Novel electroluminescent donor-acceptors based on dibenzo[*a,c*]phenazine as hole transport materials for organic electronics

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1. 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	510	12965	2.40	0.53
3	508	11370	2.38	0.38
4	540	14054	2.34	0.51
5	—	—	—	—
6	494	14239	2.47	0.50

[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	562	14779	2.26	0.49
3	552	12371	2.29	0.32
4	—	—	—	—
5	—	—	—	—
6	538	15082	2.27	0.50

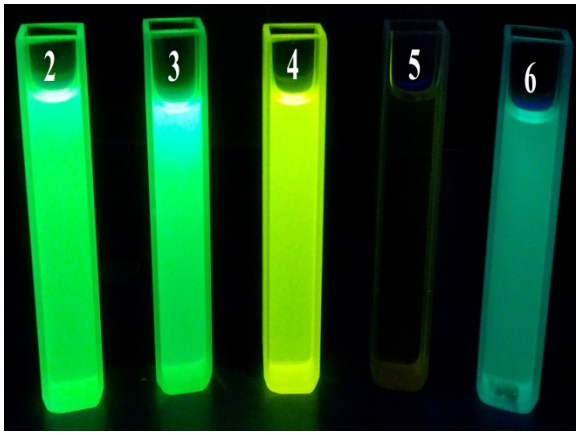
[a]Recorded in10^{-5} M dichloromethane.

c. Photophysical data of compounds **2** **6** in dimethyl sulfoxide (DMSO).

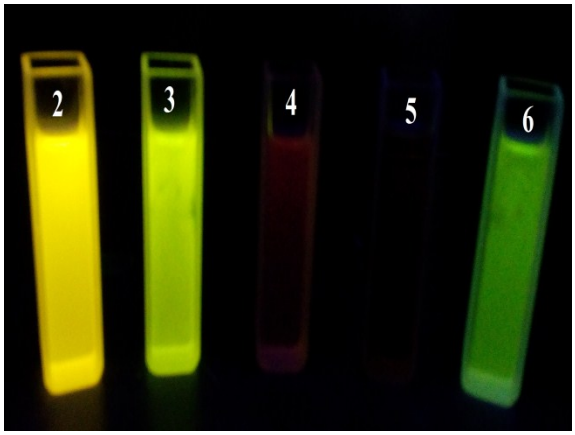
Compound	λ_{emi}[a] **nm**	**Stokes shift cm^{-1}**	E_g^{opt} **(eV)**	ϕ_F
2	587	15537	2.21	0.54
3	563	12633	2.24	0.55
4	—	—	—	—
5	—	—	—	—
6	565	11816	2.25	0.65

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

2. Emission of compounds 2 6 in various solvents under UV light (365 nm)

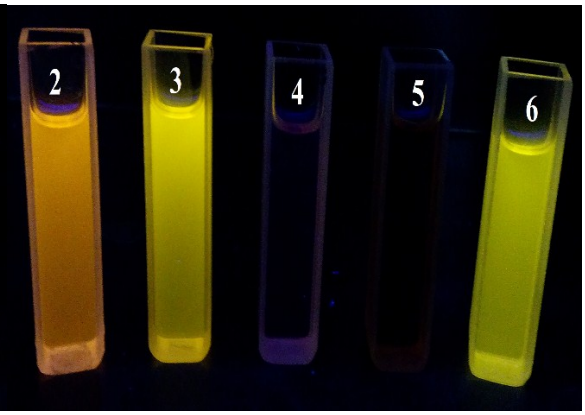


Cyclohexane



Dichloromethane

Toluene



Dimethyl sulfoxide

3. Absorption and emission spectra of compound 1in toluene

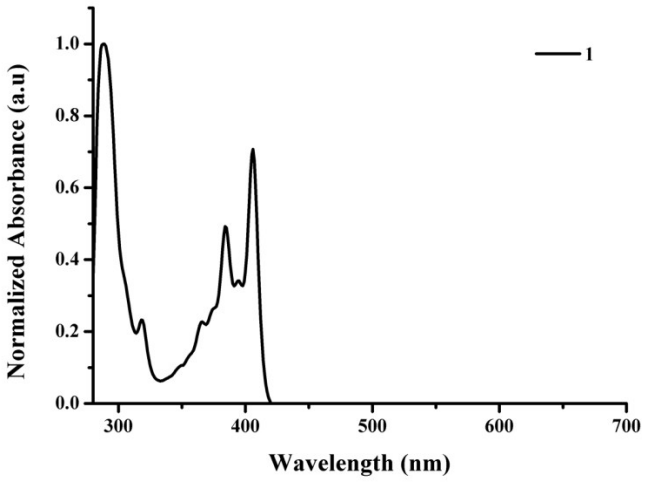


Fig. S1 Absorption spectra of **1** in toluene

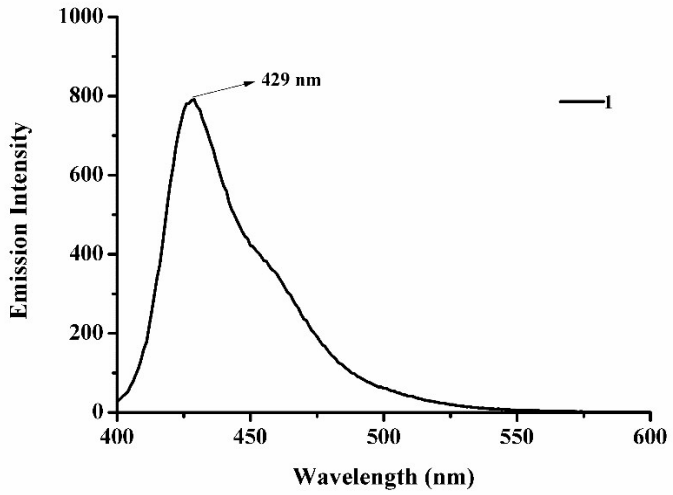
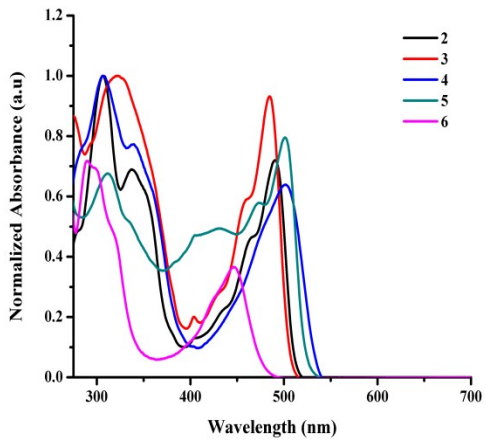


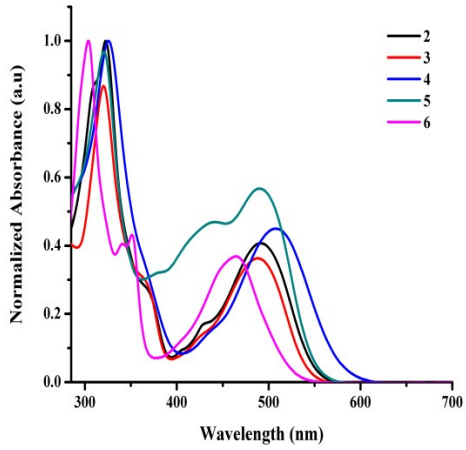
Fig. S2 Emission spectra of **1** in toluene

