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Blue-Red emitting Materials based on Pyrido[2,3–*b*]pyrazine backbone: Design and Tuning of Photophysical, Aggregation-induced emission, Electrochemical and Theoretical properties

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1. Photophysical spectra of compounds 1 in various solvents and solid film.

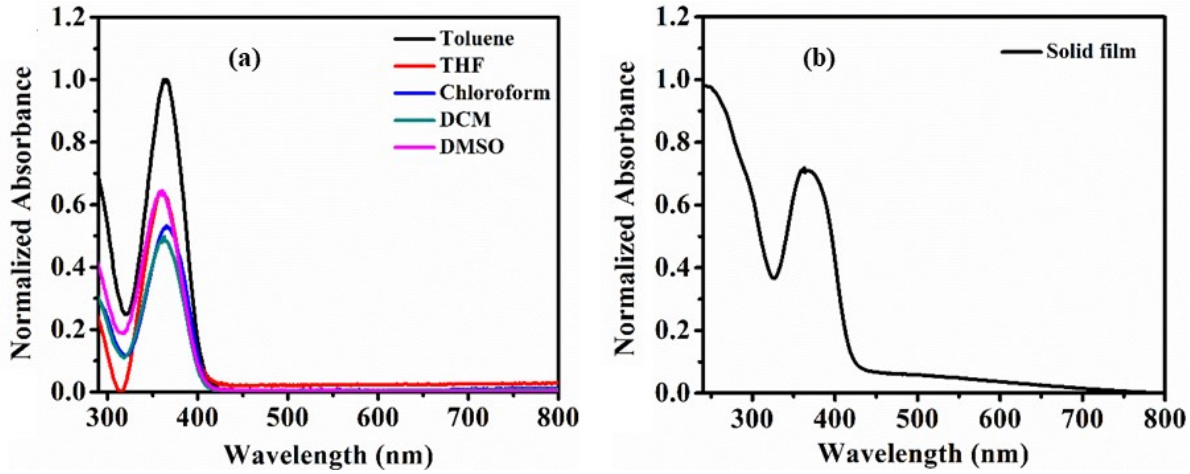


Fig. S1. UV−Vis absorption spectra of **1** in various solvents (**a**) and in solid film (**b**).

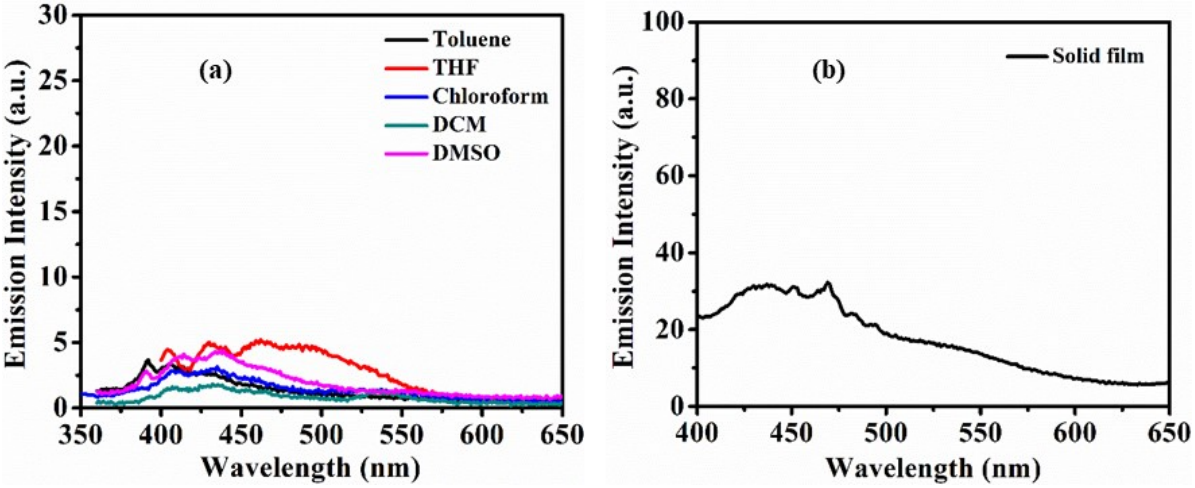


Fig. S2. Emission spectra of **1** in various solvents (**a**) and in solid film (**b**).

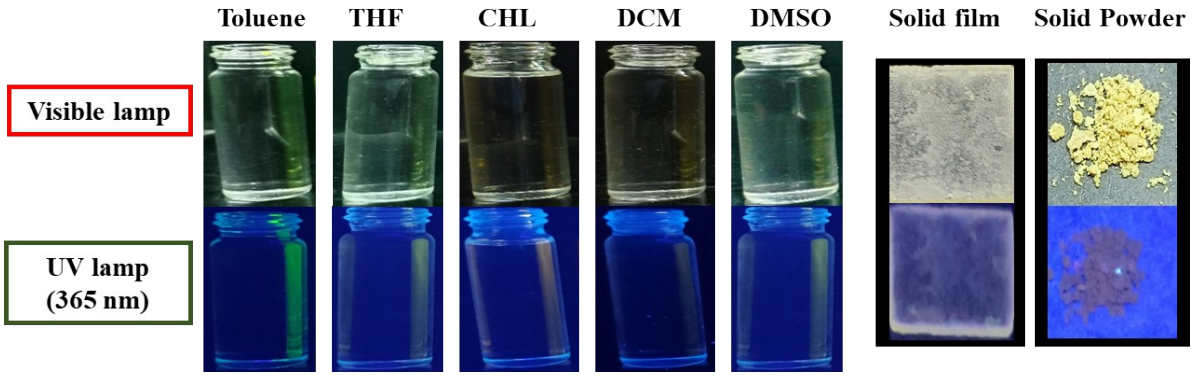


Fig. S3. Emission images of **1** in various solvents, solid film and powder.

2. Photophysical spectra of compounds 2−10 in various solvents.

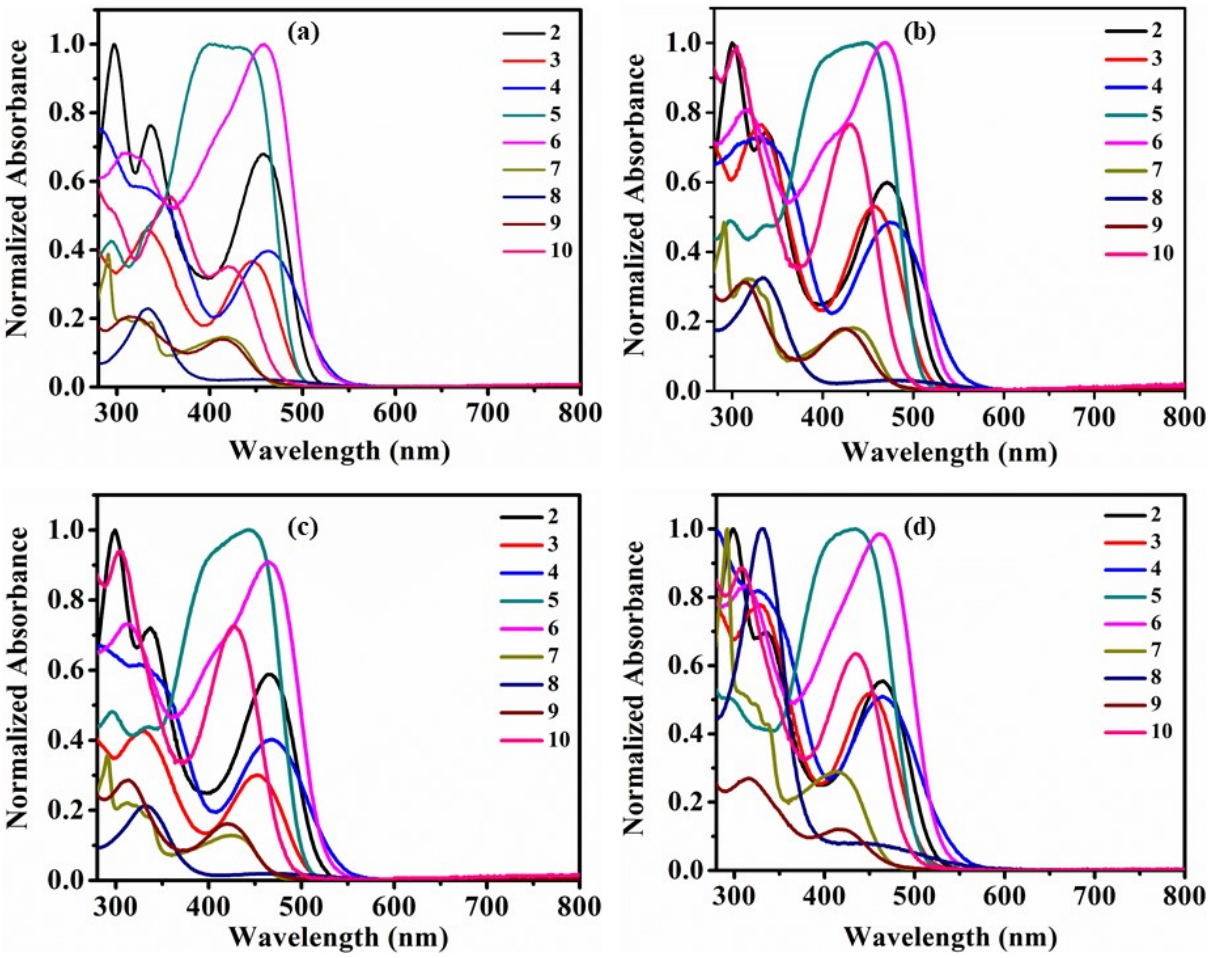


Fig. S4. UV−Vis absorption spectra of compounds **2−10** in THF (**a**) CHL (**b**) DCM (**c**) and DMSO (**d**).

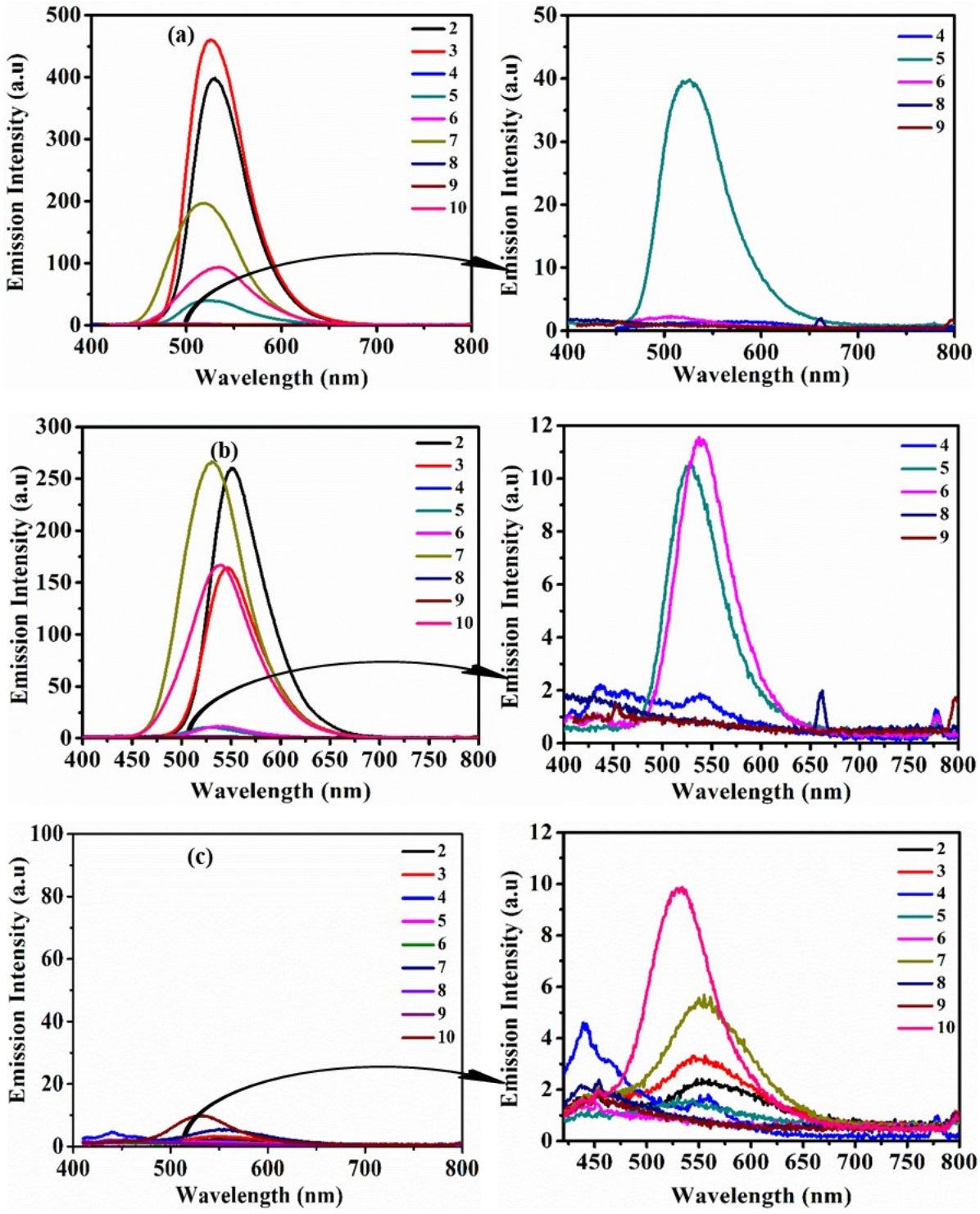


Fig. S5. Emission spectra of compounds **2**−**10** (**left**) and of weak/non emissive molecules (**right**) in THF (**a**) CHL (**b**) and DMSO (**c**) (Excitation of molecules **2**−**10** done at their respective ICT λ_{max}).

3. AIE spectrum, images and DLS plot of dyes.

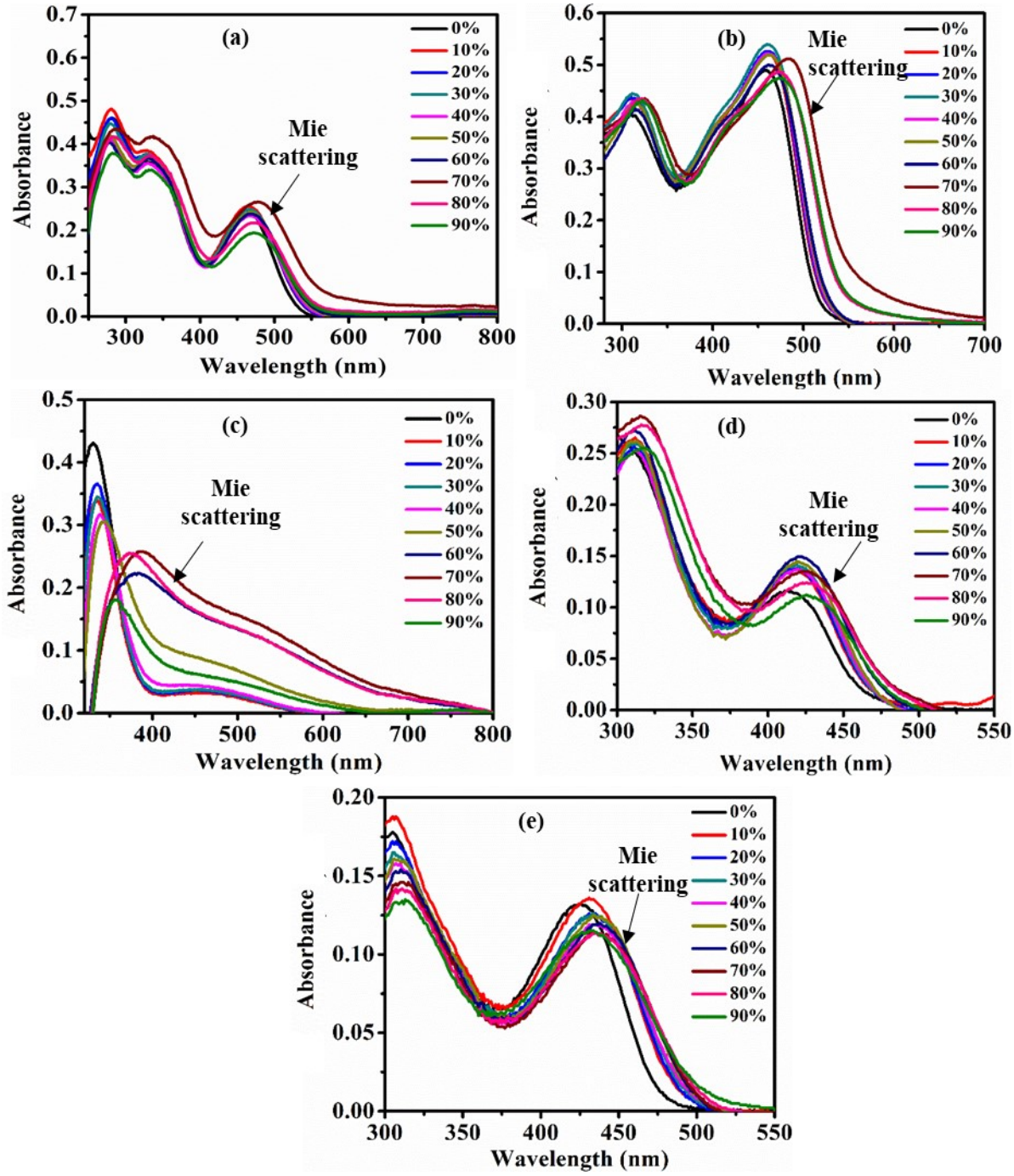


Fig. S6. Absorption spectra of **4** (**a**), **6** (**b**), **8** (**c**), **9** (**d**) and **10** (**e**) recorded in 10 μM solution of THF-H_2O mixture with increasing percentage of water fraction (f_w).

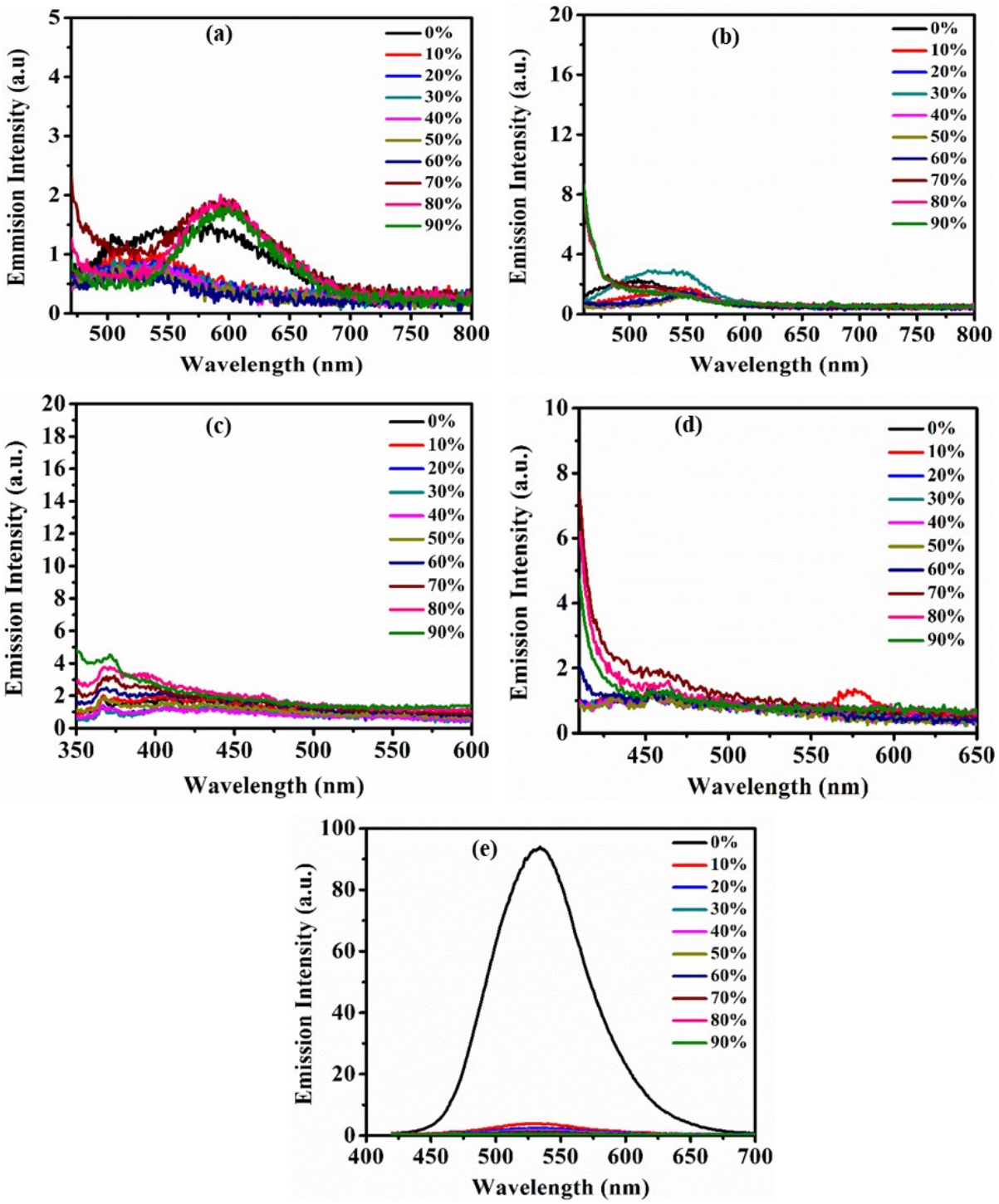


Fig. S7. Emission spectra of **4** (**a**), **6** (**b**), **8** (**c**), **9** (**d**) and **10** (**e**) recorded in 10 μM solution of THF-H_2O mixture with increasing percentage of water fraction (f_w).

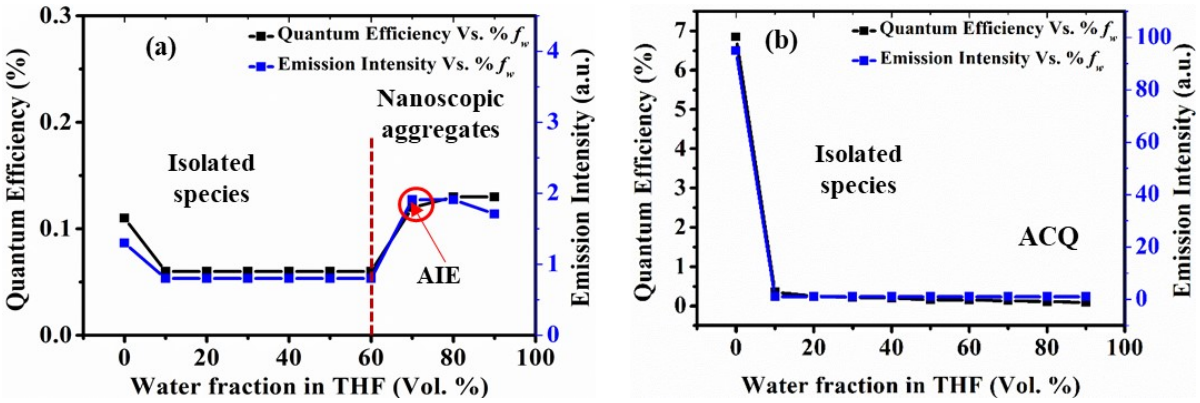


Fig. S8. Plot of percentage quantum efficiency and emission intensity versus percentage of water fraction (f_w) of **4** (**a**) and **10** (**b**) in THF/water mixture.

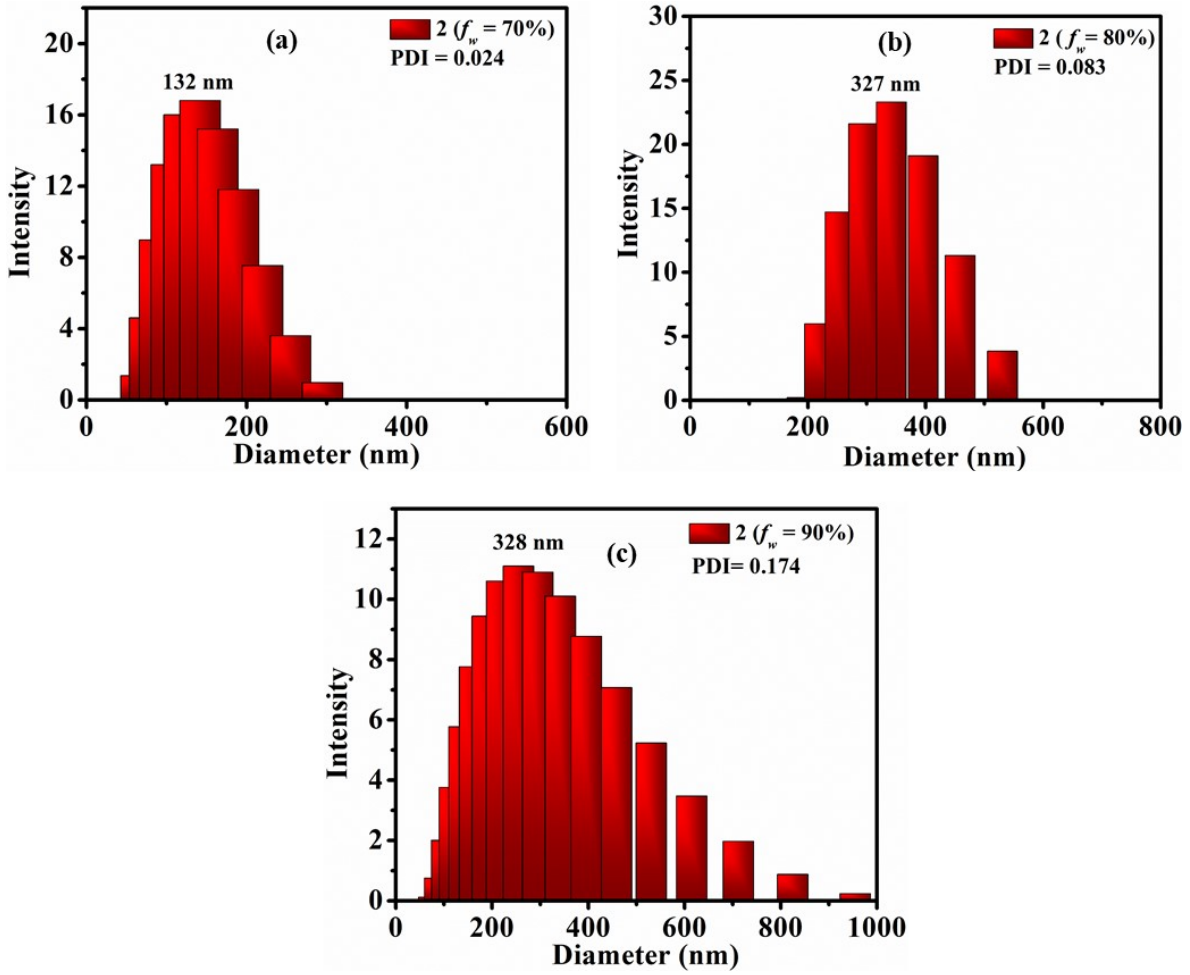


Fig. S9. DLS plot of **2** obtained from 70 (**a**), 80 (**b**) and 90% (**c**) f_w of THF–H_2O suspension.

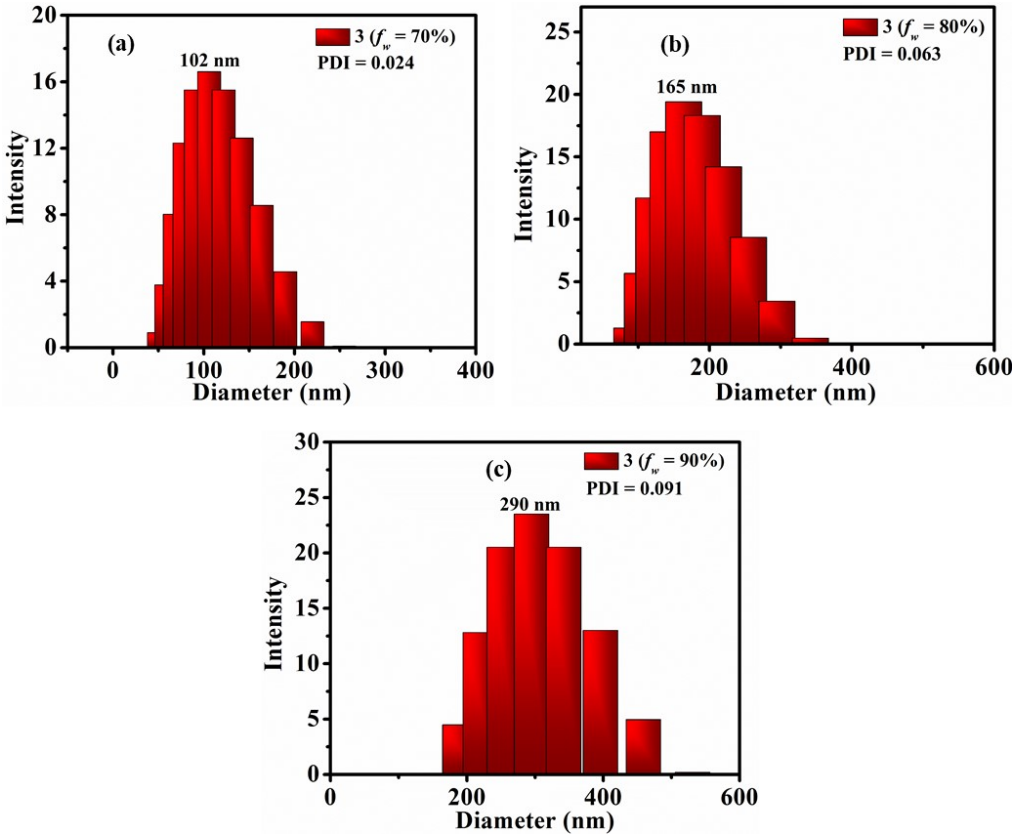


Fig. S10. DLS plot of **3** obtained from 70 (**a**), 80 (**b**) and 90% (**c**) f_w of THF–H_2O suspension.

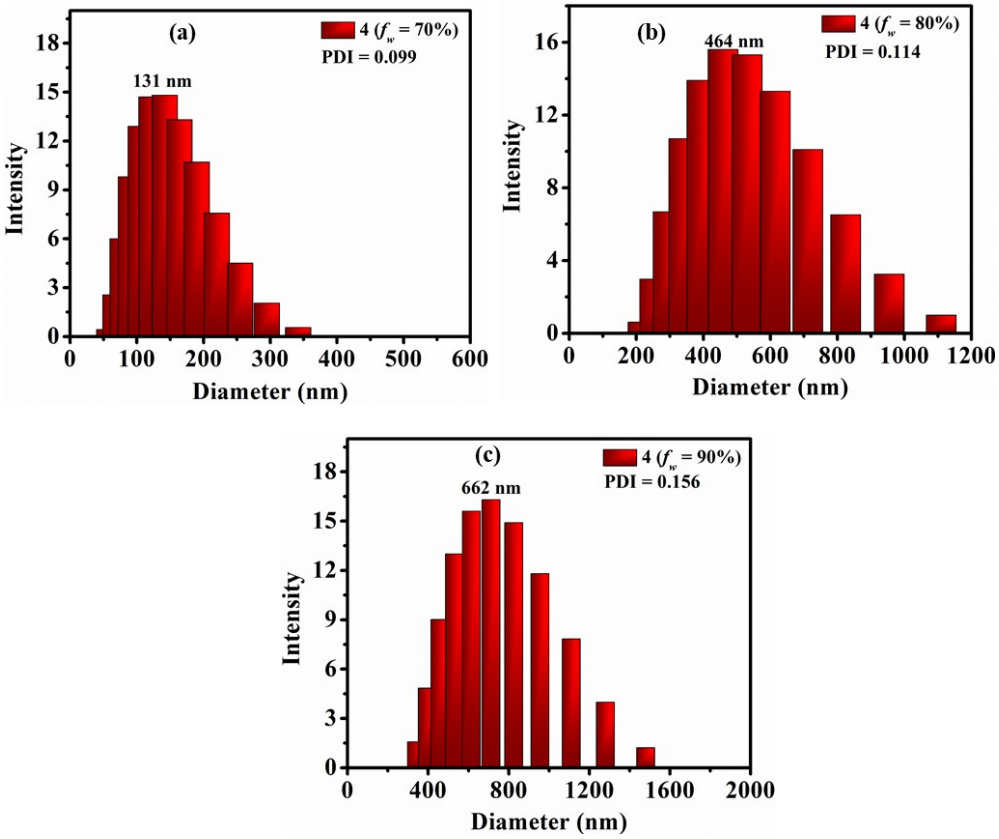


Fig S11. DLS plot of **4** obtained from 70 (**a**), 80 (**b**) and 90% (**c**) f_w of THF–H_2O suspension.

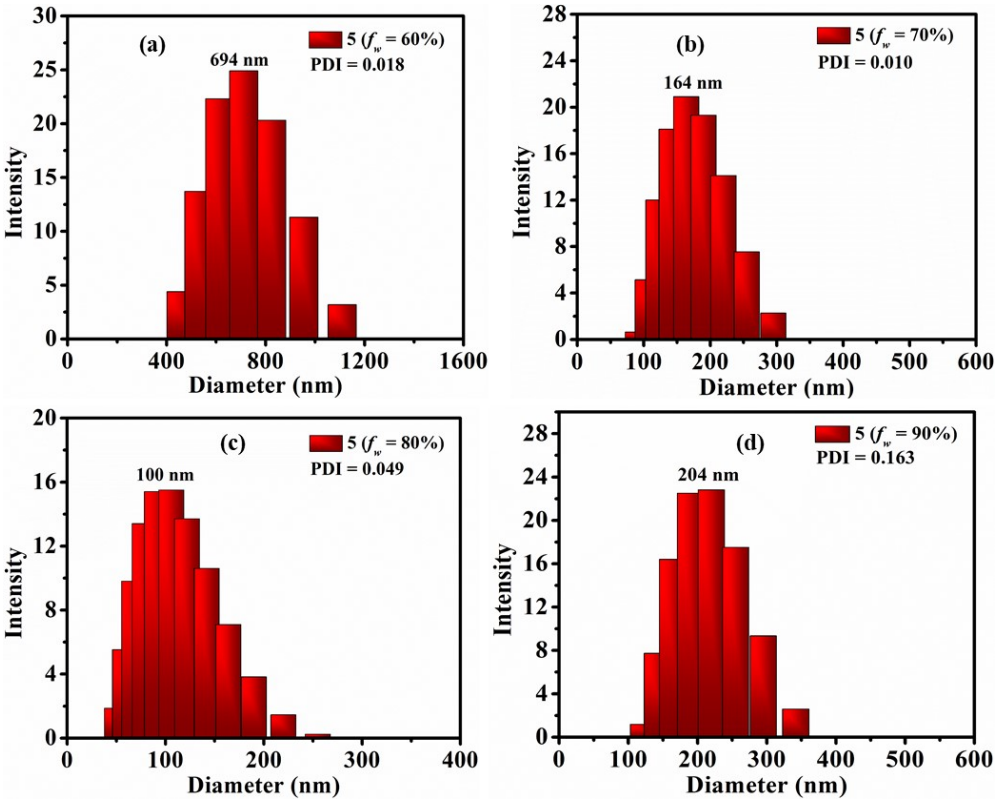


Fig S12. DLS plot of **5** obtained from 60 (**a**), 70 (**b**), 80 (**c**) and 90% (**d**) f_w of THF–H_2O suspension.

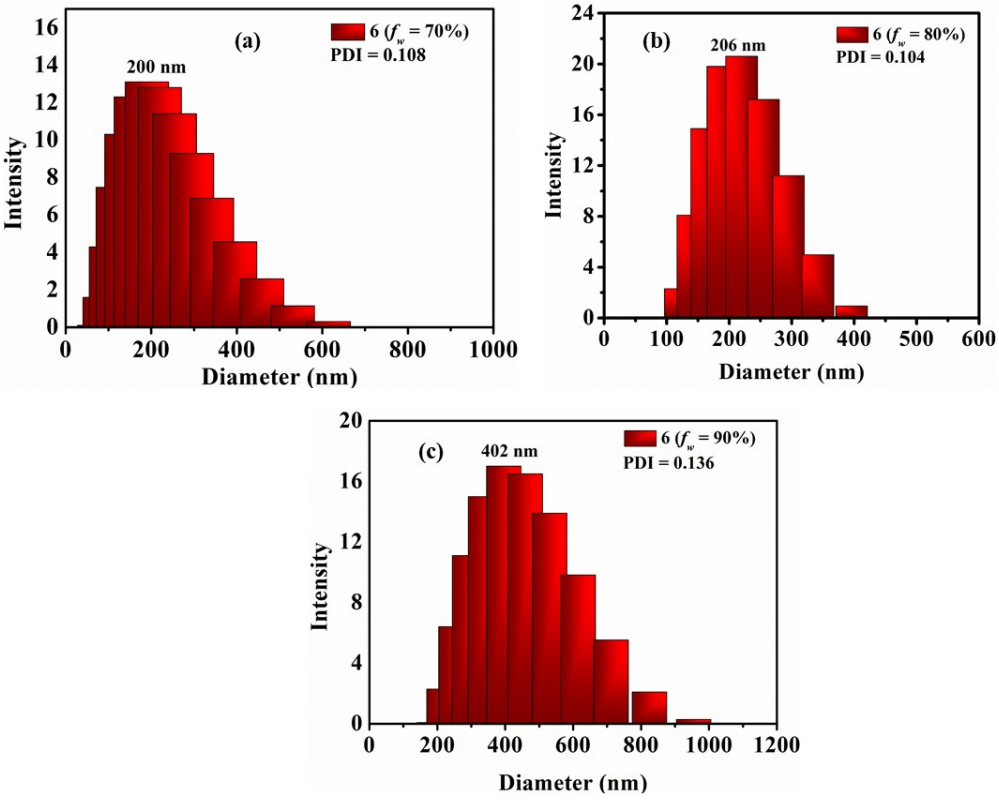


Fig S13. DLS plot of **6** obtained from 70 (**a**), 80 (**b**) and 90% (**c**) f_w of THF–H_2O suspension.

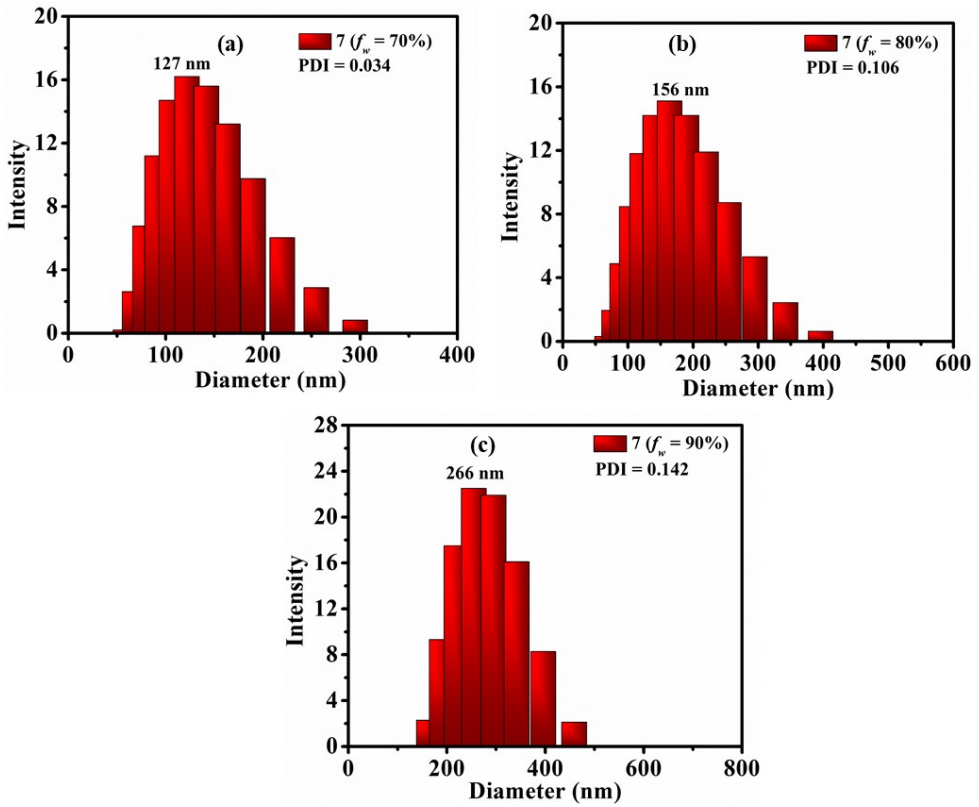


Fig. S14. DLS plot of **7** obtained from 70 (**a**), 80 (**b**) and 90% (**c**) f_w of THF–H_2O suspension.

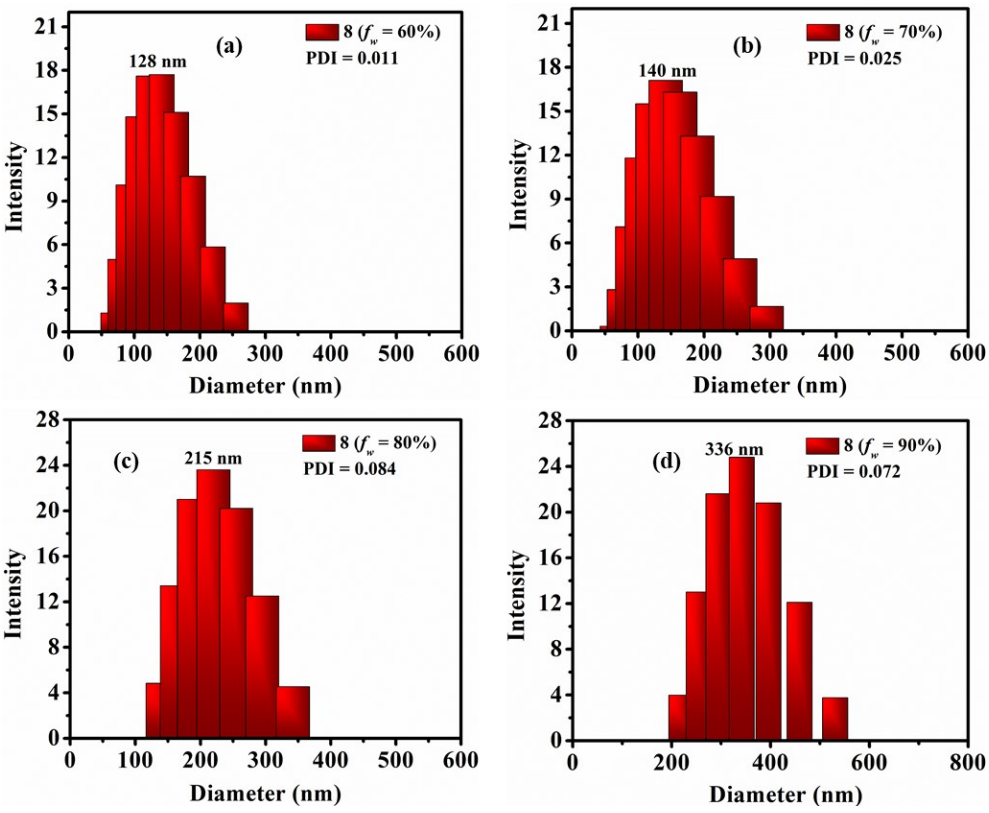


Fig. S15. DLS plot of **8** obtained from 60 (**a**), 70 (**b**), 80 (**a**) and 90% (**c**) f_w of THF–H_2O suspension.

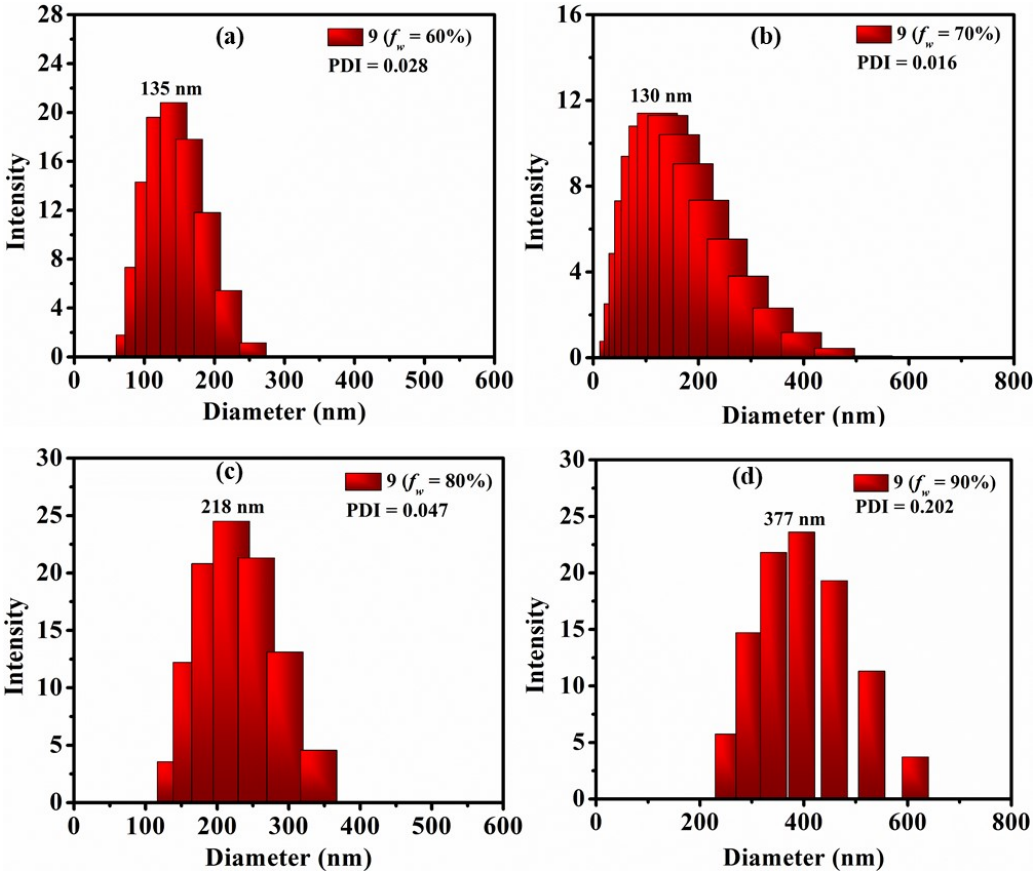


Fig. S16. DLS plot of **9** obtained from 60 (**a**), 70 (**b**), 80 (**a**) and 90% (**c**) f_w of THF–H_2O suspension.

