Electronic Supplementary Material (ESI) for RSC Advances.

Synthesis and opto-electrochemical properties of tribenzo[*a,c,i*]phenazine derivatives for hole transport materials

Azam M. Shaikh,[a] Bharat K. Sharma,[a] Sajeev Chacko[b] and Rajesh M. Kamble*[a]

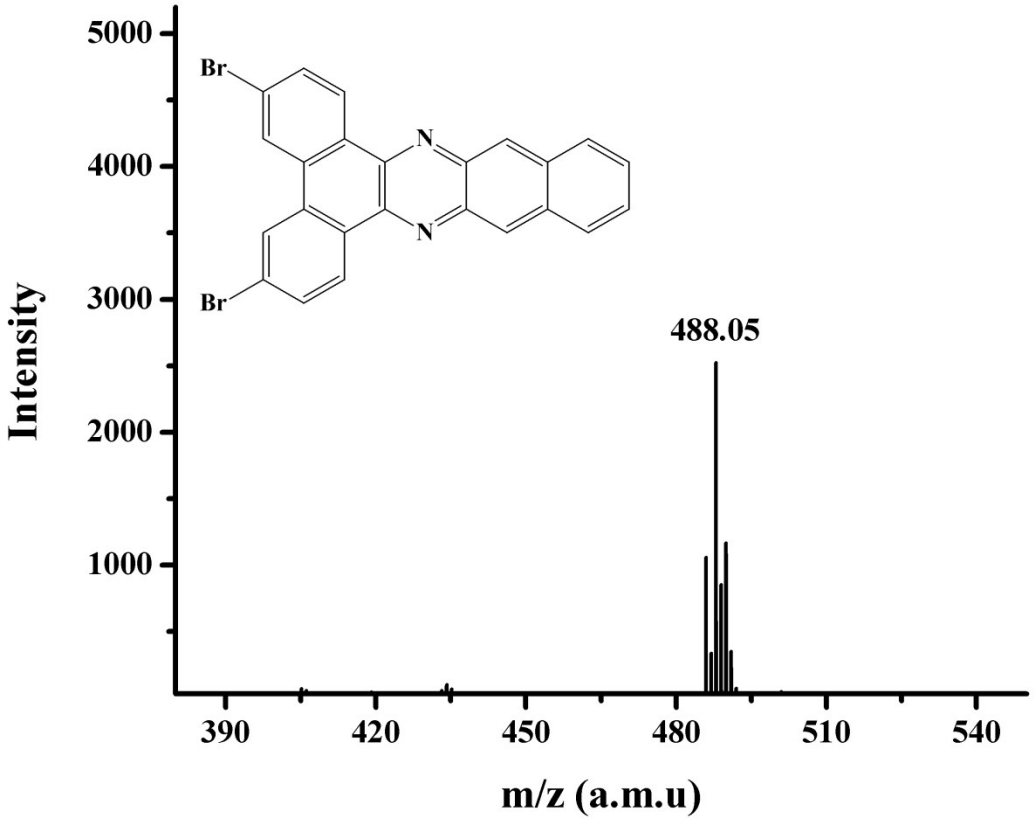
[a]*Department of Chemistry, University of Mumbai, Santacruz (East), Mumbai–400 098, India*

[b]*Department of Physics, University of Mumbai, Santacruz (East), Mumbai–400 098, India*

*Email: kamblerm@chem.mu.ac.in

Supplementary Information

1. **Mass spectra of compound 1**



2. HRMS spectra of compounds 2 6

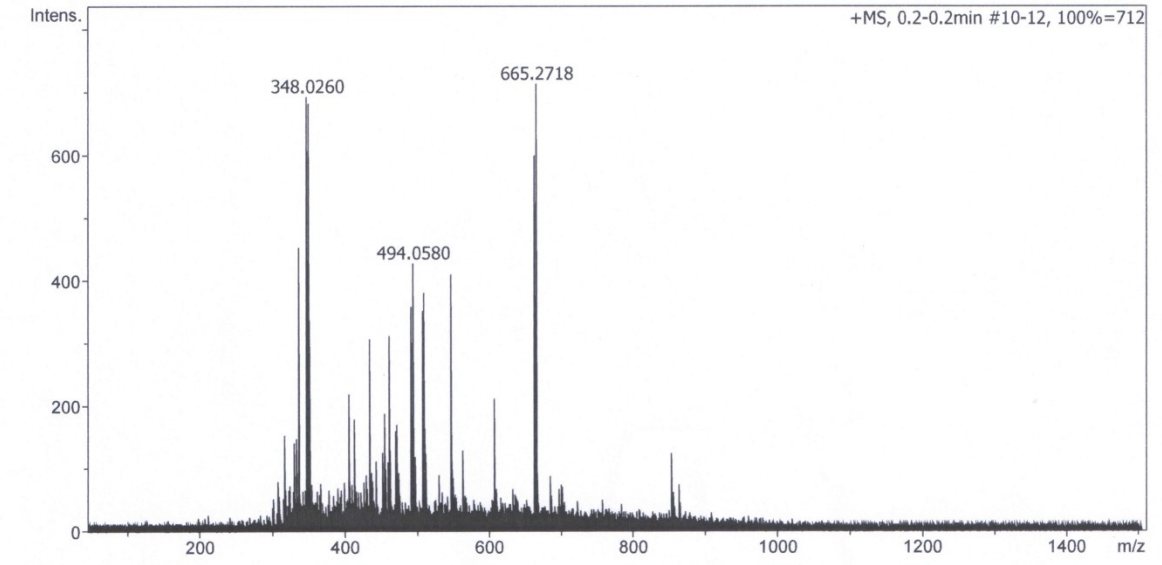
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\JULY-2016\EXT-UNI_MUMBAI-RMK-AZ-10.d	Acquisition Date	7/22/2016 4:03:35 PM
Method	Tune_pos_NAICSI-1500.m	Operator	SRKOUT
Sample Name	EXT-UNI_MUMBAI-RMK-AZ-10	Instrument	maXis impact 282001.00081
Comment	LRMS		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
665.2718	1	C48H33N4	665.2700	2.7	74.0	1	100.00	34.5	even	ok

