Impact of Donor Substituent on Optoelectrochemical properties of 6*H*-indolo[2,3-*b*]quinoxaline Amine Derivatives

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Supporting information

1. Absorption and Emission spectra of compound 1 9 in various solvents and solid film

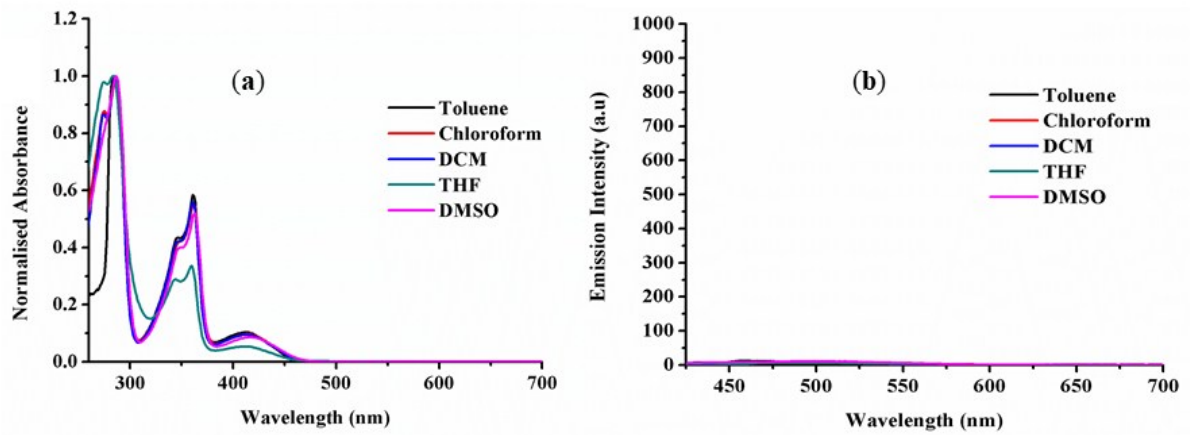


Fig. S1 Absorption spectra (**a**) and Emission spectra (**b**) of **1** in various solvent.

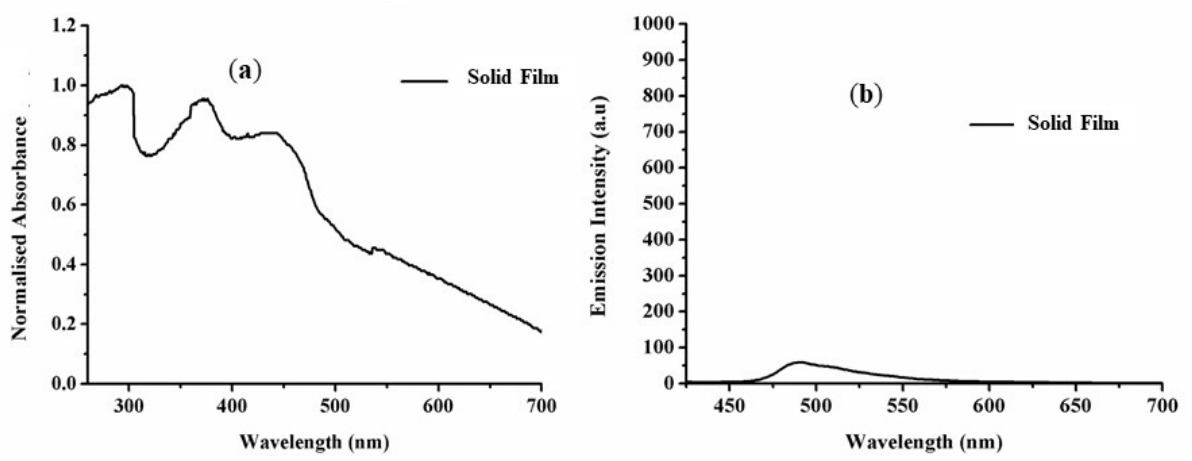


Fig. S2 Absorption spectra (**a**) and Emission spectra (**b**) of **1** in Solid Film.

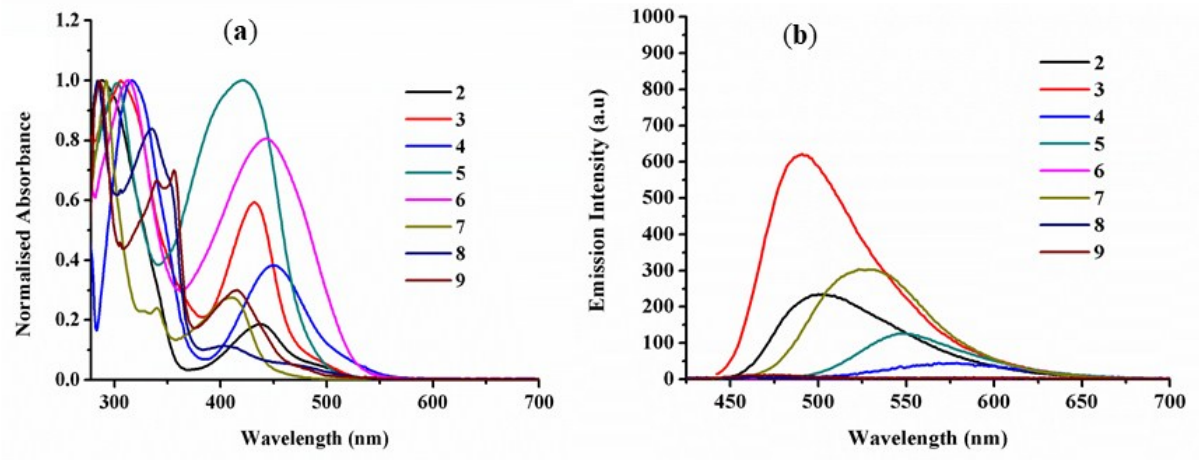


Fig. S3 Absorption spectra (**a**) and Emission spectra (**b**) of **2−9** in Toluene.

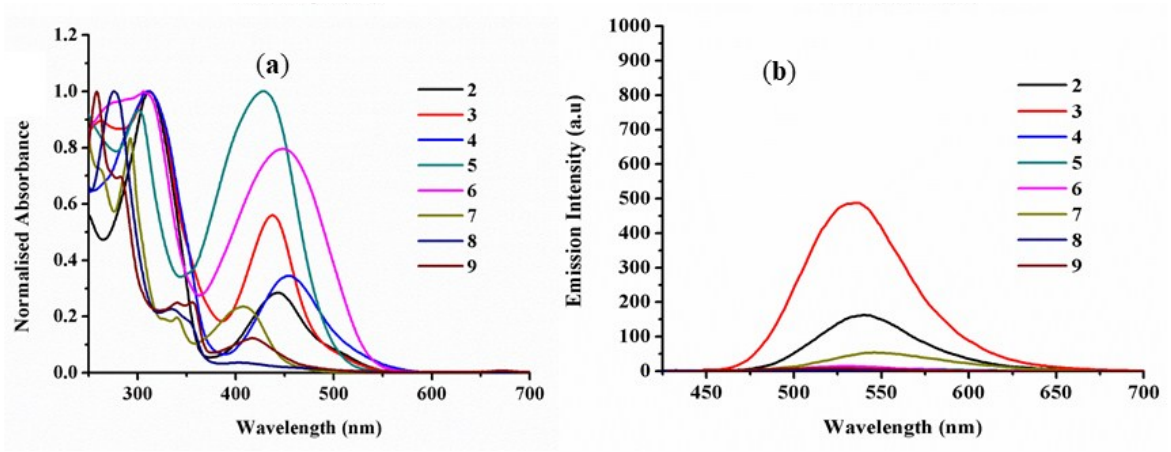


Fig. S4 Absorption spectra (**a**) and Emission spectra (**b**) of **2−9** in Chloroform.

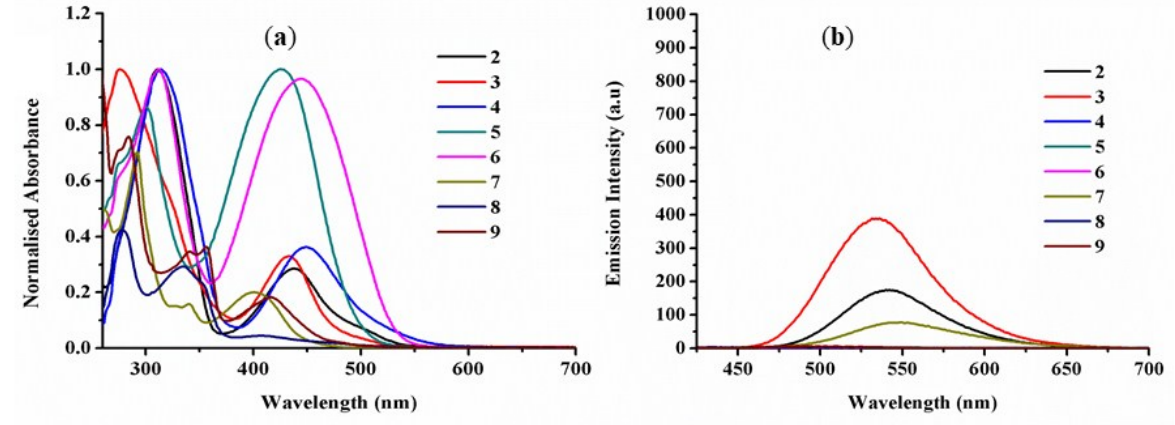


Fig. S5 Absorption spectra (**a**) and Emission spectra (**b**) of **2−9** in DCM.

Fig. S6 Absorption spectra (**a**) and Emission spectra (**b**) of **2**−**9** in THF.

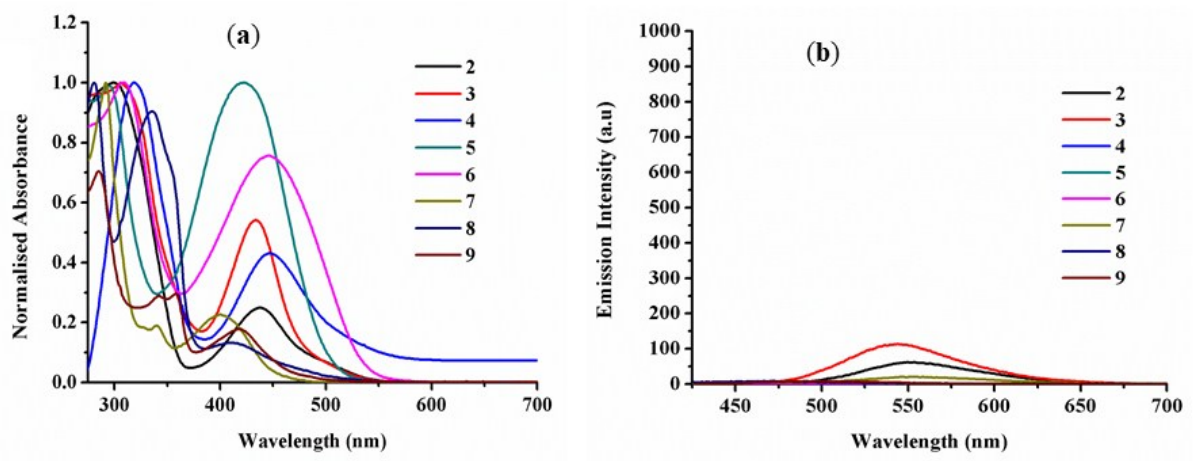


Fig. S7 Absorption spectra (**a**) and Emission spectra (**b**) of **2**−**9** in DMSO.

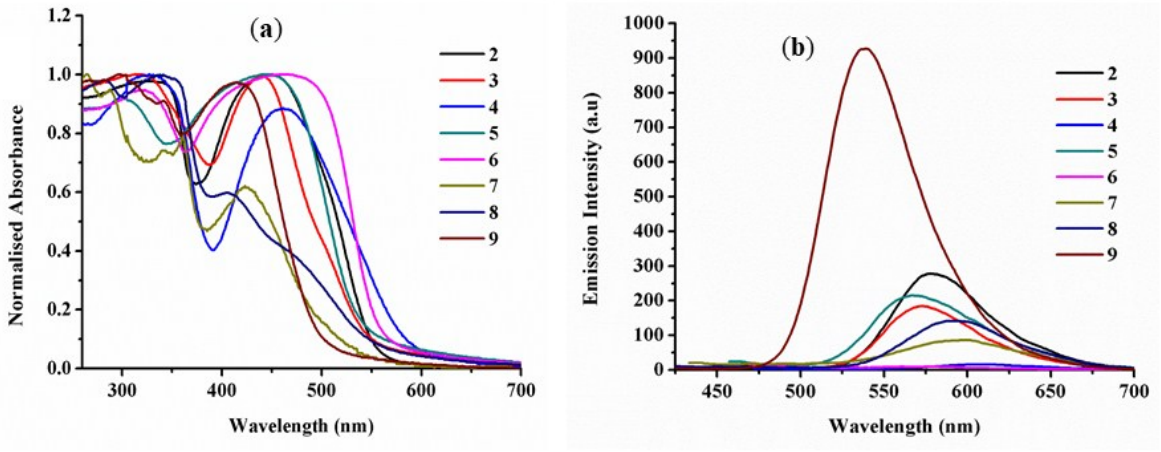


Fig. S8 Absorption spectra (**a**) and Emission spectra (**b**) of **2**−**9** in Solid Film.

2. Photophysical data of 1–9 in various solvents

Table S1 Photophysical data of **1** in various solvents:

Solvent	λ_{abs}, nm	λ_{em}, nm	Stokes shift, nm	Φ_F (%)	E_g^{opt} eV
Toluene	284, 344, 361, 412	–	–	–	–
DCM	286, 344, 361, 414	–	–	–	–
Chloroform	286, 345, 361, 416	–	–	–	–
THF	283, 346, 360, 411	–	–	–	–
DMSO	286, 346, 363, 416	–	–	–	–

Table S2 Photophysical data of **2** in various solvents:

Solvent	λ_{abs}, nm	λ_{em}, nm	Stokes shift, cm^{-1}	Φ_F (%)	E_g^{opt} eV
Toluene	289, 437	500	2883	9.25	2.63
DCM	311, 438	540	4312	5.55	2.49
Chloroform	312, 442	541	4140	3.70	2.56
THF	300, 434	517	3699	3.70	2.57
DMSO	299, 438	550	4649	1.85	2.44

Table S3 Photophysical data of **3** in various solvents:

Solvent	λ_{abs}, nm	λ_{em}, nm	Stokes shift, cm^{-1}	Φ_F (%)	E_g^{opt} eV
Toluene	306, 432	491	2781	12.96	2.69
DCM	276, 433	536	4438	9.25	2.57
Chloroform	310, 438	537	4209	5.55	2.61
THF	306, 429	507	3586	5.55	2.64
DMSO	306, 433	544	4712	1.85	2.54

Table S4 Photophysical data of **4** in various solvents:

Solvent	λ_{abs}, nm	λ_{em}, nm	Stokes shift, cm^{-1}	Φ_F (%)	E_g^{opt} eV
Toluene	316, 450	579	4951	11.13	2.42
DCM	314, 449	–	–	–	–
Chloroform	311, 454	–	–	–	–
THF	279, 445	–	–	–	–
DMSO	318, 447	–	–	–	–

Table S5 Photophysical data of **5** in various solvents:

Solvent	λ_{abs}, nm	λ_{em}, nm	Stokes shift, cm^{-1}	Φ_F (%)	E_g^{opt} eV
Toluene	302, 422	548	5448	1.85	2.48
DCM	300, 425	–	–	–	–
Chloroform	301, 428	–	–	–	–
THF	276, 417	510	4372	0.37	2.54
DMSO	295, 423	–	–	–	–

Table S6 Photophysical data of **6** in various solvents:

Solvent	λ_{abs}, nm	λ_{em}, nm	Stokes shift, cm^{-1}	Φ_F (%)	E_g^{opt} eV
Toluene	313, 443	–	–	–	–
DCM	312, 444	–	–	–	–
Chloroform	306, 447	–	–	–	–
THF	306, 439	–	–	–	–
DMSO	309, 445	–	–	–	–

Table S7 Photophysical data of **7** in various solvents:

Solvent	**λ_{abs}, nm**	**λ_{em}, nm**	**Stokes shift, cm^{-1}**	**Φ_F (%)**	**E_g^{opt} eV**
Toluene	292, 340, 410	523	5269	11.12	2.64
DCM	292, 340, 402	549	6660	1.85	2.59
Chloroform	292, 340, 407	546	6255	1.12	2.63
THF	290, 339, 400	543	6583	3.7	3.00
DMSO	292, 339, 401	550	6755	1.12	2.70

Table S8 Photophysical data of **8** in various solvents:

Solvent	**λ_{abs}, nm**	**λ_{em}, nm**	**Stokes shift, cm^{-1}**	**Φ_F (%)**	**E_g^{opt} eV**
Toluene	284, 335, 404	–	–	–	–
DCM	278, 334, 407	–	–	–	–
Chloroform	276, 335, 403	–	–	–	–
THF	276, 332, 404	–	–	–	–
DMSO	281, 336, 411	–	–	–	–

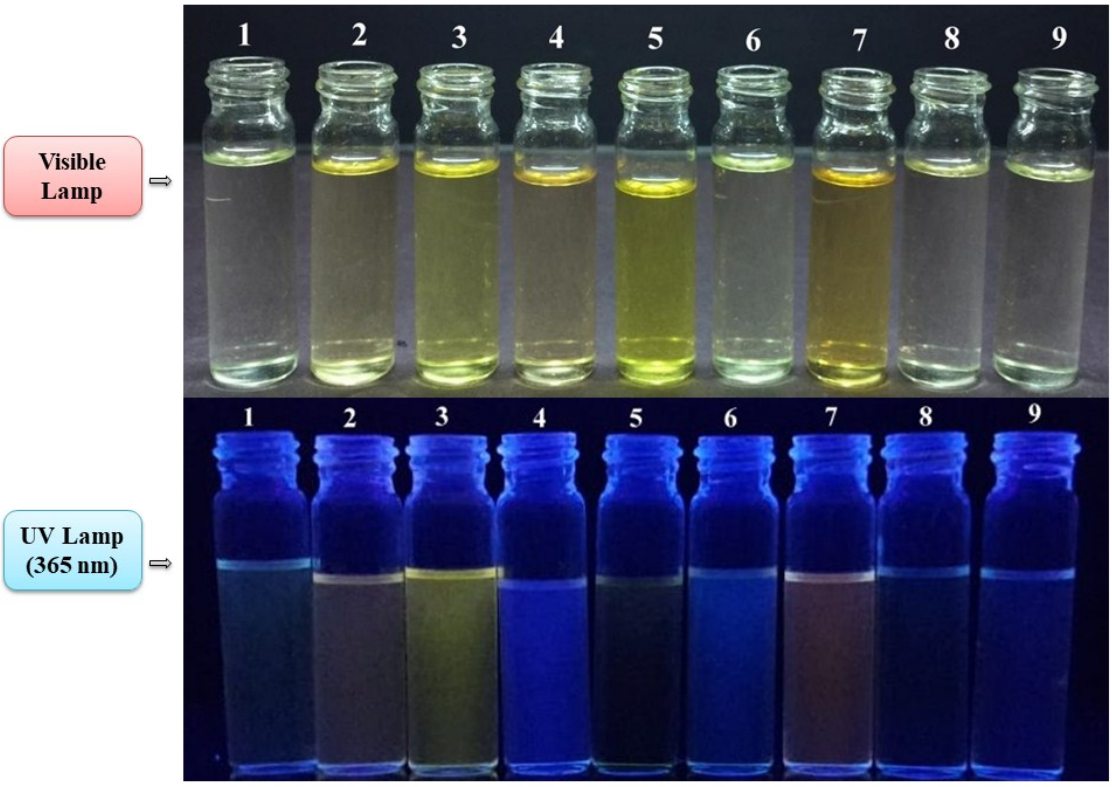
Table S9 Photophysical data of **9** in various solvents:

Solvent	**λ_{abs}, nm**	**λ_{em}, nm**	**Stokes shift, cm^{-1}**	**Φ_F (%)**	**E_g^{opt} eV**
Toluene	286, 340, 356, 416	–	–	–	–
DCM	284, 341, 356, 416	–	–	–	–
Chloroform	283, 340, 356, 417	–	–	–	–
THF	276, 339, 354, 413	–	–	–	–
DMSO	286, 342, 358, 417	–	–	–	–

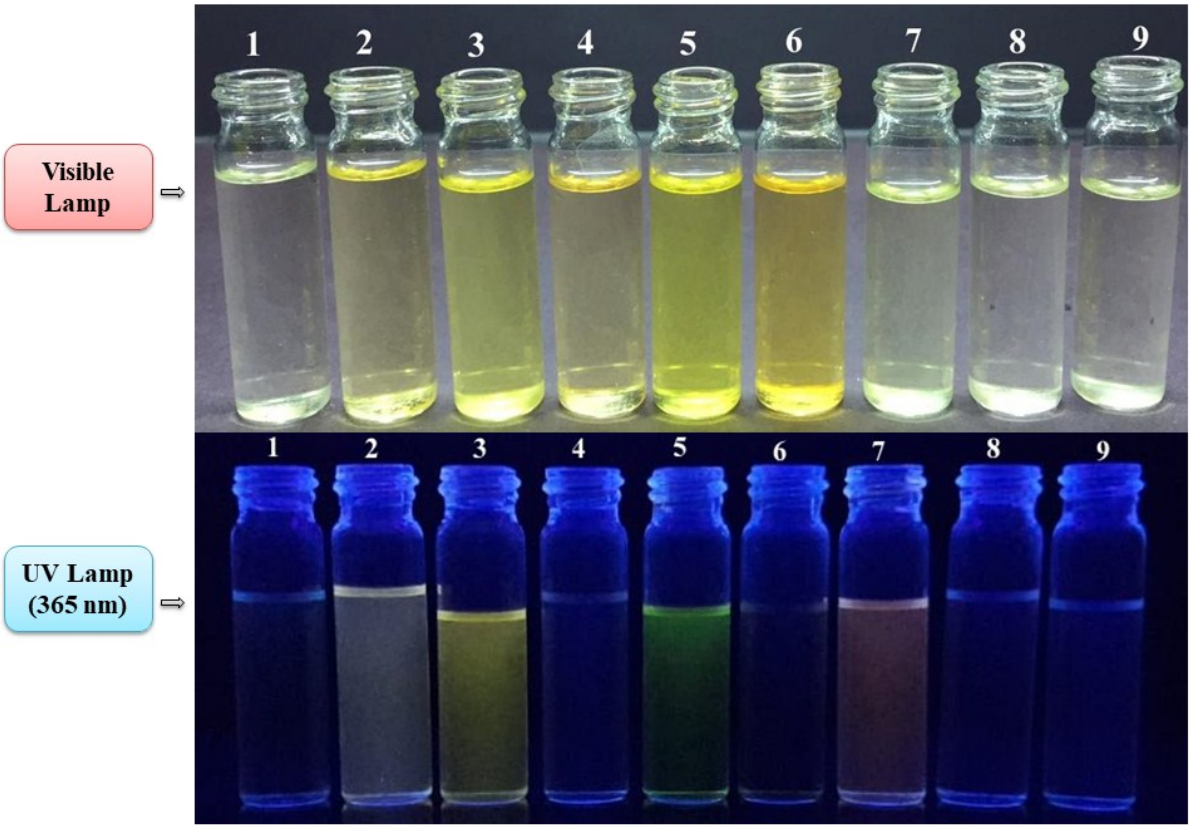
3. Emission images of 1−9 in various solvent and neat solid film