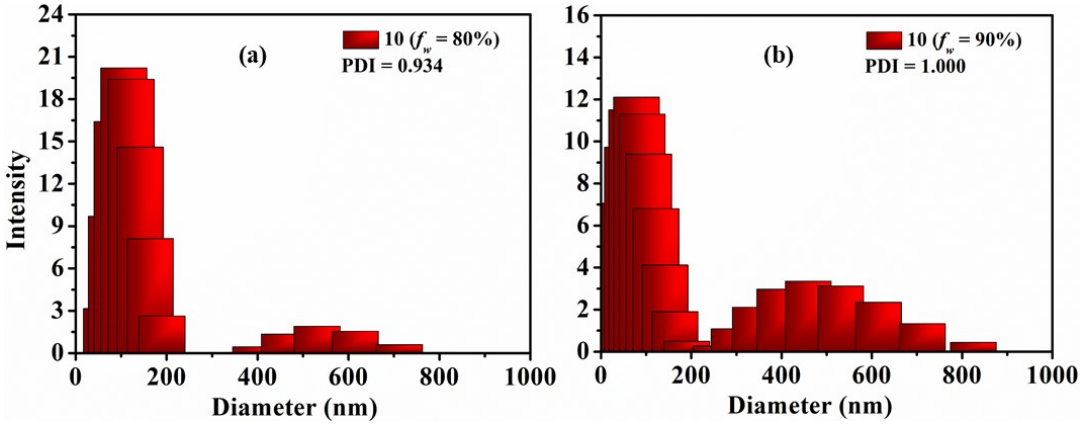


Fig. S17. DLS plot of **10** obtained from 80 (**a**) and 90% (**b**) f_w of THF–H_2O suspension.

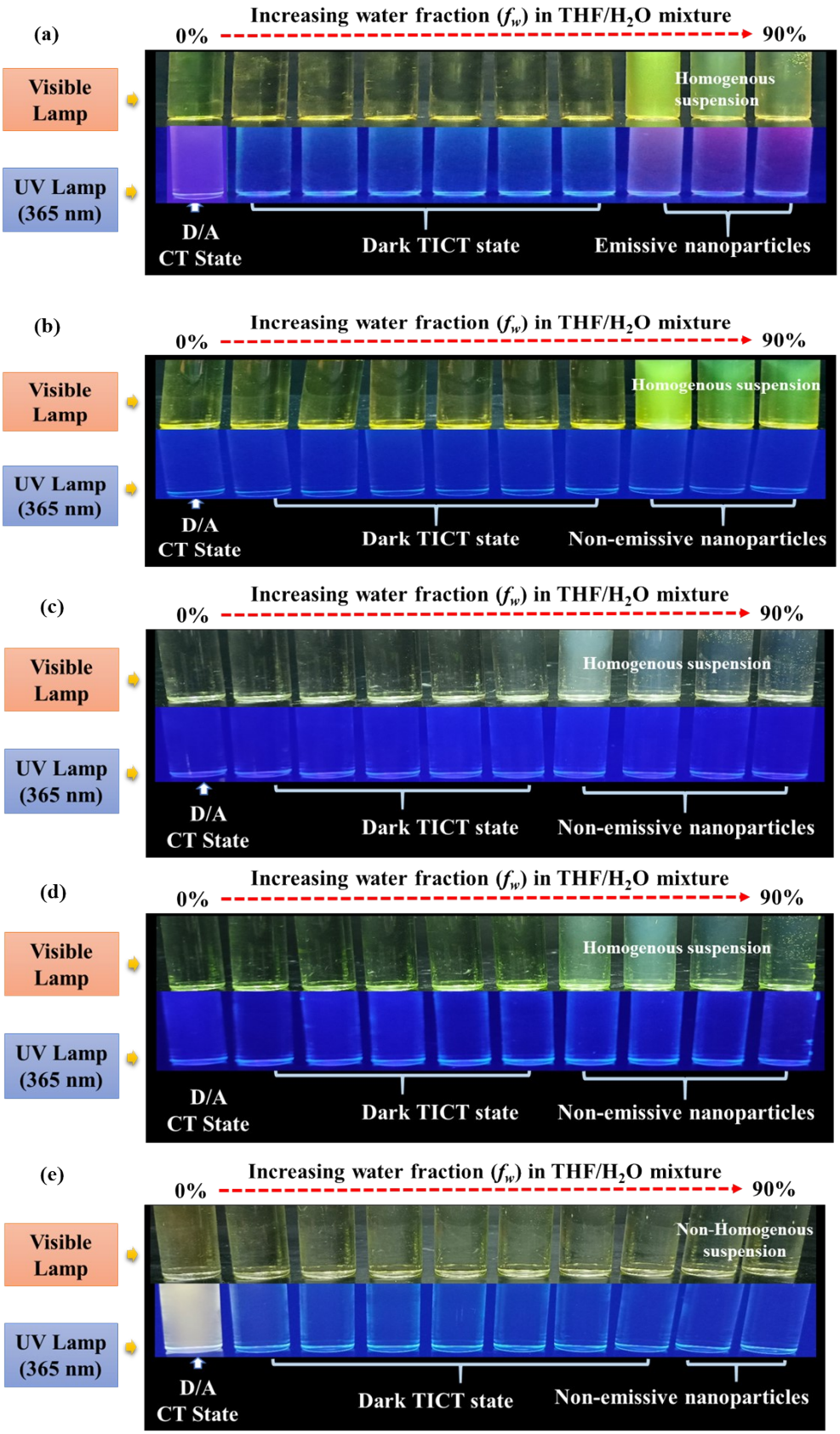


Fig. S18. Emission images of **4** (**a**), **6** (**b**), **8** (**c**), **9** (**d**) and **10** (**e**) recorded in 10 μM solution of different THF-H_2O mixture with increasing percentage of water fraction (f_w).

4. Cyclic voltammogram of compounds in anhydrous dichloromethane.

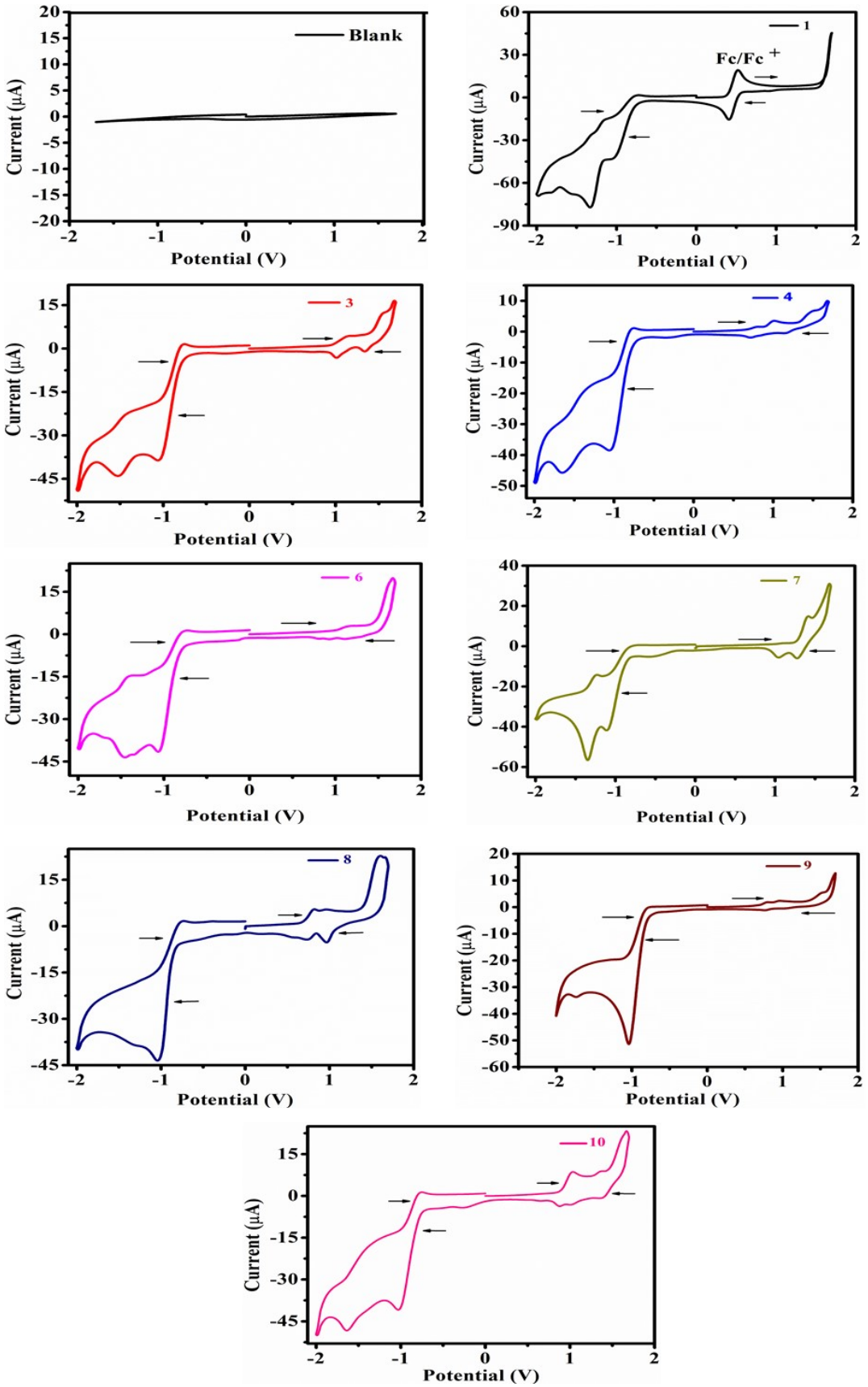


Fig. S19. Cyclic voltammogram (full scan) of blank, **1**, **3**, **4**, **6**, **7**, **8**, **9**, **10**.

5. MALDI-TOF Spectra.

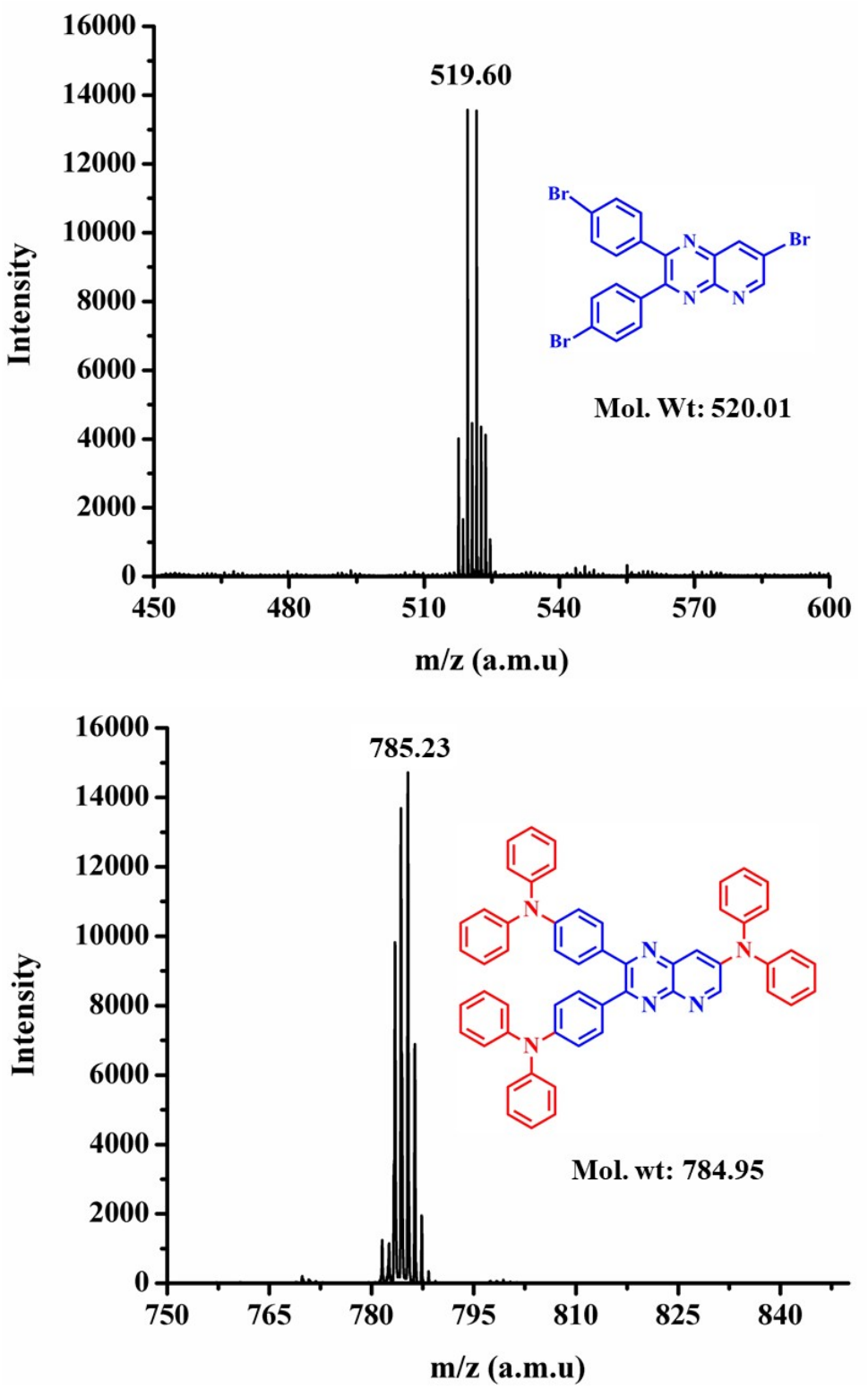


Fig. S20. MALDI-TOF spectrum of compound **1** (**above**) and **2** (**below**).

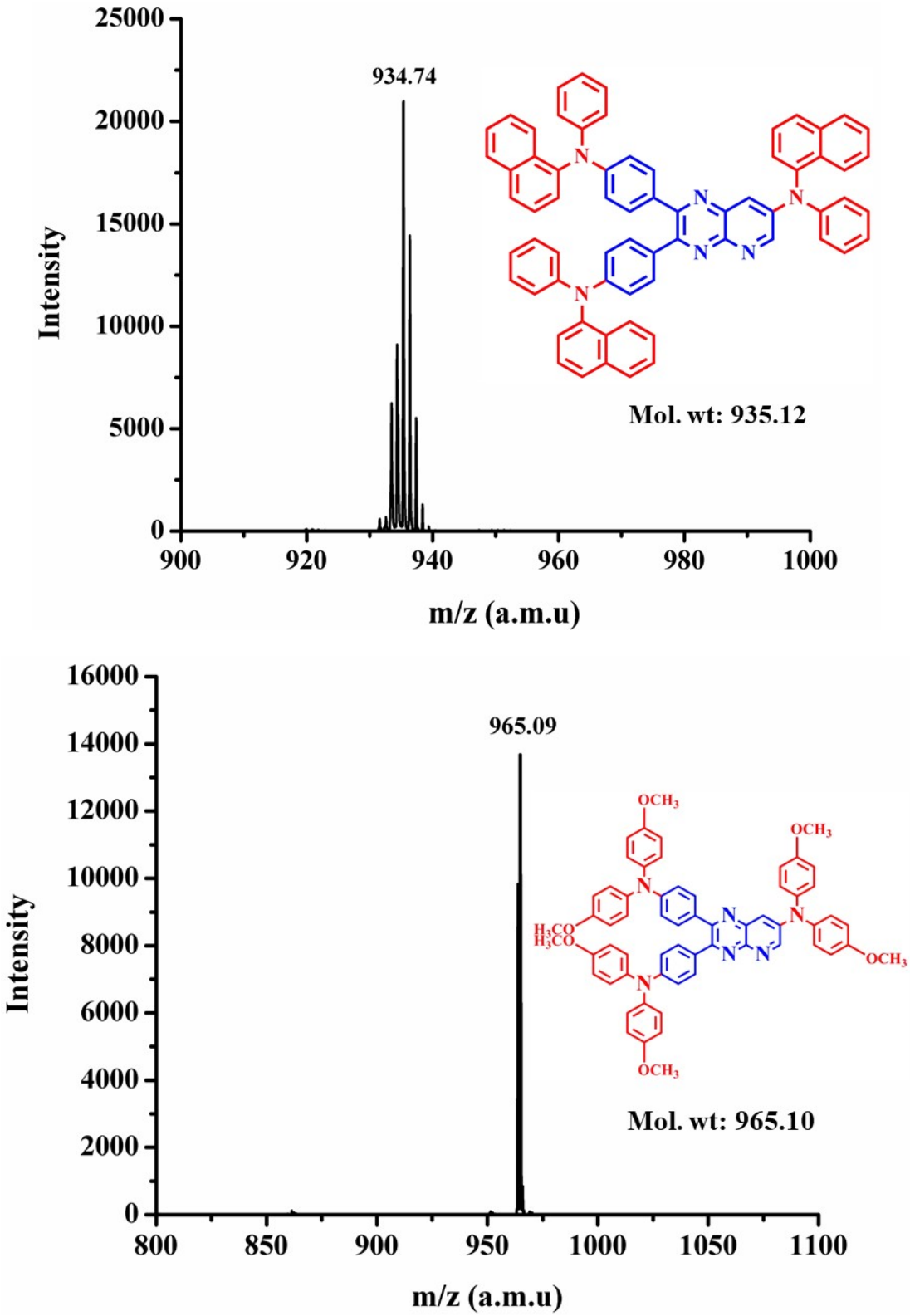


Fig. S21. MALDI-TOF spectrum of compound **3** (**above**) and **4** (**below**).

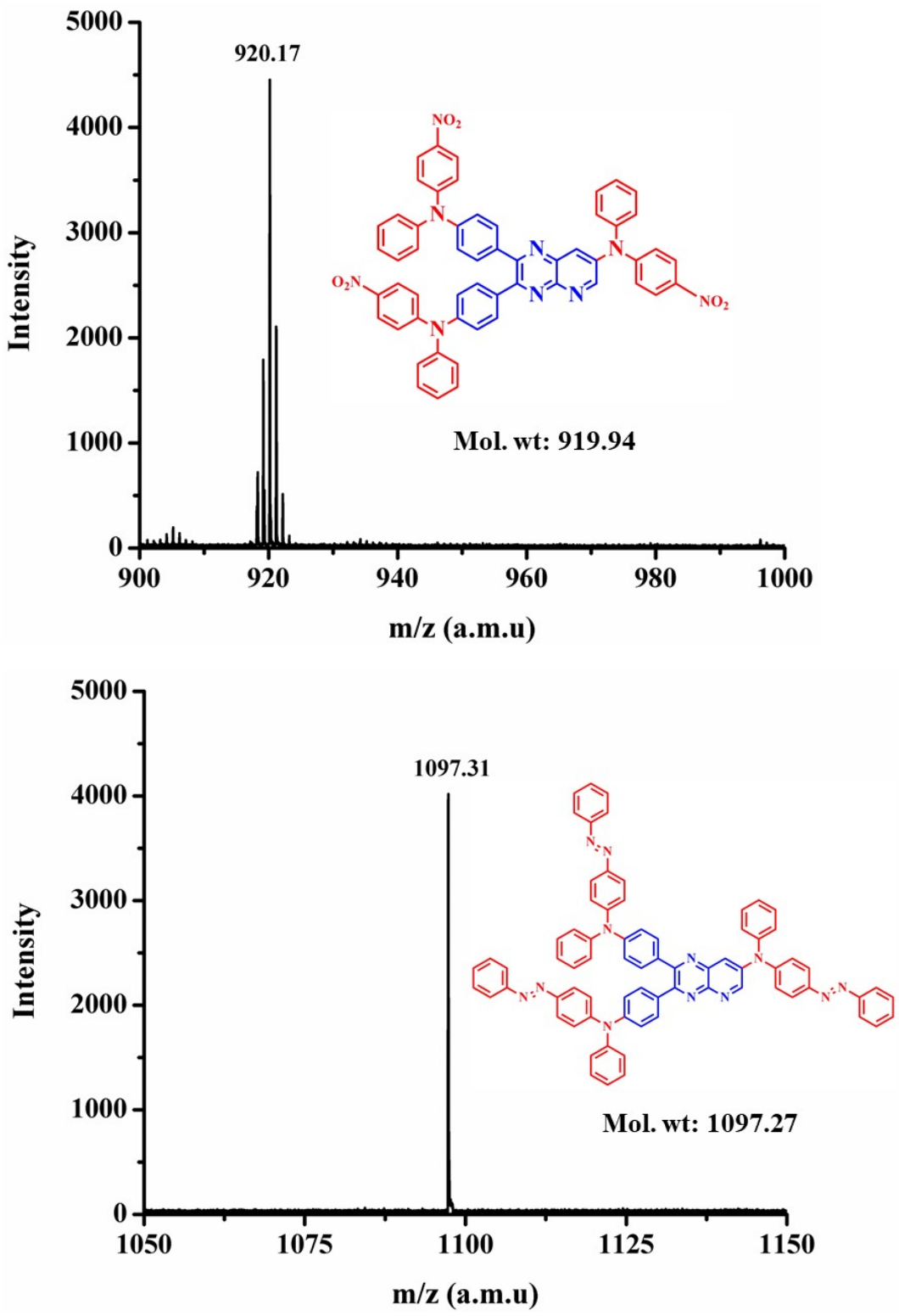


Fig. S22. MALDI-TOF spectrum of compound **5** (**above**) and **6** (**below**).

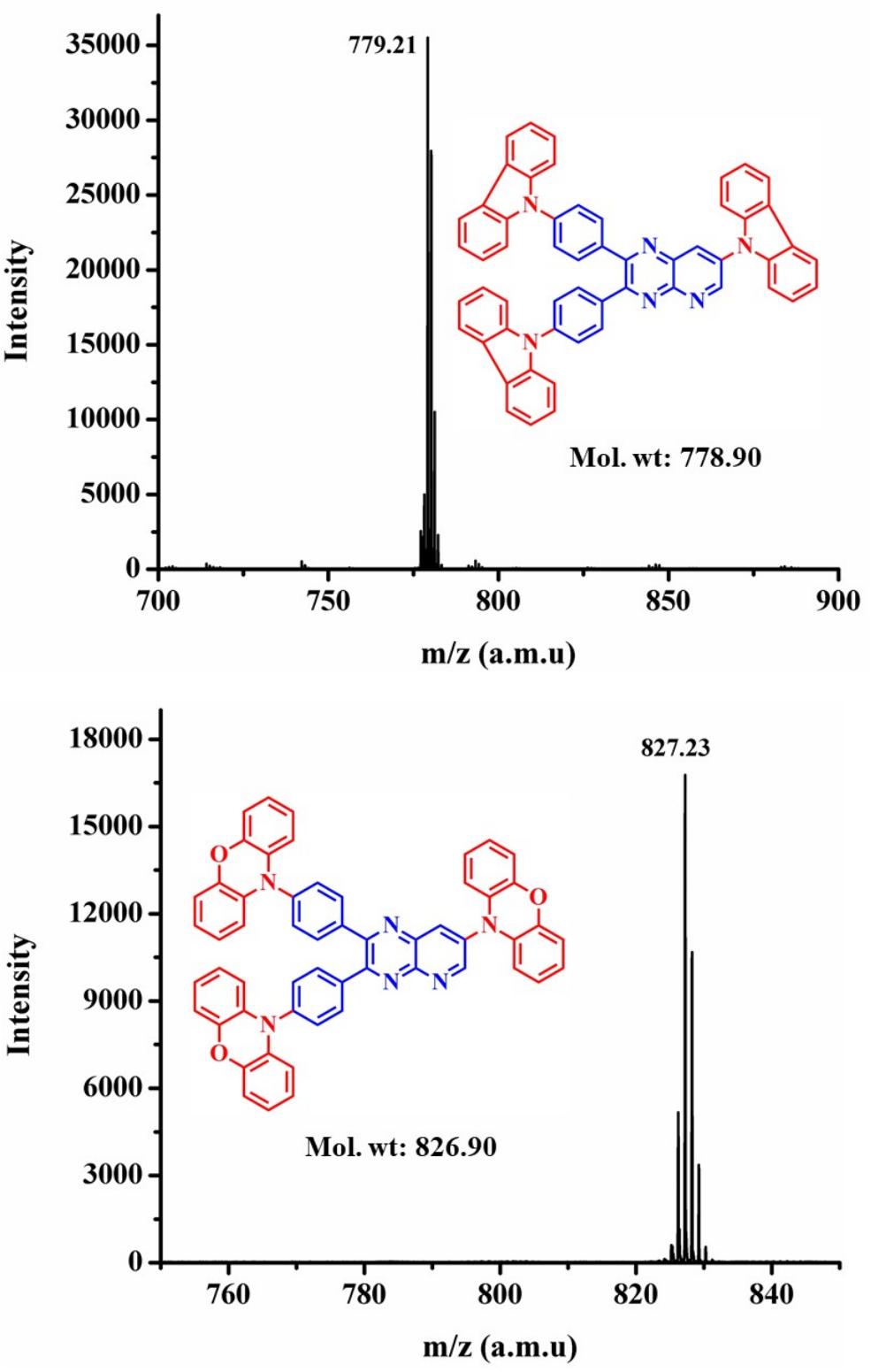


Fig. S23. MALDI-TOF spectrum of compound **7** (**above**) and **8** (**below**).

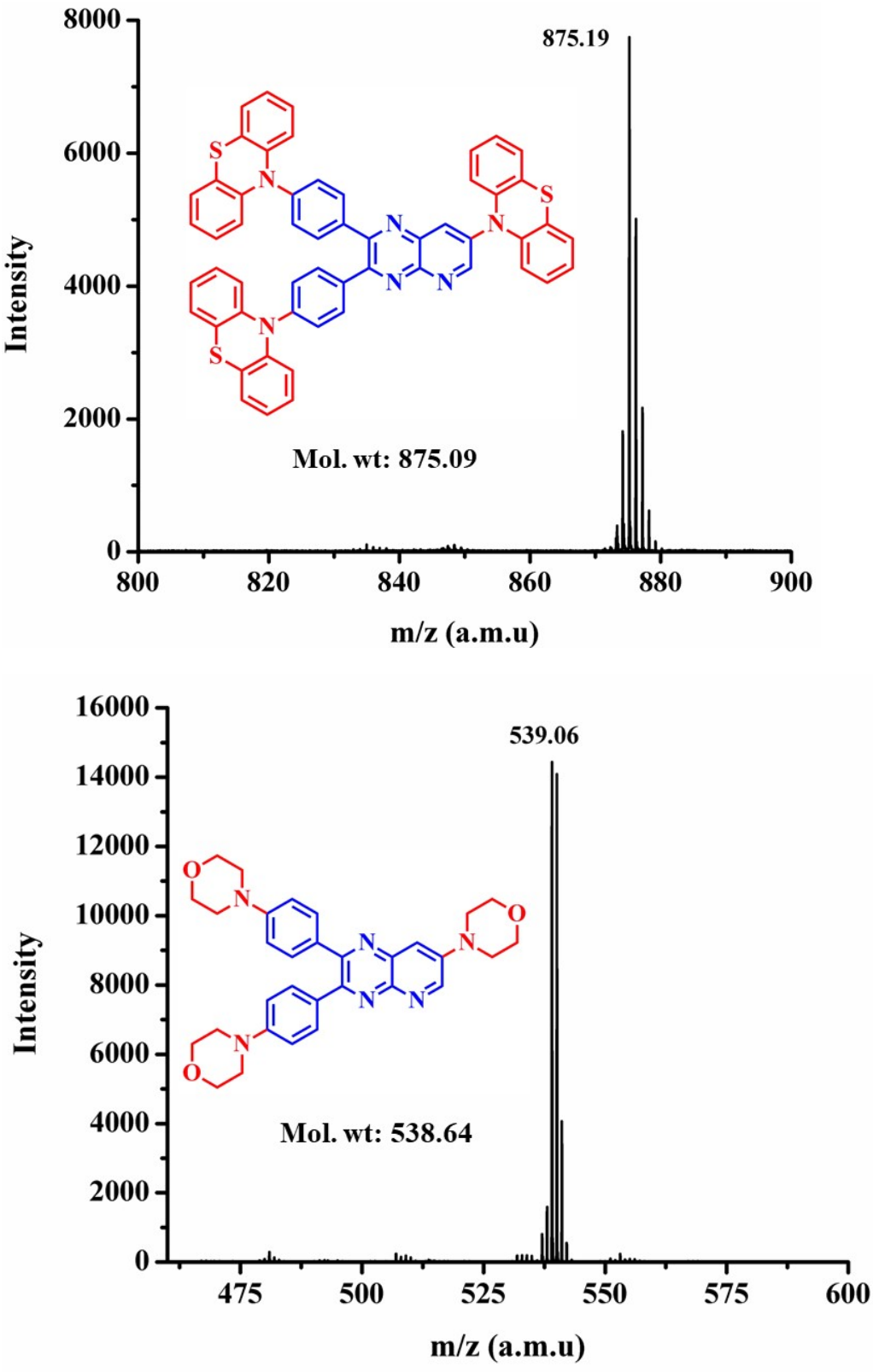


Fig. S24. MALDI-TOF spectrum of compound **9** (**above**) and **10** (**below**).

6. FT-IR Spectra.

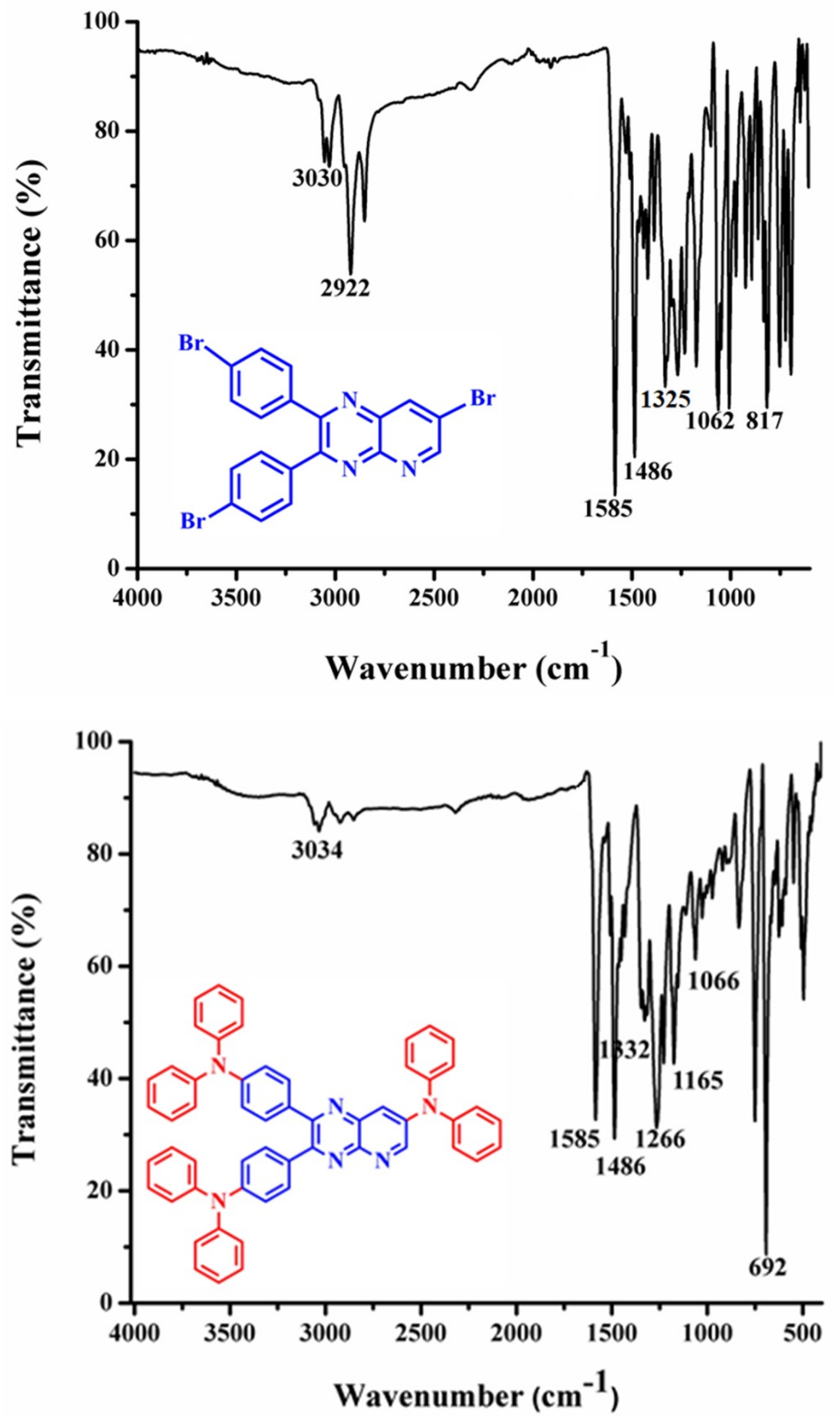
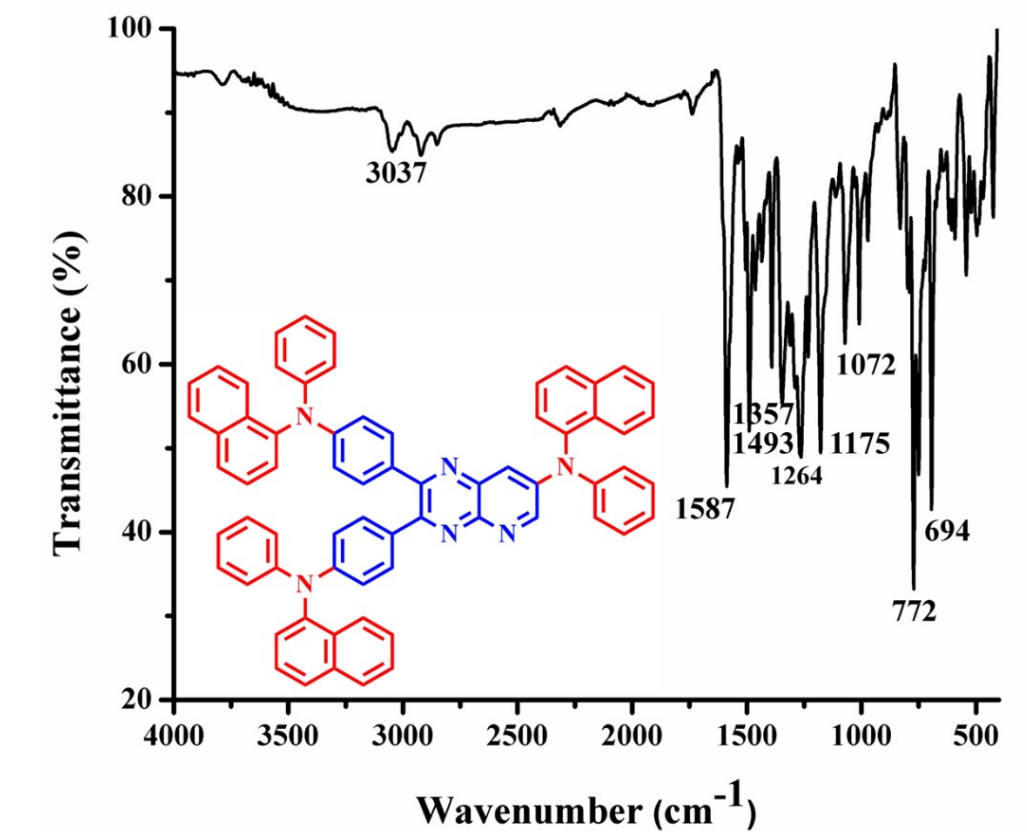


Fig. S25. FTIR spectrum of compound **1** (**above**) and **2** (**below**).



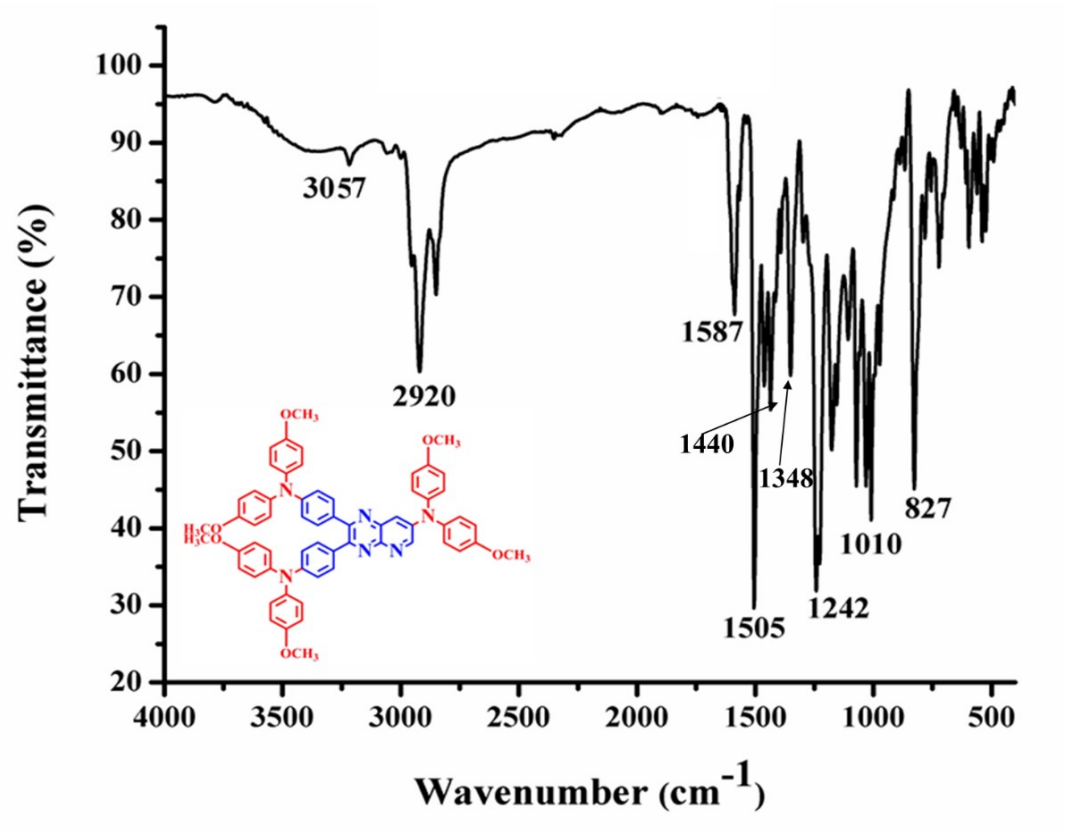
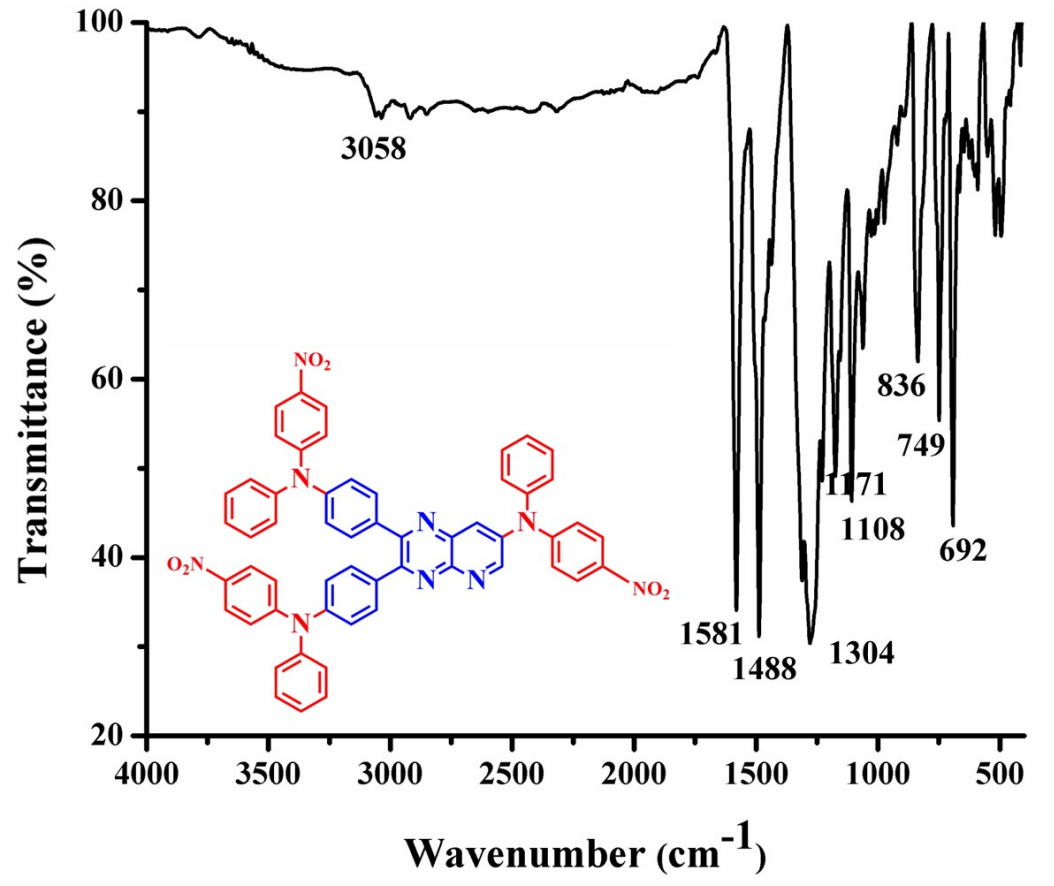


Fig. S26. FTIR spectrum of compound **3** (**above**) and **4** (**below**).



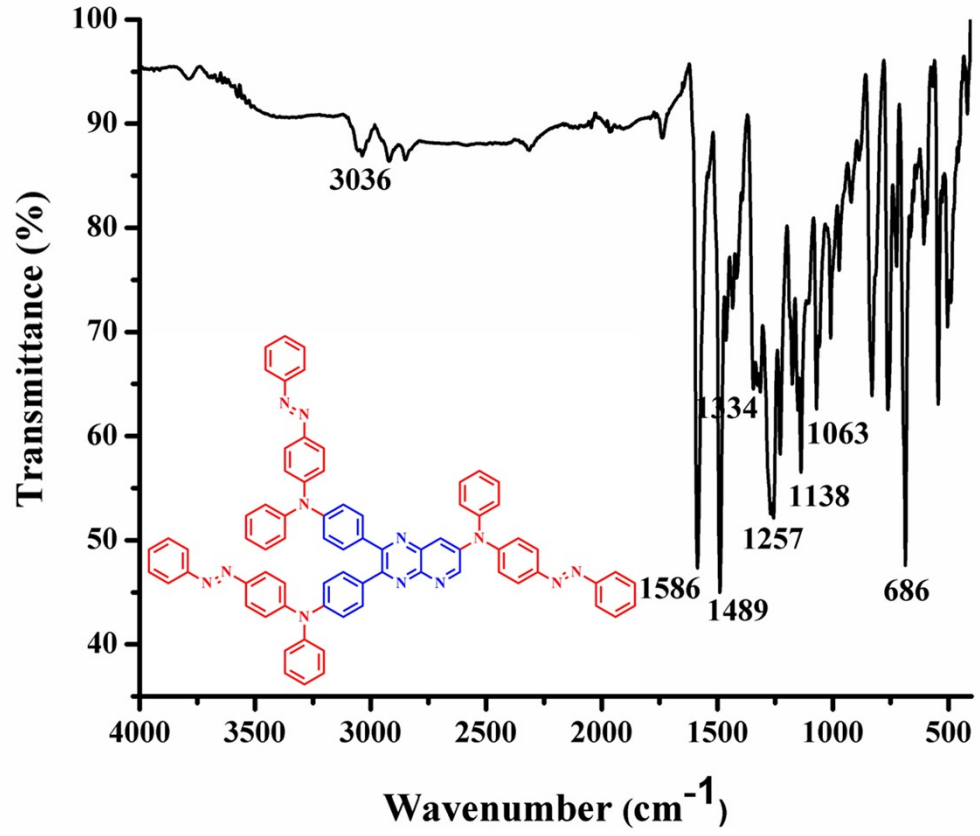


Fig. S27. FTIR spectrum of compound **5** (**above**) and **6** (**below**).