Fig. S1 HRMS spectra of compound **2**

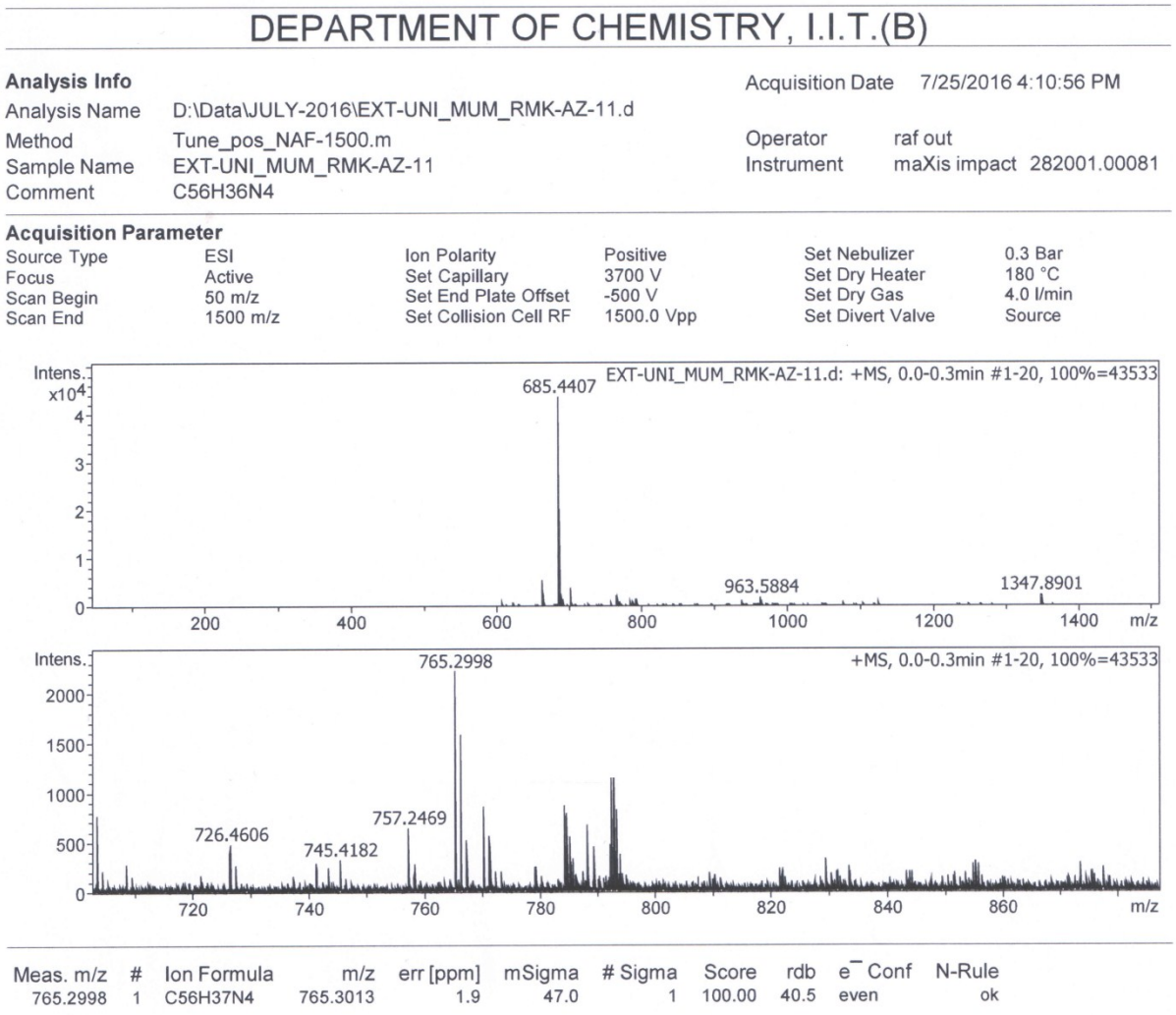


Fig. S2 HRMS spectra of compound **3**

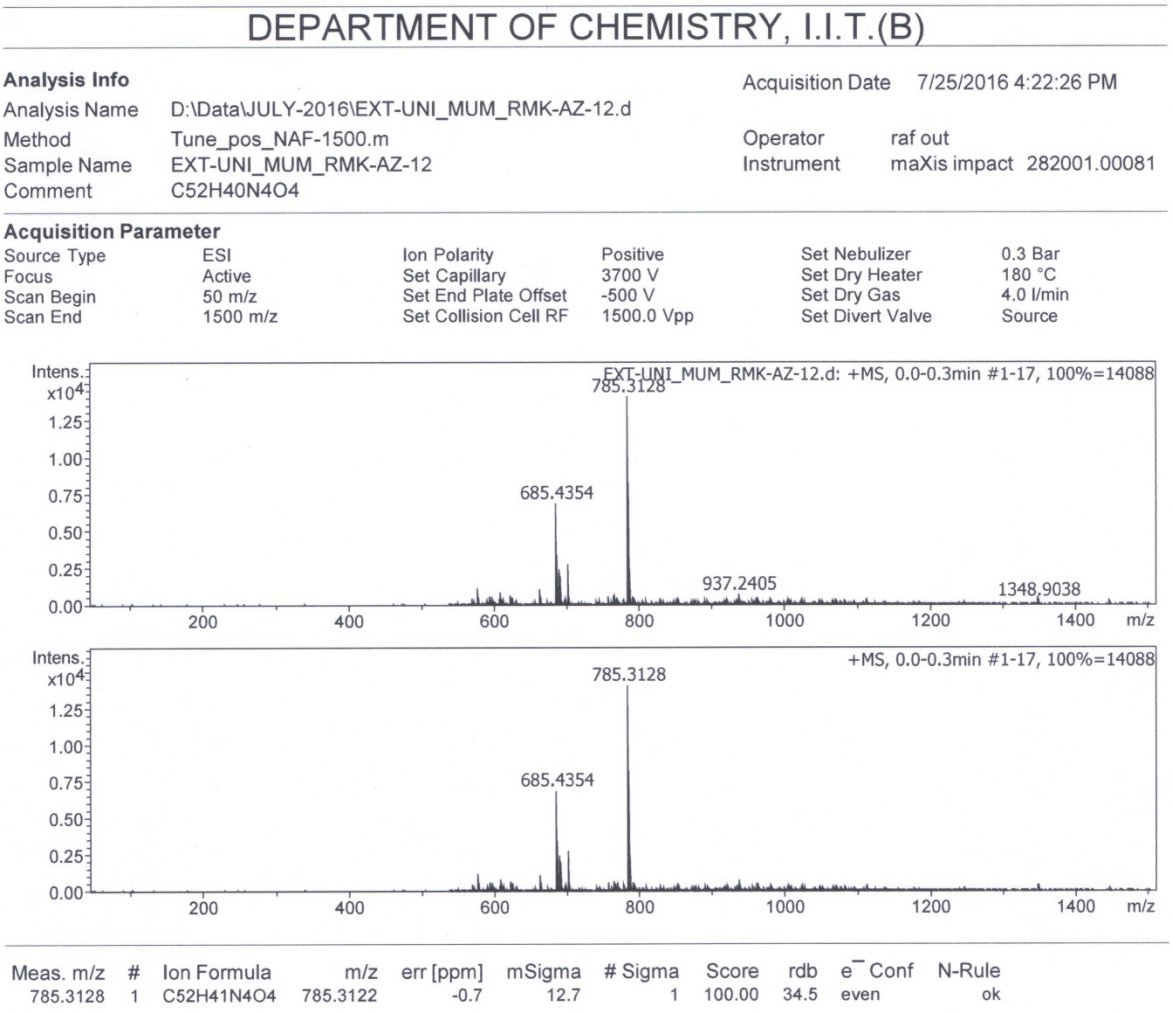


Fig. S3 HRMS spectra of compounds **4**

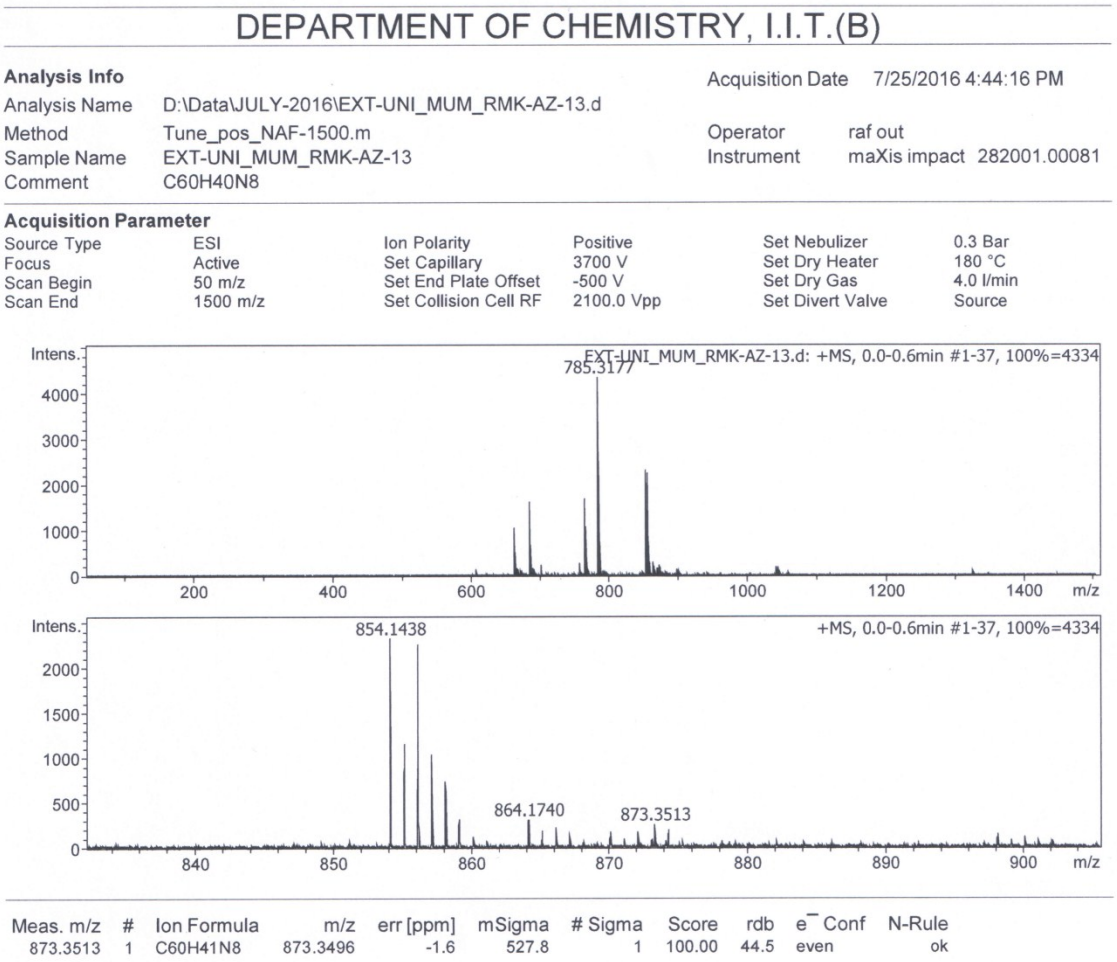


Fig. S4 HRMS spectra of compound **5**

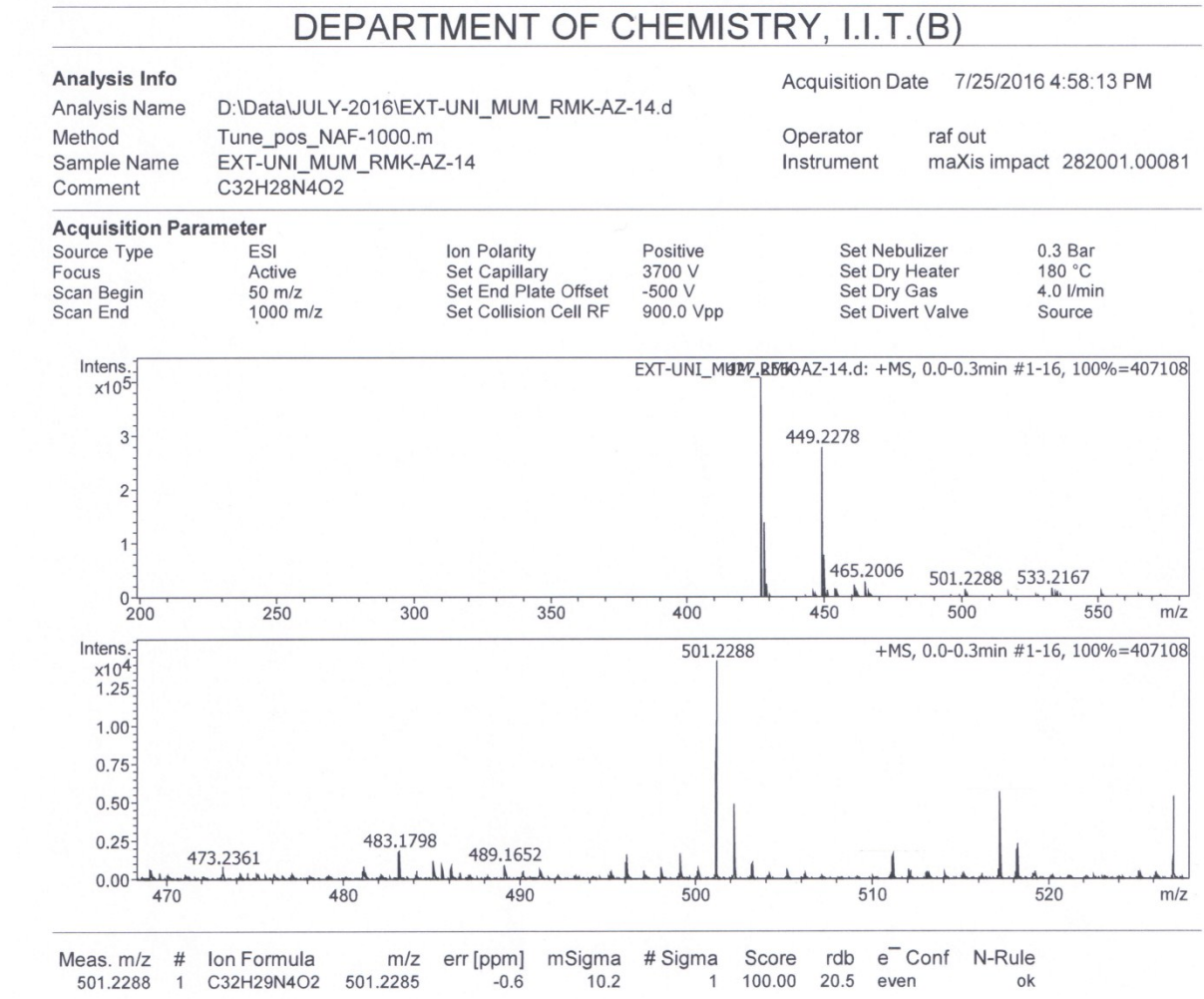


Fig. S5 HRMS spectra of compound **6**

3. FTIR Spectra of compounds 1 6

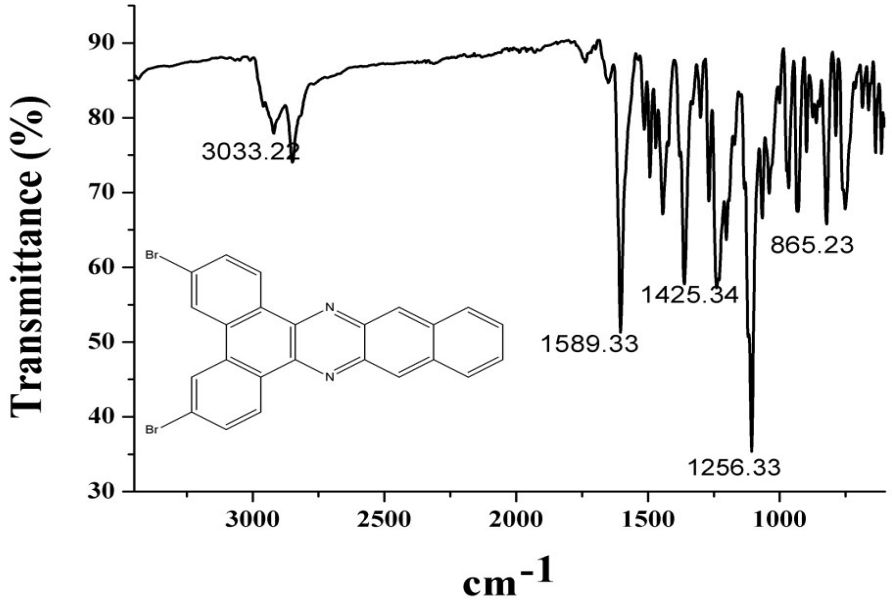


Fig. S6 FTIR Spectra of compound **1**

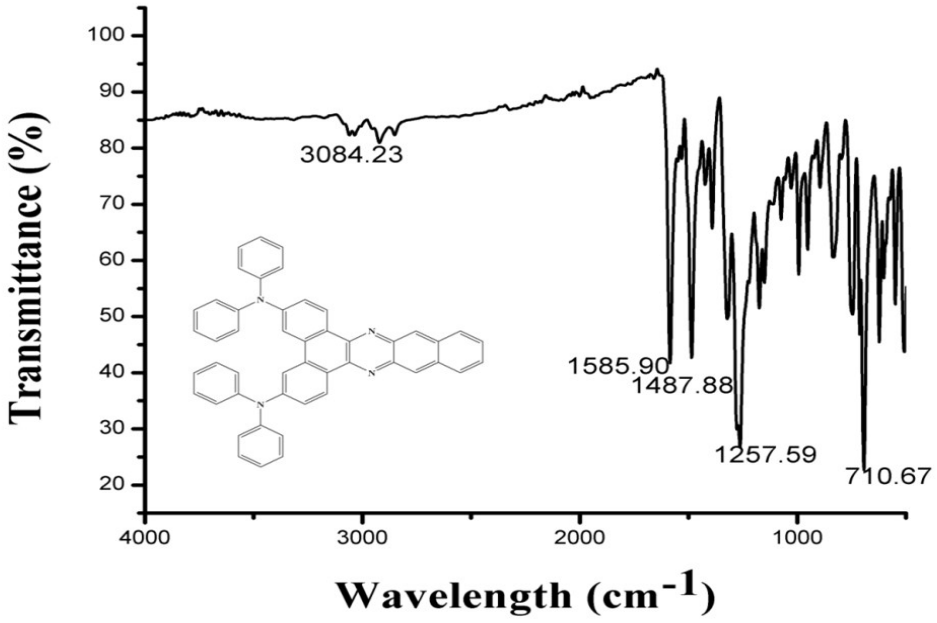


Fig. S7 FTIR Spectra of compound **2**

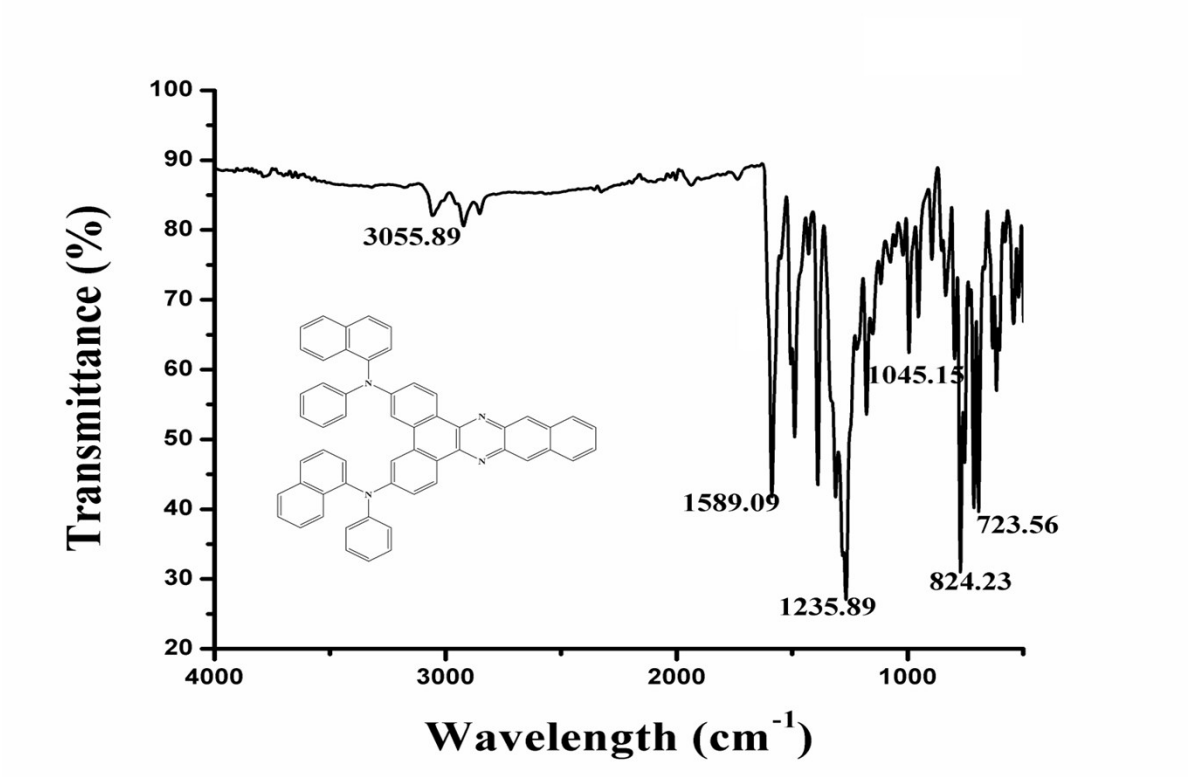


Fig. S8 FTIR Spectra of compound **3**