(a) Toluene

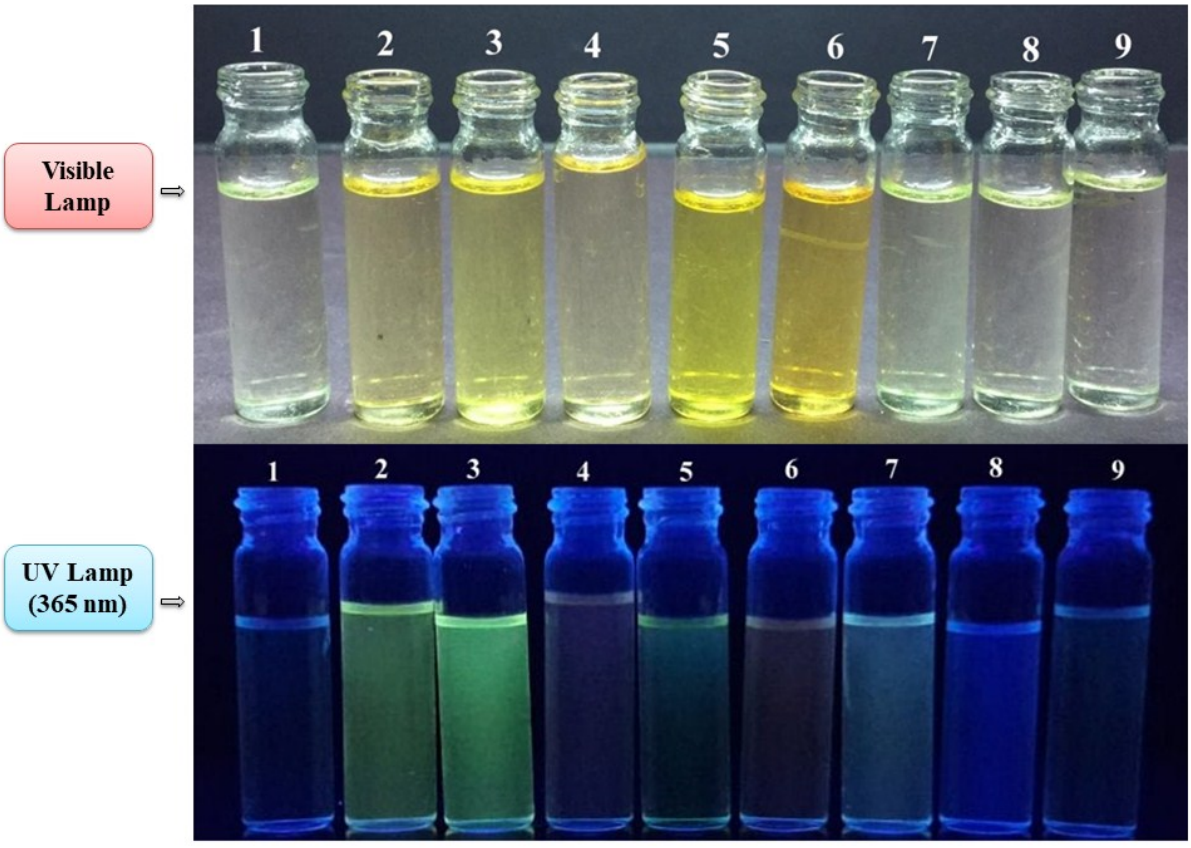
(b) Chloroform



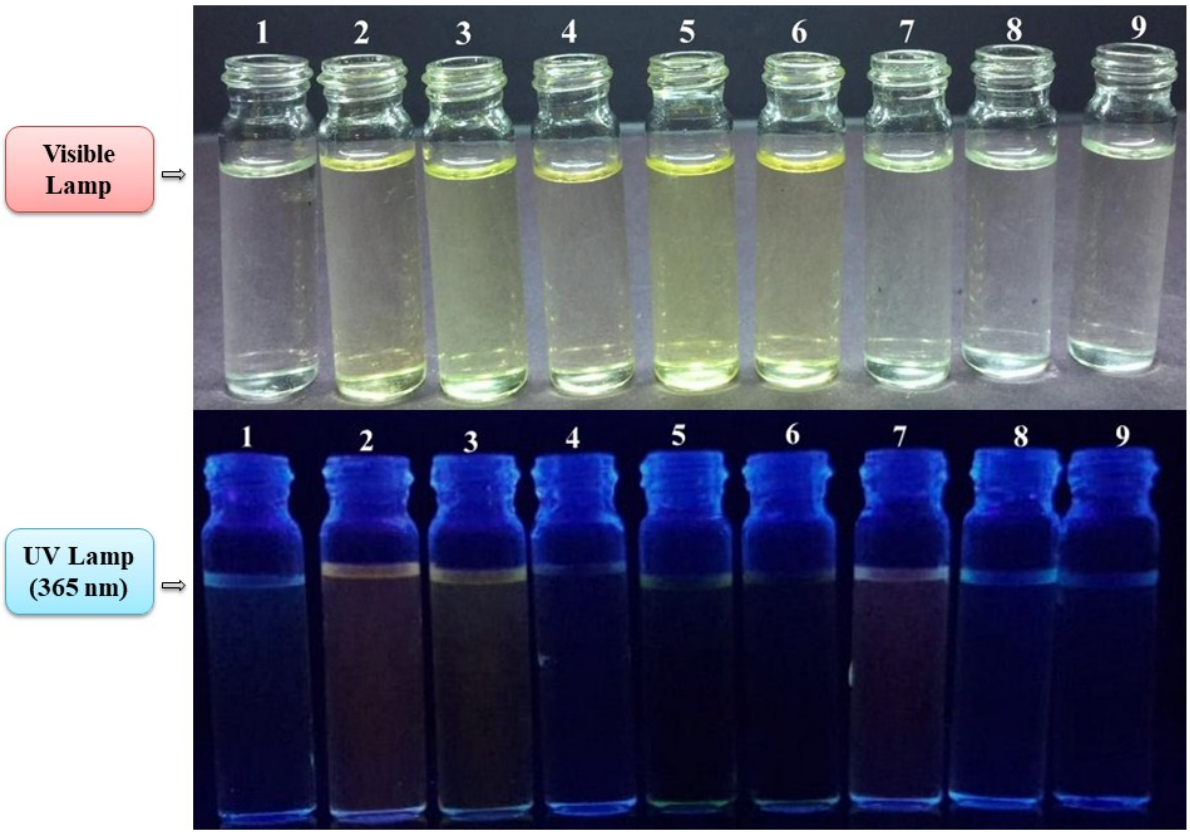
(c) Dichloromethane



(d) THF



(e) DMSO



(e) Solid Film

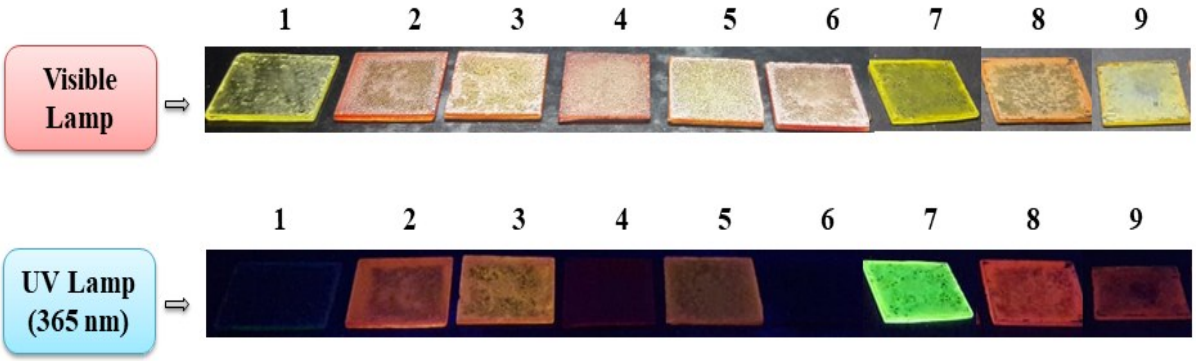


Fig. S9. Emission images of **2−9** in toluene (**a**), CHL (**b**) DCM (**c**), THF (**d**) and DMSO (**e**) and solid film (**f**) under 365 nm UV illumination

4. AIE photophysical spectrum

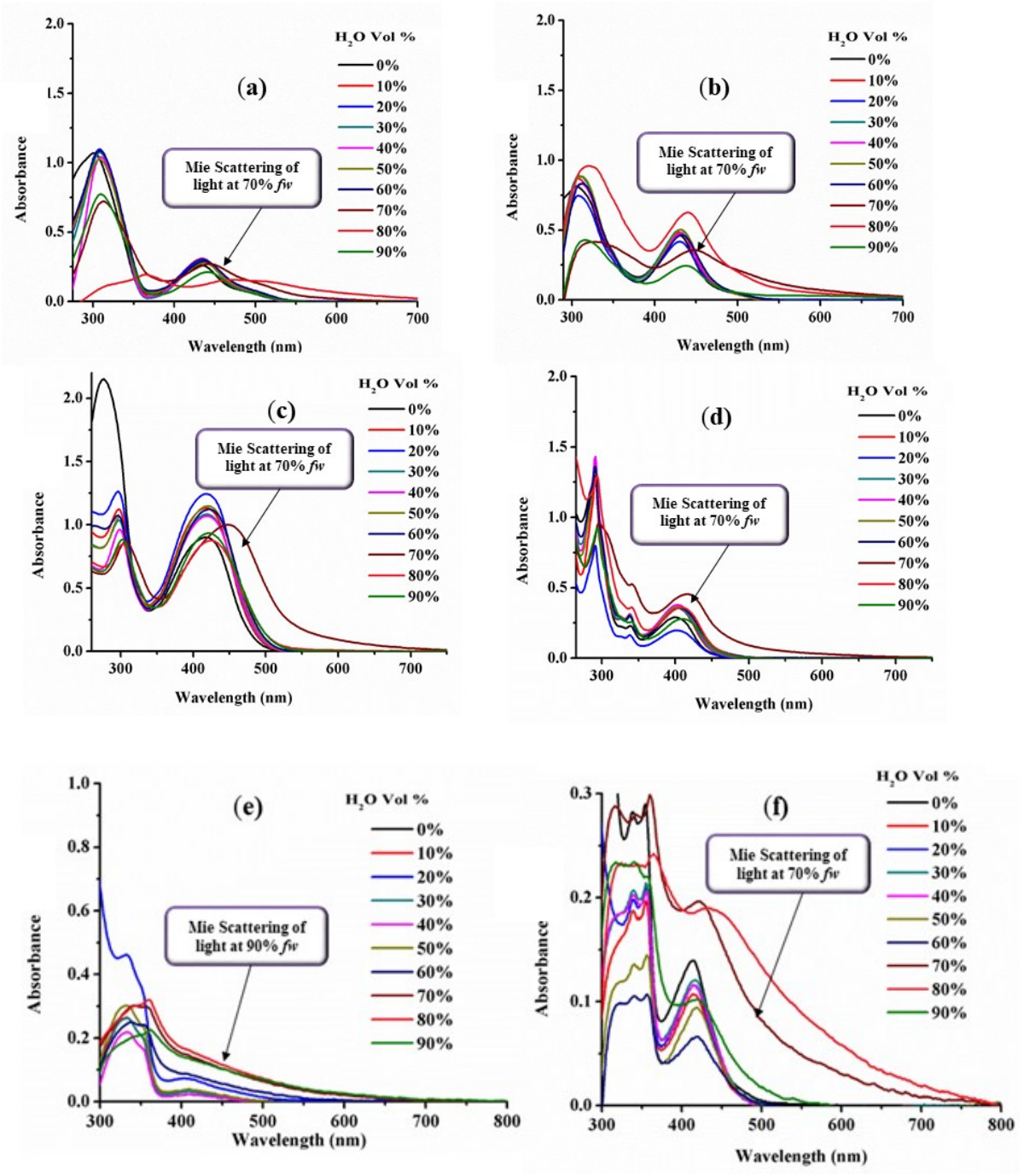


Fig. S10. Absorbance spectra of **2** (**a**), **3** (**b**), **5** (**c**), **7** (**d**), **8** (**e**) and **9** (**f**) in THF–water mixtures with different water fractions (10 μM).

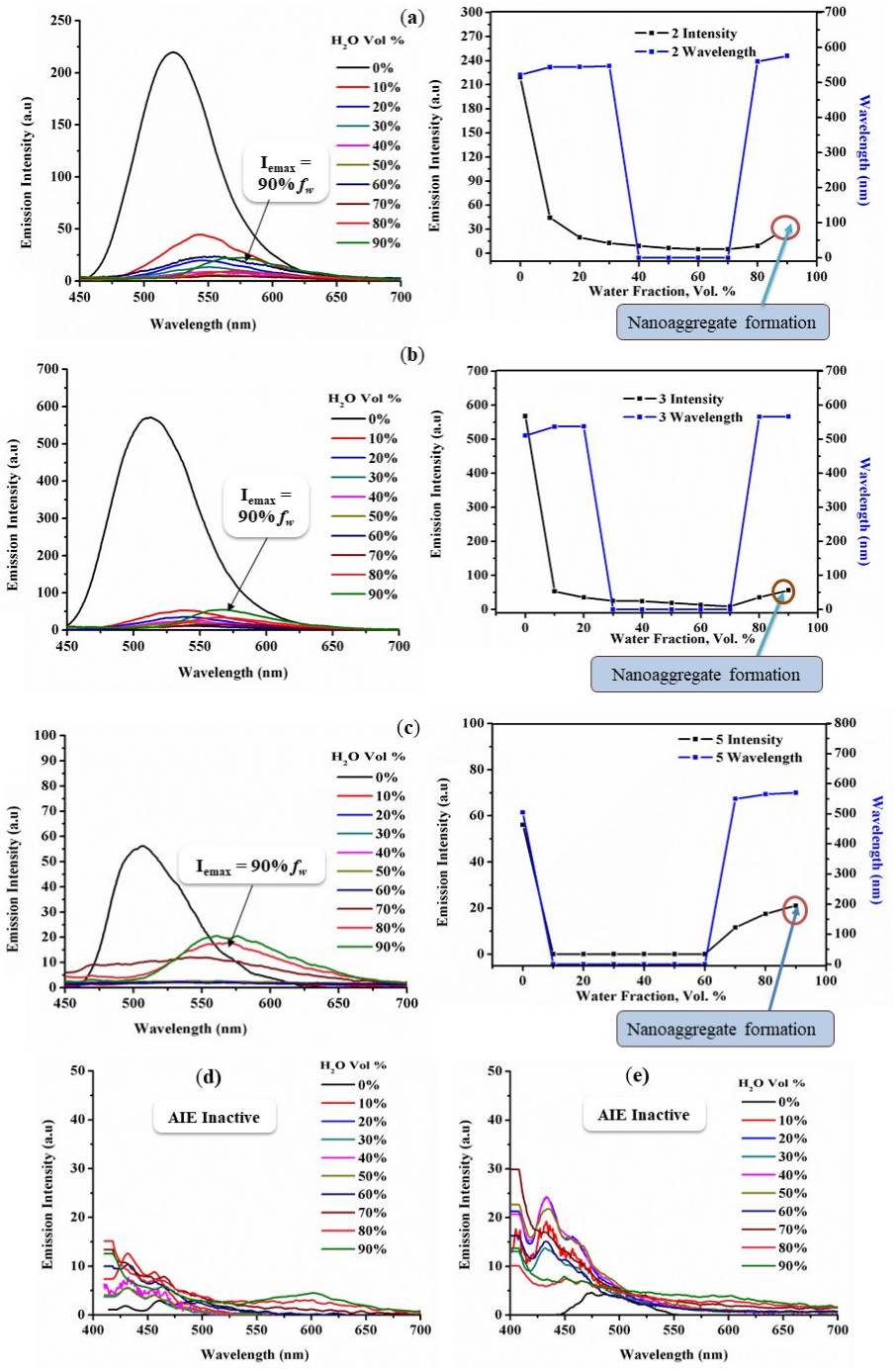


Fig. S11. Emission spectra (**left**) and Plot of wavelength and emission intensity versus % of water fraction in THF/Water mixture with different water fractions (10 μM) of **2** (**a**), **3** (**b**), and **5**(**c**) (**right**) excited at 440 nm. Emission spectra of **8** (**d**) and **8** (**e**) in THF/Water mixture with different water fractions (10 μM) excited at 390 nm.

5. Dynamic light scattering (DLS) plot

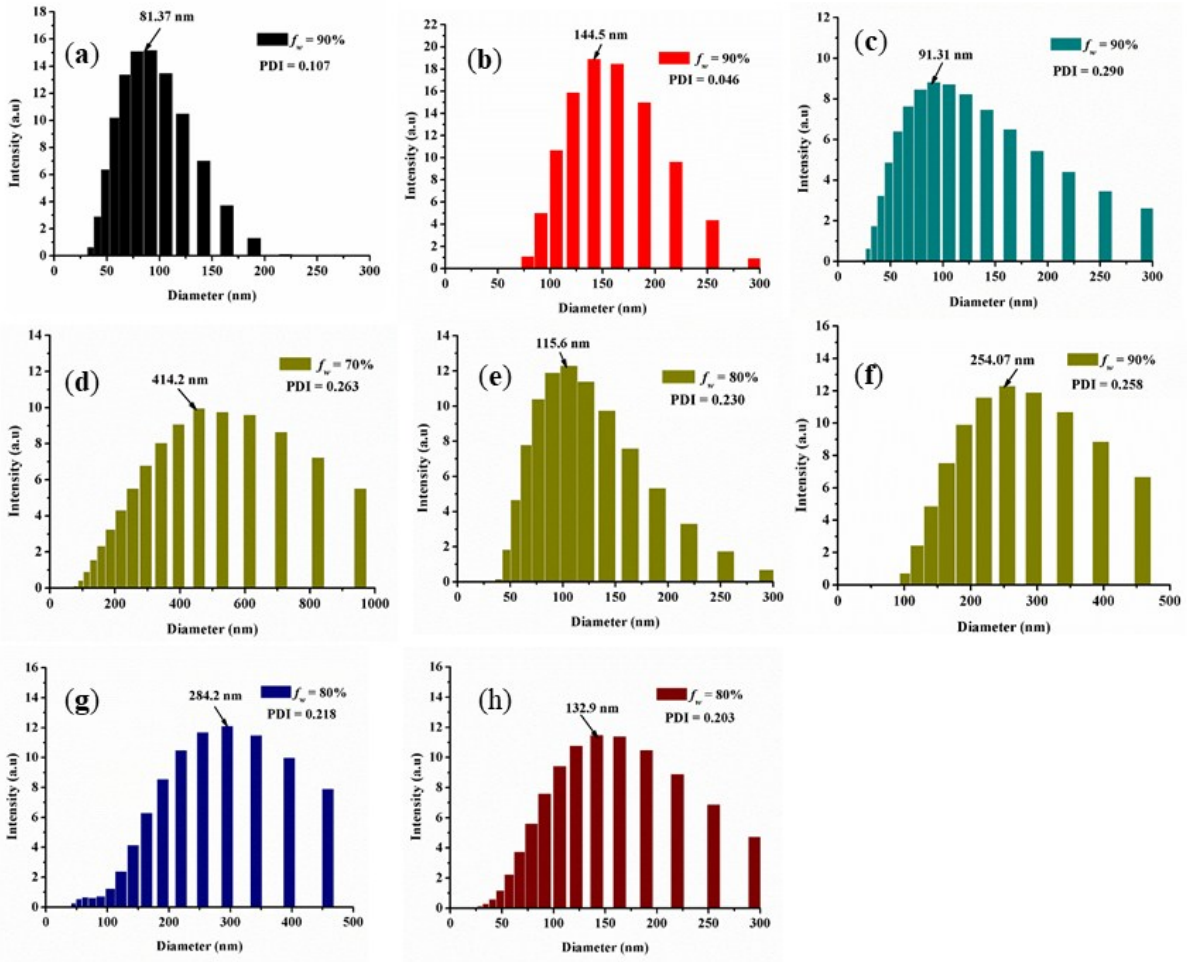


Fig. S12 DLS plot of **2** (**a**), **3** (**b**), **5** (**c**), **7** (**d**−**f**), **8** (**g**) and **9** (**h**) showing formation nanoparticle obtained from different f_w of THF−H_2O homogenous suspension.

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

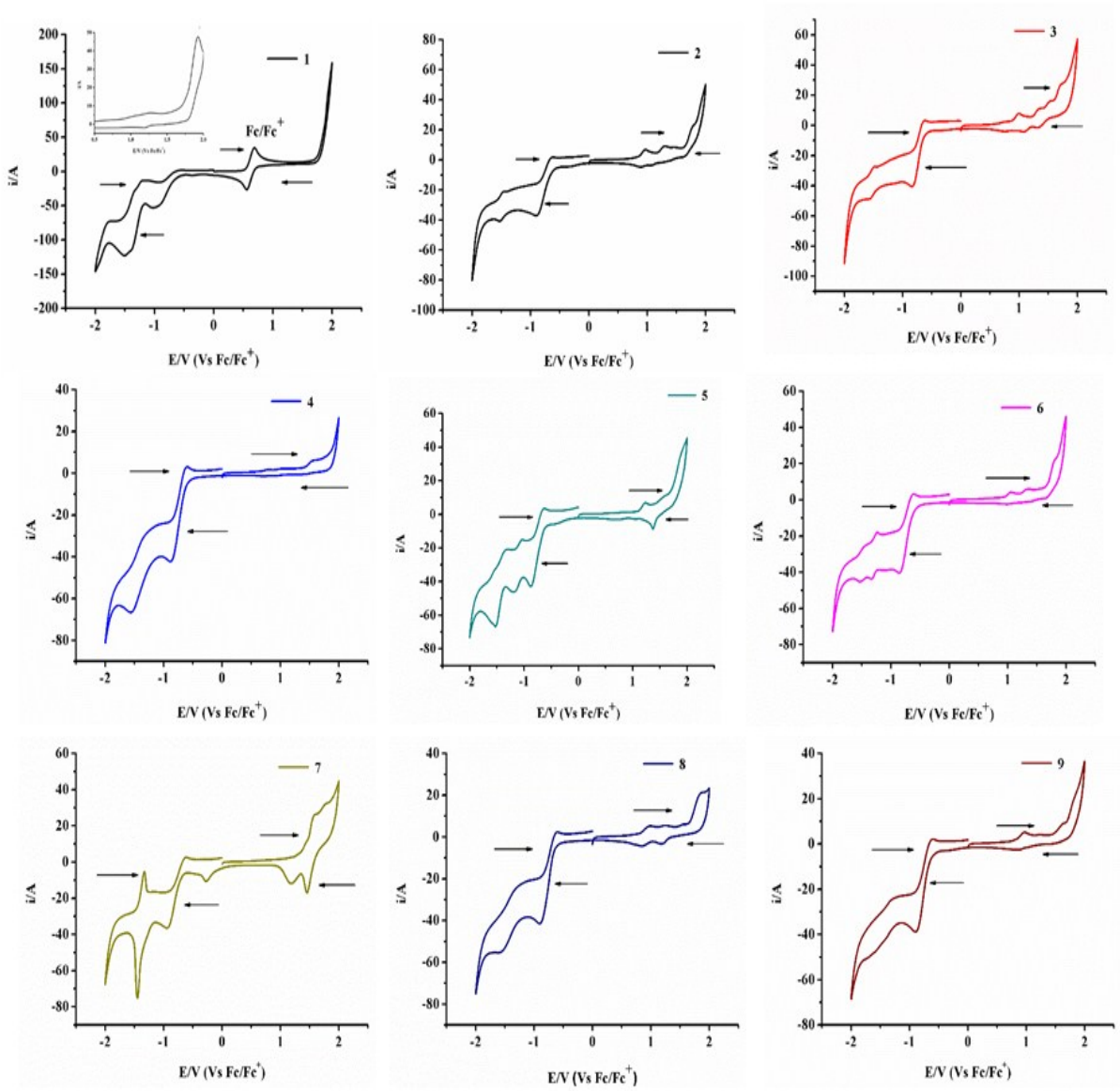


Fig. S13. Cyclic voltammogram (full scan) of compounds **1−9**.

7. TGA plot of compound 1-9

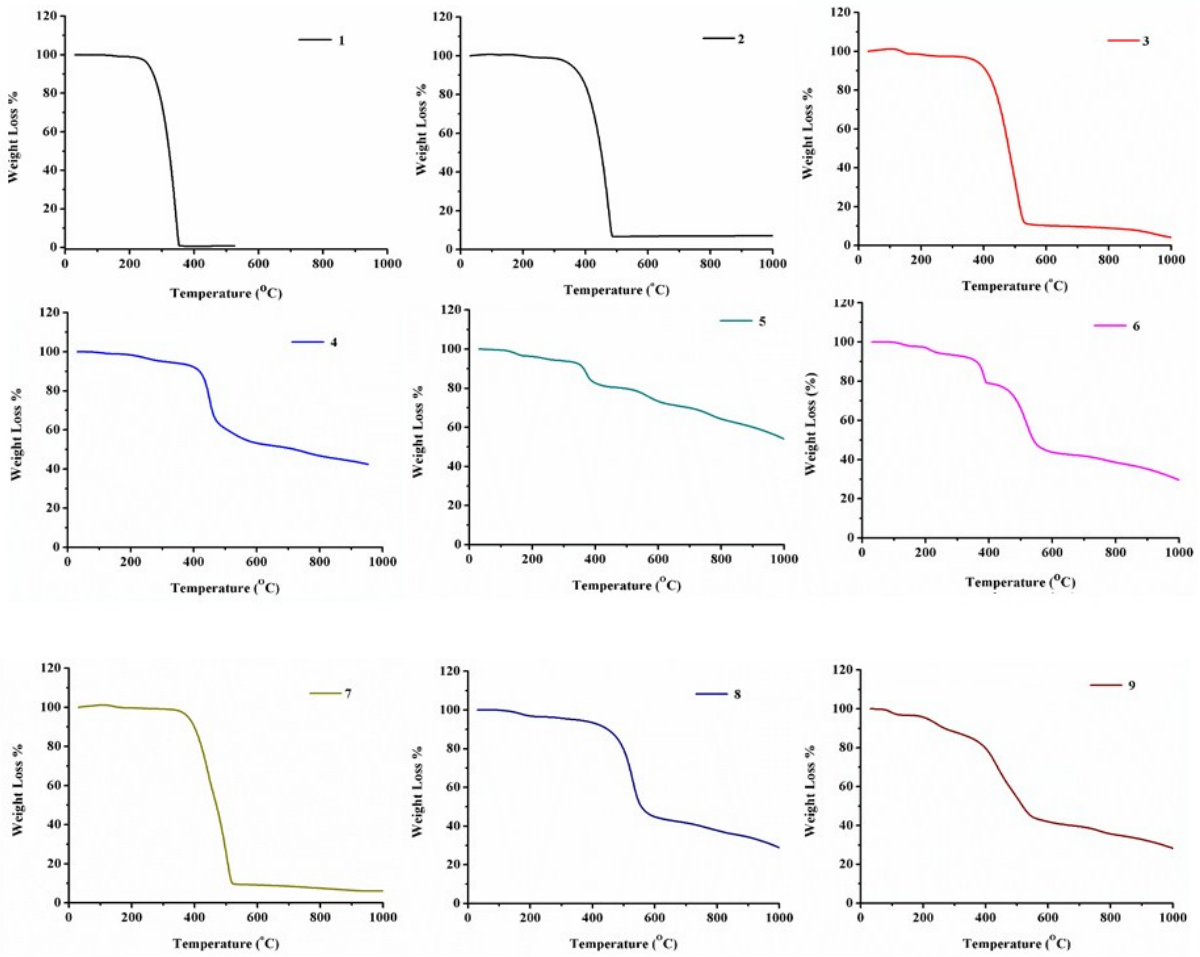


Fig. S14. TGA plot of compounds **1−9.**

8. MALDI-TOF Spectra of compounds 1−9

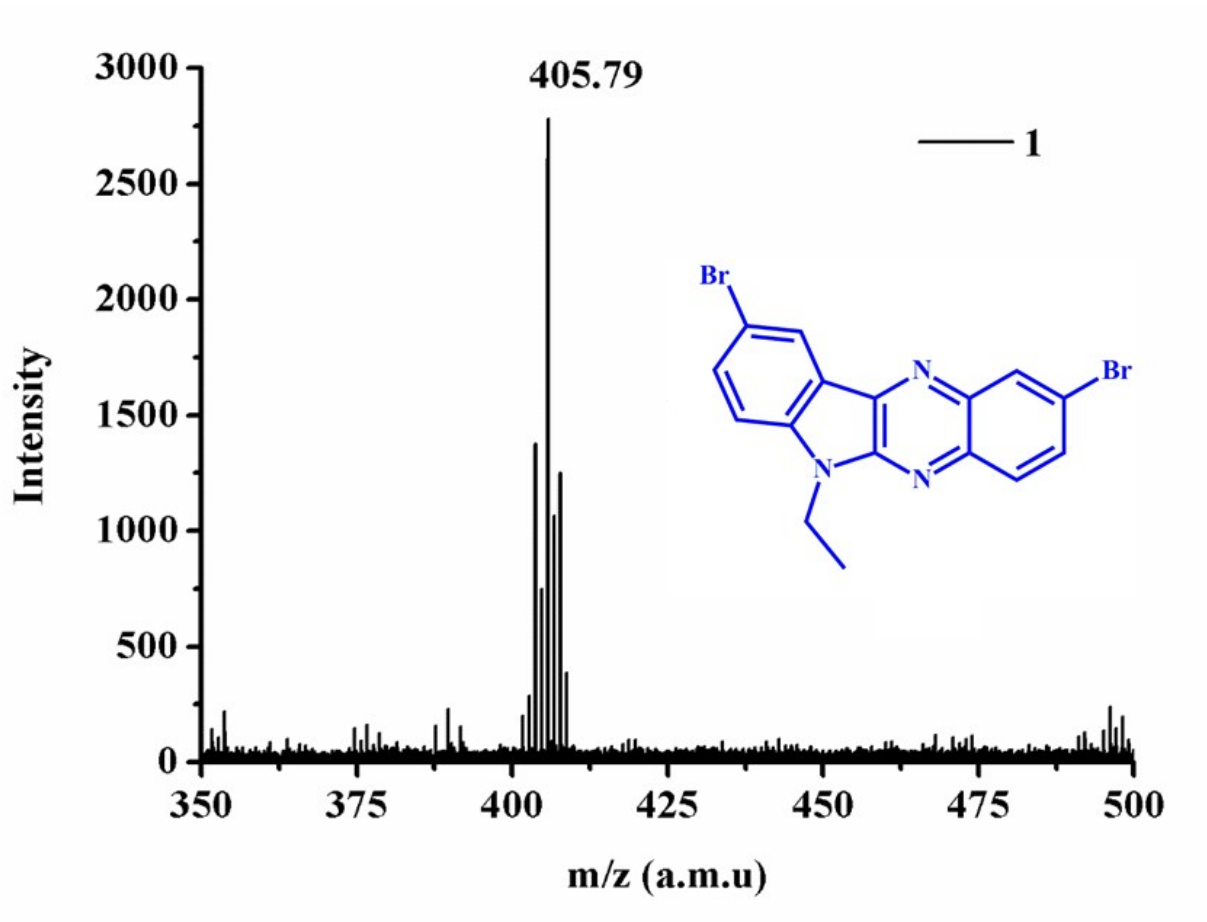


Fig. S15. MALDI-TOF spectrum of compound **1**

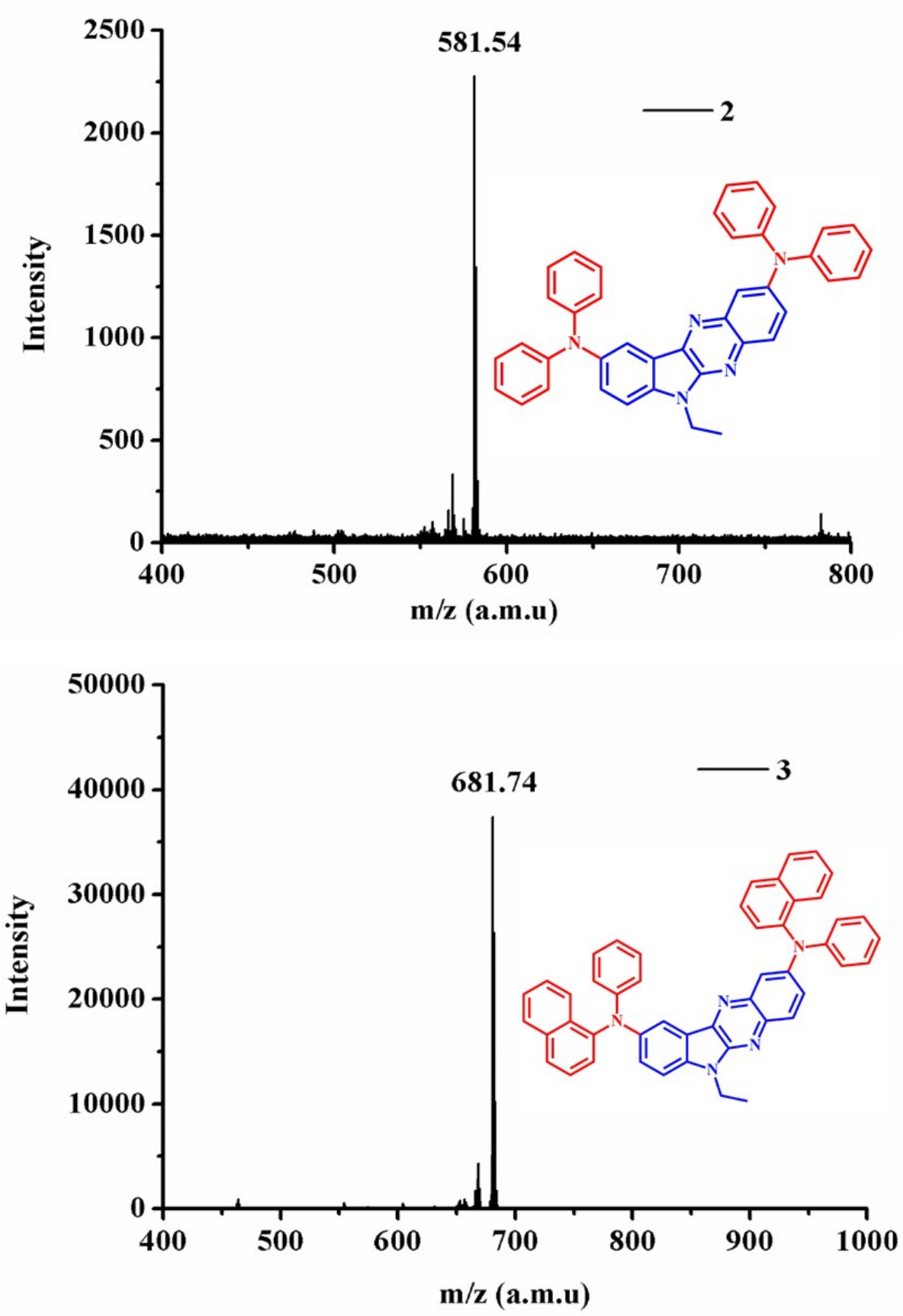


Fig. S16. MALDI-TOF spectrum of compound **2** (**above**) and **3** (**below**)