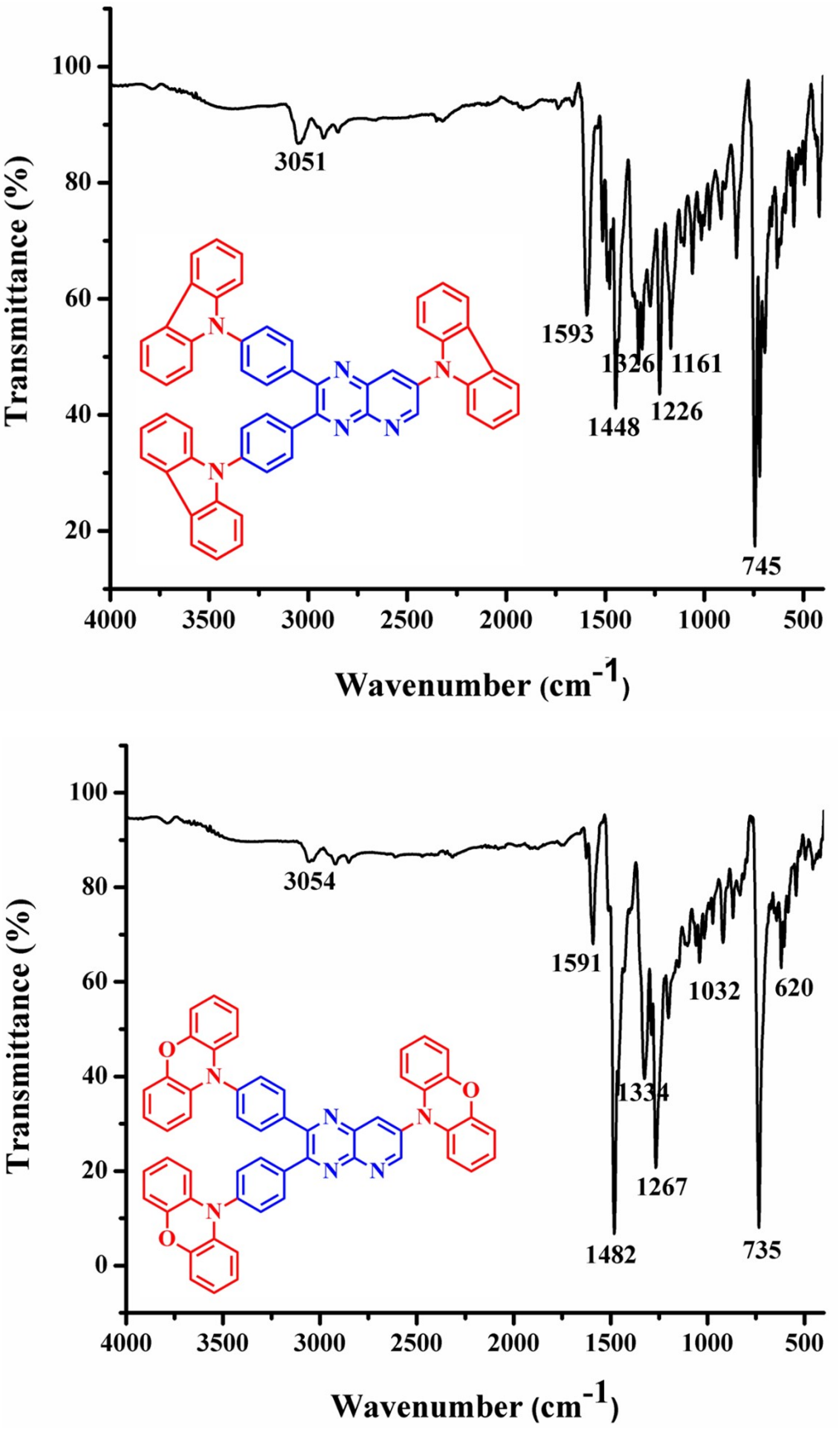


Fig. S28. FTIR spectrum of compound **7** (**above**) and **8** (**below**).

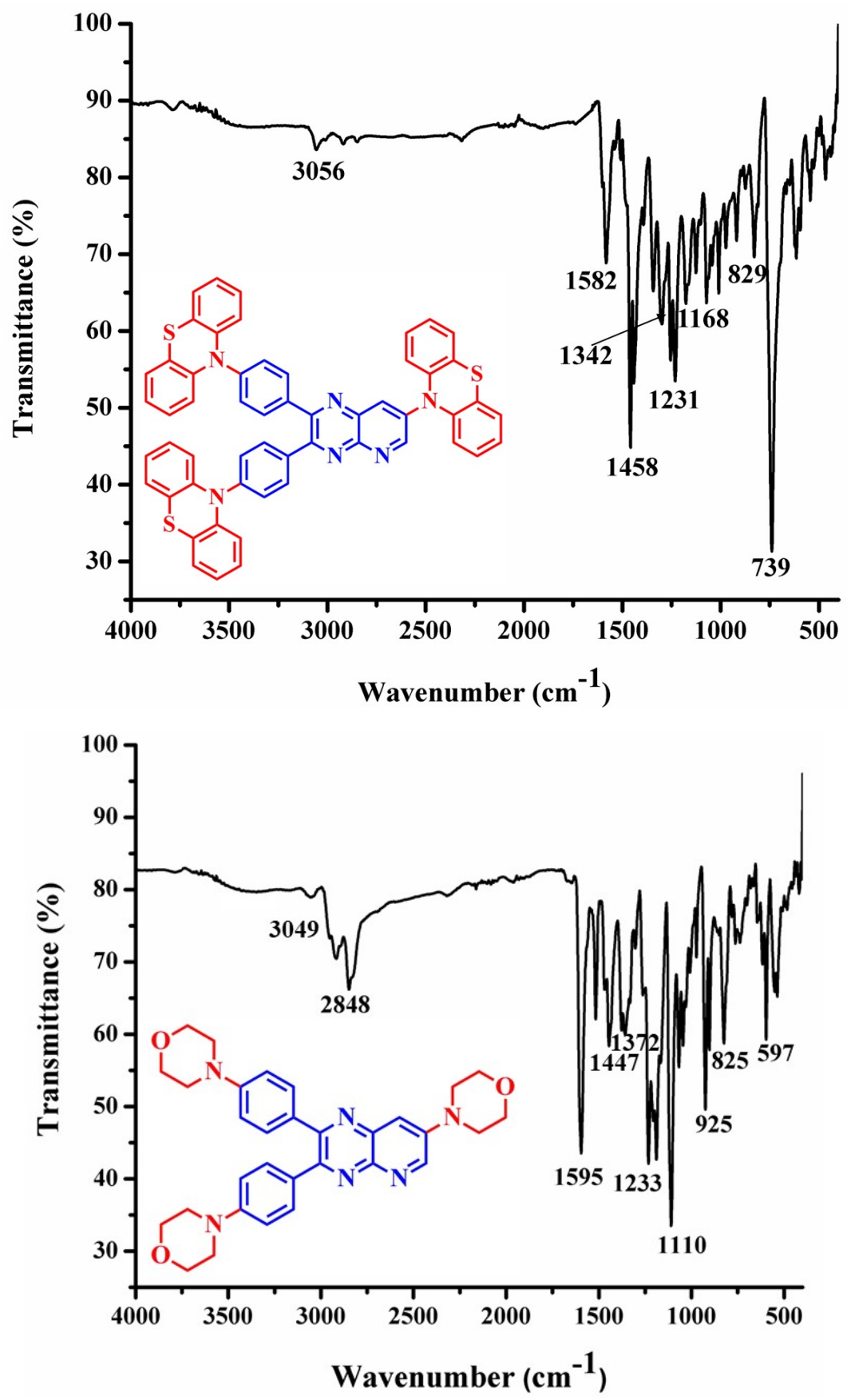


Fig. S29. FTIR spectrum of compound **9** (**above**) and **10** (**below**).

7. ^{1}H and ^{13}C NMR spectra.

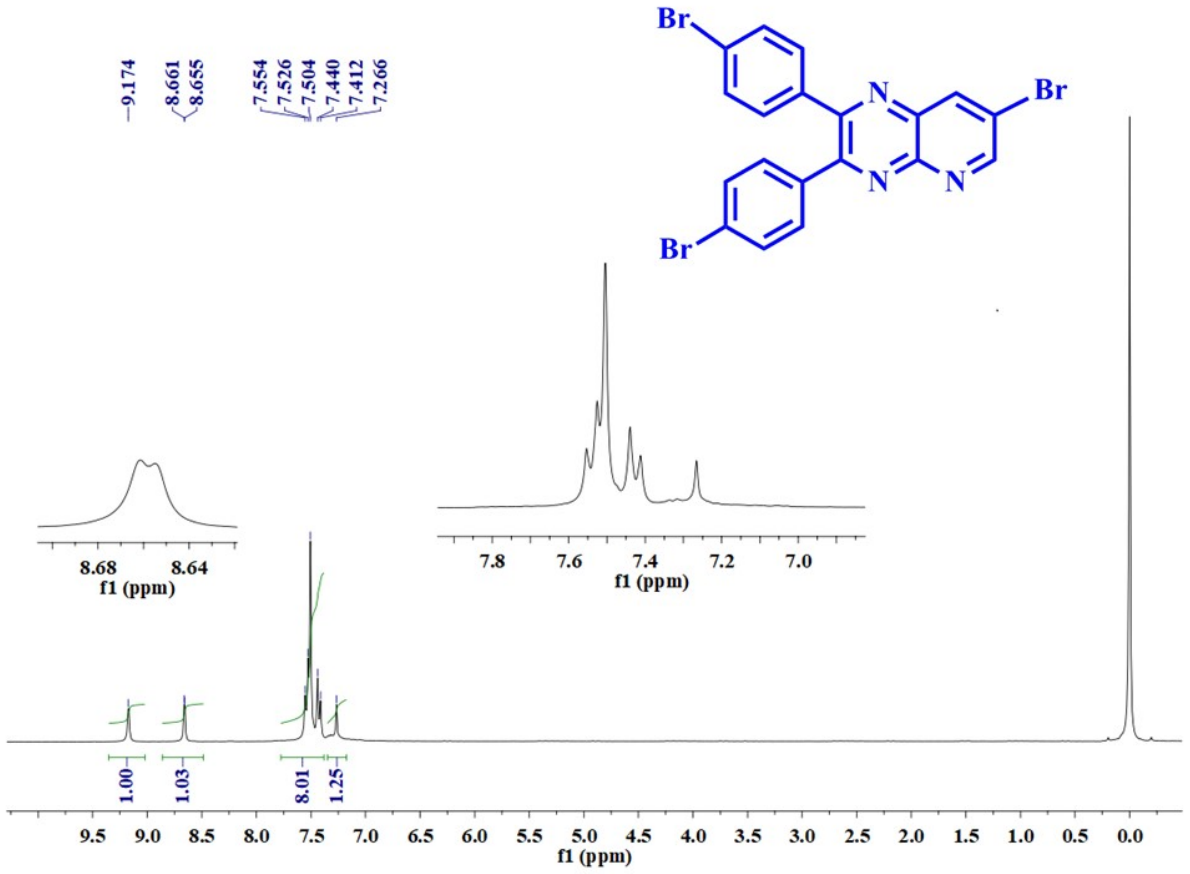


Fig. S30. ^{1}H NMR spectrum of compound **1**.

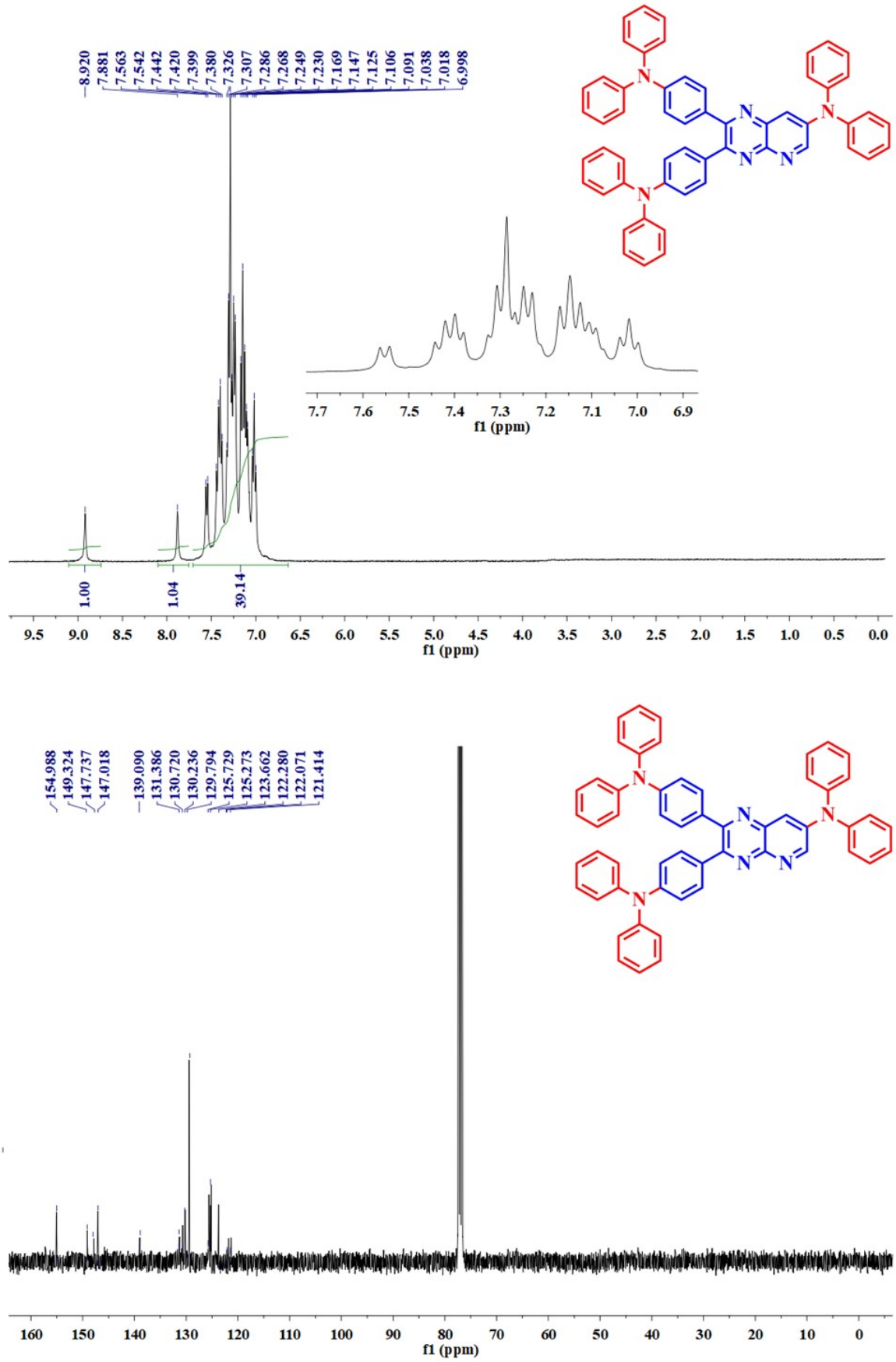


Fig. S31. ^{1}H (**above**) and ^{13}C (**below**) NMR spectrum of compound **2**.

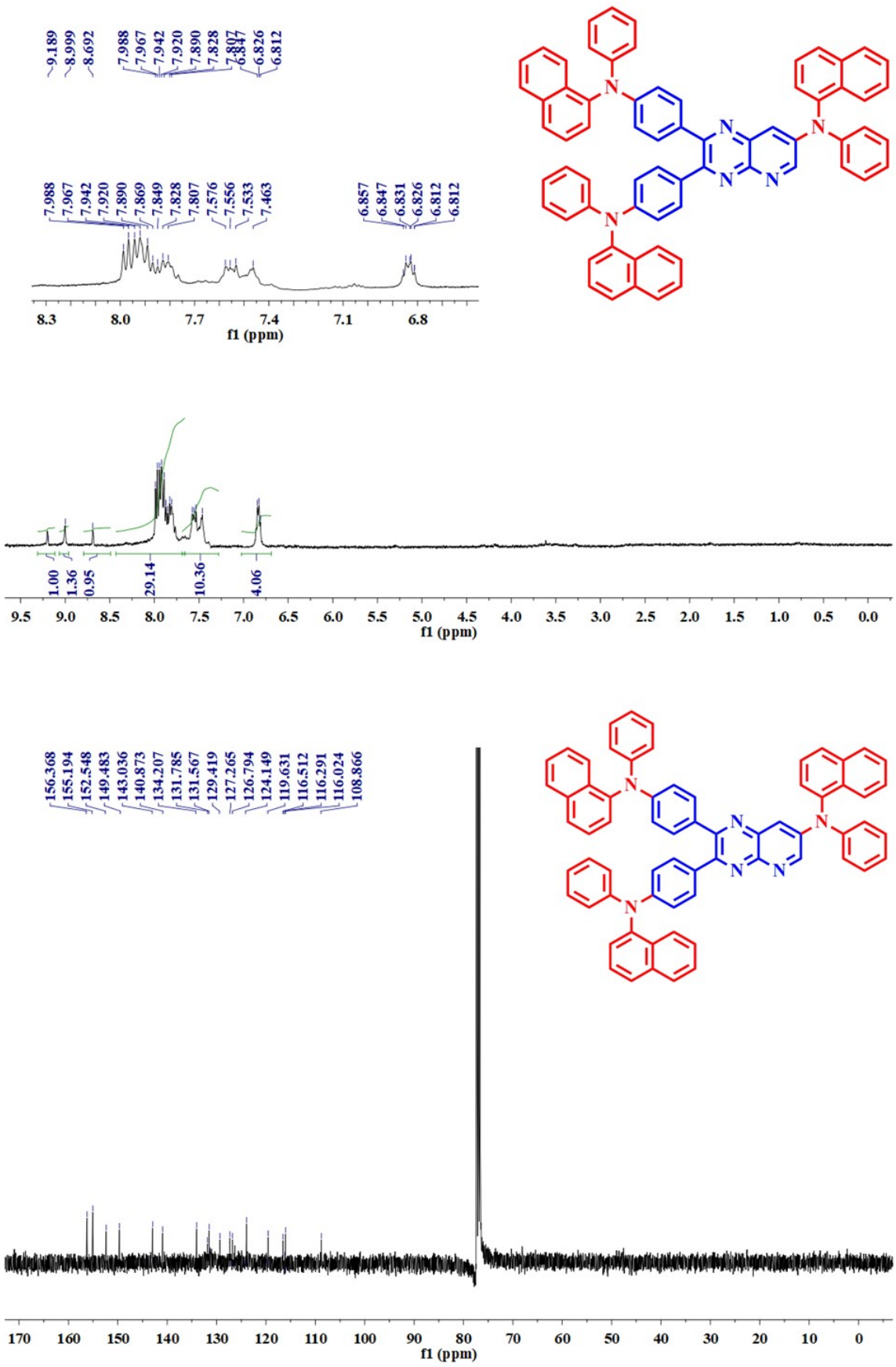


Fig. S32. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **3**.

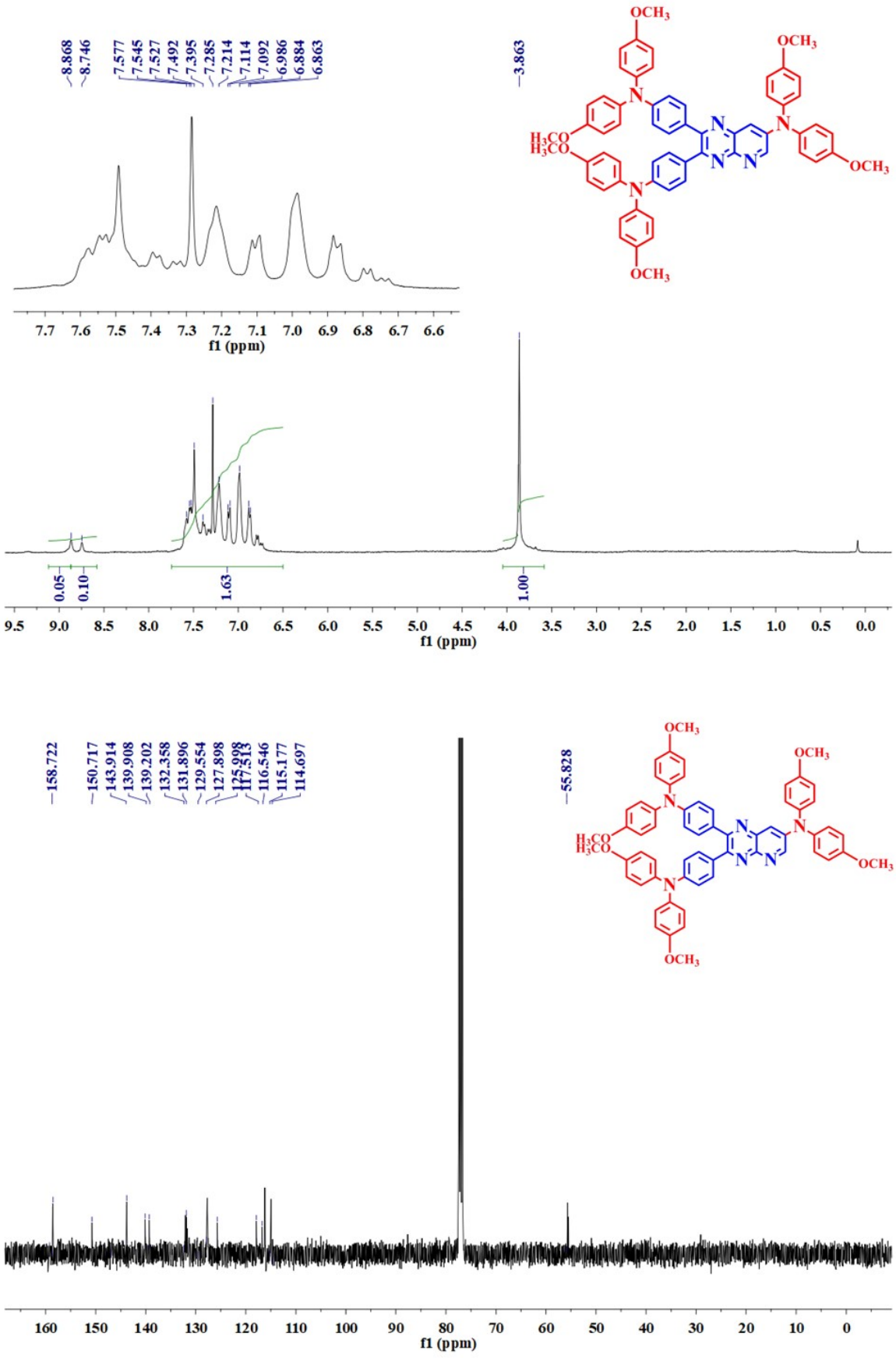


Fig. S33. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **4**.

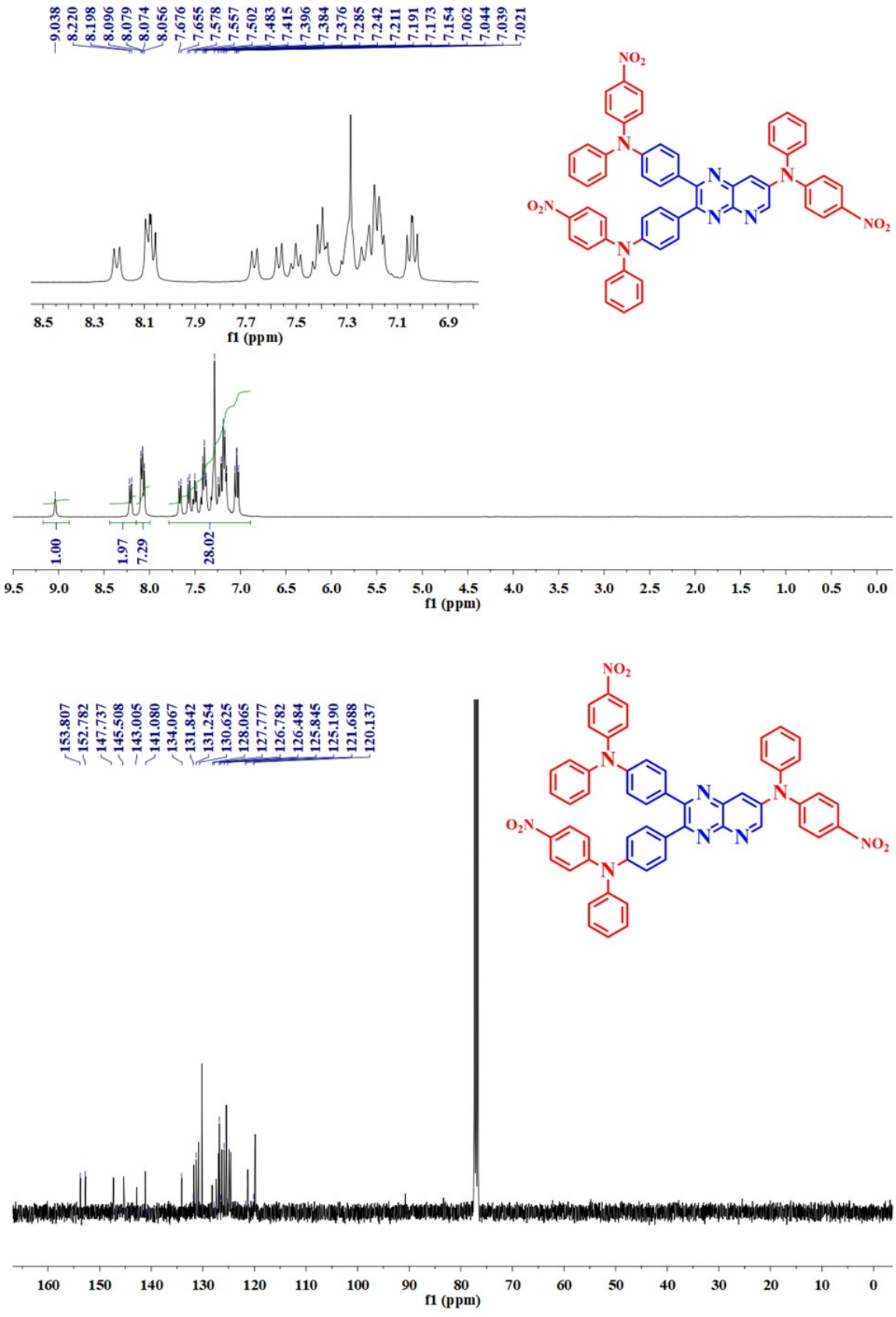


Fig. S34. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **5**.

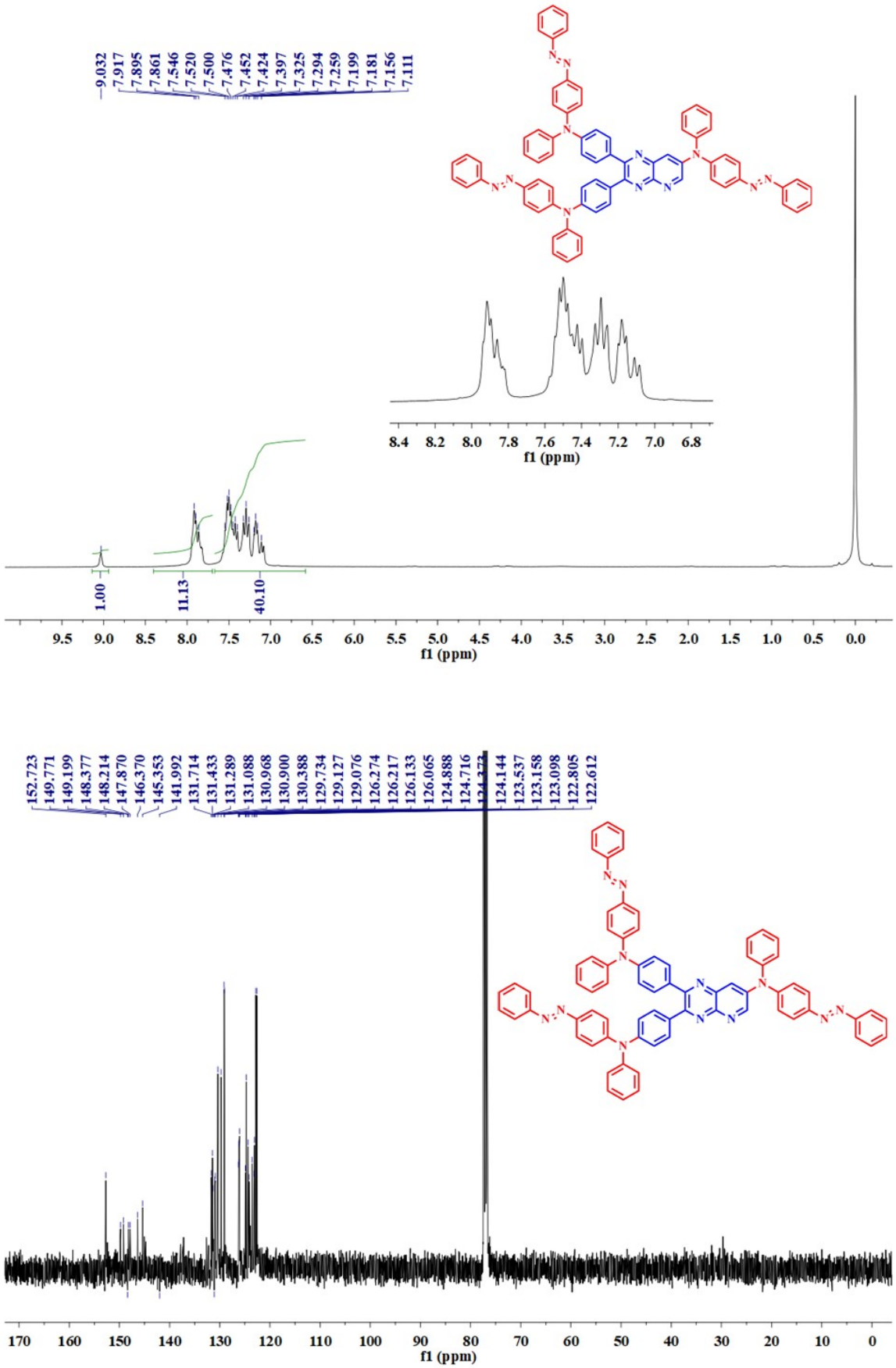


Fig. S35. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **6**.

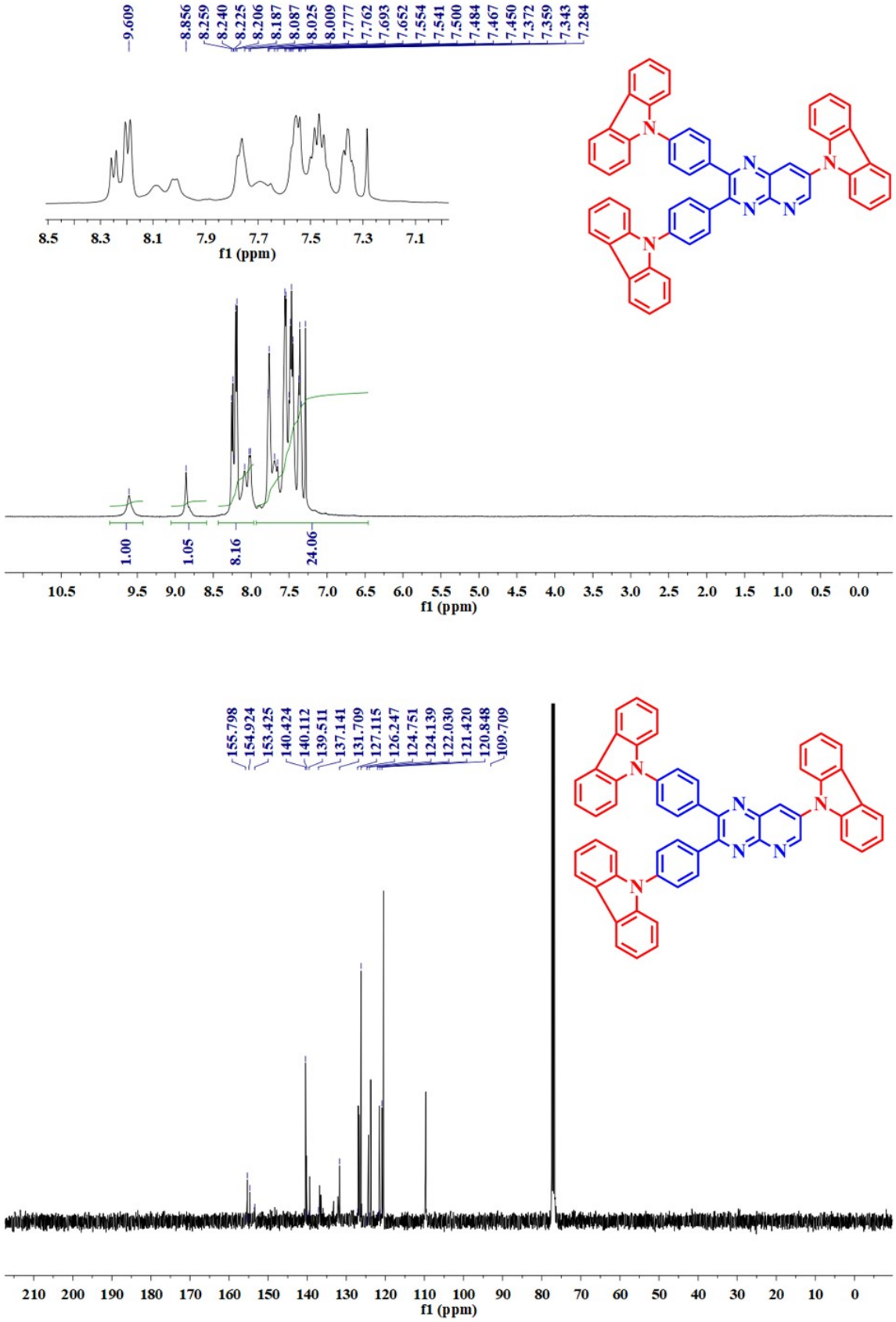


Fig. S36. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **7**.

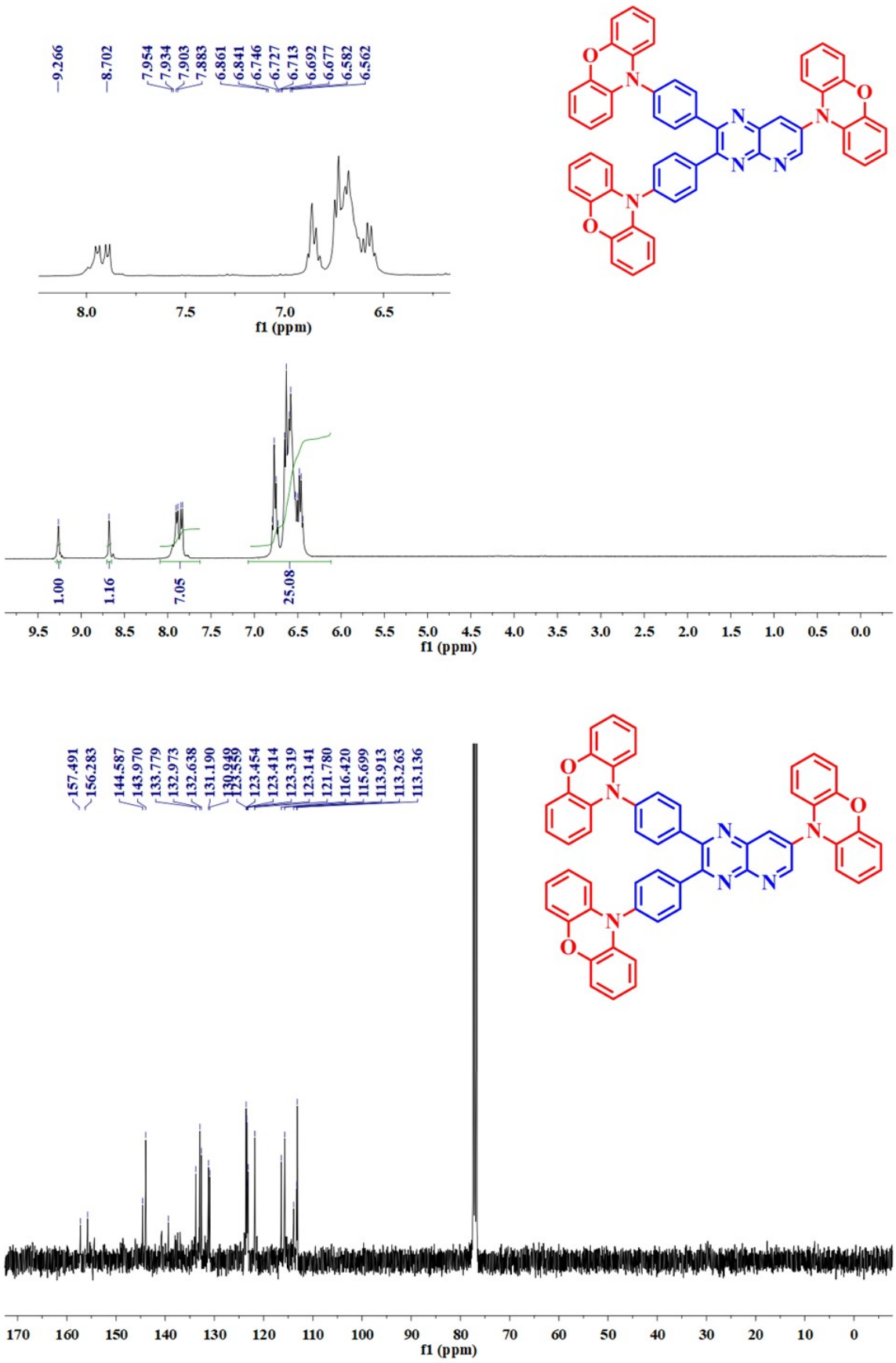


Fig. S37. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **8**.

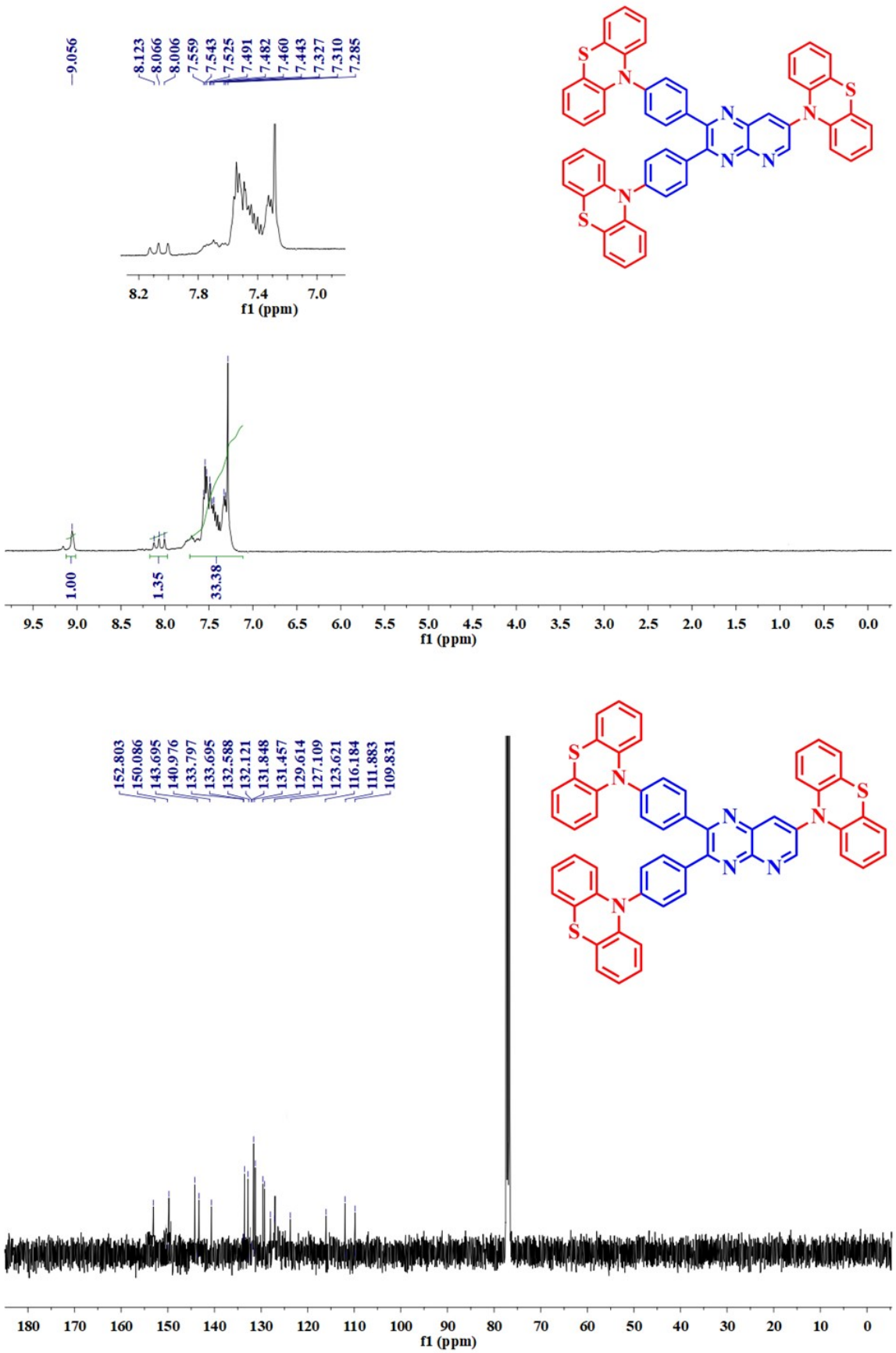


Fig. S38. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **9**.

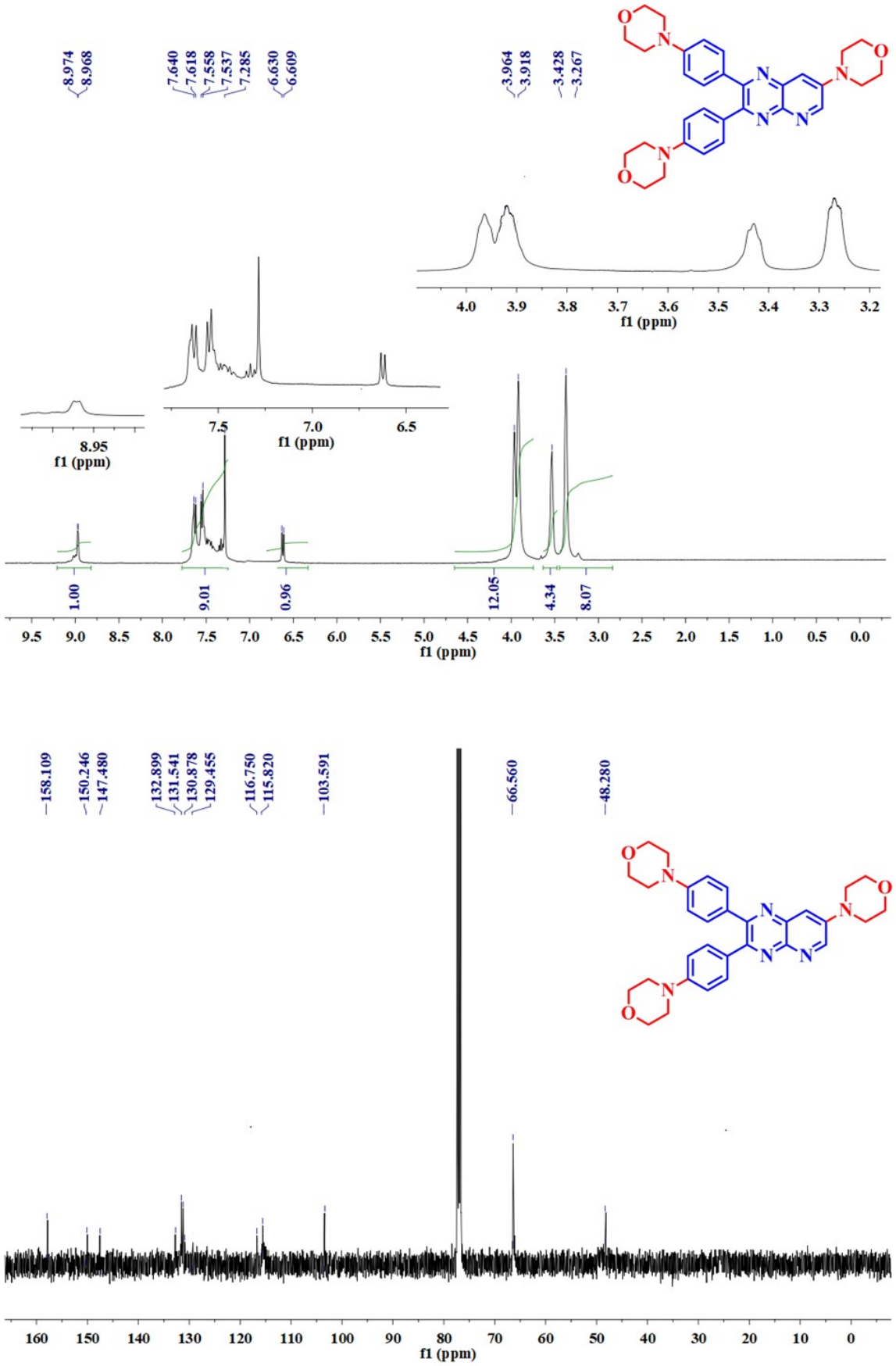


Fig. S39. ^{1}H (**above**) and ^{13}C (**below**) spectrum of compound **10**.