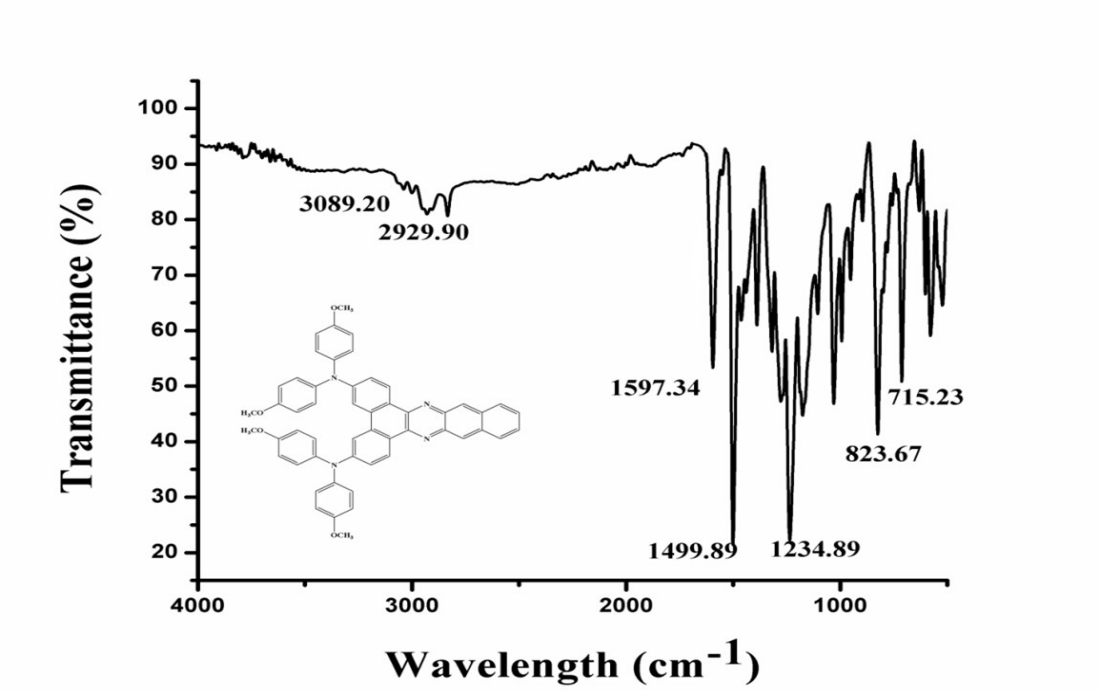


Fig. S9 FTIR Spectra of compound **4**

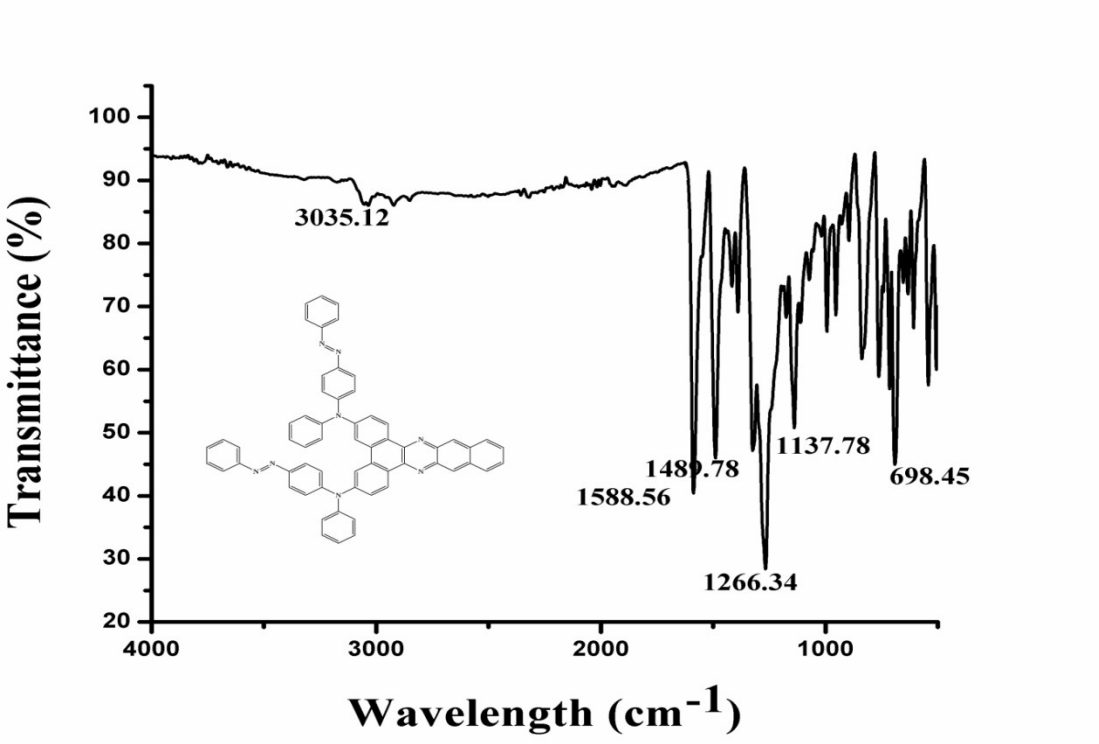


Fig. S10 FTIR Spectra of compound **5**

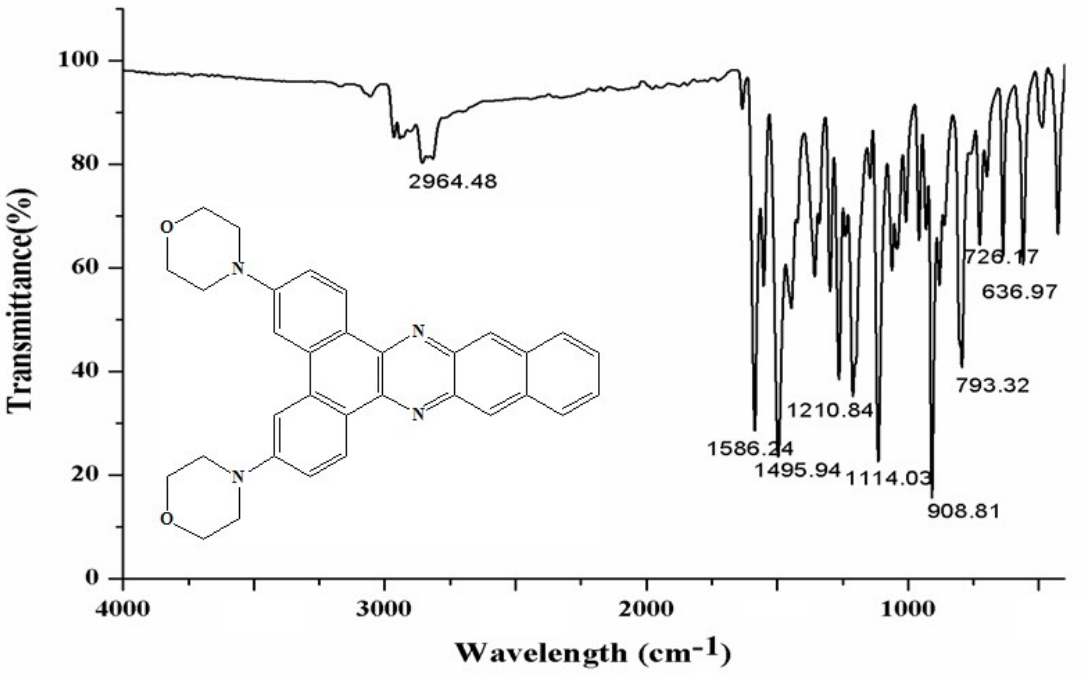


Fig. S11 FTIR Spectra of compound **6**

4. ^{1}H and ^{13}C NMR spectra of compounds 1 7

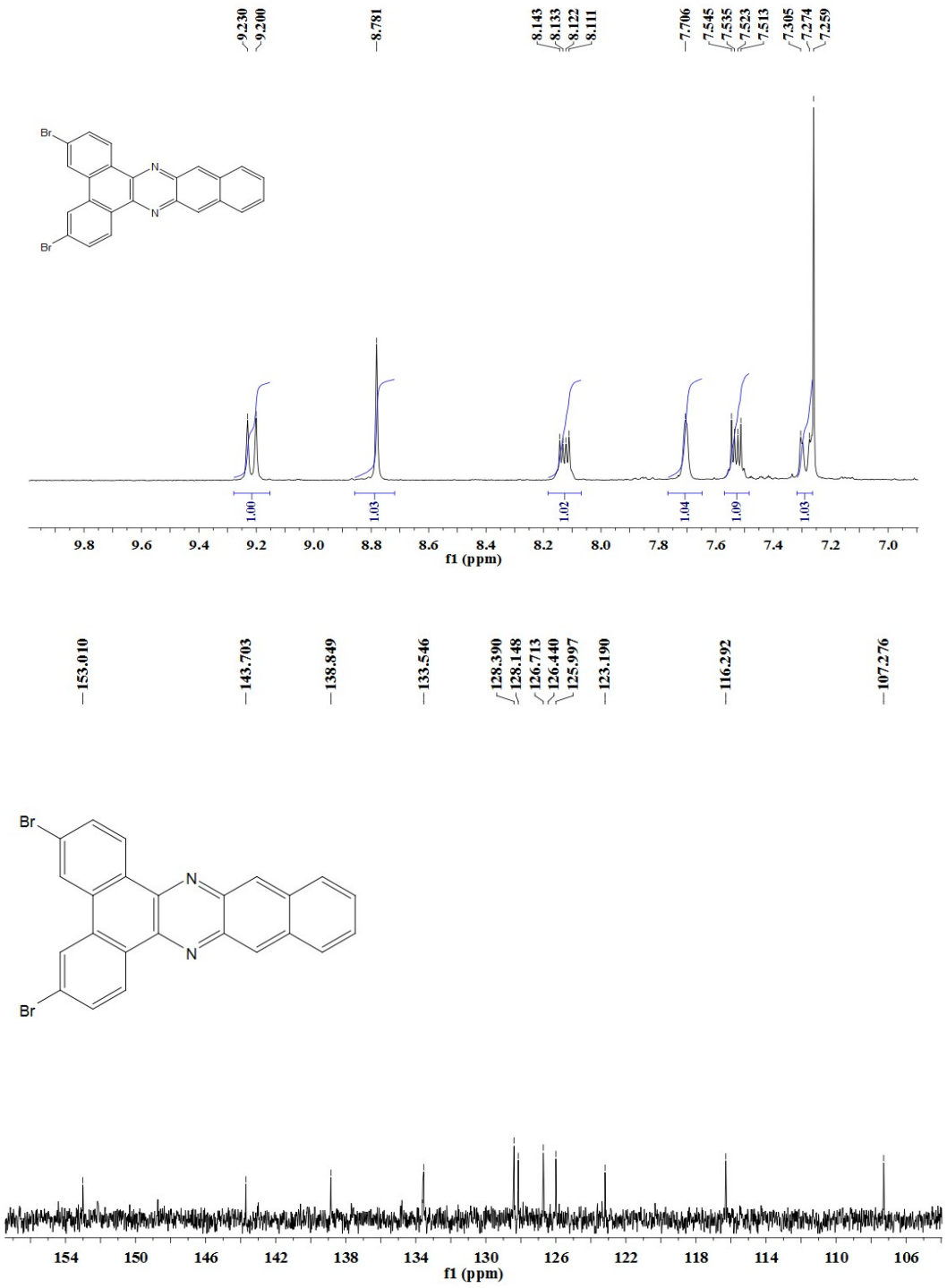


Fig. S12 ^{1}H and ^{13}C NMR spectra of compound **1** in $CDCl_3$

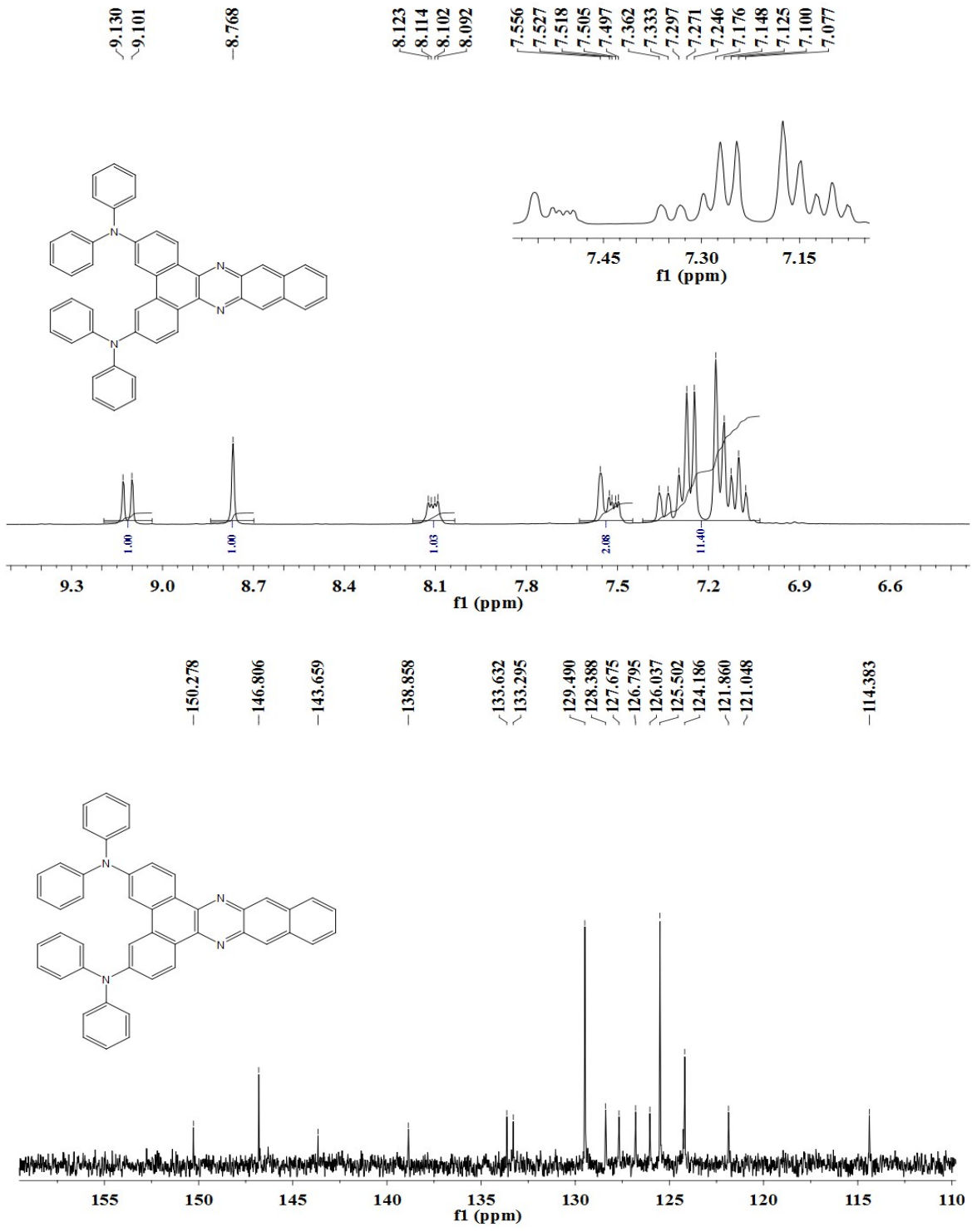


Fig. S13 ^{1}H and ^{13}C NMR spectra of compound **2** in $CDCl_3$

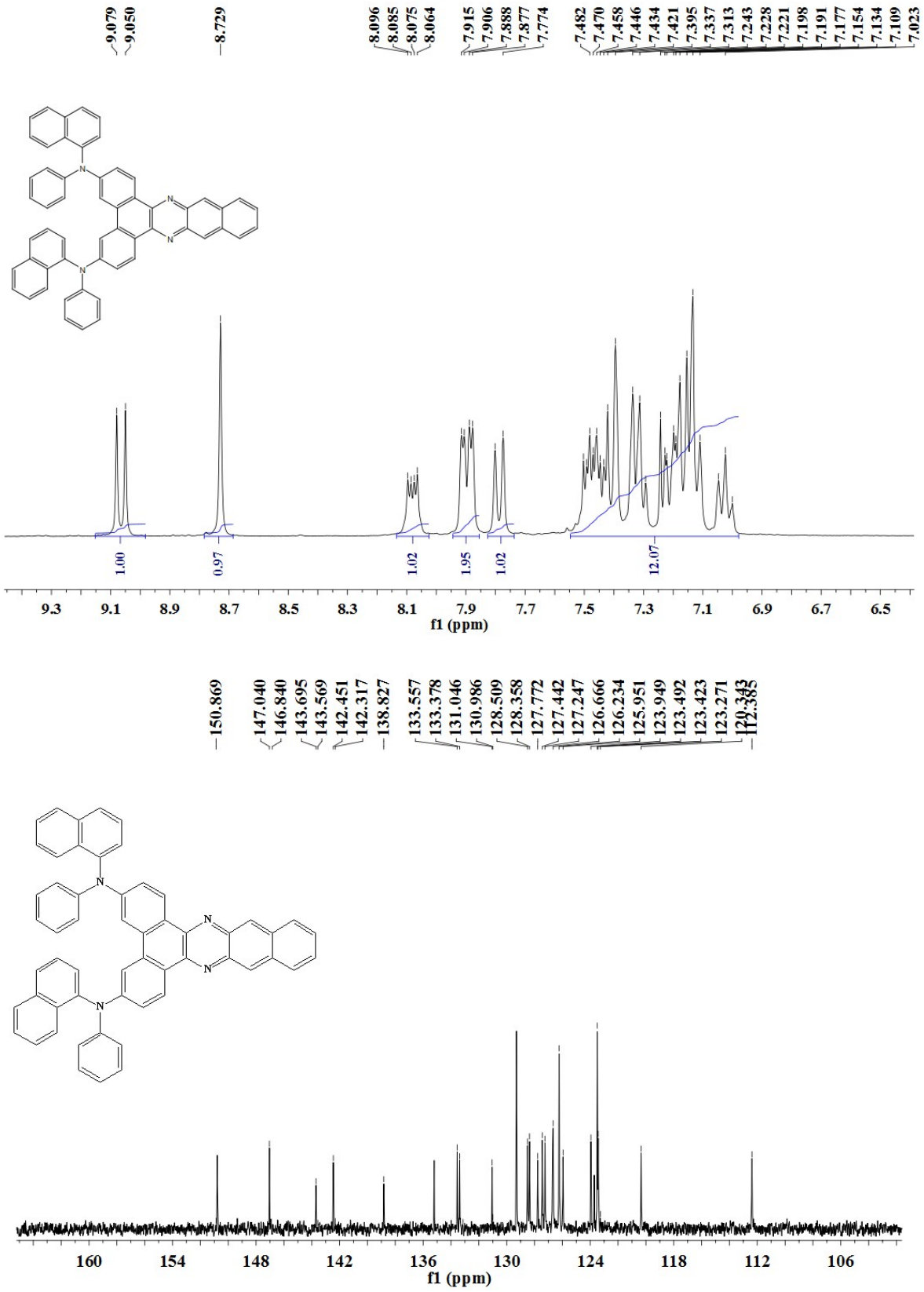


Fig. S14 ^{1}H and ^{13}C NMR spectra of compound **3** in $CDCl_3$

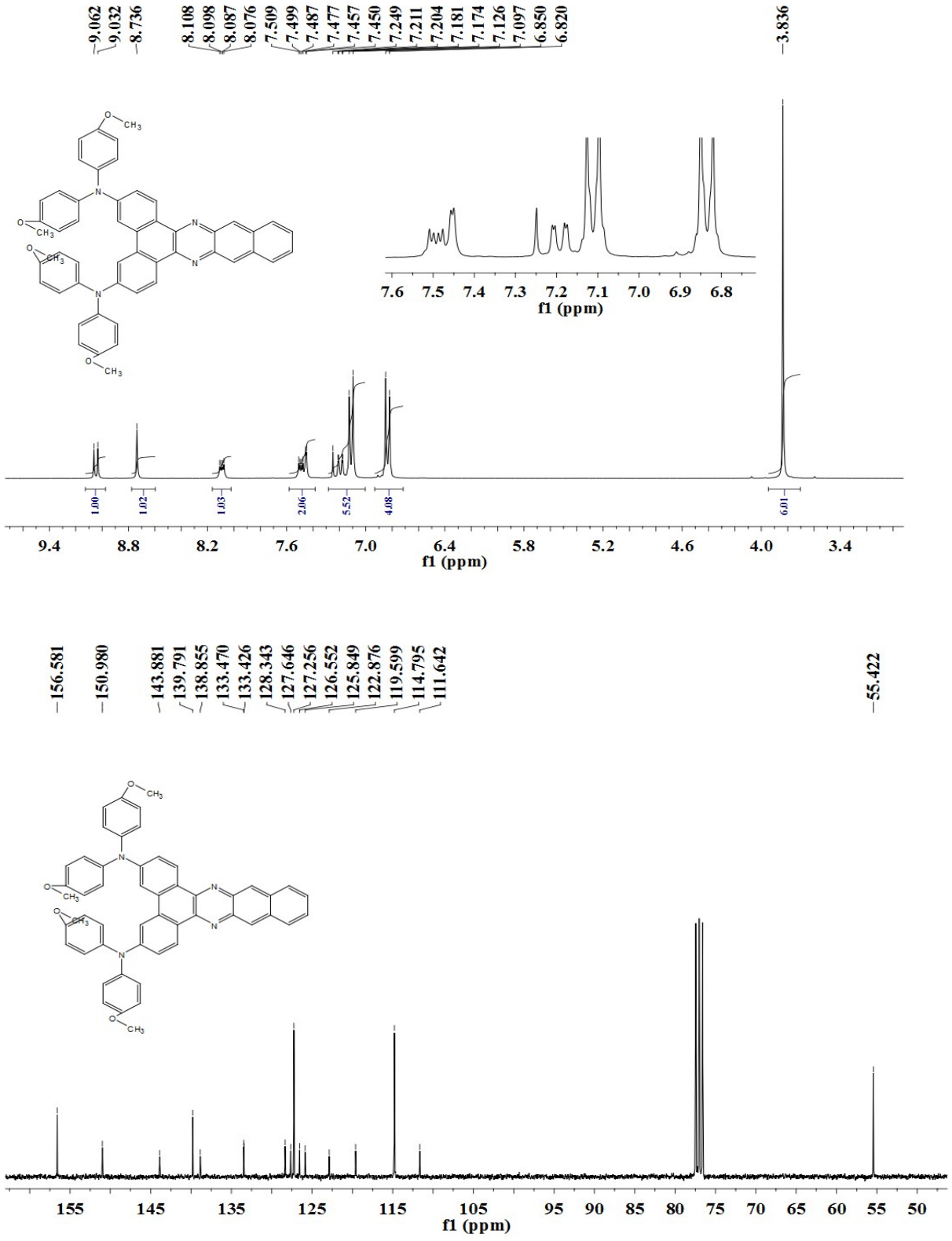