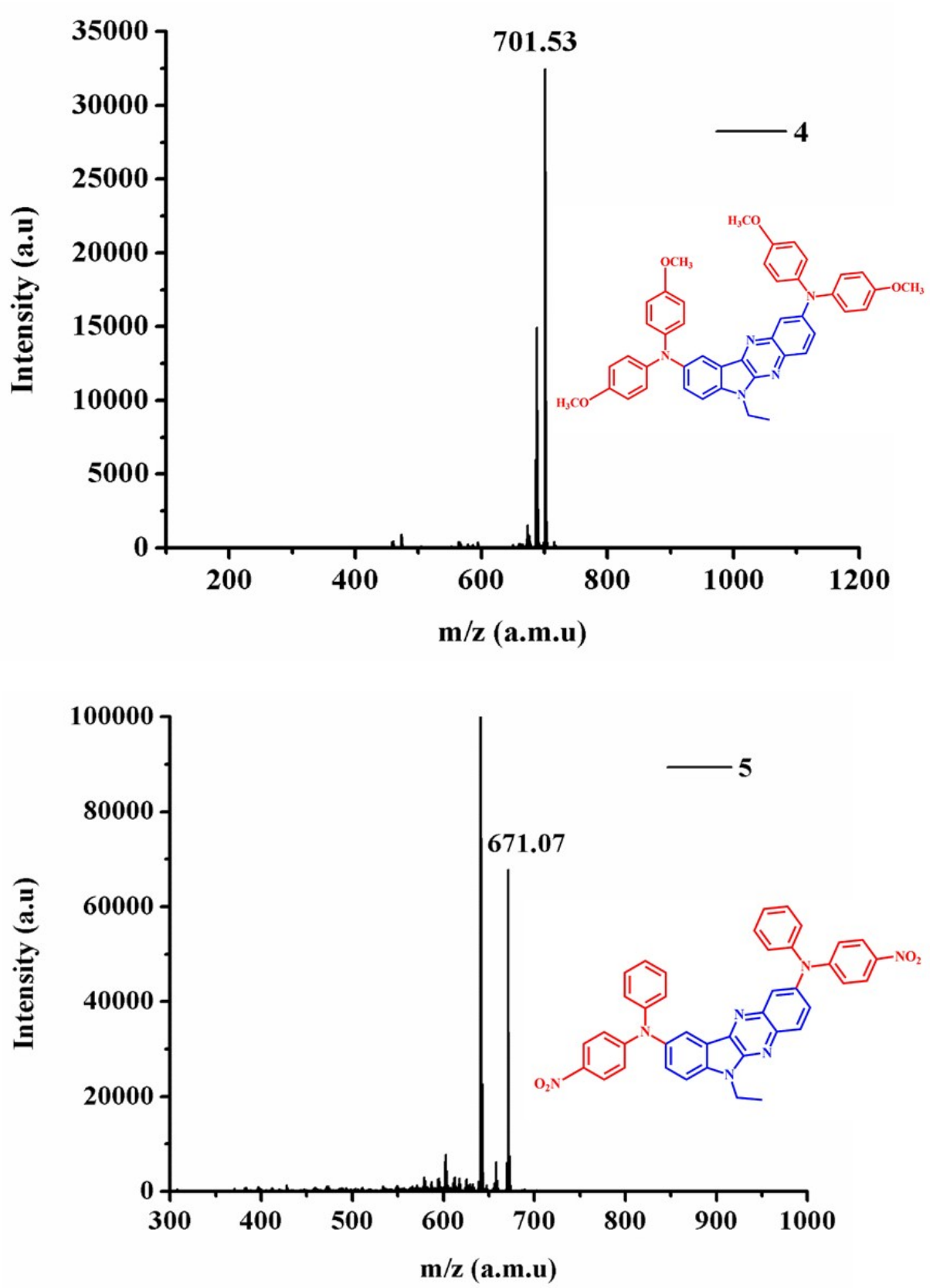


Fig. S17. MALDI-TOF spectrum of compound **4** (**above**) and **5** (**below**)

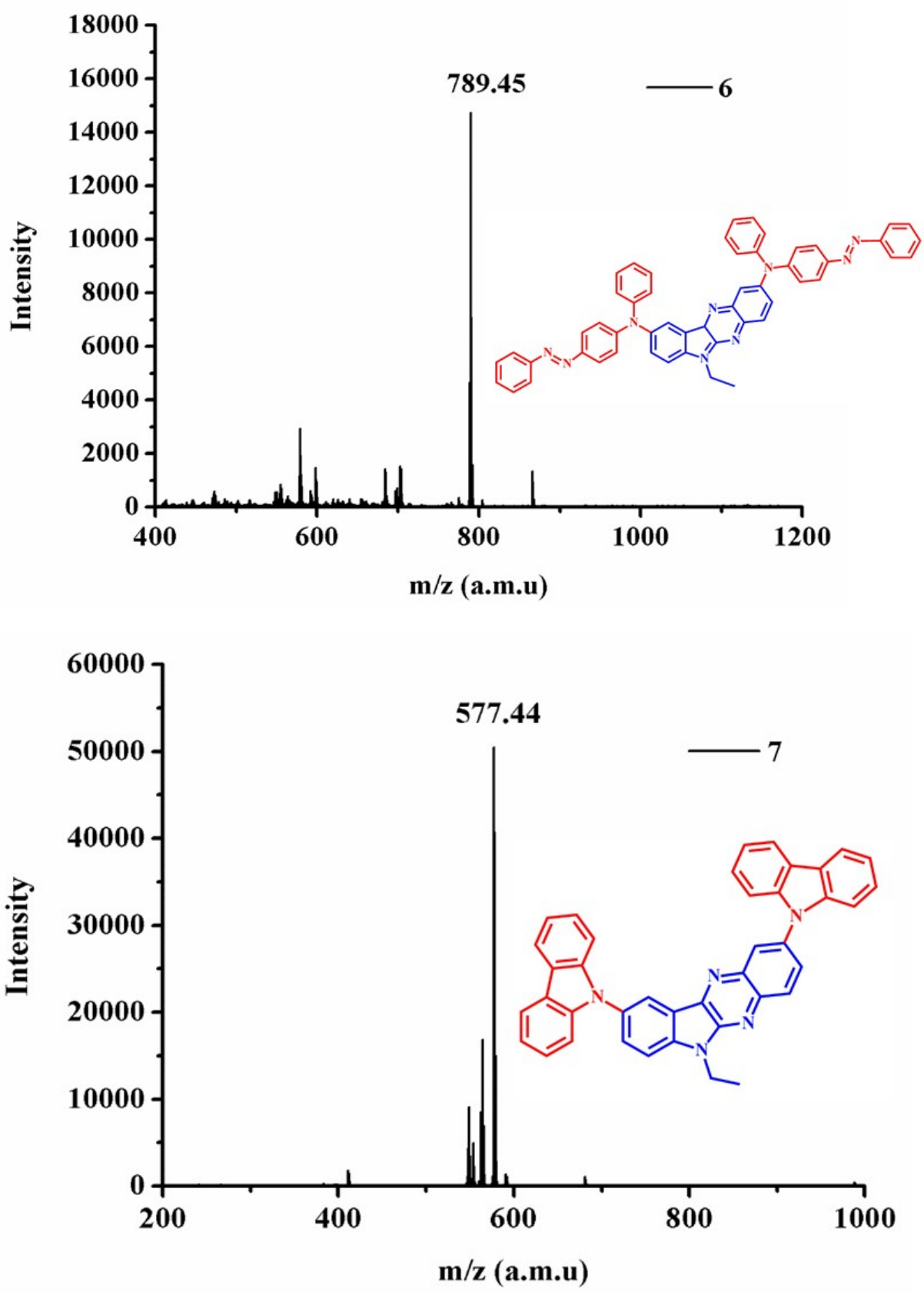


Fig. S18. MALDI-TOF spectrum of compound **6** (**above**) and **7** (**below**)

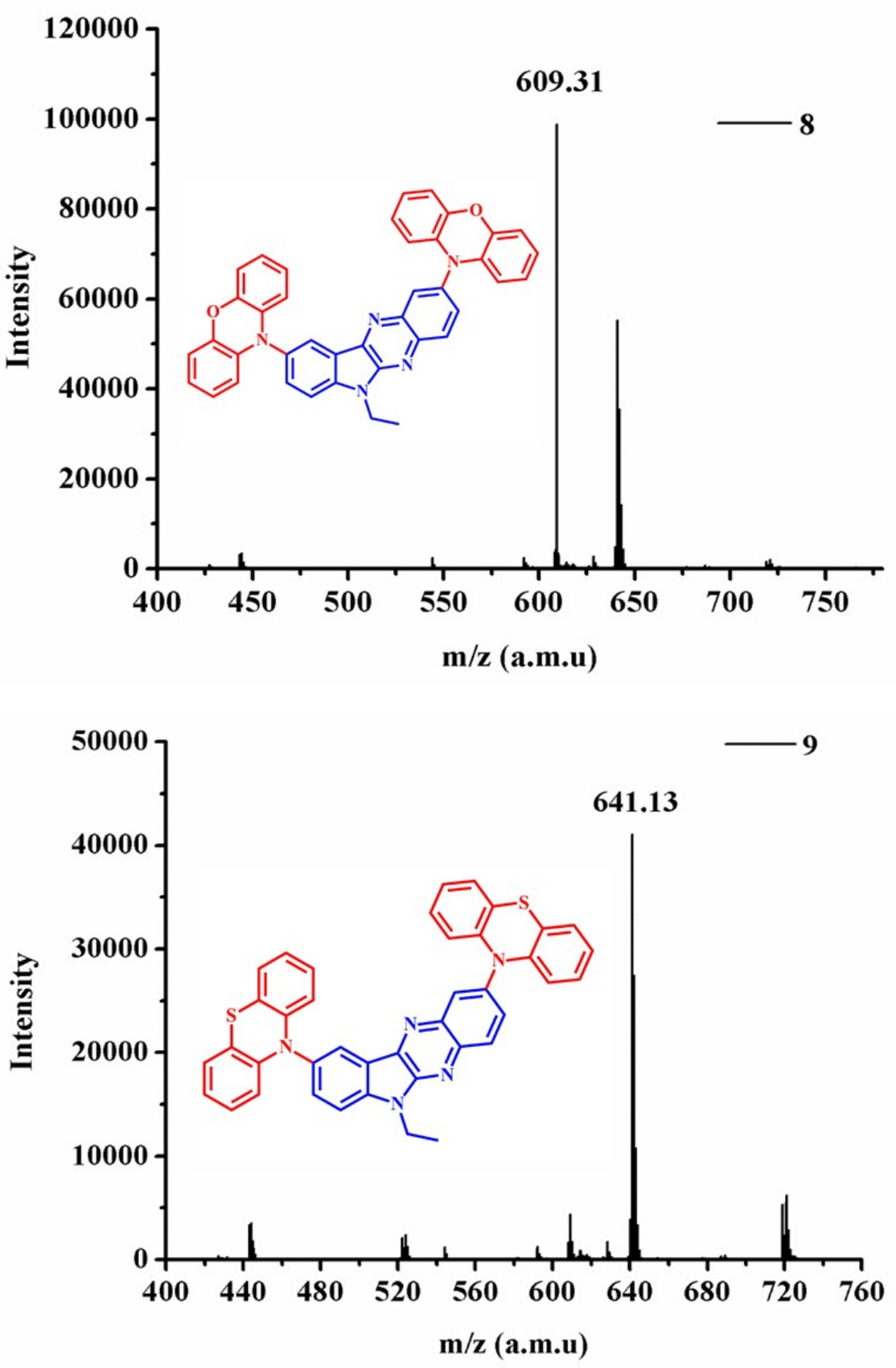


Fig. S19. MALDI-TOF spectrum of compound **8** (**above**) and **9** (**below**)

9. FT-IR Spectra of compounds 1−9

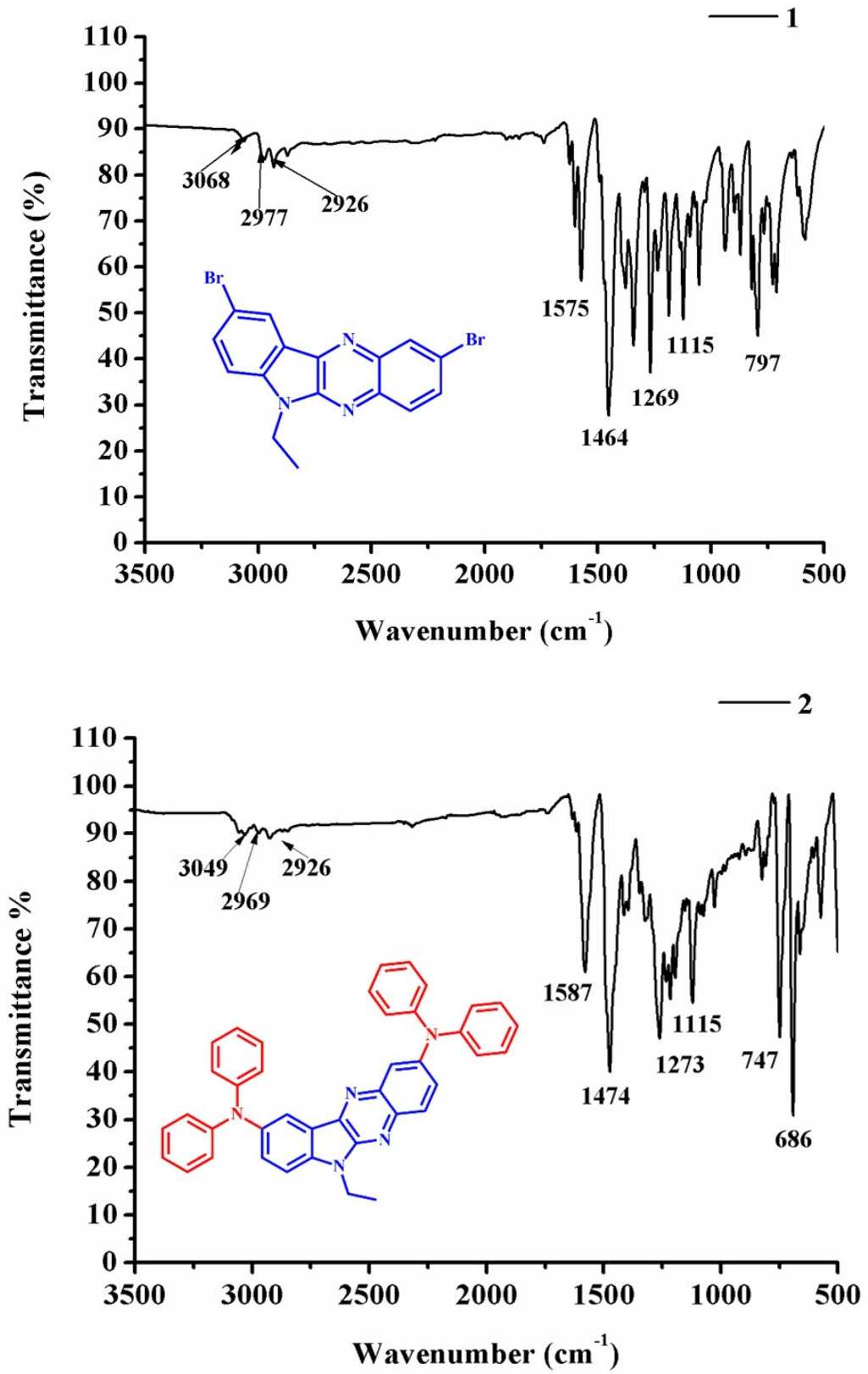


Fig. S20. FTIR spectrum of compound **1** (**above**) and **2** (**below**).

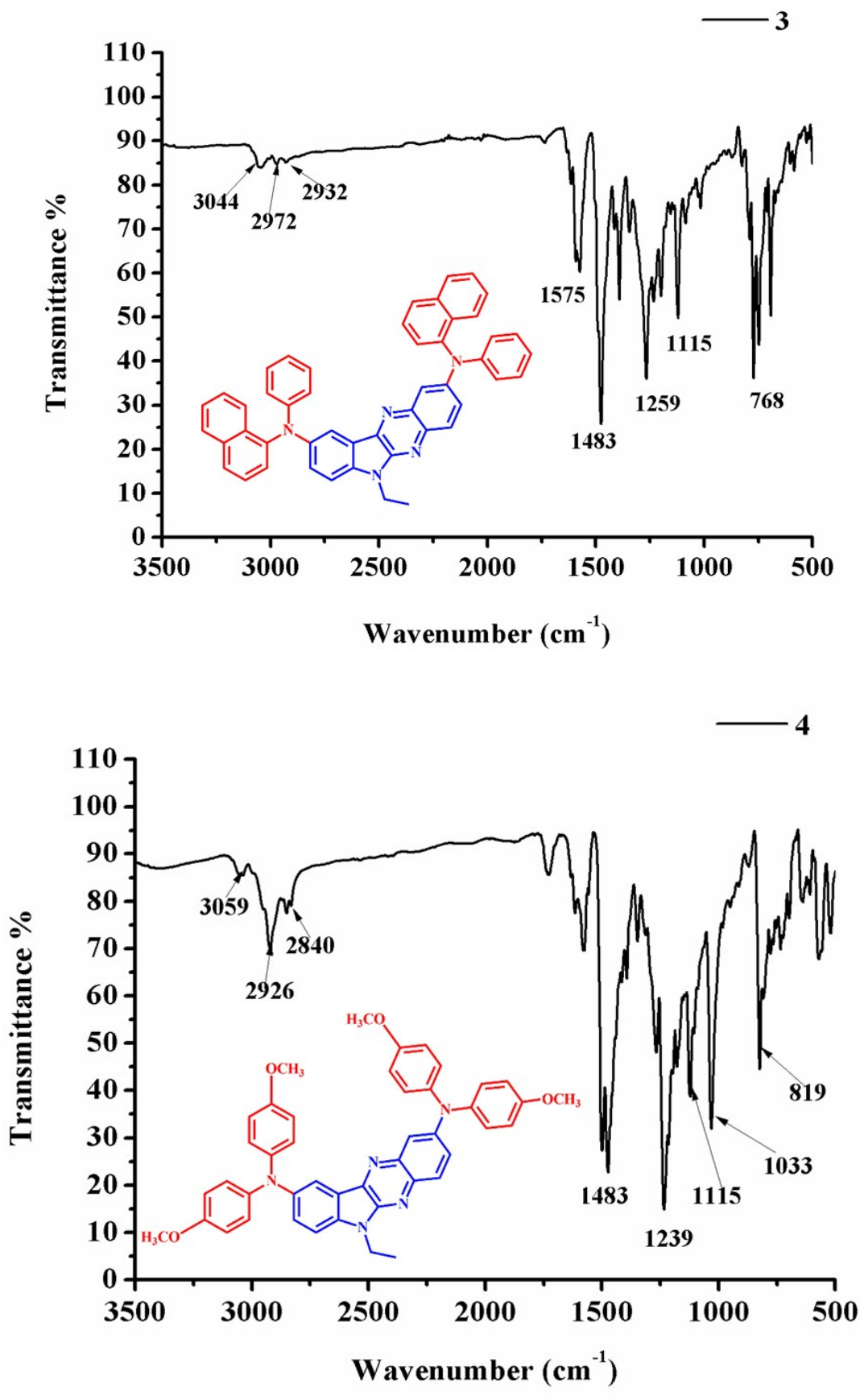


Fig. S21. FTIR spectrum of compound **3** (**above**) and **4** (**below**).

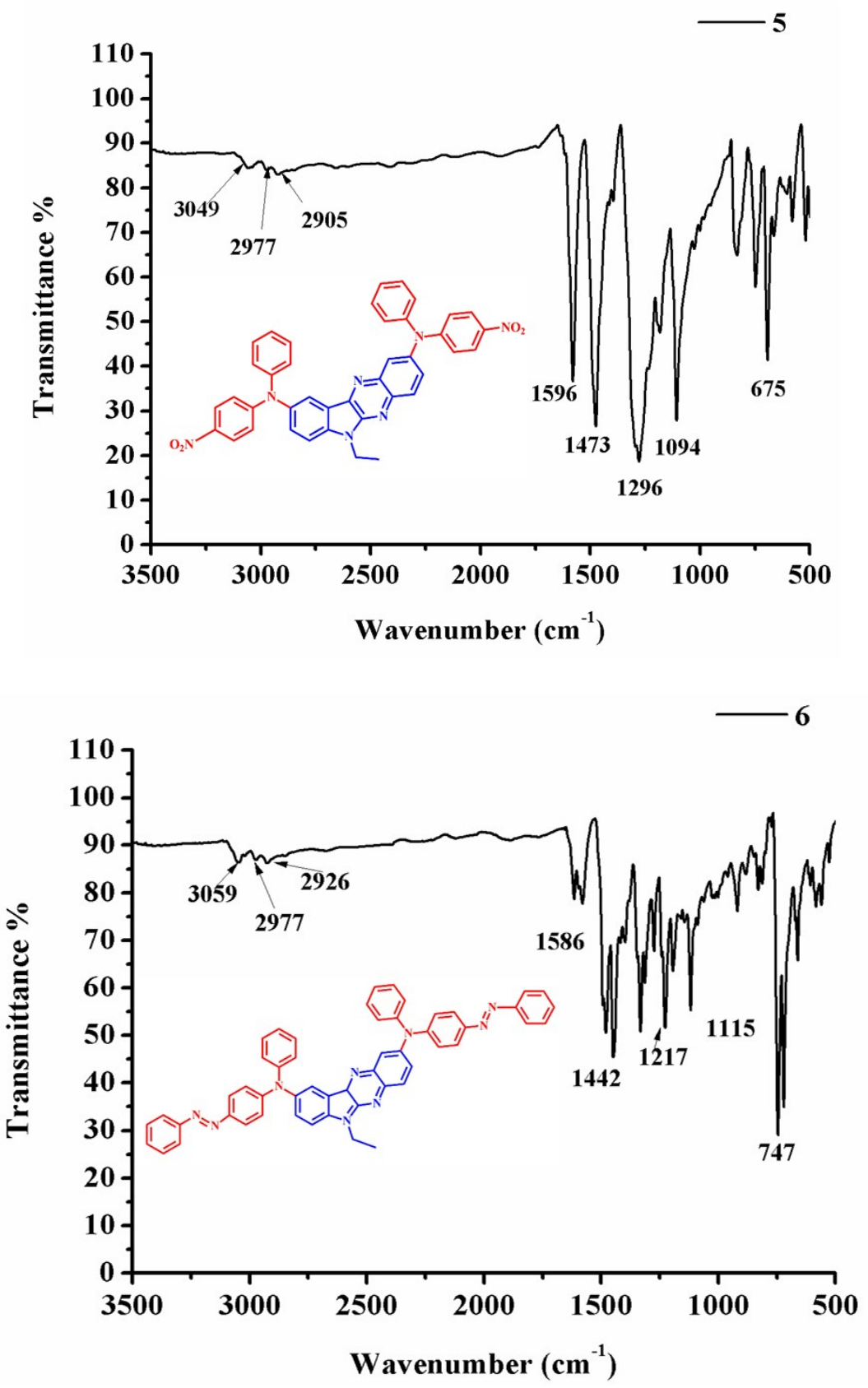


Fig. S22. FTIR spectrum of compound **5** (**above**) and **6** (**below**).