8. Simulated absorption plot in various solvents and gas phase.

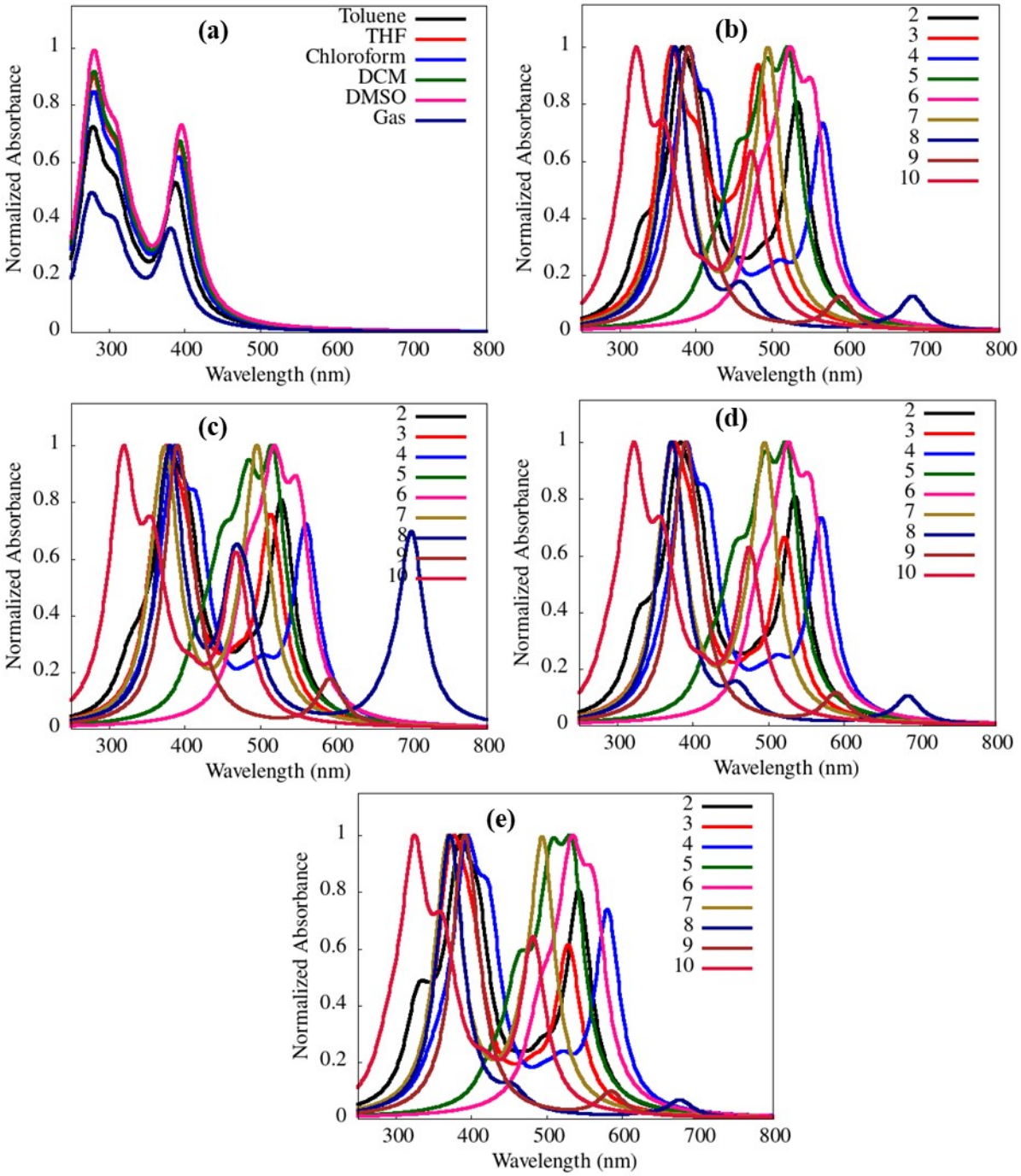


Fig. S40. Simulated absorption plot of **1** in various solvents and in gas phase (**a**), simulated absorption plot of **2**−**10** in THF (**b**), chloroform (**c**), DCM (**d**) and DMSO (**e**).

9. Vertical electronic Transition, absorption wavelength and oscillator strength in various solvents and in gas phase

Table S1. Vertical electronic Transition, absorption wavelength and oscillator strength of **1** in various solvents and in gas phase.

Molecule 1			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	390.1nm (3.2eV)	0.0042	(HOMO-2 -> LUMO) (95%)
	382.2nm (3.2eV)	0.3345	(HOMO -> LUMO) (96%)
	336.3nm (3.7eV)	0.0374	(HOMO-1 -> LUMO) (96%)
	309.8nm (4.0eV)	0.1836	(HOMO -> LUMO+1) (84%) (HOMO-3 -> LUMO) (11%)
	307.2nm (4.0eV)	0.0223	(HOMO-4 -> LUMO) (63%) (HOMO-3 -> LUMO) (25%)
	304.6nm (4.1eV)	0.0162	(HOMO-2 -> LUMO+1) (57%) (HOMO-3 -> LUMO) (27%)
	299.3nm (4.1eV)	0.0438	(HOMO-2 -> LUMO+1) (29%) (HOMO-4 -> LUMO) (27%) (HOMO-3 -> LUMO) (27%) (HOMO-3 -> LUMO) (27%)
	292.1nm (4.2eV)	0.0090	(HOMO-5 -> LUMO) (62%) (HOMO-9 -> LUMO) (16%)
	287.3nm (4.3eV)	0.0036	(HOMO-9 -> LUMO) (33%) (HOMO-5 -> LUMO) (32%) (HOMO-6 -> LUMO) (14%)
	275.3nm (4.5eV)	0.4024	(HOMO-1 -> LUMO+1) (76%)
Chloroform	392.4nm (3.2eV)	0.5825	(HOMO -> LUMO) (98%)
	381.2nm (3.3eV)	0.0021	(HOMO-2 -> LUMO) (96%)
	338.0nm (3.7eV)	0.0706	(HOMO-1 -> LUMO) (96%)
	312.2nm (4.0eV)	0.2741	(HOMO -> LUMO+1) (89%)
	310.7nm (4.0eV)	0.0215	(HOMO-3 -> LUMO) (88%)
	303.8nm (4.1eV)	0.0855	(HOMO-4 -> LUMO) (80%)
	295.6nm (4.2eV)	0.0173	(HOMO-2 -> LUMO+1) (72%)
	293.9nm (4.2eV)	0.0062	(HOMO-5 -> LUMO) (86%)
	283.8nm (4.4eV)	0.0109	(HOMO-9 -> LUMO) (54%) (HOMO-6 -> LUMO) (18%)
	277.8nm (4.5eV)	0.7119	(HOMO-1 -> LUMO+1) (87%)
Dichloromethane	394.5nm (3.1eV)	0.6372	(HOMO -> LUMO) (99%)
	379.2nm (3.3eV)	0.0017	(HOMO-2 -> LUMO) (95%)
	338.4nm (3.7eV)	0.0776	(HOMO-1 -> LUMO) (95%)
	312.6nm (4.0eV)	0.2932	(HOMO -> LUMO+1) (90%)
	311.3nm (4.0eV)	0.0234	(HOMO-3 -> LUMO) (90%)
	304.2nm (4.1eV)	0.0967	(HOMO-4 -> LUMO) (85%)

	294.7nm (4.2eV)	0.0106	(HOMO-5 -> LUMO) (58%) (HOMO-2 -> LUMO+1) (27%)
	293.9nm (4.2eV)	0.0111	(HOMO-2 -> LUMO+1) (55%) (HOMO-5 -> LUMO) (34%)
	282.7nm (4.4eV)	0.0110	(HOMO-9 -> LUMO) (52%) (HOMO-6 -> LUMO) (19%)
	278.3nm (4.5eV)	0.7734	(HOMO-1 -> LUMO+1) (87%)
Dimethylsulfoxide	396.7nm (3.1eV)	0.6947	(HOMO -> LUMO) (99%)
	376.9nm (3.3eV)	0.0017	(HOMO-2 -> LUMO) (95%)
	338.7nm (3.7eV)	0.0847	(HOMO-1 -> LUMO) (95%)
	313.0nm (4.0eV)	0.3154	(HOMO -> LUMO+1) (90%)
	311.9nm (4.0eV)	0.0265	(HOMO-3 -> LUMO) (92%)
	304.7nm (4.1eV)	0.1054	(HOMO-4 -> LUMO) (89%)
	294.9nm (4.2eV)	0.0080	(HOMO-5 -> LUMO) (90%)
	292.6nm (4.2eV)	0.0137	(HOMO-2 -> LUMO+1) (82%)
	281.6nm (4.4eV)	0.0121	(HOMO-9 -> LUMO) (48%) (HOMO-6 -> LUMO) (20%)
	278.7nm (4.4eV)	0.8360	(HOMO-1 -> LUMO+1) (87%)
Tetrahydrofuran	394.0nm (3.1eV)	0.6241	(HOMO -> LUMO) (99%)
	379.7nm (3.3eV)	0.0017	(HOMO-2 -> LUMO) (96%)
	338.3nm (3.7eV)	0.0760	(HOMO-1 -> LUMO) (95%)
	312.5nm (4.0eV)	0.2885	(HOMO -> LUMO+1) (90%)
	311.2nm (4.0eV)	0.0229	(HOMO-3 -> LUMO) (90%)
	304.1nm (4.1eV)	0.0943	(HOMO-4 -> LUMO) (84%)
	294.9nm (4.2eV)	0.0129	(HOMO-2 -> LUMO+1) (47%) (HOMO-5 -> LUMO) (35%)
	294.0nm (4.2eV)	0.0090	(HOMO-5 -> LUMO) (57%) (HOMO-2 -> LUMO+1) (35%)
	283.0nm (4.4eV)	0.0110	(HOMO-9 -> LUMO) (53%) (HOMO-6 -> LUMO) (18%)
	278.2nm (4.5eV)	0.7587	(HOMO-1 -> LUMO+1) (87%)
Toluene	388.9nm (3.2eV)	0.4837	(HOMO -> LUMO) (96%)
	384.4nm (3.2eV)	0.0109	(HOMO-2 -> LUMO) (94%)
	337.4nm (3.7eV)	0.0585	(HOMO-1 -> LUMO) (96%)
	311.5nm (4.0eV)	0.2432	(HOMO -> LUMO+1) (88%)
	309.6nm (4.0eV)	0.0200	(HOMO-3 -> LUMO) (78%) (HOMO-4 -> LUMO) (14%)
	303.5nm (4.1eV)	0.0610	(HOMO-4 -> LUMO) (62%) (HOMO-2 -> LUMO+1) (19%) (HOMO-3 -> LUMO) (10%)
	297.5nm (4.2eV)	0.0259	(HOMO-2 -> LUMO+1) (67%) (HOMO-4 -> LUMO) (17%)
	293.2nm (4.2eV)	0.0059	(HOMO-5 -> LUMO) (87%)
	285.4nm (4.3eV)	0.0095	(HOMO-9 -> LUMO) (53%) (HOMO-6 -> LUMO) (17%)
	277.0nm (4.5eV)	0.6050	(HOMO-1 -> LUMO+1) (84%)

Table S2. Vertical electronic Transition, absorption wavelength and oscillator strength of **2** in various solvents and in gas phase.

Molecule 2			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	496.6nm (2.5eV)	0.4671	(HOMO -> LUMO) (98%)
	460.2nm (2.7eV)	0.0779	(HOMO-1 -> LUMO) (99%)
	431.3nm (2.9eV)	0.0649	(HOMO-2 -> LUMO) (96%) (HOMO-2 -> LUMO) (10%)
	393.7nm (3.1eV)	0.3713	(HOMO -> LUMO+1) (95%) (HOMO-2 -> LUMO) (15%)
	384.6nm (3.2eV)	0.0066	(HOMO-3 -> LUMO) (93%) (HOMO -> LUMO+1) (18%)
	365.8nm (3.4eV)	0.4996	(HOMO-1 -> LUMO+1) (93%) (HOMO-1 -> LUMO+2) (30%) (HOMO-3 -> LUMO) (12%)
	345.8nm (3.6eV)	0.0308	(HOMO -> LUMO+2) (69%) (HOMO-1 -> LUMO+5) (11%)
	343.8nm (3.6eV)	0.0441	(HOMO-2 -> LUMO+1) (81%)
	339.8nm (3.6eV)	0.0090	(HOMO-1 -> LUMO+2) (47%) (HOMO -> LUMO+5) (44%)
	326.9nm (3.8eV)	0.0248	(HOMO -> LUMO+3) (65%) (HOMO-2 -> LUMO+3) (17%) HOMO -> LUMO+6) (11%) (HOMO-1 -> LUMO+3) (10%)
Chloroform	528.8nm (2.3eV)	0.6638	(HOMO -> LUMO) (97%)
	484.2nm (2.6eV)	0.0974	(HOMO-1 -> LUMO) (99%)
	455.0nm (2.7eV)	0.0561	(HOMO-2 -> LUMO) (96%) (HOMO-2 -> LUMO) (10%)
	405.1nm (3.1eV)	0.4489	(HOMO -> LUMO+1) (97%) (HOMO-4 -> LUMO) (13%)
	378.7nm (3.3eV)	0.6399	(HOMO-1 -> LUMO+1) (94%) (HOMO -> LUMO+1) (33%) (HOMO-4 -> LUMO) (11%)
	374.5nm (3.3eV)	0.0014	(HOMO-4 -> LUMO) (91%) (HOMO -> LUMO+2) (20%) (HOMO-1 -> LUMO+2) (10%)
	354.1nm (3.5eV)	0.0432	(HOMO-2 -> LUMO+1) (90%) (HOMO-3 -> LUMO) (25%) (HOMO -> LUMO+2) (13%)
	345.7nm (3.6eV)	0.0460	(HOMO -> LUMO+2) (75%) (HOMO-1 -> LUMO+4) (13%) (HOMO -> LUMO+2) (22%)
	339.6nm (3.7eV)	0.0113	(HOMO-1 -> LUMO+2) (50%) (HOMO -> LUMO+4) (41%)
	326.8nm (3.8eV)	0.1168	(HOMO -> LUMO+3) (58%) (HOMO-3 -> LUMO) (17%)

			(HOMO-2 -> LUMO+3) (14%) (HOMO-1 -> LUMO+2) (14%)
Dichloromethane	535.6nm (2.3eV)	0.7006	(HOMO -> LUMO) (97%)
	489.4nm (2.5eV)	0.1002	(HOMO-1 -> LUMO) (98%)
	460.2nm (2.7eV)	0.0527	(HOMO-2 -> LUMO) (96%)
	407.3nm (3.0eV)	0.4633	(HOMO -> LUMO+1) (97%) (HOMO-4 -> LUMO) (13%)
	381.4nm (3.3eV)	0.6675	(HOMO-1 -> LUMO+1) (94%) (HOMO -> LUMO+1) (33%) (HOMO-4 -> LUMO) (11%) (HOMO-4 -> LUMO) (14%) (HOMO -> LUMO+1) (11%)
	372.2nm (3.3eV)	0.0015	(HOMO-4 -> LUMO) (90%) (HOMO-2 -> LUMO) (23%)
	356.5nm (3.5eV)	0.0430	(HOMO-2 -> LUMO+1) (91%) (HOMO -> LUMO+2) (21%) (HOMO -> LUMO+5) (10%)
	345.8nm (3.6eV)	0.0509	(HOMO -> LUMO+2) (76%) (HOMO-1 -> LUMO+4) (13%) (HOMO-1 -> LUMO+1) (27%)
	339.8nm (3.6eV)	0.0130	(HOMO-1 -> LUMO+2) (50%) (HOMO -> LUMO+4) (40%)
	327.5nm (3.8eV)	0.2046	(HOMO-3 -> LUMO) (42%) (HOMO -> LUMO+3) (40%) (HOMO-1 -> LUMO+2) (17%) (HOMO-1 -> LUMO+1) (10%)
Dimethylsulfoxide	542.9nm (2.3eV)	0.7388	(HOMO -> LUMO) (96%)
	494.7nm (2.5eV)	0.1026	(HOMO-1 -> LUMO) (98%)
	465.7nm (2.7eV)	0.0491	(HOMO-2 -> LUMO) (96%) (HOMO-2 -> LUMO) (10%)
	409.4nm (3.0eV)	0.4790	(HOMO -> LUMO+1) (97%) (HOMO-4 -> LUMO) (13%)
	384.1nm (3.2eV)	0.6972	(HOMO-1 -> LUMO+1) (94%) (HOMO -> LUMO+1) (30%) (HOMO-4 -> LUMO) (27%)
	369.7nm (3.4eV)	0.0019	(HOMO-4 -> LUMO) (86%) (HOMO -> LUMO+1) (30%)
	358.9nm (3.5eV)	0.0430	(HOMO-2 -> LUMO+1) (91%) (HOMO -> LUMO+2) (24%) (HOMO -> LUMO+5) (10%) (HOMO-1 -> LUMO+2) (10%)
	345.9nm (3.6eV)	0.0570	(HOMO -> LUMO+2) (77%) (HOMO-1 -> LUMO+4) (14%) (HOMO-1 -> LUMO+2) (28%)
	340.0nm (3.6eV)	0.0158	(HOMO-1 -> LUMO+2) (50%) (HOMO -> LUMO+4) (40%)
	329.0nm (3.8eV)	0.2785	(HOMO-3 -> LUMO) (72%) (HOMO -> LUMO+3) (18%) (HOMO-1 -> LUMO+2) (16%)

			(HOMO-1 -> LUMO+1) (12%)
Tetrahydrofuran	534.0nm (2.3eV)	0.6919	(HOMO -> LUMO) (97%)
	488.1nm (2.5eV)	0.0995	(HOMO-1 -> LUMO) (98%)
	459.0nm (2.7eV)	0.0535	(HOMO-2 -> LUMO) (96%) (HOMO-2 -> LUMO) (10%)
	406.8nm (3.0eV)	0.4599	(HOMO -> LUMO+1) (97%) (HOMO-4 -> LUMO) (13%)
	380.7nm (3.3eV)	0.6609	(HOMO-1 -> LUMO+1) (94%) (HOMO-2 -> LUMO) (27%) (HOMO-5 -> LUMO) (19%)
	372.8nm (3.3eV)	0.0014	(HOMO-4 -> LUMO) (90%) (HOMO-2 -> LUMO) (23%)
	355.9nm (3.5eV)	0.0431	(HOMO-2 -> LUMO+1) (91%) (HOMO -> LUMO+2) (22%) (HOMO -> LUMO+5) (10%)
	345.8nm (3.6eV)	0.0496	(HOMO -> LUMO+2) (76%) (HOMO-1 -> LUMO+4) (13%) (HOMO-1 -> LUMO+1) (27%) (HOMO-1 -> LUMO+1) (28%)
	339.7nm (3.6eV)	0.0125	(HOMO-1 -> LUMO+2) (50%) (HOMO -> LUMO+4) (41%)
	327.3nm (3.8eV)	0.1813	(HOMO -> LUMO+3) (46%) (HOMO-3 -> LUMO) (35%) (HOMO-2 -> LUMO+3) (10%) (HOMO-1 -> LUMO+1) (11%)
Toluene	517.2nm (2.4eV)	0.5991	(HOMO -> LUMO) (97%)
	475.6nm (2.6eV)	0.0917	(HOMO-1 -> LUMO) (99%)
	446.3nm (2.8eV)	0.0611	(HOMO-2 -> LUMO) (96%)
	401.3nm (3.1eV)	0.4242	(HOMO -> LUMO+1) (97%)
	378.3nm (3.3eV)	0.0042	(HOMO-4 -> LUMO) (74%) (HOMO-3 -> LUMO) (21%)
	374.2nm (3.3eV)	0.5906	(HOMO-1 -> LUMO+1) (93%) (HOMO-1 -> LUMO+2) (30%) (HOMO-3 -> LUMO) (12%)
	350.4nm (3.5eV)	0.0438	(HOMO-2 -> LUMO+1) (88%) (HOMO -> LUMO+2) (18%) (HOMO -> LUMO+5) (10%)
	345.6nm (3.6eV)	0.0392	(HOMO -> LUMO+2) (73%) (HOMO-1 -> LUMO+2) (30%) (HOMO-1 -> LUMO+1) (24%)
	339.6nm (3.7eV)	0.0095	(HOMO-1 -> LUMO+2) (49%) (HOMO -> LUMO+5) (30%) (HOMO -> LUMO+4) (12%)
	326.3nm (3.8eV)	0.0559	(HOMO -> LUMO+3) (67%) (HOMO-2 -> LUMO+3) (17%) (HOMO-1 -> LUMO+2) (17%)

Table S3. Vertical electronic Transition, absorption wavelength and oscillator strength of **3** in various solvents and in gas phase.

Molecule 3			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	483.0nm (2.6eV)	0.4843	(HOMO -> LUMO) (97%)
	445.4nm (2.8eV)	0.0676	(HOMO-1 -> LUMO) (98%)
	423.1nm (2.9eV)	0.0409	(HOMO-2 -> LUMO) (95%)
	403.8nm (3.1eV)	0.1614	(HOMO -> LUMO+3) (34%) (HOMO -> LUMO+2) (29%) (HOMO -> LUMO+1) (21%)
	398.4nm (3.1eV)	0.0213	(HOMO -> LUMO+3) (41%) (HOMO-1 -> LUMO+2) (31%) (HOMO -> LUMO+2) (21%)
	395.6nm (3.1eV)	0.0471	(HOMO -> LUMO+1) (57%) (HOMO-2 -> LUMO+1) (17%) (HOMO -> LUMO+2) (13%)
	386.7nm (3.2eV)	0.0040	(HOMO-6 -> LUMO) (63%) (HOMO-5 -> LUMO) (29%) (HOMO -> LUMO+2) (13%)
	371.1nm (3.3eV)	0.2315	(HOMO -> LUMO+4) (43%) (HOMO-1 -> LUMO+2) (28%) (HOMO -> LUMO+2) (16%)
	367.0nm (3.4eV)	0.1383	(HOMO -> LUMO+4) (39%) (HOMO-1 -> LUMO+2) (20%) (HOMO -> LUMO+2) (17%) (HOMO-1 -> LUMO+1) (12%)
	359.4nm (3.5eV)	0.1372	(HOMO-1 -> LUMO+1) (34%) (HOMO-2 -> LUMO+1) (24%) (HOMO -> LUMO+1) (14%) (HOMO -> LUMO+4) (12%)
Chloroform	514.5nm (2.4eV)	0.6461	(HOMO -> LUMO) (97%)
	470.4nm (2.6eV)	0.0830	(HOMO-1 -> LUMO) (98%)
	446.9nm (2.8eV)	0.0340	(HOMO-2 -> LUMO) (96%)
	403.0nm (3.1eV)	0.3105	(HOMO -> LUMO+1) (52%) (HOMO -> LUMO+2) (23%) (HOMO -> LUMO+3) (11%)
	394.9nm (3.1eV)	0.0591	(HOMO -> LUMO+3) (52%) (HOMO-1 -> LUMO+2) (21%) (HOMO-1 -> LUMO+1) (14%)
	388.3nm (3.2eV)	0.1179	(HOMO -> LUMO+2) (32%) (HOMO -> LUMO+1) (27%) (HOMO-2 -> LUMO+1) (15%)
	376.9nm (3.3eV)	0.1154	(HOMO-6 -> LUMO) (58%) (HOMO -> LUMO+4) (21%)
	375.9nm (3.3eV)	0.2768	(HOMO -> LUMO+4) (47%) (HOMO-6 -> LUMO) (25%)

	366.4nm (3.4eV)	0.3067	(HOMO-1 -> LUMO+1) (46%) (HOMO -> LUMO+3) (14%) (HOMO -> LUMO+2) (12%) (HOMO-1 -> LUMO+2) (10%)
	357.9nm (3.5eV)	0.0454	(HOMO-3 -> LUMO) (74%)
Dichloromethane	521.5nm (2.4eV)	0.6750	(HOMO -> LUMO) (96%)
	476.3nm (2.6eV)	0.0852	(HOMO-1 -> LUMO) (98%)
	452.4nm (2.7eV)	0.0326	(HOMO-2 -> LUMO) (96%)
	403.3nm (3.1eV)	0.3505	(HOMO -> LUMO+1) (61%) (HOMO -> LUMO+2) (19%)
	394.4nm (3.1eV)	0.0739	(HOMO -> LUMO+3) (53%) (HOMO-1 -> LUMO+2) (18%) (HOMO-1 -> LUMO+1) (16%) (HOMO-1 -> LUMO+1) (17%)
	387.6nm (3.2eV)	0.1434	(HOMO -> LUMO+2) (36%) (HOMO -> LUMO+1) (21%) (HOMO-2 -> LUMO+1) (13%)
	377.0nm (3.3eV)	0.3982	(HOMO -> LUMO+4) (63%) (HOMO-1 -> LUMO+3) (10%)
	374.4nm (3.3eV)	0.0123	(HOMO-7 -> LUMO) (46%) (HOMO-6 -> LUMO) (38%)
	367.6nm (3.4eV)	0.3468	(HOMO-1 -> LUMO+1) (50%) (HOMO-1 -> LUMO+4) (17%) (HOMO -> LUMO+3) (14%) (HOMO -> LUMO+3) (14%)
	361.1nm (3.4eV)	0.1435	(HOMO-3 -> LUMO) (84%)
Dimethylsulfoxide	529.1nm (2.3eV)	0.7049	(HOMO -> LUMO) (96%)
	482.6nm (2.6eV)	0.0870	(HOMO-1 -> LUMO) (97%)
	458.4nm (2.7eV)	0.0317	(HOMO-2 -> LUMO) (96%)
	403.9nm (3.1eV)	0.3952	(HOMO -> LUMO+1) (69%) (HOMO -> LUMO+2) (14%)
	394.0nm (3.1eV)	0.0952	(HOMO -> LUMO+3) (52%) (HOMO-1 -> LUMO+1) (21%) (HOMO-1 -> LUMO+2) (13%)
	387.1nm (3.2eV)	0.1747	(HOMO -> LUMO+2) (37%) (HOMO -> LUMO+1) (15%) (HOMO -> LUMO+4) (11%)
	377.7nm (3.3eV)	0.4279	(HOMO -> LUMO+4) (58%) (HOMO-1 -> LUMO+3) (10%)
	372.3nm (3.3eV)	0.0091	(HOMO-7 -> LUMO) (71%)
	369.3nm (3.4eV)	0.3629	(HOMO-1 -> LUMO+1) (51%) (HOMO-1 -> LUMO+4) (17%) (HOMO -> LUMO+3) (14%)
	364.4nm (3.4eV)	0.1656	(HOMO-3 -> LUMO) (78%) (HOMO-7 -> LUMO) (11%)
Tetrahydrofuran	519.9nm (2.4eV)	0.6682	(HOMO -> LUMO) (96%)
	474.9nm (2.6eV)	0.0847	(HOMO-1 -> LUMO) (98%)
	451.1nm (2.7eV)	0.0329	(HOMO-2 -> LUMO) (96%)
	403.2nm (3.1eV)	0.3407	(HOMO -> LUMO+1) (59%)

			(HOMO -> LUMO+2) (19%)
	394.5nm (3.1eV)	0.0700	(HOMO -> LUMO+3) (53%) (HOMO-1 -> LUMO+2) (18%) (HOMO-1 -> LUMO+1) (16%)
	387.7nm (3.2eV)	0.1369	(HOMO -> LUMO+2) (35%) (HOMO -> LUMO+1) (22%) (HOMO-2 -> LUMO+1) (14%)
	376.9nm (3.3eV)	0.3872	(HOMO -> LUMO+4) (63%)
	374.9nm (3.3eV)	0.0185	(HOMO-6 -> LUMO) (57%) (HOMO-7 -> LUMO) (27%)
	367.3nm (3.4eV)	0.3399	(HOMO-1 -> LUMO+1) (49%) (HOMO-1 -> LUMO+4) (15%) (HOMO -> LUMO+3) (14%) (HOMO -> LUMO+2) (10%)
	360.3nm (3.4eV)	0.1325	(HOMO-3 -> LUMO) (84%) (HOMO -> LUMO+2) (10%)
Toluene	503.0nm (2.5eV)	0.5942	(HOMO -> LUMO) (97%)
	461.1nm (2.7eV)	0.0786	(HOMO-1 -> LUMO) (98%)
	438.0nm (2.8eV)	0.0367	(HOMO-2 -> LUMO) (96%)
	402.9nm (3.1eV)	0.2501	(HOMO -> LUMO+1) (36%) (HOMO -> LUMO+2) (28%) (HOMO -> LUMO+3) (20%)
	396.0nm (3.1eV)	0.0414	(HOMO -> LUMO+3) (48%) (HOMO-1 -> LUMO+2) (27%)
	390.2nm (3.2eV)	0.0848	(HOMO -> LUMO+1) (40%) (HOMO -> LUMO+2) (23%) (HOMO-2 -> LUMO+1) (17%)
	380.4nm (3.3eV)	0.0055	(HOMO-6 -> LUMO) (87%) (HOMO-2 -> LUMO+1) (17%)
	374.5nm (3.3eV)	0.3588	(HOMO -> LUMO+4) (71%)
	365.7nm (3.4eV)	0.1889	(HOMO-1 -> LUMO+1) (33%) (HOMO-1 -> LUMO+2) (21%) (HOMO -> LUMO+2) (20%) (HOMO -> LUMO+3) (13%)
	357.6nm (3.5eV)	0.1790	(HOMO-1 -> LUMO+3) (26%) (HOMO -> LUMO+4) (15%) (HOMO-1 -> LUMO+4) (14%) (HOMO-1 -> LUMO+1) (13%) (HOMO-1 -> LUMO+2) (11%)

Table S4. Vertical electronic Transition, absorption wavelength and oscillator strength of **4** in various solvents and in gas phase.

Molecule 4			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	517.0nm (2.4eV)	0.4673	(HOMO -> LUMO) (98%)

	469.2nm (2.6eV)	0.0809	(HOMO-1 -> LUMO) (99%)
	451.0nm (2.7eV)	0.0481	(HOMO-2 -> LUMO) (95%)
	401.9nm (3.1eV)	0.4136	(HOMO -> LUMO+1) (97%)
	380.4nm (3.3eV)	0.0184	(HOMO-4 -> LUMO) (86%)
	370.9nm (3.3eV)	0.0258	(HOMO -> LUMO+2) (56%) (HOMO -> LUMO+4) (25%)
	368.8nm (3.4eV)	0.5331	(HOMO-1 -> LUMO+1) (82%)
	365.4nm (3.4eV)	0.0702	(HOMO -> LUMO+4) (49%) (HOMO-1 -> LUMO+2) (33%) (HOMO -> LUMO+2) (10%)
	353.6nm (3.5eV)	0.0057	(HOMO -> LUMO+3) (48%) (HOMO-2 -> LUMO+1) (29%) (HOMO-2 -> LUMO+3) (12%)
	345.2nm (3.6eV)	0.0118	(HOMO-2 -> LUMO+1) (57%) (HOMO -> LUMO+3) (27%)
Chloroform	560.6nm (2.2eV)	0.6437	(HOMO -> LUMO) (97%)
	504.6nm (2.5eV)	0.1005	(HOMO-1 -> LUMO) (98%)
	482.6nm (2.6eV)	0.0499	(HOMO-2 -> LUMO) (96%)
	417.3nm (3.0eV)	0.5218	(HOMO -> LUMO+1) (97%)
	385.9nm (3.2eV)	0.7215	(HOMO-1 -> LUMO+1) (92%)
	371.0nm (3.3eV)	0.0081	(HOMO-7 -> LUMO) (64%) (HOMO-8 -> LUMO) (21%)
	368.7nm (3.4eV)	0.0299	(HOMO -> LUMO+2) (69%) (HOMO -> LUMO+4) (11%) (HOMO-1 -> LUMO+4) (10%)
	363.7nm (3.4eV)	0.0205	(HOMO-2 -> LUMO+1) (79%)
	362.6nm (3.4eV)	0.0218	(HOMO -> LUMO+4) (46%) (HOMO-1 -> LUMO+2) (36%)
	346.7nm (3.6eV)	0.0296	(HOMO -> LUMO+3) (66%) (HOMO-2 -> LUMO+3) (21%)
Dichloromethane	570.3nm (2.2eV)	0.6772	(HOMO -> LUMO) (97%)
	512.6nm (2.4eV)	0.1029	(HOMO-1 -> LUMO) (98%)
	489.7nm (2.5eV)	0.0501	(HOMO-2 -> LUMO) (96%)
	420.5nm (2.9eV)	0.5416	(HOMO -> LUMO+1) (97%)
	389.6nm (3.2eV)	0.7476	(HOMO-1 -> LUMO+1) (93%)
	369.2nm (3.4eV)	0.0093	(HOMO-8 -> LUMO) (35%) (HOMO -> LUMO+2) (21%) (HOMO-7 -> LUMO) (21%)
	368.4nm (3.4eV)	0.0280	(HOMO -> LUMO+2) (52%) (HOMO-8 -> LUMO) (14%)
	366.6nm (3.4eV)	0.0191	(HOMO-2 -> LUMO+1) (76%)
	362.4nm (3.4eV)	0.0323	(HOMO -> LUMO+4) (49%) (HOMO-1 -> LUMO+2) (38%)
	346.9nm (3.6eV)	0.0382	(HOMO -> LUMO+3) (66%) (HOMO-2 -> LUMO+3) (20%)
Dimethylsulfoxide	580.8nm (2.1eV)	0.7121	(HOMO -> LUMO) (96%)
	521.2nm (2.4eV)	0.1046	(HOMO-1 -> LUMO) (98%)
	497.3nm (2.5eV)	0.0510	(HOMO-2 -> LUMO) (96%)

	423.9nm (2.9eV)	0.5621	(HOMO -> LUMO+1) (97%)
	393.5nm (3.2eV)	0.7757	(HOMO-1 -> LUMO+1) (93%)
	370.4nm (3.3eV)	0.0086	(HOMO-2 -> LUMO+1) (87%)
	368.7nm (3.4eV)	0.0400	(HOMO -> LUMO+2) (73%) (HOMO-1 -> LUMO+4) (11%)
	366.2nm (3.4eV)	0.0151	(HOMO-8 -> LUMO) (74%) (HOMO-7 -> LUMO) (10%)
	362.3nm (3.4eV)	0.0387	(HOMO -> LUMO+4) (49%) (HOMO-1 -> LUMO+2) (39%)
	347.4nm (3.6eV)	0.0627	(HOMO -> LUMO+3) (61%) (HOMO-2 -> LUMO+3) (18%) (HOMO-3 -> LUMO) (12%)
Tetrahydrofuran	568.0nm (2.2eV)	0.6692	(HOMO -> LUMO) (97%)
	510.6nm (2.4eV)	0.1024	(HOMO-1 -> LUMO) (98%)
	488.0nm (2.5eV)	0.0500	(HOMO-2 -> LUMO) (96%)
	419.8nm (3.0eV)	0.5369	(HOMO -> LUMO+1) (97%)
	388.8nm (3.2eV)	0.7414	(HOMO-1 -> LUMO+1) (93%)
	369.5nm (3.4eV)	0.0074	(HOMO-8 -> LUMO) (39%) (HOMO-7 -> LUMO) (33%) (HOMO -> LUMO+2) (10%)
	368.5nm (3.4eV)	0.0310	(HOMO -> LUMO+2) (62%)
	366.0nm (3.4eV)	0.0172	(HOMO-2 -> LUMO+1) (82%)
	362.4nm (3.4eV)	0.0309	(HOMO -> LUMO+4) (49%) (HOMO-1 -> LUMO+2) (38%)
	346.8nm (3.6eV)	0.0355	(HOMO -> LUMO+3) (66%) (HOMO-2 -> LUMO+3) (21%)
Toluene	544.7nm (2.3eV)	0.5850	(HOMO -> LUMO) (97%)
	491.6nm (2.5eV)	0.0952	(HOMO-1 -> LUMO) (99%)
	471.0nm (2.6eV)	0.0498	(HOMO-2 -> LUMO) (96%)
	411.9nm (3.0eV)	0.4868	(HOMO -> LUMO+1) (97%)
	379.8nm (3.3eV)	0.6761	(HOMO-1 -> LUMO+1) (91%)
	374.4nm (3.3eV)	0.0099	(HOMO-7 -> LUMO) (72%) (HOMO-6 -> LUMO) (17%)
	369.2nm (3.4eV)	0.0256	(HOMO -> LUMO+2) (66%) (HOMO -> LUMO+4) (16%) (HOMO-1 -> LUMO+4) (10%)
	363.4nm (3.4eV)	0.0297	(HOMO -> LUMO+4) (50%) (HOMO-1 -> LUMO+2) (37%)
	358.8nm (3.5eV)	0.0067	(HOMO-2 -> LUMO+1) (78%)
	346.7nm (3.6eV)	0.0218	(HOMO -> LUMO+3) (64%) (HOMO-2 -> LUMO+3) (19%) (HOMO-2 -> LUMO+1) (11%)

Table S5. Vertical electronic Transition, absorption wavelength and oscillator strength of **5** in various solvents and in gas phase.

Molecule 5			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	487.1nm (2.5eV)	0.6340	(HOMO -> LUMO) (94%)
	452.3nm (2.7eV)	0.1608	(HOMO-1 -> LUMO) (91%)
	432.2nm (2.9eV)	0.2074	(HOMO -> LUMO+1) (77%)
	428.0nm (2.9eV)	0.1395	(HOMO-2 -> LUMO) (83%)
	418.0nm (3.0eV)	0.1828	(HOMO -> LUMO+2) (73%) (HOMO -> LUMO+1) (15%)
	413.4nm (3.0eV)	0.1000	(HOMO -> LUMO+3) (82%)
	405.5nm (3.1eV)	0.1770	(HOMO-1 -> LUMO+1) (81%)
	391.6nm (3.2eV)	0.0940	(HOMO-1 -> LUMO+2) (72%) (HOMO-1 -> LUMO+3) (23%)
	389.6nm (3.2eV)	0.0357	(HOMO-3 -> LUMO) (59%) (HOMO-1 -> LUMO+3) (13%)
	386.6nm (3.2eV)	0.0453	(HOMO-1 -> LUMO+3) (56%) (HOMO-3 -> LUMO) (20%) (HOMO-1 -> LUMO+2) (13%)
Chloroform	517.9nm (2.4eV)	0.9370	(HOMO -> LUMO) (85%)
	484.6nm (2.6eV)	0.6763	(HOMO -> LUMO+1) (49%) (HOMO-1 -> LUMO) (22%) (HOMO -> LUMO+2) (13%)
	469.1nm (2.6eV)	0.0929	(HOMO -> LUMO+2) (73%) (HOMO -> LUMO+1) (11%)
	466.4nm (2.7eV)	0.0116	(HOMO-1 -> LUMO) (62%) (HOMO -> LUMO+1) (30%)
	450.7nm (2.8eV)	0.3718	(HOMO-1 -> LUMO+1) (48%) (HOMO-2 -> LUMO) (32%) (HOMO -> LUMO+3) (11%)
	448.3nm (2.8eV)	0.0504	(HOMO-2 -> LUMO) (40%) (HOMO -> LUMO+3) (30%)
	443.8nm (2.8eV)	0.0174	(HOMO -> LUMO+3) (48%) (HOMO-1 -> LUMO+1) (27%) (HOMO-2 -> LUMO) (13%)
	434.2nm (2.9eV)	0.1080	(HOMO-1 -> LUMO+2) (86%)
	418.2nm (3.0eV)	0.0829	(HOMO-1 -> LUMO+3) (68%)
	411.5nm (3.0eV)	0.0917	(HOMO-2 -> LUMO+1) (36%) (HOMO-2 -> LUMO+3) (21%) (HOMO-1 -> LUMO+3) (19%) (HOMO-2 -> LUMO+2) (15%)
Dichloromethane	525.7nm (2.4eV)	0.9769	(HOMO -> LUMO) (82%)
	494.9nm (2.5eV)	0.7633	(HOMO -> LUMO+1) (55%) (HOMO-1 -> LUMO) (15%) (HOMO -> LUMO+2) (12%) (HOMO-1 -> LUMO+1) (10%)
	480.8nm (2.6eV)	0.0863	(HOMO -> LUMO+2) (71%)
	472.4nm (2.6eV)	0.0108	(HOMO-1 -> LUMO) (67%) (HOMO -> LUMO+1) (23%)

	458.5nm (2.7eV)	0.3010	(HOMO-1 -> LUMO+1) (60%) (HOMO-2 -> LUMO) (15%) (HOMO -> LUMO+3) (12%)
	454.6nm (2.7eV)	0.1135	(HOMO-2 -> LUMO) (56%) (HOMO -> LUMO+3) (16%)
	450.9nm (2.7eV)	0.0378	(HOMO -> LUMO+3) (60%) (HOMO-1 -> LUMO+1) (16%) (HOMO-2 -> LUMO) (10%)
	443.0nm (2.8eV)	0.0968	(HOMO-1 -> LUMO+2) (82%)
	423.9nm (2.9eV)	0.0800	(HOMO-1 -> LUMO+3) (67%)
	417.1nm (3.0eV)	0.0699	(HOMO-2 -> LUMO+1) (32%) (HOMO-1 -> LUMO+3) (21%) (HOMO-2 -> LUMO+2) (20%) (HOMO-2 -> LUMO+3) (19%)
Dimethylsulfoxide	534.5nm (2.3eV)	1.0080	(HOMO -> LUMO) (80%)
	506.5nm (2.4eV)	0.8499	(HOMO -> LUMO+1) (62%) (HOMO-1 -> LUMO) (11%) (HOMO-1 -> LUMO+1) (10%)
	493.6nm (2.5eV)	0.0887	(HOMO -> LUMO+2) (71%)
	479.3nm (2.6eV)	0.0159	(HOMO-1 -> LUMO) (70%) (HOMO -> LUMO+1) (18%)
	467.0nm (2.7eV)	0.2444	(HOMO-1 -> LUMO+1) (65%) (HOMO -> LUMO+3) (10%) (HOMO-2 -> LUMO) (10%) (HOMO -> LUMO+1) (10%)
	461.8nm (2.7eV)	0.1507	(HOMO-2 -> LUMO) (62%) (HOMO -> LUMO+2) (11%)
	458.1nm (2.7eV)	0.0765	(HOMO -> LUMO+3) (72%) (HOMO-1 -> LUMO+1) (10%)
	452.1nm (2.7eV)	0.0779	(HOMO-1 -> LUMO+2) (74%)
	429.7nm (2.9eV)	0.0777	(HOMO-1 -> LUMO+3) (65%) (HOMO-2 -> LUMO+2) (12%)
	422.8nm (2.9eV)	0.0492	(HOMO-2 -> LUMO+2) (31%) (HOMO-1 -> LUMO+3) (23%) (HOMO-2 -> LUMO+1) (23%) (HOMO-2 -> LUMO+3) (16%)
Tetrahydrofuran	523.8nm (2.4eV)	0.9683	(HOMO -> LUMO) (83%)
	492.4nm (2.5eV)	0.7430	(HOMO -> LUMO+1) (54%) (HOMO-1 -> LUMO) (17%) (HOMO -> LUMO+2) (13%) (HOMO-1 -> LUMO+1) (10%)
	478.0nm (2.6eV)	0.0870	(HOMO -> LUMO+2) (71%) (HOMO -> LUMO+1) (10%)
	470.9nm (2.6eV)	0.0105	(HOMO-1 -> LUMO) (66%) (HOMO -> LUMO+1) (24%)
	456.6nm (2.7eV)	0.3163	(HOMO-1 -> LUMO+1) (58%) (HOMO-2 -> LUMO) (17%) (HOMO -> LUMO+3) (13%)
	453.1nm (2.7eV)	0.1010	(HOMO-2 -> LUMO) (53%)

			(HOMO -> LUMO+3) (19%)
	449.2nm (2.8eV)	0.0313	(HOMO -> LUMO+3) (57%) (HOMO-1 -> LUMO+1) (18%) (HOMO-2 -> LUMO) (11%)
	440.9nm (2.8eV)	0.1002	(HOMO-1 -> LUMO+2) (84%)
	422.6nm (2.9eV)	0.0806	(HOMO-1 -> LUMO+3) (67%)
	415.7nm (3.0eV)	0.0750	(HOMO-2 -> LUMO+1) (33%) (HOMO-1 -> LUMO+3) (20%) (HOMO-2 -> LUMO+3) (20%) (HOMO-2 -> LUMO+2) (19%)
Toluene	505.8nm (2.5eV)	0.8480	(HOMO -> LUMO) (89%)
	469.2nm (2.6eV)	0.4910	(HOMO-1 -> LUMO) (47%) (HOMO -> LUMO+1) (31%)
	456.1nm (2.7eV)	0.0726	(HOMO -> LUMO+1) (46%) (HOMO-1 -> LUMO) (42%)
	450.2nm (2.8eV)	0.1034	(HOMO -> LUMO+2) (74%) (HOMO -> LUMO+1) (16%)
	440.4nm (2.8eV)	0.2651	(HOMO-2 -> LUMO) (80%)
	436.7nm (2.8eV)	0.1259	(HOMO -> LUMO+3) (61%) (HOMO-1 -> LUMO+1) (26%)
	431.1nm (2.9eV)	0.0414	(HOMO-1 -> LUMO+1) (53%) (HOMO -> LUMO+3) (29%)
	419.1nm (3.0eV)	0.1124	(HOMO-1 -> LUMO+2) (88%)
	407.9nm (3.0eV)	0.0863	(HOMO-1 -> LUMO+3) (70%)
	401.5nm (3.1eV)	0.1329	(HOMO-2 -> LUMO+1) (40%) (HOMO-2 -> LUMO+3) (22%) (HOMO-1 -> LUMO+3) (16%) (HOMO-2 -> LUMO+2) (12%)

Table S6. Vertical electronic Transition, absorption wavelength and oscillator strength of **6** in various solvents and in gas phase.