Fig. S15 ^{1}H and ^{13}C NMR spectra of compound **4** in $CDCl_3$

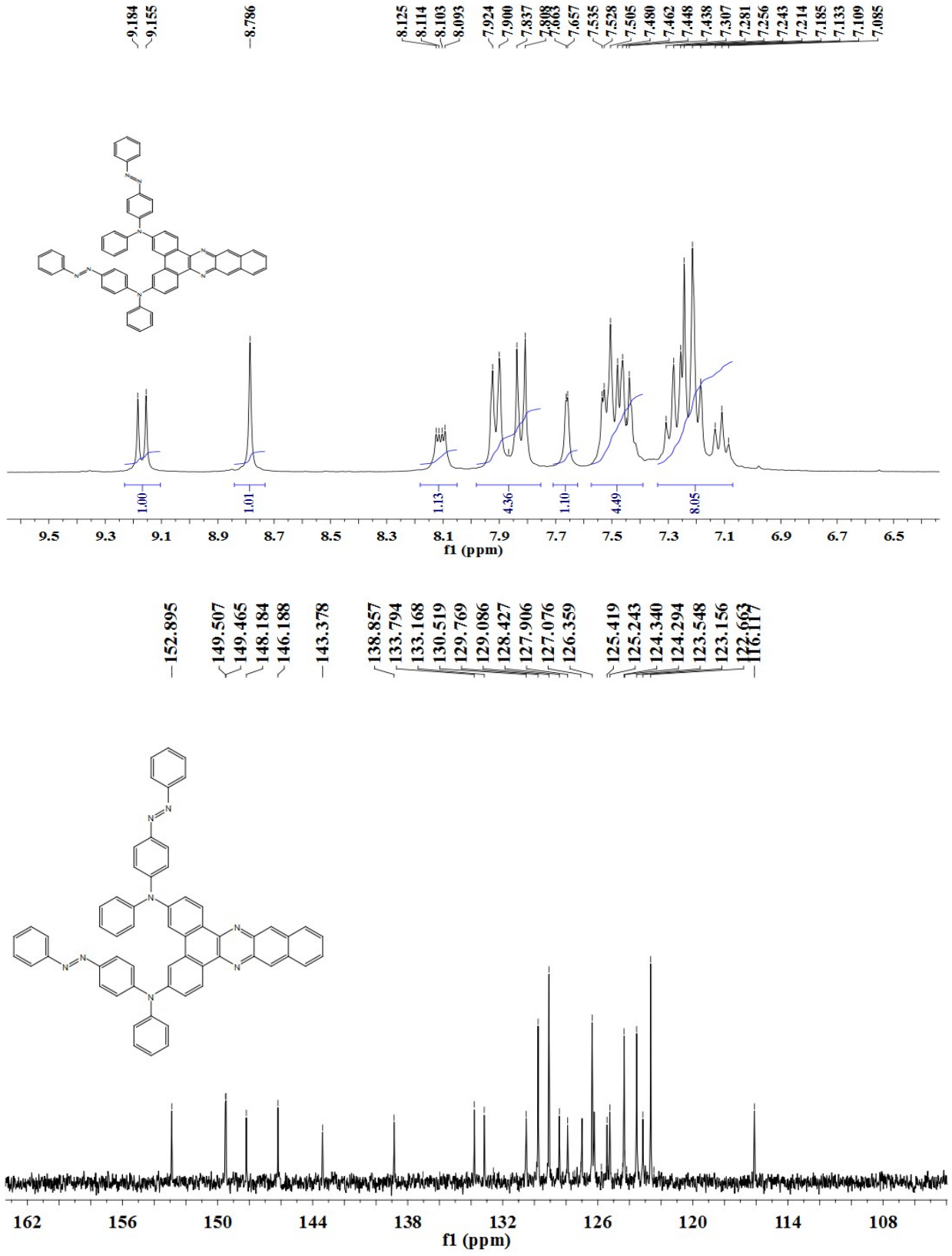


Fig. S16 ^{1}H and ^{13}C NMR spectra of compound **5** in $CDCl_3$

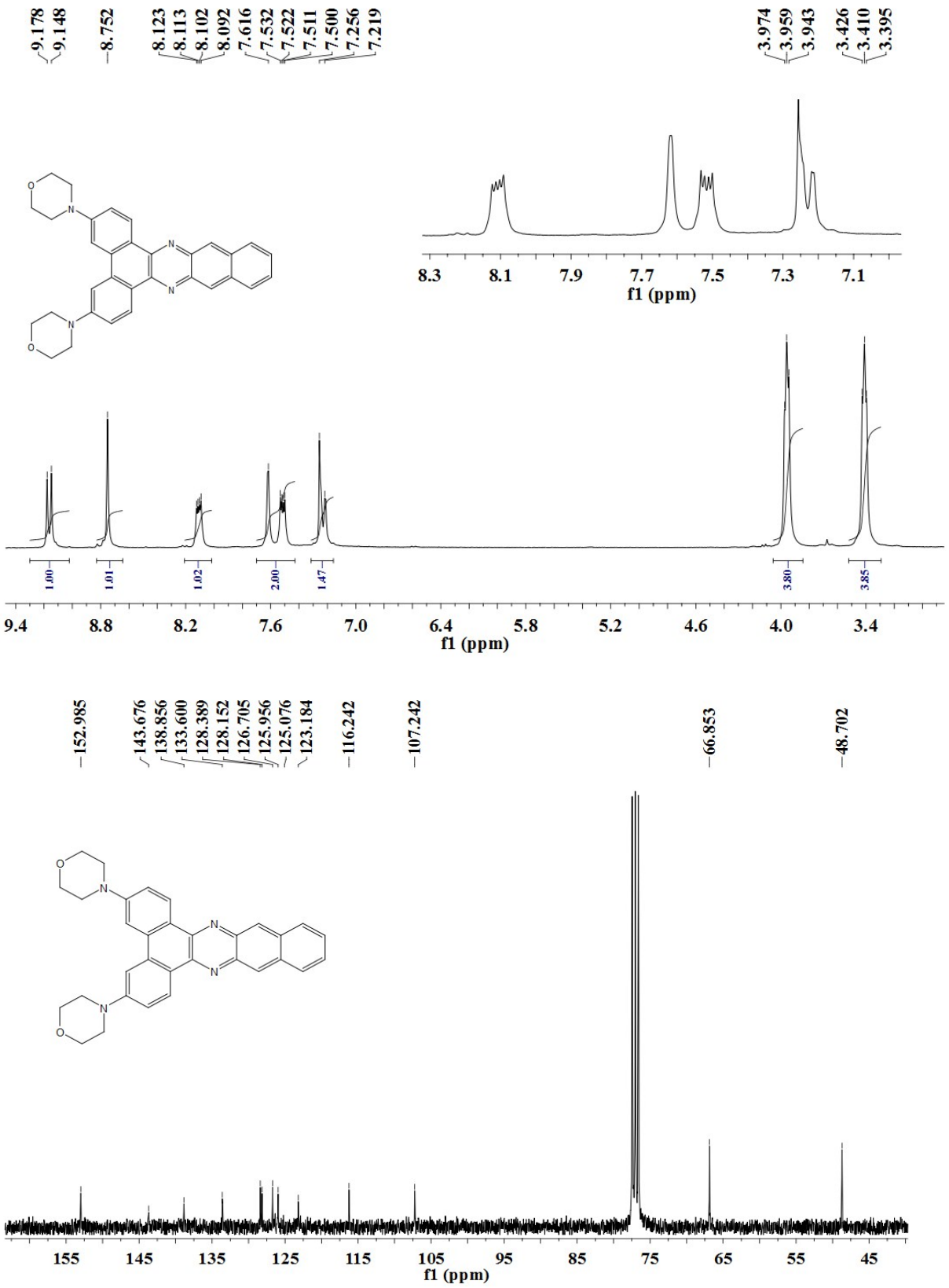


Fig. S17 ^{1}H and ^{13}C NMR spectra of compound **6** in $CDCl_3$

5. Photophysical data of compounds 2 6 in various solvents

a. Photophysical data of compounds **2-6** in Cyclohexane.

Compound	**λ_{emi}[a] nm**	**Stokes shift cm^{-1}**	E_g^{opt} **(eV)**	ϕ_F
2	515	11832	2.48	0.10
3	512	11816	2.46	0.07
4	550	12587	2.34	0.11
5	—	—	—	—
6	507	14883	2.49	0.21

[a]Recorded in10^{-5} M cyclohexane.

b**.** Photophysical data of compounds **2-6** in dichloromethane.