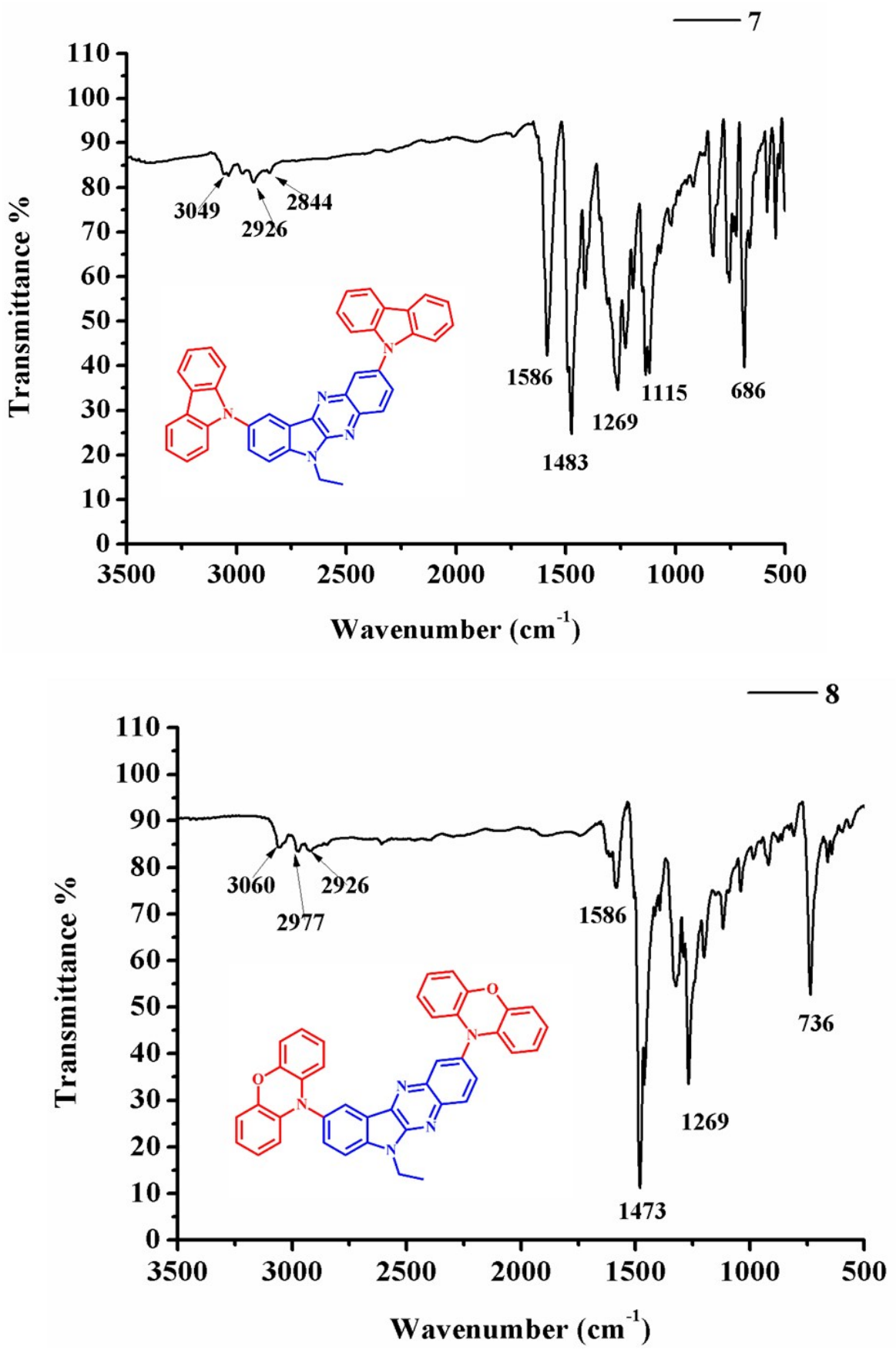


Fig. S23. FTIR spectrum of compound **7** (**above**) and **8** (**below**).

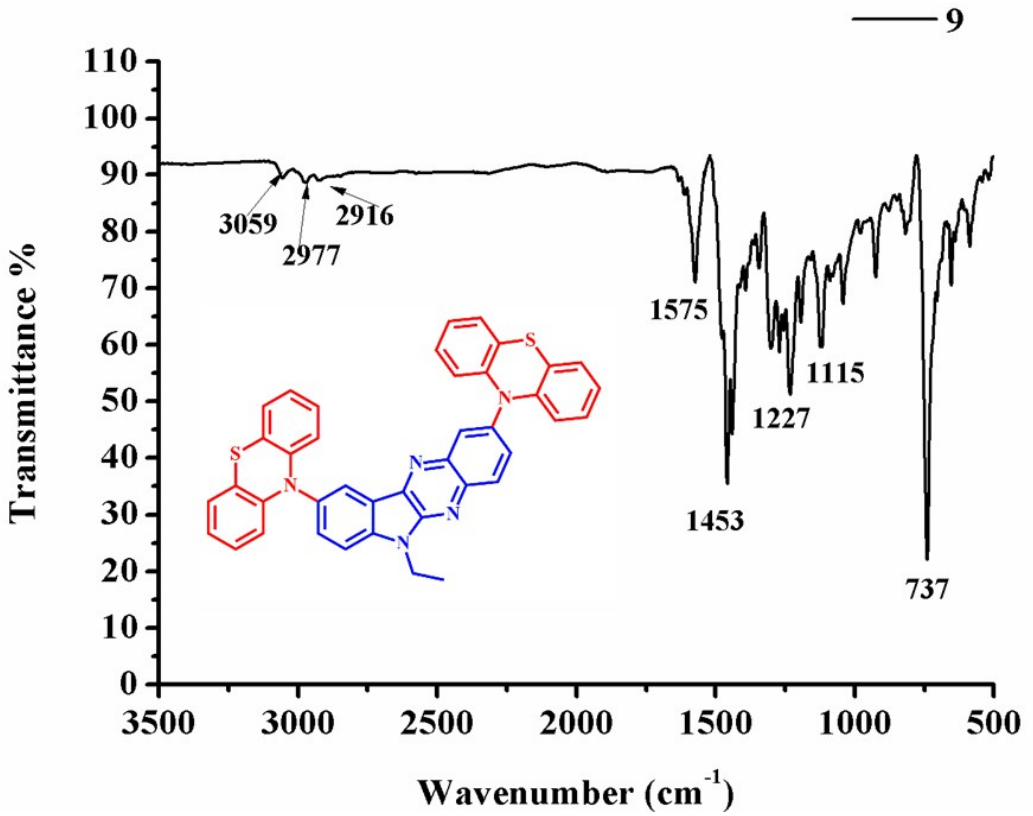


Fig. S24. FTIR spectrum of compound **9**.

10. ^{1}H spectra of compounds 1 – 9

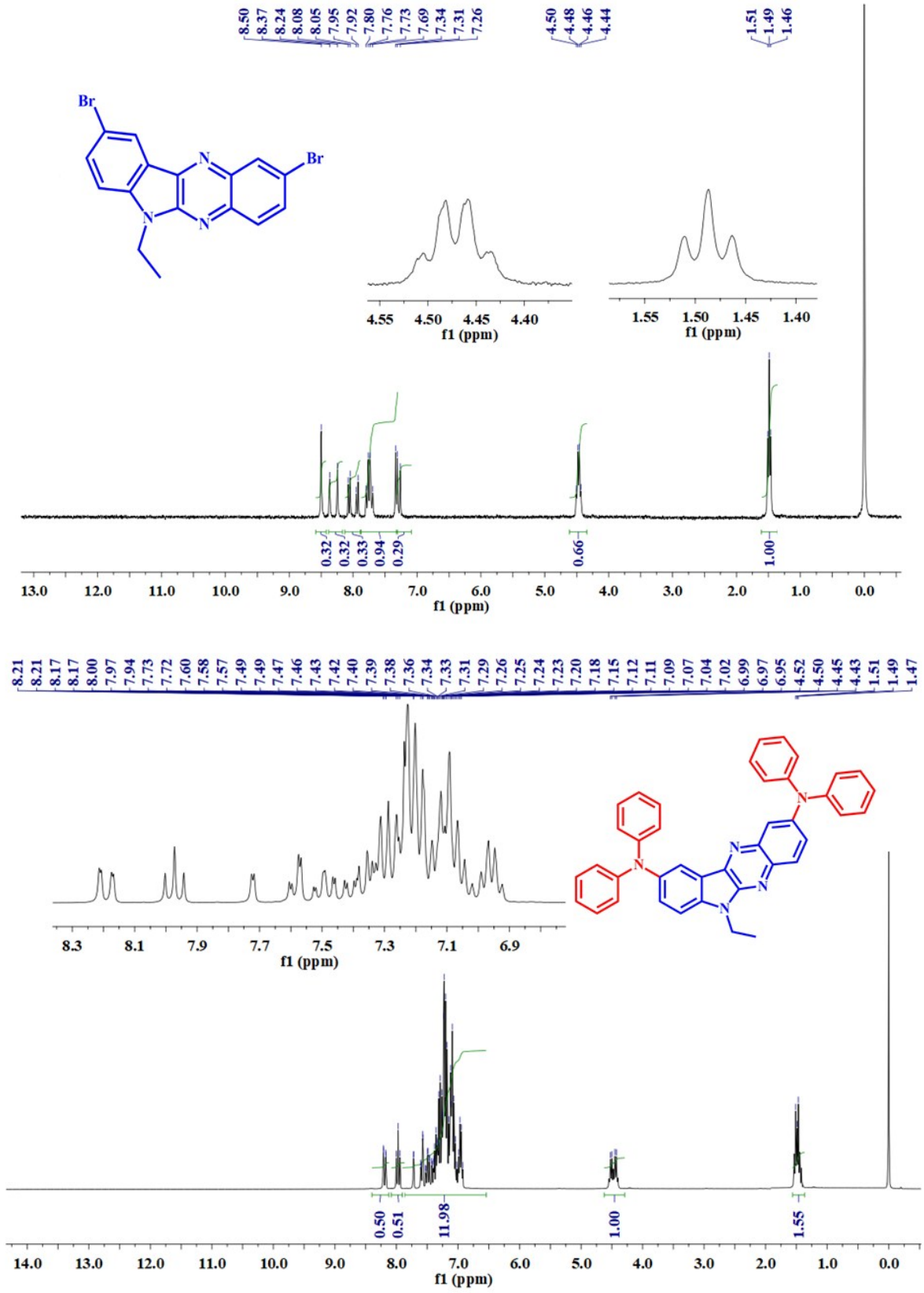


Fig. S25. ^{1}H NMR spectrum of compound **1** (**above**) and **2** (**below**).

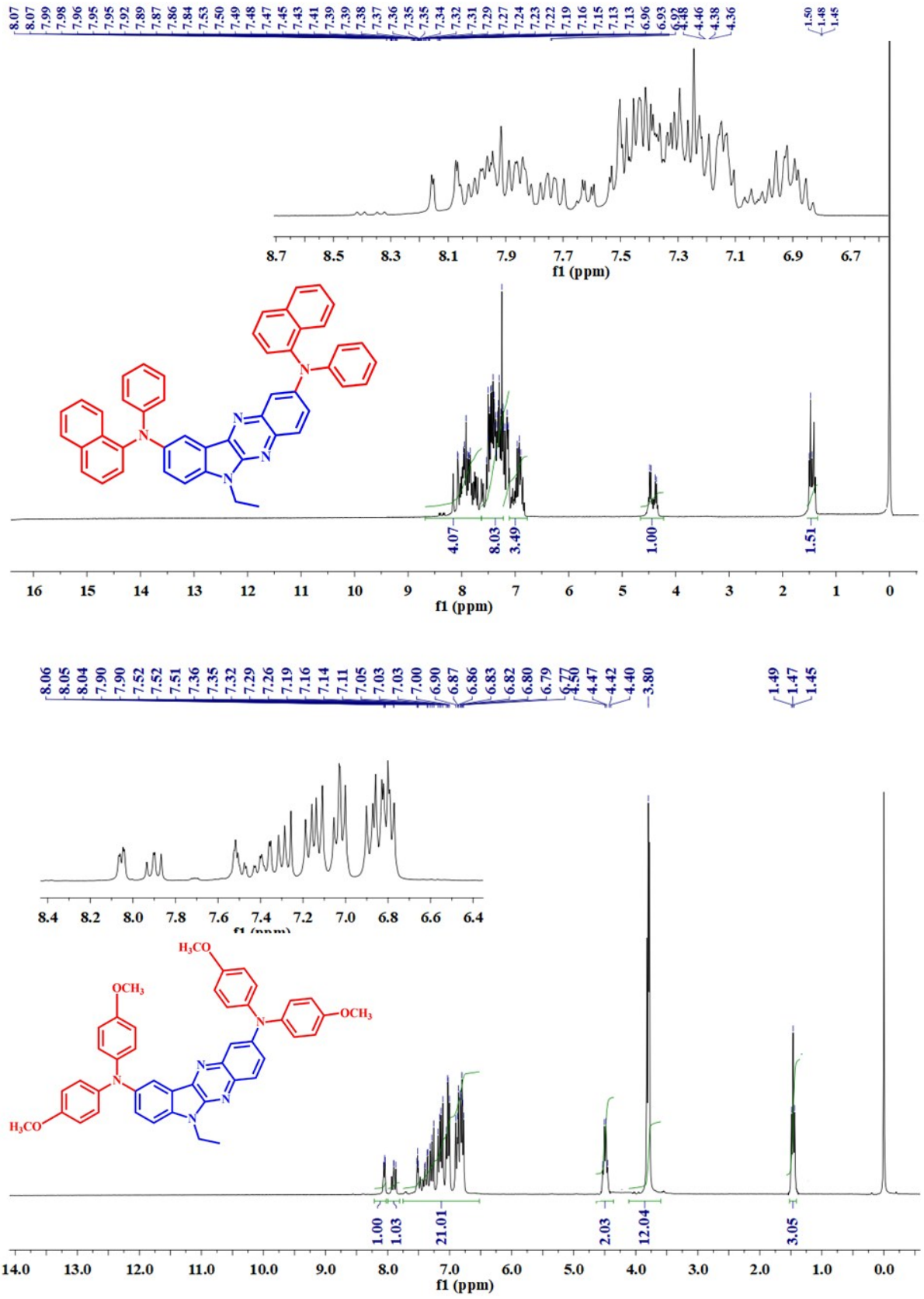


Fig. S26. ^{1}H NMR spectrum of compound **3** (**above**) and **4** (**below**).

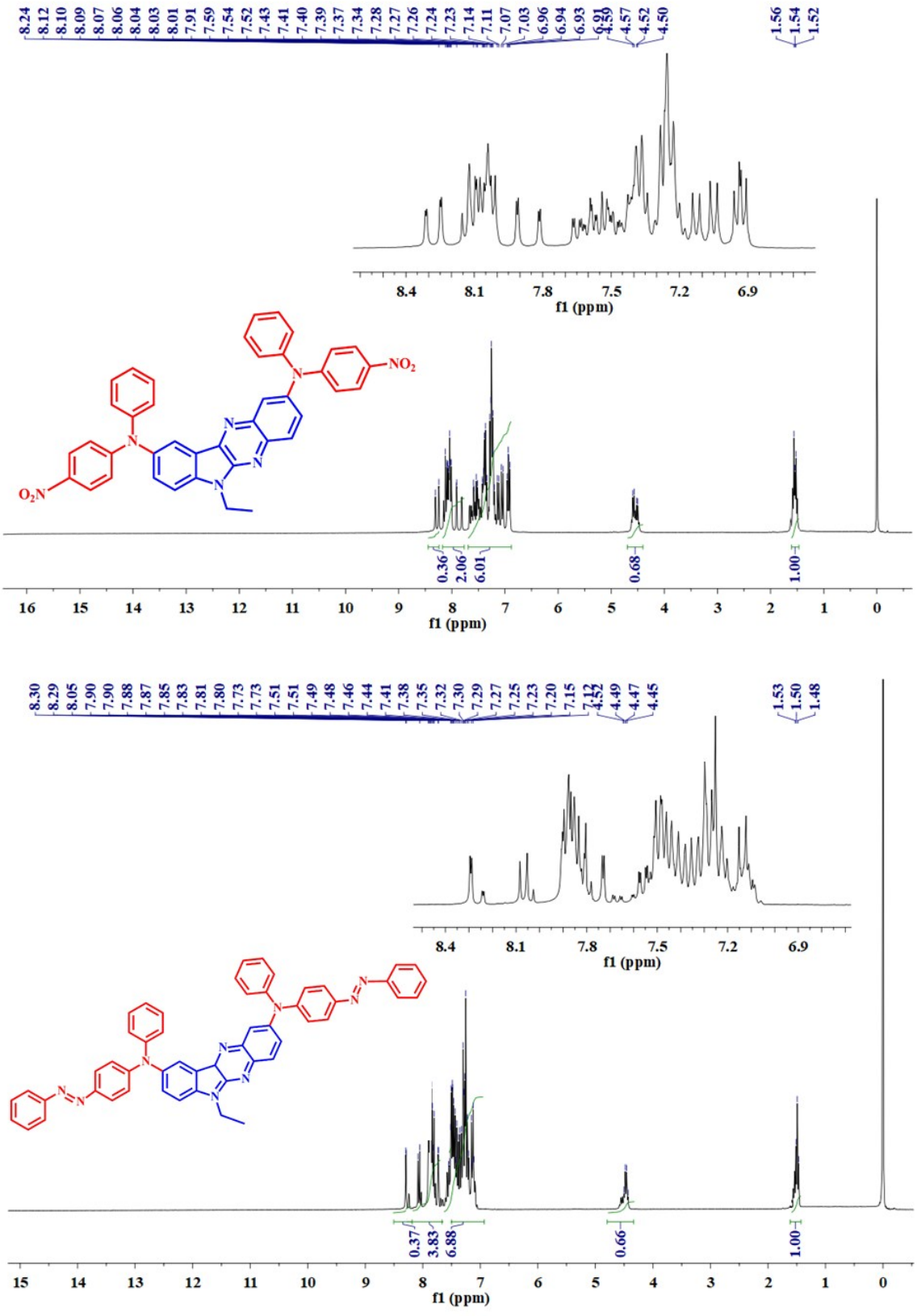
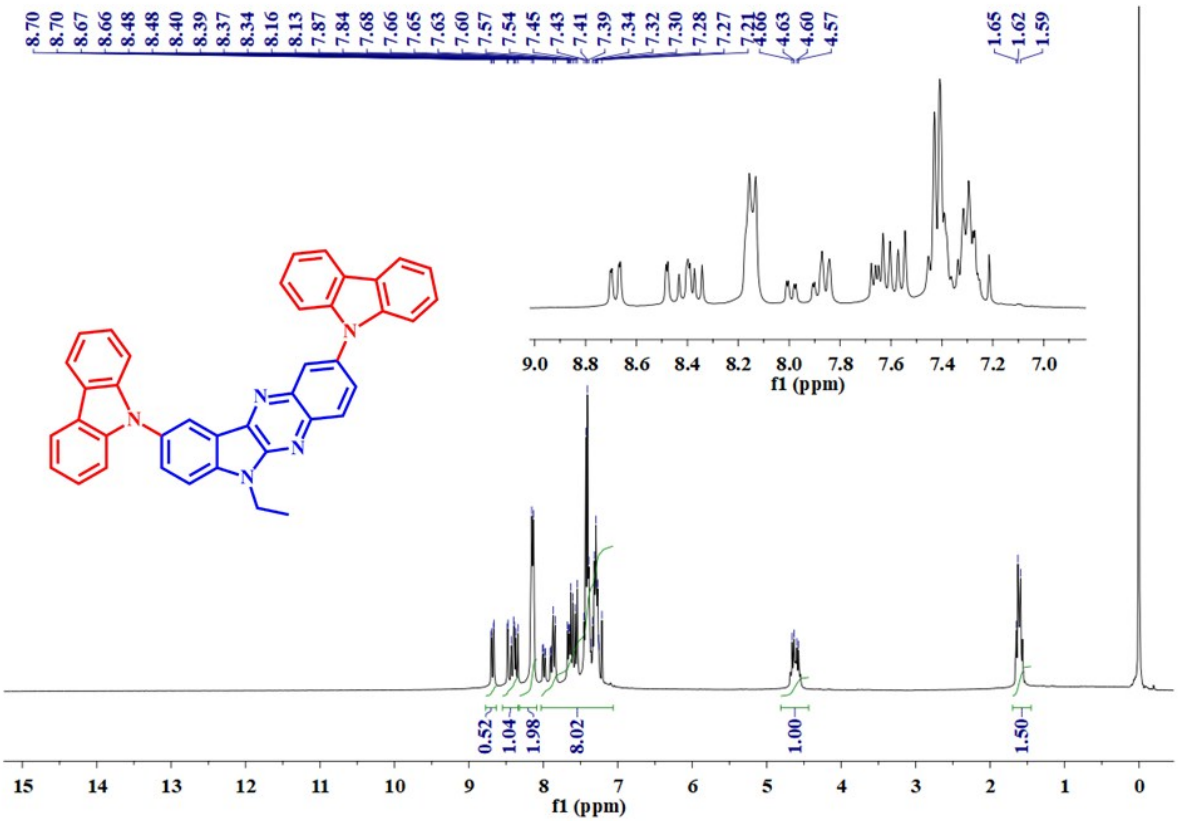


Fig. S27. ^{1}H NMR spectrum of compound **5** (**above**) and **6** (**below**).



^{1}H NMR spectrum of compound **7**.

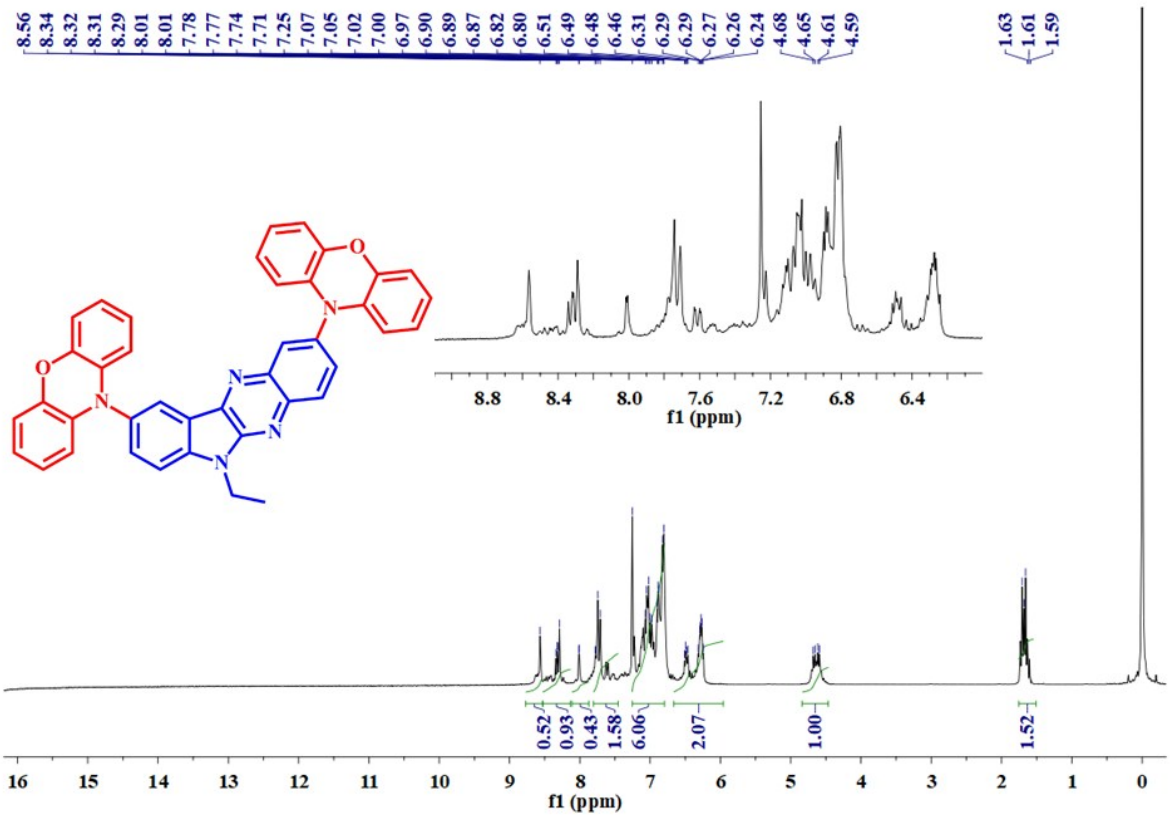


Fig. S28. ^{1}H NMR spectrum of compound **7** (**above**) and **8** (**below**).

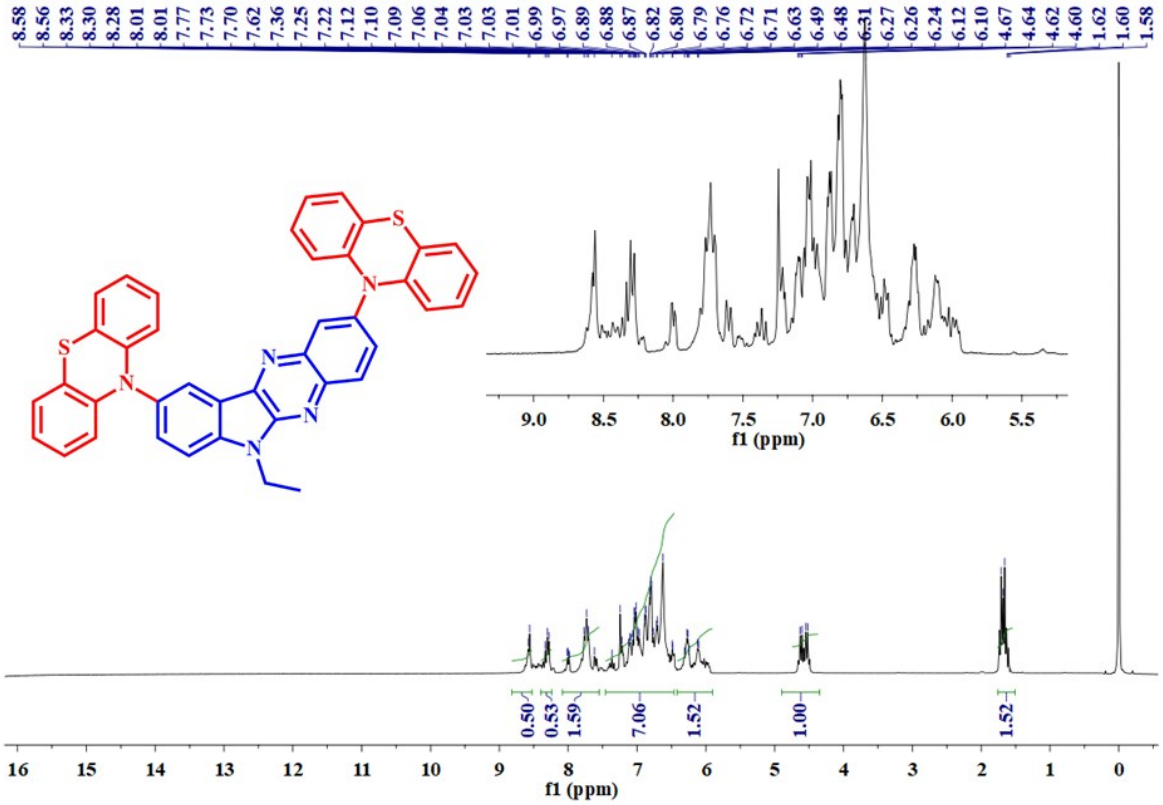


Fig. S29. ^{1}H NMR spectrum of compound **9**.