Molecule 6			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	523.8nm (2.4eV)	0.8738	(HOMO -> LUMO) (87%)
	489.8nm (2.5eV)	0.6088	(HOMO-1 -> LUMO) (57%) (HOMO -> LUMO+1) (16%)
	485.7nm (2.6eV)	0.0009	(HOMO-5 -> LUMO) (54%) (HOMO-5 -> LUMO+1) (18%) (HOMO-5 -> LUMO+2) (16%) (HOMO-5 -> LUMO+3) (10%)
	484.1nm (2.6eV)	0.0081	(HOMO-4 -> LUMO+1) (67%) (HOMO-4 -> LUMO+3) (10%)
	483.8nm (2.6eV)	0.0025	(HOMO-3 -> LUMO+2) (63%) (HOMO-3 -> LUMO+3) (21%)

	477.7nm (2.6eV)	0.1107	(HOMO -> LUMO+1) (64%) (HOMO-1 -> LUMO) (21%)
	467.6nm (2.7eV)	0.2662	(HOMO -> LUMO+2) (71%) (HOMO -> LUMO+1) (11%)
	459.7nm (2.7eV)	0.5877	(HOMO-2 -> LUMO) (56%) (HOMO-1 -> LUMO+1) (19%)
	457.6nm (2.7eV)	0.0668	(HOMO -> LUMO+3) (89%)
	450.3nm (2.8eV)	0.0598	(HOMO-1 -> LUMO+1) (61%) (HOMO-2 -> LUMO) (22%)
Chloroform	551.0nm (2.3eV)	1.1829	(HOMO -> LUMO) (83%)
	518.7nm (2.4eV)	1.2286	(HOMO -> LUMO+1) (33%) (HOMO-1 -> LUMO) (31%) (HOMO -> LUMO+2) (16%) (HOMO-1 -> LUMO+1) (15%)
	498.9nm (2.5eV)	0.2214	(HOMO -> LUMO+2) (57%) (HOMO-2 -> LUMO) (10%)
	494.4nm (2.5eV)	0.0556	(HOMO-1 -> LUMO) (52%) (HOMO -> LUMO+1) (36%)
	483.2nm (2.6eV)	0.4364	(HOMO-2 -> LUMO) (28%) (HOMO -> LUMO+3) (23%) (HOMO-1 -> LUMO+1) (22%)
	479.7nm (2.6eV)	0.0868	(HOMO-5 -> LUMO) (42%) (HOMO-5 -> LUMO+2) (14%) (HOMO-5 -> LUMO+3) (12%) (HOMO-5 -> LUMO+1) (11%)
	478.1nm (2.6eV)	0.0283	(HOMO-4 -> LUMO+1) (67%)
	477.6nm (2.6eV)	0.002	(HOMO-3 -> LUMO+2) (71%)
	477.0nm (2.6eV)	0.0559	(HOMO-2 -> LUMO) (39%) (HOMO -> LUMO+3) (17%) (HOMO -> LUMO+2) (10%)
	470.0nm (2.6eV)	0.0336	(HOMO -> LUMO+3) (39%) (HOMO-1 -> LUMO+1) (37%) (HOMO -> LUMO+1) (10%)
Dichloromethane	556.7nm (2.2eV)	1.2312	(HOMO -> LUMO) (82%)
	525.7nm (2.4eV)	1.3247	(HOMO -> LUMO+1) (36%) (HOMO-1 -> LUMO) (27%) (HOMO-1 -> LUMO+1) (16%) (HOMO -> LUMO+2) (15%)
	507.5nm (2.4eV)	0.227	(HOMO -> LUMO+2) (53%) (HOMO-2 -> LUMO) (14%)
	498.1nm (2.5eV)	0.0661	(HOMO-1 -> LUMO) (57%) (HOMO -> LUMO+1) (30%)
	488.1nm (2.5eV)	0.4831	(HOMO -> LUMO+3) (30%) (HOMO-2 -> LUMO) (28%) (HOMO-1 -> LUMO+1) (25%)
	480.8nm (2.6eV)	0.0537	(HOMO-2 -> LUMO) (40%) (HOMO -> LUMO+3) (14%) (HOMO -> LUMO+2) (14%)
	478.8nm (2.6eV)	0.025	(HOMO-5 -> LUMO) (49%)

			(HOMO-5 -> LUMO+2) (17%) (HOMO-5 -> LUMO+3) (14%) (HOMO-5 -> LUMO+1) (11%)
	476.8nm (2.6eV)	0.0046	(HOMO-4 -> LUMO+1) (78%) (HOMO-5 -> LUMO+1) (11%) (HOMO-4 -> LUMO+3) (10%)
	476.4nm (2.6eV)	0.0031	(HOMO-3 -> LUMO+2) (73%) (HOMO-3 -> LUMO) (10%)
	473.6nm (2.6eV)	0.033	(HOMO -> LUMO+3) (38%) (HOMO-1 -> LUMO+1) (36%) (HOMO -> LUMO+1) (11%)
Dimethylsulfoxide	562.8nm (2.2eV)	1.2772	(HOMO -> LUMO) (80%)
	533.5nm (2.3eV)	1.4096	(HOMO -> LUMO+1) (39%) (HOMO-1 -> LUMO) (24%) (HOMO-1 -> LUMO+1) (16%) (HOMO -> LUMO+2) (14%)
	517.1nm (2.4eV)	0.2542	(HOMO -> LUMO+2) (51%) (HOMO-2 -> LUMO) (17%) (HOMO-1 -> LUMO+1) (10%)
	502.3nm (2.5eV)	0.0856	(HOMO-1 -> LUMO) (60%) (HOMO -> LUMO+1) (23%)
	493.8nm (2.5eV)	0.4261	(HOMO -> LUMO+3) (34%) (HOMO-2 -> LUMO) (25%) (HOMO-1 -> LUMO+1) (24%)
	484.5nm (2.6eV)	0.0647	(HOMO-2 -> LUMO) (45%) (HOMO -> LUMO+2) (17%) (HOMO -> LUMO+3) (11%) (HOMO -> LUMO) (10%)
	478.0nm (2.6eV)	0.0364	(HOMO-1 -> LUMO+1) (23%) (HOMO-5 -> LUMO) (22%) (HOMO -> LUMO+3) (19%)
	477.1nm (2.6eV)	0.0089	(HOMO-5 -> LUMO) (31%) (HOMO -> LUMO+3) (17%) (HOMO-1 -> LUMO+1) (14%) (HOMO-5 -> LUMO+2) (11%)
	475.5nm (2.6eV)	0.0022	(HOMO-4 -> LUMO+1) (73%)
	475.1nm (2.6eV)	0.0026	(HOMO-3 -> LUMO+2) (66%) (HOMO-3 -> LUMO) (10%)
Tetrahydrofuran	555.3nm (2.2eV)	1.22	(HOMO -> LUMO) (82%)
	524.0nm (2.4eV)	1.303	(HOMO -> LUMO+1) (35%) (HOMO-1 -> LUMO) (28%) (HOMO-1 -> LUMO+1) (15%) (HOMO -> LUMO+2) (15%)
	505.4nm (2.5eV)	0.2236	(HOMO -> LUMO+2) (54%) (HOMO-2 -> LUMO) (13%)
	497.2nm (2.5eV)	0.0635	(HOMO-1 -> LUMO) (56%) (HOMO -> LUMO+1) (31%)
	486.9nm (2.5eV)	0.489	(HOMO -> LUMO+3) (29%) (HOMO-2 -> LUMO) (29%)

			(HOMO-1 -> LUMO+1) (25%)
	480.1nm (2.6eV)	0.0427	(HOMO-2 -> LUMO) (33%) (HOMO -> LUMO+3) (14%) (HOMO -> LUMO+2) (12%)
	478.9nm (2.6eV)	0.0399	(HOMO-5 -> LUMO) (43%) (HOMO-5 -> LUMO+2) (15%) (HOMO-5 -> LUMO+3) (12%) (HOMO-2 -> LUMO) (11%) (HOMO-5 -> LUMO+1) (10%)
	477.1nm (2.6eV)	0.0055	(HOMO-4 -> LUMO+1) (78%) (HOMO-2 -> LUMO) (11%) (HOMO-4 -> LUMO+3) (10%)
	476.7nm (2.6eV)	0.0034	(HOMO-3 -> LUMO+2) (74%) (HOMO-5 -> LUMO+1) (10%) (HOMO-3 -> LUMO) (10%)
	472.8nm (2.6eV)	0.0332	(HOMO -> LUMO+3) (38%) (HOMO-1 -> LUMO+1) (36%) (HOMO -> LUMO+1) (11%)
Toluene	541.3nm (2.3eV)	1.0898	(HOMO -> LUMO) (84%)
	507.6nm (2.4eV)	1.039	(HOMO-1 -> LUMO) (39%) (HOMO -> LUMO+1) (28%) (HOMO -> LUMO+2) (15%) (HOMO-1 -> LUMO+1) (13%)
	488.5nm (2.5eV)	0.0996	(HOMO-1 -> LUMO) (46%) (HOMO -> LUMO+2) (10%)
	485.8nm (2.6eV)	0.179	(HOMO -> LUMO+2) (54%) (HOMO -> LUMO+1) (20%)
	482.4nm (2.6eV)	0.0058	(HOMO-5 -> LUMO) (48%) (HOMO-5 -> LUMO+2) (16%) (HOMO-5 -> LUMO+1) (14%) (HOMO-5 -> LUMO+3) (13%)
	480.1nm (2.6eV)	0.0013	(HOMO-4 -> LUMO+1) (74%) (HOMO-4 -> LUMO+3) (11%)
	479.6nm (2.6eV)	0.0275	(HOMO-3 -> LUMO+2) (71%) (HOMO-3 -> LUMO+3) (12%)
	473.7nm (2.6eV)	0.5867	(HOMO-2 -> LUMO) (43%) (HOMO-1 -> LUMO+1) (26%) (HOMO -> LUMO+3) (15%)
	470.9nm (2.6eV)	0.0346	(HOMO -> LUMO+3) (36%) (HOMO-2 -> LUMO) (31%)
	463.9nm (2.7eV)	0.038	(HOMO-1 -> LUMO+1) (41%) (HOMO -> LUMO+3) (34%)

Table S7. Vertical electronic Transition, absorption wavelength and oscillator strength of **7** in various solvents and in gas phase.

Molecule 7

Phase	Wavelength	oscillator strength	Assignment
Gas	497.1nm (2.5eV)	0.2626	(HOMO -> LUMO) (86%) (HOMO-2 -> LUMO) (13%)
	481.4nm (2.6eV)	0.0509	(HOMO-1 -> LUMO) (94%)
	472.5nm (2.6eV)	0.0116	(HOMO-2 -> LUMO) (82%) (HOMO -> LUMO) (12%)
	421.8nm (2.9eV)	0.0000	(HOMO-3 -> LUMO) (100%) (HOMO -> LUMO) (12%)
	419.6nm (3.0eV)	0.0001	(HOMO-5 -> LUMO) (100%) (HOMO -> LUMO) (12%)
	415.5nm (3.0eV)	0.0000	(HOMO-4 -> LUMO) (100%) (HOMO -> LUMO) (12%)
	389.1nm (3.2eV)	0.0149	(HOMO-7 -> LUMO) (51%) (HOMO-8 -> LUMO) (29%) (HOMO-9 -> LUMO) (12%)
	385.2nm (3.2eV)	0.1490	(HOMO -> LUMO+1) (92%) (HOMO-9 -> LUMO) (12%)
	375.5nm (3.3eV)	0.1348	(HOMO-1 -> LUMO+1) (95%) (HOMO-9 -> LUMO) (12%)
	360.0nm (3.4eV)	0.0347	(HOMO-2 -> LUMO+1) (95%) (HOMO-9 -> LUMO) (12%)
Chloroform	496.6nm (2.5eV)	0.4146	(HOMO -> LUMO) (76%) (HOMO-2 -> LUMO) (23%)
	474.1nm (2.6eV)	0.0462	(HOMO-1 -> LUMO) (99%) (HOMO-2 -> LUMO) (23%)
	469.7nm (2.6eV)	0.0008	(HOMO-2 -> LUMO) (76%) (HOMO -> LUMO) (23%)
	416.2nm (3.0eV)	0.0002	(HOMO-5 -> LUMO) (100%) (HOMO -> LUMO) (23%)
	408.1nm (3.0eV)	0.0000	(HOMO-3 -> LUMO) (100%) (HOMO -> LUMO) (23%)
	405.4nm (3.1eV)	0.0000	(HOMO-4 -> LUMO) (100%) (HOMO -> LUMO) (23%)
	380.6nm (3.3eV)	0.0535	(HOMO-7 -> LUMO) (49%) (HOMO-9 -> LUMO) (21%) (HOMO -> LUMO+1) (20%)
	378.2nm (3.3eV)	0.1734	(HOMO -> LUMO+1) (77%) (HOMO-7 -> LUMO) (13%)
	369.5nm (3.4eV)	0.2161	(HOMO-1 -> LUMO+1) (94%)
	357.1nm (3.5eV)	0.0235	(HOMO-2 -> LUMO+1) (94%)
Dichloromethane	495.9nm (2.5eV)	0.4414	(HOMO -> LUMO) (74%) (HOMO-2 -> LUMO) (24%)
	471.9nm (2.6eV)	0.0448	(HOMO-1 -> LUMO) (95%)
	468.1nm (2.6eV)	0.0040	(HOMO-2 -> LUMO) (73%) (HOMO -> LUMO) (22%)
	414.7nm (3.0eV)	0.0003	(HOMO-5 -> LUMO) (100%) (HOMO -> LUMO) (22%)
	404.7nm (3.1eV)	0.0000	(HOMO-3 -> LUMO) (100%)

			(HOMO -> LUMO) (22%)
	402.7nm (3.1eV)	0.0000	(HOMO-4 -> LUMO) (100%) (HOMO -> LUMO) (22%)
	378.6nm (3.3eV)	0.0676	(HOMO-7 -> LUMO) (48%) (HOMO -> LUMO+1) (25%) (HOMO-9 -> LUMO) (19%)
	376.4nm (3.3eV)	0.1736	(HOMO -> LUMO+1) (72%) (HOMO-7 -> LUMO) (16%)
	367.8nm (3.4eV)	0.2352	(HOMO-1 -> LUMO+1) (94%)
	356.0nm (3.5eV)	0.0168	(HOMO-2 -> LUMO+1) (93%)
Dimethylsulfoxide	494.9nm (2.5eV)	0.4689	(HOMO -> LUMO) (73%) (HOMO-2 -> LUMO) (25%)
	469.5nm (2.6eV)	0.0407	(HOMO-1 -> LUMO) (82%)
	465.6nm (2.7eV)	0.0120	(HOMO-2 -> LUMO) (65%) (HOMO -> LUMO) (18%) (HOMO-1 -> LUMO) (16%)
	412.7nm (3.0eV)	0.0003	(HOMO-5 -> LUMO) (100%) (HOMO -> LUMO) (18%)
	400.7nm (3.1eV)	0.0000	(HOMO-3 -> LUMO) (100%) (HOMO -> LUMO) (18%)
	399.6nm (3.1eV)	0.0000	(HOMO-4 -> LUMO) (100%) (HOMO -> LUMO) (18%)
	376.4nm (3.3eV)	0.0821	(HOMO-7 -> LUMO) (47%) (HOMO -> LUMO+1) (30%) (HOMO-9 -> LUMO) (17%)
	374.4nm (3.3eV)	0.1753	(HOMO -> LUMO+1) (67%) (HOMO-7 -> LUMO) (20%)
	365.9nm (3.4eV)	0.2550	(HOMO-1 -> LUMO+1) (94%)
	354.7nm (3.5eV)	0.0058	(HOMO-2 -> LUMO+1) (91%)
Tetrahydrofuran	496.1nm (2.5eV)	0.4351	(HOMO -> LUMO) (75%) (HOMO-2 -> LUMO) (24%)
	472.5nm (2.6eV)	0.0454	(HOMO-1 -> LUMO) (96%) (HOMO-2 -> LUMO) (24%)
	468.5nm (2.6eV)	0.0029	(HOMO-2 -> LUMO) (74%) (HOMO -> LUMO) (23%)
	415.1nm (3.0eV)	0.0003	(HOMO-5 -> LUMO) (100%) (HOMO -> LUMO) (23%)
	405.5nm (3.1eV)	0.0000	(HOMO-3 -> LUMO) (100%) (HOMO -> LUMO) (23%)
	403.4nm (3.1eV)	0.0000	(HOMO-4 -> LUMO) (100%) (HOMO -> LUMO) (23%)
	379.1nm (3.3eV)	0.0641	(HOMO-7 -> LUMO) (49%) (HOMO -> LUMO+1) (24%) (HOMO-9 -> LUMO) (20%)
	376.9nm (3.3eV)	0.1735	(HOMO -> LUMO+1) (73%) (HOMO-7 -> LUMO) (16%)
	368.2nm (3.4eV)	0.2306	(HOMO-1 -> LUMO+1) (94%)
	356.3nm (3.5eV)	0.0187	(HOMO-2 -> LUMO+1) (93%)
Toluene	497.2nm (2.5eV)	0.3662	(HOMO -> LUMO) (78%)

			(HOMO-2 -> LUMO) (20%)
	477.3nm (2.6eV)	0.0463	(HOMO-1 -> LUMO) (97%) (HOMO-2 -> LUMO) (20%)
	471.5nm (2.6eV)	0.0016	(HOMO-2 -> LUMO) (77%) (HOMO -> LUMO) (20%)
	418.1nm (3.0eV)	0.0002	(HOMO-5 -> LUMO) (100%) (HOMO -> LUMO) (20%)
	413.4nm (3.0eV)	0.0000	(HOMO-3 -> LUMO) (100%) (HOMO -> LUMO) (20%)
	409.4nm (3.0eV)	0.0000	(HOMO-4 -> LUMO) (100%) (HOMO -> LUMO) (20%)
	383.7nm (3.2eV)	0.0338	(HOMO-7 -> LUMO) (51%) (HOMO-8 -> LUMO) (29%) (HOMO-9 -> LUMO) (12%)
	381.0nm (3.3eV)	0.1705	(HOMO -> LUMO+1) (84%) (HOMO -> LUMO+1) (12%)
	371.9nm (3.3eV)	0.1852	(HOMO-1 -> LUMO+1) (95%)
	358.5nm (3.5eV)	0.0305	(HOMO-2 -> LUMO+1) (94%)

Table S8. Vertical electronic Transition, absorption wavelength and oscillator strength of **8** in various solvents and in gas phase.

Molecule 8			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	714.2nm (1.7eV)	0.0242	(HOMO-2 -> LUMO) (65%) (HOMO -> LUMO) (34%)
	711.3nm (1.7eV)	0.0038	(HOMO -> LUMO) (65%) (HOMO-2 -> LUMO) (34%)
	693.6nm (1.8eV)	0.0011	(HOMO-1 -> LUMO) (99%) (HOMO-2 -> LUMO) (34%)
	506.7nm (2.4eV)	0.0051	(HOMO -> LUMO+1) (97%) (HOMO-2 -> LUMO) (34%)
	500.1nm (2.5eV)	0.0055	(HOMO-1 -> LUMO+1) (97%) (HOMO-2 -> LUMO) (34%)
	473.7nm (2.6eV)	0.0164	(HOMO-2 -> LUMO+1) (98%) (HOMO-2 -> LUMO) (34%)
	396.2nm (3.1eV)	0.0023	(HOMO-5 -> LUMO) (48%) (HOMO-11 -> LUMO) (36%)
	392.4nm (3.2eV)	0.0033	(HOMO-3 -> LUMO) (98%) (HOMO-11 -> LUMO) (36%)
	387.5nm (3.2eV)	0.003	(HOMO-4 -> LUMO) (97%) (HOMO-11 -> LUMO) (36%)
	386.8nm (3.2eV)	0.0008	(HOMO -> LUMO+2) (76%) (HOMO -> LUMO+4) (15%)
Chloroform	691.4nm (1.8eV)	0.0344	(HOMO-2 -> LUMO) (99%)

	657.0nm (1.9eV)	0.0021	(HOMO -> LUMO) (99%)
	646.9nm (1.9eV)	0.0015	(HOMO-1 -> LUMO) (99%)
	473.5nm (2.6eV)	0.0072	(HOMO -> LUMO+1) (94%)
	471.1nm (2.6eV)	0.0085	(HOMO-1 -> LUMO+1) (94%)
	459.7nm (2.7eV)	0.0219	(HOMO-2 -> LUMO+1) (97%)
	386.6nm (3.2eV)	0.0077	(HOMO-5 -> LUMO) (52%) (HOMO-7 -> LUMO) (20%) (HOMO-10 -> LUMO) (10%)
	378.0nm (3.3eV)	0.0489	(HOMO-5 -> LUMO) (43%) (HOMO-7 -> LUMO) (21%) (HOMO-10 -> LUMO) (11%)
	373.9nm (3.3eV)	0.073	(HOMO-3 -> LUMO) (86%)
	370.5nm (3.3eV)	0.0205	(HOMO-4 -> LUMO) (94%)
Dichloromethane	684.8nm (1.8eV)	0.0356	(HOMO-2 -> LUMO) (99%)
	645.4nm (1.9eV)	0.0025	(HOMO -> LUMO) (99%)
	637.1nm (1.9eV)	0.0015	(HOMO-1 -> LUMO) (99%)
	466.6nm (2.7eV)	0.0076	(HOMO -> LUMO+1) (88%)
	464.9nm (2.7eV)	0.0096	(HOMO-1 -> LUMO+1) (88%)
	455.9nm (2.7eV)	0.0227	(HOMO-2 -> LUMO+1) (97%)
	384.1nm (3.2eV)	0.0109	(HOMO-5 -> LUMO) (51%) (HOMO-7 -> LUMO) (26%) (HOMO-9 -> LUMO) (12%)
	376.2nm (3.3eV)	0.1034	(HOMO-5 -> LUMO) (40%) (HOMO-7 -> LUMO) (26%) (HOMO-9 -> LUMO) (12%)
	371.2nm (3.3eV)	0.2225	(HOMO-3 -> LUMO) (59%) (HOMO-6 -> LUMO) (28%)
	366.9nm (3.4eV)	0.0351	(HOMO-4 -> LUMO) (82%) (HOMO-3 -> LUMO) (10%)
Dimethylsulfoxide	676.9nm (1.8eV)	0.0369	(HOMO-2 -> LUMO) (99%)
	633.2nm (2.0eV)	0.0029	(HOMO -> LUMO) (98%)
	626.8nm (2.0eV)	0.0014	(HOMO-1 -> LUMO) (98%)
	459.4nm (2.7eV)	0.008	(HOMO -> LUMO+1) (71%) (HOMO-1 -> LUMO+1) (26%)
	458.0nm (2.7eV)	0.0111	(HOMO-1 -> LUMO+1) (71%) (HOMO -> LUMO+1) (26%)
	451.4nm (2.7eV)	0.0234	(HOMO-2 -> LUMO+1) (97%) (HOMO -> LUMO+1) (26%)
	381.4nm (3.3eV)	0.0191	(HOMO-5 -> LUMO) (49%) (HOMO-7 -> LUMO) (26%) (HOMO-9 -> LUMO) (17%)
	374.8nm (3.3eV)	0.2936	(HOMO-5 -> LUMO) (28%) (HOMO-6 -> LUMO) (26%) (HOMO-7 -> LUMO) (19%) (HOMO-9 -> LUMO) (12%) (HOMO-3 -> LUMO) (10%)
	370.1nm (3.3eV)	0.2801	(HOMO-6 -> LUMO) (43%) (HOMO-5 -> LUMO) (21%) (HOMO-3 -> LUMO) (19%)

	363.0nm (3.4eV)	0.0316	(HOMO-4 -> LUMO) (52%) (HOMO-3 -> LUMO) (24%) (HOMO -> LUMO+2) (12%)
Tetrahydrofuran	686.4nm (1.8eV)	0.0353	(HOMO-2 -> LUMO) (99%)
	648.2nm (1.9eV)	0.0024	(HOMO -> LUMO) (99%)
	639.5nm (1.9eV)	0.0015	(HOMO-1 -> LUMO) (99%)
	468.3nm (2.6eV)	0.0076	(HOMO -> LUMO+1) (90%)
	466.4nm (2.7eV)	0.0093	(HOMO-1 -> LUMO+1) (90%)
	456.8nm (2.7eV)	0.0226	(HOMO-2 -> LUMO+1) (97%)
	384.8nm (3.2eV)	0.0099	(HOMO-5 -> LUMO) (51%) (HOMO-7 -> LUMO) (25%)
	376.6nm (3.3eV)	0.0841	(HOMO-5 -> LUMO) (41%) (HOMO-7 -> LUMO) (26%)
	371.7nm (3.3eV)	0.177	(HOMO-3 -> LUMO) (68%) (HOMO-6 -> LUMO) (21%)
	367.8nm (3.4eV)	0.0319	(HOMO-4 -> LUMO) (86%)
Toluene	700.7nm (1.8eV)	0.0322	(HOMO-2 -> LUMO) (98%)
	676.5nm (1.8eV)	0.0015	(HOMO -> LUMO) (99%)
	663.3nm (1.9eV)	0.0013	(HOMO-1 -> LUMO) (99%)
	485.2nm (2.6eV)	0.0065	(HOMO -> LUMO+1) (96%)
	481.4nm (2.6eV)	0.0072	(HOMO-1 -> LUMO+1) (96%)
	465.3nm (2.7eV)	0.0202	(HOMO-2 -> LUMO+1) (98%)
	390.3nm (3.2eV)	0.0048	(HOMO-5 -> LUMO) (52%) (HOMO-7 -> LUMO) (20%) (HOMO-10 -> LUMO) (10%) (HOMO-8 -> LUMO) (13%)
	381.1nm (3.3eV)	0.0273	(HOMO-5 -> LUMO) (40%) (HOMO-11 -> LUMO) (18%) (HOMO-8 -> LUMO) (13%) (HOMO-3 -> LUMO) (10%)
	380.1nm (3.3eV)	0.0084	(HOMO-3 -> LUMO) (88%) (HOMO-8 -> LUMO) (13%)
	376.5nm (3.3eV)	0.007	(HOMO-4 -> LUMO) (98%) (HOMO-8 -> LUMO) (13%)

Table S9. Vertical electronic Transition, absorption wavelength and oscillator strength of **9** in various solvents and in gas phase.

Molecule 9			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	626.9nm (2.0eV)	0.0005	(HOMO -> LUMO) (99%)
	610.0nm (2.0eV)	0.0012	(HOMO-1 -> LUMO) (99%)
	601.8nm (2.1eV)	0.0354	(HOMO-2 -> LUMO) (98%)
	464.8nm (2.7eV)	0.0001	(HOMO -> LUMO+1) (97%)
	458.5nm (2.7eV)	0.0003	(HOMO-1 -> LUMO+1) (97%)

	422.2nm (2.9eV)	0.0121	(HOMO-2 -> LUMO+1) (97%)
	414.0nm (3.0eV)	0.0029	(HOMO-3 -> LUMO) (76%) (HOMO-5 -> LUMO) (15%)
	412.4nm (3.0eV)	0.0107	(HOMO-5 -> LUMO) (57%) (HOMO-3 -> LUMO) (23%)
	406.6nm (3.0eV)	0.0011	(HOMO-4 -> LUMO) (97%) (HOMO-11 -> LUMO) (10%)
	394.5nm (3.1eV)	0.0315	(HOMO-11 -> LUMO) (42%) (HOMO-5 -> LUMO) (24%) (HOMO-10 -> LUMO) (21%)
Chloroform	593.1nm (2.1eV)	0.0510	(HOMO-2 -> LUMO) (98%)
	586.8nm (2.1eV)	0.0004	(HOMO -> LUMO) (99%)
	578.9nm (2.1eV)	0.0007	(HOMO-1 -> LUMO) (99%)
	438.1nm (2.8eV)	0.0002	(HOMO -> LUMO+1) (97%)
	436.9nm (2.8eV)	0.0006	(HOMO-1 -> LUMO+1) (97%)
	414.0nm (3.0eV)	0.0193	(HOMO-2 -> LUMO+1) (97%)
	405.9nm (3.1eV)	0.0533	(HOMO-5 -> LUMO) (86%)
	395.0nm (3.1eV)	0.0028	(HOMO-3 -> LUMO) (96%)
	392.1nm (3.2eV)	0.0143	(HOMO-4 -> LUMO) (90%)
	389.1nm (3.2eV)	0.254	(HOMO-11 -> LUMO) (33%) (HOMO-6 -> LUMO) (29%)
Dichloromethane	589.9nm (2.1eV)	0.0539	(HOMO-2 -> LUMO) (98%)
	577.5nm (2.1eV)	0.0005	(HOMO -> LUMO) (99%)
	571.8nm (2.2eV)	0.0008	(HOMO-1 -> LUMO) (99%)
	432.2nm (2.9eV)	0.0007	(HOMO-1 -> LUMO+1) (97%)
	432.1nm (2.9eV)	0.0003	(HOMO -> LUMO+1) (97%)
	411.8nm (3.0eV)	0.0211	(HOMO-2 -> LUMO+1) (97%)
	404.1nm (3.1eV)	0.078	(HOMO-5 -> LUMO) (88%)
	390.8nm (3.2eV)	0.0601	(HOMO-3 -> LUMO) (75%)
	389.5nm (3.2eV)	0.2707	(HOMO-6 -> LUMO) (34%) (HOMO-3 -> LUMO) (22%) (HOMO-4 -> LUMO) (18%) (HOMO-11 -> LUMO) (12%)
	388.2nm (3.2eV)	0.1305	(HOMO-4 -> LUMO) (76%) (HOMO-6 -> LUMO) (19%) (HOMO-4 -> LUMO) (18%)
Dimethylsulfoxide	585.9nm (2.1eV)	0.0571	(HOMO-2 -> LUMO) (98%)
	567.1nm (2.2eV)	0.0006	(HOMO -> LUMO) (99%)
	563.7nm (2.2eV)	0.0009	(HOMO-1 -> LUMO) (99%)
	427.1nm (2.9eV)	0.0009	(HOMO-1 -> LUMO+1) (97%)
	425.6nm (2.9eV)	0.0004	(HOMO -> LUMO+1) (97%)
	409.1nm (3.0eV)	0.0234	(HOMO-2 -> LUMO+1) (97%)
	402.1nm (3.1eV)	0.1298	(HOMO-5 -> LUMO) (89%)
	390.5nm (3.2eV)	0.527	(HOMO-6 -> LUMO) (73%) (HOMO-9 -> LUMO) (10%)
	385.8nm (3.2eV)	0.0266	(HOMO-3 -> LUMO) (82%)
	384.7nm (3.2eV)	0.0086	(HOMO-4 -> LUMO) (84%) (HOMO-3 -> LUMO) (10%)

Tetrahydrofuran	590.8nm (2.1eV)	0.0532	(HOMO-2 -> LUMO) (98%)
	579.8nm (2.1eV)	0.0005	(HOMO -> LUMO) (99%)
	573.6nm (2.2eV)	0.0008	(HOMO-1 -> LUMO) (99%)
	433.6nm (2.9eV)	0.0003	(HOMO -> LUMO+1) (97%)
	433.4nm (2.9eV)	0.0007	(HOMO-1 -> LUMO+1) (97%)
	412.3nm (3.0eV)	0.0207	(HOMO-2 -> LUMO+1) (97%)
	404.5nm (3.1eV)	0.0707	(HOMO-5 -> LUMO) (87%)
	391.8nm (3.2eV)	0.0175	(HOMO-3 -> LUMO) (88%)
	389.9nm (3.2eV)	0.1482	(HOMO-4 -> LUMO) (51%) (HOMO-6 -> LUMO) (17%) (HOMO-11 -> LUMO) (12%)
	388.6nm (3.2eV)	0.2539	(HOMO-4 -> LUMO) (45%) (HOMO-6 -> LUMO) (34%) (HOMO-11 -> LUMO) (10%)
Toluene	601.4nm (2.1eV)	0.0011	(HOMO -> LUMO) (99%)
	597.2nm (2.1eV)	0.0451	(HOMO-2 -> LUMO) (98%)
	590.1nm (2.1eV)	0.0006	(HOMO-1 -> LUMO) (98%)
	447.7nm (2.8eV)	0.0002	(HOMO -> LUMO+1) (97%)
	444.6nm (2.8eV)	0.0005	(HOMO-1 -> LUMO+1) (97%)
	417.3nm (3.0eV)	0.0166	(HOMO-2 -> LUMO+1) (97%)
	408.6nm (3.0eV)	0.0313	(HOMO-5 -> LUMO) (81%) (HOMO-11 -> LUMO) (11%)
	401.8nm (3.1eV)	0.0012	(HOMO-3 -> LUMO) (97%) (HOMO-11 -> LUMO) (11%)
	397.3nm (3.1eV)	0.0024	(HOMO-4 -> LUMO) (97%) (HOMO-11 -> LUMO) (11%)
	390.8nm (3.2eV)	0.0898	(HOMO-11 -> LUMO) (49%) (HOMO-5 -> LUMO) (14%)

Table S10. Vertical electronic Transition, absorption wavelength and oscillator strength of **10** in various solvents and in gas phase.

Molecule 10			
Phase	**Wavelength**	**oscillator strength**	**Assignment**
Gas	439.5nm (2.8eV)	0.3671	(HOMO -> LUMO) (98%)
	387.4nm (3.2eV)	0.0570	(HOMO-1 -> LUMO) (99%)
	382.0nm (3.2eV)	0.0021	(HOMO-3 -> LUMO) (75%) (HOMO-2 -> LUMO) (23%)
	347.7nm (3.6eV)	0.0724	(HOMO-2 -> LUMO) (73%) (HOMO-3 -> LUMO) (23%)
	345.6nm (3.6eV)	0.3339	(HOMO -> LUMO+1) (98%) (HOMO-3 -> LUMO) (23%)
	307.3nm (4.0eV)	0.5892	(HOMO-1 -> LUMO+1) (90%)
	301.1nm (4.1eV)	0.0476	(HOMO -> LUMO+2) (82%)
	298.4nm (4.2eV)	0.0262	(HOMO-4 -> LUMO) (63%)

			(HOMO-3 -> LUMO+1) (12%)
	296.3nm (4.2eV)	0.0009	(HOMO-3 -> LUMO+1) (42%) (HOMO-2 -> LUMO+1) (25%) (HOMO-4 -> LUMO) (21%)
	284.4nm (4.4eV)	0.0022	(HOMO-3 -> LUMO+1) (30%) (HOMO-2 -> LUMO+1) (24%) (HOMO -> LUMO+3) (14%) (HOMO-5 -> LUMO) (10%)
Chloroform	468.6nm (2.6eV)	0.5669	(HOMO -> LUMO) (99%)
	408.2nm (3.0eV)	0.0783	(HOMO-1 -> LUMO) (99%)
	378.0nm (3.3eV)	0.0389	(HOMO-2 -> LUMO) (60%) (HOMO-3 -> LUMO) (38%)
	359.8nm (3.4eV)	0.0800	(HOMO-3 -> LUMO) (52%) (HOMO-2 -> LUMO) (34%) (HOMO -> LUMO+1) (11%)
	357.1nm (3.5eV)	0.4133	(HOMO -> LUMO+1) (87%)
	319.4nm (3.9eV)	0.7905	(HOMO-1 -> LUMO+1) (96%)
	303.7nm (4.1eV)	0.0571	(HOMO -> LUMO+2) (66%) (HOMO-4 -> LUMO) (22%)
	303.1nm (4.1eV)	0.0261	(HOMO-4 -> LUMO) (69%) (HOMO -> LUMO+2) (20%)
	296.3nm (4.2eV)	0.0073	(HOMO-2 -> LUMO+1) (68%) (HOMO -> LUMO+3) (10%) (HOMO-3 -> LUMO+1) (10%)
	285.4nm (4.3eV)	0.0136	(HOMO-6 -> LUMO) (81%)
Dichloromethane	475.1nm (2.6eV)	0.6088	(HOMO -> LUMO) (99%)
	412.9nm (3.0eV)	0.0817	(HOMO-1 -> LUMO) (99%)
	379.4nm (3.3eV)	0.0567	(HOMO-2 -> LUMO) (74%) (HOMO-3 -> LUMO) (23%)
	360.9nm (3.4eV)	0.1963	(HOMO -> LUMO+1) (45%) (HOMO-3 -> LUMO) (39%) (HOMO-2 -> LUMO) (14%)
	358.9nm (3.5eV)	0.3013	(HOMO -> LUMO+1) (53%) (HOMO-3 -> LUMO) (34%) (HOMO-2 -> LUMO) (10%)
	322.1nm (3.8eV)	0.8240	(HOMO-1 -> LUMO+1) (96%) (HOMO-3 -> LUMO) (24%)
	304.5nm (4.1eV)	0.0370	(HOMO-4 -> LUMO) (58%) (HOMO -> LUMO+2) (31%)
	304.0nm (4.1eV)	0.0538	(HOMO -> LUMO+2) (55%) (HOMO-4 -> LUMO) (33%)
	297.5nm (4.2eV)	0.0090	(HOMO-2 -> LUMO+1) (72%) (HOMO -> LUMO+3) (10%)
	286.5nm (4.3eV)	0.1084	(HOMO-5 -> LUMO) (50%) (HOMO -> LUMO+3) (33%)
Dimethylsulfoxide	482.3nm (2.6eV)	0.6534	(HOMO -> LUMO) (99%)
	417.9nm (3.0eV)	0.0848	(HOMO-1 -> LUMO) (99%)
	381.9nm (3.2eV)	0.0726	(HOMO-2 -> LUMO) (85%) (HOMO-3 -> LUMO) (13%)

	362.8nm (3.4eV)	0.4014	(HOMO -> LUMO+1) (88%)
	359.2nm (3.5eV)	0.1029	(HOMO-3 -> LUMO) (74%) (HOMO-2 -> LUMO) (12%)
	325.0nm (3.8eV)	0.8578	(HOMO-1 -> LUMO+1) (97%) (HOMO-2 -> LUMO) (12%)
	305.5nm (4.1eV)	0.0175	(HOMO-4 -> LUMO) (86%)
	304.9nm (4.1eV)	0.0839	(HOMO -> LUMO+2) (82%)
	299.0nm (4.1eV)	0.0108	(HOMO-2 -> LUMO+1) (75%) (HOMO -> LUMO+3) (10%)
	288.5nm (4.3eV)	0.1261	(HOMO-5 -> LUMO) (61%) (HOMO -> LUMO+3) (29%)
Tetrahydrofuran	473.6nm (2.6eV)	0.5987	(HOMO -> LUMO) (99%)
	411.7nm (3.0eV)	0.0809	(HOMO-1 -> LUMO) (99%)
	379.0nm (3.3eV)	0.0525	(HOMO-2 -> LUMO) (71%) (HOMO-3 -> LUMO) (27%)
	360.6nm (3.4eV)	0.1469	(HOMO-3 -> LUMO) (46%) (HOMO -> LUMO+1) (32%)
	358.5nm (3.5eV)	0.3496	(HOMO -> LUMO+1) (66%) (HOMO-3 -> LUMO) (24%)
	321.5nm (3.9eV)	0.8161	(HOMO-1 -> LUMO+1) (96%) (HOMO-3 -> LUMO) (24%)
	304.3nm (4.1eV)	0.0441	(HOMO-4 -> LUMO) (47%) (HOMO -> LUMO+2) (42%)
	303.8nm (4.1eV)	0.0447	(HOMO -> LUMO+2) (44%) (HOMO-4 -> LUMO) (44%)
	297.2nm (4.2eV)	0.0086	(HOMO-2 -> LUMO+1) (71%) (HOMO -> LUMO+3) (10%)
	286.1nm (4.3eV)	0.0360	(HOMO-6 -> LUMO) (67%) (HOMO-5 -> LUMO) (10%)
Toluene	457.9nm (2.7eV)	0.4965	(HOMO -> LUMO) (99%)
	400.6nm (3.1eV)	0.0718	(HOMO-1 -> LUMO) (99%)
	378.0nm (3.3eV)	0.0158	(HOMO-3 -> LUMO) (60%) (HOMO-2 -> LUMO) (38%)
	356.5nm (3.5eV)	0.0734	(HOMO-2 -> LUMO) (59%) (HOMO-3 -> LUMO) (37%)
	353.2nm (3.5eV)	0.4035	(HOMO -> LUMO+1) (96%) (HOMO-3 -> LUMO) (37%)
	315.0nm (3.9eV)	0.7298	(HOMO-1 -> LUMO+1) (95%) (HOMO-3 -> LUMO) (37%)
	302.6nm (4.1eV)	0.0570	(HOMO -> LUMO+2) (79%)
	301.3nm (4.1eV)	0.0174	(HOMO-4 -> LUMO) (82%)
	295.2nm (4.2eV)	0.0041	(HOMO-2 -> LUMO+1) (56%) (HOMO-3 -> LUMO+1) (23%)
	285.4nm (4.3eV)	0.0008	(HOMO-3 -> LUMO+1) (55%) (HOMO -> LUMO+3) (13%)

10. Optimized structures and geometrical parameter of compounds.

Table S11. Geometrical parameter of compound 1

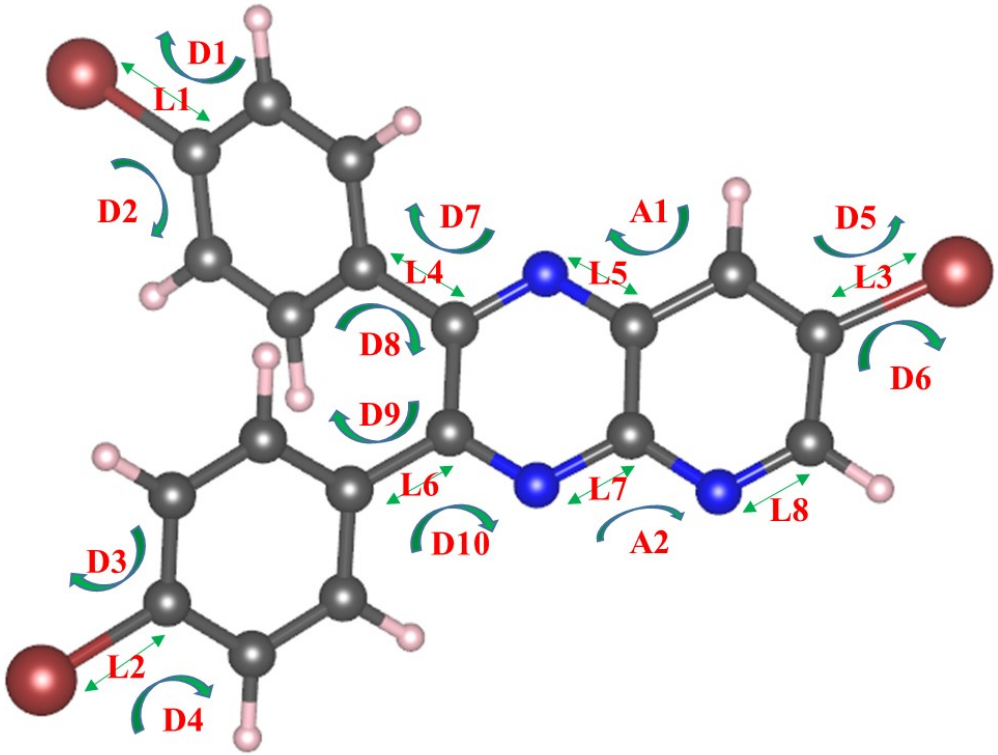


Fig. S41. Optimized structures of 1.

bond length (A°)						Dihedral/bond angle					
	S0	S1	Δ (S1-S0)	T1	Δ (T1−S0)		S0	S1	Δ (S1-S0)	T1	Δ (T1−S0)

L1	1.9149	1.9065	-0.0084	1.9036	-0.0113	**D1**	0.1824	0.0568	-0.1256	0.4380	0.2556
L2	1.9149	1.9031	-0.0118	1.9129	-0.0020	**D2**	0.8265	1.2261	0.3996	1.3809	0.5544
L3	1.9087	1.9119	0.0032	1.9121	0.0034	**D3**	0.8406	1.2022	0.3616	0.8540	0.0134
L4	1.4876	1.4788	-0.0088	1.4213	-0.0663	**D4**	0.2463	0.3196	0.0733	0.1188	-0.1275
L5	1.3548	1.3465	-0.0083	1.3235	-0.0313	**D5**	0.7996	1.9148	1.1152	0.9960	0.1964
L6	1.4881	1.4832	-0.0049	1.4805	-0.0076	**D6**	0.6123	1.1020	0.4897	2.8543	2.2420
L7	1.3513	1.3426	-0.0087	1.3860	0.0347	**D7**	40.8533	33.7297	-7.1236	16.3733	-24.4800
L8	1.3123	1.3341	0.0218	1.3490	0.0367	**D8**	42.9209	35.7434	-7.1775	9.6854	-33.2355
						D9	40.7539	31.7454	-9.0085	31.6121	-9.1418
						D10	38.4461	34.2487	-4.1974	30.0701	-8.3760
						A1	120.2957	121.2161	0.9204	121.0276	0.7319
						A2	117.6290	118.3440	0.7150	117.9450	0.3160