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

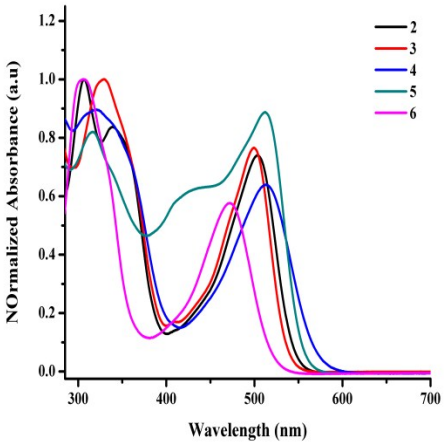
a. Absorption spectra of compound 2 6



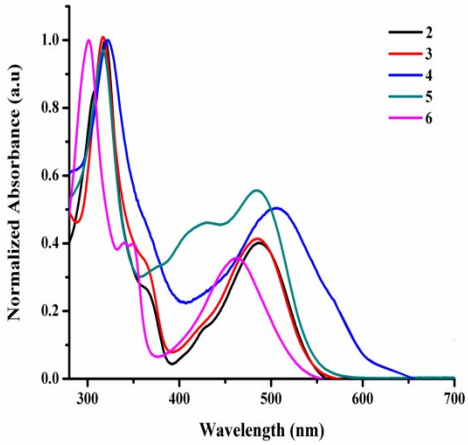
(**a**) Cyclohexane



(**b**) Dichloromethane

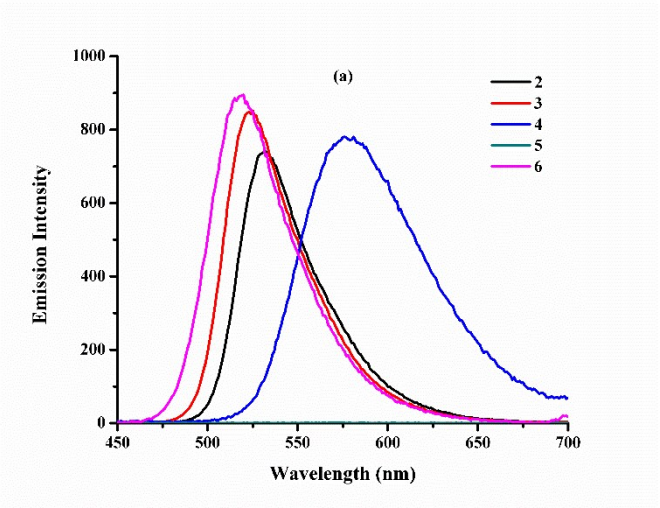


(**c**)Dimethyl sulfoxide

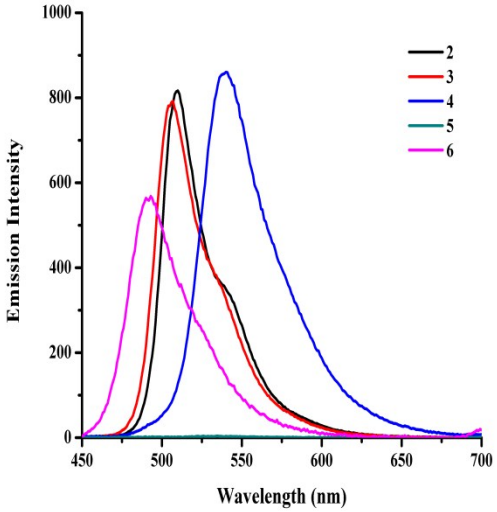


(**d**) Methanol

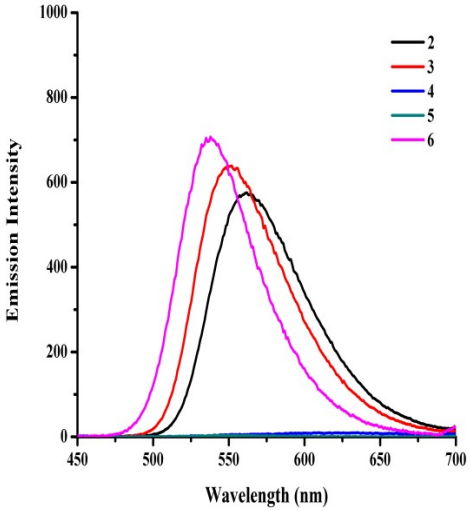
b. Emission spectra of compounds 2 6



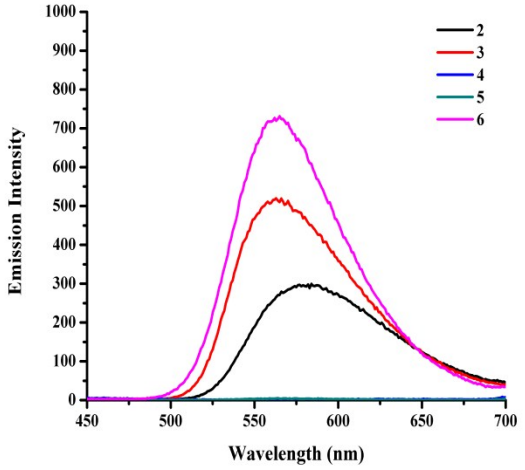
(a) Toluene



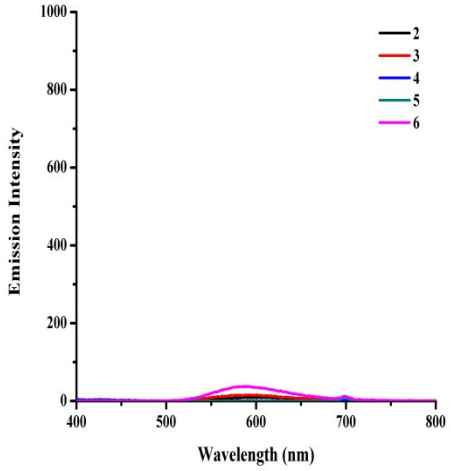
(**b**) Cyclohexane



(**c**) Dichloromethane

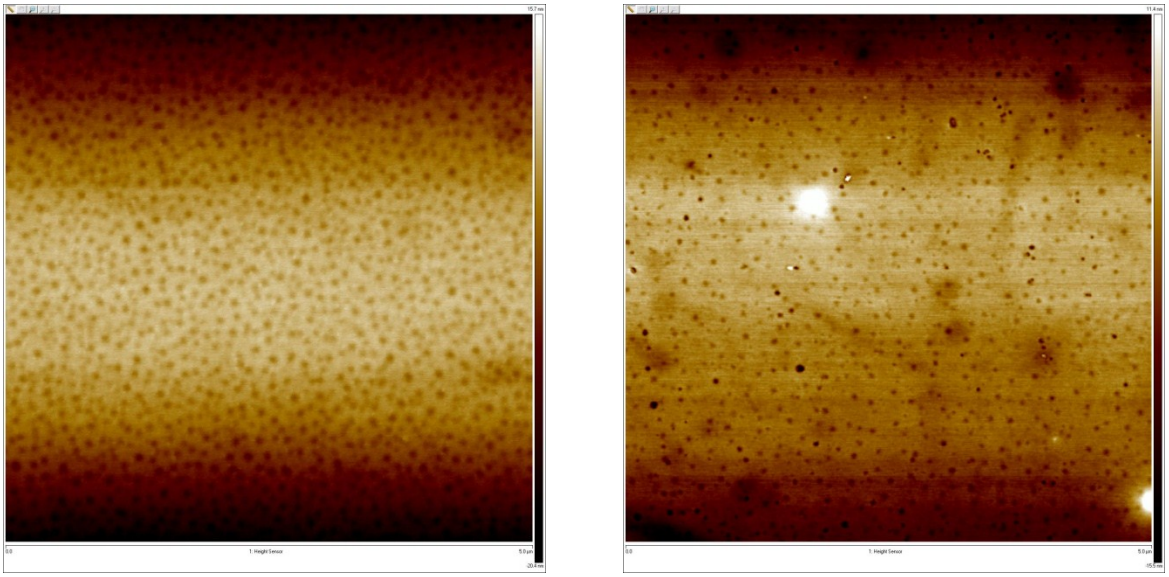


(**d**) Dimethyl sulfoxide

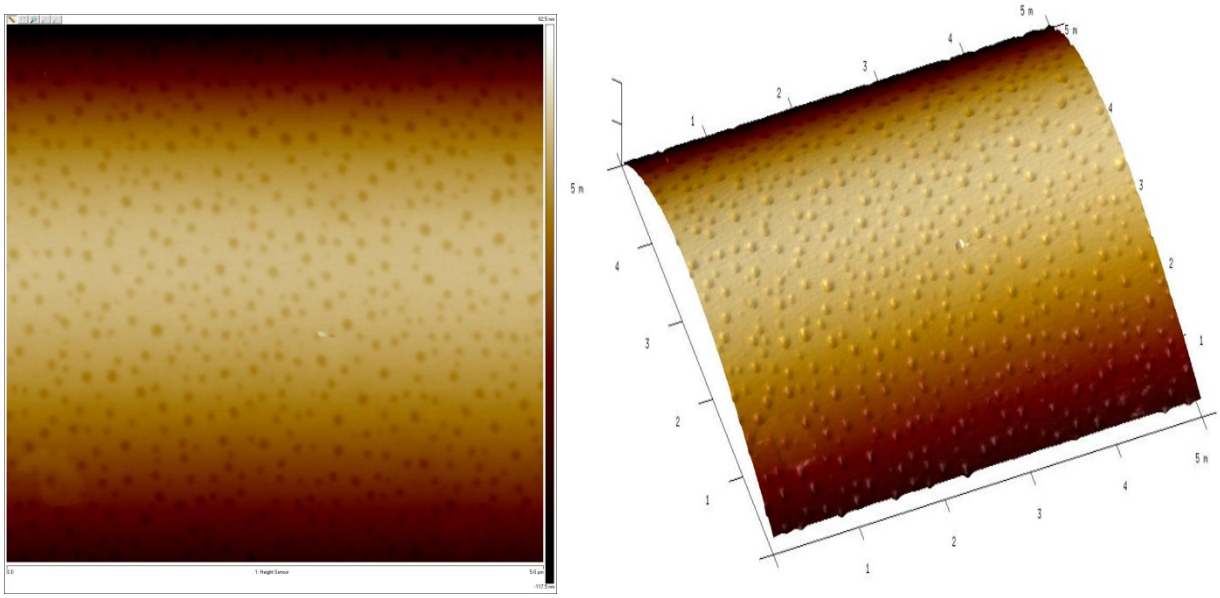


(**e**) Methanol

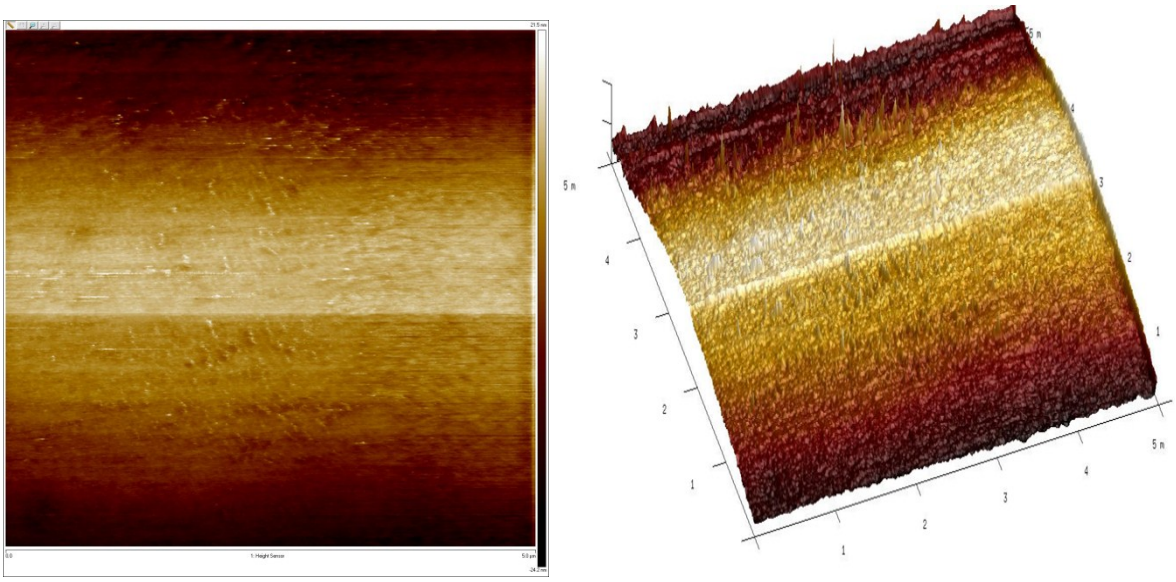
5. Tapping mode AFM topographical image of compound **2 6**



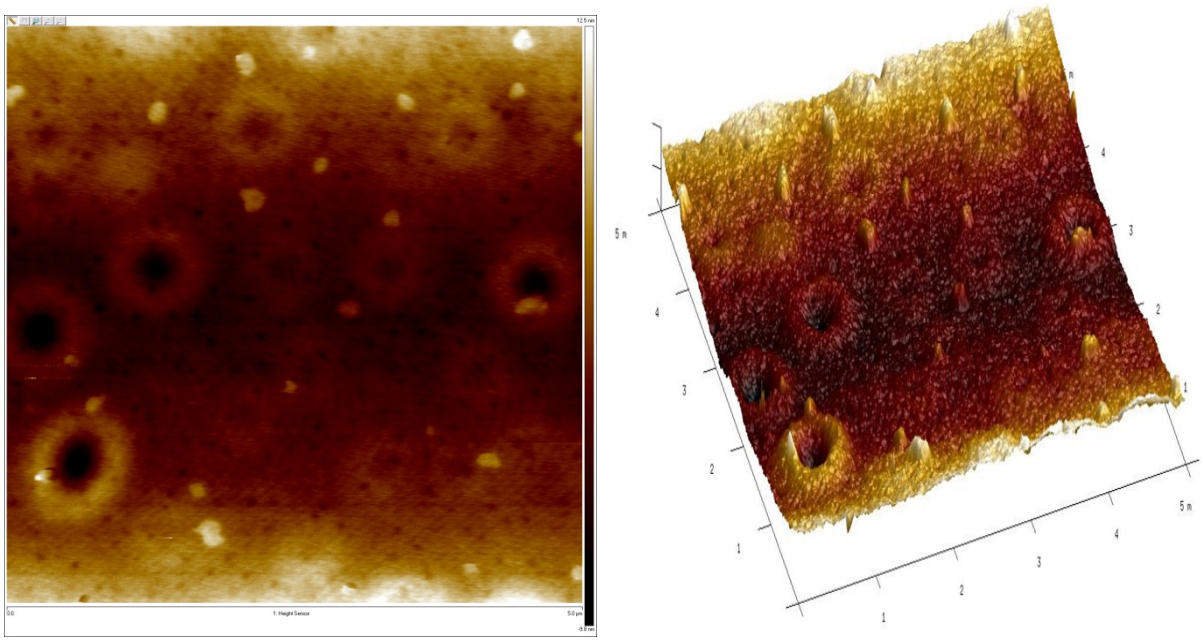
AFM topographical image (2D) of compound **2** and **3**



AFM topographical image **2D** (left) and **3D** (right) of compound **4**

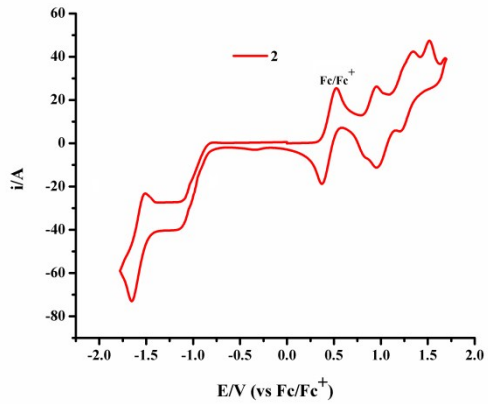


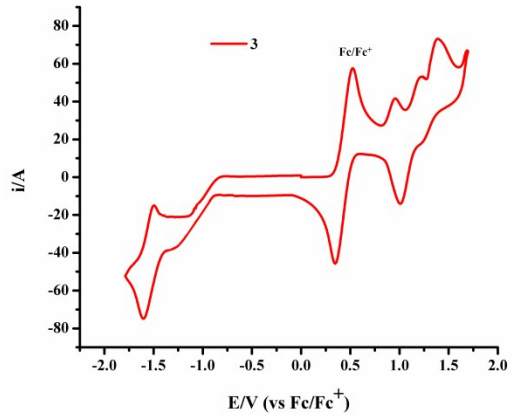
AFM topographical image **2D** (left) and **3D** (right) of compound **5**

