	2.36418	-5.06793	2.43183	-0.13372	-0.04783
C	-3.12331	6.256965	2.03438	-0.13666	-0.04548
C	-4.31853	6.595385	2.66615	-0.28328	-0.03591
C	-4.68962	7.927765	2.81124	-0.23931	-0.05609
C	-3.8399	8.923668	2.33526	0.35231	-0.06312
C	-2.62336	8.59331	1.74197	-0.20209	-0.25792
C	-0.70537	9.137587	-0.08881	-0.19107	-0.25793
C	-0.22389	9.946915	-1.11551	0.31003	-0.06301
C	0.51787	9.399804	-2.16013	-0.24231	-0.05583
C	0.7518	8.02898	-2.17922	-0.34208	-0.03636
C	0.23569	7.208017	-1.17838	-0.142	-0.0451
C	-5.19542	-4.45488	-2.65692	0.02685	-0.25857
C	-6.58839	-4.42983	-2.6561	0.24731	-0.06413
C	-7.27649	-3.26353	-2.32913	-0.25627	-0.05752
C	-6.55379	-2.1152	-2.02387	-0.32509	-0.03671
C	-5.16088	-2.12213	-2.06453	-0.14579	-0.04645
C	-2.34397	-4.16269	-3.33069	0.07551	-0.04412
C	-1.10722	-3.7989	-3.88095	-0.21623	-0.04806
C	-0.43855	-4.64479	-4.76368	-0.3707	-0.03694
C	-0.99968	-5.8599	-5.14099	-0.21096	-0.05671
C	-2.2316	-6.23169	-4.60737	0.30073	-0.06332
C	-2.88537	-5.40979	-3.69183	-0.11484	-0.25828
S	-4.35421	-6.00723	-2.88324	-0.52969	0.55945
S	-1.47853	9.89211	1.32624	-0.51832	0.55989
S	5.87112	-6.21341	0.75707	-0.52769	0.55934
H	1.94121	4.101666	2.99961	0.19914	0.07201

H	0.87601	6.3318	2.6229	0.1848	0.07994
H	-1.7027	4.631071	-0.36217	0.20382	0.09214
H	-0.79133	-1.49671	1.12791	0.24503	0.0744
H	-2.02749	-3.32234	0.01156	0.18662	0.07923
H	-2.47564	-0.89986	-3.48841	0.18837	0.08127
H	-1.26793	0.950073	-2.36444	0.22701	0.07374
H	1.94648	-0.15404	3.22849	0.23149	0.07385
H	3.38079	-2.16321	3.47212	0.1883	0.08126
H	3.21393	-2.7983	-0.75712	0.18669	0.07931
H	1.74823	-0.82225	-1.00509	0.23979	0.0744
H	5.53979	-1.46647	1.98494	0.19295	0.07038
H	7.96577	-1.15266	2.08127	0.17534	0.05544
H	9.50178	-3.08379	1.72839	0.15613	0.05393
H	8.53973	-5.32218	1.23805	0.17528	0.06076
H	4.34906	-8.33672	1.90452	0.17464	0.06088
H	2.07882	-8.42519	2.91217	0.15939	0.05421
H	0.80687	-6.30532	3.22622	0.17454	0.05514
H	1.79865	-4.15999	2.58673	0.1525	0.06784
H	-2.86233	5.214028	1.92365	0.19371	0.06892
H	-4.9628	5.804876	3.03343	0.17594	0.05574
H	-5.62453	8.194008	3.28949	0.1582	0.05437
H	-4.10659	9.969158	2.44061	0.17629	0.06109
H	-0.41653	11.01314	-1.07905	0.1759	0.06112
H	0.90646	10.03923	-2.9436	0.15814	0.05438
H	1.3292	7.58382	-2.98133	0.17546	0.05556
H	0.41962	6.143647	-1.22046	0.19015	0.06913
H	-7.13023	-5.33847	-2.89307	0.17604	0.06077
H	-8.35972	-3.25825	-2.31155	0.15599	0.05394
H	-7.06875	-1.1981	-1.76168	0.17625	0.05545
H	-4.62169	-1.21459	-1.832	0.19031	0.07051
H	-0.65527	-2.85561	-3.60916	0.15086	0.06781
H	0.52217	-4.33914	-5.16198	0.17583	0.05513
H	-0.48851	-6.51476	-5.83634	0.15874	0.05418
H	-2.68576	-7.17686	-4.88252	0.17568	0.06087

Table S10. Cartesian coordinates of optimized structure of molecule **9**.