Table S12. Geometrical parameter of compound 2

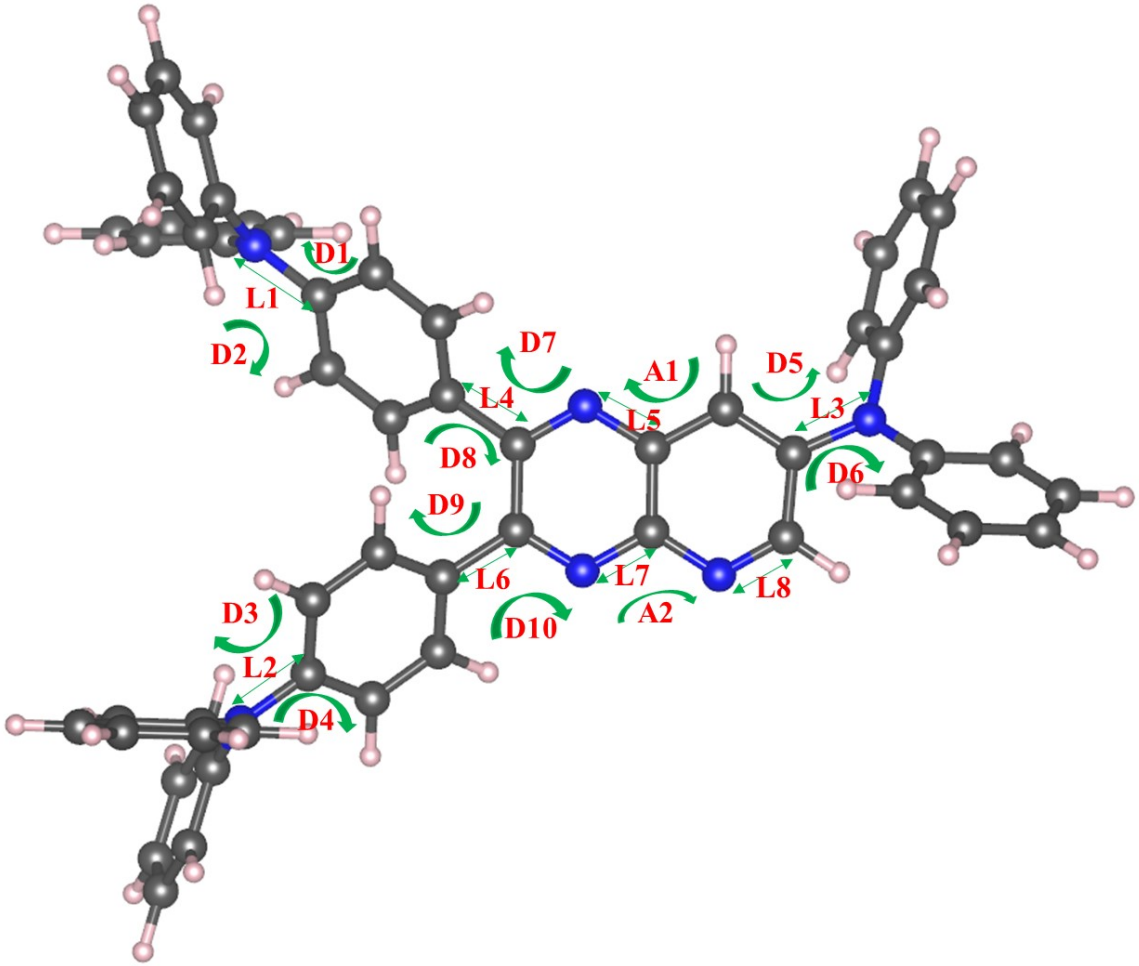


Fig. S42. Optimized structures of 2.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4152	1.4119	-0.0033	1.4045	-0.0107	D1	0.3144	0.2275	-0.0869	0.7228	0.4084
L2	1.4155	1.4386	0.0231	1.4118	-0.0037	D2	0.2395	0.3954	0.1559	0.4201	0.1806
L3	1.4088	1.4331	0.0243	1.4177	0.0089	D3	0.3385	0.2422	-0.0963	0.3099	-0.0286
L4	1.4856	1.4961	0.0105	1.4337	-0.0519	D4	0.4134	0.0701	-0.3433	0.3961	-0.0173
L5	1.3561	1.3582	0.0021	1.3302	-0.0259	D5	31.3151	55.8533	24.5382	38.4535	7.1384
L6	1.4853	1.4925	0.0073	1.4802	-0.0051	D6	40.4395	56.8019	16.3624	45.3444	4.9049
L7	1.3482	1.3499	0.0017	1.3674	0.0192	D7	38.9861	46.8688	7.8827	17.8650	-21.1211
L8	1.3099	1.3362	0.0263	1.3364	0.0265	D8	41.3275	46.4259	5.0984	17.6952	-23.6323
						D9	39.6448	40.6841	1.0393	34.2018	-5.4430
						D10	37.0100	37.8284	0.8184	33.7137	-3.2963
						A1	120.4218	120.8046	0.3828	121.1327	0.7109
						A2	117.8987	117.9245	0.0258	118.1182	0.2195

Table S13. Geometrical parameter of compound 3

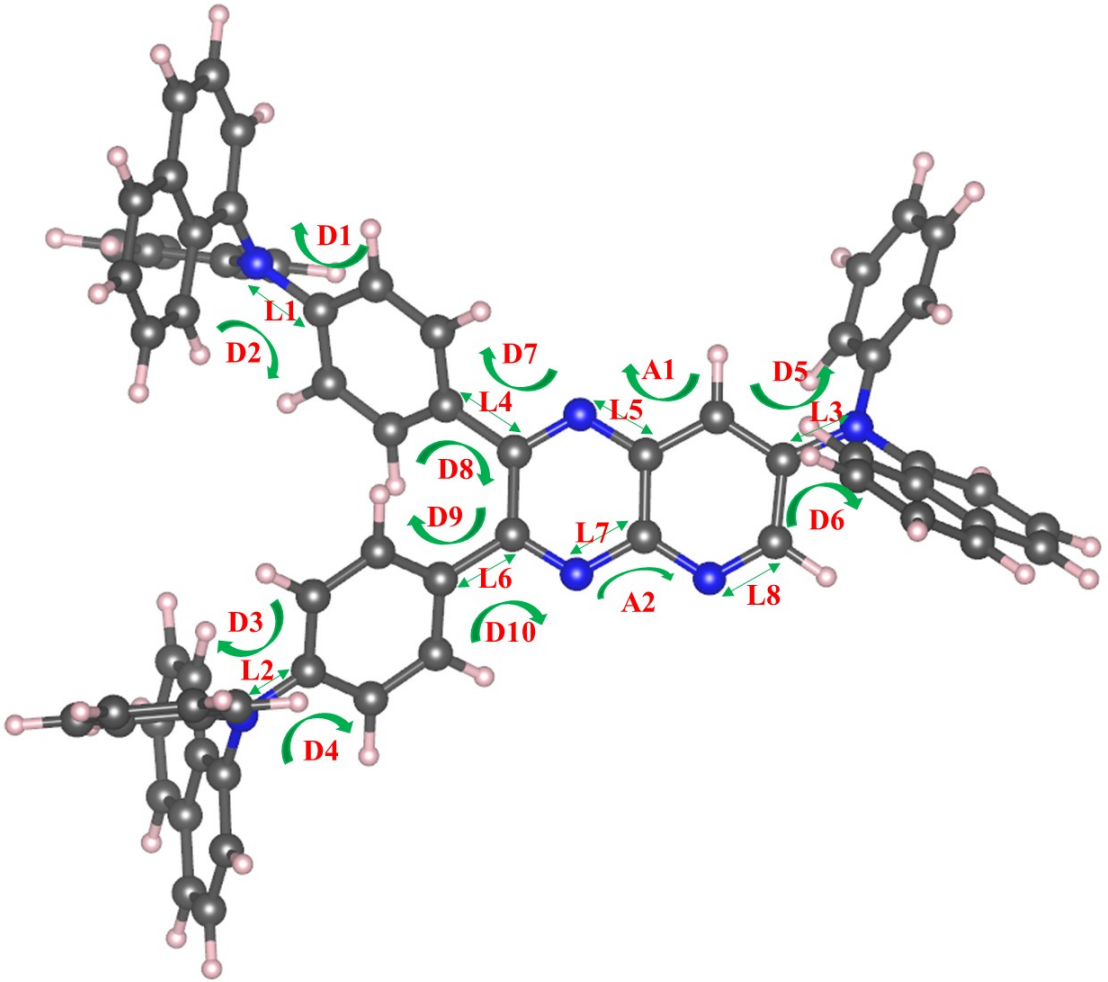


Fig. S43. Optimized structures of 3.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4140	1.4371	0.0231	1.4177	0.0037	D1	1.6683	0.4434	-1.2249	1.1794	-0.4889
L2	1.4135	1.4324	0.0189	1.4075	-0.0061	D2	1.6824	0.5070	-1.1754	1.2388	-0.4436
L3	1.4054	1.4316	0.0261	1.3996	-0.0059	D3	1.7048	0.8709	-0.8339	2.2840	0.5792
L4	1.4858	1.4963	0.0104	1.4850	-0.0008	D4	1.7650	1.0084	-0.7566	2.0713	0.3063
L5	1.3575	1.3581	0.0006	1.3726	0.0152	D5	30.2056	53.7046	23.4990	36.8129	6.6073
L6	1.4855	1.4915	0.0060	1.4509	-0.0346	D6	25.3288	38.7218	13.3930	28.9324	3.6036
L7	1.3493	1.3492	-0.0001	1.3178	-0.0315	D7	40.9439	48.4595	7.5156	43.1033	2.1594
L8	1.3112	1.3378	0.0266	1.3204	0.0092	D8	43.1948	49.4972	6.3024	44.0414	0.8466
						D9	40.1406	37.4082	-2.7324	22.2475	-17.8931
						D10	37.5008	34.3973	-3.1035	20.4502	-17.0506
						A1	120.2917	120.7245	0.4328	120.7430	0.4513
						A2	117.9584	118.0943	0.1359	117.9999	0.0415

Table S14. Geometrical parameter of compound 4

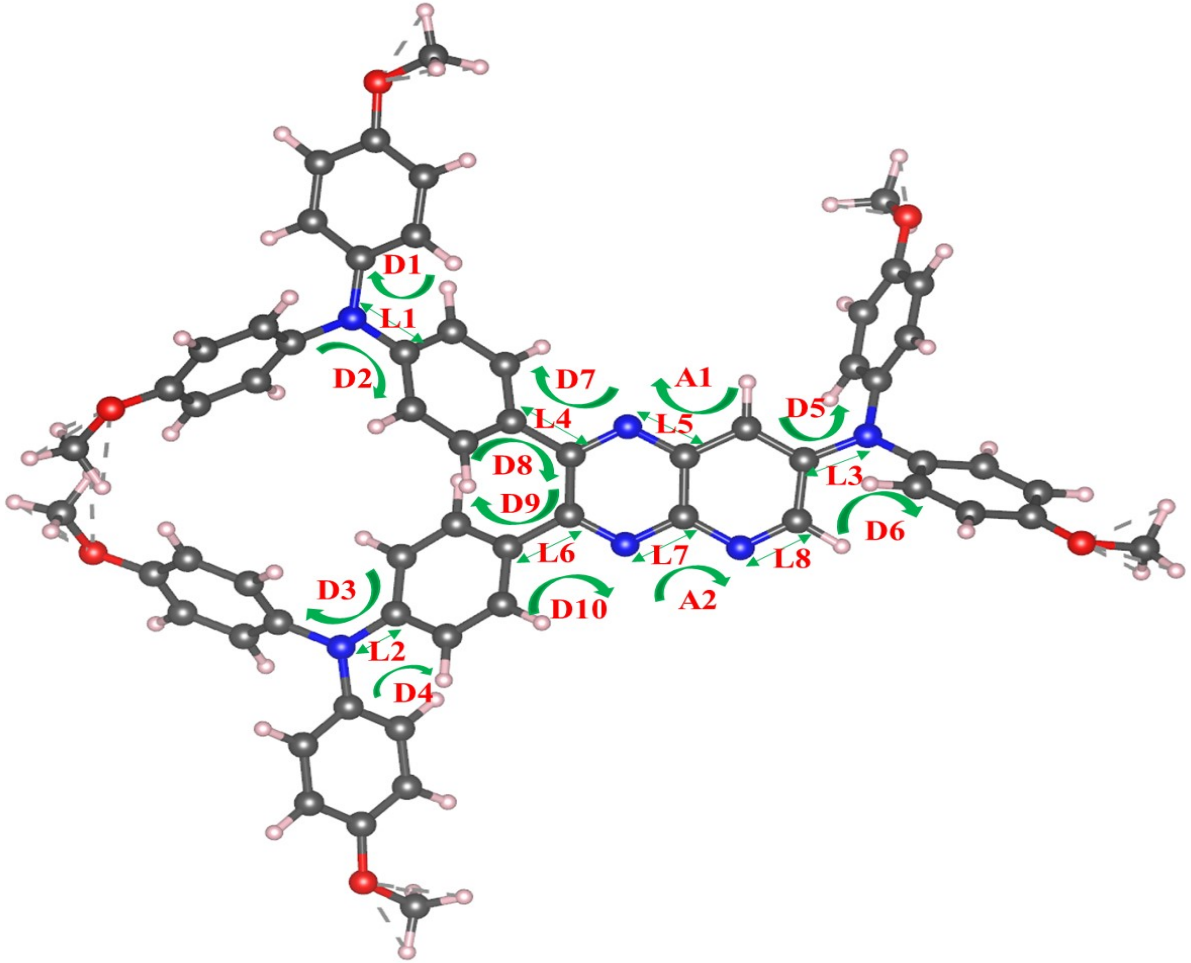


Fig. S44. Optimized structures of 4.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4085	1.4451	0.0366	1.4205	0.0120	D1	1.2672	0.6961	-0.5711	0.2560	-1.0112
L2	1.4096	1.4447	0.0352	1.4268	0.0172	D2	0.5944	0.1583	-0.4361	2.7902	2.1958
L3	1.4025	1.4294	0.0270	1.4244	0.0219	D3	0.5383	0.8207	0.2824	2.1537	1.6154
L4	1.4833	1.4952	0.0119	1.4695	-0.0138	D4	1.2430	0.0323	-1.2107	1.0713	-0.1717
L5	1.3570	1.3578	0.0008	1.3470	-0.0100	D5	28.1185	54.7603	26.6418	51.1673	23.0488
L6	1.4834	1.4934	0.0100	1.4195	-0.0639	D6	35.7866	50.5830	14.7964	45.5948	9.8082
L7	1.3484	1.3512	0.0028	1.3557	0.0073	D7	38.3836	46.2741	7.8905	27.4579	-10.9257
L8	1.3103	1.3376	0.0273	1.3399	0.0296	D8	41.1943	47.4796	6.2853	29.0186	-12.1757
						D9	39.1936	41.3603	2.1667	39.1886	-0.0050
						D10	36.2516	38.9900	2.7384	37.9663	1.7147
						A1	120.3953	120.7369	0.3416	120.5924	0.1971
						A2	117.9506	117.9851	0.0345	118.3185	0.3679

Table S15. Geometrical parameter of compound 5

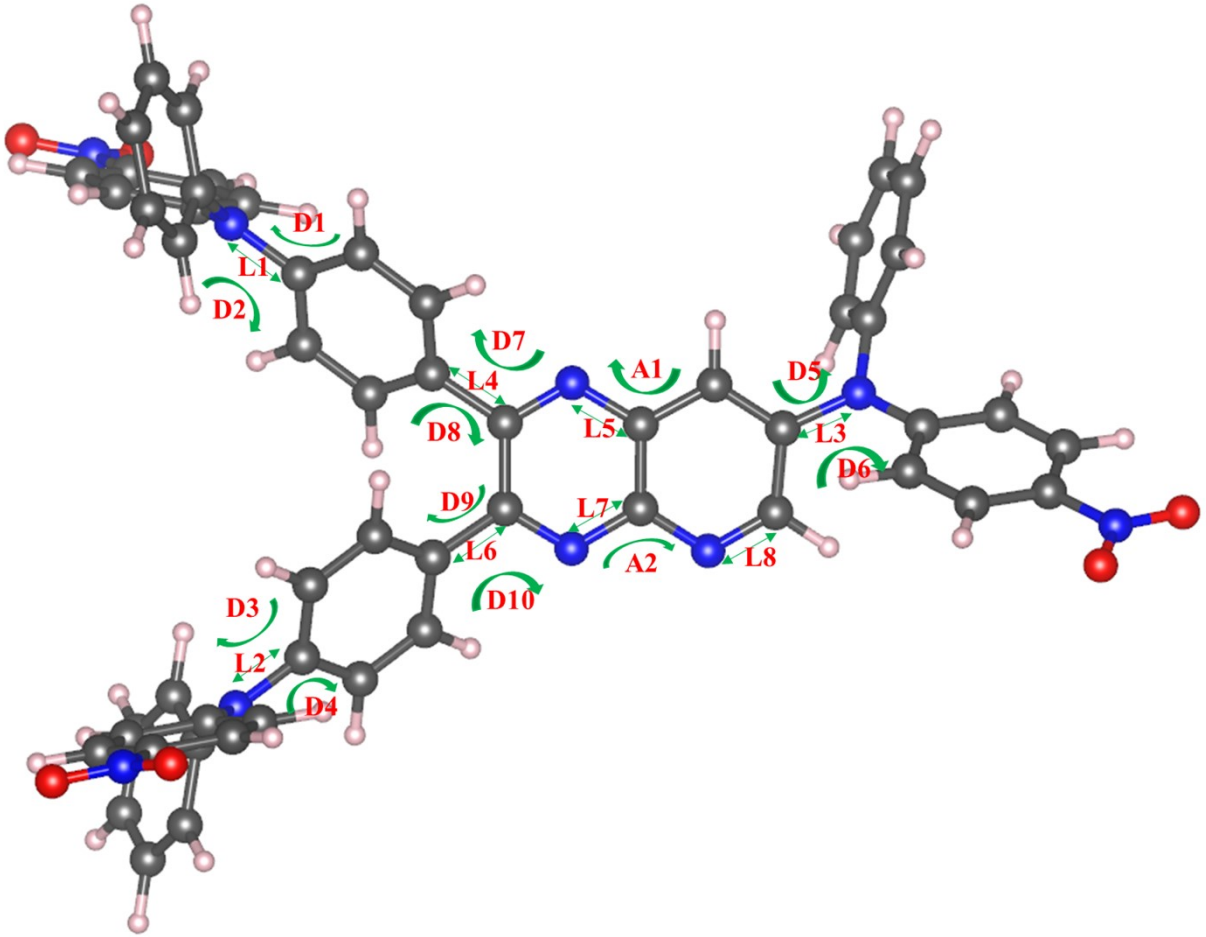


Fig. S45. Optimized structures of 5.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4232	1.4371	0.0139	1.4239	0.0007	D1	0.9165	0.5625	-0.3540	0.8208	-0.0957
L2	1.4230	1.4372	0.0143	1.4129	-0.0101	D2	1.0082	0.5949	-0.4133	0.8265	-0.1817
L3	1.4160	1.4345	0.0185	1.3995	-0.0164	D3	1.0552	0.5647	-0.4905	0.8550	-0.2002
L4	1.4866	1.4959	0.0092	1.4869	0.0003	D4	0.9772	0.8751	-0.1021	0.9998	0.0226
L5	1.3558	1.3587	0.0029	1.3772	0.0214	D5	37.8804	57.2233	19.3429	35.1716	-2.7088
L6	1.4864	1.4909	0.0045	1.4442	-0.0422	D6	46.0290	59.1118	13.0828	35.6971	-10.3319
L7	1.3487	1.3468	-0.0020	1.3138	-0.0349	D7	40.3486	45.4832	5.1346	42.0182	1.6696
L8	1.3097	1.3334	0.0237	1.3138	0.0041	D8	42.4416	47.1988	4.7572	43.8264	1.3848
						D9	39.9903	35.7808	-4.2095	16.3872	-23.6031
						D10	37.5033	32.8197	-4.6836	16.3403	-21.1630
						A1	120.4181	120.8529	0.4348	120.8834	0.4653
						A2	117.7940	117.9072	0.1132	118.0414	0.2474

Table S16. Geometrical parameter of compound 6

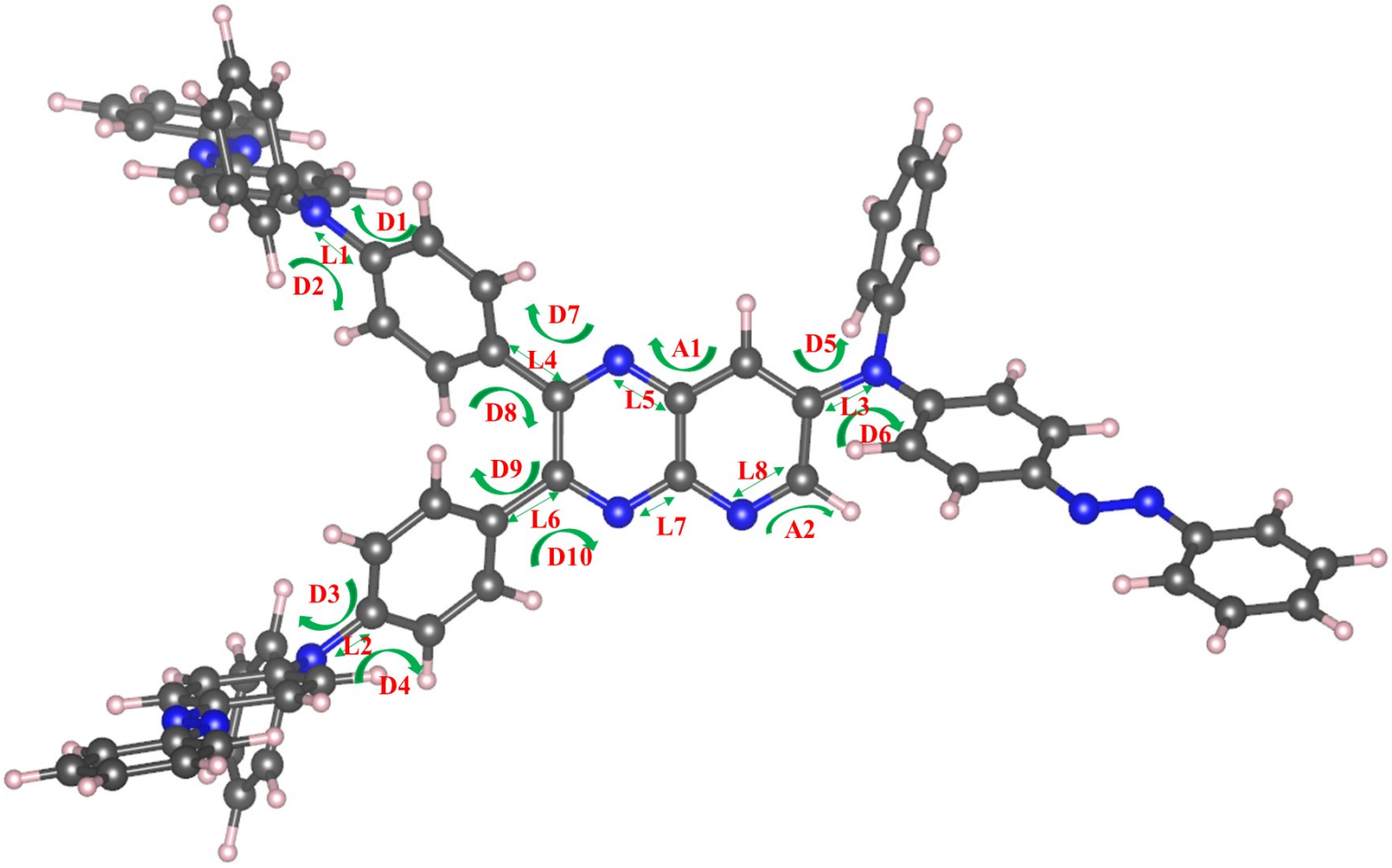


Fig. S46. Optimized structures of 6.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4185	1.4442	0.0258	1.4442	0.0257	D1	0.6841	0.4795	-0.2046	0.7332	0.0491
L2	1.4197	1.4395	0.0197	1.4437	0.0240	D2	0.6020	0.2611	-0.3409	0.4405	-0.1615
L3	1.4122	1.4351	0.0229	1.4354	0.0231	D3	0.6738	0.9016	0.2278	1.1450	0.4712
L4	1.4860	1.4945	0.0086	1.4944	0.0084	D4	0.7116	0.8039	0.0923	0.3708	-0.3408
L5	1.3558	1.3586	0.0028	1.3620	0.0062	D5	34.8923	57.3494	22.4571	57.4601	22.5678
L6	1.4861	1.4913	0.0052	1.4906	0.0045	D6	44.3035	59.4906	15.1871	59.1851	14.8816
L7	1.3484	1.3487	0.0004	1.3478	-0.0006	D7	39.1993	43.7766	4.5773	43.1826	3.9833
L8	1.3095	1.3346	0.0251	1.3280	0.0185	D8	41.3557	45.4951	4.1394	45.6709	4.3152
						D9	41.0727	37.9032	-3.1695	37.9887	-3.0840
						D10	38.4912	35.1211	-3.3701	35.1263	-3.3649
						A1	120.4148	120.8161	0.4013	120.7981	0.3833
						A2	117.8258	117.9232	0.0974	118.2001	0.3743

Table S17. Geometrical parameter of compound 7

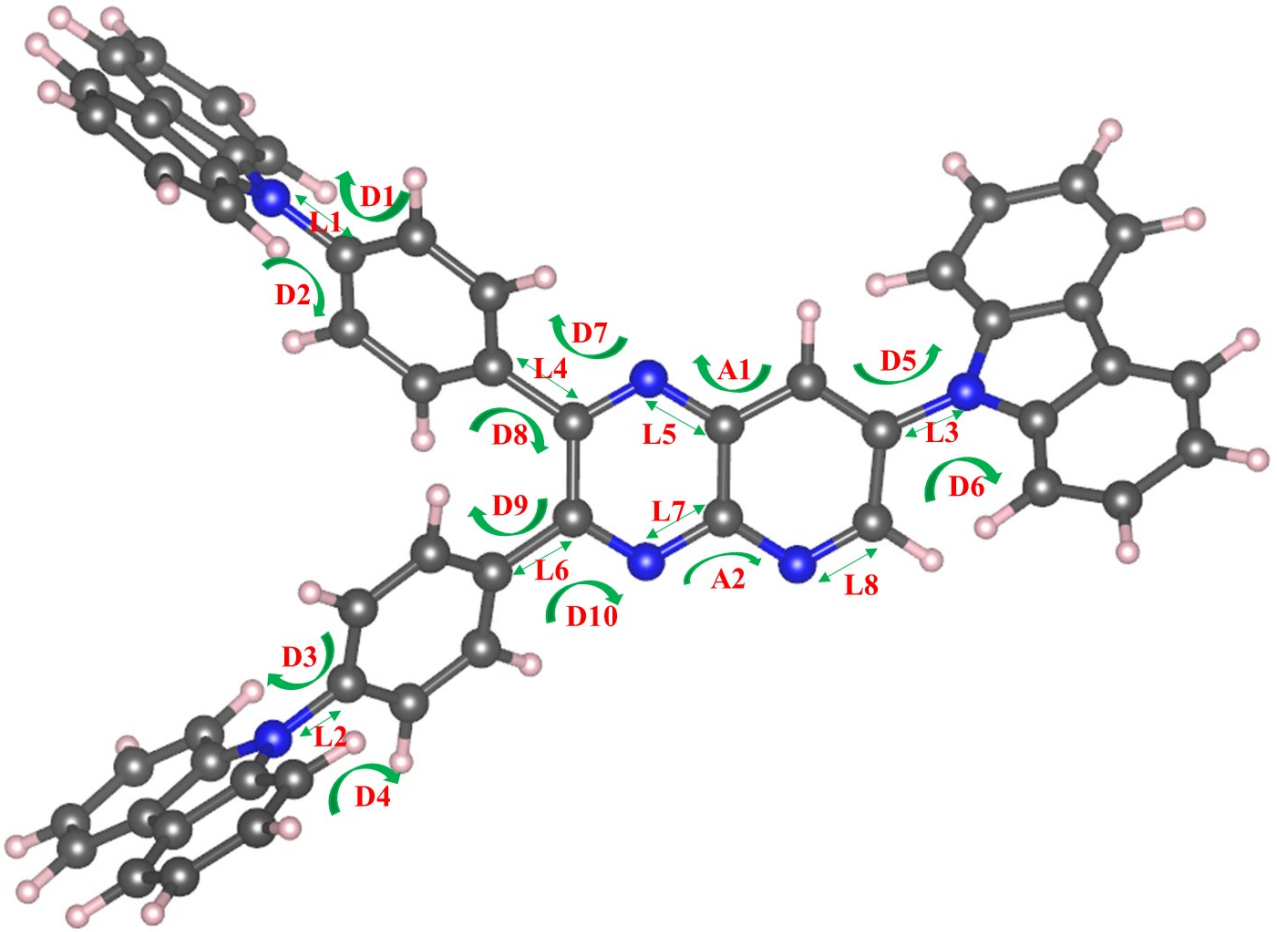


Fig. S47. Optimized structures of 7.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4187	1.4511	0.0324	1.4269	0.0082	D1	1.1391	0.9720	-0.1671	0.2584	-0.8807
L2	1.4191	1.4300	0.0109	1.4232	0.0041	D2	0.4297	0.6489	0.2192	0.6165	0.1868
L3	1.4123	1.4319	0.0196	1.4494	0.0372	D3	0.3252	1.4711	1.1459	0.2755	-0.0497
L4	1.4878	1.4945	0.0067	1.4899	0.0021	D4	1.2359	1.2089	-0.0270	0.6258	-0.6101
L5	1.3557	1.3584	0.0028	1.3535	-0.0022	D5	53.9308	91.4481	37.5173	104.6692	50.7384
L6	1.4881	1.4899	0.0018	1.4847	-0.0034	D6	54.9546	94.7202	39.7656	104.9653	50.0107
L7	1.3509	1.3506	-0.0003	1.3365	-0.0144	D7	40.1962	42.5602	2.3640	41.3216	1.1254
L8	1.3117	1.3365	0.0248	1.3323	0.0206	D8	43.2270	44.1363	0.9093	43.1554	-0.0716
						D9	41.1704	41.8328	0.6624	37.6262	-3.5442
						D10	38.6737	39.7314	1.0577	35.5318	-3.1419
						A1	120.3893	120.8464	0.4571	120.6350	0.2457
						A2	117.6886	117.7999	0.1113	118.1954	0.5068

Table S18. Geometrical parameter of compound 8

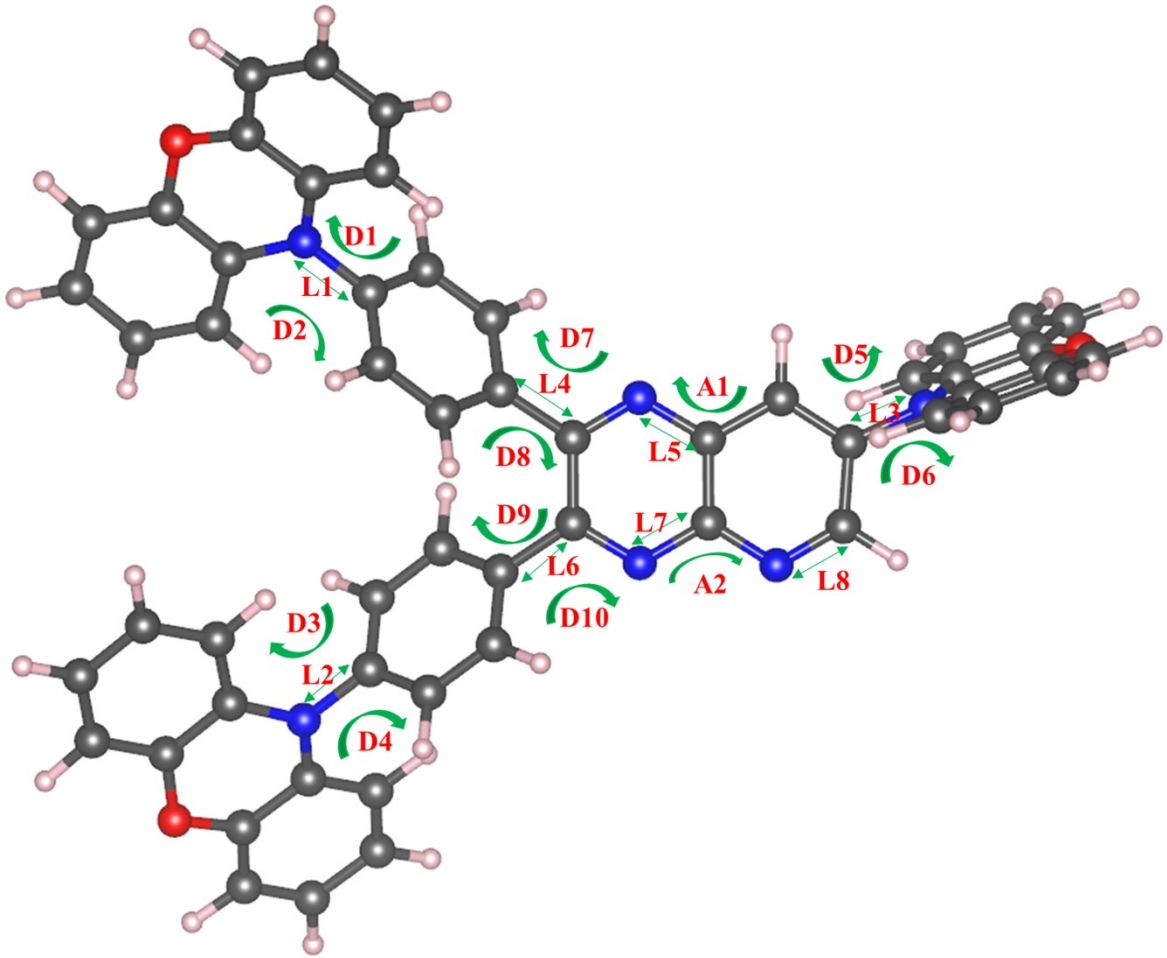


Fig. S48. Optimized structures of 8.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4320	1.4359	0.0039	1.4737	0.0417	D1	1.3203	0.9598	-0.3605	0.5779	-0.7424
L2	1.4319	1.4360	0.0041	1.4261	-0.0058	D2	0.3367	0.1477	-0.1890	0.4215	0.0848
L3	1.4243	1.4264	0.0021	1.4368	0.0125	D3	0.3296	0.5697	0.2401	0.6216	0.2920
L4	1.4887	1.4885	-0.0002	1.4926	0.0039	D4	0.5908	0.2333	-0.3575	1.2146	0.6238
L5	1.3556	1.3520	-0.0036	1.3605	0.0049	D5	76.8210	90.3690	13.5480	85.2848	8.4638
L6	1.4890	1.4875	-0.0015	1.4918	0.0028	D6	78.1824	90.5746	12.3922	95.3551	17.1727
L7	1.3525	1.3431	-0.0094	1.3480	-0.0045	D7	41.5648	39.3690	-2.1958	45.5437	3.9789
L8	1.3130	1.3363	0.0233	1.3363	0.0233	D8	43.8467	41.6366	-2.2101	47.2652	3.4185
						D9	42.3689	40.7106	-1.6583	35.6730	-6.6959
						D10	40.0162	38.1919	-1.8243	32.5773	-7.4389
						A1	120.3935	120.6469	0.2534	120.7605	0.3670
						A2	117.6046	117.9917	0.3871	117.8931	0.2885

Table S19. Geometrical parameter of compound 9

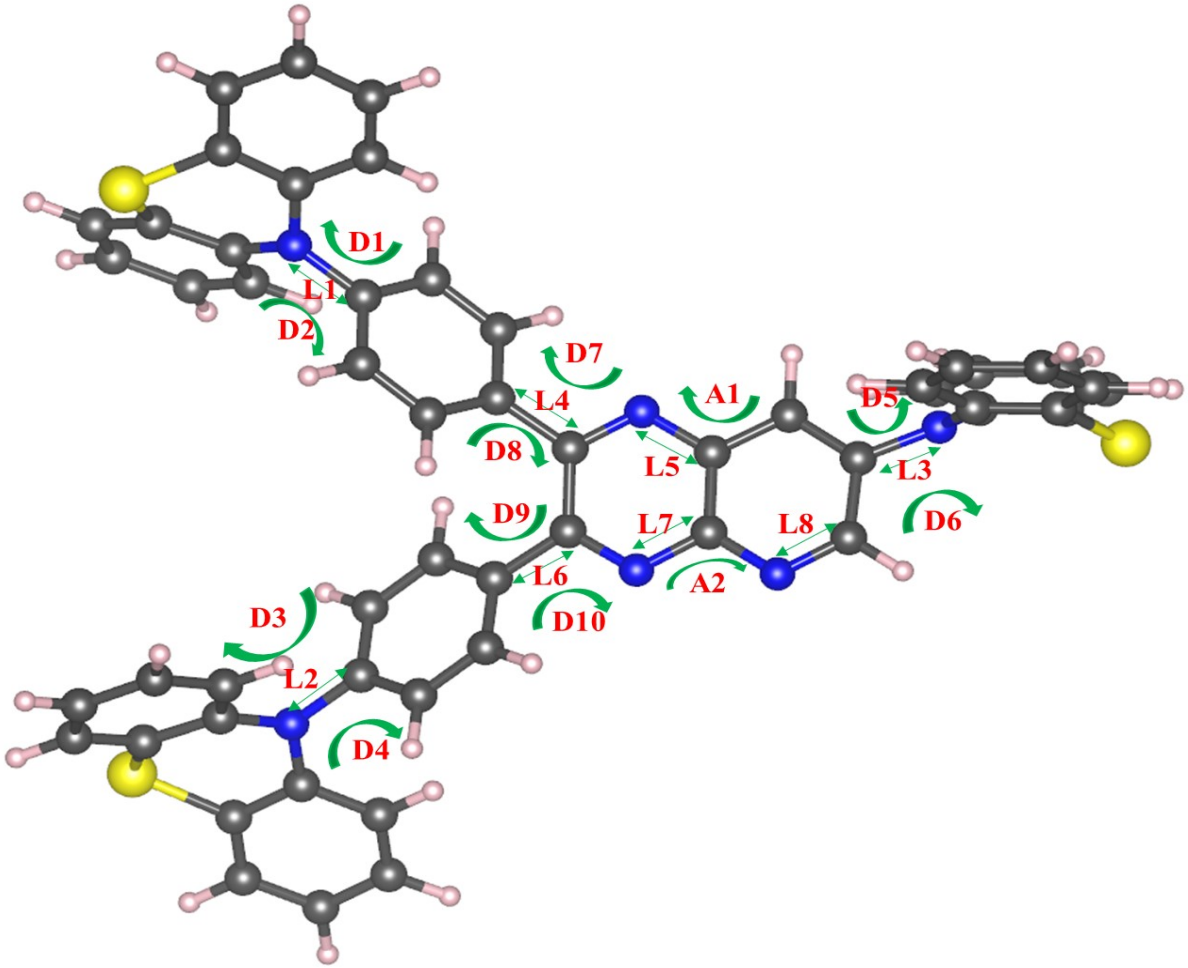


Fig. S49. Optimized structures of 9.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4440	1.4739	0.0299	1.4484	0.0044	D1	0.1108	0.4540	0.3432	0.2333	0.1225
L2	1.4441	1.4493	0.0052	1.4485	0.0044	D2	0.3489	0.0414	-0.3075	0.3668	0.0179
L3	1.4347	1.4492	0.0145	1.4719	0.0372	D3	0.6046	1.3037	0.6991	0.6908	0.0862
L4	1.4858	1.4911	0.0053	1.4870	0.0011	D4	0.0754	0.4747	0.3993	0.0598	-0.0156
L5	1.3684	1.3717	0.0033	1.3661	-0.0023	D5	74.9529	84.2732	9.3203	91.1960	16.2431
L6	1.4860	1.4894	0.0033	1.4857	-0.0004	D6	80.4305	95.1588	14.7283	90.5097	10.0792
L7	1.3626	1.3646	0.0020	1.3541	-0.0085	D7	36.0243	34.0942	-1.9301	33.9983	-2.0260
L8	1.3276	1.3517	0.0241	1.3504	0.0228	D8	37.8189	36.0046	-1.8143	35.9799	-1.8390
						D9	36.0819	37.0720	0.9901	33.9603	-2.1216
						D10	34.2386	35.2679	1.0293	31.8650	-2.3736
						A1	120.5657	120.9260	0.3603	120.7657	0.2000
						A2	118.0289	118.0189	-0.0100	118.2318	0.2029

Table S20. Geometrical parameter of compound 10

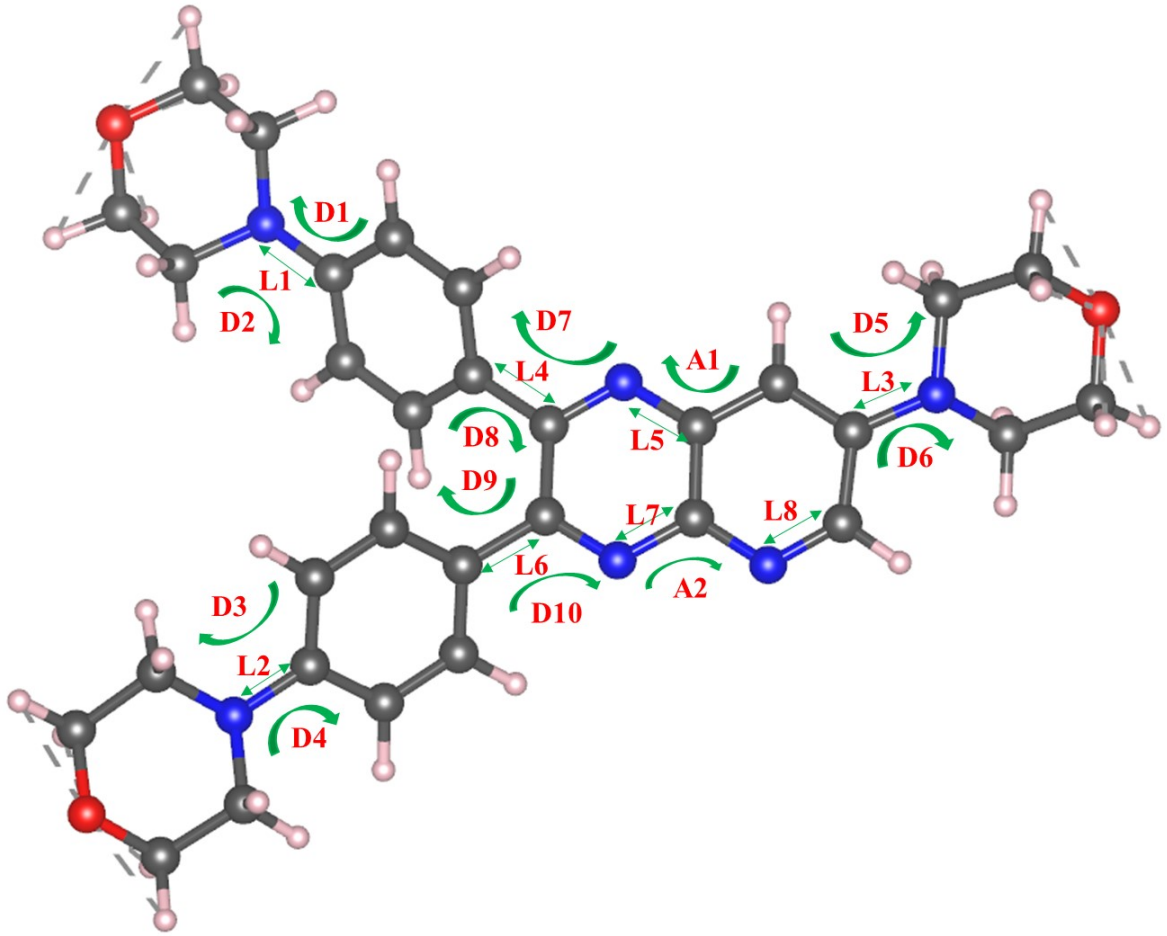


Fig. S50. Optimized structures of 10.

bond length (A°)						Dihedral/bond angle					
	S0	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**		**S0**	**S1**	**Δ (S1-S0)**	**T1**	**Δ (T1−S0)**
L1	1.4060	1.3924	-0.0136	1.3917	-0.0144	D1	2.6211	10.4854	7.8643	4.8245	2.2034
L2	1.4062	1.3977	-0.0085	1.3989	-0.0073	D2	44.8850	33.8340	-11.0510	39.5211	-5.3639
L3	1.4028	1.4144	0.0117	1.4066	0.0039	D3	3.4528	5.6301	2.1773	2.3283	-1.1245
L4	1.4842	1.4985	0.0143	1.4262	-0.0580	D4	45.3724	34.3049	-11.0675	40.6142	-4.7582
L5	1.3556	1.3545	-0.0012	1.3247	-0.0309	D5	5.9054	6.5143	0.6089	5.8128	-0.0926
L6	1.4847	1.4972	0.0124	1.4752	-0.0095	D6	50.4757	50.5818	0.1061	50.0750	-0.4007
L7	1.3479	1.3529	0.0050	1.3714	0.0235	D7	38.5825	72.8334	34.2509	17.0017	-21.5808
L8	1.3087	1.3357	0.0270	1.3372	0.0285	D8	40.9980	73.5959	32.5979	15.3071	-25.6909
						D9	39.0231	31.5779	-7.4452	30.7217	-8.3014
						D10	36.2154	27.9397	-8.2757	29.9631	-6.2523
						A1	120.3056	120.4938	0.1882	120.8793	0.5737
						A2	117.9428	118.1216	0.1788	118.2587	0.3159

11. Frontier molecular orbital of compounds.

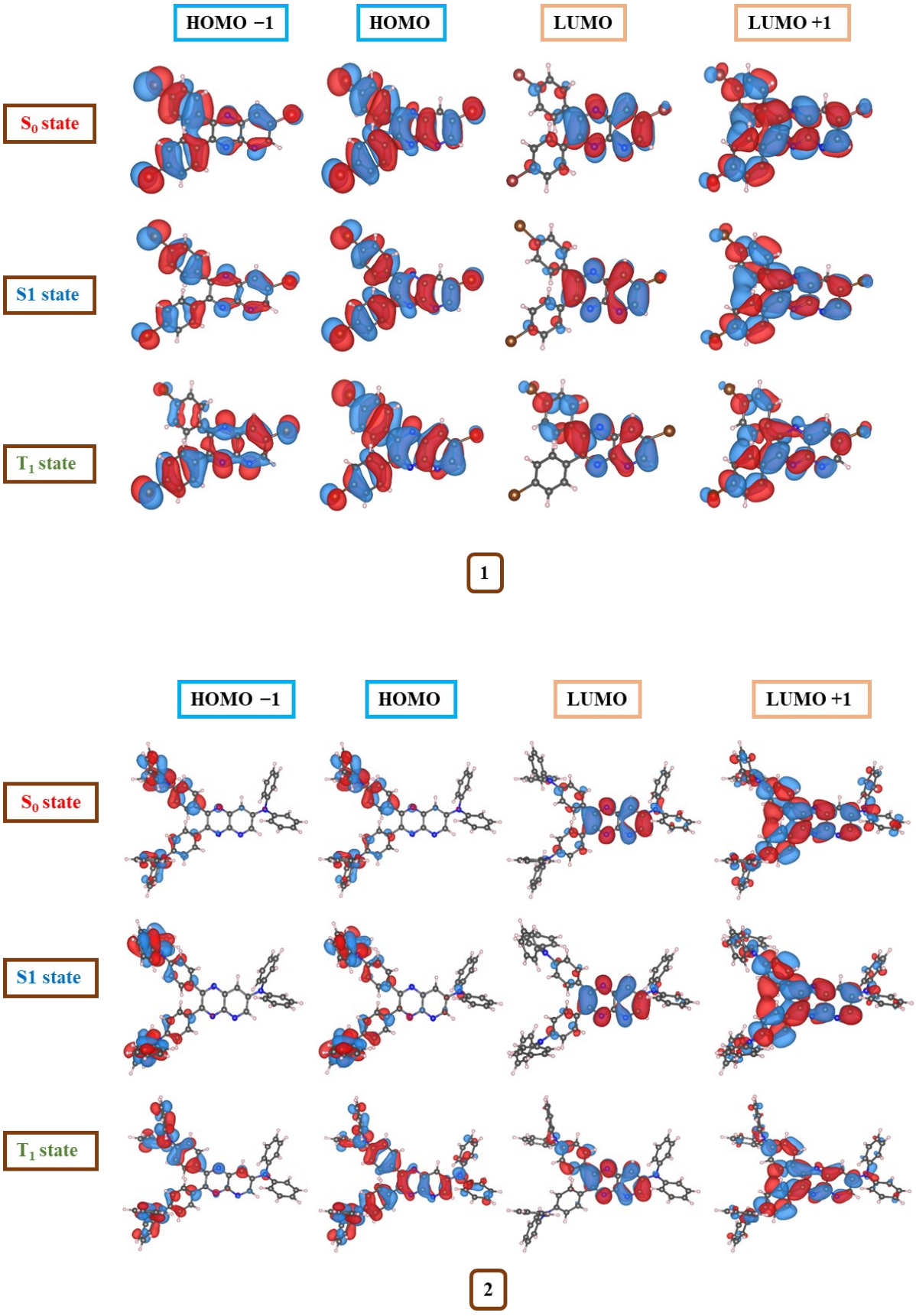


Fig. S51. Frontier molecular orbitals of compound **1** and **2**.