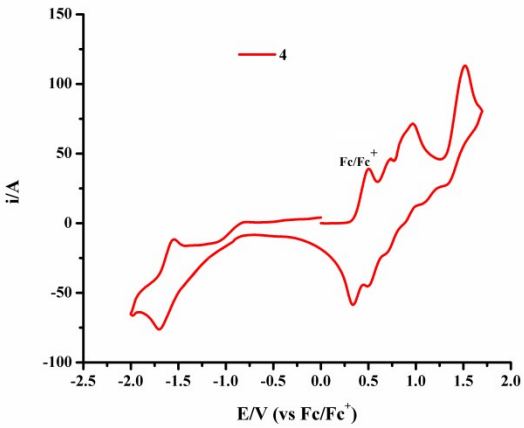


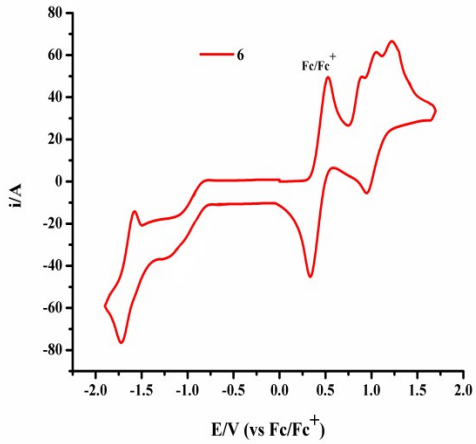
AFM topographical image **2D** (left) and **3D** (right) of compound **6**

6. Cyclic Voltammogram of compounds **2 6**

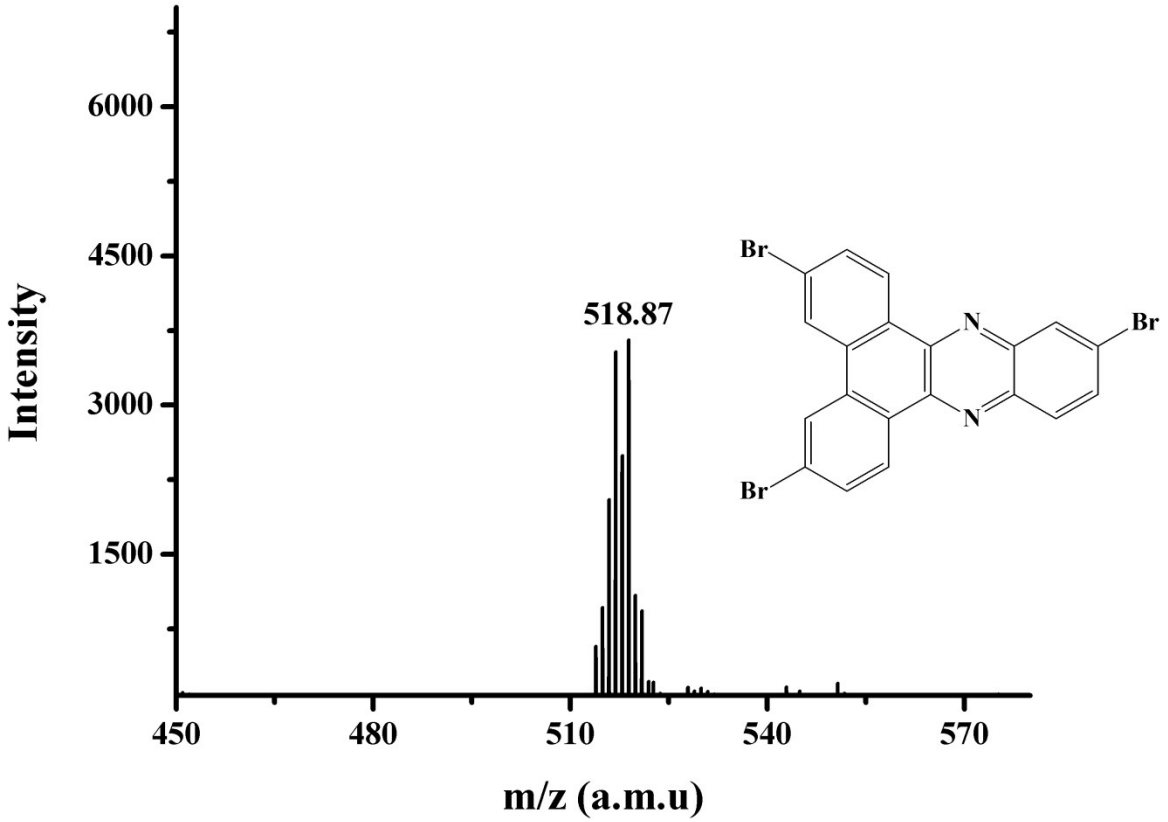








6. Mass spectra of compound 1



7. HRMS spectra of compounds 2 6.

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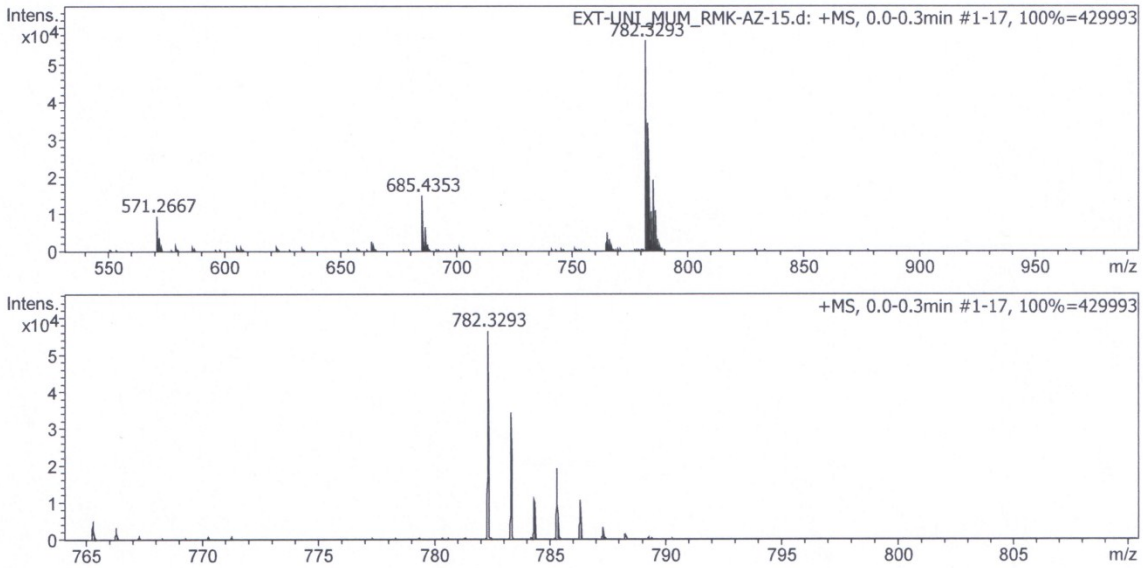
Analysis Info

Analysis Name	D:\Data\JULY-2016\EXT-UNI_MUM_RMK-AZ-15.d	Acquisition Date	7/25/2016 5:31:38 PM
Method	Tune_pos_NAF-1500.m	Operator	raf out
Sample Name	EXT-UNI_MUM_RMK-AZ-15	Instrument	maXis impact 282001.00081
Comment	C56H39N5		

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
782.3293	1	C56H40N5	782.3278	-1.9	19.9	1	100.00	39.5	even	ok

Fig. S3 HRMS Spectra of compound **2**

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Analysis Info

Analysis Name	D:\Data\JULY-2016\EXT-UNI_MUM_RMK-AZ-16.d	Acquisition Date	7/25/2016 5:44:47 PM
Method	Tune_pos_NAF-1500.m	Operator	raf out
Sample Name	EXT-UNI_MUM_RMK-AZ-16	Instrument	maXis impact 282001.00081
Comment	C68H45N5		

Acquisition Parameter

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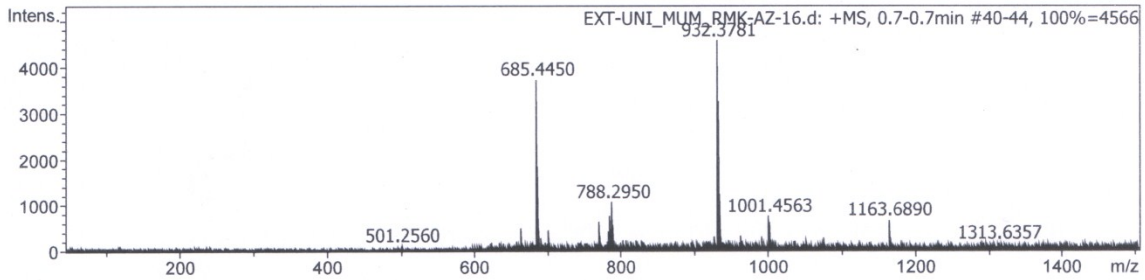
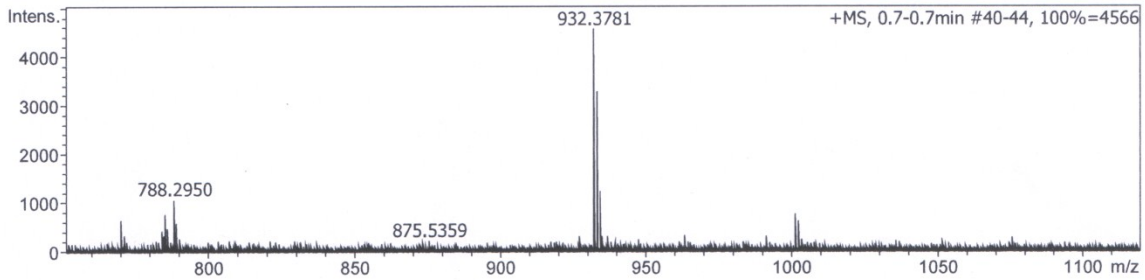
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
932.3781	1	C68H46N5	932.3646	0.9	717.9	1	100.00	45.5	even	ok

Fig. S4 HRMS Spectra of compound **3**

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Analysis Info

Analysis Name	D:\Data\JULY-2016\EXT-UNI_MUM-RMK-AZ-17.d	Acquisition Date	8/1/2016 4:19:42 PM
Method	Tune_pos_NAICSI-1500.m	Operator	gkl-in
Sample Name	EXT-UNI_MUM-RMK-AZ-17	Instrument	maXis impact 282001.00081
Comment	C62H51N5O6		

Acquisition Parameter

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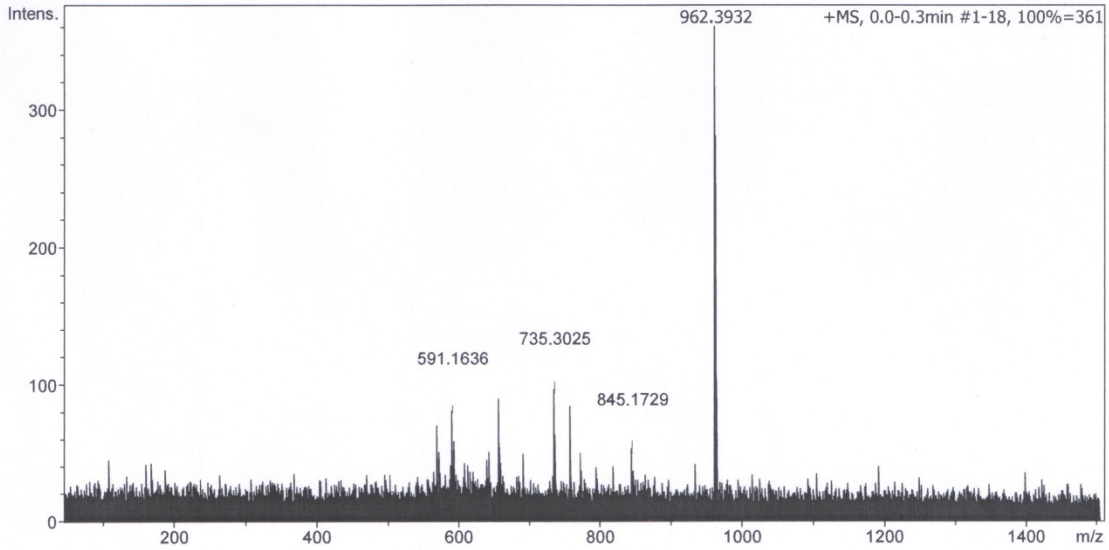
Scan End	1500 m/z	Set Collision Cell RF	2100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
962.3932	1	C62H52N5O6	962.3912	-2.0	48.4	1	100.00	39.5	even	ok

Fig. S5 HRMS Spectra of compound **4**

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

Analysis Info

Analysis Name	D:\Data\JULY-2016\EXT-UNI_MUM-RMK-AZ-18.d	Acquisition Date	8/1/2016 4:40:58 PM
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Sample Name	EXT-UNI_MUM-RMK-AZ-18	Instrument	maXis impact 282001.00081
Comment	C74H51N11		