Compound	**λ_{emi}[a] nm**	**Stokes shift cm^{-1}**	E_g^{opt} **(eV)**	ϕ_F
2	625	15055	2.37	0.17
3	613	14936	2.39	0.12
4	—	—	—	—
5	—	—	—	—
6	589	16025	2.39	0.20

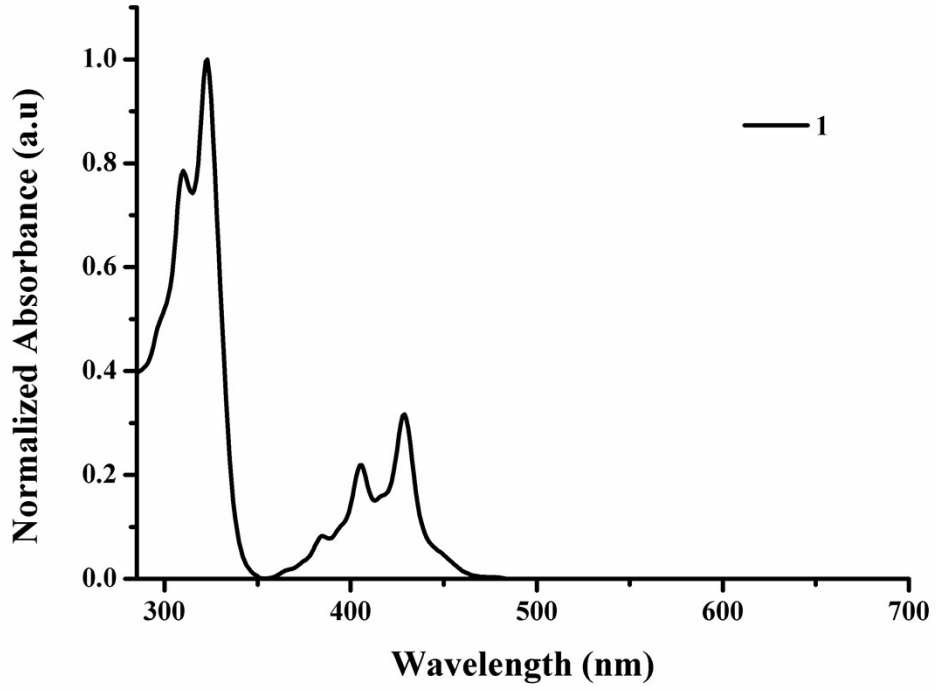
[a]Recorded in10^{-5} M dichloromethane.

c**.** Photophysical data of compounds **2-6** in dimethyl sulfoxide.

Compound	λ_{emi}[a] **nm**	**Stokes shift cm^{-1}**	E_g^{opt} **(eV)**	ϕ_F
2	552	12748	2.38	0.15
3	540	12634	2.39	0.13
4	—	—	—	—
5	—	—	—	—
6	538	13985	2.42	0.19

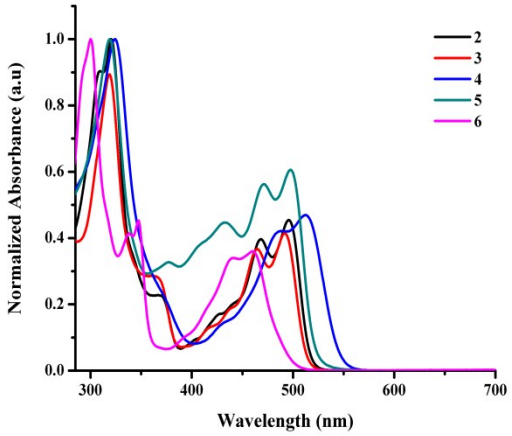
[a]Recorded in10^{-5} M dimethyl sulfoxide.

6. Absorption spectra of compound **1** in toluene

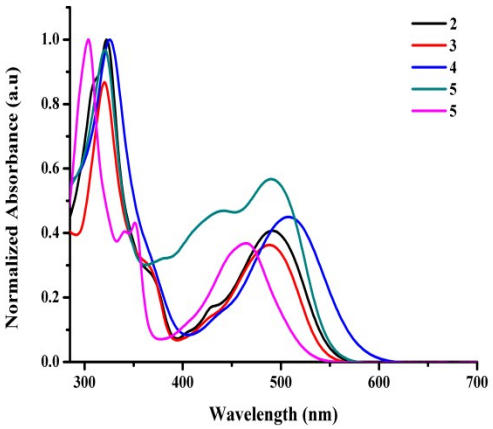


7. Absorption and Emission spectra of compound 2 6 in various solvents

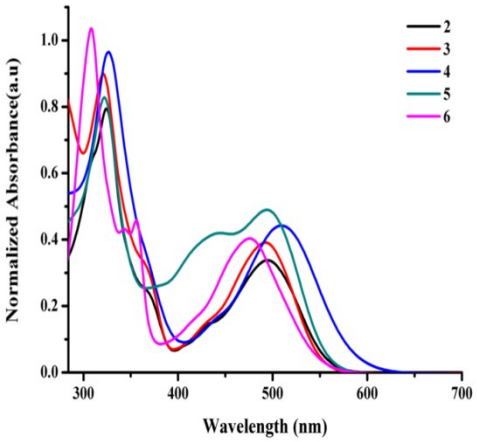
a. Absorption spectra of compound 2 6



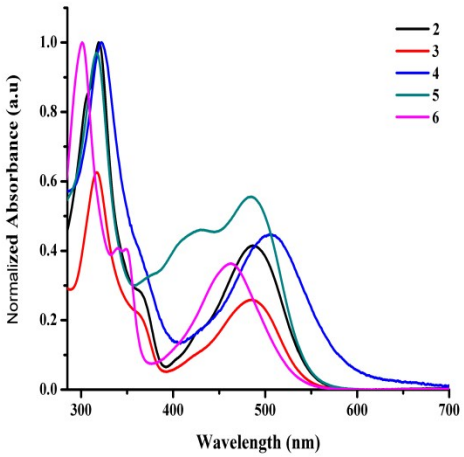
(a) Cyclohexane



(**b**) Dichloromethane

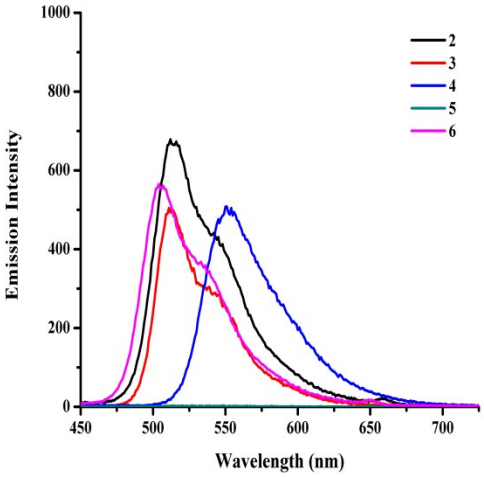


(**c**) dimethyl sulfoxide

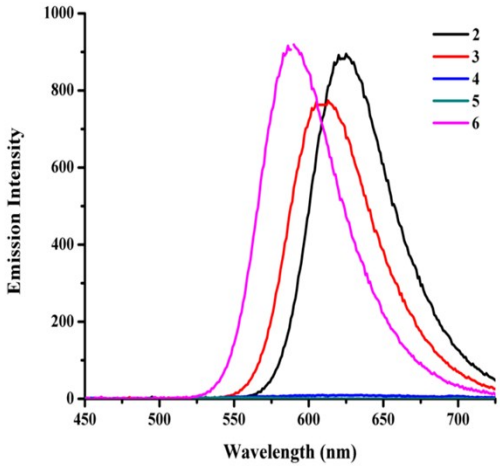


(**d**) methanol

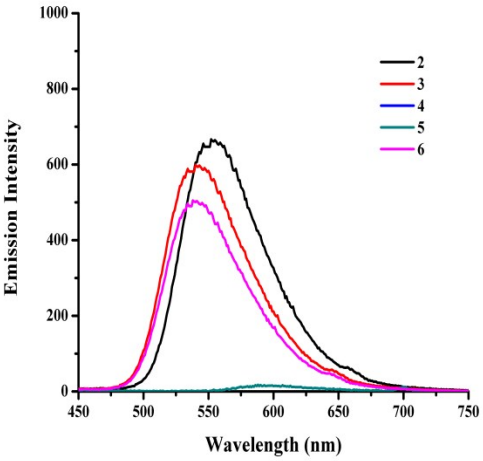
Fluorescence spectra of compound 2 6



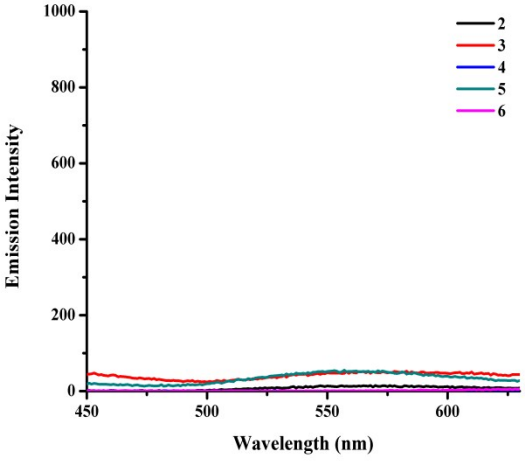
(**a**) Cyclohexane



(**b**) Dichloromethane



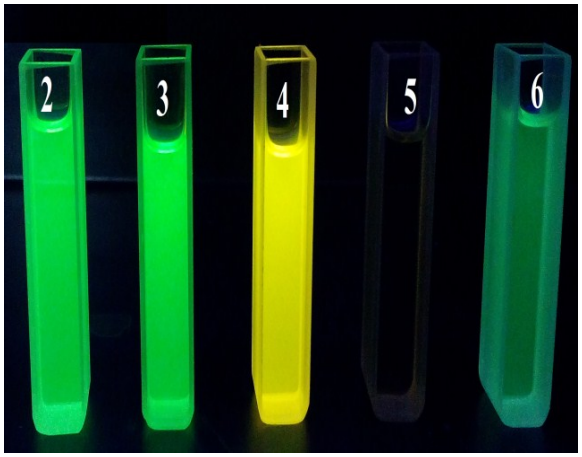
(**c**) Dimethyl sulfoxide



(**d**) Methanol

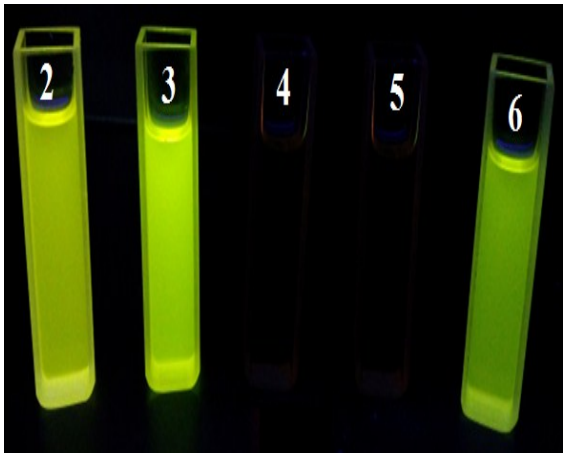
8. Emission of compounds 2 6 under UV light (365 nm)