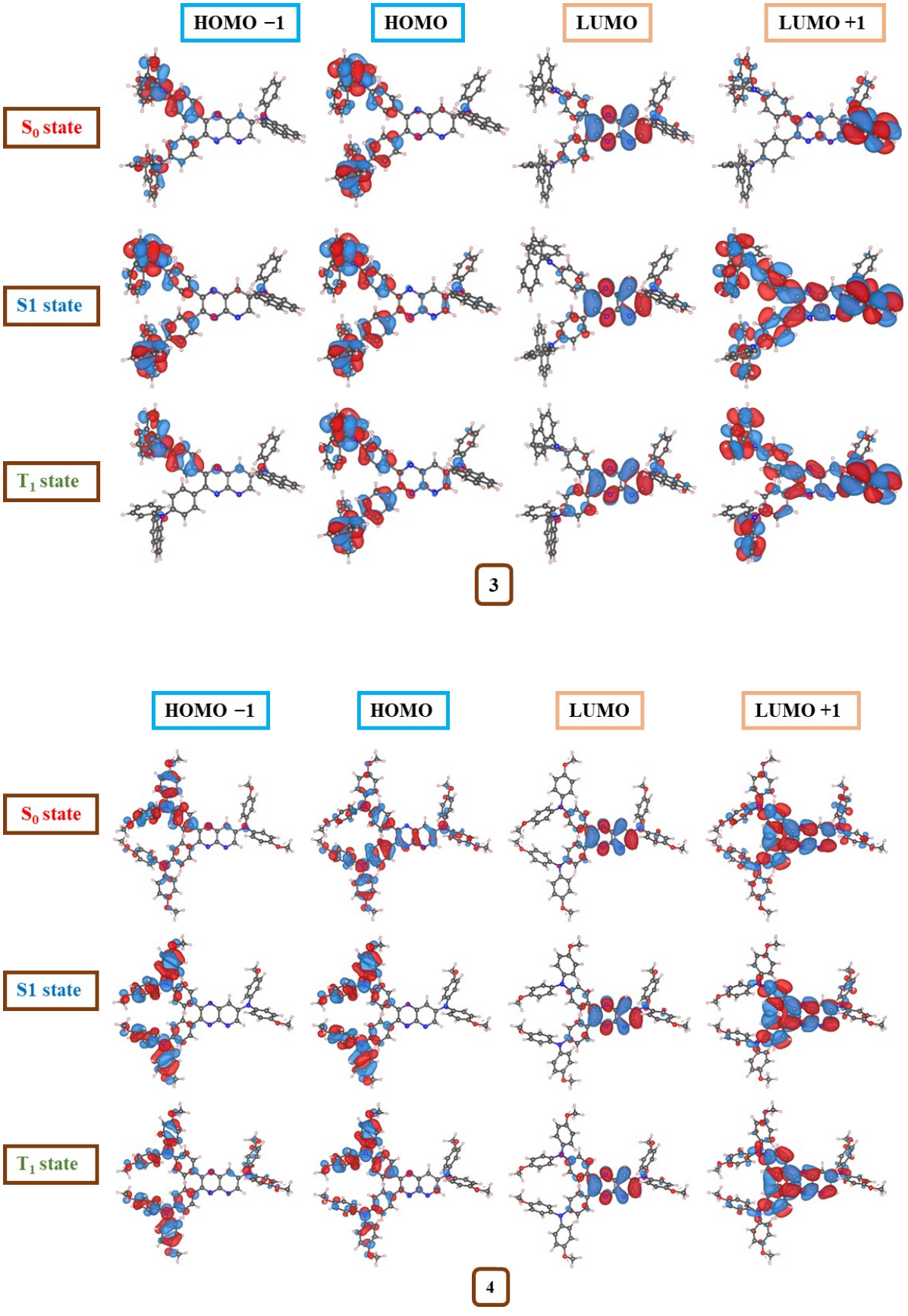


Fig. S52. Frontier molecular orbitals of compound **3** and **4**.

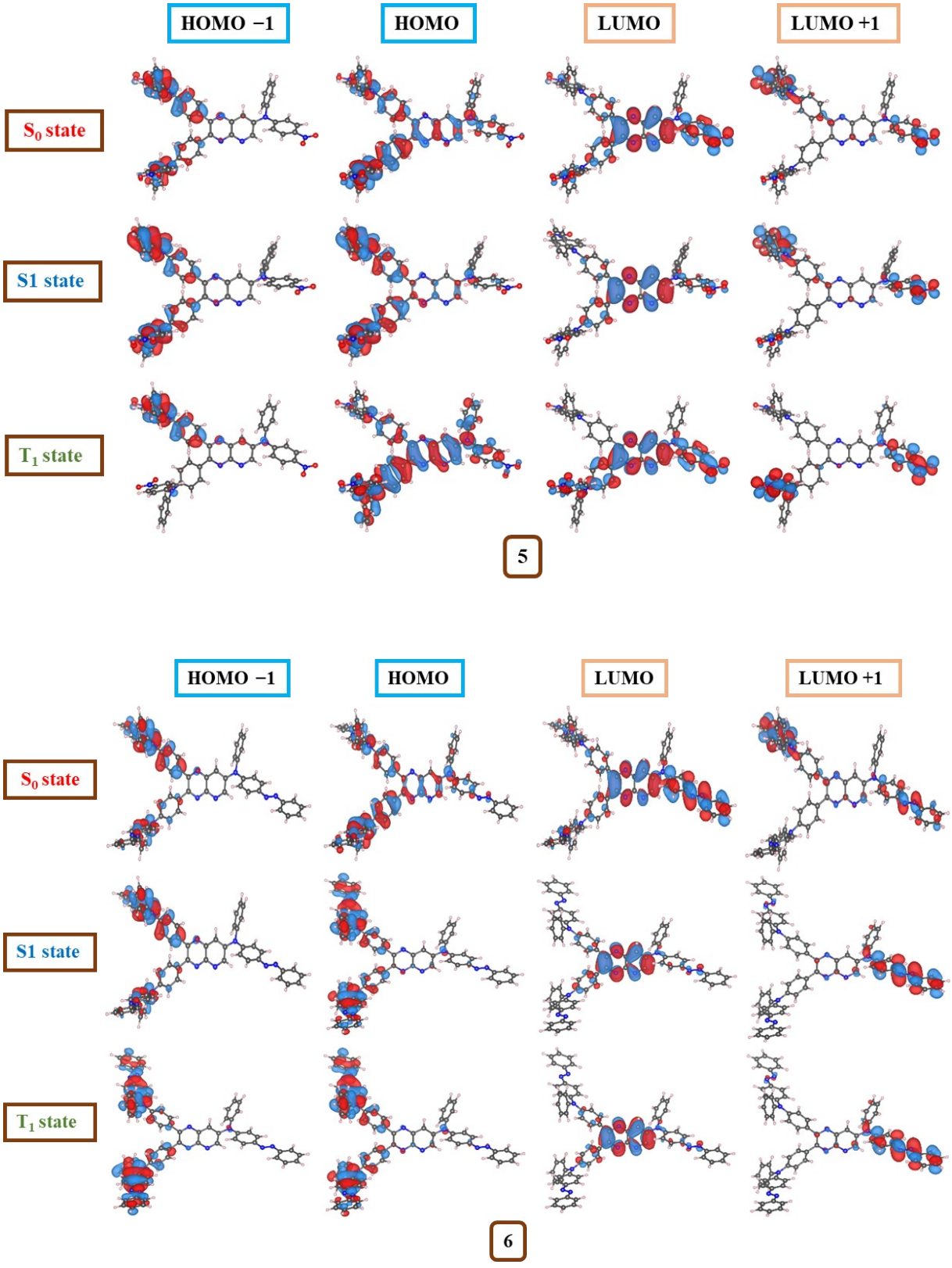


Fig. S53. Frontier molecular orbitals of compound **5** and **6**.

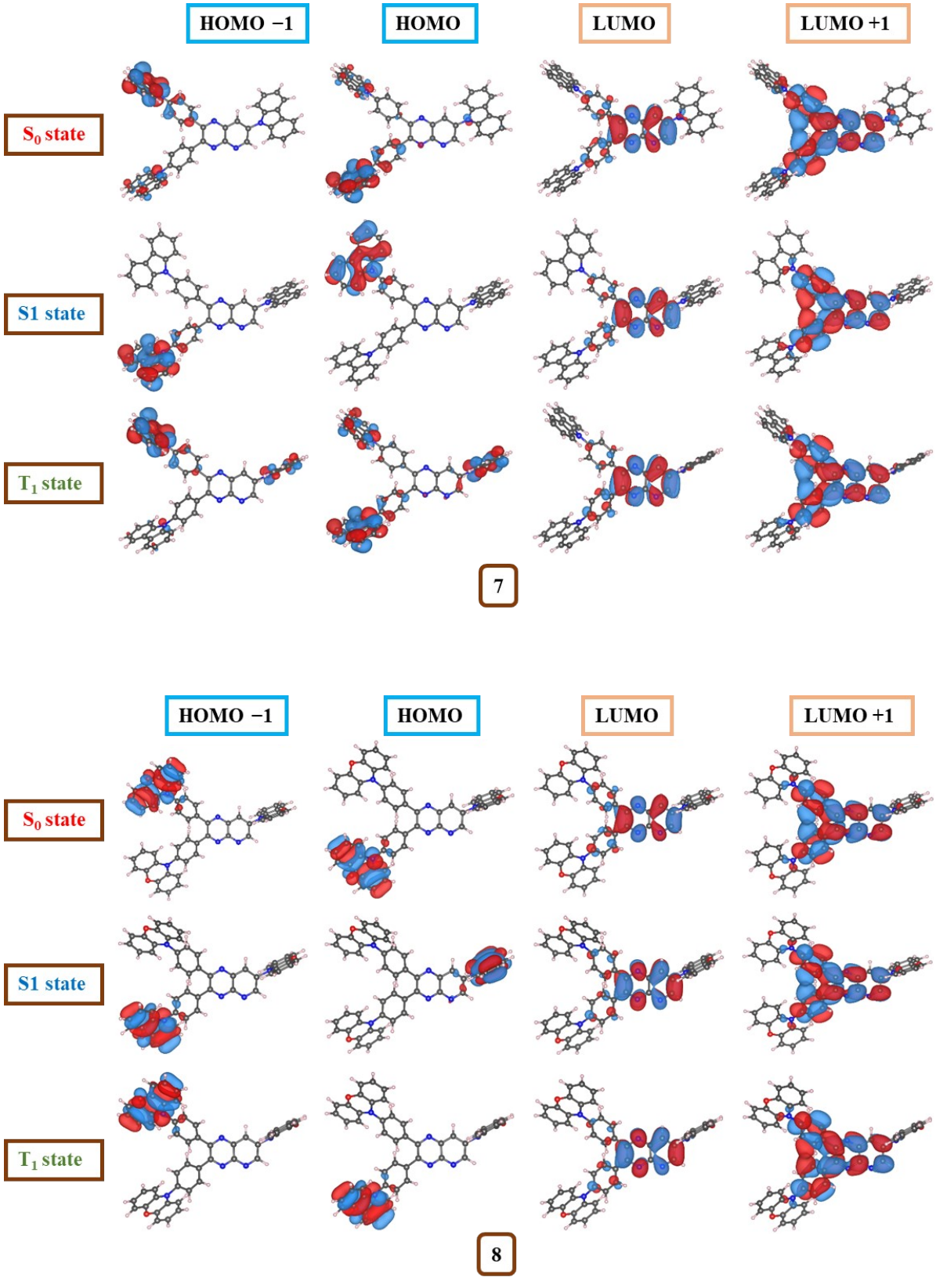


Fig. S54. Frontier molecular orbitals of compound **7** and **8**.

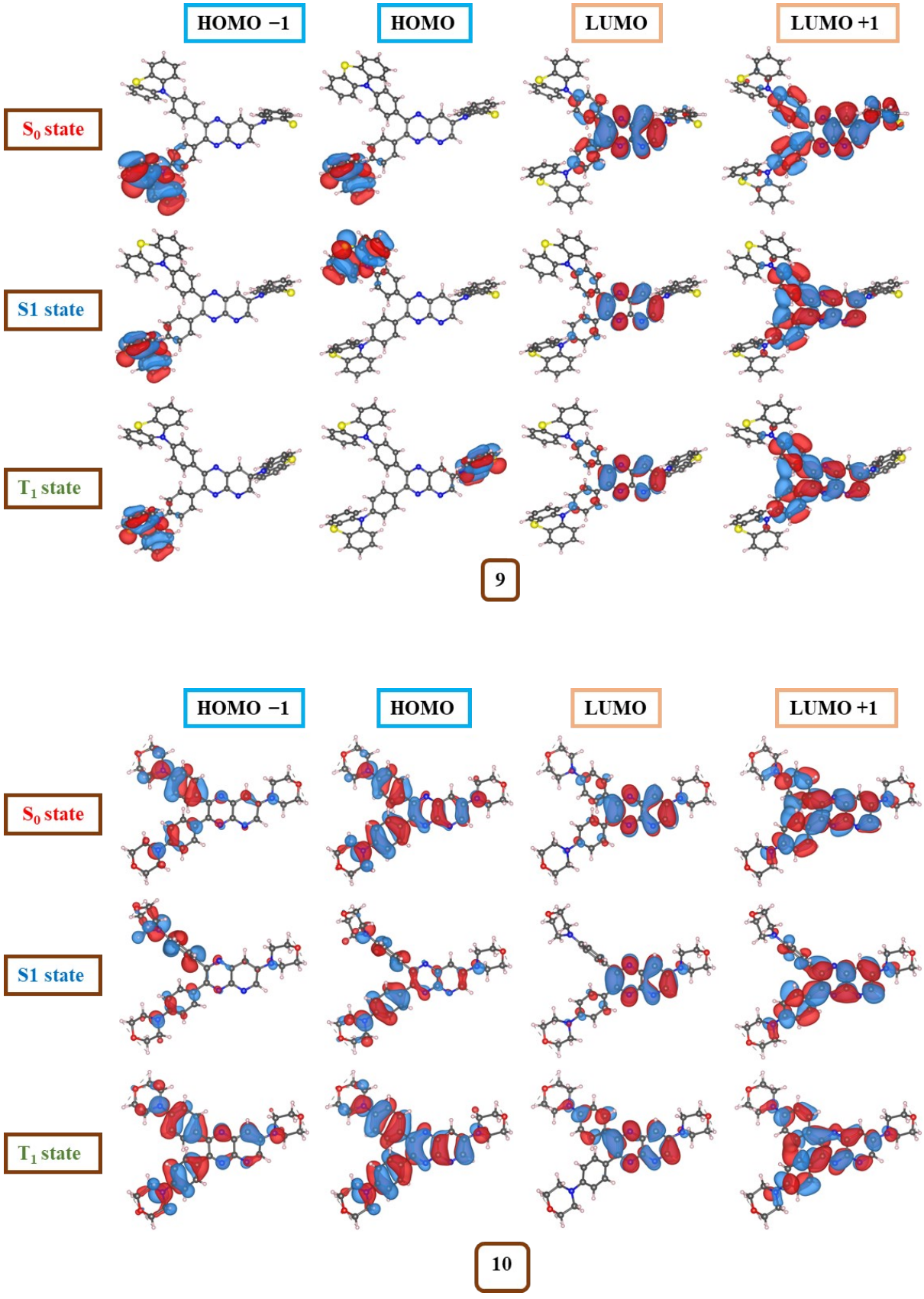


Fig. S55. Frontier molecular orbitals of compound **9** and **10**.

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

Table S21. Cartesian coordinates of optimized structure of molecule **1**.

Total energy: −23.758 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	-0.7503	1.1058	3.4132	-0.3607	-0.0726
C	0.3885	0.9517	4.1982	0.0526	-0.2363
C	1.6184	0.6375	3.6264	-0.1347	-0.0743
C	1.7020	0.4751	2.2474	-0.3865	-0.0070
C	0.5666	0.5984	1.4365	0.4735	-0.0851
C	-0.6564	0.9217	2.0373	-0.2004	-0.0114
C	-2.6065	-1.0598	-0.9992	-0.3261	-0.0019
C	-3.6351	-1.8930	-0.5732	-0.1587	-0.0735
C	-3.4041	-2.7693	0.4839	0.0532	-0.2356
C	-2.1647	-2.8236	1.1146	-0.3304	-0.0737
C	-1.1501	-1.9707	0.6909	-0.1916	-0.0121
C	-1.3574	-1.0738	-0.3646	0.4501	-0.0845
N	1.7585	1.0515	-0.5702	0.2097	-0.0320
C	0.7010	0.4704	-0.0395	-0.4344	-0.0317
C	-0.2674	-0.2049	-0.8857	-0.5440	-0.0296
N	-0.2001	-0.1038	-2.1982	0.1992	-0.0123
C	0.8385	0.5620	-2.7498	-0.6440	-0.0568
C	1.8668	1.0863	-1.9202	0.6470	-0.0551
N	0.8701	0.6696	-4.1028	0.0329	-0.0446
C	1.9104	1.2535	-4.6497	0.1928	-0.0246
C	3.0006	1.7703	-3.8988	-0.2012	-0.2534
C	2.9877	1.6972	-2.5308	-0.2738	-0.0212
Br	4.4589	2.5746	-4.8312	-0.1380	0.2900
Br	0.2611	1.1814	6.0950	-0.1668	0.2730
Br	-4.8119	-3.9252	1.0747	-0.1680	0.2723
H	-1.6977	1.3668	3.8663	0.2390	0.0635
H	2.4987	0.5261	4.2462	0.2405	0.0622
H	2.6574	0.2513	1.7894	0.2074	0.0737
H	-1.5455	1.0456	1.4316	0.2076	0.0760
H	-2.7649	-0.3930	-1.8375	0.2250	0.0764
H	-4.6003	-1.8659	-1.0618	0.2402	0.0625
H	-1.9904	-3.5214	1.9231	0.2404	0.0631
H	-0.1868	-2.0217	1.1829	0.2100	0.0752
H	1.9229	1.3346	-5.7325	0.2716	0.0646
H	3.7816	2.0947	-1.9117	0.2667	0.0769

Table S22. Cartesian coordinates of optimized structure of molecule **2**.

Total energy: −6.752 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	2.5925	1.6381	0.0901	-0.0068	-0.0324
C	3.0489	1.7426	-1.2331	-0.5824	-0.0414
C	2.1703	1.3941	-2.2708	0.0633	-0.0335
C	0.8839	0.9563	-1.9895	-0.1462	-0.0059
C	0.4279	0.8346	-0.6695	0.1560	-0.0951
C	1.3066	1.1919	0.3624	-0.3198	-0.0087
C	-0.6901	-1.4328	2.8688	-0.0923	-0.0010
C	0.1293	-2.2394	3.6449	0.0725	-0.0331
C	1.2304	-2.8977	3.0752	-0.6338	-0.0470
C	1.4769	-2.7217	1.7051	-0.0056	-0.0339
C	0.6563	-1.9067	0.9372	-0.3419	-0.0100
C	-0.4382	-1.2382	1.5028	0.1697	-0.0945
N	-1.8817	0.9462	-1.2205	0.2710	-0.0420
C	-0.9777	0.4323	-0.4062	-0.6495	-0.0348
C	-1.3823	-0.4286	0.6904	-0.7383	-0.0392
N	-2.6604	-0.5652	0.9979	0.2313	-0.0183
C	-3.5872	0.0231	0.2155	-0.5152	-0.0607
C	-3.1939	0.7314	-0.9533	0.6678	-0.0512
N	-4.8948	-0.1155	0.5642	0.0147	-0.0488
C	-5.7989	0.3907	-0.2371	-0.0729	0.0162
C	-5.5166	1.0665	-1.4685	-0.7338	-0.0594
C	-4.1904	1.2389	-1.8134	0.0682	0.0038
N	-6.5825	1.5610	-2.2457	0.7571	-0.0947
N	4.3606	2.1938	-1.5139	0.7857	-0.0948
C	-6.4208	2.7582	-3.0058	-0.5338	-0.0596
C	4.9490	3.2254	-0.7295	-0.3531	-0.0598
C	5.0985	1.6286	-2.5917	-0.4823	-0.0588
C	-7.7744	0.7953	-2.3953	-0.3617	-0.0615
C	4.2099	4.3625	-0.3759	-0.0154	-0.0392
C	4.7903	5.3651	0.3955	-0.1759	-0.0399
C	6.1172	5.2608	0.8121	-0.4484	-0.0582
C	6.8577	4.1349	0.4535	-0.2538	-0.0370
C	6.2801	3.1203	-0.3043	0.1792	-0.0362
C	5.8165	2.4520	-3.4690	0.1115	-0.0353
C	6.5455	1.8958	-4.5161	-0.2172	-0.0375
C	6.5591	0.5159	-4.7156	-0.4480	-0.0577
C	5.8408	-0.3058	-3.8474	-0.2111	-0.0386
C	5.1224	0.2413	-2.7884	0.0971	-0.0390
C	-9.0233	1.4307	-2.3764	0.0942	-0.0351
C	-10.1894	0.6876	-2.5270	-0.4162	-0.0352

C	-10.1322	-0.6976	-2.6841	-0.3478	-0.0546
C	-8.8916	-1.3320	-2.6991	-0.2778	-0.0337
C	-7.7181	-0.5938	-2.5665	0.3441	-0.0407
C	-5.9049	3.9122	-2.4028	0.1015	-0.0341
C	-5.7464	5.0787	-3.1443	-0.3327	-0.0368
C	-6.1137	5.1176	-4.4896	-0.3643	-0.0535
C	-6.6358	3.9727	-5.0887	-0.3266	-0.0355
C	-6.7827	2.7965	-4.3573	0.3112	-0.0337
N	2.0662	-3.7265	3.8616	0.7829	-0.0965
C	2.3831	-3.3642	5.2006	-0.4671	-0.0550
C	2.5985	-4.9296	3.3189	-0.3268	-0.0591
C	3.9413	-5.2698	3.5310	0.2091	-0.0372
C	4.4572	-6.4527	3.0091	-0.2698	-0.0388
C	3.6507	-7.3062	2.2572	-0.4434	-0.0582
C	2.3156	-6.9668	2.0392	-0.1954	-0.0383
C	1.7879	-5.7937	2.5703	-0.0047	-0.0376
C	2.7341	-2.0454	5.5190	0.1177	-0.0384
C	3.0425	-1.6978	6.8309	-0.2256	-0.0389
C	3.0229	-2.6581	7.8420	-0.4391	-0.0582
C	2.6822	-3.9730	7.5267	-0.2008	-0.0381
C	2.3568	-4.3254	6.2201	0.0829	-0.0365
H	3.2504	1.9098	0.9063	0.1631	0.0756
H	2.4982	1.4757	-3.2998	0.1749	0.0729
H	0.2083	0.7188	-2.8020	0.2198	0.0710
H	0.9857	1.1215	1.3946	0.2623	0.0749
H	-1.5559	-0.9584	3.3138	0.2400	0.0732
H	-0.0873	-2.3718	4.6978	0.1799	0.0761
H	2.3133	-3.2302	1.2421	0.1593	0.0752
H	0.8736	-1.7947	-0.1178	0.2589	0.0756
H	-6.8358	0.2823	0.0687	0.2387	0.0796
H	-3.8895	1.7668	-2.7097	0.2277	0.0888
H	3.1821	4.4542	-0.7060	0.1797	0.0738
H	4.2050	6.2392	0.6593	0.1866	0.0545
H	6.5681	6.0463	1.4072	0.1557	0.0529
H	7.8887	4.0374	0.7750	0.1873	0.0558
H	6.8576	2.2436	-0.5719	0.1599	0.0748
H	5.8015	3.5256	-3.3247	0.1593	0.0746
H	7.0947	2.5474	-5.1867	0.1884	0.0558
H	7.1227	0.0865	-5.5357	0.1502	0.0533
H	5.8499	-1.3814	-3.9850	0.1882	0.0551
H	4.5758	-0.4023	-2.1096	0.1325	0.0721
H	-9.0726	2.5046	-2.2427	0.1732	0.0762
H	-11.1486	1.1928	-2.5075	0.1868	0.0560
H	-11.0433	-1.2740	-2.7933	0.1635	0.0538

H	-8.8316	-2.4070	-2.8273	0.1876	0.0561
H	-6.7568	-1.0926	-2.5956	0.1938	0.0747
H	-5.6292	3.8900	-1.3553	0.1826	0.0750
H	-5.3464	5.9648	-2.6642	0.1890	0.0555
H	-5.9948	6.0296	-5.0628	0.1591	0.0536
H	-6.9205	3.9879	-6.1349	0.1871	0.0563
H	-7.1817	1.9066	-4.8291	0.1724	0.0773
H	4.5745	-4.6058	4.1071	0.1598	0.0757
H	5.4986	-6.7008	3.1818	0.1847	0.0548
H	4.0564	-8.2239	1.8476	0.1556	0.0518
H	1.6745	-7.6256	1.4640	0.1874	0.0546
H	0.7471	-5.5408	2.4075	0.1816	0.0747
H	2.7627	-1.2978	4.7356	0.1320	0.0742
H	3.3134	-0.6730	7.0601	0.1868	0.0546
H	3.2700	-2.3854	8.8614	0.1487	0.0523
H	2.6558	-4.7290	8.3037	0.1865	0.0548
H	2.0834	-5.3465	5.9824	0.1581	0.0745

Table S23. Cartesian coordinates of optimized structure of molecule **3**.

Total energy: −8.023 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	-0.6967	-2.7260	-1.4028	-0.1360	-0.0435
C	-2.0695	-2.9408	-1.1921	-0.4533	-0.0453
C	-2.8609	-1.8488	-0.8065	-0.1183	-0.0339
C	-2.2972	-0.5899	-0.6440	-0.1256	-0.0007
C	-0.9279	-0.3734	-0.8381	0.2833	-0.0960
C	-0.1411	-1.4675	-1.2260	-0.3980	-0.0088
C	1.1050	-0.5710	1.5908	-0.4171	-0.0098
C	1.8722	-1.4226	2.3721	-0.1676	-0.0450
C	3.2745	-1.4114	2.2818	-0.5144	-0.0449
C	3.8743	-0.5127	1.3869	-0.0737	-0.0339
C	3.0981	0.3419	0.6156	-0.0660	0.0038
C	1.6994	0.3250	0.6901	0.2953	-0.0956
N	-1.1049	1.9600	-1.2463	0.3014	-0.0537
C	-0.3712	0.9989	-0.7174	-0.6183	-0.0268
C	0.9098	1.3017	-0.1031	-0.5595	-0.0322
N	1.4294	2.5124	-0.1999	0.2675	-0.0301
C	0.7131	3.4852	-0.8010	-0.4689	-0.0574
C	-0.5995	3.2194	-1.2793	0.4306	-0.0473
N	1.2715	4.7195	-0.8984	-0.0050	-0.0483
C	0.5546	5.6799	-1.4300	-0.3383	0.0191
C	-0.7881	5.5329	-1.9082	-0.0540	-0.0556

C	-1.3577	4.2751	-1.8229	-0.1219	-0.0069
N	-1.4662	6.6436	-2.4391	0.6735	-0.1049
N	-2.6318	-4.2305	-1.3330	0.7285	-0.1062
C	-3.8075	-4.5700	-0.5880	-0.5104	-0.0501
C	-1.0982	7.9711	-2.0398	-0.4224	-0.0532
C	-2.4545	6.4974	-3.4570	0.0014	-0.0523
C	-2.2036	-5.1214	-2.3557	-0.0151	-0.0514
N	4.0570	-2.3025	3.0510	0.7354	-0.1060
C	5.3608	-2.6774	2.5910	-0.5062	-0.0495
C	3.6947	-2.6474	4.3834	-0.0855	-0.0527
C	-2.1823	-6.5020	-2.1107	0.1348	-0.0347
C	-1.7884	-7.3883	-3.1080	-0.3983	-0.0372
C	-1.3956	-6.9179	-4.3609	-0.4531	-0.0613
C	-1.4128	-5.5458	-4.6069	-0.1299	-0.0385
C	-1.8205	-4.6523	-3.6202	-0.0500	-0.0447
C	3.9395	-3.9450	4.8544	0.1088	-0.0337
C	3.6165	-4.2919	6.1625	-0.3588	-0.0379
C	3.0319	-3.3596	7.0193	-0.4697	-0.0609
C	2.7837	-2.0694	6.5530	-0.0907	-0.0388
C	3.1178	-1.7090	5.2503	-0.0209	-0.0434
C	-2.2653	5.6123	-4.5264	0.0174	-0.0399
C	-3.2350	5.4940	-5.5178	-0.2925	-0.0360
C	-4.3965	6.2641	-5.4694	-0.4183	-0.0557
C	-4.5805	7.1544	-4.4128	-0.3877	-0.0352
C	-3.6229	7.2681	-3.4089	0.0412	-0.0310
C	-1.2912	8.4002	-0.6879	-0.1930	-0.0577
C	-0.8920	9.7303	-0.3324	0.4592	-0.0609
C	-0.3542	10.5882	-1.3259	-0.2269	-0.0257
C	-0.2146	10.1559	-2.6222	-0.3740	-0.0352
C	-0.5810	8.8409	-2.9769	0.1046	-0.0200
C	6.4768	-2.2668	3.2901	0.1050	-0.0222
C	7.7737	-2.6234	2.8644	-0.3482	-0.0358
C	7.9481	-3.3786	1.7306	-0.1778	-0.0290
C	6.8280	-3.8301	0.9855	0.3805	-0.0619
C	5.5058	-3.4920	1.4223	0.0611	-0.0557
C	-3.7412	-4.7071	0.8356	0.0479	-0.0555
C	-4.9431	-5.0265	1.5475	0.3851	-0.0620
C	-6.1499	-5.2263	0.8282	-0.1821	-0.0288
C	-6.1729	-5.1178	-0.5408	-0.3502	-0.0365
C	-4.9995	-4.7820	-1.2487	0.1220	-0.0228
C	-4.8903	-5.1596	2.9606	-0.0708	-0.0292
C	-3.7085	-5.0027	3.6424	-0.5341	-0.0418
C	-2.5186	-4.7106	2.9370	-0.1768	-0.0355
C	-2.5343	-4.5649	1.5700	-0.1546	-0.0139

C	-1.8799	7.5789	0.3101	-0.1484	-0.0165
C	-2.0434	8.0379	1.5956	-0.1600	-0.0321
C	-1.6268	9.3407	1.9525	-0.5095	-0.0399
C	-1.0683	10.1660	1.0077	0.0792	-0.0271
C	6.9838	-4.6333	-0.1754	-0.0761	-0.0292
C	5.8916	-5.0965	-0.8673	-0.4979	-0.0425
C	4.5871	-4.7808	-0.4230	-0.1895	-0.0364
C	4.3987	-3.9980	0.6914	-0.1671	-0.0142
H	-0.0648	-3.5523	-1.7033	0.1251	0.0743
H	-3.9218	-1.9871	-0.6399	0.1985	0.0763
H	-2.9279	0.2476	-0.3718	0.2279	0.0721
H	0.9213	-1.3375	-1.3928	0.2621	0.0751
H	0.0270	-0.6069	1.6886	0.2655	0.0742
H	1.3840	-2.1025	3.0588	0.1211	0.0733
H	4.9531	-0.4789	1.3023	0.2009	0.0767
H	3.5784	1.0506	-0.0478	0.2454	0.0747
H	1.0296	6.6539	-1.5023	0.2566	0.0797
H	-2.3606	4.0678	-2.1736	0.2203	0.0860
H	-2.4786	-6.8746	-1.1375	0.1616	0.0746
H	-1.7786	-8.4524	-2.8993	0.1865	0.0549
H	-1.0835	-7.6102	-5.1340	0.1599	0.0522
H	-1.1217	-5.1646	-5.5796	0.1897	0.0550
H	-1.8444	-3.5897	-3.8277	0.1875	0.0742
H	4.3868	-4.6757	4.1911	0.1605	0.0746
H	3.8139	-5.3002	6.5094	0.1881	0.0548
H	2.7760	-3.6339	8.0361	0.1591	0.0521
H	2.3405	-1.3297	7.2108	0.1904	0.0550
H	2.9350	-0.6998	4.9025	0.1897	0.0750
H	-1.3605	5.0194	-4.5799	0.1850	0.0740
H	-3.0734	4.8049	-6.3393	0.1903	0.0560
H	-5.1469	6.1725	-6.2458	0.1602	0.0532
H	-5.4799	7.7580	-4.3604	0.1874	0.0555
H	-3.7747	7.9560	-2.5858	0.1589	0.0754
H	-0.0605	11.5942	-1.0458	0.1521	0.0604
H	0.1932	10.8162	-3.3790	0.1848	0.0571
H	-0.4531	8.5000	-3.9976	0.1543	0.0767
H	6.3476	-1.6587	4.1778	0.1535	0.0769
H	8.6315	-2.2827	3.4329	0.1811	0.0565
H	8.9440	-3.6452	1.3930	0.1481	0.0596
H	-7.0524	-5.4727	1.3773	0.1480	0.0597
H	-7.0960	-5.2754	-1.0871	0.1814	0.0564
H	-5.0281	-4.6840	-2.3276	0.1537	0.0768
H	-5.8054	-5.3947	3.4942	0.1494	0.0595
H	-3.6825	-5.1087	4.7211	0.1669	0.0547

H	-1.5864	-4.6041	3.4802	0.1736	0.0555
H	-1.6180	-4.3425	1.0393	0.0628	0.0754
H	-2.2053	6.5805	0.0499	0.2007	0.0758
H	-2.4965	7.3963	2.3429	0.1811	0.0567
H	-1.7554	9.6866	2.9719	0.1619	0.0552
H	-0.7558	11.1709	1.2714	0.1502	0.0601
H	7.9878	-4.8803	-0.5044	0.1493	0.0595
H	6.0256	-5.7102	-1.7510	0.1658	0.0545
H	3.7295	-5.1626	-0.9655	0.1729	0.0551
H	3.3965	-3.7619	1.0240	0.0485	0.0754

Table S24. Cartesian coordinates of optimized structure of molecule **4**.

Total energy: −8.647 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	0.6124	2.8466	-1.6746	0.1260	-0.0435
C	1.4053	3.3452	-0.6248	-0.6768	-0.0375
C	1.7602	2.4616	0.4095	0.0650	-0.0426
C	1.3326	1.1413	0.3943	-0.3582	-0.0068
C	0.5625	0.6354	-0.6618	0.1104	-0.0993
C	0.2226	1.5163	-1.6984	-0.0462	-0.0047
C	-1.4306	0.0743	1.7746	-0.3530	-0.0092
C	-1.9319	0.5042	2.9957	0.0880	-0.0436
C	-1.6178	-0.1794	4.1827	-0.6972	-0.0389
C	-0.7888	-1.3122	4.0922	0.0802	-0.0417
C	-0.3226	-1.7535	2.8636	-0.0054	-0.0009
C	-0.6209	-1.0660	1.6778	0.1162	-0.0982
N	0.3390	-1.3416	-1.9605	0.2842	-0.0468
C	0.2140	-0.8030	-0.7607	-0.5902	-0.0352
C	-0.1830	-1.6190	0.3728	-0.6503	-0.0418
N	-0.2216	-2.9362	0.2666	0.2748	-0.0220
C	0.0063	-3.5010	-0.9364	-0.5752	-0.0678
C	0.2028	-2.6859	-2.0860	0.6708	-0.0509
N	-0.0174	-4.8582	-1.0181	-0.0134	-0.0455
C	0.1155	-5.4061	-2.2010	-0.2132	0.0102
C	0.2886	-4.6816	-3.4260	-0.2732	-0.0557
C	0.3330	-3.3013	-3.3473	-0.0221	-0.0028
N	0.3825	-5.3806	-4.6403	0.7777	-0.0988
N	-2.1281	0.2419	5.4273	0.8774	-0.0994
N	1.8382	4.6854	-0.6211	0.8700	-0.0999
C	2.1377	5.3605	0.5992	-0.5439	-0.0743
C	2.0668	5.3817	-1.8464	-0.7629	-0.0771
C	-2.4705	1.6053	5.6614	-0.5579	-0.0727

C	-2.4106	-0.7092	6.4542	-0.7464	-0.0778
C	-0.0582	-4.7766	-5.8578	-0.7401	-0.0760
C	1.0435	-6.6437	-4.7020	-0.6433	-0.0780
C	-3.7124	1.9416	6.2221	0.1194	-0.0167
C	-4.0463	3.2631	6.4717	-0.0480	-0.0253
C	-3.1535	4.2918	6.1506	-0.9990	-0.0293
C	-1.9165	3.9711	5.5867	0.2400	-0.0740
C	-1.5795	2.6360	5.3583	0.2773	-0.0233
C	-3.1446	-1.8650	6.1865	0.2036	-0.0203
C	-3.4234	-2.7908	7.1926	0.1187	-0.0695
C	-2.9851	-2.5536	8.4976	-0.7642	-0.0280
C	-2.2582	-1.3898	8.7765	-0.0738	-0.0270
C	-1.9682	-0.4863	7.7663	0.0882	-0.0173
C	3.3544	6.0420	0.7539	0.1192	-0.0155
C	3.6461	6.7190	1.9272	-0.0740	-0.0250
C	2.7343	6.7195	2.9891	-1.0073	-0.0281
C	1.5220	6.0396	2.8498	0.2683	-0.0737
C	1.2278	5.3774	1.6568	0.2521	-0.0223
C	2.8275	4.8151	-2.8697	0.2077	-0.0213
C	3.0511	5.4989	-4.0654	0.1314	-0.0701
C	2.5280	6.7822	-4.2411	-0.7676	-0.0282
C	1.7755	7.3631	-3.2132	-0.0747	-0.0267
C	1.5416	6.6682	-2.0373	0.1039	-0.0168
C	2.2787	-6.8465	-4.0679	0.2052	-0.0240
C	2.9151	-8.0761	-4.1331	-0.2032	-0.0244
C	2.3451	-9.1316	-4.8549	-0.6850	-0.0277
C	1.1232	-8.9356	-5.5040	0.1883	-0.0673
C	0.4792	-7.7017	-5.4154	0.0378	-0.0173
C	0.7918	-4.7033	-6.9703	0.1742	-0.0161
C	0.3579	-4.1323	-8.1567	-0.1059	-0.0256
C	-0.9337	-3.6018	-8.2564	-0.7286	-0.0272
C	-1.7871	-3.6644	-7.1517	0.1417	-0.0689
C	-1.3486	-4.2588	-5.9683	0.1296	-0.0187
O	3.1189	7.4075	4.1059	-0.1367	-0.1756
O	2.6922	7.5427	-5.3641	-0.1597	-0.1774
C	3.4495	7.0083	-6.4407	-0.3248	0.0560
O	-1.2627	-3.0515	-9.4622	-0.1578	-0.1766
O	3.0540	-10.2985	-4.8675	-0.1562	-0.1759
O	-3.5802	5.5616	6.4257	-0.1374	-0.1764
O	-3.2110	-3.3857	9.5573	-0.1596	-0.1775
C	-3.9421	-4.5834	9.3346	-0.3270	0.0560
C	-2.7162	6.6465	6.1259	-0.3531	0.0528
C	2.5170	-11.4107	-5.5699	-0.3220	0.0564
C	-2.5584	-2.4903	-9.6206	-0.3244	0.0565

H	3.4442	7.7723	-7.2164	0.1766	0.0536
H	4.4835	6.8044	-6.1413	0.1517	0.0451
H	2.9966	6.0911	-6.8332	0.1528	0.0452
H	3.2356	-12.2186	-5.4422	0.1786	0.0540
H	1.5504	-11.7166	-5.1549	0.1519	0.0455
H	2.4030	-11.1931	-6.6377	0.1507	0.0448
H	-2.5954	-2.1100	-10.6401	0.1763	0.0539
H	-3.3410	-3.2454	-9.4875	0.1516	0.0450
H	-2.7252	-1.6649	-8.9198	0.1545	0.0457
C	2.2363	7.4453	5.2167	-0.3505	0.0535
H	2.7415	8.0354	5.9797	0.1840	0.0547
H	1.2867	7.9273	4.9574	0.1607	0.0434
H	2.0408	6.4405	5.6081	0.1717	0.0444
H	-3.9980	-5.0821	10.3009	0.1764	0.0534
H	-4.9561	-4.3731	8.9768	0.1507	0.0449
H	-3.4316	-5.2371	8.6188	0.1544	0.0456
H	-3.2528	7.5466	6.4220	0.1833	0.0544
H	-1.7801	6.5816	6.6924	0.1616	0.0433
H	-2.4915	6.6964	5.0544	0.1709	0.0440
H	0.3143	3.5065	-2.4793	0.1832	0.0727
H	2.3854	2.8100	1.2215	0.1916	0.0735
H	1.6366	0.4861	1.2017	0.2489	0.0743
H	-0.3625	1.1445	-2.5308	0.2281	0.0709
H	-1.7069	0.6182	0.8794	0.2434	0.0731
H	-2.5849	1.3668	3.0302	0.1874	0.0731
H	-0.5243	-1.8538	4.9916	0.1894	0.0733
H	0.2876	-2.6468	2.8100	0.2414	0.0737
H	0.0812	-6.4912	-2.2393	0.2446	0.0763
H	0.4775	-2.6785	-4.2210	0.2348	0.0858
H	-4.4154	1.1549	6.4685	0.1885	0.0762
H	-5.0044	3.5228	6.9057	0.2041	0.0692
H	-1.2008	4.7423	5.3349	0.0883	0.0537
H	-0.6129	2.3969	4.9311	0.1802	0.0750
H	-3.4964	-2.0530	5.1791	0.1744	0.0774
H	-3.9905	-3.6781	6.9453	0.2068	0.0604
H	-1.9184	-1.2197	9.7911	0.2059	0.0688
H	-1.3979	0.4075	7.9904	0.1737	0.0751
H	4.0708	6.0422	-0.0589	0.1866	0.0761
H	4.5846	7.2466	2.0476	0.2050	0.0694
H	0.7932	6.0277	3.6493	0.0918	0.0541
H	0.2803	4.8619	1.5533	0.1827	0.0752
H	3.2443	3.8235	-2.7386	0.1739	0.0770
H	3.6420	5.0244	-4.8374	0.2080	0.0602
H	1.3722	8.3575	-3.3628	0.2063	0.0689

H	0.9510	7.1236	-1.2511	0.1751	0.0752
H	2.7385	-6.0338	-3.5179	0.1975	0.0764
H	3.8666	-8.2367	-3.6408	0.2085	0.0702
H	0.6556	-9.7316	-6.0678	0.2010	0.0601
H	-0.4727	-7.5604	-5.9134	0.1738	0.0752
H	1.7966	-5.1032	-6.9016	0.1793	0.0763
H	1.0116	-4.0745	-9.0187	0.2061	0.0693
H	-2.7939	-3.2717	-7.1993	0.2092	0.0604
H	-2.0197	-4.3131	-5.1193	0.1846	0.0758

Table S25. Cartesian coordinates of optimized structure of molecule **5**.