Acquisition Parameter

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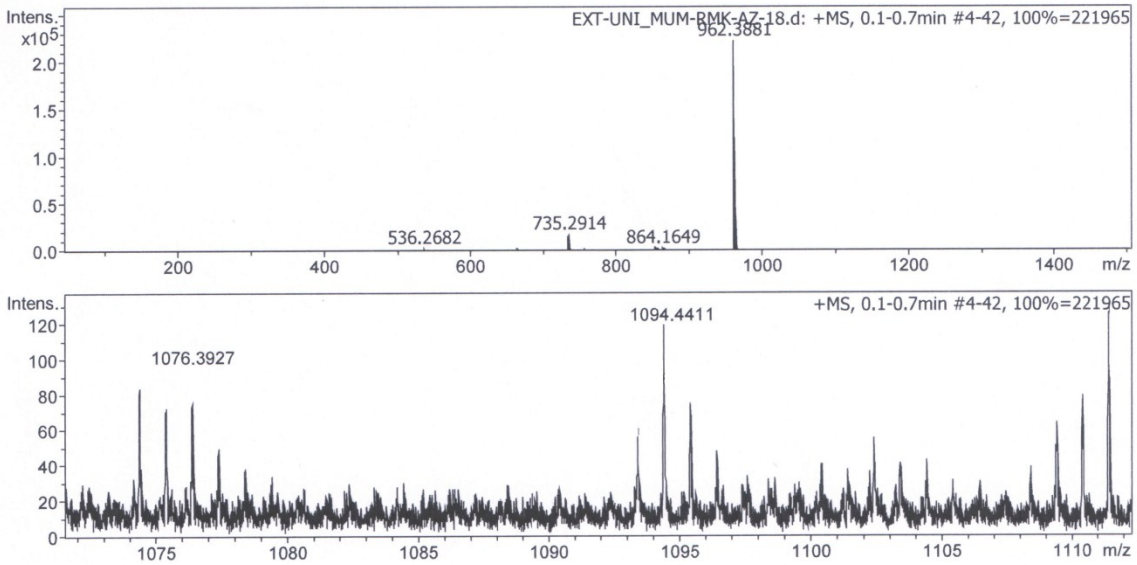
Scan End	1500 m/z	Set Collision Cell RF	2100.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
1094.4411	1	C74H52N11	1094.4323	-5.2	n.a.	n.a.	n.a.	55.0	odd	ok

Fig. S6 HRMS Spectra of compound **5**

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Analysis Info

Analysis Name	D:\Data\JULY-2016\EXT-UNI_MUM-RMK-AZ-19.d	Acquisition Date	8/1/2016 4:34:43 PM
Method	Tune_pos_NAICSI-1500.m	Operator	gkl-in
Sample Name	EXT-UNI_MUM-RMK-AZ-19	Instrument	maXis impact 282001.00081
Comment	C32H33N5O3		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
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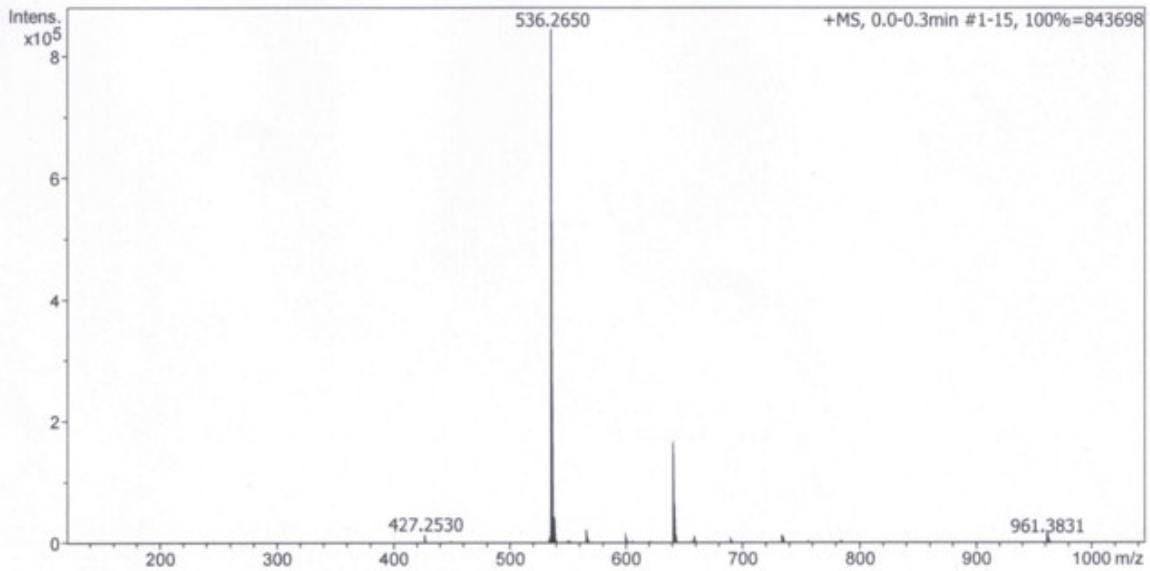
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
536.2650	1	C32H34N5O3	536.2656	1.1	32.4	1	100.00	18.5	even	ok