Total energy: –1740.31850225Hartrees

Atom	x	y	z	Mulliken charges	Lowdin Charges
C	-0.730878	0.297	0.42527	-0.37205	-0.034
C	0.114748	-0.65656	1.12239	-0.55276	-0.04693

N	-0.267877	-1.16109	2.28139	0.22928	-0.03803
C	-1.495515	-0.84671	2.75758	-0.32823	-0.06912
C	-2.384074	-0.03292	2.0014	0.4151	-0.0436
N	-1.954521	0.54978	0.84987	0.26198	-0.04902
C	-1.949134	-1.36652	3.99088	-0.2235	-0.00446
C	-3.222207	-1.10594	4.43611	0.44994	-0.04626
C	-4.130778	-0.29718	3.68279	-0.82949	-0.03646
C	-3.687078	0.22321	2.47102	-0.44119	-0.04264
C	-0.288513	1.07879	-0.75843	0.09491	-0.09886
C	1.409222	-1.15793	0.59394	0.18059	-0.09899
C	0.990375	1.64897	-0.84822	-0.5905	-0.00769
C	1.351422	2.44547	-1.92276	0.06453	-0.04757
C	0.455868	2.69706	-2.98099	-0.84648	-0.04359
C	-0.824951	2.12321	-2.89101	0.36133	-0.06393
C	-1.187947	1.34976	-1.79365	0.07517	-0.00253
C	2.4825	-1.38605	1.46845	-0.19384	-0.00576
C	3.687325	-1.89963	1.01788	-0.04008	-0.04993
C	3.873536	-2.24477	-0.33604	-0.7374	-0.04459
C	2.7875	-2.04429	-1.20578	0.21003	-0.06261
C	1.59026	-1.50206	-0.7484	-0.24448	-0.00841
N	0.835107	3.53224	-4.04803	0.25545	-0.16338
N	5.117028	-2.73046	-0.78322	0.24513	-0.16354
N	-5.416966	-0.01	4.1677	0.2357	-0.16015
C	-0.167284	3.88673	-5.04969	-0.01461	-0.03146
C	0.316841	5.07705	-5.87382	-0.53917	0.02527
O	1.578802	4.82532	-6.47787	-0.11578	-0.23137
C	2.557307	4.52794	-5.48962	-0.36772	0.02313
C	2.154794	3.31828	-4.65509	-0.14585	-0.01731
C	-5.829243	-0.52801	5.47087	-0.08794	-0.02882
C	-7.053075	0.23227	5.97741	-0.44418	0.02468
O	-8.125205	0.19574	5.0465	-0.10803	-0.22953
C	-7.72453	0.76544	3.80685	-0.34741	0.02378
C	-6.53121	0.02741	3.21288	-0.21046	-0.01481
C	5.299574	-2.96059	-2.2142	-0.0351	-0.03213
C	6.783533	-3.11969	-2.5346	-0.53048	0.02449
O	7.383632	-4.15608	-1.76947	-0.1169	-0.23097
C	7.243156	-3.89545	-0.37844	-0.35239	0.02302
C	5.777723	-3.76842	0.01911	-0.17319	-0.01696
H	-1.27804	-1.99791	4.56151	0.1865	0.06827
H	-3.540531	-1.54894	5.36921	0.18122	0.05932
H	-4.301624	0.87638	1.8667	0.20386	0.0698
H	1.70851	1.49235	-0.05267	0.2387	0.07406