Toluene

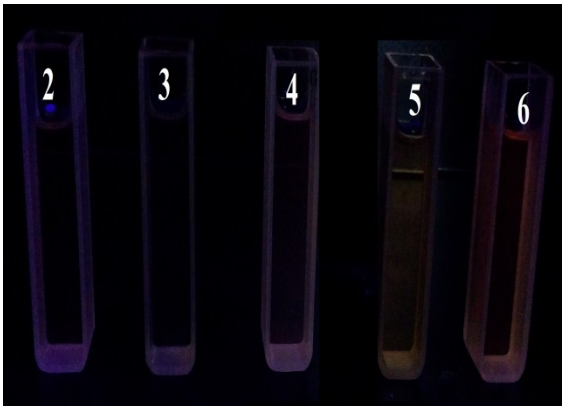


Cyclohexane

Dichloromethane

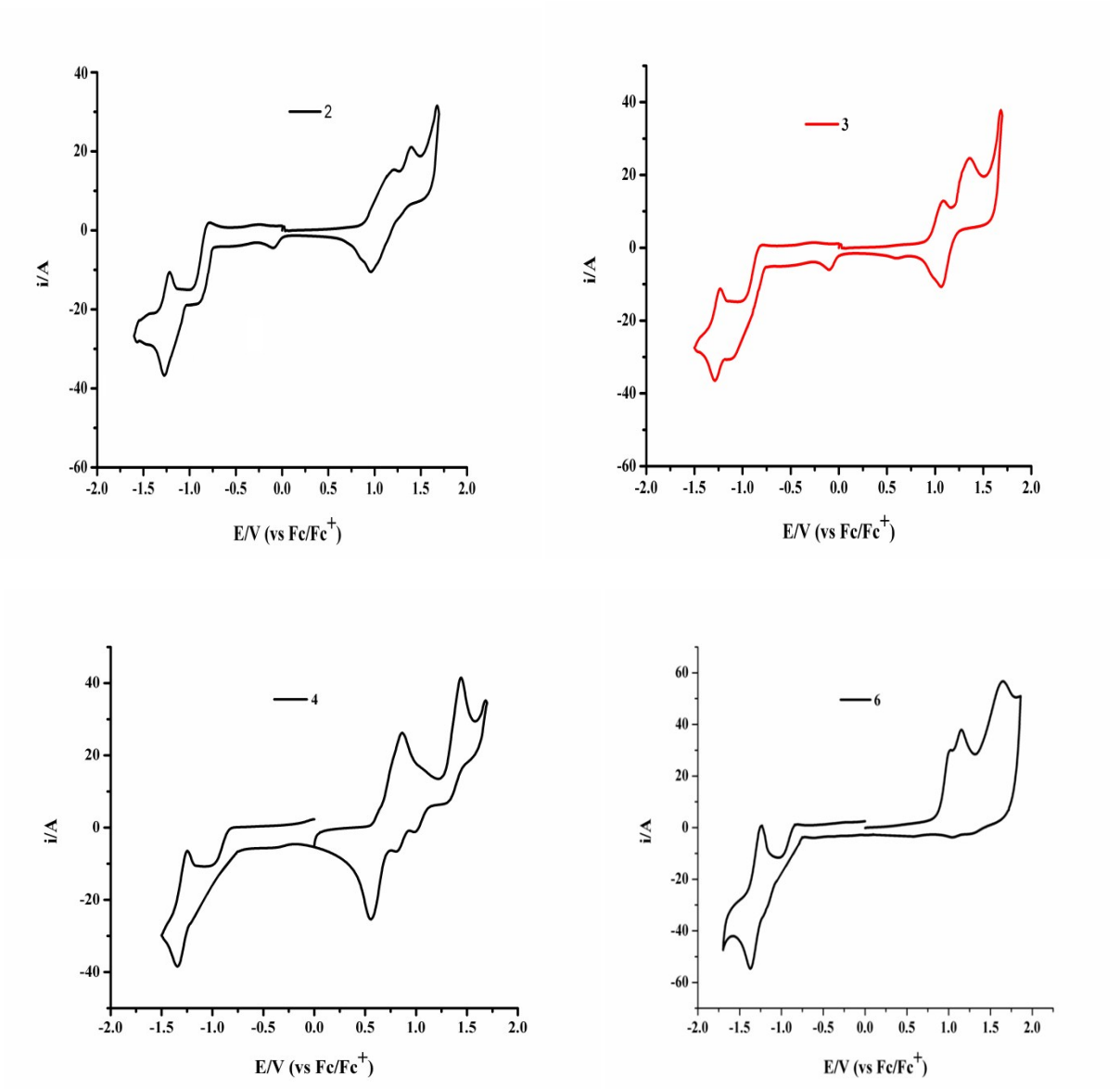


Dimethyl sulfoxide

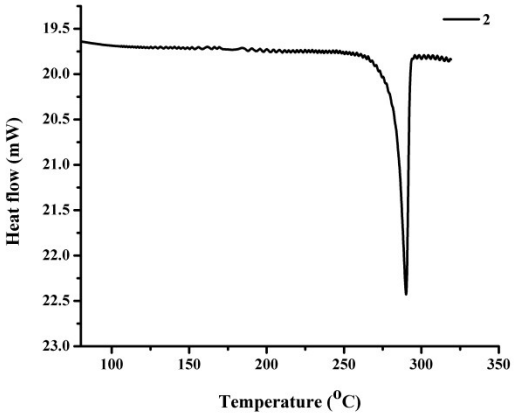


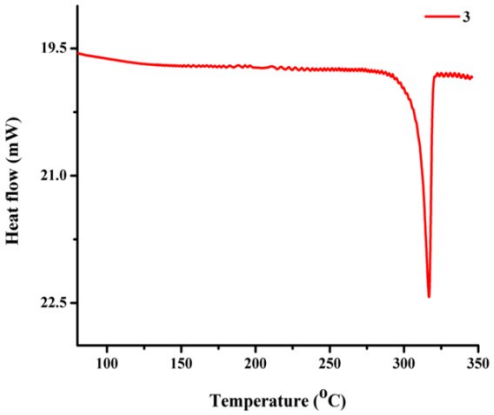
Methanol

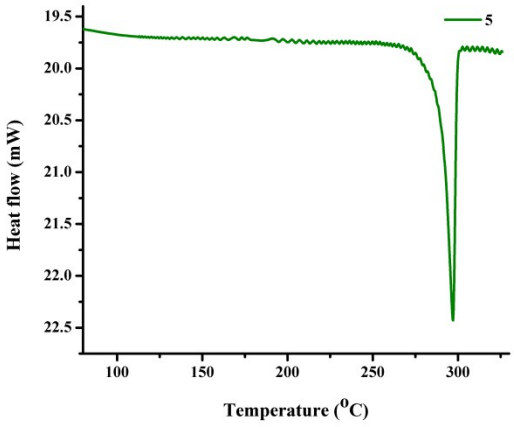
9. Cyclic voltammogram of compounds 2−6

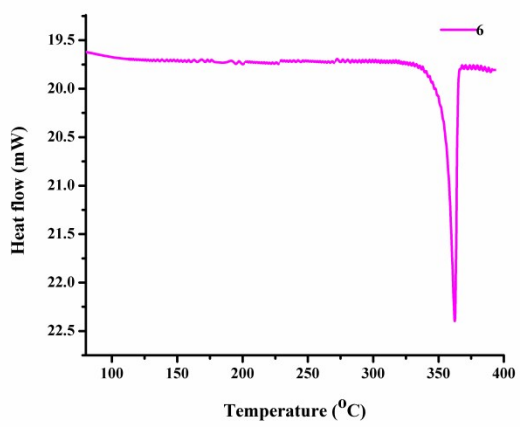


10. DSC Plots of compounds 2, 3, 5, 6.









11. Optimized structures of compounds of **2 6**

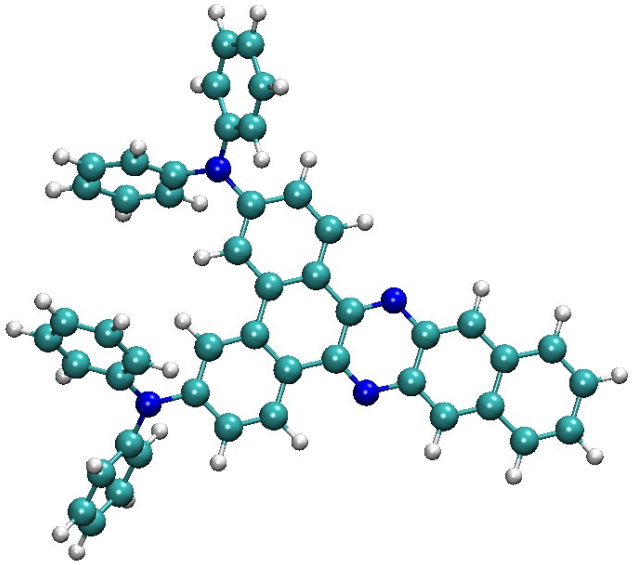


Fig. S18 Optimized structure of compound **2**

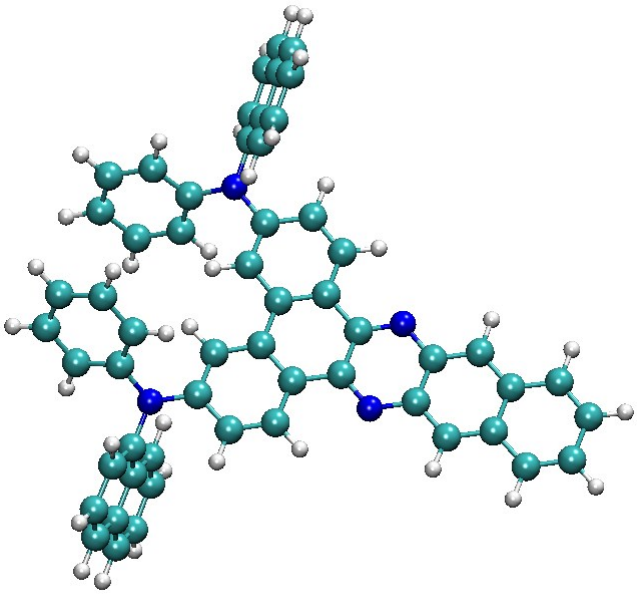


Fig. S19 Optimized structure of compound **3**

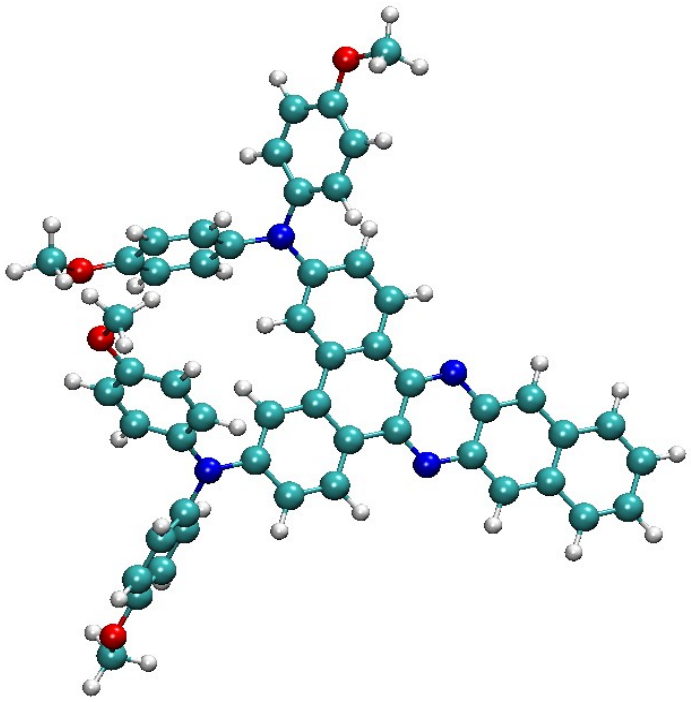


Fig. S20 Optimized structure of compound **4**

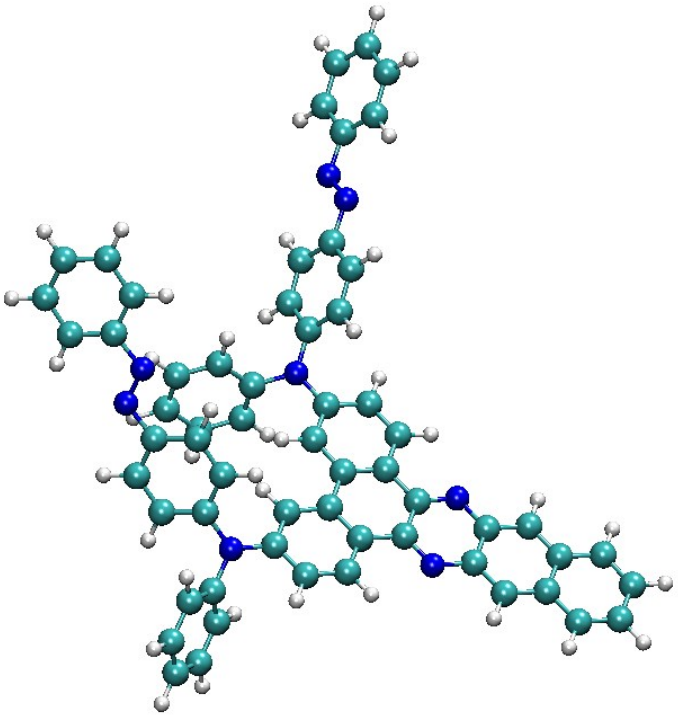


Fig. S21 Optimized structure of compound **5**

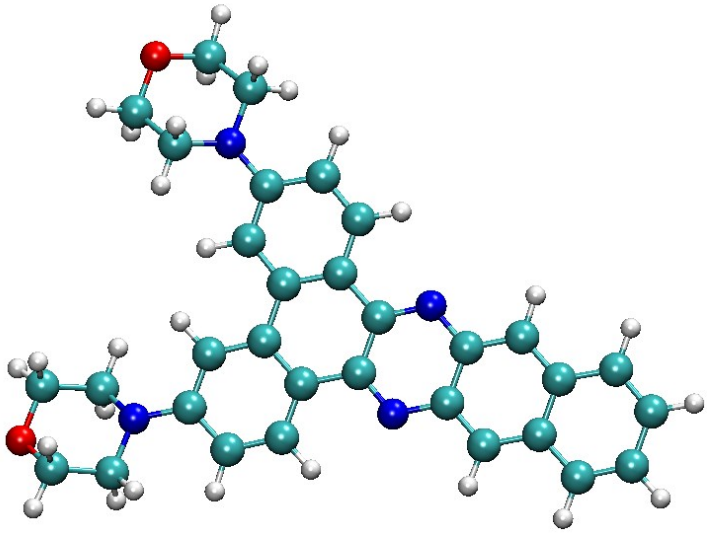


Fig. S22 Optimized structure of compound **6**

12. Cartesian coordinates and Mulliken and Lowdin charges of compounds **2 6**

Table S1. Cartesian coordinates and Mulliken and Lowdin charges of optimized structure of compound **2**

Total energy: 2067.36384755 Hartrees

Atom	Cartesian Coordinates			Mulliken charges	Lowdin charges
	x	y	z		
C	-1.86943	4.15878	3.408169	0.302431	0.071094
C	-1.91956	2.96258	2.685618	-0.18615	-0.09621
C	-2.99202	2.062106	2.812493	0.007546	-0.00174
C	-4.05861	2.400816	3.686471	-0.04266	-0.05447
C	-4.00655	3.615014	4.399622	-0.08397	-0.04084
C	-2.93681	4.48052	4.27452	-0.13368	-0.09487
C	-3.03836	0.793579	2.053196	0.008095	-0.00159
C	-4.13849	-0.08844	2.219388	-0.04351	-0.05494
C	-5.2309	0.250448	3.122752	0.064857	0.031062
C	-5.19454	1.502619	3.853176	0.064811	0.030998
C	-2.0081	0.419893	1.17224	-0.18661	-0.0969
C	-2.05185	-0.77648	0.449034	0.30603	0.071692
C	-3.15438	-1.64136	0.623191	-0.13577	-0.09554
C	-4.16827	-1.29741	1.496325	-0.08341	-0.04064
N	-6.24855	-0.59807	3.262038	-0.3738	-0.11413
C	-7.27669	-0.26257	4.11301	0.113334	0.006586
C	-7.24466	0.985444	4.8325	0.113169	0.006536
N	-6.18244	1.84685	4.678177	-0.37369	-0.11402
C	-8.35852	-1.13204	4.281447	-0.11993	-0.06505
C	-9.41692	-0.80687	5.140699	-0.00215	-0.02016
C	-9.38601	0.452165	5.863789	-0.00211	-0.0202
C	-8.29743	1.317819	5.690399	-0.11983	-0.06501
C	-10.5378	-1.67812	5.33312	-0.13093	-0.0662
C	-11.5609	-1.33676	6.178595	-0.15214	-0.07925
C	-11.5308	-0.09828	6.889268	-0.15216	-0.07927
C	-10.4783	0.765996	6.736109	-0.13096	-0.06621
N	-0.75512	5.033608	3.279952	-0.96833	-0.13351
N	-1.00795	-1.11385	-0.4556	-0.9681	-0.13356
C	-0.943	6.452743	3.309792	0.216049	0.055922
C	0.56637	4.502889	3.11768	0.208691	0.054636

C	-0.59954	-2.47798	-0.61193	0.211014	0.055345
C	-0.35679	-0.09591	-1.22628	0.209315	0.054694
C	1.435061	5.043689	2.156595	-0.11589	-0.09061
C	2.726814	4.535559	2.012862	-0.15948	-0.07258
C	3.164447	3.4747	2.810999	-0.13118	-0.08942
C	2.298409	2.93052	3.76444	-0.16231	-0.07341
C	1.011263	3.443712	3.925774	-0.11597	-0.09142
C	-0.06601	7.26886	4.04288	-0.12101	-0.09226
C	-0.24429	8.652434	4.061038	-0.16188	-0.07318
C	-1.30434	9.240818	3.364525	-0.13205	-0.09075
C	-2.18216	8.429548	2.639496	-0.16153	-0.07313
C	-2.00088	7.046621	2.601882	-0.11989	-0.09333
C	-0.37435	-3.0068	-1.89314	-0.11887	-0.09137
C	0.033633	-4.33244	-2.04383	-0.16191	-0.07323
C	0.208366	-5.15214	-0.9247	-0.13181	-0.0901
C	-0.02063	-4.62891	0.351413	-0.16205	-0.07327
C	-0.41301	-3.29951	0.511703	-0.11644	-0.09236
C	1.04153	-0.08742	-1.35021	-0.11619	-0.09048
C	1.672345	0.892289	-2.11811	-0.15926	-0.07252
C	0.922652	1.883239	-2.75827	-0.13126	-0.0894
C	-0.46985	1.880739	-2.6299	-0.16236	-0.0734
C	-1.10926	0.895025	-1.87766	-0.11629	-0.09164
H	-1.10356	2.745071	2.015717	0.215248	0.08932
H	-4.82565	3.842697	5.065074	0.179206	0.094732
H	-2.9068	5.397653	4.84399	0.179065	0.091008
H	-1.14969	1.057858	1.038543	0.216149	0.089239
H	-3.205	-2.56381	0.063964	0.179466	0.090995
H	-5.02178	-1.94405	1.633642	0.17912	0.094714
H	-8.35616	-2.06212	3.729304	0.167478	0.08987
H	-8.24774	2.261124	6.217305	0.167461	0.08987
H	-10.5591	-2.6164	4.793326	0.157475	0.084296
H	-12.4009	-2.00482	6.314097	0.149266	0.083196
H	-12.3487	0.152242	7.551645	0.14925	0.083191
H	-10.4539	1.705028	7.274492	0.157501	0.084306
H	1.094438	5.856161	1.530673	0.174885	0.089551
H	3.385841	4.961284	1.267782	0.150461	0.082683
H	4.163787	3.078706	2.692576	0.150736	0.081561
H	2.628166	2.11414	4.393324	0.151989	0.083324
H	0.348884	3.030979	4.67334	0.176523	0.089944
H	0.746127	6.815767	4.593365	0.176352	0.089587
H	0.438578	9.268926	4.630641	0.150848	0.082857