11. ^{13}C NMR and DEPT-135 spectra of compounds 1 – 9

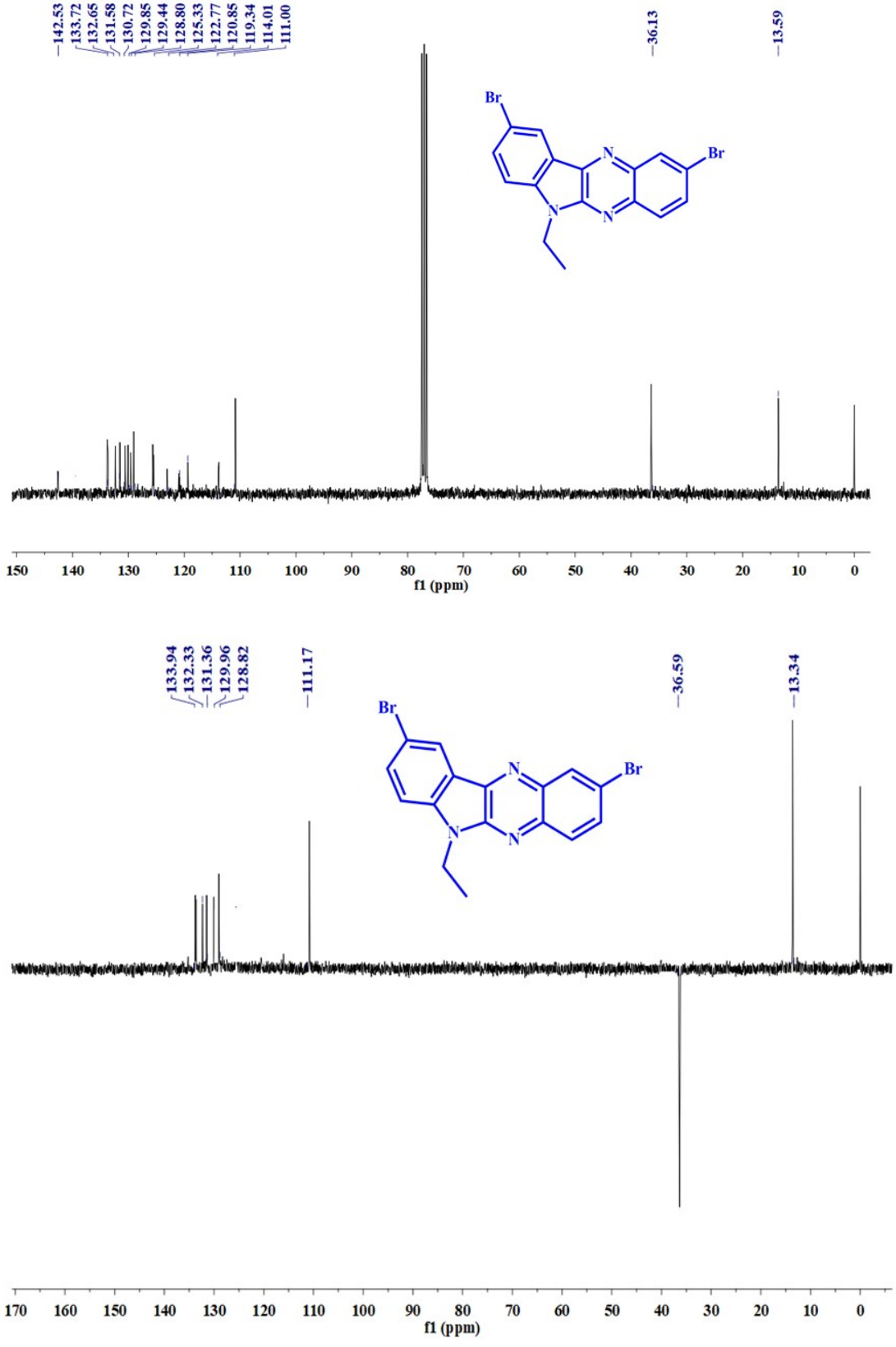


Fig. S30. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **1**.

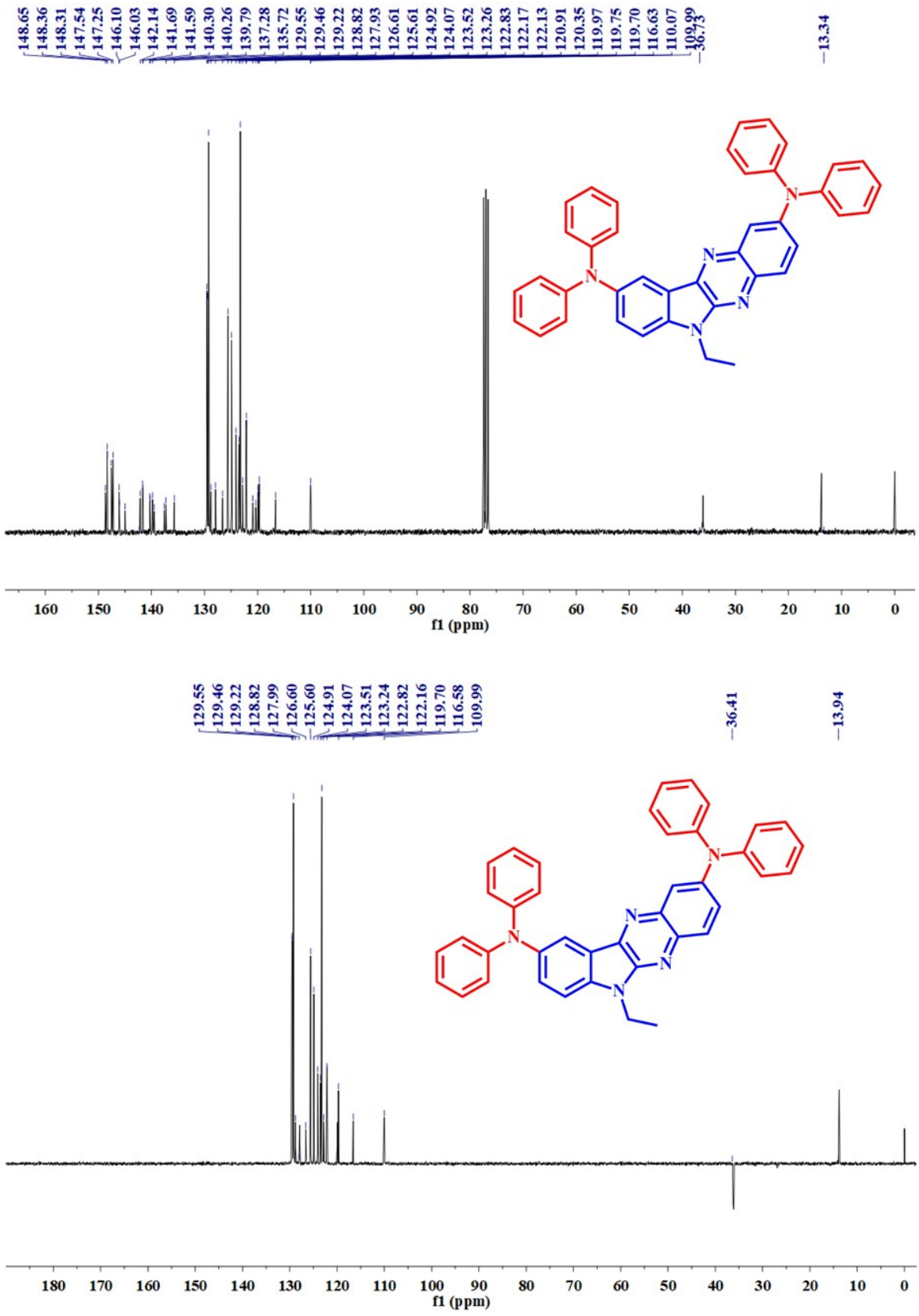


Fig. S31. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **2**.

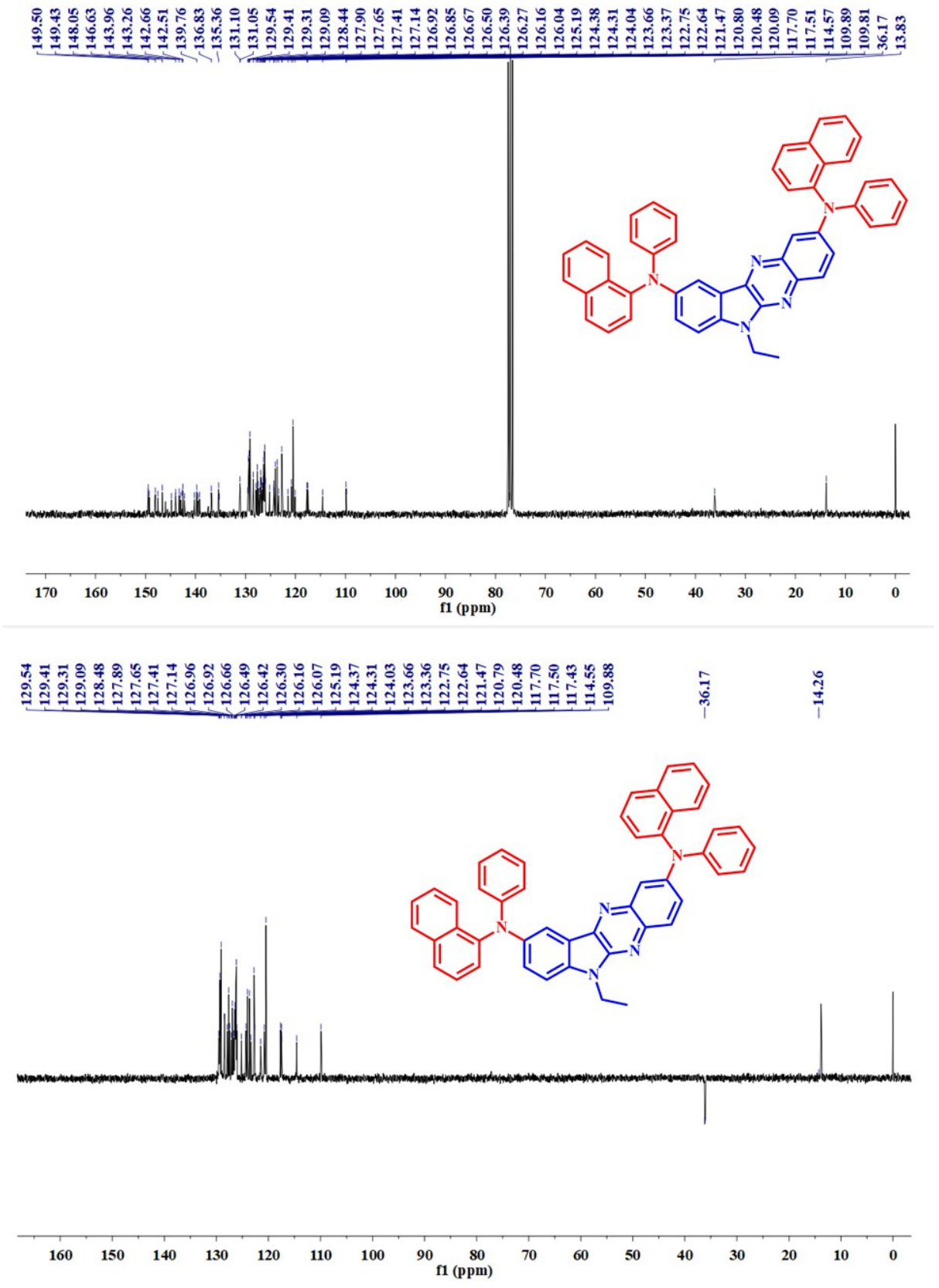


Fig. S32. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **3**.

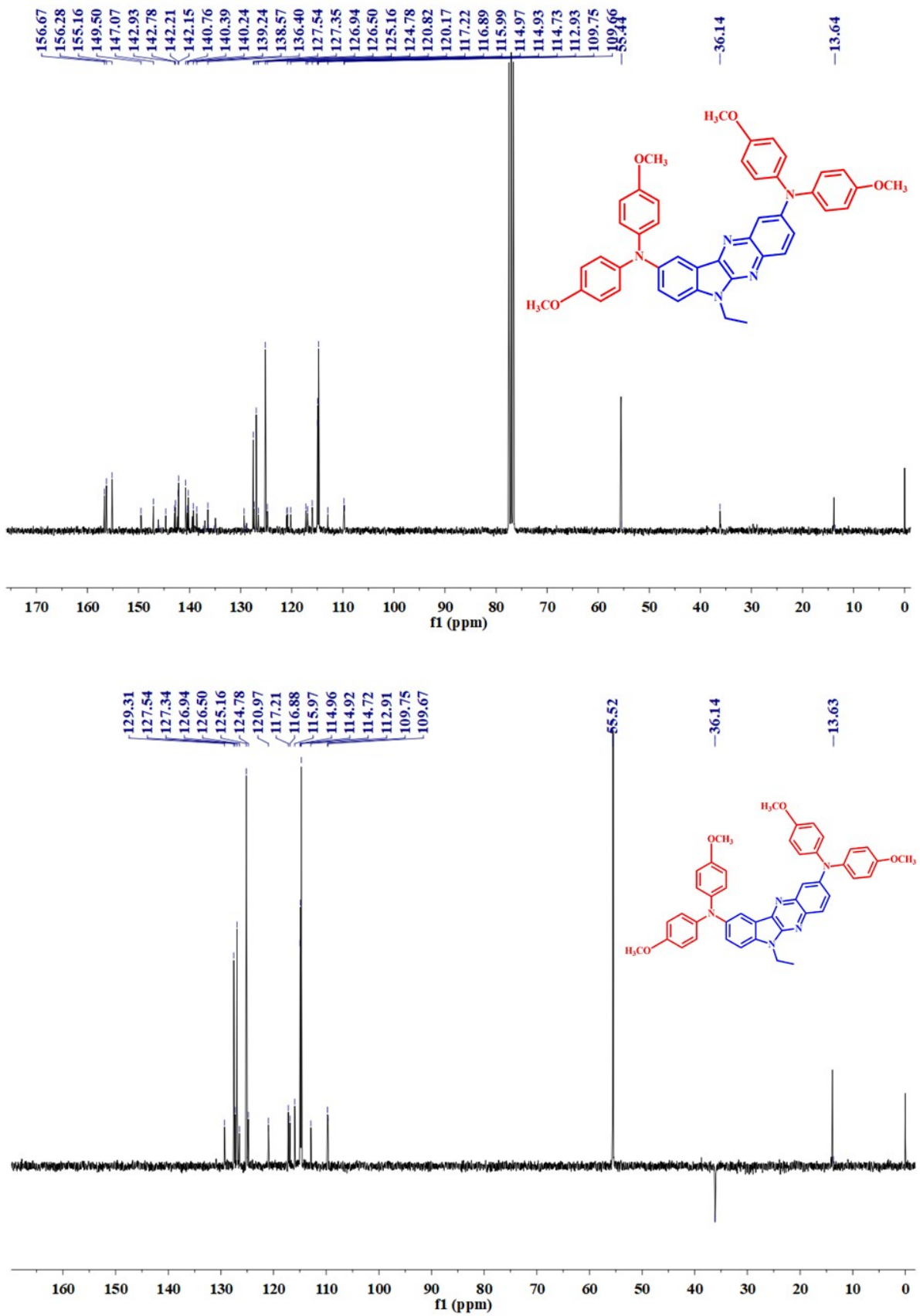


Fig. S33. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **4**.

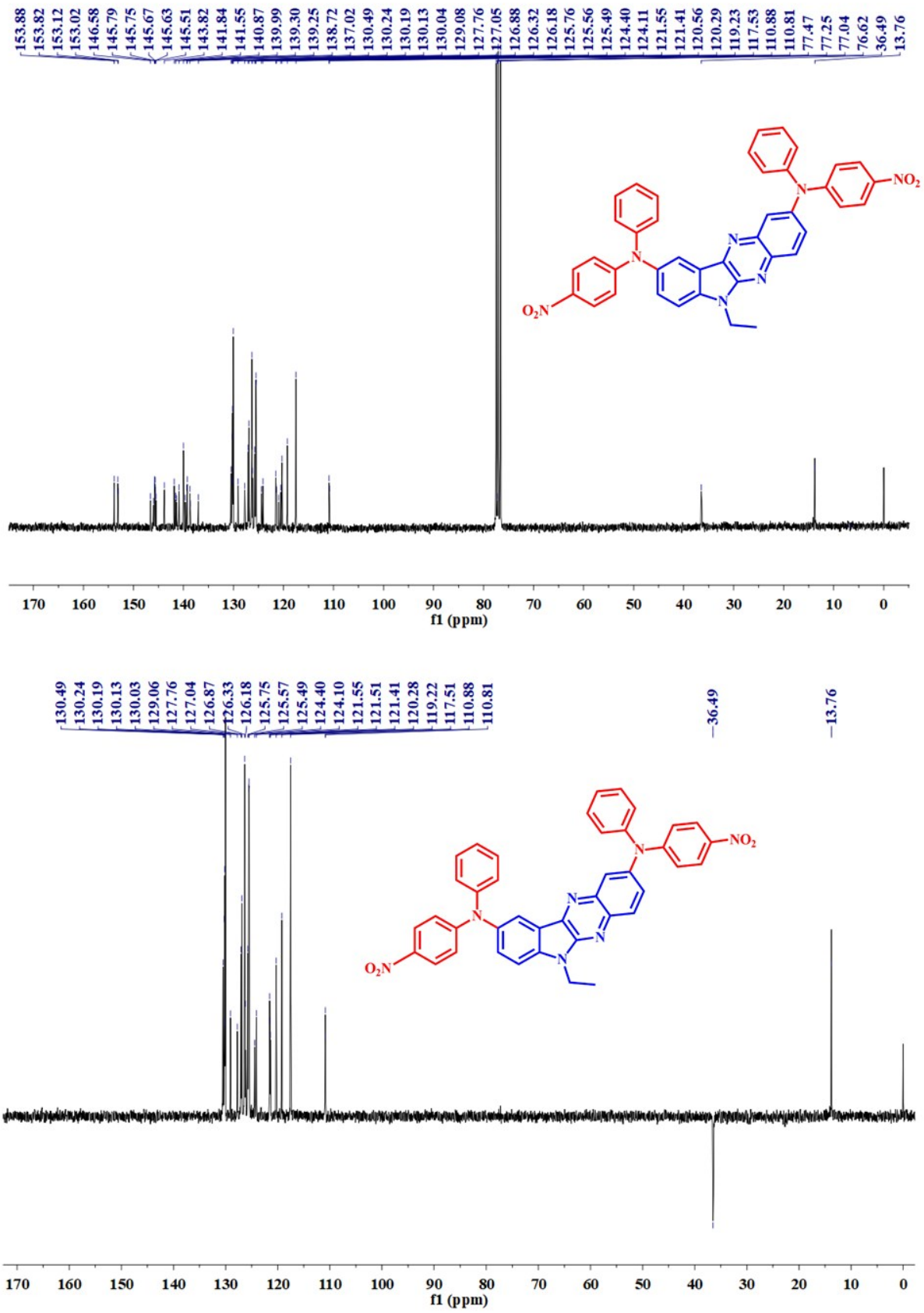
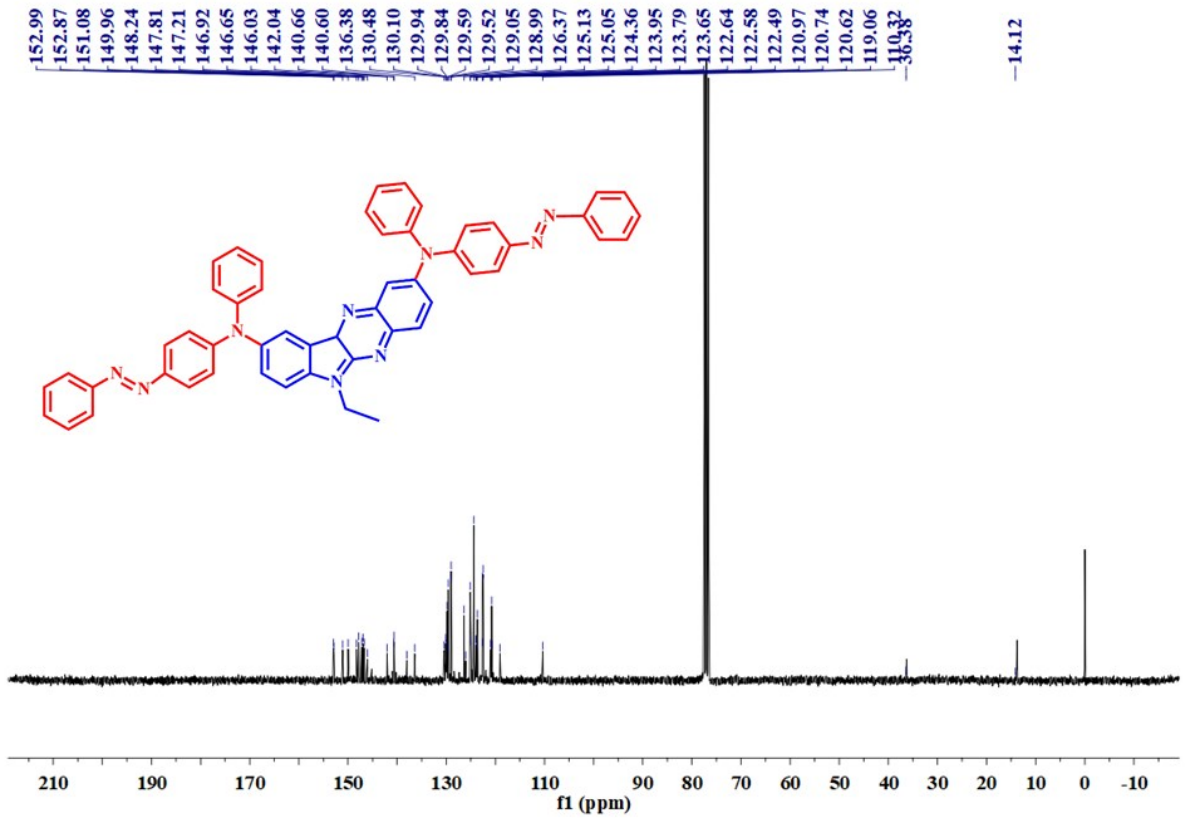


Fig. S34. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **5**.



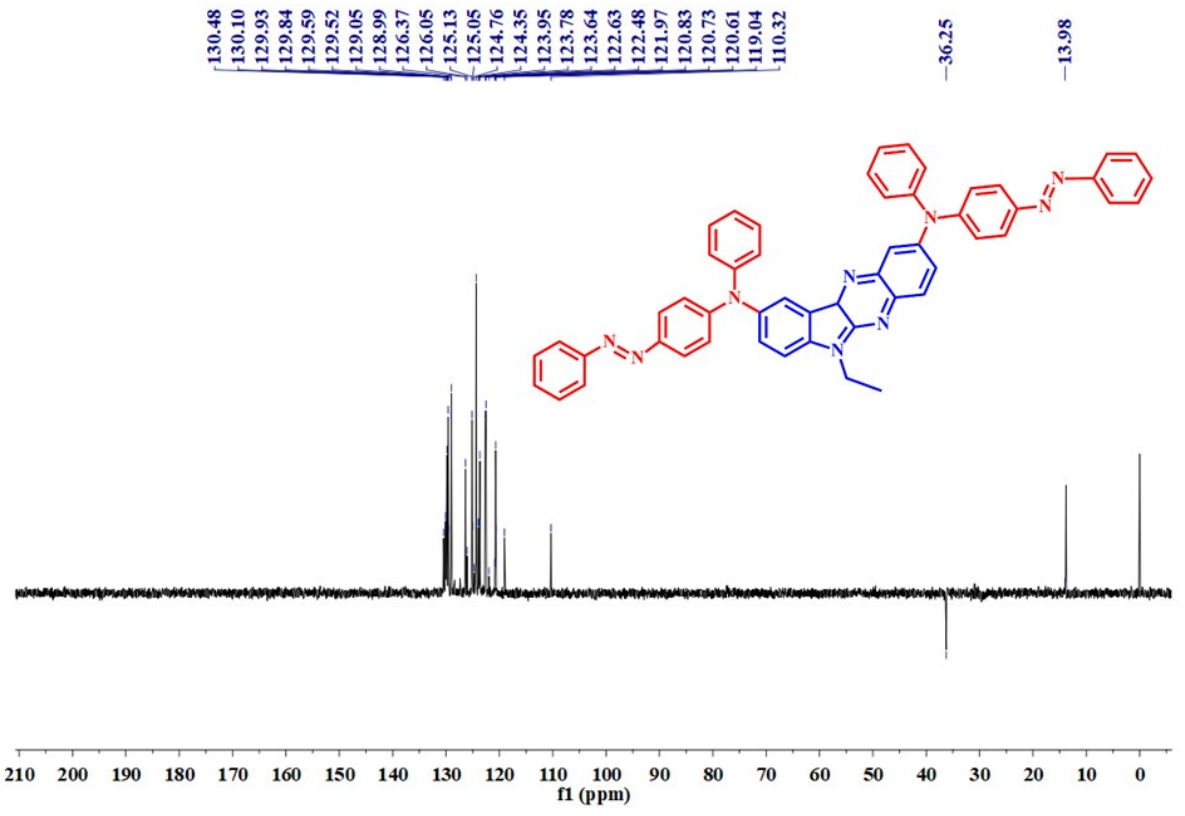


Fig. S35. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **6**.