Fig. S7 HRMS Spectra of compound **6**

8. FTIR Spectra of compounds 1 6

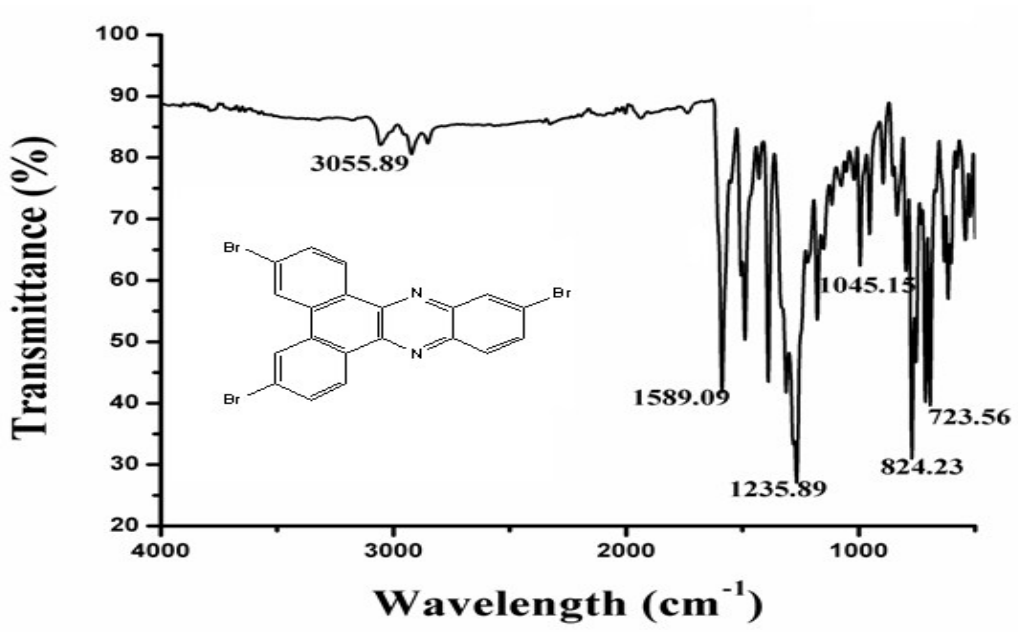


Fig. S8 FTIR Spectra of compound **1**

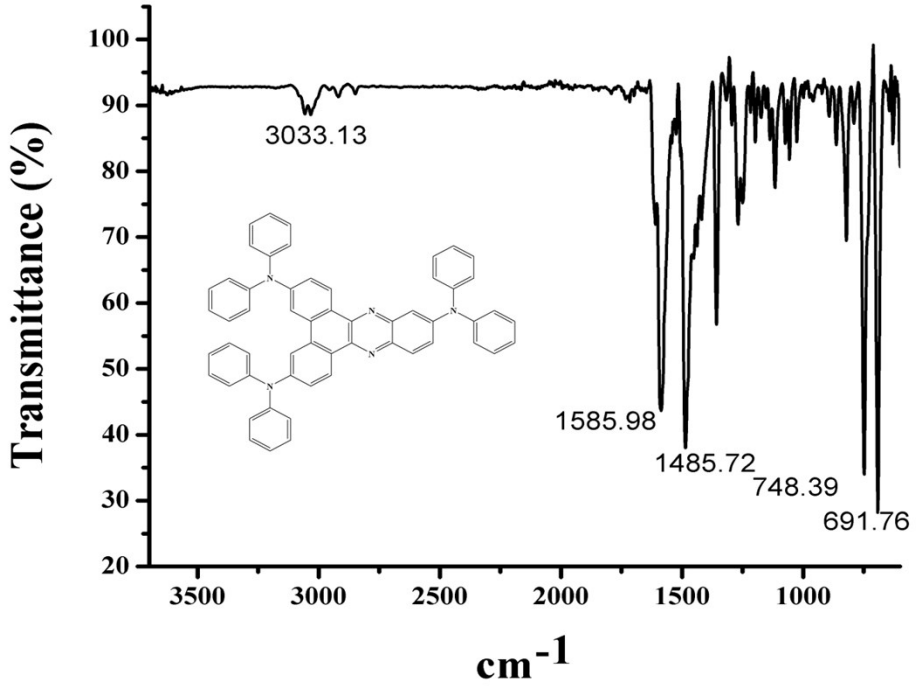


Fig. S9 FTIR Spectra of compound **2**

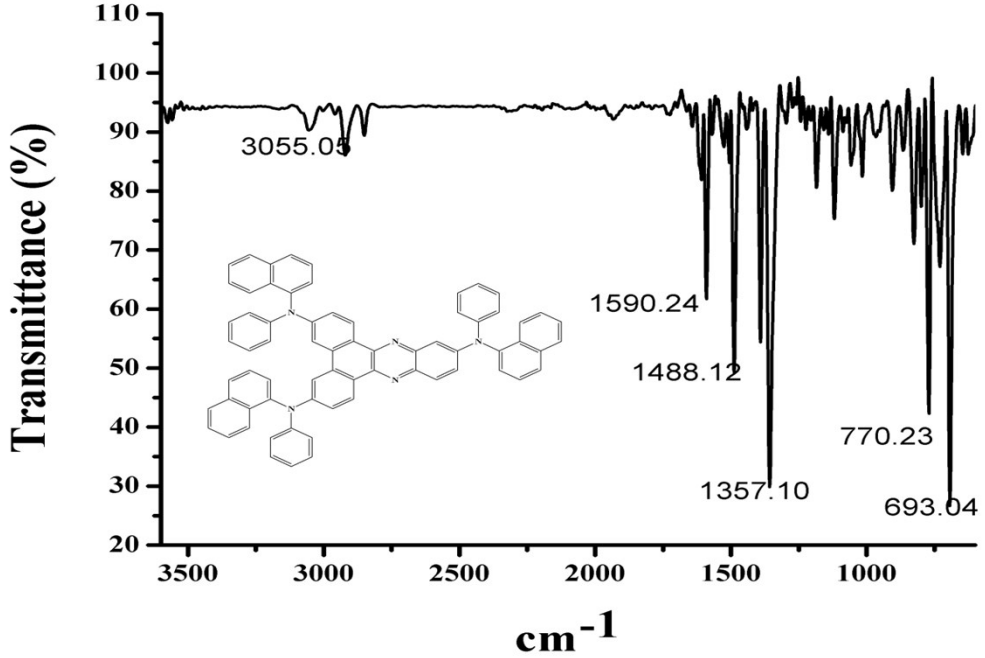


Fig. S10 FTIR Spectra of compound **3**

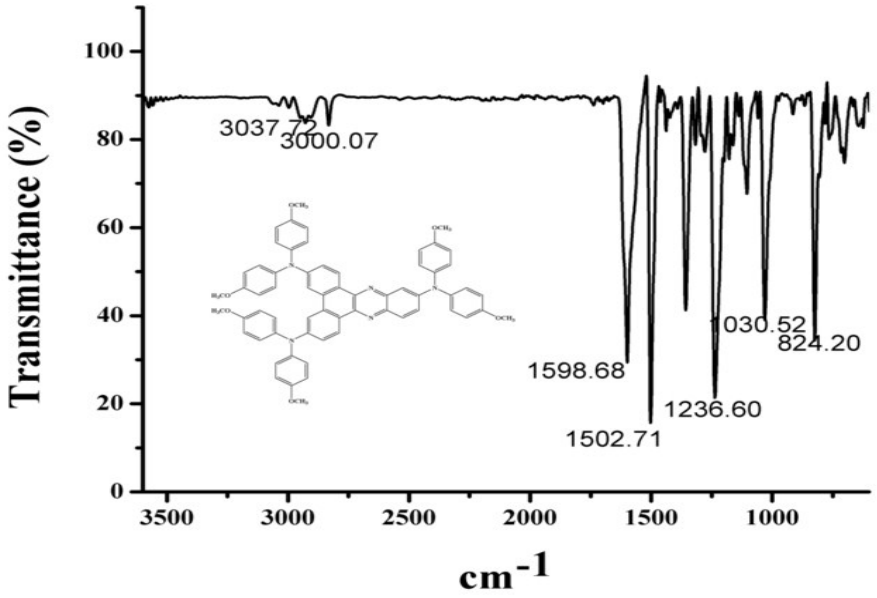


Fig. S11 FTIR Spectra of compound **4**

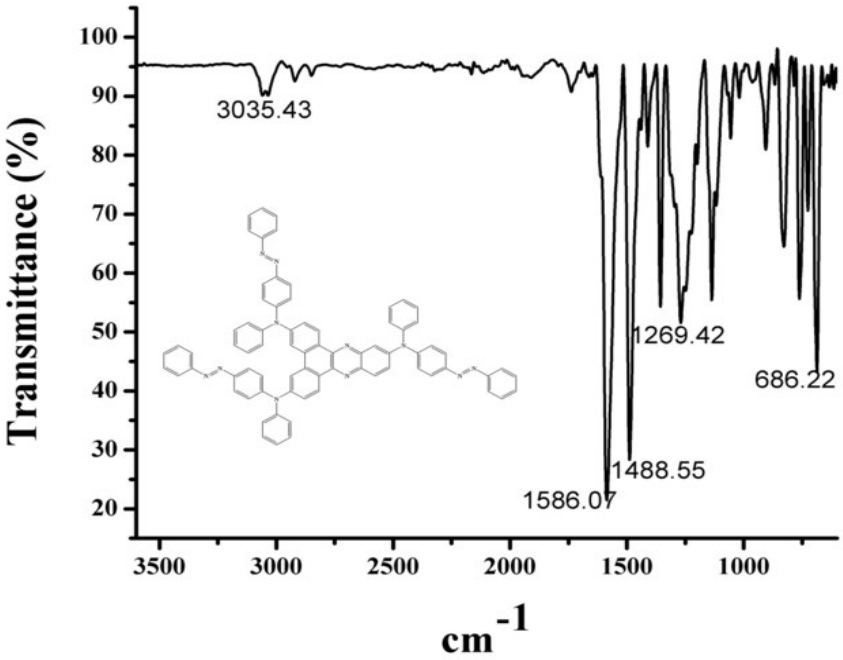


Fig. S12 FTIR Spectra of compound **5**

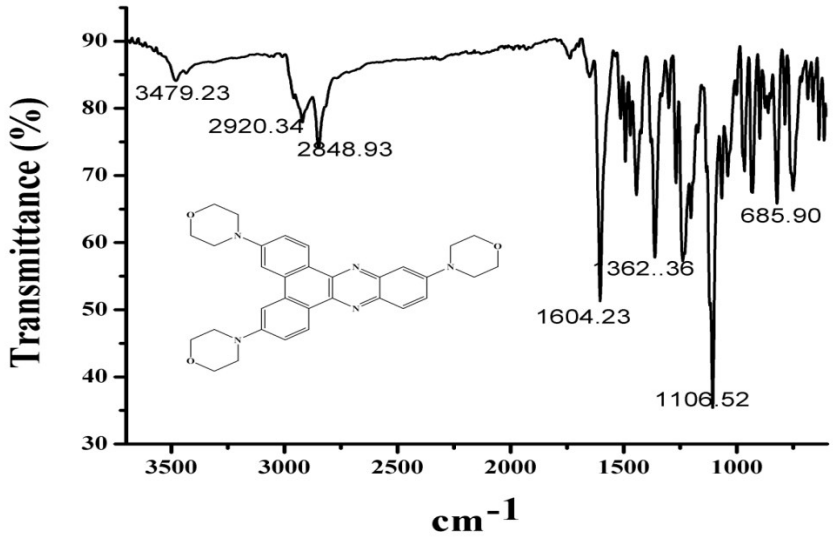


Fig. S13 FTIR Spectra of compound **6**

9. ^{1}H and ^{13}C NMR spectra of compounds 1 6

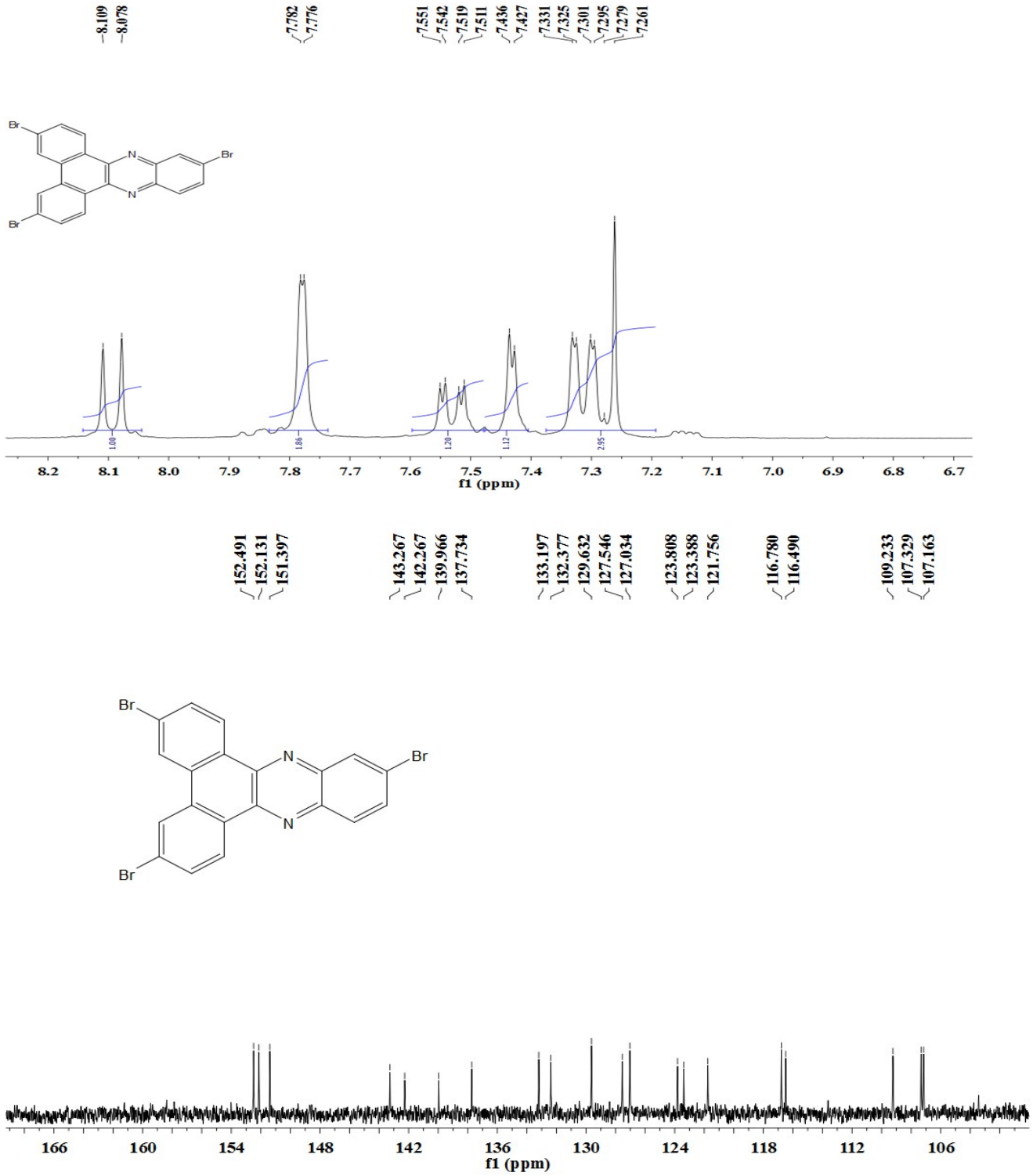


Fig. S14 ^{1}H and ^{13}C NMR spectra of compound **1** in $CDCl_3$.

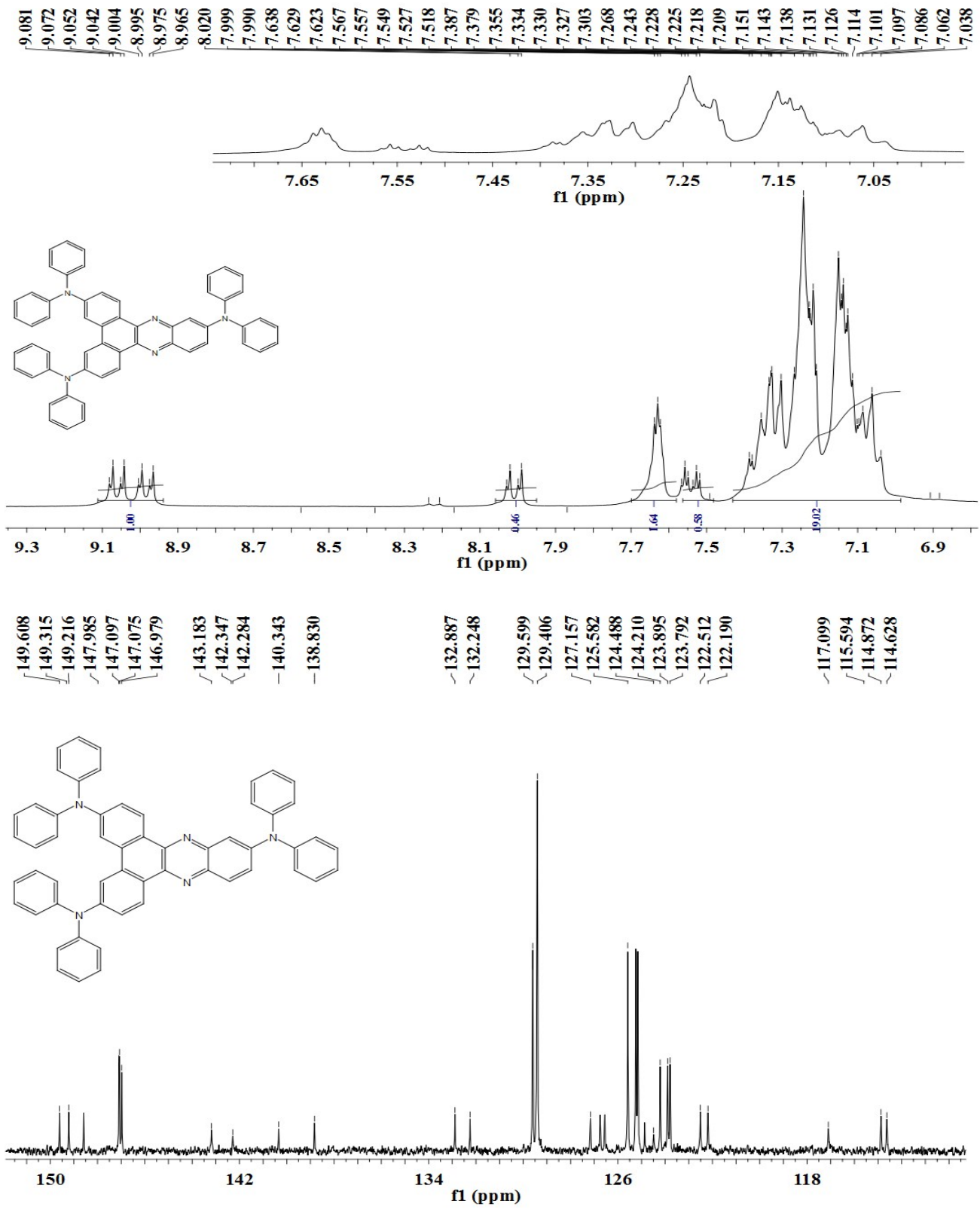


Fig. S15 ^{1}H and ^{13}C NMR spectra of compound **2** in $CDCl_3$.