H	2.331951	2.90452	-1.92236	0.1502	0.05992
H	-1.54945	2.26946	-3.68054	0.17196	0.05885
H	-2.188028	0.93689	-1.73918	0.23269	0.07085
H	2.363273	-1.1424	2.51723	0.21553	0.07082
H	4.501212	-2.01171	1.72315	0.15804	0.0584
H	2.857558	-2.32639	-2.24731	0.17237	0.05967
H	0.778326	-1.37205	-1.45374	0.23866	0.0734
H	-1.09448	4.17001	-4.54736	0.13757	0.06066
H	-0.386137	3.04045	-5.72301	0.1692	0.06153
H	0.383791	5.96667	-5.23062	0.14732	0.05676
H	-0.381348	5.2823	-6.68716	0.18762	0.05541
H	2.702757	5.40014	-4.83525	0.14589	0.056
H	3.487738	4.32857	-6.02431	0.1807	0.05518
H	2.902361	3.15673	-3.87978	0.11468	0.05421
H	2.138508	2.42217	-5.29796	0.17331	0.06462
H	-5.023506	-0.38321	6.19245	0.12584	0.0589
H	-6.061041	-1.6053	5.42429	0.17055	0.06276
H	-6.776706	1.2767	6.18462	0.14735	0.05684
H	-7.422926	-0.22298	6.89782	0.18599	0.05589
H	-7.473801	1.827	3.94939	0.14631	0.0565
H	-8.584033	0.69279	3.13818	0.17994	0.05606
H	-6.226783	0.53561	2.29998	0.10436	0.05568
H	-6.833081	-0.99764	2.94223	0.19077	0.06658
H	4.918028	-2.10083	-2.769	0.13167	0.05963
H	4.754109	-3.85731	-2.55428	0.17169	0.06185
H	7.304904	-2.16959	-2.34595	0.14957	0.05606
H	6.915887	-3.39117	-3.58346	0.18461	0.05531
H	7.78189	-2.97251	-0.11717	0.14025	0.05566
H	7.706615	-4.7347	0.14324	0.18371	0.0555
H	5.718665	-3.51825	1.07734	0.10769	0.05412
H	5.275555	-4.73971	-0.12394	0.18379	0.06599

13. Vertical electronic Transition in implicit water of 1−9.

Molecule 1

376.1nm	0.6831	(HOMO→LUMO)	(98%)
349.7nm	0.0059	(HOMO-2 → LUMO) (HOMO-3 → LUMO)	(51%) (33%)
332.0nm	0.0323	(HOMO-1 → LUMO)	(86%)
307.3nm	0.4349	(HOMO → LUMO+1)	(92%)
301.4nm	0.0226	(HOMO-3 → LUMO) (HOMO-2 → LUMO)	(54%) (38%)
294.9nm	0.0041	(HOMO-4 →LUMO) (HOMO-2 → LUMO)	(95%) (38%)
291.0nm	0.2854	(HOMO-1 → LUMO+1) (HOMO-5 → LUMO) (HOMO-2 → LUMO+1)	(48%) (51%) (51%)
280.2nm	0.0278	(HOMO-2 → LUMO+1) (HOMO-3 → LUMO+1) (HOMO-5 → LUMO) (HOMO-6 → LUMO)	(33%) (26%) (15%) (12%)
279.8nm	0.1918	(HOMO-6 → LUMO) (HOMO-2 → LUMO+1)	(53%) (11%)
276.3nm	1.0545	(HOMO-5 → LUMO) (HOMO-1 → LUMO+1) (HOMO-6 → LUMO)	(38%) (35%) (18%)

Molecule 2

504.3nm	0.7615	(HOMO → LUMO)	(96%)
459.0nm	0.1127	(HOMO-1 → LUMO)	(97%)
439.9nm	0.0269	(HOMO-2 → LUMO)	(96%)
400.4nm	0.5388	(HOMO → LUMO+1)	(96%)
377.0nm	0.6757	(HOMO-1 → LUMO+1)	(93%)
356.6nm	0.0101	(HOMO-2 → LUMO+1)	(90%)
347.1nm	0.0527	(HOMO → LUMO+2) (HOMO-1 → LUMO+3)	(71%) (11%)
344.3nm	0.0157	(HOMO-6 → LUMO) (HOMO-4 → LUMO) (HOMO-10 → LUMO)	(38%) (25%) (14%)
341.0nm	0.0260	(HOMO-1 → LUMO+2) (HOMO → LUMO+3)	(49%) (36%)
327.6nm	0.3035	(HOMO → LUMO+7) (HOMO-2 → LUMO+7) (HOMO-1 → LUMO+7)	(70%) (13%) (11%)