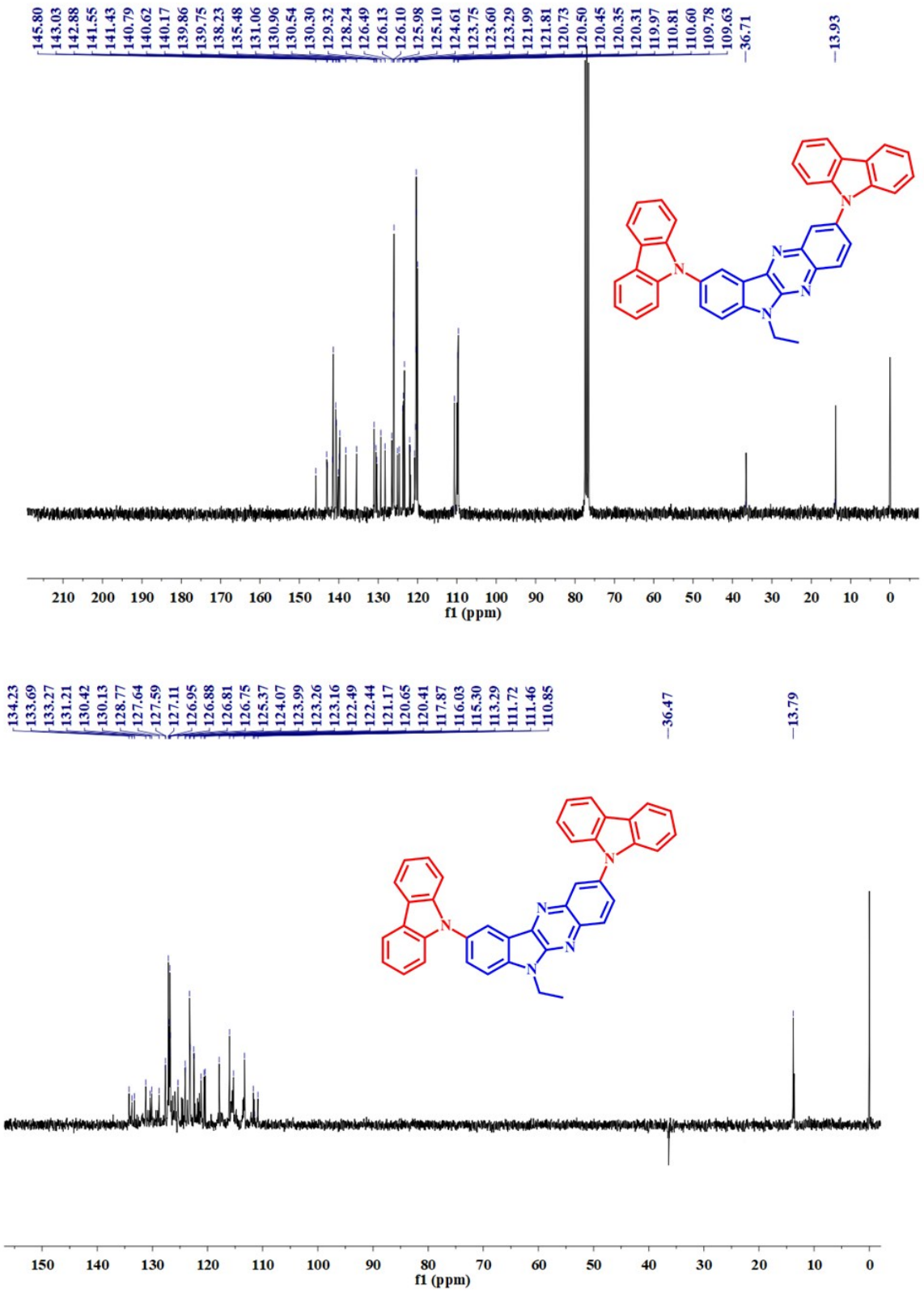


Fig. S36. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **7**.

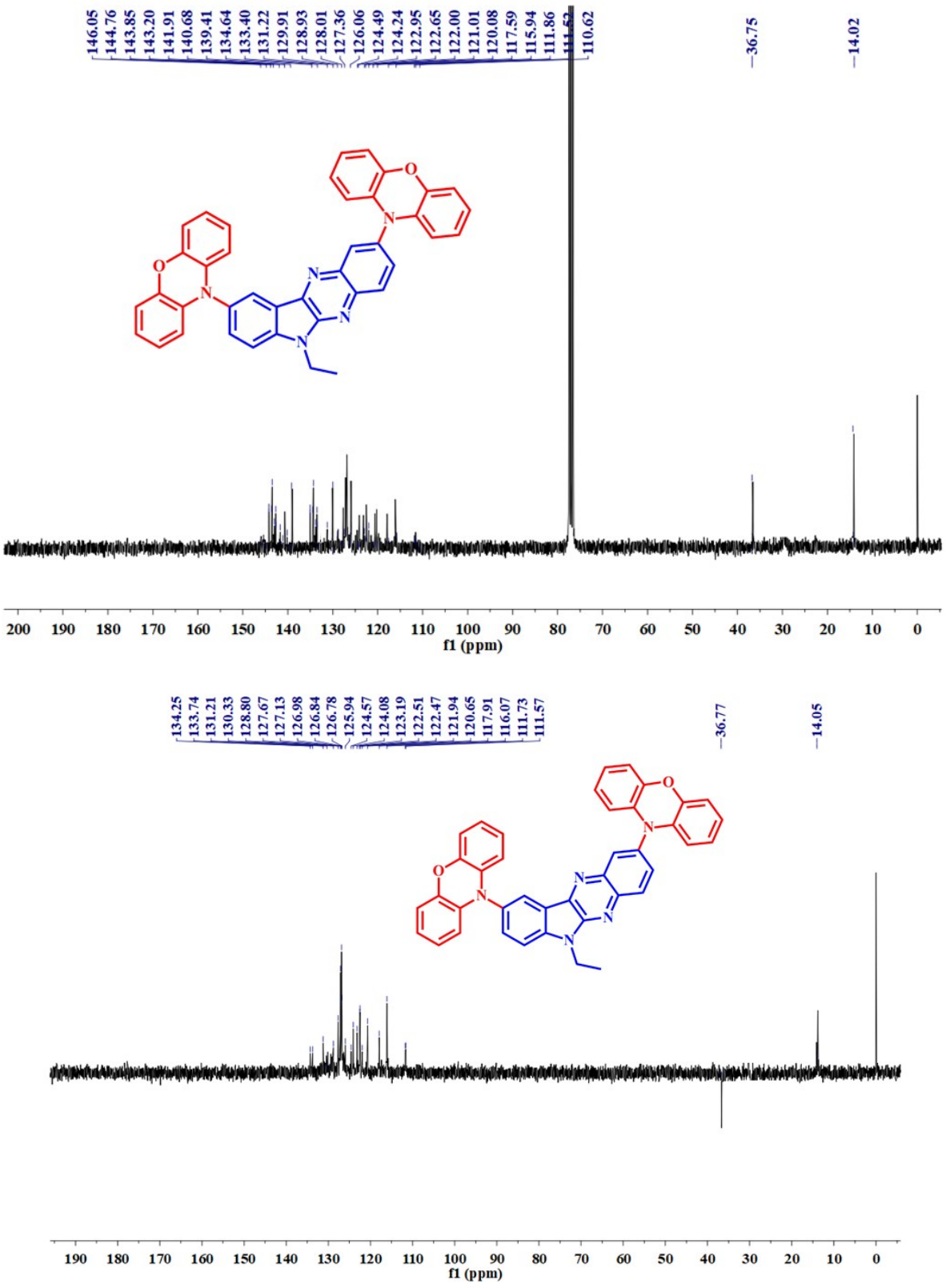


Fig. S37. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **8**.

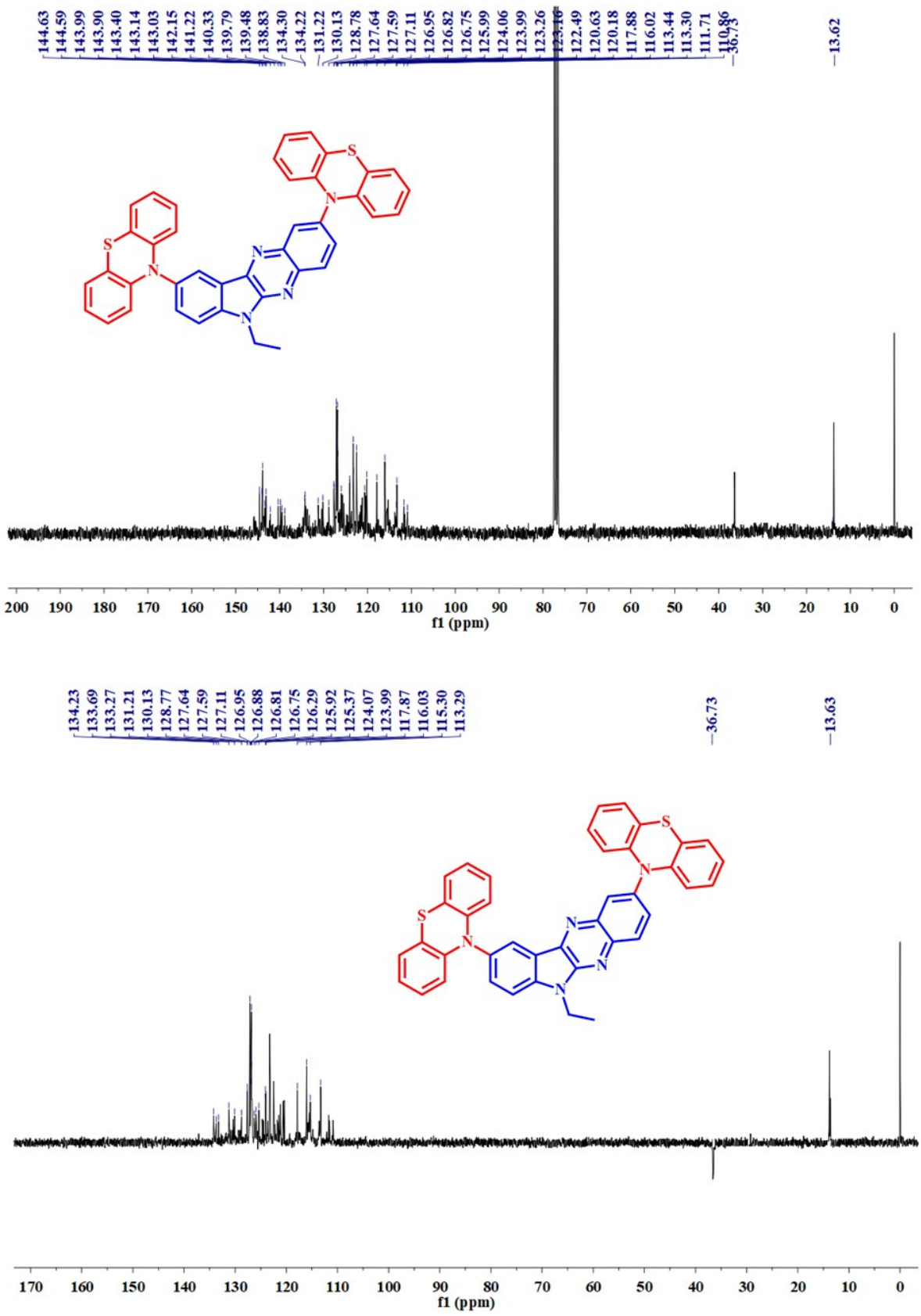


Fig. S38. ^{13}C (**above**) and DEPT-135 (**below**) NMR spectrum of compound **9**.

12. Optimized structures of compounds 1 9

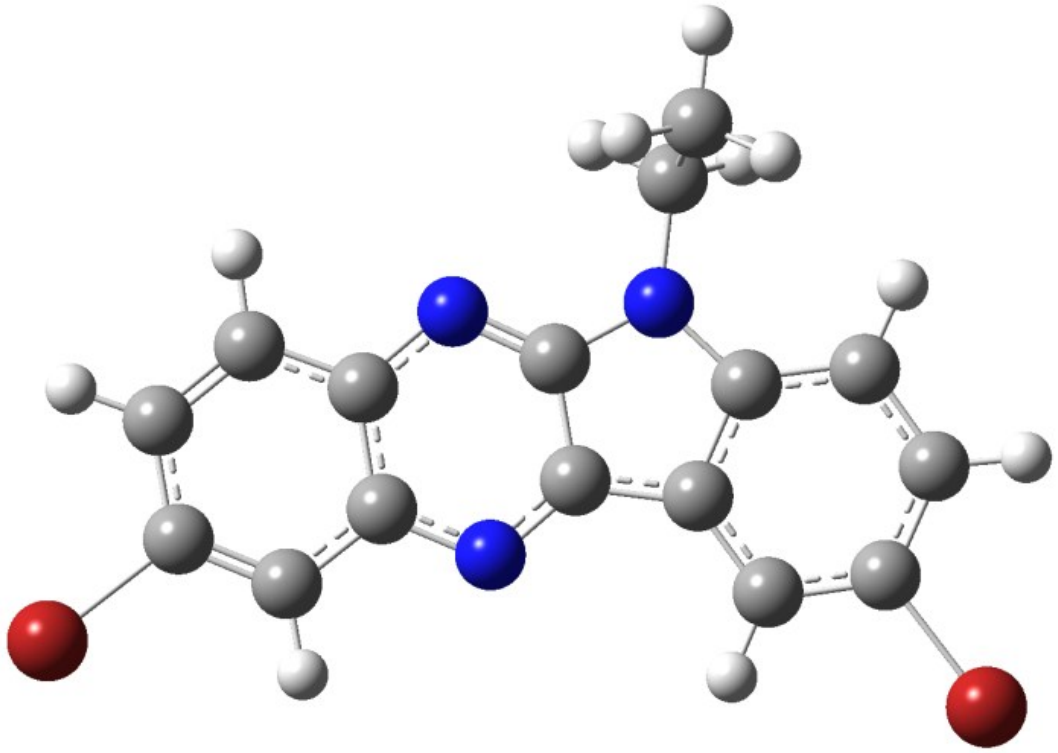


Fig. S39. Optimized structure of **1**.

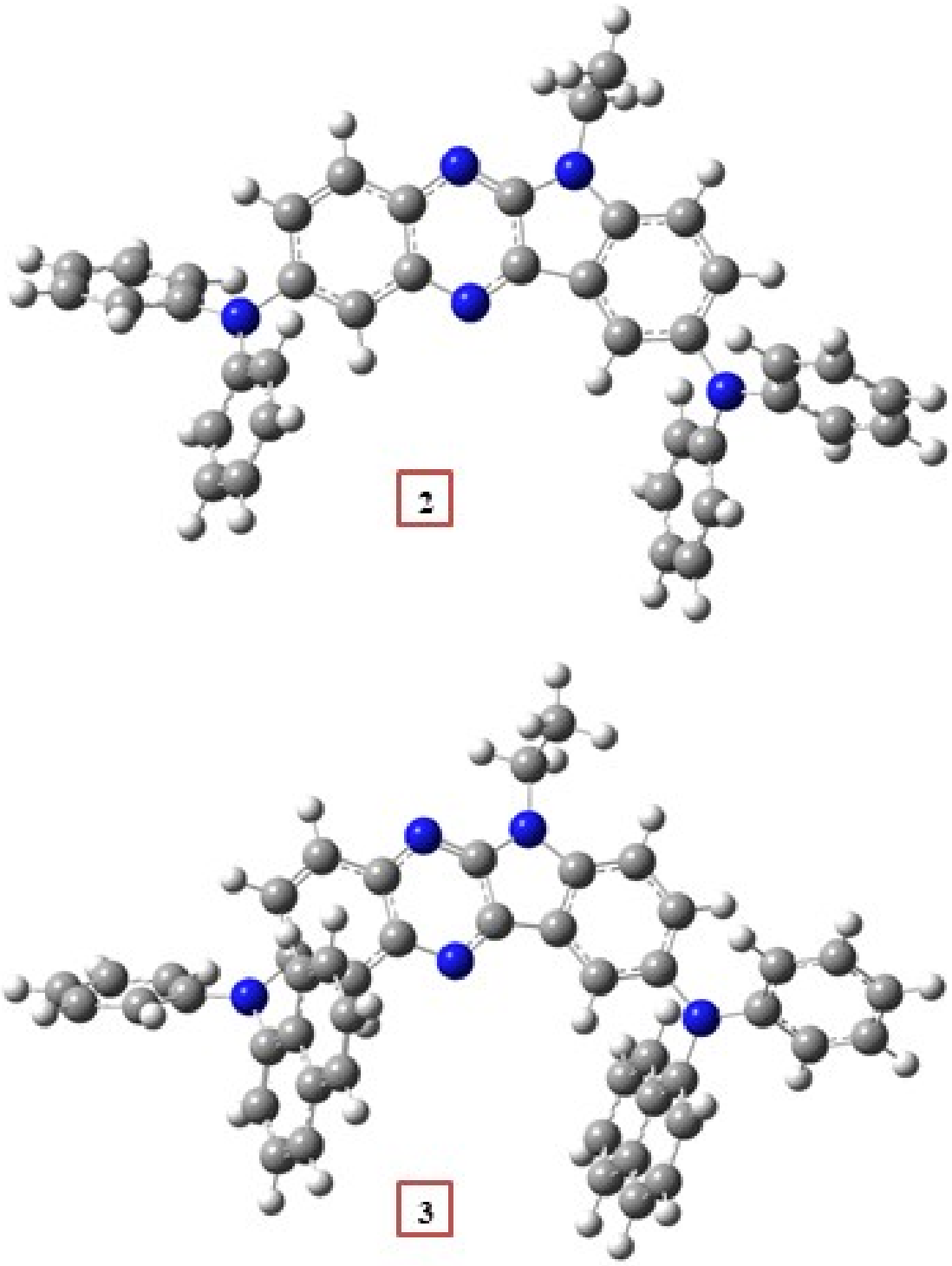


Fig. S40. Optimized structure of **2** and **3.**

Fig. S41. Optimized structure of **4** and **5**.

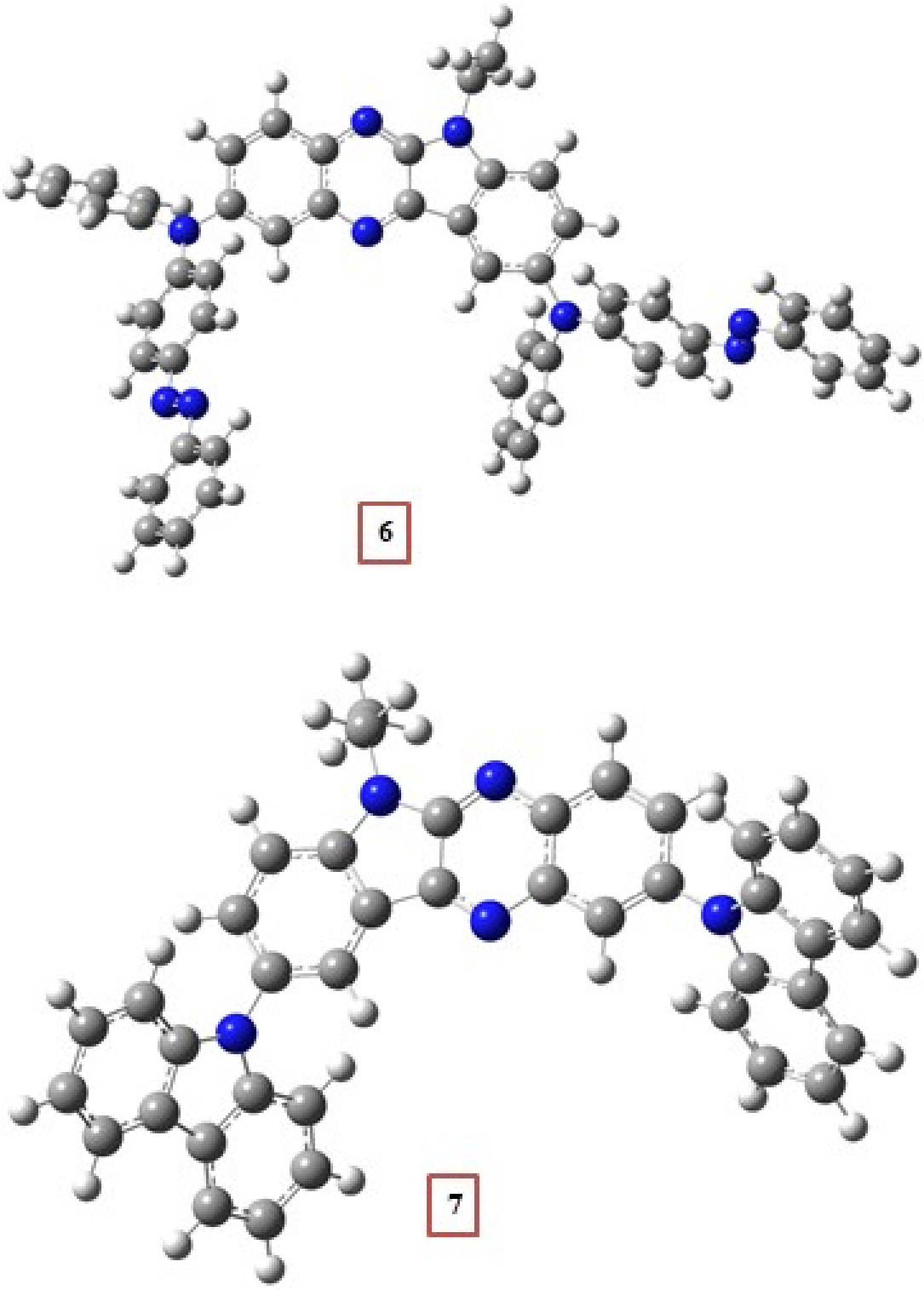


Fig. S42. Optimized structure of **6** and **7**.

Fig. S43. Optimized structure of **8** and **9**.

13. Frontier molecular orbital of compounds 1 9

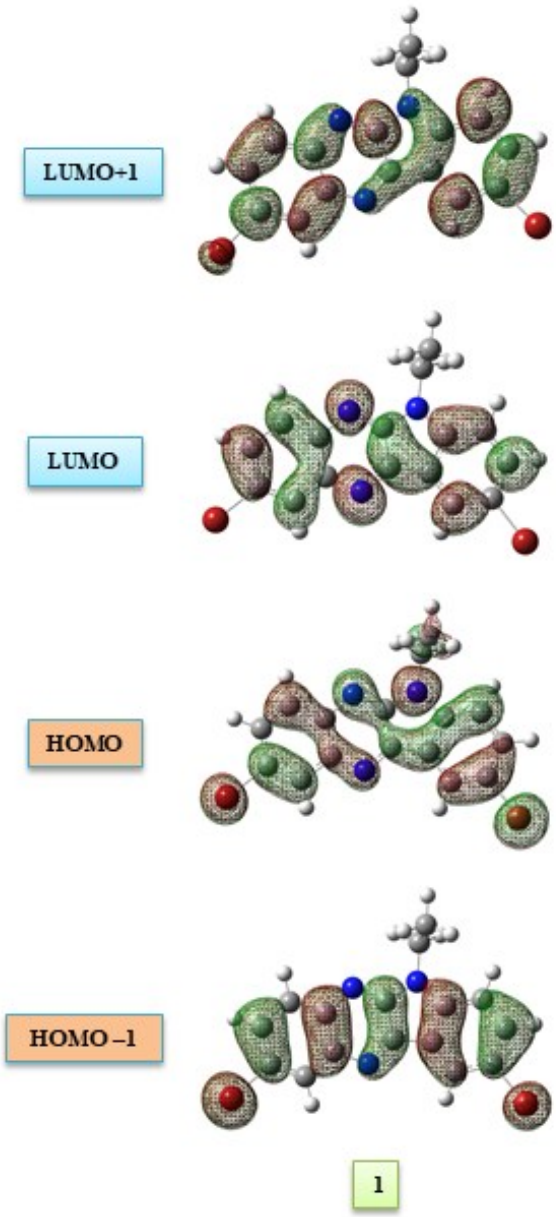


Fig. S44. Frontier molecular orbitals of compound **1**.

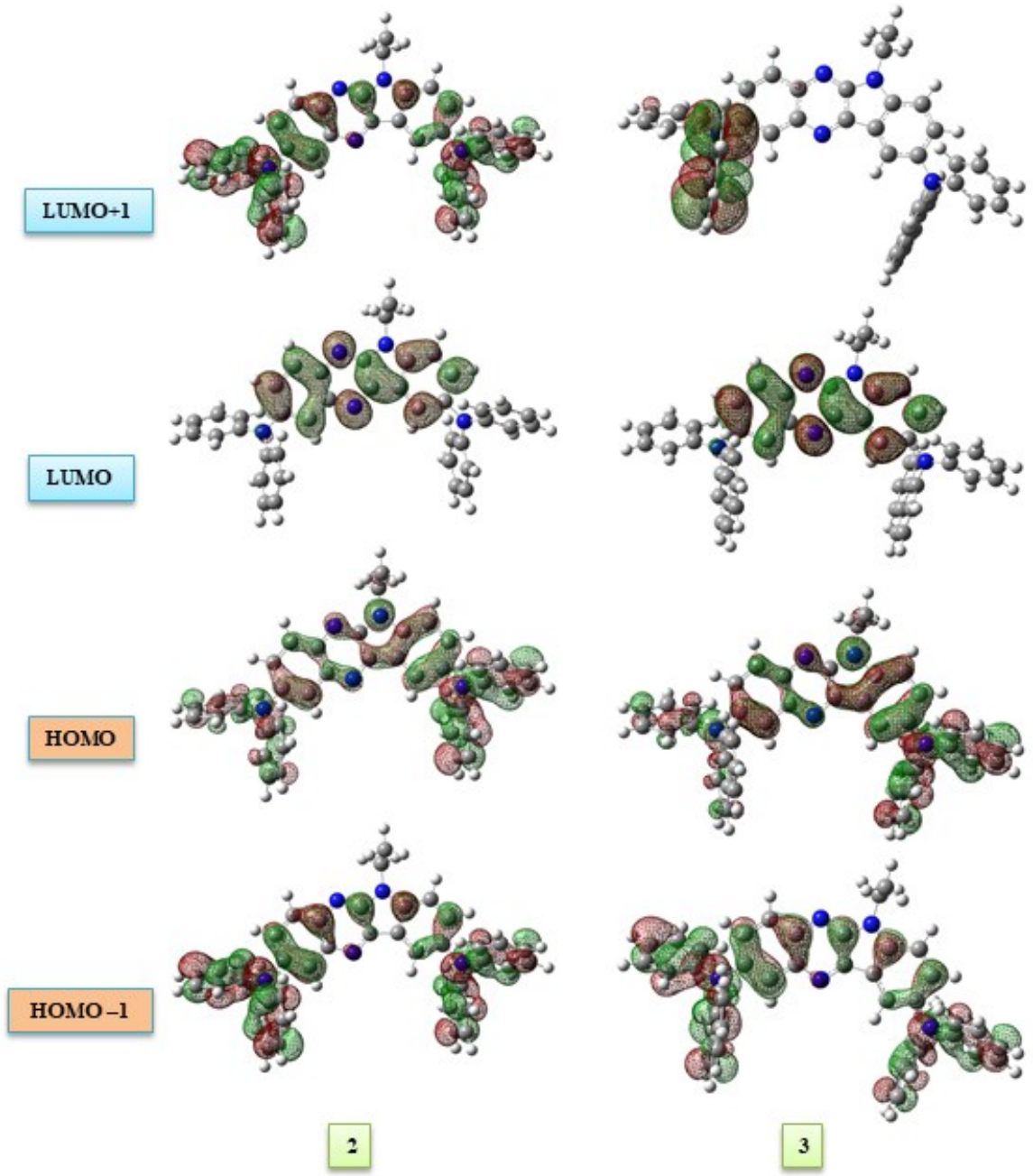


Fig. S45. Frontier molecular orbitals of compound **2** and **3**.