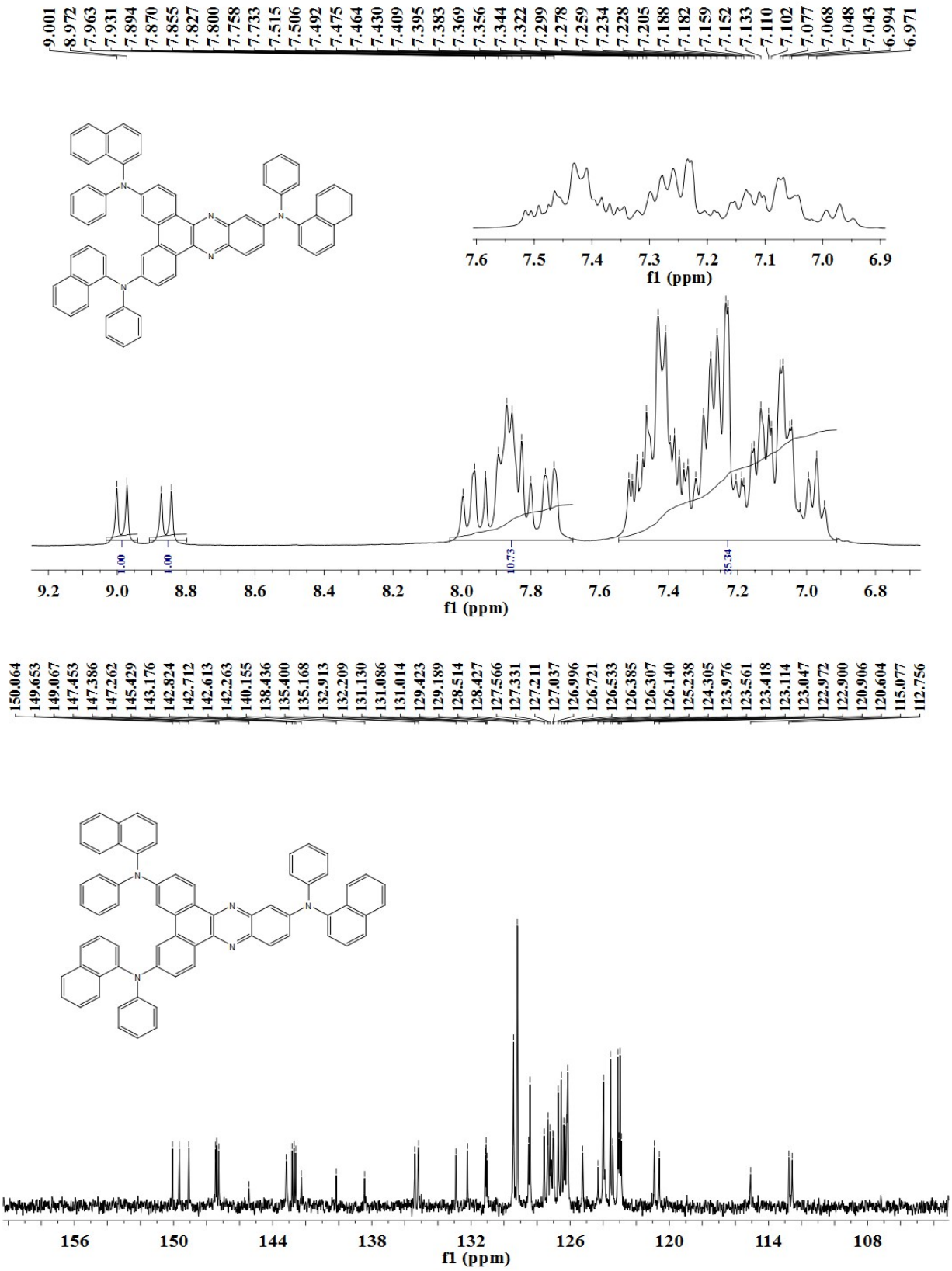


Fig. S16 ^{1}H and ^{13}C NMR spectra of compound **3** in $CDCl_3$.

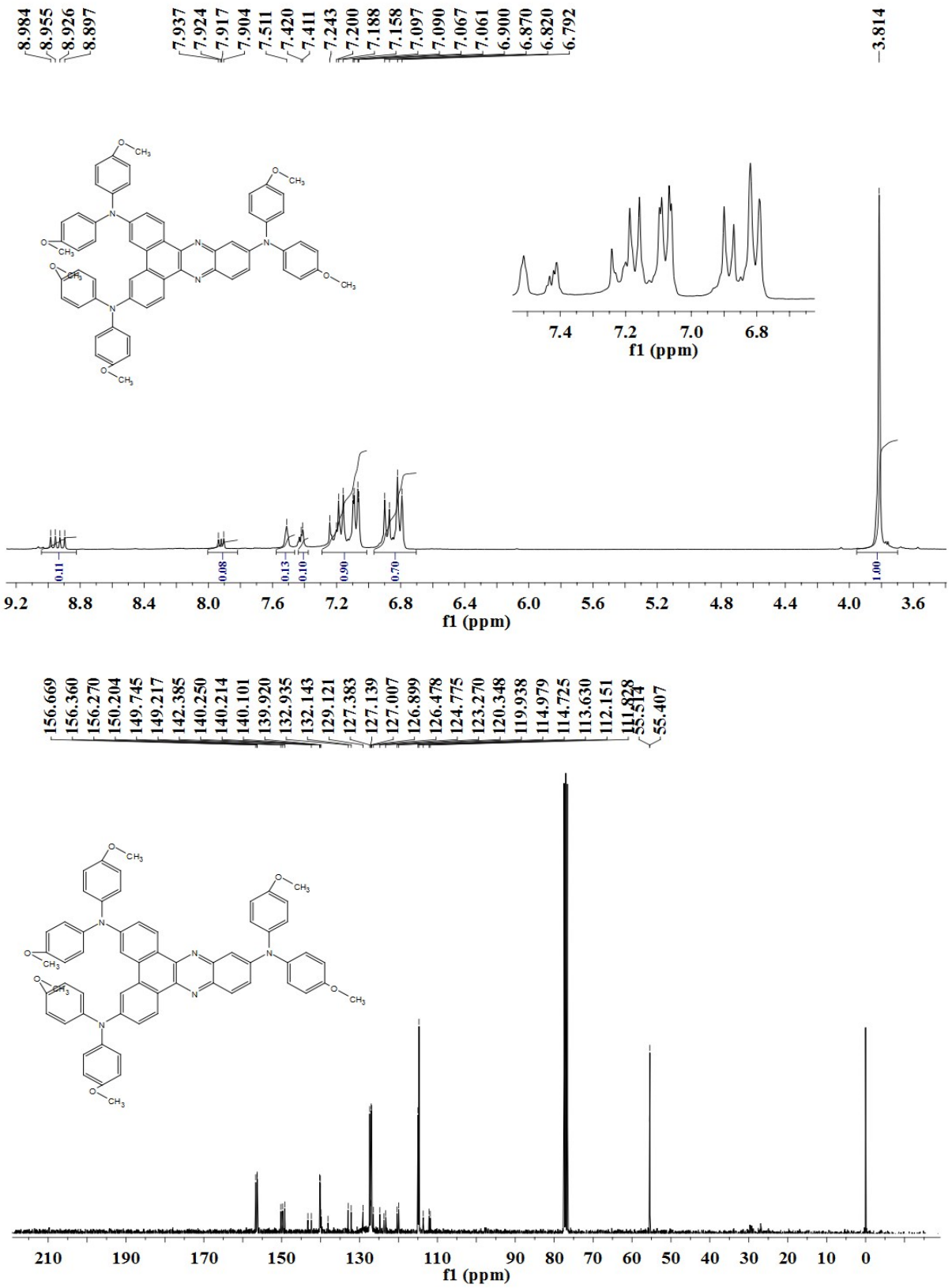


Fig. S17 ^{1}H and ^{13}C NMR spectra of compound **4** in $CDCl_3$.

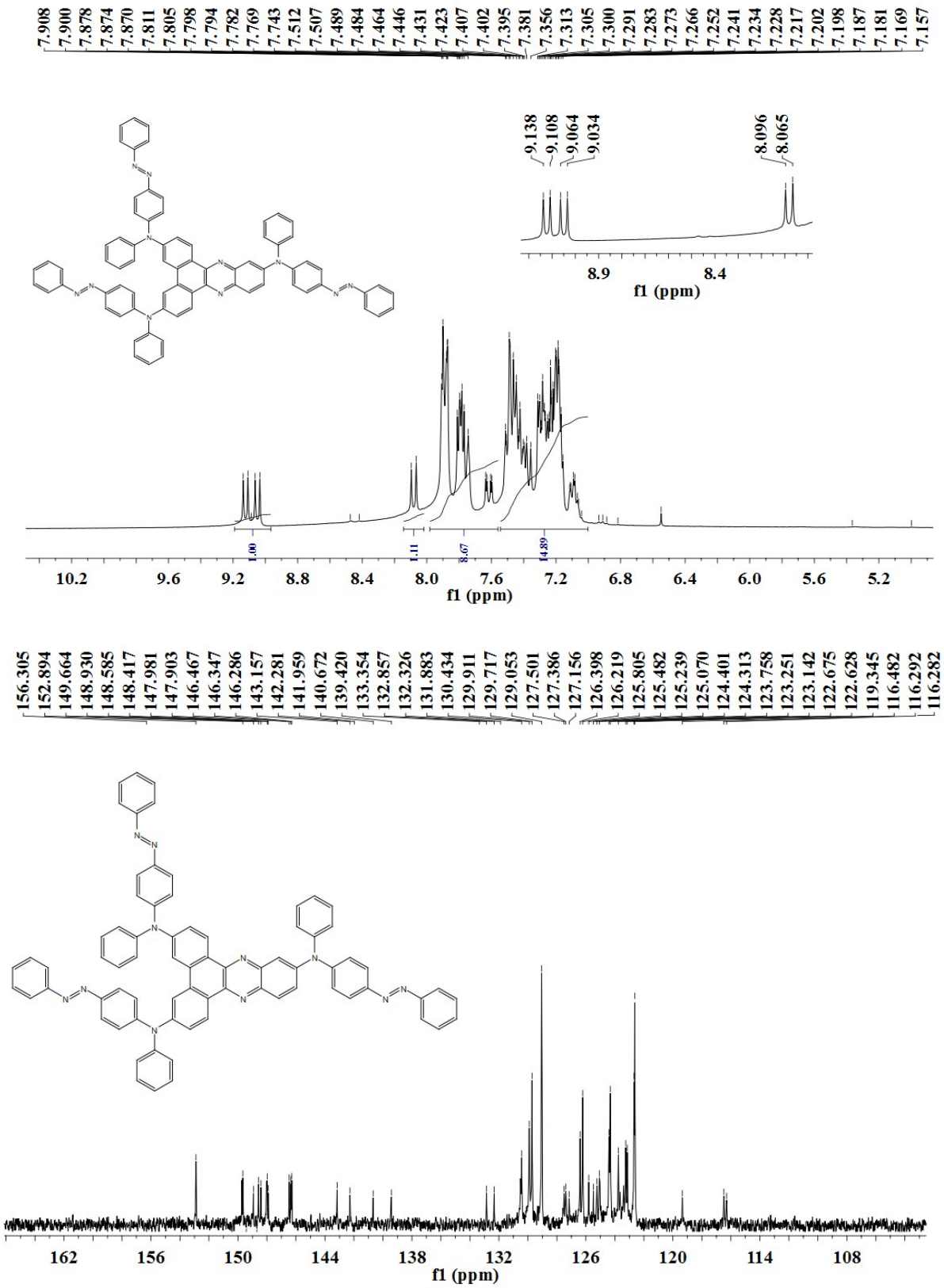


Fig. S18 ^{1}H and ^{13}C NMR spectra of compound **5** in $CDCl_3$.