Molecule 3

489.1nm	0.7793	(HOMO → LUMO)	(96%)
443.1nm	0.1380	(HOMO-1 → LUMO)	(95%)
424.2nm	0.0263	(HOMO-2 → LUMO)	(96%)
404.6nm	0.2987	(HOMO → LUMO+1)	(71%)
395.3nm	0.2400	(HOMO → LUMO+3) (HOMO-1 → LUMO+1) (HOMO-1→ LUMO+3)	(47%) (18%) (14%)
389.7nm	0.1600	(HOMO → LUMO+2) (HOMO-2 → LUMO+1)	(50%) (10%)
380.6nm	0.1435	(HOMO → LUMO+4) (HOMO-1 → LUMO+3)	(71%) (11%)
367.9nm	0.5209	(HOMO-1 → LUMO+1) (HOMO-1 → LUMO+4) (HOMO → LUMO+3)	(59%) (18%) (16%)
355.7nm	0.0578	(HOMO-1 → LUMO+3) (HOMO → LUMO+3) (HOMO → LUMO+4)	(45%) (18%) (13%)
353.5nm	0.0040	(HOMO-1 → LUMO+2) (HOMO-2 → LUMO+1) (HOMO → LUMO+2)	(34%) (29%) (21%)

Molecule 4

535.6nm	0.7159	(HOMO → LUMO)	(96%)
487.4nm	0.1214	(HOMO-1 → LUMO)	(98%)
468.5nm	0.0227	(HOMO-2 → LUMO)	(96%)
416.3nm	0.5881	(HOMO → LUMO+1)	(96%)
391.1nm	0.6944	(HOMO-1 → LUMO+1)	(93%)
371.9nm	0.0487	(HOMO-2 → LUMO+1) (HOMO → LUMO+2)	(62%) (23%)
370.3nm	0.0304	(HOMO → LUMO+2) (HOMO-2 → LUMO+1)	(50%) (27%)
364.2nm	0.0300	(HOMO-1 → LUMO+2) (HOMO → LUMO+3)	(49%) (35%)
346.9nm	0.0772	(HOMO → LUMO+4) (HOMO-2 → LUMO+4)	(60%) (29%)
343.6nm	0.0146	(HOMO-8 → LUMO) (HOMO-7 → LUMO) (HOMO-9 → LUMO)	(56%) (12%) (10%)

Molecule 5

550.2nm	1.2040	(HOMO → LUMO)	(73%)
533.0nm	1.3723	(HOMO → LUMO+1) (HOMO-1 → LUMO+1)	(56%) (17%)
524.6nm	0.4151	(HOMO → LUMO+2) (HOMO-1 → LUMO+1) (HOMO-2 → LUMO)	(60%) (16%) (14%)
492.2nm	0.0576	(HOMO-1 → LUMO) (HOMO → LUMO+1)	(58%) (21%)
490.4nm	0.1715	(HOMO-1 → LUMO+1) (HOMO → LUMO+1) (HOMO-1 → LUMO)	(45%) (15%) (13%)
478.7nm	0.0544	(HOMO-1 → LUMO+2) (HOMO-2 → LUMO) (HOMO → LUMO+2)	(33%) (28%) (18%)
477.2nm	0.0049	(HOMO-5 → LUMO) (HOMO-5 → LUMO+2)	(73%) (14%)
474.8nm	0.0150	(HOMO-4 → LUMO+1) (HOMO-3 → LUMO+1)	(63%) (14%)
474.4nm	0.0092	(HOMO-3 → LUMO+2) (HOMO-4 → LUMO+2) (HOMO-3 → LUMO+1)	(46%) (19%) (12%)
472.8nm	0.2701	(HOMO → LUMO+3)	(77%)