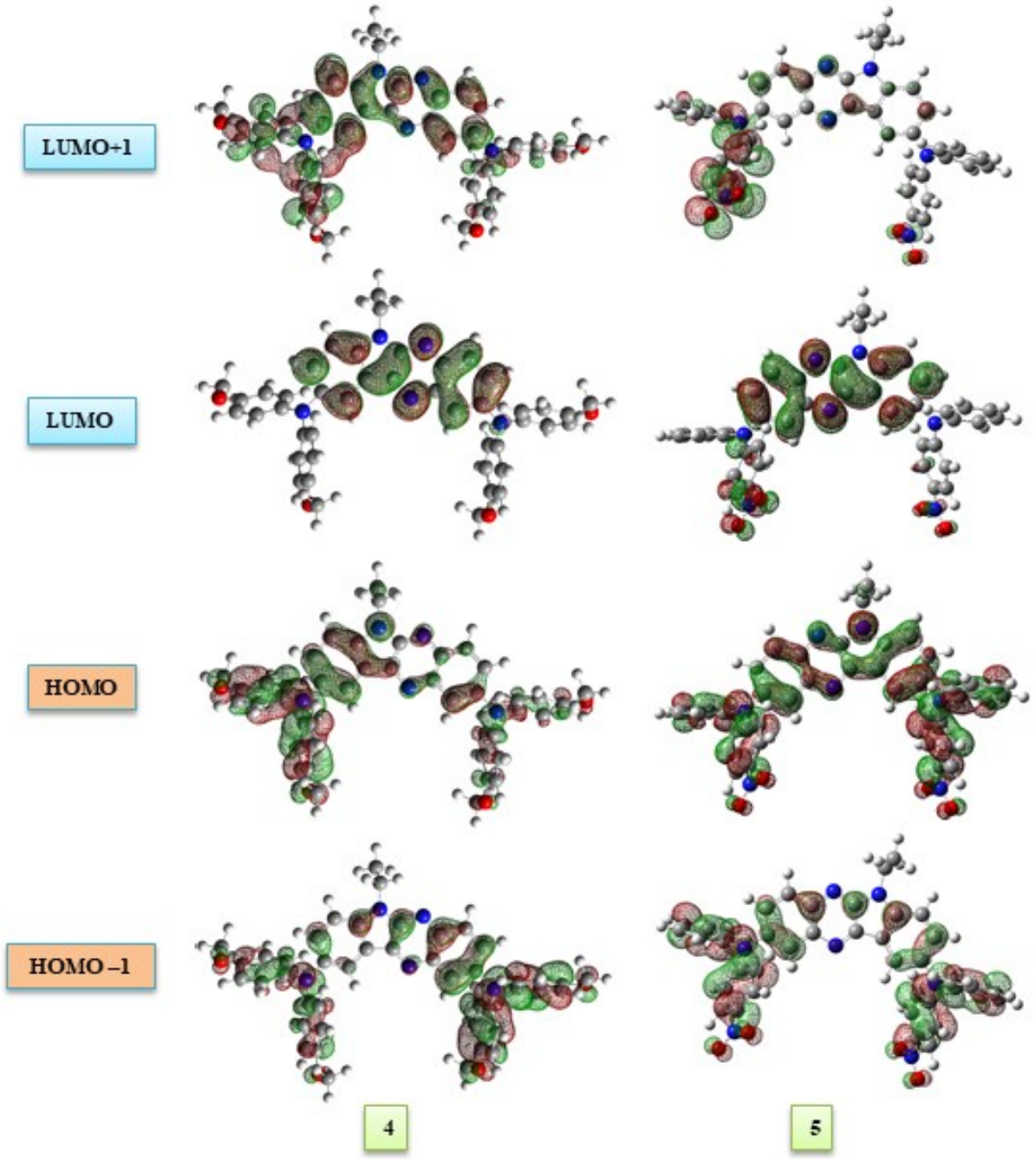


Fig. S46. Frontier molecular orbitals of compound **4** and **5**.

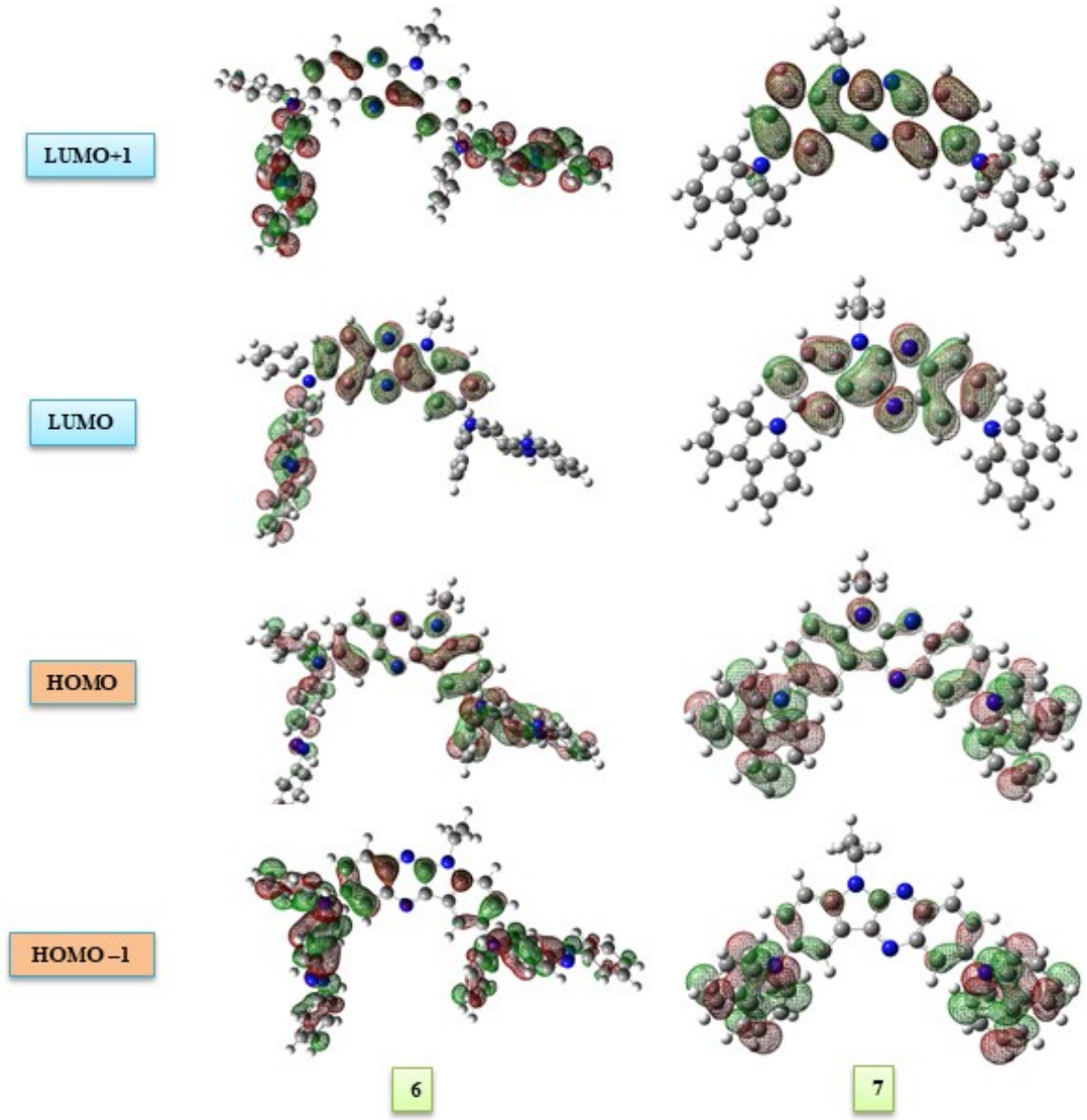


Fig. S47. Frontier molecular orbitals of compound **6** and **7**.

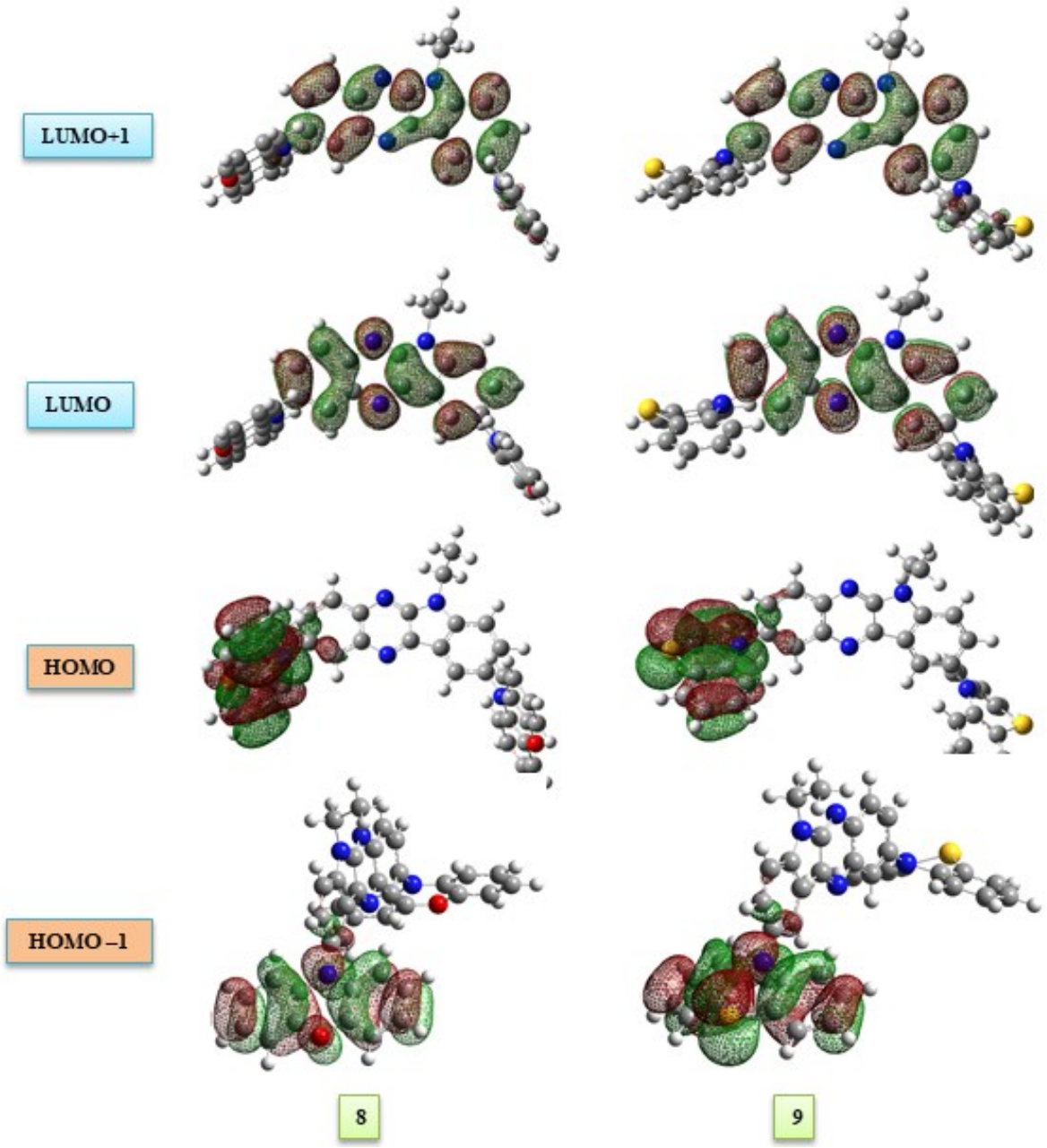


Fig. S48. Frontier molecular orbitals of compound **8** and **9**.

14. Cartesian coordinates and Mulliken Charges of compounds 1 9

Table S10. Cartesian coordinates of optimized structure of molecule **1**.

Total energy: –5929.09 Hartrees

	x	y	z	Mulliken charges
C	3.97012	-0.84594	-0.03373	-0.213892
C	4.5395	0.43029	-0.13693	-0.019008
C	3.7276	1.56684	-0.21209	-0.068338
C	2.34241	1.38548	-0.18273	0.267383
C	1.77382	0.08215	-0.07835	-0.137359
C	2.59501	-1.04591	-0.00304	0.070033
N	1.3168	2.34543	-0.25368	-0.53459
C	0.09944	1.68862	-0.18852	0.44192
C	0.3377	0.2632	-0.08098	0.094646
N	-1.09839	2.24227	-0.22233	-0.37259
C	-2.14903	1.34892	-0.14967	0.098463
C	-1.92782	-0.07051	-0.04197	0.092924
N	-0.65645	-0.60826	-0.00834	-0.341073
C	1.47734	3.79982	-0.33472	-0.103691
C	-3.47957	1.83764	-0.18038	-0.069404
C	-4.54877	0.96722	-0.10851	-0.021705
C	-4.31046	-0.42278	-0.00284	-0.200286
C	-3.04108	-0.9466	0.03132	0.003251
C	1.76281	4.45028	1.02655	-0.286243
Br	5.15327	-2.38924	0.07027	-0.041055
Br	-5.84424	-1.61446	0.09546	-0.033313
H	5.61752	0.53382	-0.15717	0.127467
H	4.17285	2.55177	-0.28896	0.124473
H	2.17005	-2.03859	0.07536	0.119729
H	2.28149	4.01534	-1.04771	0.134948
H	0.54572	4.18938	-0.75375	0.142842
H	-3.62491	2.90855	-0.26199	0.115469
H	-5.56721	1.33466	-0.13199	0.127247
H	-2.85505	-2.00965	0.11213	0.12309
H	1.88088	5.53335	0.90867	0.120111
H	0.93497	4.2691	1.7191	0.122888
H	2.67953	4.05342	1.47568	0.115663

Table S11. Cartesian coordinates of optimized structure of molecule **2**.

Total energy: –1817.14 Hartrees

	x	y	z	Mulliken charges
C	-0.84281	0.97381	0.01103	0.09092
C	-0.35303	2.29759	-0.08868	-0.076044
C	-1.20605	3.4033	-0.06987	-0.06713
C	-2.58057	3.17136	0.02473	0.260445
C	-3.08928	1.84279	0.11028	-0.124108
C	-2.2238	0.74799	0.116	-0.009199
N	-3.64643	4.0904	0.0431	-0.536332
C	-4.83173	3.37937	0.15128	0.43058
C	-4.53087	1.96424	0.19352	0.089054
N	-6.05213	3.88269	0.20297	-0.376341
C	-7.05819	2.94363	0.29893	0.093896
C	-6.779	1.53103	0.3465	0.096492
N	-5.48412	1.04842	0.29141	-0.347372
C	-3.55114	5.55016	0.00172	-0.100868
N	0.07571	-0.12585	-0.00109	-0.506861
C	-8.41017	3.36744	0.35894	-0.071383
C	-9.4328	2.45063	0.46042	-0.087595
C	-9.16301	1.04586	0.49208	0.139332
C	-7.84703	0.60698	0.43113	-0.093339
N	-10.24563	0.12786	0.60698	-0.502699
C	-0.18167	-1.25308	-0.83955	0.125196
C	1.22939	-0.09002	0.83815	0.129779
C	-11.46226	0.3592	-0.10654	0.113042
C	2.46715	-0.58112	0.37861	-0.096818
C	3.59247	-0.53923	1.20497	-0.103694
C	3.51244	0.00573	2.49266	-0.108814
C	2.28552	0.50255	2.94888	-0.10419
C	1.15035	0.45064	2.13611	-0.102697
C	0.07081	-2.56021	-0.38082	-0.095724
C	-0.18181	-3.65764	-1.20731	-0.103324
C	-0.70499	-3.47638	-2.49352	-0.107647
C	-0.96684	-2.17824	-2.94813	-0.102459
C	-0.70178	-1.07336	-2.13552	-0.096234
C	-12.70348	0.08551	0.49894	-0.08959
C	-13.89163	0.30767	-0.20064	-0.102674
C	-13.8657	0.81991	-1.50408	-0.106252
C	-12.63295	1.09827	-2.1062	-0.101861
C	-11.438	0.86234	-1.42095	-0.096159
C	-10.09805	-1.06525	1.38622	0.099306
C	-10.52909	-2.30396	0.87888	-0.086564
C	-10.39843	-3.46292	1.64901	-0.102158
C	-9.82311	-3.40736	2.92398	-0.104356
C	-9.38558	-2.17558	3.42714	-0.100928

C	-9.52772	-1.00978	2.67101	-0.077212
C	-3.22782	6.17242	1.36811	-0.286932
H	0.7166	2.45001	-0.17732	0.118554
H	-0.80167	4.4067	-0.14018	0.1153
H	-2.6149	-0.25941	0.19508	0.10836
H	-2.79164	5.82359	-0.74016	0.131058
H	-4.51757	5.91235	-0.35977	0.13928
H	-8.60739	4.43329	0.33807	0.10498
H	-10.46064	2.78741	0.52447	0.125102
H	-7.59968	-0.44697	0.44963	0.113424
H	2.54015	-0.99058	-0.62247	0.117237
H	4.53859	-0.92184	0.83443	0.106045
H	4.39045	0.04199	3.12902	0.102805
H	2.2058	0.9209	3.94762	0.105688
H	0.19989	0.82283	2.50118	0.116469
H	0.46023	-2.70855	0.61986	0.116741
H	0.01707	-4.65879	-0.83735	0.105943
H	-0.90744	-4.3319	-3.12931	0.102886
H	-1.36902	-2.02159	-3.94429	0.105879
H	-0.89552	-0.07033	-2.49821	0.114232
H	-12.72869	-0.29733	1.51283	0.116855
H	-14.84084	0.09222	0.28009	0.10728
H	-14.79112	0.99785	-2.04173	0.104474
H	-12.5977	1.48684	-3.11927	0.107611
H	-10.48565	1.06153	-1.89922	0.119178
H	-10.96192	-2.3519	-0.11399	0.115531
H	-10.73471	-4.41249	1.24451	0.107452
H	-9.71601	-4.30989	3.51655	0.104923
H	-8.9428	-2.11864	4.41658	0.107767
H	-9.19827	-0.05607	3.06752	0.114856
H	-3.15952	7.26285	1.28029	0.116498
H	-4.01386	5.93482	2.09175	0.120975
H	-2.27536	5.80028	1.76082	0.114134

Table S12. Cartesian coordinates of optimized structure of molecule **3**.

Total energy: –2124.49 Hartrees

	x	y	z	Mulliken charges
C	0.49918	0.89198	0	0.122904
C	0.99749	2.21623	-0.08188	-0.08597
C	0.14883	3.31831	-0.19701	-0.06651
C	-1.22802	3.08692	-0.25801	0.261246
C	-1.74233	1.76087	-0.19687	-0.133885

C	-0.88454	0.66759	-0.05746	-0.022382
N	-2.28797	4.00428	-0.39171	-0.536231
C	-3.47716	3.29235	-0.40748	0.430111
C	-3.18326	1.87977	-0.29083	0.088859
N	-4.69542	3.79227	-0.51629	-0.377029
C	-5.70468	2.85239	-0.51573	0.092655
C	-5.43375	1.44304	-0.3956	0.091762
N	-4.14202	0.9637	-0.28199	-0.34795
C	-2.18723	5.46244	-0.45432	-0.100719
N	1.41264	-0.20386	0.10417	-0.509004
C	-7.0546	3.27336	-0.62956	-0.068632
C	-8.08238	2.35736	-0.62687	-0.092378
C	-7.81826	0.95369	-0.52455	0.146972
C	-6.50528	0.51812	-0.41024	-0.098157
N	-8.906	0.03724	-0.48798	-0.505009
C	1.07159	-1.46457	-0.49892	0.041141
C	2.53204	-0.14467	0.98796	0.140814
C	-10.05967	0.22359	-1.31025	0.133015
C	3.71852	-0.82987	0.65991	-0.095999
C	4.81627	-0.79298	1.5218	-0.106278
C	4.76068	-0.06469	2.71707	-0.109001
C	3.58478	0.62083	3.04375	-0.106322
C	2.47491	0.57821	2.19544	-0.110388
C	0.97635	-1.58424	-1.92762	-0.032815
C	0.61003	-2.85987	-2.48467	-0.061742
C	0.38358	-3.96645	-1.61833	-0.052241
C	0.51282	-3.82532	-0.25213	-0.101504
C	0.84875	-2.56998	0.30774	-0.036941
C	-11.32403	-0.18013	-0.84011	-0.092432
C	-12.45707	-0.02016	-1.64011	-0.105696
C	-12.35489	0.55532	-2.91321	-0.106451
C	-11.09959	0.95961	-3.38201	-0.104632
C	-9.95656	0.78822	-2.59582	-0.104009
C	-8.75802	-1.21137	0.21471	0.037035
C	-8.64616	-1.22506	1.64654	-0.024056
C	-8.4872	-2.49359	2.30709	-0.062235
C	-8.47244	-3.69012	1.53576	-0.050577
C	-8.61005	-3.64326	0.16397	-0.101592
C	-8.74559	-2.39943	-0.49785	-0.034339
C	-8.70665	-0.0446	2.43986	-0.036116
C	-8.59515	-0.10915	3.81477	-0.106143
C	-8.41692	-1.35668	4.46565	-0.093211
C	-8.36801	-2.52034	3.72622	-0.07203
C	-2.00594	6.11352	0.92512	-0.287303

C	1.25	-0.50568	-2.8158	-0.033799
C	1.14612	-0.66945	-4.18308	-0.108165
C	0.76237	-1.91958	-4.73214	-0.09319
C	0.5045	-2.98872	-3.89933	-0.073133
H	2.06972	2.3725	-0.05003	0.120293
H	0.56063	4.31977	-0.25056	0.114539
H	-1.28649	-0.33649	0.00163	0.109146
H	-1.35472	5.72181	-1.11915	0.130373
H	-3.11084	5.81583	-0.92092	0.13885
H	-7.24757	4.3377	-0.70341	0.104649
H	-9.11008	2.6941	-0.69553	0.124025
H	-6.26236	-0.53358	-0.32782	0.111225
H	3.77144	-1.3848	-0.26993	0.11439
H	5.72246	-1.32657	1.2518	0.105287
H	5.61774	-0.03304	3.38161	0.101929
H	3.52211	1.18103	3.97182	0.105151
H	1.563	1.09705	2.4673	0.117561
H	0.11283	-4.92418	-2.05286	0.095086
H	0.34137	-4.67108	0.40568	0.107457
H	0.93158	-2.46155	1.38362	0.104606
H	-11.40947	-0.61309	0.15018	0.115227
H	-13.42448	-0.33604	-1.26211	0.106408
H	-13.23833	0.68413	-3.5297	0.103504
H	-11.00324	1.39625	-4.37136	0.106926
H	-8.98527	1.08309	-2.97624	0.119954
H	-8.35596	-4.6407	2.04788	0.09589
H	-8.60056	-4.55749	-0.42028	0.108121
H	-8.83802	-2.36717	-1.57795	0.104974
H	-8.8454	0.91015	1.94803	0.113577
H	-8.64574	0.80064	4.40439	0.105731
H	-8.32491	-1.39128	5.5465	0.106047
H	-8.24105	-3.48076	4.21774	0.097595
H	-1.92612	7.20192	0.82257	0.11585
H	-2.86324	5.89087	1.56815	0.120759
H	-1.10042	5.74888	1.4218	0.113684
H	1.54536	0.4506	-2.40292	0.113798
H	1.36136	0.1633	-4.84509	0.104401
H	0.67852	-2.03184	-5.80841	0.105497
H	0.21964	-3.95245	-4.31193	0.097173

Table S13. Cartesian coordinates of optimized structure of molecule **4**.

Total energy: –2275.34 Hartrees

	x	y	z	Mulliken charges
C	4.15797	-0.87654	0.50783	0.115709
C	4.62267	-2.21033	0.61044	-0.088672
C	3.75653	-3.30305	0.53271	-0.069858
C	2.39152	-3.05162	0.37476	0.258241
C	1.90632	-1.71486	0.28463	-0.126259
C	2.78541	-0.63212	0.33842	-0.022218
N	1.31496	-3.95525	0.29009	-0.536362
C	0.14669	-3.22506	0.13321	0.427289
C	0.46877	-1.8142	0.12723	0.086996
N	-1.0767	-3.70956	0.01254	-0.37729
C	-2.06294	-2.7547	-0.12113	0.091732
C	-1.76339	-1.34542	-0.13438	0.093488
N	-0.46582	-0.88294	-0.00572	-0.349284
N	5.0879	0.20627	0.58193	-0.508426
C	-3.41594	-3.15683	-0.25758	-0.074318
C	-4.41924	-2.22472	-0.39952	-0.098163
C	-4.13144	-0.82184	-0.39888	0.162928
C	-2.81219	-0.40504	-0.26272	-0.107182
N	-5.19305	0.10746	-0.55785	-0.503706
C	4.77426	1.36951	1.35181	0.105684
C	6.3227	0.13539	-0.13381	0.10529
C	-6.47867	-0.1576	0.01391	0.081699
C	-4.97633	1.35801	-1.22513	0.085079
C	7.52527	0.56992	0.46213	-0.088267
C	8.72672	0.50686	-0.23613	-0.095609
C	8.76067	-0.01061	-1.54002	0.168546
C	7.57755	-0.45588	-2.1417	-0.13279
C	6.36775	-0.37023	-1.44267	-0.09395
C	5.06021	2.658	0.85496	-0.08954
C	4.7661	3.79029	1.60766	-0.095897
C	4.15884	3.66431	2.8661	0.169579
C	3.85786	2.3924	3.36815	-0.131141
C	4.17668	1.2556	2.61676	-0.088667
C	-5.43171	2.56154	-0.652	-0.082398
C	-5.24375	3.77441	-1.30782	-0.095586
C	-4.57885	3.81238	-2.54253	0.172618
C	-4.11346	2.6241	-3.12057	-0.13025
C	-4.3244	1.40568	-2.46631	-0.069988
C	-7.65193	0.0874	-0.72827	-0.078859
C	-8.90404	-0.15929	-0.17567	-0.09475
C	-9.01263	-0.67428	1.12575	0.171514
C	-7.85625	-0.92752	1.8734	-0.131081
C	-6.59919	-0.65656	1.31969	-0.082835

C	1.38762	-5.41602	0.31429	-0.099966
C	1.7601	-6.0248	-1.04581	-0.287051
O	3.89654	4.86026	3.53274	-0.39186
C	3.26136	4.80312	4.8348	-0.128668
O	-4.43226	5.07569	-3.10993	-0.390257
C	-3.73868	5.19206	-4.37866	-0.129161
O	10.01628	-0.03934	-2.14581	-0.391732
C	10.12092	-0.54474	-3.50042	-0.128418
O	-10.3107	-0.89815	1.5783	-0.390179
C	-10.49937	-1.42847	2.91506	-0.128885
H	5.68401	-2.38087	0.74991	0.118077
H	4.14417	-4.31283	0.60799	0.112997
H	2.41057	0.381	0.2553	0.10755
H	-3.62924	-4.2199	-0.26266	0.102706
H	-5.44592	-2.54782	-0.52272	0.125133
H	-2.5477	0.64466	-0.25393	0.112117
H	7.50846	0.95848	1.47397	0.115113
H	9.65503	0.84007	0.21308	0.109465
H	7.57641	-0.85387	-3.14918	0.117291
H	5.45098	-0.70007	-1.91832	0.114525
H	5.51462	2.76326	-0.12345	0.114715
H	4.98282	4.78436	1.23438	0.10911
H	3.39132	2.26862	4.33778	0.117517
H	3.95446	0.27226	3.01558	0.112956
H	-5.93486	2.53763	0.30793	0.113612
H	-5.59017	4.70638	-0.87692	0.110376
H	-3.60143	2.62846	-4.07486	0.11921
H	-3.97328	0.48601	-2.92062	0.114258
H	-7.57159	0.4722	-1.73857	0.114218
H	-9.81256	0.02557	-0.73672	0.110919
H	-7.9152	-1.31703	2.88234	0.119227
H	-5.70566	-0.83619	1.90718	0.116808
H	2.11101	-5.71116	1.08357	0.129667
H	0.40169	-5.7696	0.62886	0.138063
H	1.80904	-7.11733	-0.97095	0.115238
H	1.009	-5.7655	-1.79854	0.120414
H	2.73363	-5.66126	-1.39226	0.113482
H	3.15538	5.84136	5.14775	0.134106
H	2.27245	4.3322	4.77649	0.119006
H	3.88204	4.261	5.55877	0.117631
H	-3.73925	6.25706	-4.60811	0.135051
H	-2.70606	4.83068	-4.30302	0.120153
H	-4.2617	4.64336	-5.17129	0.118763
H	11.17749	-0.46689	-3.75475	0.134428

H	9.80277	-1.59278	-3.56199	0.117281
H	9.52769	0.05826	-4.1987	0.118428
H	-11.57801	-1.52214	3.03603	0.135337
H	-10.02844	-2.41304	3.02383	0.118798
H	-10.10042	-0.74619	3.67544	0.119386

Table S14. Cartesian coordinates of optimized structure of molecule **5**.