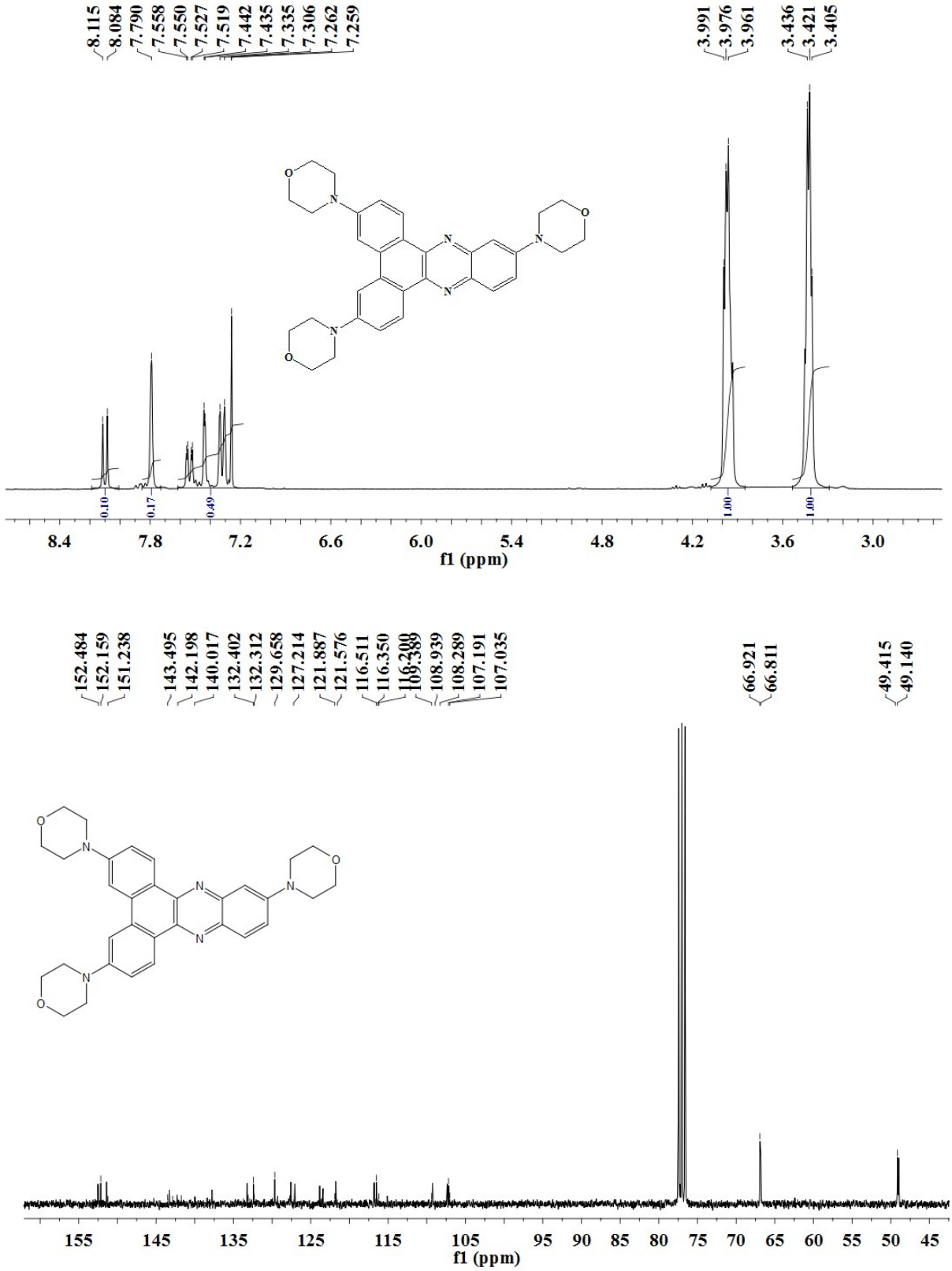


Fig. S19 ^{1}H and ^{13}C NMR spectra of compound **6** in $CDCl_3$.

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

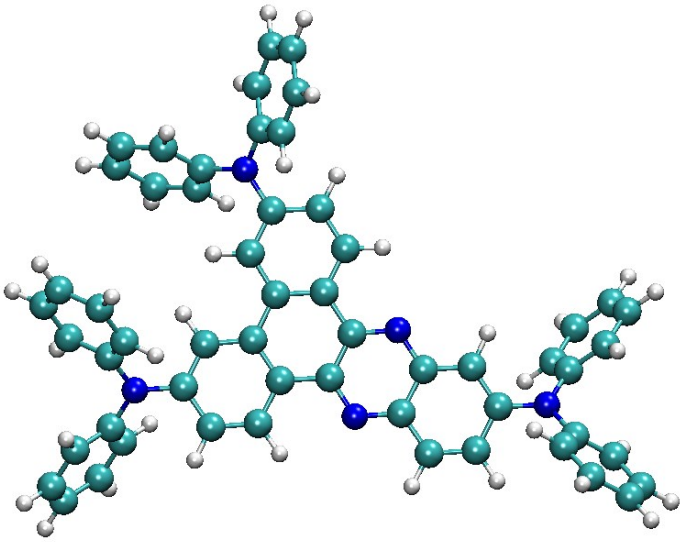


Fig. S20 Optimized structure of compound **2**

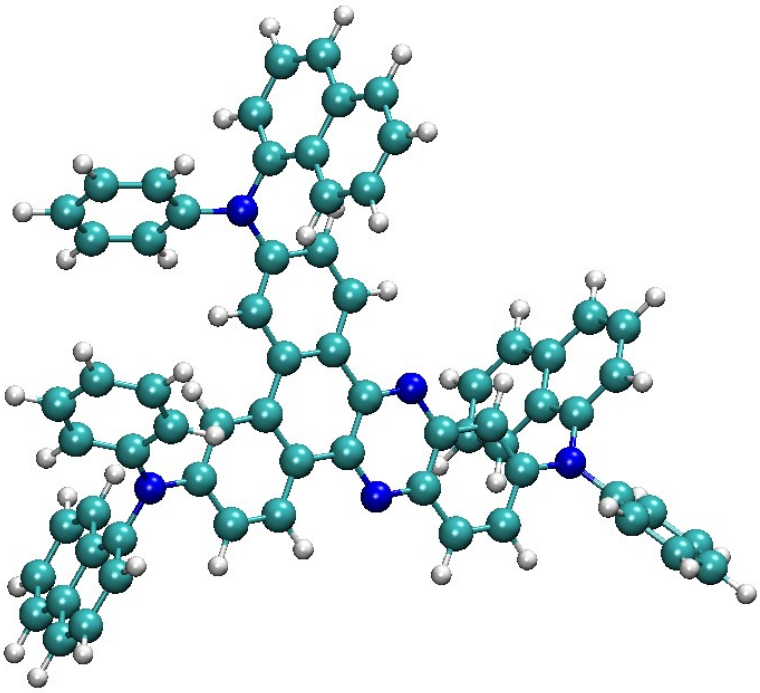


Fig. S21 Optimized structure of compound **3**

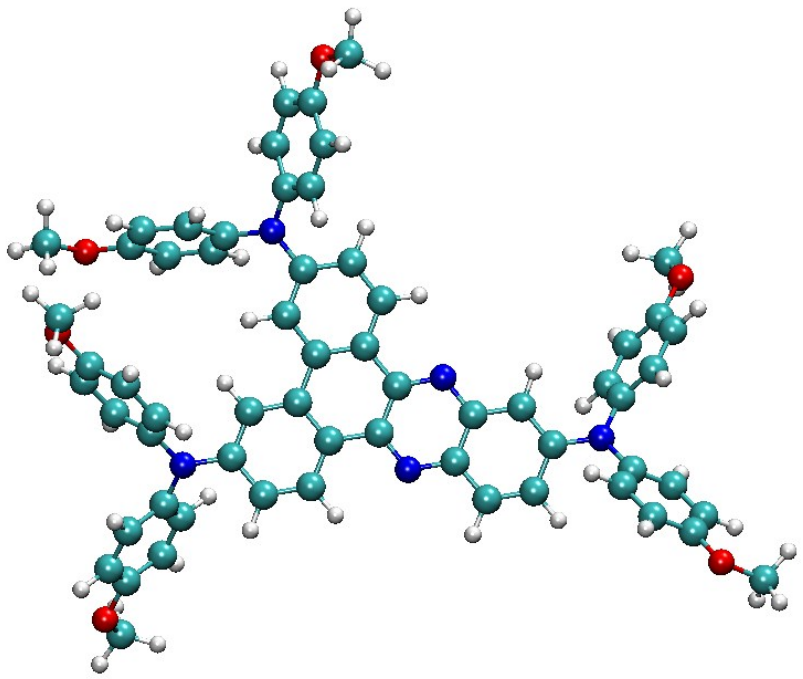


Fig. S22 Optimized structure of compound **4**

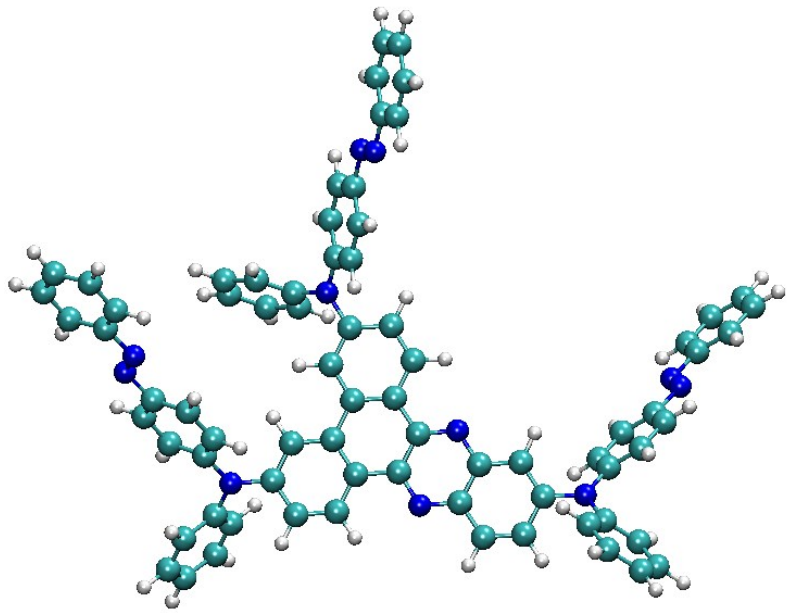


Fig. S23 Optimized structure of compound **5**

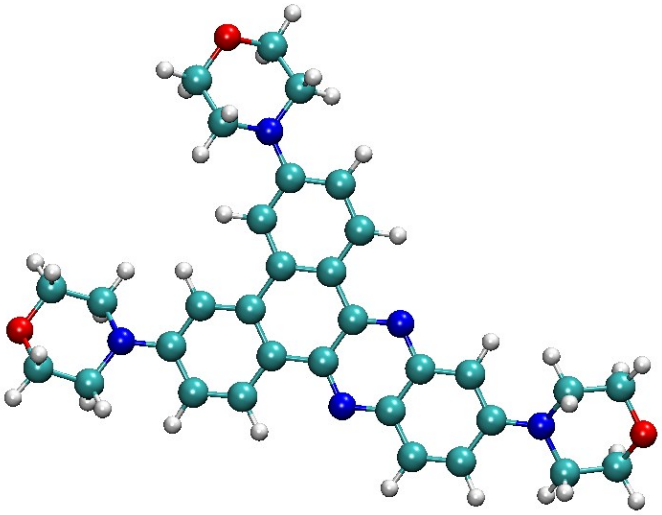


Fig. S24 Optimized structure of compound **6**

11. Cartesian coordinates of compounds of **2** **6**

Table S1. Cartesian coordinates of optimized structure of compound **2**

Total energy: 2431.16599750 Hartrees

Atom	x	y	z
C	-4.814272	-2.107246	8.423454
C	-5.684190	-1.159842	7.878440
C	-5.391159	-0.484929	6.678601
C	-4.182520	-0.802743	6.003337
C	-3.314402	-1.765379	6.557487
C	-3.612009	-2.405549	7.744711
C	-6.310248	0.518057	6.104183
C	-5.976261	1.160897	4.882474
C	-4.735182	0.836283	4.195166
C	-3.840772	-0.140917	4.751937
C	-7.514408	0.872789	6.740854
C	-8.390410	1.811978	6.191345
C	-8.049078	2.434913	4.970510
C	-6.861927	2.114856	4.341030
N	-4.441472	1.458496	3.041531
C	-3.277819	1.142032	2.410602
C	-2.381221	0.172063	2.965358
N	-2.689565	-0.456738	4.139258
C	-2.927853	1.774717	1.187310
C	-1.753995	1.459092	0.551433
C	-0.859418	0.478455	1.095287
C	-1.183340	-0.151704	2.286089
N	-9.614602	2.131144	6.845023