Molecule 6

455.1nm	0.4956	(HOMO → LUMO) (HOMO-2 → LUMO)	(81%) (16%)
430.2nm	0.0505	(HOMO-1 → LUMO) (HOMO-2 → LUMO)	(75%) (16%)
426.5nm	0.0221	(HOMO-2 → LUMO) (HOMO-1 → LUMO) (HOMO → LUMO)	(67%) (22%) (10%)
380.5nm	0.0004	(HOMO-5 → LUMO) (HOMO-1 → LUMO)	(100%) (22%)
369.1nm	0.0000	(HOMO-3 → LUMO) (HOMO-1 → LUMO)	(99%) (22%)
369.0nm	0.0000	(HOMO-4 → LUMO) (HOMO-1 → LUMO)	(99%) (22%)
364.9nm	0.2899	(HOMO → LUMO+1) (HOMO-1 → LUMO)	(96%) (22%)
355.7nm	0.2677	(HOMO-1 → LUMO+1) (HOMO → LUMO)	(93%) (10%)
348.9nm	0.0198	(HOMO-11 → LUMO) (HOMO-9 → LUMO) (HOMO-7 → LUMO) (HOMO-10 → LUMO)	(34%) (21%) (20%) (16%)
346.8nm	0.0073	(HOMO-2 →LUMO+1) (HOMO-7 → LUMO)	(90%) (20%)

Molecule 7

584.9nm	0.0000	(HOMO-2 → LUMO)	(99%)
559.8nm	0.0009	(HOMO → LUMO)	(99%)
556.1nm	0.0000	(HOMO-1 → LUMO)	(99%)
442.1nm	0.0036	(HOMO → LUMO+1)	(96%)
440.2nm	0.0017	(HOMO-1 → LUMO+1)	(96%)
431.1nm	0.0004	(HOMO-2 → LUMO+1)	(98%)
362.4nm	0.0001	(HOMO → LUMO+2) (HOMO → LUMO+3)	(68%) (21%)
360.5nm	0.0000	(HOMO-1 → LUMO+2) (HOMO-1 → LUMO+3)	(67%) (23%)
354.8nm	0.6874	(HOMO-6 → LUMO)	(91%)
350.1nm	0.0104	(HOMO-11 → LUMO) (HOMO-7 → LUMO) (HOMO-12 → LUMO) (HOMO-9 → LUMO)	(35%) (20%) (15%) (12%)

Molecule 8

529.9nm	0.0013	(HOMO-2 → LUMO)	(99%)
501.6nm	0.0006	(HOMO → LUMO)	(99%)
501.1nm	0.0009	(HOMO-1 → LUMO)	(99%)
403.2nm	0.0005	(HOMO-1 → LUMO+1)	(95%)
402.9nm	0.0002	(HOMO → LUMO+1)	(95%)
397.2nm	0.0001	(HOMO-2 → LUMO+1)	(98%)
362.5nm	0.0606	(HOMO-5 → LUMO)	(94%)
359.1nm	0.6655	(HOMO-6 → LUMO)	(92%)
352.5nm	0.0056	(HOMO-13 → LUMO) (HOMO-4 → LUMO) (HOMO-7 → LUMO) (HOMO-3 → LUMO)	(50%) (19%) (12%) (11%)
350.2nm	0.0001	(HOMO-3 →LUMO) (HOMO-4 → LUMO) (HOMO-7 → LUMO)	(64%) (35%) (12%)

Molecule 9

463.0nm	0.6499	(HOMO → LUMO)	(99%)
405.4nm	0.0497	(HOMO-1 → LUMO)	(98%)
379.4nm	0.0843	(HOMO-2 → LUMO)	(94%)
352.1nm	0.5445	(HOMO → LUMO+1)	(95%)
340.6nm	0.0435	(HOMO-3 →LUMO) (HOMO-4 → LUMO) (HOMO-5 → LUMO)	(50%) (29%) (10%)
322.2nm	0.7996	(HOMO-1 → LUMO+1) (HOMO-4 → LUMO)	(95%) (29%)
306.2nm	0.0820	(HOMO → LUMO+2) (HOMO-5 → LUMO)	(89%) (10%)
300.9nm	0.2604	(HOMO-2 → LUMO+1) (HOMO-3 → LUMO) (HOMO-4 → LUMO)	(52%) (15%) (15%)
294.7nm	0.0041	(HOMO-5 → LUMO) (HOMO-4 → LUMO) (HOMO-1 → LUMO+2)	(37%) (32%) (11%)
289.1nm	0.2709	(HOMO-2 → LUMO+1) (HOMO-3 → LUMO) (HOMO-5 → LUMO) (HOMO-4 → LUMO)	(38%) (22%) (20%) (10%)