Total energy: −8.444 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	0.8749	0.5698	-0.5215	-0.6362	-0.0331
C	1.3000	0.3179	0.8432	-0.6735	-0.0343
N	2.4658	0.7623	1.2754	0.2851	-0.0142
C	3.2106	1.5385	0.4621	-0.4495	-0.0584
C	2.7180	1.9130	-0.8181	0.7305	-0.0492
N	1.5620	1.3889	-1.2948	0.2961	-0.0353
N	4.4177	1.9633	0.9218	0.0263	-0.0383
C	5.1088	2.7766	0.1628	-0.1443	0.0173
C	4.6768	3.2667	-1.1103	-0.4643	-0.0604
C	3.4717	2.8125	-1.6023	-0.0392	0.0203
C	-0.2969	-0.0856	-1.1600	0.1844	-0.0860
C	0.4735	-0.3952	1.8520	0.1891	-0.0855
C	-0.5627	-1.4514	-0.9931	-0.4019	-0.0082
C	-1.6188	-2.0612	-1.6568	-0.0422	-0.0298
C	-2.4438	-1.3189	-2.5125	-0.5632	-0.0485
C	-2.1819	0.0462	-2.6868	0.0496	-0.0219
C	-1.1193	0.6475	-2.0258	-0.0647	-0.0006
C	1.0966	-1.2312	2.7892	-0.0572	0.0044
C	0.3655	-1.8606	3.7869	0.0930	-0.0210
C	-1.0167	-1.6567	3.8891	-0.6191	-0.0478
C	-1.6454	-0.8127	2.9640	-0.0637	-0.0311
C	-0.9091	-0.1927	1.9633	-0.4228	-0.0093
N	5.5149	4.1380	-1.8471	0.7732	-0.0860
C	5.6243	3.9499	-3.2655	-0.6351	-0.0654
C	6.1498	5.2302	-1.2305	-0.4466	-0.0281
N	-3.5411	-1.9306	-3.1813	0.8207	-0.0863
C	-3.4158	-3.1896	-3.7879	-0.4307	-0.0260
N	-1.7661	-2.3118	4.9061	0.8245	-0.0862
C	-2.7528	-1.6335	5.6375	-0.4256	-0.0259

C	-1.4907	-3.6911	5.1757	-0.5274	-0.0644
C	-4.5230	-4.0572	-3.8714	0.1219	-0.0315
C	-4.4065	-5.2975	-4.4754	-0.0513	0.0141
C	-3.1774	-5.6918	-5.0006	-0.5413	-0.0761
C	-2.0662	-4.8528	-4.9327	-0.0165	0.0129
C	-2.1863	-3.6103	-4.3338	-0.0748	-0.0342
C	5.3166	4.9941	-4.1424	0.2470	-0.0303
C	5.4255	4.8022	-5.5175	-0.2713	-0.0322
C	5.8255	3.5675	-6.0265	-0.3555	-0.0410
C	6.1236	2.5240	-5.1508	-0.4142	-0.0311
C	6.0303	2.7129	-3.7747	0.2269	-0.0259
C	7.3674	5.7226	-1.7389	0.0191	-0.0282
C	7.9971	6.8009	-1.1416	-0.0458	0.0156
C	7.4193	7.3979	-0.0225	-0.5248	-0.0720
C	6.2160	6.9307	0.5004	-0.1236	0.0167
C	5.5827	5.8570	-0.1046	0.0696	-0.0347
C	-2.6429	-0.2516	5.8920	-0.0776	-0.0336
C	-3.6194	0.4148	6.6123	0.0007	0.0132
C	-4.7182	-0.2932	7.0966	-0.5505	-0.0762
C	-4.8461	-1.6621	6.8683	-0.0582	0.0137
C	-3.8719	-2.3256	6.1422	0.1383	-0.0316
C	-1.4776	-4.6202	4.1308	0.1509	-0.0293
C	-1.1919	-5.9580	4.3900	-0.2830	-0.0333
C	-0.9299	-6.3829	5.6918	-0.4453	-0.0439
C	-0.9473	-5.4572	6.7346	-0.1699	-0.0333
C	-1.2184	-4.1155	6.4806	0.0968	-0.0317
N	-3.0524	-7.0052	-5.6359	-0.2084	0.1551
O	-4.0582	-7.7065	-5.7064	-0.0074	-0.1908
O	-1.9483	-7.3335	-6.0623	-0.0064	-0.1917
N	8.0864	8.5398	0.6114	-0.1960	0.1555
N	-5.7521	0.4108	7.8577	-0.2071	0.1550
C	-4.7924	-1.2350	-3.2181	-0.5452	-0.0644
C	-5.4523	-1.0325	-4.4348	0.1061	-0.0324
C	-6.6682	-0.3550	-4.4638	-0.1761	-0.0335
C	-7.2280	0.1401	-3.2865	-0.4487	-0.0438
C	-6.5655	-0.0537	-2.0751	-0.2724	-0.0327
C	-5.3565	-0.7431	-2.0368	0.1568	-0.0292
H	6.0791	3.0890	0.5401	0.2340	0.0804
H	3.0961	3.1068	-2.5745	0.2503	0.0898
H	0.0602	-2.0489	-0.3388	0.2471	0.0759
H	-1.8067	-3.1182	-1.5125	0.1720	0.0770
H	-2.8112	0.6320	-3.3457	0.1934	0.0778
H	-0.9089	1.6972	-2.1885	0.2272	0.0741
H	2.1696	-1.3678	2.7388	0.2484	0.0769

H	0.8653	-2.5079	4.4971	0.1963	0.0782
H	-2.7128	-0.6412	3.0319	0.1689	0.0764
H	-1.4209	0.4578	1.2651	0.2464	0.0749
H	-5.4736	-3.7545	-3.4529	0.1868	0.0783
H	-5.2505	-5.9711	-4.5328	0.2631	0.0816
H	-1.1280	-5.1758	-5.3629	0.2601	0.0814
H	-1.3289	-2.9516	-4.2955	0.2077	0.0779
H	4.9962	5.9505	-3.7461	0.1694	0.0768
H	5.1857	5.6167	-6.1913	0.1979	0.0586
H	5.9039	3.4193	-7.0971	0.1678	0.0569
H	6.4409	1.5626	-5.5382	0.1955	0.0586
H	6.2716	1.9063	-3.0924	0.1856	0.0760
H	7.8191	5.2491	-2.6005	0.1975	0.0789
H	8.9367	7.1784	-1.5210	0.2629	0.0822
H	5.7818	7.4220	1.3603	0.2606	0.0827
H	4.6353	5.5109	0.2872	0.2265	0.0773
H	-1.7811	0.2936	5.5308	0.2088	0.0785
H	-3.5344	1.4728	6.8195	0.2612	0.0815
H	-5.7123	-2.1863	7.2481	0.2621	0.0814
H	-3.9752	-3.3861	5.9543	0.1871	0.0782
H	-1.6897	-4.2901	3.1207	0.1464	0.0742
H	-1.1855	-6.6713	3.5737	0.1940	0.0575
H	-0.7125	-7.4255	5.8920	0.1593	0.0562
H	-0.7360	-5.7764	7.7488	0.2000	0.0582
H	-1.2191	-3.3941	7.2893	0.1594	0.0765
H	-5.0115	-1.4065	-5.3514	0.1593	0.0763
H	-7.1721	-0.2028	-5.4115	0.1998	0.0582
H	-8.1715	0.6724	-3.3131	0.1601	0.0564
H	-6.9958	0.3225	-1.1539	0.1946	0.0579
H	-4.8451	-0.9019	-1.0949	0.1422	0.0744
O	9.1331	8.9406	0.1106	-0.0079	-0.1878
O	7.5609	9.0303	1.6061	-0.0045	-0.1870
O	-5.6255	1.6226	8.0127	-0.0069	-0.1913
O	-6.6901	-0.2488	8.2981	-0.0086	-0.1916

Table S26. Cartesian coordinates of optimized structure of molecule **6**.

Total energy: −9.570 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	-1.2784	-4.2742	8.1082	-0.9145	-0.0467
C	-1.3715	-5.4548	7.3518	-0.0967	-0.0314
C	-2.5977	-5.8738	6.8528	-0.3915	-0.0085
C	-3.7659	-5.1337	7.0878	0.2229	-0.0894

C	-3.6665	-3.9635	7.8527	0.0231	-0.0022
C	-2.4433	-3.5309	8.3493	0.1656	-0.0282
C	-3.4542	-7.3498	2.2661	0.1776	-0.0267
C	-2.7107	-6.2072	1.9332	-0.8848	-0.0472
C	-2.8212	-5.0652	2.7408	-0.1186	-0.0321
C	-3.6502	-5.0740	3.8577	-0.4709	-0.0102
C	-4.3917	-6.2151	4.2022	0.2195	-0.0891
C	-4.2854	-7.3440	3.3765	0.0279	0.0013
C	-5.0957	-5.6118	6.6304	-0.5510	-0.0331
C	-5.3479	-6.2310	5.3408	-0.5771	-0.0362
N	-6.5029	-6.8311	5.1040	0.2765	-0.0167
C	-7.4746	-6.7726	6.0375	-0.4642	-0.0610
C	-7.2760	-6.0279	7.2330	0.5948	-0.0503
N	-6.0673	-5.4840	7.5151	0.2942	-0.0397
N	-8.6488	-7.4152	5.7844	0.0127	-0.0416
C	-9.6167	-7.2961	6.6607	-0.1538	0.0173
C	-9.5396	-6.5226	7.8650	-0.3961	-0.0602
C	-8.3430	-5.8924	8.1443	-0.1078	0.0126
N	10.6423	-6.4761	8.7346	0.7712	-0.0878
N	-0.0286	-3.8251	8.6209	0.8662	-0.0885
N	-1.8553	-6.2106	0.7900	0.8753	-0.0882
C	0.2707	-2.4299	8.5792	-0.4254	-0.0612
C	0.9132	-4.7382	9.1604	-0.4694	-0.0406
C	10.4277	-6.4602	10.1487	-0.5854	-0.0615
C	11.9523	-6.3030	8.2350	-0.3073	-0.0433
C	0.7626	-1.7766	9.7168	0.0871	-0.0329
C	1.0561	-0.4164	9.6650	-0.1549	-0.0366
C	0.8495	0.3085	8.4918	-0.4641	-0.0511
C	0.3517	-0.3400	7.3640	-0.2239	-0.0361
C	0.0697	-1.7018	7.4002	0.0892	-0.0330
C	11.0137	-5.4710	10.9424	0.0331	-0.0321
C	10.8046	-5.4648	12.3211	-0.1960	-0.0346
C	-9.9977	-6.4349	12.9172	-0.4162	-0.0483
C	-9.4070	-7.4187	12.1226	-0.2544	-0.0341
C	-9.6257	-7.4374	10.7491	0.2000	-0.0299
C	0.4814	-5.8535	9.9060	-0.0102	-0.0318
C	1.3912	-6.7398	10.4476	0.0653	-0.0030
C	2.7711	-6.5346	10.2702	-0.9783	-0.1060
C	3.1995	-5.4258	9.5374	0.0303	-0.0032
C	2.2898	-4.5404	8.9837	0.1867	-0.0381
C	12.2025	-5.5306	7.0934	0.2014	-0.0412
C	13.5024	-5.3825	6.6194	-0.0456	-0.0006
C	14.5805	-5.9852	7.2808	-0.9567	-0.1027
C	14.3253	-6.7575	8.4303	0.0495	-0.0009

C	13.0336	-6.9145	8.8942	-0.0476	-0.0276
N	3.7868	-7.3658	10.7893	0.1014	-0.0484
N	3.3978	-8.3761	11.4282	0.0852	-0.0574
C	4.4197	-9.2177	11.9343	-0.3375	-0.0935
C	5.7965	-8.9922	11.7792	0.1519	-0.0205
C	6.7051	-9.8877	12.3263	-0.2286	-0.0424
C	6.2627	-11.0102	13.0286	-0.3273	-0.0407
C	4.8983	-11.2365	13.1832	-0.1816	-0.0473
C	3.9797	-10.3444	12.6383	-0.0314	-0.0209
N	15.8622	-5.7628	6.7243	0.1116	-0.0479
N	16.8200	-6.2915	7.3380	0.0768	-0.0547
C	18.1083	-6.0897	6.7863	-0.3441	-0.0936
C	18.3881	-5.3418	5.6292	0.1391	-0.0191
C	19.7011	-5.2184	5.1927	-0.2109	-0.0416
C	20.7439	-5.8325	5.8937	-0.3241	-0.0391
C	20.4681	-6.5751	7.0413	-0.1790	-0.0468
C	19.1541	-6.7035	7.4875	-0.0274	-0.0199
C	-1.7957	-5.0857	-0.0649	-0.4733	-0.0397
C	-1.0523	-7.3652	0.5186	-0.4391	-0.0612
C	-0.2884	-7.9629	1.5324	0.0963	-0.0327
C	0.4760	-9.0903	1.2570	-0.2201	-0.0364
C	0.5053	-9.6301	-0.0241	-0.4691	-0.0511
C	-0.2470	-9.0353	-1.0347	-0.1393	-0.0365
C	-1.0293	-7.9143	-0.7698	0.0703	-0.0326
C	-2.9586	-4.3248	-0.3198	-0.0073	-0.0318
C	-2.9145	-3.2286	-1.1617	0.0840	-0.0026
C	-1.7060	-2.8708	-1.7779	-0.9709	-0.1055
C	-0.5557	-3.6285	-1.5330	0.0282	-0.0033
C	-0.5937	-4.7185	-0.6828	0.2003	-0.0390
N	-1.5564	-1.7821	-2.6607	0.0972	-0.0502
N	-2.6350	-1.1046	-2.8141	0.0810	-0.0598
C	-2.4727	-0.0135	-3.7109	-0.3305	-0.0924
C	-1.2738	0.2819	-4.3767	0.1592	-0.0208
C	-1.2282	1.3684	-5.2343	-0.2380	-0.0428
C	-2.3597	2.1626	-5.4369	-0.3237	-0.0411
C	-3.5463	1.8683	-4.7762	-0.1856	-0.0475
C	-3.6089	0.7804	-3.9114	-0.0348	-0.0210
H	-0.4794	-6.0402	7.1587	0.1772	0.0765
H	-2.6434	-6.7880	6.2718	0.2525	0.0753
H	-4.5657	-3.3980	8.0691	0.2236	0.0731
H	-2.3860	-2.6187	8.9358	0.1867	0.0763
H	-3.3837	-8.2366	1.6433	0.1871	0.0768
H	-2.2567	-4.1715	2.4900	0.1733	0.0761
H	-3.7187	-4.1777	4.4629	0.2457	0.0743

H	-4.8807	-8.2175	3.6058	0.2430	0.0757
H	10.5365	-7.8344	6.4484	0.2363	0.0797
H	-8.1881	-5.3169	9.0478	0.2332	0.0885
H	0.9141	-2.3371	10.6332	0.1632	0.0757
H	1.4361	0.0798	10.5511	0.1927	0.0563
H	1.0741	1.3675	8.4582	0.1529	0.0542
H	0.1938	0.2120	6.4445	0.1920	0.0564
H	-0.3078	-2.2094	6.5179	0.1409	0.0742
H	11.6333	-4.7122	10.4806	0.1630	0.0762
H	11.2647	-4.6915	12.9277	0.1943	0.0569
H	-9.8315	-6.4244	13.9890	0.1560	0.0548
H	-8.7839	-8.1817	12.5751	0.1935	0.0570
H	-9.1754	-8.2073	10.1361	0.1748	0.0751
H	-0.5804	-6.0083	10.0638	0.1991	0.0758
H	1.0568	-7.5872	11.0306	0.2363	0.0732
H	4.2643	-5.2790	9.4013	0.1989	0.0683
H	2.6397	-3.6881	8.4127	0.1759	0.0755
H	11.3825	-5.0387	6.5827	0.2220	0.0751
H	13.7052	-4.7818	5.7395	0.1981	0.0695
H	15.1540	-7.2343	8.9340	0.2321	0.0736
H	12.8461	-7.5186	9.7722	0.1872	0.0760
H	6.1266	-8.1182	11.2347	0.1794	0.0697
H	7.7683	-9.7118	12.2069	0.1848	0.0540
H	6.9809	-11.7026	13.4520	0.1478	0.0534
H	4.5489	-12.1063	13.7275	0.1831	0.0543
H	2.9134	-10.4981	12.7457	0.1533	0.0650
H	17.5720	-4.8726	5.0969	0.1804	0.0701
H	19.9180	-4.6408	4.3004	0.1860	0.0544
H	21.7655	-5.7306	5.5443	0.1484	0.0537
H	21.2738	-7.0533	7.5878	0.1839	0.0545
H	18.9131	-7.2750	8.3764	0.1545	0.0652
H	-0.3006	-7.5396	2.5323	0.1387	0.0740
H	1.0615	-9.5405	2.0492	0.1912	0.0562
H	1.1065	-10.5042	-0.2342	0.1521	0.0541
H	-0.2395	-9.4510	-2.0356	0.1933	0.0564
H	-1.6241	-7.4599	-1.5576	0.1622	0.0759
H	-3.8984	-4.6141	0.1421	0.2030	0.0762
H	-3.8080	-2.6496	-1.3702	0.2367	0.0733
H	0.3678	-3.3358	-2.0116	0.1984	0.0682
H	0.3052	-5.2921	-0.4924	0.1760	0.0753
H	-0.4070	-0.3459	-4.2096	0.1791	0.0696
H	-0.3059	1.6011	-5.7521	0.1846	0.0539
H	-2.3112	3.0079	-6.1103	0.1474	0.0533
H	-4.4238	2.4832	-4.9333	0.1828	0.0542

H	-4.5209	0.5267	-3.3844	0.1545	0.0651

Table S27. Cartesian coordinates of optimized structure of molecule **7**.

Total energy: −6.743 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	0.1444	-1.1342	-0.2920	-0.4776	-0.0323
C	-0.4321	-0.5450	-1.4873	-0.5723	-0.0309
N	-0.6433	-1.2773	-2.5636	0.2634	-0.0129
C	-0.4010	-2.6052	-2.5089	-0.5301	-0.0547
C	0.0238	-3.2016	-1.2901	0.7198	-0.0509
N	0.3143	-2.4391	-0.2075	0.2959	-0.0323
N	-0.6093	-3.3318	-3.6375	0.0216	-0.0397
C	-0.4361	-4.6300	-3.5660	-0.0265	0.0250
C	-0.0663	-5.3319	-2.3798	-0.6344	-0.0486
C	0.1687	-4.6056	-1.2349	0.0299	0.0307
C	1.6097	1.0295	3.1202	-0.6649	-0.0375
C	0.8748	-0.1488	3.2840	0.1556	-0.0179
C	0.3894	-0.8286	2.1739	-0.0896	-0.0033
C	0.6169	-0.3465	0.8783	0.2610	-0.0821
C	1.3639	0.8283	0.7239	-0.3724	-0.0081
C	1.8552	1.5105	1.8306	-0.0861	-0.0168
C	-1.1137	2.8762	-2.9387	0.1690	-0.0166
C	-1.7743	3.5180	-1.8865	-0.6849	-0.0378
C	-1.9874	2.8299	-0.6885	-0.0680	-0.0171
C	-1.5352	1.5237	-0.5428	-0.4023	-0.0089
C	-0.8610	0.8765	-1.5864	0.2576	-0.0811
C	-0.6682	1.5692	-2.7895	-0.0781	0.0013
N	0.0784	-6.7361	-2.4207	0.6994	-0.0300
N	2.1069	1.7269	4.2511	0.7541	-0.0293
N	-2.2306	4.8534	-2.0357	0.7605	-0.0296
C	1.3415	2.1987	5.3243	0.2387	-0.0216
C	2.1967	2.8492	6.2470	0.2281	-0.0638
C	3.5380	2.7644	5.7095	0.1035	-0.0640
C	3.4454	2.0682	4.4796	0.1464	-0.0218
C	-3.5497	5.2911	-1.8698	0.1818	-0.0218
C	-3.6015	6.6884	-2.0951	0.1494	-0.0641
C	-2.2542	7.1139	-2.4094	0.2072	-0.0639
C	-1.4368	5.9579	-2.3655	0.2151	-0.0217
C	-0.8964	-7.6442	-2.8578	0.2556	-0.0232
C	-0.3738	-8.9561	-2.7644	0.2244	-0.0627
C	0.9740	-8.8382	-2.2480	0.1625	-0.0628
C	1.2198	-7.4595	-2.0429	0.2570	-0.0202

C	4.7872	3.1964	6.1645	-0.2123	-0.0222
C	5.9166	2.9275	5.4002	-0.3379	-0.0608
C	5.8090	2.2234	4.1908	-0.4384	-0.0378
C	4.5778	1.7822	3.7153	-0.3451	-0.0516
C	-0.0375	2.1319	5.5294	-0.2732	-0.0524
C	-0.5501	2.7117	6.6859	-0.5071	-0.0379
C	0.2849	3.3485	7.6170	-0.3612	-0.0607
C	1.6559	3.4238	7.4010	-0.1940	-0.0220
C	-4.6989	4.5550	-1.5775	-0.3353	-0.0511
C	-5.9052	5.2434	-1.4928	-0.4417	-0.0379
C	-5.9722	6.6303	-1.6984	-0.3418	-0.0612
C	-4.8265	7.3558	-2.0036	-0.2215	-0.0225
C	-1.6791	8.3536	-2.7037	-0.2212	-0.0223
C	-0.3116	8.4267	-2.9424	-0.3439	-0.0612
C	0.4860	7.2735	-2.8820	-0.5042	-0.0382
C	-0.0612	6.0273	-2.5917	-0.2851	-0.0521
C	-2.2033	-7.4054	-3.2843	-0.3048	-0.0505
C	-2.9777	-8.5046	-3.6439	-0.3927	-0.0348
C	-2.4700	-9.8107	-3.5735	-0.3829	-0.0575
C	-1.1730	-10.0428	-3.1303	-0.3040	-0.0207
C	1.9787	-9.7669	-1.9617	-0.2700	-0.0208
C	3.2033	-9.3142	-1.4847	-0.3665	-0.0578
C	3.4340	-7.9427	-1.2989	-0.4488	-0.0351
C	2.4503	-6.9976	-1.5754	-0.2900	-0.0498
H	-0.5833	-5.1973	-4.4812	0.2376	0.0801
H	0.4603	-5.0741	-0.3030	0.2289	0.0895
H	0.7028	-0.5369	4.2806	0.2032	0.0773
H	-0.1582	-1.7539	2.3036	0.2169	0.0739
H	1.5674	1.2164	-0.2664	0.2519	0.0755
H	2.4222	2.4240	1.6998	0.2051	0.0782
H	-0.9699	3.3986	-3.8767	0.2019	0.0777
H	-2.4988	3.3238	0.1286	0.2035	0.0779
H	-1.7144	1.0072	0.3919	0.2561	0.0748
H	-0.1845	1.0634	-3.6158	0.2379	0.0765
H	4.8752	3.7309	7.1039	0.1312	0.0605
H	6.8906	3.2583	5.7413	0.1609	0.0527
H	6.7030	2.0143	3.6143	0.1703	0.0541
H	4.5080	1.2291	2.7873	0.1690	0.0671
H	-0.6926	1.6515	4.8138	0.1551	0.0658
H	-1.6183	2.6720	6.8674	0.1707	0.0541
H	-0.1464	3.7893	8.5081	0.1618	0.0528
H	2.2971	3.9261	8.1168	0.1341	0.0606
H	-4.6605	3.4832	-1.4293	0.1714	0.0674
H	-6.8119	4.6936	-1.2670	0.1698	0.0541

H	-6.9277	7.1362	-1.6242	0.1606	0.0526
H	-4.8834	8.4254	-2.1731	0.1316	0.0604
H	-2.2911	9.2480	-2.7414	0.1322	0.0604
H	0.1460	9.3817	-3.1723	0.1612	0.0526
H	1.5521	7.3526	-3.0628	0.1704	0.0539
H	0.5648	5.1455	-2.5400	0.1538	0.0660
H	-2.6126	-6.4040	-3.3313	0.1866	0.0678
H	-3.9954	-8.3448	-3.9811	0.1721	0.0555
H	-3.0994	-10.6447	-3.8608	0.1640	0.0537
H	-0.7885	-11.0545	-3.0647	0.1329	0.0611
H	1.8065	-10.8266	-2.1134	0.1339	0.0612
H	3.9900	-10.0240	-1.2575	0.1641	0.0536
H	4.3982	-7.6085	-0.9334	0.1714	0.0552
H	2.6445	-5.9419	-1.4343	0.1813	0.0670

Table S28. Cartesian coordinates of optimized structure of molecule **8**.

Total energy: −7.365 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	3.3400	0.8713	-1.3220	-0.6704	-0.0581
C	3.4285	0.1166	-0.1517	0.0336	-0.0073
C	2.2947	-0.1105	0.6212	-0.1041	-0.0055
C	1.0479	0.3869	0.2219	0.1734	-0.0765
C	0.9656	1.1337	-0.9607	-0.4615	-0.0122
C	2.1036	1.3842	-1.7197	-0.0135	-0.0130
C	-1.2852	-2.0004	-2.6661	-0.0041	-0.0138
C	-2.4299	-1.5306	-3.3128	-0.6788	-0.0575
C	-3.2406	-0.5865	-2.6812	-0.0392	-0.0067
C	-2.9142	-0.1231	-1.4114	-0.0876	-0.0007
C	-1.7547	-0.5706	-0.7652	0.1331	-0.0762
C	-0.9438	-1.5154	-1.4081	-0.4662	-0.0128
C	-0.1360	0.2033	1.1055	-0.4911	-0.0337
C	-1.4676	-0.1093	0.6211	-0.4974	-0.0292
N	-2.5110	-0.0390	1.4230	0.2842	-0.0098
C	-2.3117	0.2416	2.7309	-0.5739	-0.0522
C	-0.9882	0.3868	3.2309	0.5415	-0.0551
N	0.0769	0.3920	2.3924	0.3212	-0.0266
N	-3.4069	0.3365	3.5281	0.0214	-0.0397
C	-3.2066	0.5383	4.8099	0.0100	0.0342
C	-1.9234	0.6627	5.4167	-1.0535	-0.0689
C	-0.8078	0.5947	4.6180	0.0006	0.0396
N	-1.8372	0.8620	6.8243	0.7195	-0.0802
N	-2.7892	-2.0244	-4.6080	0.7361	-0.0802

N	4.5211	1.1384	-2.0864	0.7326	-0.0800
C	5.3064	2.2712	-1.7817	0.2937	-0.0234
C	6.4526	2.5292	-2.5512	-0.0054	-0.0010
O	6.8362	1.6889	-3.5782	-0.1492	-0.0971
C	5.9224	0.7549	-4.0266	-0.0589	-0.0011
C	4.7642	0.4484	-3.2927	0.2902	-0.0238
C	-1.4719	-0.1966	7.6867	0.5881	-0.0216
C	-1.5031	0.0199	9.0741	-0.0074	0.0004
O	-1.9048	1.2247	9.6158	-0.1341	-0.0949
C	-2.1028	2.2935	8.7657	0.0040	0.0002
C	-2.0812	2.1411	7.3701	0.4546	-0.0246
C	-2.1196	-1.5611	-5.7593	0.3822	-0.0234
C	-2.4914	-2.0747	-7.0132	-0.0567	-0.0009
O	-3.5126	-2.9953	-7.1442	-0.1457	-0.0973
C	-3.9832	-3.6107	-6.0005	-0.0375	-0.0010
C	-3.6468	-3.1395	-4.7208	0.4011	-0.0234
C	5.0013	3.1518	-0.7403	-0.3344	-0.0487
C	5.8216	4.2488	-0.4690	-0.2740	-0.0457
C	6.9516	4.4895	-1.2404	-0.2267	-0.0542
C	7.2610	3.6231	-2.2907	-0.3057	-0.0268
C	6.2140	0.1026	-5.2129	-0.2684	-0.0263
C	5.3604	-0.8913	-5.6956	-0.2377	-0.0542
C	4.2163	-1.2147	-4.9770	-0.2579	-0.0450
C	3.9186	-0.5485	-3.7865	-0.2311	-0.0518
C	-1.1128	-0.5925	-5.7192	-0.2396	-0.0519
C	-0.4928	-0.1550	-6.8915	-0.2593	-0.0456
C	-0.8653	-0.6819	-8.1217	-0.2467	-0.0547
C	-1.8707	-1.6494	-8.1758	-0.2913	-0.0266
C	-4.8244	-4.6981	-6.1667	-0.3422	-0.0271
C	-5.3654	-5.3430	-5.0527	-0.2273	-0.0544
C	-5.0436	-4.8895	-3.7797	-0.3165	-0.0453
C	-4.1865	-3.7997	-3.6136	-0.3329	-0.0482
C	-2.3374	3.5284	9.3474	-0.3689	-0.0244
C	-2.5633	4.6498	8.5472	-0.2423	-0.0503
C	-2.5381	4.5179	7.1647	-0.2669	-0.0438
C	-2.2918	3.2743	6.5799	-0.2064	-0.0484
C	-1.1012	-1.4631	7.2279	-0.2552	-0.0496
C	-0.7617	-2.4784	8.1241	-0.3369	-0.0437
C	-0.7839	-2.2430	9.4928	-0.2349	-0.0511
C	-1.1576	-0.9838	9.9642	-0.3227	-0.0239
H	4.3916	-0.2767	0.1520	0.1845	0.0794
H	2.3691	-0.6718	1.5443	0.2213	0.0735
H	0.0151	1.5451	-1.2778	0.2467	0.0753
H	2.0408	1.9852	-2.6193	0.1958	0.0815

H	-0.6698	-2.7492	-3.1509	0.1919	0.0810
H	-4.1307	-0.2308	-3.1865	0.1842	0.0797
H	-3.5593	0.5848	-0.9062	0.2439	0.0763
H	-0.0561	-1.8945	-0.9169	0.2443	0.0746
H	-4.0868	0.6097	5.4442	0.2253	0.0827
H	0.1930	0.7082	5.0176	0.2074	0.0932
H	4.1225	2.9760	-0.1343	0.1766	0.0717
H	5.5646	4.9113	0.3490	0.1764	0.0549
H	7.5911	5.3394	-1.0357	0.1570	0.0541
H	8.1330	3.7762	-2.9151	0.1840	0.0699
H	7.1194	0.3784	-5.7401	0.1868	0.0700
H	5.5961	-1.4030	-6.6207	0.1693	0.0545
H	3.5432	-1.9847	-5.3349	0.1644	0.0552
H	3.0259	-0.8104	-3.2343	0.1185	0.0685
H	-0.8172	-0.1730	-4.7669	0.1188	0.0685
H	0.2839	0.5980	-6.8300	0.1637	0.0548
H	-0.3870	-0.3485	-9.0345	0.1687	0.0543
H	-2.1944	-2.0794	-9.1161	0.1867	0.0699
H	-5.0512	-5.0214	-7.1755	0.1836	0.0698
H	-6.0290	-6.1884	-5.1878	0.1565	0.0540
H	-5.4533	-5.3778	-2.9034	0.1763	0.0551
H	-3.9420	-3.4559	-2.6173	0.1836	0.0721
H	-2.3445	3.5922	10.4288	0.1872	0.0708
H	-2.7522	5.6117	9.0078	0.1602	0.0552
H	-2.7047	5.3783	6.5277	0.1760	0.0559
H	-2.2647	3.1867	5.5018	0.1954	0.0701
H	-1.0846	-1.6631	6.1651	0.1843	0.0685
H	-0.4821	-3.4516	7.7388	0.1745	0.0556
H	-0.5197	-3.0254	10.1936	0.1604	0.0551
H	-1.1968	-0.7631	11.0241	0.1867	0.0709

Table S29. Cartesian coordinates of optimized structure of molecule **9**.

Total energy: −10.036 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	0.6101	2.3453	-2.9038	0.1997	0.0651
C	1.0405	1.0380	-3.1822	-0.1234	-0.1254
C	1.0799	0.0806	-2.1673	-0.1368	-0.0924
C	0.6745	0.4034	-0.8585	0.0715	-0.0283
C	0.2533	1.7190	-0.5864	-0.1386	-0.0977
C	0.2237	2.6795	-1.5991	-0.0864	-0.1025
C	-3.2464	0.7849	2.7894	-0.1234	-0.1248
C	-4.0634	0.9207	1.6554	0.1991	0.0653

C	-3.5797	0.5146	0.4047	-0.0872	-0.1038
C	-2.2900	-0.0058	0.2826	-0.1402	-0.0988
C	-1.4598	-0.1343	1.4123	0.0711	-0.0298
C	-1.9619	0.2530	2.6696	-0.1379	-0.0883
C	0.7983	-0.6191	0.2124	0.1145	0.0408
C	-0.1117	-0.7550	1.3373	0.1080	0.0442
N	0.2178	-1.5244	2.3789	-0.3644	-0.1116
C	1.3623	-2.2624	2.3338	0.2159	0.0519
C	2.1544	-2.2693	1.1509	0.2106	-0.0020
N	1.8701	-1.4128	0.1223	-0.4437	-0.1316
N	1.6890	-3.0117	3.4335	-0.3370	-0.1241
C	2.7574	-3.7954	3.3505	0.0437	-0.0207
C	3.5804	-3.9083	2.1857	0.1999	0.0411
C	3.2830	-3.1248	1.0857	-0.0697	-0.0930
N	4.6940	-4.8115	2.2342	-0.8453	-0.1481
N	0.5678	3.3615	-3.9288	-0.8389	-0.1476
N	-5.3996	1.4604	1.7477	-0.8391	-0.1473
C	1.7546	4.1104	-4.1938	0.3325	0.0678
C	1.6906	5.3757	-4.8075	-0.2706	-0.1670
S	0.0560	6.1559	-5.1219	0.3951	0.2320
C	-0.8991	4.6217	-5.4605	-0.2709	-0.1667
C	-0.5769	3.4323	-4.7795	0.3353	0.0684
C	5.8880	-4.3605	2.8800	0.3201	0.0635
C	6.7740	-5.2711	3.4821	-0.2675	-0.1646
S	6.3227	-7.0504	3.5643	0.4039	0.2377
C	5.4053	-7.1533	1.9730	-0.2720	-0.1645
C	4.6479	-6.0540	1.5251	0.3381	0.0687
C	-5.5683	2.8778	1.7199	0.3352	0.0685
C	-6.7998	3.4534	1.3536	-0.2706	-0.1668
S	-8.1612	2.3827	0.7369	0.3932	0.2307
C	-7.8020	0.8970	1.7589	-0.2709	-0.1672
C	-6.4700	0.5769	2.0837	0.3330	0.0678
C	-4.5104	3.7450	2.0558	-0.1155	-0.1441
C	-4.6831	5.1316	2.0285	-0.1450	-0.1090
C	-5.9205	5.6872	1.6925	-0.1020	-0.1247
C	-6.9817	4.8371	1.3640	-0.1621	-0.1127
C	-8.8560	0.0580	2.1238	-0.1625	-0.1135
C	-8.6018	-1.1512	2.7797	-0.1025	-0.1252
C	-7.2817	-1.4979	3.0802	-0.1459	-0.1087
C	-6.2285	-0.6408	2.7493	-0.1171	-0.1428
C	5.4035	-8.3627	1.2758	-0.1611	-0.1111
C	4.6024	-8.5217	0.1406	-0.1006	-0.1211
C	3.8193	-7.4502	-0.2958	-0.1461	-0.1070
C	3.8510	-6.2258	0.3782	-0.1112	-0.1422

C	6.2112	-2.9911	2.9188	-0.1080	-0.1383
C	7.3766	-2.5510	3.5524	-0.1439	-0.1077
C	8.2578	-3.4688	4.1313	-0.1003	-0.1193
C	7.9565	-4.8341	4.0814	-0.1633	-0.1115
C	3.0246	3.6083	-3.8492	-0.1162	-0.1432
C	4.1825	4.3453	-4.1128	-0.1456	-0.1093
C	4.1051	5.5867	-4.7499	-0.1025	-0.1250
C	2.8503	6.0933	-5.1046	-0.1626	-0.1131
C	-1.9920	4.6848	-6.3262	-0.1618	-0.1124
C	-2.8242	3.5734	-6.4961	-0.1019	-0.1242
C	-2.5358	2.3954	-5.8021	-0.1448	-0.1087
C	-1.4195	2.3190	-4.9645	-0.1155	-0.1442
H	1.3477	0.7803	-4.1902	0.1537	0.1314
H	1.4343	-0.9224	-2.3727	0.1582	0.1341
H	-0.0387	1.9983	0.4189	0.1525	0.1292
H	-0.0927	3.6947	-1.3885	0.1591	0.1367
H	-3.6243	1.0902	3.7593	0.1550	0.1322
H	-4.2238	0.6061	-0.4624	0.1576	0.1360
H	-1.9369	-0.3253	-0.6905	0.1495	0.1277
H	-1.3373	0.1179	3.5444	0.1711	0.1402
H	3.0089	-4.3890	4.2237	0.1795	0.1370
H	3.8942	-3.1239	0.1909	0.1772	0.1461
H	-3.5487	3.3338	2.3334	0.1356	0.1258
H	-3.8463	5.7744	2.2819	0.1281	0.1186
H	-6.0612	6.7624	1.6813	0.1277	0.1196
H	-7.9504	5.2446	1.0947	0.1417	0.1280
H	-9.8716	0.3467	1.8749	0.1413	0.1277
H	-9.4222	-1.8085	3.0461	0.1270	0.1192
H	-7.0632	-2.4338	3.5840	0.1301	0.1197
H	-5.2147	-0.9219	3.0027	0.1439	0.1291
H	6.0148	-9.1824	1.6377	0.1454	0.1297
H	4.5904	-9.4684	-0.3882	0.1314	0.1214
H	3.1860	-7.5561	-1.1705	0.1321	0.1206
H	3.2430	-5.4085	0.0147	0.1333	0.1246
H	5.5486	-2.2710	2.4549	0.1376	0.1259
H	7.5972	-1.4891	3.5799	0.1333	0.1213
H	9.1681	-3.1315	4.6147	0.1317	0.1216
H	8.6284	-5.5630	4.5216	0.1455	0.1297
H	3.1063	2.6425	-3.3678	0.1406	0.1278
H	5.1461	3.9371	-3.8259	0.1285	0.1189
H	5.0024	6.1560	-4.9664	0.1274	0.1194
H	2.7642	7.0567	-5.5958	0.1420	0.1280
H	-2.1988	5.6125	-6.8491	0.1423	0.1282
H	-3.6831	3.6326	-7.1555	0.1285	0.1200

H	-3.1728	1.5242	-5.9158	0.1287	0.1189
H	-1.2051	1.3932	-4.4468	0.1350	0.1255

Table S30. Cartesian coordinates of optimized structure of molecule **10**.

Total energy: −4.842 eV

Atom	x	y	z	Mulliken Charges	Lowdin Charges
C	-0.0318	0.7430	-0.7718	-0.5428	-0.0326
C	0.9837	1.0767	0.2107	-0.6702	-0.0387
N	1.7289	2.1581	0.0613	0.2267	-0.0213
C	1.4663	2.9952	-0.9621	-0.4462	-0.0680
C	0.3638	2.7527	-1.8236	0.6431	-0.0485
N	-0.3477	1.6031	-1.7243	0.2570	-0.0478
N	2.2556	4.0941	-1.1056	-0.0133	-0.0455
C	1.9571	4.9451	-2.0539	0.1967	0.0073
C	0.8604	4.8149	-2.9711	-1.0323	-0.0609
C	0.0643	3.6915	-2.8363	0.0426	-0.0221
C	-0.7448	-0.5580	-0.8164	-0.0482	-0.1015
C	1.2386	0.2888	1.4430	0.1225	-0.1006
C	-0.0901	-1.7797	-0.5985	-0.5329	-0.0070
C	-0.7570	-2.9876	-0.7211	0.0607	-0.0477
C	-2.1277	-3.0383	-1.0467	-0.7657	-0.0419
C	-2.7824	-1.8120	-1.2652	0.3601	-0.0639
C	-2.0963	-0.6063	-1.1702	0.0453	-0.0025
C	2.5481	0.1736	1.9355	-0.1425	-0.0003
C	2.8222	-0.5067	3.1096	-0.0368	-0.0488
C	1.7905	-1.0851	3.8771	-0.7565	-0.0425
C	0.4757	-0.9401	3.3998	0.2821	-0.0632
C	0.2128	-0.2788	2.2044	-0.2357	-0.0075
N	0.6217	5.8365	-3.9022	0.2398	-0.1600
N	-2.7812	-4.2751	-1.1885	0.2490	-0.1613
N	2.0902	-1.8061	5.0466	0.2475	-0.1621
C	-4.1732	-4.2820	-1.6327	-0.0249	-0.0310
C	-4.5757	-5.6848	-2.0808	-0.5241	0.0251
O	-4.3567	-6.6514	-1.0623	-0.1133	-0.2302
C	-2.9872	-6.6721	-0.6812	-0.3695	0.0231
C	-2.5290	-5.3092	-0.1767	-0.1477	-0.0170
C	3.0585	-1.2256	5.9867	-0.1706	-0.0160
C	3.5505	-2.2844	6.9659	-0.3543	0.0234
O	2.4685	-2.8992	7.6547	-0.1163	-0.2308
C	1.5684	-3.5010	6.7344	-0.5302	0.0245
C	1.0023	-2.4867	5.7446	-0.0371	-0.0317
C	-0.6096	5.7659	-4.6874	-0.0460	-0.0304

C	-0.8689	7.1059	-5.3703	-0.5322	0.0265
O	0.2311	7.5093	-6.1755	-0.1202	-0.2298
C	1.4132	7.6212	-5.3933	-0.3528	0.0243
C	1.7570	6.3001	-4.7156	-0.1989	-0.0157
H	2.5913	5.8252	-2.1155	0.2201	0.0631
H	-0.7706	3.4789	-3.4904	0.2395	0.0741
H	0.9651	-1.7909	-0.3541	0.2411	0.0745
H	-0.1954	-3.9039	-0.5923	0.1529	0.0599
H	-3.8367	-1.7860	-1.5040	0.1648	0.0588
H	-2.6211	0.3218	-1.3623	0.2387	0.0707
H	3.3580	0.6245	1.3752	0.2347	0.0736
H	3.8539	-0.6080	3.4218	0.1588	0.0589
H	-0.3605	-1.3257	3.9667	0.1736	0.0597
H	-0.8171	-0.1845	1.8825	0.2463	0.0734
H	-4.2838	-3.6070	-2.4837	0.1381	0.0604
H	-4.8544	-3.9418	-0.8344	0.1721	0.0620
H	-4.0084	-5.9600	-2.9821	0.1479	0.0569
H	-5.6414	-5.7140	-2.3139	0.1879	0.0558
H	-2.3674	-6.9810	-1.5359	0.1472	0.0562
H	-2.8956	-7.4189	0.1094	0.1814	0.0556
H	-1.4659	-5.3576	0.0540	0.1133	0.0541
H	-3.0646	-5.0676	0.7565	0.1753	0.0651
H	3.9126	-0.8225	5.4447	0.1081	0.0547
H	2.5956	-0.3971	6.5473	0.1860	0.0664
H	4.1309	-3.0488	6.4283	0.1408	0.0558
H	4.1860	-1.8298	7.7279	0.1844	0.0558
H	2.0813	-4.3042	6.1850	0.1498	0.0562
H	0.7636	-3.9386	7.3275	0.1847	0.0554
H	0.3874	-3.0223	5.0182	0.1314	0.0596
H	0.3549	-1.7729	6.2816	0.1732	0.0622
H	-1.4455	5.5427	-4.0203	0.1524	0.0626
H	-0.5570	4.9699	-5.4486	0.1704	0.0635
H	-1.0749	7.8738	-4.6104	0.1536	0.0575
H	-1.7302	7.0302	-6.0360	0.1903	0.0566
H	1.2860	8.4076	-4.6349	0.1409	0.0569
H	2.2117	7.9150	-6.0765	0.1892	0.0568
H	2.6374	6.4381	-4.0886	0.1184	0.0554
H	2.0047	5.5496	-5.4837	0.1814	0.0669