Total energy: –2226.25 Hartrees

	x	y	z	Mulliken charges
C	4.18883	0.96395	0.171	0.052177
C	4.69812	2.28094	0.12489	-0.06114
C	3.85597	3.3905	0.02539	-0.062105
C	2.47872	3.16358	-0.04572	0.264705
C	1.95412	1.83821	-0.00488	-0.118967
C	2.8062	0.73985	0.11424	0.013458
N	1.42586	4.08719	-0.16689	-0.535821
C	0.23134	3.38523	-0.19296	0.437835
C	0.51441	1.96841	-0.09352	0.093075
N	-0.98205	3.89584	-0.29726	-0.373509
C	-2.00007	2.96441	-0.30514	0.0972
C	-1.73756	1.55226	-0.19531	0.106209
N	-0.44981	1.06039	-0.09172	-0.344095
C	1.53651	5.54794	-0.21169	-0.102836
N	5.10218	-0.14121	0.29886	-0.498652
C	-3.34479	3.39959	-0.4211	-0.066048
C	-4.37995	2.49027	-0.41963	-0.07026
C	-4.12249	1.09037	-0.31028	0.092
C	-2.81649	0.63622	-0.21126	-0.065335
N	-5.22837	0.179	-0.31766	-0.496182
C	5.07481	-1.20567	-0.61903	0.21705
C	6.03723	-0.11639	1.39084	0.081717
C	-6.23853	0.35423	-1.32761	0.058464
C	-5.31625	-0.87747	0.61101	0.208668
C	7.40429	-0.35534	1.16561	-0.071575
C	8.30677	-0.31037	2.23173	-0.098181
C	7.86178	-0.00987	3.52519	-0.098005
C	6.50214	0.24022	3.74676	-0.100769
C	5.59067	0.18283	2.68871	-0.077686
C	5.54215	-2.49239	-0.25311	-0.122206
C	5.51475	-3.54118	-1.16169	-0.055253
C	5.0162	-3.32558	-2.45247	0.142741
C	4.54272	-2.06542	-2.83755	-0.054791

C	4.57216	-1.01574	-1.93005	-0.121252
C	-6.00629	-2.0687	0.28153	-0.120912
C	-6.10848	-3.10572	1.19947	-0.05339
C	-5.51915	-2.97004	2.46176	0.143431
C	-4.82785	-1.80353	2.81125	-0.053639
C	-4.72865	-0.76608	1.89444	-0.112058
C	-7.59757	0.40196	-0.97241	-0.063006
C	-8.57054	0.58364	-1.95881	-0.097226
C	-8.19898	0.73638	-3.30076	-0.096657
C	-6.84433	0.7	-3.65197	-0.098337
C	-5.86552	0.50395	-2.67317	-0.070396
C	1.70647	6.18082	1.17697	-0.286306
N	4.9903	-4.4195	-3.40155	0.14506
O	4.51282	-4.20218	-4.55807	-0.311477
O	5.44756	-5.54584	-3.03488	-0.310712
N	-5.62742	-4.05145	3.42145	0.145716
O	-5.06558	-3.91149	4.5511	-0.309007
O	-6.28053	-5.08765	3.08878	-0.308536
H	5.77166	2.42495	0.17191	0.119678
H	4.2704	4.39135	-0.00382	0.120778
H	2.40479	-0.26591	0.15908	0.111949
H	2.37732	5.80701	-0.86535	0.134437
H	0.62051	5.91156	-0.6849	0.142442
H	-3.52713	4.46524	-0.4975	0.110607
H	-5.40682	2.82846	-0.49546	0.123305
H	-2.58476	-0.41968	-0.14219	0.117538
H	7.75226	-0.57277	0.16178	0.119731
H	9.35986	-0.49737	2.04808	0.113483
H	8.56605	0.02999	4.34935	0.110958
H	6.14683	0.46993	4.74609	0.112649
H	4.53598	0.36575	2.86137	0.116959
H	5.91218	-2.66388	0.74928	0.136812
H	5.85958	-4.52918	-0.8862	0.138651
H	4.1713	-1.92504	-3.84413	0.137933
H	4.2184	-0.03859	-2.23214	0.133717
H	-6.44898	-2.17763	-0.70005	0.136911
H	-6.62449	-4.024	0.95184	0.139443
H	-4.39209	-1.7221	3.79829	0.138923
H	-4.20602	0.14092	2.16899	0.135648
H	-7.88327	0.29806	0.06863	0.118768
H	-9.6178	0.61821	-1.67668	0.114247
H	-8.95674	0.88294	-4.06308	0.111919
H	-6.5476	0.81323	-4.68956	0.113882
H	-4.81646	0.46265	-2.94447	0.118061

H	1.79234	7.2695	1.08648	0.120122
H	0.84144	5.95662	1.80886	0.122252
H	2.60526	5.80768	1.6794	0.115017

Table S15. Cartesian coordinates of optimized structure of molecule **6**.

Total energy: –2498.33 Hartrees

	x	y	z	Mulliken charges
C	3.18586	-1.96573	1.00997	0.076241
C	3.83607	-3.02191	0.33	-0.06703
C	3.14158	-3.89274	-0.51239	-0.063718
C	1.7631	-3.71088	-0.65238	0.263907
C	1.09329	-2.66147	0.04201	-0.124428
C	1.80316	-1.78426	0.86263	-0.001056
N	0.8351	-4.44553	-1.41246	-0.536277
C	-0.41838	-3.88199	-1.23197	0.434081
C	-0.30523	-2.761	-0.32269	0.090662
N	-1.55049	-4.28323	-1.78158	-0.375123
C	-2.65845	-3.54382	-1.42206	0.095728
C	-2.56496	-2.42269	-0.52245	0.101612
N	-1.35758	-2.03757	0.0308	-0.345626
C	-3.92965	-3.88451	-1.95045	-0.068628
C	-5.04973	-3.1565	-1.61467	-0.081052
C	-4.96338	-2.04912	-0.71506	0.119159
C	-3.73254	-1.70221	-0.17615	-0.082369
N	3.94411	-1.09332	1.86146	-0.500459
C	1.11933	-5.58086	-2.29277	-0.101915
C	1.65653	-5.15745	-3.66771	-0.286737
N	-6.14772	-1.3191	-0.39369	-0.499769
C	-7.35931	-2.04136	-0.13532	0.084452
C	-6.12347	0.09683	-0.27971	0.15915
C	3.46534	-0.83919	3.18847	0.096956
C	5.13635	-0.49582	1.38855	0.178382
C	3.44991	0.46965	3.70389	-0.079107
C	2.97192	0.7092	4.99457	-0.100206
C	2.4881	-0.34418	5.78042	-0.101753
C	2.49269	-1.64554	5.26409	-0.101088
C	2.98345	-1.89669	3.98017	-0.084246
C	6.20393	-0.21251	2.26883	-0.111299
C	7.37201	0.36932	1.78896	-0.05443
C	7.5178	0.67724	0.42534	0.033171
C	6.45478	0.39699	-0.45733	-0.02857
C	5.28371	-0.17659	0.01592	-0.114914

C	-6.91506	0.75226	0.68569	-0.106539
C	-6.89947	2.14059	0.77852	-0.053504
C	-6.09256	2.90904	-0.07641	0.036266
C	-5.29779	2.25747	-1.0416	-0.025658
C	-5.31569	0.87403	-1.14383	-0.095938
C	-8.57449	-1.61574	-0.70187	-0.075254
C	-9.75092	-2.32574	-0.45091	-0.0997
C	-9.73025	-3.47464	0.35043	-0.101505
C	-8.51981	-3.90394	0.90735	-0.099819
C	-7.34064	-3.19005	0.67524	-0.083549
N	8.74855	1.26034	0.04706	-0.215976
N	8.8888	1.51859	-1.20136	-0.228509
C	10.13022	2.10915	-1.57153	0.044502
N	-6.15121	4.31104	0.10755	-0.216103
N	-5.40097	5.00901	-0.66238	-0.225438
C	-5.46654	6.41864	-0.47483	0.044185
C	10.28278	2.38993	-2.93889	-0.06277
C	11.4641	2.96894	-3.40852	-0.104369
C	12.49828	3.26969	-2.51339	-0.094435
C	12.34581	2.98935	-1.14569	-0.107382
C	11.16928	2.41191	-0.67082	-0.037349
C	-4.63995	7.17922	-1.31736	-0.061385
C	-4.62719	8.5723	-1.21537	-0.104098
C	-5.44075	9.21048	-0.27094	-0.093461
C	-6.26771	8.44976	0.57175	-0.107248
C	-6.2849	7.05933	0.47503	-0.035986
H	4.90376	-3.1502	0.46764	0.121626
H	3.66652	-4.6893	-1.0269	0.11847
H	1.29208	-0.9795	1.37768	0.109714
H	-3.98472	-4.72308	-2.63516	0.107498
H	-6.014	-3.41307	-2.0372	0.124899
H	-3.62792	-0.87498	0.51483	0.116698
H	1.83049	-6.24089	-1.78245	0.132653
H	0.17835	-6.12622	-2.40521	0.140579
H	1.85883	-6.04206	-4.28226	0.118126
H	0.92233	-4.53688	-4.19091	0.121671
H	2.58607	-4.5857	-3.5749	0.115029
H	3.80725	1.2897	3.09135	0.118997
H	2.96324	1.72388	5.37984	0.110224
H	2.11017	-0.15279	6.77919	0.106983
H	2.12272	-2.47052	5.86462	0.108864
H	2.9952	-2.90648	3.58561	0.114113
H	6.11189	-0.45833	3.31958	0.124711
H	8.20186	0.58476	2.45289	0.107599

H	6.56774	0.65188	-1.50403	0.111445
H	4.46394	-0.37255	-0.66503	0.126494
H	-7.53054	0.16919	1.35985	0.124034
H	-7.49741	2.65814	1.52029	0.108432
H	-4.68844	2.85848	-1.70528	0.113066
H	-4.71231	0.37927	-1.89567	0.126377
H	-8.5891	-0.73515	-1.33421	0.118884
H	-10.68263	-1.98806	-0.89353	0.110778
H	-10.64498	-4.02722	0.53743	0.107984
H	-8.49289	-4.78908	1.53492	0.110361
H	-6.40643	-3.51415	1.12005	0.118735
H	9.46343	2.14491	-3.60553	0.105488
H	11.57878	3.18493	-4.46584	0.108847
H	13.41736	3.71963	-2.87558	0.10956
H	13.14891	3.22399	-0.45379	0.110254
H	11.02999	2.18746	0.37954	0.110178
H	-4.02191	6.65435	-2.03724	0.106802
H	-3.98711	9.15768	-1.86746	0.109555
H	-5.43278	10.29288	-0.18939	0.110175
H	-6.89718	8.94745	1.30301	0.110701
H	-6.91396	6.45268	1.11479	0.110717

Table S16. Cartesian coordinates of optimized structure of molecule **7**.

Total energy: – 1814.77 Hartrees

	x	y	z	Mulliken charges
C	-4.14932	0.51787	-0.0501	0.105822
C	-4.63991	1.81536	-0.31738	-0.070115
C	-3.77943	2.89598	-0.52599	-0.068512
C	-2.40381	2.65455	-0.48525	0.266175
C	-1.8983	1.34655	-0.22845	-0.122436
C	-2.76951	0.28073	0.00117	-0.003809
N	-1.33415	3.55122	-0.65774	-0.535739
C	-0.14878	2.8465	-0.52406	0.439746
C	-0.45442	1.45727	-0.25024	0.091111
N	1.07404	3.33516	-0.61889	-0.373911
C	2.08056	2.40895	-0.43098	0.097249
C	1.79489	1.02332	-0.16172	0.102559
N	0.49775	0.55408	-0.07218	-0.343937
C	-1.42454	4.98004	-0.96873	-0.102973
N	-5.0697	-0.5509	0.16235	-0.599246
C	3.43388	2.82397	-0.50863	-0.070438
C	4.45724	1.91691	-0.33348	-0.081975

C	4.1758	0.54678	-0.05188	0.131679
C	2.86288	0.11463	0.03575	-0.075344
N	5.25507	-0.36346	0.12028	-0.600808
C	-5.13992	-1.73946	-0.5912	0.226304
C	-6.19046	-2.54825	-0.07328	-0.096686
C	-6.46544	-3.7866	-0.66947	-0.054421
C	-5.70362	-4.19776	-1.76487	-0.120413
C	-4.67406	-3.37972	-2.27079	-0.107592
C	-4.37939	-2.14138	-1.69434	-0.080313
C	6.34128	-0.19184	1.00359	0.226444
C	7.21656	-1.30611	0.87394	-0.098912
C	8.37152	-1.37344	1.66443	-0.05258
C	8.63572	-0.34527	2.57148	-0.119735
C	7.75008	0.74239	2.69978	-0.107313
C	6.59155	0.83268	1.92324	-0.080484
C	-1.66997	5.25764	-2.45892	-0.286275
C	-6.06445	-0.59569	1.15854	0.22768
C	-6.77739	-1.82204	1.03893	-0.097195
C	5.42935	-1.58362	-0.56783	0.227669
C	6.63907	-2.18787	-0.12501	-0.098675
C	-6.36574	0.33375	2.16001	-0.082855
C	-7.4088	0.02856	3.03853	-0.107721
C	-8.13252	-1.17512	2.92728	-0.120627
C	-7.81944	-2.1039	1.93277	-0.054466
C	4.63822	-2.17133	-1.56071	-0.07712
C	5.06509	-3.38925	-2.09699	-0.107668
C	6.25287	-4.0076	-1.66009	-0.119178
C	7.0446	-3.41024	-0.67758	-0.053918
H	-5.71257	1.96462	-0.36805	0.126777
H	-4.17885	3.88309	-0.72735	0.120448
H	-2.38646	-0.70856	0.22239	0.117213
H	-2.22176	5.41374	-0.35393	0.13386
H	-0.47751	5.42463	-0.6511	0.142066
H	3.63159	3.8675	-0.72479	0.110756
H	5.49098	2.23032	-0.42201	0.130527
H	2.61953	-0.91478	0.26832	0.123209
H	-7.26241	-4.41656	-0.28654	0.095442
H	-5.90563	-5.15502	-2.23406	0.101771
H	-4.09719	-3.71561	-3.12663	0.104458
H	-3.5889	-1.51592	-2.09259	0.113703
H	9.04892	-2.21722	1.57713	0.096143
H	9.52702	-0.38567	3.18887	0.102387
H	7.96651	1.52548	3.41946	0.104786
H	5.90903	1.66607	2.0412	0.116338

H	-1.7391	6.33716	-2.63445	0.119431
H	-0.84632	4.86416	-3.06276	0.122347
H	-2.60068	4.79475	-2.80405	0.115323
H	-5.80678	1.25719	2.25869	0.111624
H	-7.66206	0.73306	3.8245	0.10388
H	-8.9375	-1.38185	3.62483	0.101708
H	-8.3736	-3.03428	1.85577	0.095636
H	3.7258	-1.70158	-1.90796	0.118059
H	4.46677	-3.86593	-2.86688	0.104922
H	6.55427	-4.955	-2.09462	0.102263
H	7.96435	-3.88416	-0.34895	0.095871

Table S17. Cartesian coordinates of optimized structure of molecule **8**.

Total energy: –1965.20 Hartrees

	x	y	z	Mulliken charges
C	4.15233	0.46149	-0.1657	-0.041355
C	4.64117	1.71862	-0.5819	-0.016825
C	3.77993	2.76353	-0.92754	-0.063722
C	2.40474	2.52587	-0.8496	0.265063
C	1.89912	1.26042	-0.42841	-0.109319
C	2.77434	0.22731	-0.08675	0.038516
N	1.33517	3.38729	-1.14993	-0.535359
C	0.14961	2.70743	-0.9246	0.440302
C	0.45532	1.36531	-0.4711	0.092879
N	-1.07203	3.17709	-1.094	-0.373513
C	-2.08069	2.27835	-0.80367	0.097365
C	-1.79368	0.94186	-0.34944	0.116366
N	-0.49733	0.49157	-0.18584	-0.341015
C	1.42527	4.78349	-1.5875	-0.10326
N	5.08489	-0.57839	0.17493	-0.573515
C	-3.43263	2.67735	-0.95539	-0.064505
C	-4.45636	1.79626	-0.67264	-0.021498
C	-4.17394	0.47572	-0.21771	-0.033635
C	-2.86489	0.06073	-0.05648	-0.017139
N	-5.26446	-0.41554	0.06866	-0.570876
C	5.56173	-1.46279	-0.82651	0.246127
C	5.54423	-0.71551	1.51003	0.246577
C	-5.94191	-0.32736	1.31179	0.246463
C	6.50174	-1.70411	1.81458	0.141833
C	6.9838	-1.87733	3.10482	-0.112542
C	6.51866	-1.05599	4.14114	-0.109939
C	5.57053	-0.07081	3.86012	-0.110846

C	5.08585	0.09909	2.55585	-0.11029
C	5.12038	-1.40848	-2.15681	-0.110326
C	5.6225	-2.30082	-3.11414	-0.110903
C	6.57081	-3.26156	-2.75888	-0.109934
C	7.0182	-3.32755	-1.43206	-0.112476
C	6.51911	-2.44039	-0.48812	0.142187
C	-5.54381	0.55216	2.32951	-0.11049
C	-6.24482	0.60688	3.54207	-0.110898
C	-7.34923	-0.21848	3.76005	-0.109642
C	-7.75219	-1.10717	2.75373	-0.112605
C	-7.05624	-1.15573	1.55353	0.142174
C	-5.698	-1.35368	-0.90426	0.249138
C	-6.81407	-2.16899	-0.62798	0.140344
C	-7.28028	-3.10025	-1.54604	-0.112564
C	-6.6395	-3.24276	-2.78432	-0.109601
C	-5.53559	-2.44094	-3.07921	-0.110703
C	-5.06763	-1.50352	-2.14818	-0.109561
C	1.6632	5.76235	-0.42891	-0.286222
O	7.01815	-2.56026	0.82309	-0.384585
O	-7.5149	-2.0734	0.5896	-0.384133
H	5.71477	1.86387	-0.6297	0.113049
H	4.17526	3.722	-1.24284	0.122068
H	2.39841	-0.73817	0.23164	0.104815
H	2.2258	4.85678	-2.33249	0.135149
H	0.48023	5.00998	-2.08835	0.143005
H	-3.62696	3.68577	-1.30169	0.111793
H	-5.49253	2.09281	-0.7915	0.112076
H	-2.62996	-0.93829	0.29108	0.108514
H	7.71891	-2.65463	3.2772	0.113062
H	6.89553	-1.19115	5.14875	0.10465
H	5.19839	0.57267	4.65034	0.103558
H	4.34854	0.8647	2.34985	0.122639
H	4.38277	-0.66932	-2.4427	0.122834
H	5.26357	-2.23692	-4.13594	0.103568
H	6.96125	-3.95401	-3.4962	0.104636
H	7.75247	-4.05729	-1.11173	0.113084
H	-4.68431	1.19203	2.17463	0.124093
H	-5.91622	1.29713	4.31181	0.103747
H	-7.89355	-0.17975	4.69695	0.104605
H	-8.60093	-1.76876	2.88095	0.113081
H	-8.14229	-3.69865	-1.27569	0.113049
H	-7.00376	-3.96988	-3.50137	0.104589
H	-5.02832	-2.53616	-4.03342	0.10387
H	-4.20977	-0.88845	-2.38828	0.124232

H	1.72987	6.78743	-0.8104	0.120481
H	0.83729	5.71657	0.28773	0.122636
H	2.59316	5.5348	0.10313	0.115574

Table S18. Cartesian coordinates of optimized structure of molecule **9**.

Total energy: –2611.15 Hartrees

9	x	y	z	Mulliken charges
C	4.16103	0.56422	-0.17349	-0.015889
C	4.64182	1.85904	-0.46125	-0.017113
C	3.7765	2.93278	-0.68771	-0.067827
C	2.40232	2.68719	-0.62247	0.2683
C	1.90286	1.38321	-0.33395	-0.097194
C	2.78273	0.3218	-0.10956	-0.017762
N	1.32833	3.5733	-0.81814	-0.535868
C	0.14619	2.87032	-0.65411	0.439987
C	0.45883	1.48771	-0.35144	0.094259
N	-1.07801	3.35252	-0.75632	-0.373162
C	-2.08229	2.42522	-0.55329	0.097333
C	-1.78824	1.04816	-0.25159	0.126363
N	-0.48961	0.58557	-0.15209	-0.342685
C	1.41272	5.00815	-1.10641	-0.10291
N	5.12347	-0.48929	0.04966	-0.562131
C	-3.43662	2.83417	-0.64219	-0.069263
C	-4.45549	1.92501	-0.44258	-0.019033
C	-4.16795	0.56287	-0.14379	-0.011974
C	-2.85501	0.13591	-0.05139	-0.063872
N	-5.27712	-0.34006	0.05276	-0.560584
C	5.48979	-1.32671	-1.04765	0.292931
C	5.50527	-0.79634	1.39094	0.293861
C	-5.75294	-1.09413	-1.0628	0.290608
C	6.72367	-1.44583	1.66674	-0.263743
C	7.08241	-1.78611	2.97197	-0.073293
C	6.25425	-1.44029	4.04501	-0.097065
C	5.05632	-0.76733	3.79011	-0.113267
C	4.67828	-0.45961	2.48024	-0.089464
C	4.64741	-1.47188	-2.16709	-0.089019
C	5.01008	-2.29639	-3.23568	-0.113294
C	6.20781	-3.01568	-3.20407	-0.096883
C	7.05092	-2.88589	-2.09541	-0.073477
C	6.70711	-2.03411	-1.04449	-0.263213
C	-4.91871	-1.37625	-2.16168	-0.085695
C	-5.39077	-2.11882	-3.24754	-0.113044

C	-6.69513	-2.62067	-3.25226	-0.096503
C	-7.53163	-2.35487	-2.16295	-0.073542
C	-7.07346	-1.58107	-1.09553	-0.262089
C	-5.73502	-0.59067	1.38205	0.292572
C	-7.05365	-1.02213	1.62185	-0.262737
C	-7.49604	-1.30972	2.91398	-0.073444
C	-6.64543	-1.12442	4.00894	-0.096608
C	-5.34304	-0.66752	3.78943	-0.113211
C	-4.88674	-0.41616	2.49251	-0.086548
C	1.66313	5.86001	0.14596	-0.286467
S	7.92241	-1.75138	0.30615	0.173167
S	-8.2536	-1.10178	0.23065	0.173623
H	5.71485	2.00836	-0.50279	0.11655
H	4.16928	3.91926	-0.9044	0.12192
H	2.40447	-0.67071	0.10881	0.111114
H	2.20501	5.16064	-1.84826	0.135192
H	0.46215	5.28502	-1.57011	0.142853
H	-3.63733	3.8745	-0.87029	0.111732
H	-5.49445	2.22736	-0.50852	0.114869
H	-2.60898	-0.89562	0.17303	0.114366
H	8.01976	-2.3043	3.14434	0.113137
H	6.54465	-1.69133	5.05933	0.105978
H	4.40187	-0.48692	4.60907	0.106694
H	3.73982	0.04882	2.30246	0.126321
H	3.70917	-0.93413	-2.20403	0.126341
H	4.34401	-2.38098	-4.08822	0.106758
H	6.48654	-3.66554	-4.02638	0.106013
H	7.98806	-3.43042	-2.04935	0.113165
H	-3.90057	-1.00982	-2.16778	0.126572
H	-4.72769	-2.31211	-4.08452	0.106801
H	-7.06045	-3.20752	-4.08795	0.106002
H	-8.5492	-2.73047	-2.14512	0.113107
H	-8.51256	-1.65967	3.05904	0.113137
H	-6.99844	-1.33209	5.01317	0.105956
H	-4.66916	-0.51445	4.62611	0.106729
H	-3.87011	-0.07802	2.34122	0.126896
H	1.72516	6.91956	-0.12668	0.120269
H	0.84507	5.73835	0.86282	0.122482
H	2.59902	5.57945	0.64088	0.115914

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

Molecule 1

Wavelength (nm)	Oscillator strength	Assignments	
426.52	0.0418	HOMO → LUMO	(69.90 %)
349.83	0.0029	HOMO − 4→ LUMO	(70.13 %)
346.62	0.4875	HOMO − 3→ LUMO HOMO − 2→ LUMO	(13.03 %) (66.83 %)

Molecule 2

Wavelength (nm)	Oscillator strength	Assignments	
544.63	0.0396	HOMO → LUMO	(70.22%)
490.11	0.2049	HOMO − 1→ LUMO	(70.18%)
359.65	0.0310	HOMO − 2→ LUMO HOMO → LUMO +1	(70.18%) (70.18%)

Molecule 3

Wavelength (nm)	Oscillator strength	Assignments	
530.70	0.0295	HOMO → LUMO	(70.18%)
471.98	0.2476	HOMO − 1→ LUMO	(70.11%)
407.07	0.0828	HOMO − 1→ LUMO +2 HOMO → LUMO +2	(21.07%) (66.20%)

Molecule 4

Wavelength (nm)	Oscillator strength	Assignments	
593.81	0.0255	HOMO → LUMO	(70.32 %)
531.91	0.1945	HOMO − 1→ LUMO	(70.29 %)
374.55	0.1148	HOMO − 2→ LUMO HOMO → LUMO +1	(50.22 %) (46.92 %)

Molecule 5

Wavelength (nm)	Oscillator strength	Assignments	
505.48	0.1225	HOMO → LUMO HOMO → LUMO +1 HOMO → LUMO +2	(57.50 %) (13.45 %) (37.80 %)
467.68	0.2818	HOMO → LUMO +2	(51.07 %)
464.26	0.2548	HOMO − 1→ LUMO +2 HOMO → LUMO +1	(11.78 %) (66.97 %)

Molecule 6

Wavelength (nm)	Oscillator strength	Assignments	
543.01	0.1186	HOMO → LUMO HOMO → LUMO +2	(58.11 %) (38.41 %)
512.32	0.6367	HOMO − 1→ LUMO HOMO → LUMO HOMO → LUMO +1	(40.05 %) (12.09 %) (49.65 %)
500.29	0.7905	HOMO → LUMO +1 HOMO → LUMO +2	(39.08 %) (41.06 %)

Molecule 7

Wavelength (nm)	Oscillator strength	Assignments	
490.61	0.0460	HOMO → LUMO	(70.14 %)
464.46	0.1068	HOMO − 1→ LUMO	(70.32 %)
397.90	0.0003	HOMO − 3→ LUMO	(70.33 %)

Molecule 8

Wavelength (nm)	Oscillator strength	Assignments	
644.06	0.0062	HOMO → LUMO	(70.41%)
631.13	0.0002	HOMO − 1→ LUMO	(70.43 %)
407.87	0.454	HOMO − 2→ LUMO	(69.68 %)

Molecule 9

Wavelength (nm)	Oscillator strength	Assignments	
544.70	0.0005	HOMO → LUMO	(70.27%)
535.73	0.0001	HOMO − 1→ LUMO	(70.32 %)
411.04	0.0437	HOMO − 2→ LUMO	(69.82 %)