H	-1.44365	10.31301	3.386285	0.151268	0.081727
H	-3.00226	8.873087	2.090421	0.151674	0.083228
H	-2.67212	6.424346	2.02737	0.178164	0.089724
H	-0.52156	-2.37823	-2.75982	0.175827	0.089648
H	0.202652	-4.72741	-3.03688	0.151163	0.082979
H	0.518348	-6.1812	-1.04488	0.151437	0.081837
H	0.11858	-5.25135	1.225453	0.151918	0.08332
H	-0.57523	-2.89345	1.500024	0.177552	0.089777
H	1.623471	-0.84558	-0.84579	0.174659	0.089539
H	2.750856	0.887494	-2.20471	0.150484	0.082692
H	1.4148	2.644866	-3.34759	0.150778	0.081577
H	-1.06167	2.638312	-3.12648	0.15206	0.083348
H	-2.18659	0.886255	-1.79277	0.176674	0.089927

Table S2. Cartesian coordinates and Mulliken and Lowdin charges of optimized structure of compound **3**

Total energy: 2374.63457150 Hartrees

Atom	Cartesian Coordinates			Mulliken charges	Lowdin charges
	x	y	z		
C	-0.36366	6.628363	-3.04239	0.328925	0.073846
C	0.620423	5.646487	-2.86856	-0.19607	-0.10487
C	1.736469	5.554005	-3.71712	0.006329	-0.00076
C	1.873438	6.504779	-4.76336	-0.04303	-0.05805
C	0.888243	7.498312	-4.92076	-0.08167	-0.03655
C	-0.21231	7.565393	-4.08757	-0.14226	-0.10101
C	2.768108	4.508486	-3.53529	0.005978	-0.00075
C	3.878753	4.452574	-4.41893	-0.04205	-0.05805
C	4.020087	5.423003	-5.49705	0.065713	0.031665
C	3.016384	6.45674	-5.6662	0.065653	0.031623
C	2.674231	3.547807	-2.51428	-0.19597	-0.10498
C	3.651695	2.560705	-2.33314	0.329564	0.073969
C	4.748229	2.518032	-3.22138	-0.14226	-0.1011
C	4.847191	3.446126	-4.24077	-0.082	-0.03652
N	5.071261	5.345083	-6.31167	-0.3741	-0.11528
C	5.19511	6.272418	-7.32146	0.113219	0.006388
C	4.203271	7.304644	-7.48352	0.113029	0.006379
N	3.121396	7.365411	-6.63462	-0.37413	-0.11523

C	6.286436	6.217194	-8.19343	-0.12025	-0.06563
C	6.432705	7.154852	-9.2251	-0.00214	-0.02065
C	5.434759	8.197322	-9.38627	-0.00222	-0.02066
C	4.34274	8.244742	-8.50877	-0.12028	-0.06557
C	7.539947	7.12287	-10.1335	-0.13135	-0.06645
C	7.660785	8.052224	-11.1335	-0.15258	-0.08013
C	6.67976	9.077948	-11.2915	-0.15263	-0.08014
C	5.603674	9.146835	-10.4456	-0.1312	-0.06645
N	-1.48012	6.700889	-2.17031	-0.97053	-0.13554
N	3.531926	1.601597	-1.29501	-0.97009	-0.13584
C	4.176698	0.318038	-1.42113	0.114244	0.05609
C	2.906034	1.9189	-0.04506	0.216397	0.058328
C	-2.04695	5.526862	-1.57405	0.215705	0.05815
C	-2.17121	7.952806	-1.9876	0.116564	0.056109
C	-3.48055	8.073979	-2.4143	-0.09963	-0.08128
C	-4.19141	9.284063	-2.24436	-0.15949	-0.07872
C	-3.58119	10.37198	-1.66152	-0.10259	-0.06982
C	-2.23828	10.2892	-1.20034	-0.04066	-0.02223
C	-1.51474	9.055351	-1.34668	0.019635	-0.03005
C	-2.49039	5.56648	-0.24245	-0.11934	-0.0912
C	-3.07308	4.439777	0.338455	-0.15786	-0.07167
C	-3.21115	3.256377	-0.39231	-0.12884	-0.08977
C	-2.76877	3.213947	-1.71787	-0.16352	-0.07325
C	-2.19888	4.340812	-2.31148	-0.12536	-0.09672
C	5.204343	-0.01314	-0.55796	-0.09942	-0.08092
C	5.851039	-1.26734	-0.64487	-0.15954	-0.07873
C	5.47384	-2.17783	-1.60632	-0.10239	-0.06959
C	4.416209	-1.88191	-2.51002	-0.04047	-0.02227
C	3.737525	-0.61792	-2.41532	0.021304	-0.0299
C	2.080697	0.971326	0.581315	-0.11985	-0.09145
C	1.492531	1.256221	1.813991	-0.15783	-0.07164
C	1.706325	2.490949	2.433123	-0.12877	-0.08987
C	2.526304	3.436836	1.810562	-0.16366	-0.07324
C	3.131399	3.154087	0.585463	-0.12487	-0.09676
C	3.993921	-2.81613	-3.49757	-0.1657	-0.06932
C	2.945249	-2.53037	-4.34243	-0.13015	-0.07812
C	2.262996	-1.29338	-4.23338	-0.17361	-0.0755
C	2.649121	-0.36078	-3.2952	-0.05408	-0.06664
C	-1.5937	11.39386	-0.57538	-0.16578	-0.06938
C	-0.30523	11.28889	-0.10209	-0.13012	-0.07811
C	0.39847	10.06547	-0.22601	-0.17355	-0.07554

C	-0.19012	8.97703	-0.83252	-0.05304	-0.06654
H	0.505126	4.954824	-2.05011	0.22286	0.08773
H	1.012222	8.206661	-5.72601	0.178097	0.094577
H	-0.96116	8.328812	-4.23641	0.17897	0.09084
H	1.828482	3.550446	-1.84621	0.222653	0.087715
H	5.510081	1.763042	-3.0973	0.178639	0.090765
H	5.683851	3.426691	-4.92282	0.178079	0.094569
H	7.015072	5.430963	-8.04886	0.166797	0.089539
H	3.583544	9.009048	-8.60596	0.16681	0.089543
H	8.283127	6.344847	-10.0124	0.156816	0.083961
H	8.502721	8.015323	-11.812	0.14841	0.082746
H	6.793773	9.802111	-12.0872	0.148412	0.082745
H	4.85899	9.923793	-10.5642	0.156826	0.083964
H	-3.95906	7.227654	-2.88704	0.162354	0.090231
H	-5.21434	9.350509	-2.58964	0.150176	0.08467
H	-4.11764	11.30462	-1.54083	0.154502	0.083235
H	-2.37648	6.477758	0.327358	0.175078	0.08939
H	-3.409	4.484957	1.365979	0.149835	0.082564
H	-3.65652	2.382188	0.062545	0.150279	0.081346
H	-2.8796	2.306978	-2.29752	0.150791	0.082729
H	-1.8735	4.30787	-3.34132	0.178254	0.089208
H	5.513253	0.704097	0.189601	0.162135	0.090225
H	6.65341	-1.49852	0.042689	0.150257	0.084701
H	5.973843	-3.13493	-1.68446	0.154519	0.083254
H	1.905251	0.019993	0.099445	0.17522	0.089357
H	0.858211	0.516368	2.284034	0.149777	0.082539
H	1.243127	2.712509	3.384862	0.150235	0.081321
H	2.708593	4.392176	2.284904	0.150743	0.082712
H	3.77822	3.881987	0.117087	0.17815	0.089185
H	4.513775	-3.76342	-3.56932	0.155492	0.082493
H	2.634886	-3.24984	-5.08833	0.149046	0.083006
H	1.432351	-1.08149	-4.89322	0.148617	0.083789
H	2.123562	0.578741	-3.21692	0.191397	0.090961
H	-2.14109	12.32283	-0.47488	0.155446	0.082476
H	0.172491	12.13675	0.370421	0.149051	0.083002
H	1.40622	9.987377	0.159491	0.14863	0.083794
H	0.3524	8.048037	-0.92101	0.191298	0.090987

Table S3. Cartesian coordinates and Mulliken and Lowdin charges of optimized structure of compound **4**

Total energy: 2525.42118500 Hartrees

Atom	Cartesian Coordinates			Mulliken charges	Lowdin charges
	x	y	z		
C	-2.04378	3.738805	-4.50576	0.336478	0.076628
C	-1.16047	4.139275	-3.49475	-0.21784	-0.10916
C	-0.62474	5.436799	-3.44359	0.001218	0.000485
C	-1.0223	6.37601	-4.43043	-0.03735	-0.06102
C	-1.90588	5.964799	-5.44937	-0.08483	-0.04002
C	-2.40453	4.677856	-5.50085	-0.14461	-0.10349
C	0.320319	5.842637	-2.38066	-0.00015	0.000615
C	0.782321	7.183269	-2.32228	-0.03883	-0.06014
C	0.359275	8.157319	-3.31923	0.067216	0.031876
C	-0.5331	7.74692	-4.38906	0.067098	0.03197
C	0.798594	4.924157	-1.43097	-0.21171	-0.10765
C	1.687463	5.300239	-0.41628	0.333788	0.075733
C	2.110983	6.64816	-0.35089	-0.14545	-0.10312
C	1.669036	7.557365	-1.29225	-0.08476	-0.04009
N	0.812204	9.408058	-3.24311	-0.376	-0.1178
C	0.41937	10.31281	-4.20357	0.113174	0.00597
C	-0.46251	9.904722	-5.26746	0.113499	0.00623
N	-0.92301	8.608711	-5.32775	-0.37596	-0.11814
C	0.877266	11.63258	-4.1514	-0.12198	-0.06673
C	0.493721	12.56796	-5.12256	-0.00213	-0.02134
C	-0.39259	12.1561	-6.19635	-0.00177	-0.02117
C	-0.84929	10.83139	-6.24011	-0.12205	-0.06683
C	0.948862	13.92594	-5.09545	-0.13188	-0.06689
C	0.561034	14.82082	-6.05849	-0.15308	-0.08118
C	-0.31022	14.41562	-7.11488	-0.15302	-0.08108
C	-0.77087	13.12635	-7.17995	-0.13188	-0.0669
N	-2.55581	2.419908	-4.53365	-0.96453	-0.13308
N	2.152873	4.350221	0.52596	-0.96508	-0.13389
C	3.456232	4.470827	1.114508	0.202596	0.03565
C	1.368574	3.189642	0.842352	0.195287	0.036568
C	-3.84603	2.134648	-5.09196	0.208857	0.03696

C	-1.83145	1.346597	-3.90781	0.183147	0.030626
C	-2.44142	0.549577	-2.93449	-0.10423	-0.0749
C	-1.74283	-0.49494	-2.32055	-0.16512	-0.12979
C	-0.41118	-0.73663	-2.67155	0.259401	0.102811
C	0.20689	0.053712	-3.65108	-0.17945	-0.09656
C	-0.49895	1.078323	-4.26889	-0.08937	-0.07416
C	-4.96036	2.922025	-4.77874	-0.11175	-0.08008
C	-6.21748	2.635634	-5.32064	-0.17217	-0.13212
C	-6.37161	1.533411	-6.16658	0.252327	0.096317
C	-5.26595	0.729635	-6.47363	-0.17544	-0.09532
C	-4.01592	1.03203	-5.94877	-0.10676	-0.0749
C	3.623856	4.294682	2.499673	-0.10485	-0.07546
C	4.884193	4.384522	3.077149	-0.17522	-0.09529
C	6.002788	4.670284	2.283628	0.253378	0.097375
C	5.850833	4.852414	0.905664	-0.17211	-0.13117
C	4.582429	4.739475	0.327896	-0.10642	-0.07749
C	0.041605	3.318116	1.268258	-0.10218	-0.07382
C	-0.731	2.189245	1.556821	-0.1621	-0.12896
C	-0.16401	0.916803	1.440201	0.256634	0.097486
C	1.168431	0.777415	1.035384	-0.16348	-0.09215
C	1.924481	1.903504	0.732331	-0.10135	-0.07081
O	0.382879	-1.73381	-2.11452	-0.52891	-0.22816
O	7.217342	4.751656	2.962917	-0.52316	-0.22934
O	-0.8491	-0.27737	1.691513	-0.54481	-0.2311
O	-7.57671	1.148627	-6.75341	-0.52328	-0.22975
H	-0.90442	3.420557	-2.73437	0.223777	0.088506
H	-2.17705	6.690352	-6.20166	0.175675	0.09325
H	-3.067	4.383199	-6.30077	0.180143	0.089351
H	0.496721	3.891283	-1.48131	0.223833	0.088762
H	2.779727	6.96223	0.436459	0.179136	0.089352
H	1.990591	8.5875	-1.25592	0.175988	0.093353
H	1.537509	11.91163	-3.34129	0.165233	0.088771
H	-1.5109	10.49719	-7.02796	0.165271	0.088825
H	1.609617	14.2314	-4.29387	0.155835	0.083454
H	0.913403	15.84321	-6.02502	0.147419	0.082214
H	-0.60423	15.13726	-7.86542	0.14747	0.082235
H	-1.43154	12.81719	-7.98014	0.155904	0.083486
H	-3.4674	0.74562	-2.65558	0.16369	0.08774
H	-2.2362	-1.09252	-1.56935	0.172213	0.085943
H	1.232284	-0.16172	-3.91376	0.170159	0.093265
H	-0.02395	1.68265	-5.02902	0.170115	0.091374

H	-4.84654	3.765923	-4.11312	0.174596	0.09021
H	-7.05639	3.265504	-5.06517	0.171542	0.086532
H	-5.40994	-0.11412	-7.13264	0.169747	0.093347
H	-3.16243	0.416607	-6.19533	0.171363	0.091328
H	2.760608	4.086067	3.115668	0.168704	0.090154
H	5.027236	4.251224	4.139535	0.169644	0.093304
H	6.69939	5.065833	0.27311	0.17276	0.087184
H	4.469329	4.865319	-0.73959	0.175672	0.091233
H	-0.39197	4.303597	1.364469	0.171466	0.091405
H	-1.75497	2.318766	1.873299	0.173422	0.087099
H	1.585561	-0.21489	0.948203	0.176694	0.094369
H	2.948553	1.794136	0.405085	0.171401	0.092524
C	-2.20205	-0.20898	2.216777	-0.29409	-0.03043
C	8.424036	5.046662	2.212032	-0.29169	-0.02903
C	-8.76835	1.93344	-6.48891	-0.29134	-0.0291
C	-0.17736	-2.57858	-1.06867	-0.32173	-0.03734
H	-2.50095	-1.24071	2.370195	0.197975	0.08324
H	-2.22768	0.325186	3.168833	0.187046	0.070644
H	-2.88038	0.269088	1.506687	0.184648	0.067305
H	9.21923	5.064792	2.949747	0.200552	0.085114
H	8.629506	4.271549	1.470093	0.182193	0.067698
H	8.357104	6.019902	1.720212	0.182543	0.06803
H	-9.55807	1.448707	-7.0531	0.200405	0.084979
H	-9.01994	1.927156	-5.42567	0.1806	0.066836
H	-8.64991	2.963393	-6.83359	0.18254	0.067957
H	0.622466	-3.26244	-0.80411	0.193817	0.082963
H	-0.46412	-1.98737	-0.19751	0.226937	0.07517
H	-1.03334	-3.14665	-1.44111	0.173642	0.065139

Table S4. Cartesian coordinates and Mulliken and Lowdin charges of optimized structure of compound **5**

Total energy: 2748.34276402 Hartrees

Atom	Cartesian Coordinates			Mulliken charges	Lowdin charges
	x	y	z		
C	-1.59749	-7.28921	1.692705	0.305124	0.069725
C	-2.03284	-8.0678	2.768201	-0.19114	-0.09376

C	-1.38086	-9.25959	3.132385	0.01017	-0.00211
C	-0.23476	-9.65532	2.395621	-0.03997	-0.05124
C	0.190884	-8.86909	1.306262	-0.08256	-0.04037
C	-0.47518	-7.71256	0.948497	-0.1313	-0.09205
C	-1.8427	-10.0806	4.271477	0.003876	-0.00156
C	-1.11359	-11.2377	4.651483	-0.03877	-0.05111
C	0.070207	-11.6443	3.90304	0.067113	0.030413
C	0.503149	-10.8575	2.764889	0.065233	0.030404
C	-3.00486	-9.75496	4.992021	-0.18986	-0.09563
C	-3.42721	-10.5081	6.090978	0.306602	0.069256
C	-2.67699	-11.6401	6.474892	-0.13635	-0.09285
C	-1.55089	-11.9953	5.755973	-0.08135	-0.03936
N	0.729785	-12.7413	4.27217	-0.37264	-0.11204
C	1.839413	-13.1189	3.550992	0.113798	0.006842
C	2.27002	-12.3361	2.420237	0.112686	0.00686
N	1.574852	-11.2064	2.055026	-0.37228	-0.1116
C	2.554389	-14.2649	3.912728	-0.11854	-0.06403
C	3.686726	-14.6649	3.190308	-0.00167	-0.01934
C	4.120562	-13.8754	2.050918	-0.00258	-0.01936
C	3.398696	-12.7285	1.694488	-0.11845	-0.06367
C	4.4388	-15.834	3.53731	-0.13046	-0.06589
C	5.542914	-16.2035	2.814672	-0.15139	-0.07778
C	5.969642	-15.4268	1.694504	-0.15153	-0.0778
C	5.280809	-14.301	1.326267	-0.13016	-0.06557
N	-2.29104	-6.09463	1.34402	-0.9652	-0.12522
N	-4.60474	-10.1477	6.807976	-0.9677	-0.12496
C	-3.7212	-6.04187	1.494611	0.17191	0.047013
C	-1.59344	-4.93962	0.900178	0.262283	0.070433
C	-4.98298	-8.78526	6.963739	0.255609	0.06867
C	-5.46157	-11.1792	7.325112	0.183147	0.049865
C	-0.32634	-4.61326	1.420452	-0.13419	-0.10179
C	0.342345	-3.48077	0.972213	-0.12649	-0.05552
C	-0.23437	-2.6409	0.008425	0.059572	-0.03845
C	-1.50459	-2.95833	-0.50695	-0.05003	-0.05858
C	-2.17281	-4.09086	-0.06943	-0.13968	-0.09246
C	-4.31414	-5.01695	2.245595	-0.10059	-0.08281
C	-5.70151	-4.97129	2.393027	-0.16	-0.06935
C	-6.50613	-5.95069	1.803592	-0.12737	-0.08149
C	-5.91427	-6.97582	1.058911	-0.1659	-0.07407
C	-4.52871	-7.021	0.898084	-0.09729	-0.08518
C	-6.33569	-8.40675	6.880194	-0.13204	-0.0986

C	-6.69844	-7.07288	7.025708	-0.12312	-0.05524
C	-5.72804	-6.08569	7.246775	0.06183	-0.03719
C	-4.37534	-6.46175	7.346436	-0.05224	-0.06001
C	-4.0095	-7.79168	7.212808	-0.13752	-0.09224
C	-5.90726	-11.1211	8.653983	-0.10396	-0.08482
C	-6.74804	-12.1161	9.153901	-0.16343	-0.07251
C	-7.1393	-13.185	8.341643	-0.12805	-0.08354
C	-6.6884	-13.2477	7.019901	-0.16293	-0.07237
C	-5.86016	-12.2476	6.508142	-0.10392	-0.08649
N	-6.20658	-4.75585	7.354548	-0.26038	-0.05479
N	-5.31534	-3.84747	7.506519	-0.26865	-0.06297
C	-5.80204	-2.51192	7.613627	0.043502	-0.02439
C	-7.16168	-2.15636	7.588726	-0.04508	-0.0714
C	-7.52432	-0.81689	7.695487	-0.15236	-0.07638
C	-6.54219	0.175328	7.827897	-0.14024	-0.06999
C	-5.19015	-0.17904	7.854776	-0.14619	-0.07931
C	-4.8209	-1.52015	7.748774	-0.117	-0.0662
N	0.535758	-1.51501	-0.37587	-0.25858	-0.0536
N	0.006987	-0.74138	-1.25006	-0.26851	-0.06341
C	0.790813	0.385801	-1.63441	0.045141	-0.02309
C	2.062867	0.683295	-1.11613	-0.04356	-0.07028
C	2.741848	1.812531	-1.56428	-0.15213	-0.0765
C	2.163762	2.651648	-2.52771	-0.14091	-0.0712
C	0.898312	2.35544	-3.04279	-0.14668	-0.08037
C	0.213045	1.225045	-2.59677	-0.11703	-0.06676
H	-2.88452	-7.7198	3.329903	0.216124	0.090343
H	1.052832	-9.20472	0.749757	0.181883	0.096005
H	-0.14281	-7.13189	0.100843	0.182865	0.092267
H	-3.6046	-8.91001	4.696118	0.222928	0.090214
H	-2.98613	-12.2243	7.328972	0.1802	0.091958
H	-0.97008	-12.8618	6.034039	0.180467	0.095736
H	2.209025	-14.8335	4.765482	0.16852	0.090412
H	3.698998	-12.1218	0.850929	0.169386	0.090799
H	4.114405	-16.4217	4.386691	0.158472	0.084796
H	6.100943	-17.0889	3.088531	0.150618	0.083929
H	6.844135	-15.7363	1.137961	0.150828	0.084022
H	5.603056	-13.7111	0.477582	0.158972	0.085049
H	0.120709	-5.24251	2.175478	0.185679	0.092145
H	1.312965	-3.2144	1.365786	0.162392	0.089518
H	-1.93637	-2.31169	-1.25545	0.17539	0.091614
H	-3.14212	-4.3387	-0.47683	0.182745	0.091602

H	-3.68882	-4.26919	2.712678	0.177201	0.092473
H	-6.14923	-4.18186	2.981241	0.162593	0.088257
H	-7.58016	-5.91686	1.924823	0.154764	0.0839
H	-6.53036	-7.73453	0.59502	0.15434	0.084366
H	-4.06832	-7.80688	0.315761	0.172635	0.090303
H	-7.08939	-9.15664	6.691576	0.181506	0.092264
H	-7.73172	-6.76488	6.952383	0.161369	0.088971
H	-3.63753	-5.69812	7.539569	0.177288	0.092173
H	-2.97196	-8.07846	7.304198	0.185113	0.092107
H	-5.59251	-10.3013	9.284119	0.176059	0.091005
H	-7.0862	-12.0625	10.18007	0.155632	0.085176
H	-7.78545	-13.9585	8.733599	0.155112	0.083893
H	-6.98973	-14.0681	6.382351	0.155611	0.085121
H	-5.52152	-12.2885	5.482554	0.177433	0.091196
H	-7.90078	-2.93604	7.486659	0.174591	0.088329
H	-8.5702	-0.54011	7.67692	0.154337	0.082923
H	-6.83164	1.214473	7.910076	0.155099	0.083159
H	-4.43042	0.583874	7.957229	0.155251	0.084354
H	-3.78485	-1.82692	7.765961	0.162509	0.08723
H	2.48878	0.023817	-0.37574	0.175099	0.0888
H	3.721339	2.043596	-1.16674	0.153738	0.082632
H	2.697345	3.527669	-2.87172	0.153602	0.082368
H	0.449757	3.000528	-3.78616	0.153044	0.083213
H	-0.76632	0.968502	-2.97478	0.160945	0.086516

Table S5. Cartesian coordinates and Mulliken and Lowdin charges of optimized structure of compound **6**

Total energy: 1605.64834179 Hartrees

Atom	Cartesian Coordinates			Mulliken charges	Lowdin charges
	x	y	z		
C	-2.06344	0.485868	-0.33247	0.374937	0.077209
C	-2.20396	0.751756	1.040202	-0.21778	-0.11399
C	-3.44386	1.036723	1.632476	-0.00493	0.003626
C	-4.59921	1.063939	0.806708	-0.05119	-0.06247
C	-4.45889	0.804863	-0.56831	-0.08766	-0.03392

C	-3.23043	0.517497	-1.13403	-0.16398	-0.11931
C	-3.57238	1.321318	3.081192	-0.00481	0.003801
C	-4.85381	1.587538	3.632605	-0.05159	-0.06272
C	-6.04236	1.602002	2.79038	0.071253	0.032294
C	-5.91308	1.34866	1.368076	0.070771	0.032247
C	-2.46033	1.325529	3.937295	-0.21822	-0.11457
C	-2.5645	1.590786	5.313499	0.377129	0.077447
C	-3.8531	1.855569	5.838279	-0.16517	-0.11965
C	-4.96057	1.846061	5.010687	-0.08815	-0.03379
N	-7.22975	1.851141	3.339885	-0.37679	-0.11719
C	-8.34206	1.871317	2.52841	0.113968	0.006341
C	-8.21218	1.630226	1.11389	0.113621	0.006306
N	-6.97613	1.369434	0.565955	-0.37672	-0.11711
C	-9.60304	2.127959	3.074238	-0.12091	-0.06614
C	-10.747	2.157103	2.264387	-0.00209	-0.02078
C	-10.6155	1.917822	0.838294	-0.00208	-0.02079
C	-9.34753	1.659611	0.299076	-0.12089	-0.0661
C	-12.0515	2.417024	2.796016	-0.13153	-0.06661
C	-13.1543	2.441294	1.982508	-0.15258	-0.08017
C	-13.0249	2.20673	0.579832	-0.15261	-0.08018
C	-11.7962	1.953679	0.027869	-0.13148	-0.06659
N	-1.42428	1.570813	6.138658	-0.66596	-0.19042
N	-0.7972	0.219396	-0.88652	-0.66594	-0.19099
C	-0.60686	0.197213	-2.34549	-0.18532	-0.04848
C	0.837655	0.561754	-2.68727	-0.10472	0.026234
O	1.780851	-0.31139	-1.99797	-0.46354	-0.28802
C	1.606045	-0.22275	-0.55232	-0.09749	0.024042
C	0.184584	-0.61478	-0.16462	-0.20272	-0.04074
C	-1.56058	1.615892	7.60376	-0.18538	-0.04858
C	-0.35641	0.943774	8.262443	-0.10548	0.026146
O	0.894944	1.53925	7.808582	-0.46326	-0.28787
C	1.027369	1.420436	6.360654	-0.09797	0.024057
C	-0.13639	2.114368	5.662117	-0.20196	-0.04087
H	-1.31465	0.773084	1.648047	0.198999	0.07498
H	-5.3519	0.820158	-1.17528	0.176637	0.093974
H	-3.17953	0.289937	-2.18765	0.170043	0.083527
H	-1.49036	1.080877	3.537434	0.20029	0.074929
H	-3.98255	2.09553	6.882203	0.170122	0.083482
H	-5.94263	2.057186	5.407086	0.17662	0.093989
H	-9.67154	2.304554	4.1392	0.165722	0.089
H	-9.22047	1.476058	-0.75932	0.165739	0.089008

H	-12.1479	2.595068	3.85966	0.15649	0.083781
H	-14.1332	2.639233	2.398529	0.148426	0.08275
H	-13.9078	2.230659	-0.04499	0.148428	0.08275
H	-11.6963	1.775267	-1.03539	0.1565	0.083784
H	-1.2671	0.930042	-2.8061	0.196208	0.085126
H	-0.84377	-0.79118	-2.76507	0.183452	0.064904
H	1.032694	1.603254	-2.40848	0.170348	0.060737
H	1.03244	0.42749	-3.7486	0.184877	0.077232
H	1.821627	0.798411	-0.21783	0.167061	0.058688
H	2.333987	-0.90809	-0.12444	0.182007	0.076442
H	0.05251	-0.50349	0.907965	0.181203	0.078779
H	0.02531	-1.67405	-0.41196	0.186878	0.068876
H	-2.46006	1.078359	7.898732	0.196305	0.085125
H	-1.64432	2.65102	7.965167	0.183832	0.065097
H	-0.35654	-0.12735	8.031525	0.170563	0.060805
H	-0.37571	1.082127	9.340807	0.185085	0.07739
H	1.059581	0.361455	6.080317	0.167217	0.058873
H	1.974397	1.893015	6.110843	0.182103	0.076543
H	-0.0493	1.982091	4.587414	0.181051	0.078745
H	-0.08785	3.192719	5.87027	0.187023	0.068996