N	-5.129690	-2.758902	9.649525
C	-5.785573	-2.041124	10.701909
C	-4.816227	-4.143444	9.831965
C	-10.356449	1.113624	7.528158
C	-10.111316	3.473526	6.831406
N	0.353849	0.193547	0.412374
C	-6.863351	-2.619712	11.391054
C	-7.489167	-1.924668	12.426682
C	-7.062257	-0.641148	12.778927
C	-5.994102	-0.059933	12.088669
C	-5.352316	-0.754724	11.063118
C	-4.279325	-4.594352	11.049240
C	-3.988792	-5.946657	11.230994
C	-4.211888	-6.865479	10.200910
C	-4.738969	-6.417724	8.985958
C	-5.048855	-5.069750	8.801789
C	0.382444	0.141414	-1.017616
C	1.541900	-0.126190	1.150197
C	-10.891415	1.360589	8.802589
C	-11.625433	0.372420	9.459859
C	-11.823524	-0.877248	8.865712
C	-11.286362	-1.127324	7.599087
C	-10.565639	-0.139191	6.928209
C	-11.475581	3.721958	6.607273
C	-11.960200	5.030126	6.603026
C	-11.093781	6.108625	6.805910
C	-9.734451	5.864002	7.022726
C	-9.244242	4.557811	7.045227
C	2.321670	-1.236881	0.793335

C	3.486890	-1.533104	1.502653
C	3.880000	-0.738343	2.582762
C	3.099673	0.364694	2.943944
C	1.942917	0.676588	2.229979
C	1.462238	0.697011	-1.724089
C	1.494334	0.637471	-3.117090
C	0.447891	0.039467	-3.826718
C	-0.629792	-0.509290	-3.126150
C	-0.661637	-0.469668	-1.731356
H	-6.603825	-0.959120	8.403924
H	-2.396594	-1.977812	6.030192
H	-2.926678	-3.128239	8.162667
H	-7.784448	0.420693	7.681492
H	-8.723236	3.154999	4.530711
H	-6.590727	2.579693	3.405158
H	-3.605762	2.517014	0.790488
H	-1.481605	1.957298	-0.367250
H	-0.538572	-0.896711	2.726402
H	-7.203628	-3.606764	11.112247
H	-8.319244	-2.382133	12.948687
H	-7.553617	-0.102334	13.577577
H	-5.650160	0.930459	12.356261
H	-4.518011	-0.309254	10.540231
H	-4.093448	-3.884655	11.842761
H	-3.575684	-6.279415	12.174134
H	-3.978946	-7.911999	10.342563
H	-4.922730	-7.119541	8.183132
H	-5.471138	-4.730346	7.866730
H	-10.727924	2.321412	9.269485

H	-12.030479	0.576113	10.442320
H	-12.387064	-1.643421	9.380463
H	-11.439460	-2.087989	7.125259
H	-10.164456	-0.330314	5.943051
H	-12.145024	2.891041	6.436289
H	-13.013395	5.206331	6.428036
H	-11.471340	7.121979	6.795422
H	-9.054711	6.689539	7.187962
H	-8.195399	4.371815	7.227445
H	2.012675	-1.860284	-0.033637
H	4.079198	-2.392568	1.217678
H	4.779528	-0.974078	3.134873
H	3.397229	0.990591	3.774784
H	1.347161	1.535690	2.503734
H	2.265501	1.171238	-1.178491
H	2.331884	1.069672	-3.648580
H	0.473153	0.001013	-4.907158
H	-1.441284	-0.982561	-3.663024
H	-1.486540	-0.913085	-1.192073

Table S2. Cartesian coordinates of optimized structure of compound **3**

Total energy: 2892.07198924 Hartrees

Atom	x	y	z
C	8.057408	1.622258	-9.850136
C	7.763365	2.974152	-9.639952
C	7.033945	3.410651	-8.519179
C	6.612298	2.443985	-7.566805
C	6.922300	1.086914	-7.781570

C	7.624248	0.673827	-8.897593
C	6.715334	4.837624	-8.304674
C	5.989179	5.229743	-7.147792
C	5.567624	4.237375	-6.170074
C	5.873218	2.849237	-6.379365
C	7.095581	5.829821	-9.226316
C	6.799849	7.181798	-9.021511
C	6.077257	7.554685	-7.867242
C	5.682152	6.591323	-6.958627
N	4.895400	4.635832	-5.077636
C	4.511324	3.694914	-4.172532
C	4.807248	2.309423	-4.381157
N	5.492365	1.913799	-5.495666
C	3.801891	4.072675	-3.000382
C	3.414187	3.127257	-2.085681
C	3.723886	1.739369	-2.281038
C	4.408085	1.349537	-3.420776
N	7.193010	8.164482	-9.970076
N	8.804047	1.206972	-10.984732
C	9.572033	-0.011466	-10.931727
C	8.703781	1.885979	-12.242259
C	6.434360	9.383272	-10.095523
C	8.410937	8.046796	-10.713924
N	3.271910	0.786999	-1.329642
C	9.221675	-1.071287	-11.747427
C	9.956032	-2.279094	-11.726413
C	11.029330	-2.424566	-10.876343
C	11.430368	-1.357177	-10.026217
C	10.704566	-0.116320	-10.057677

C	9.852745	2.068382	-13.028931
C	9.762990	2.698970	-14.270214
C	8.533216	3.168394	-14.740146
C	7.388140	2.989742	-13.958202
C	7.466022	2.345886	-12.722686
C	3.020003	-0.570685	-1.745308
C	3.269989	1.079299	0.071036
C	7.021378	10.587723	-9.754820
C	6.309795	11.803424	-9.875192
C	5.007856	11.804862	-10.323190
C	4.367045	10.589841	-10.692086
C	5.089757	9.350722	-10.593720
C	8.451343	8.457082	-12.056780
C	9.639365	8.373682	-12.783218
C	10.800335	7.869881	-12.190060
C	10.762731	7.459556	-10.854076
C	9.583002	7.553851	-10.115205
C	2.253286	0.560695	0.890902
C	2.252364	0.822745	2.260447
C	3.252919	1.614462	2.833443
C	4.264470	2.132331	2.020278
C	4.283423	1.860935	0.651077
C	3.833891	-1.587794	-1.284122
C	3.606210	-2.929933	-1.666783
C	2.572266	-3.242657	-2.520155
C	1.705661	-2.227640	-3.012404
C	1.916659	-0.863043	-2.613392
C	3.029921	10.568780	-11.179839
C	2.434440	9.389590	-11.567308

C	3.155105	8.172057	-11.490244
C	4.448514	8.152241	-11.015207
C	12.550529	-1.476146	-9.155894
C	12.950058	-0.422411	-8.365241
C	12.248320	0.807489	-8.414551
C	11.153663	0.956921	-9.238162
C	0.616545	-2.529751	-3.877721
C	-0.233810	-1.541459	-4.319800
C	-0.036745	-0.199881	-3.909081
C	1.011638	0.131178	-3.078343
H	8.121169	3.688835	-10.362973
H	6.584741	0.371612	-7.046780
H	7.841525	-0.373199	-9.047275
H	7.624488	5.558343	-10.125477
H	5.839126	8.594092	-7.696944
H	5.133012	6.864858	-6.070265
H	3.568893	5.119580	-2.866721
H	2.857768	3.418187	-1.206987
H	4.654676	0.315725	-3.607133
H	8.369824	-0.967548	-12.404944
H	9.657310	-3.092000	-12.374512
H	11.587448	-3.351845	-10.847657
H	10.806698	1.715352	-12.663736
H	10.657426	2.832804	-14.864232
H	8.467624	3.663804	-15.699179
H	6.428175	3.338958	-14.315251
H	6.574766	2.195876	-12.130506
H	8.038815	10.590159	-9.389365
H	6.794321	12.730361	-9.599273

H	4.455193	12.732150	-10.406330
H	7.553256	8.837540	-12.522225
H	9.653070	8.692867	-13.817051
H	11.718029	7.798967	-12.757742
H	11.657003	7.077870	-10.379051
H	9.565783	7.249986	-9.078493
H	1.471784	-0.041489	0.449804
H	1.462365	0.416568	2.878295
H	3.245359	1.821264	3.894871
H	5.051786	2.736177	2.452095
H	5.081913	2.245311	0.032898
H	4.655467	-1.345488	-0.624542
H	4.260731	-3.705675	-1.292871
H	2.400953	-4.267253	-2.825127
H	2.488351	11.504319	-11.244700
H	1.417440	9.388133	-11.936316
H	2.683790	7.251446	-11.807576
H	4.991486	7.220957	-10.960576
H	13.088701	-2.415580	-9.131000
H	13.803502	-0.526823	-7.708604
H	12.576291	1.634706	-7.799362
H	10.624594	1.897177	-9.270414
H	0.466461	-3.558553	-4.180647
H	-1.057516	-1.785251	-4.977426
H	-0.716455	0.568993	-4.251369
H	1.154608	1.154693	-2.766706

Table S3. Cartesian coordinates of optimized structure of compound **4**

Total energy: 3118.25066717 Hartrees

Atom	x	y	z
C	-1.784548	0.021110	-7.919493
C	-2.475143	1.238207	-7.891907
C	-2.350048	2.143370	-6.822584
C	-1.464059	1.822900	-5.760695
C	-0.780191	0.589833	-5.789286
C	-0.937499	-0.301719	-6.831810
C	-3.100609	3.414412	-6.791397
C	-2.887746	4.332342	-5.729369
C	-1.953969	4.015375	-4.659383
C	-1.256493	2.757393	-4.664767
C	-4.051230	3.735106	-7.777673
C	-4.763196	4.938032	-7.756670
C	-4.514456	5.857682	-6.711486
C	-3.602142	5.548425	-5.721333
N	-1.764408	4.901680	-3.667962
C	-0.897089	4.582758	-2.668426
C	-0.206221	3.327704	-2.665529
N	-0.404422	2.431949	-3.680060
C	-0.664711	5.490053	-1.600207
C	0.205136	5.169755	-0.588715
C	0.912530	3.920826	-0.587939
C	0.698747	3.021874	-1.623305
N	-5.718240	5.231689	-8.765824
N	-1.937259	-0.871599	-9.008135
C	-3.114298	-0.817980	-9.833368

C	-0.885837	-1.769184	-9.390639
C	-5.571963	4.680394	-10.082648
C	-6.900382	5.983834	-8.464178
N	1.795549	3.625820	0.480672
C	-3.005242	-0.611392	-11.211809
C	-4.143126	-0.560455	-12.023209
C	-5.409401	-0.701428	-11.447520
C	-5.528681	-0.912537	-10.066399
C	-4.392385	-0.978472	-9.269545
C	0.439933	-1.332347	-9.498943
C	1.457312	-2.212147	-9.883077
C	1.145421	-3.540094	-10.188447
C	-0.180272	-3.983689	-10.097954
C	-1.182491	-3.110281	-9.695184
C	2.547485	4.668061	1.115821
C	2.025945	2.266940	0.884500
C	-4.387777	4.865737	-10.805226
C	-4.230505	4.310306	-12.078378
C	-5.277294	3.578278	-12.646292
C	-6.472720	3.401336	-11.940609
C	-6.615175	3.942177	-10.668021
C	-7.343400	6.988919	-9.343570
C	-8.500129	7.708767	-9.071610
C	-9.231006	7.452046	-7.904593
C	-8.800496	6.460427	-7.018418
C	-7.647407	5.724566	-7.308519
C	0.953070	1.416141	1.173119
C	1.172333	0.091831	1.562728
C	2.481223	-0.384585	1.688532

C	3.561957	0.463270	1.416096
C	3.336148	1.772836	1.009318
C	2.656038	4.715453	2.510622
C	3.409130	5.711650	3.139249
C	4.047858	6.687377	2.367783
C	3.940537	6.653228	0.971662
C	3.208425	5.647925	0.351867
O	-10.368620	8.238249	-7.720569
O	-5.221122	2.972732	-13.907369
O	2.074345	-4.499302	-10.591980
O	2.816549	-1.681017	2.077216
O	4.815389	7.729635	2.886788
H	-3.108061	1.480063	-8.729332
H	-0.129472	0.357232	-4.959537
H	-0.415505	-1.246706	-6.820789
H	-4.262418	3.036204	-8.570118
H	-5.041617	6.800028	-6.691673
H	-3.408129	6.240320	-4.915389
H	-1.205868	6.425711	-1.605821
H	0.360522	5.855543	0.230758
H	1.210993	2.073117	-1.664044
H	-2.025643	-0.490094	-11.653019
H	-4.030349	-0.395504	-13.083874
H	-6.517649	-1.028967	-9.647712
H	-4.484925	-1.146958	-8.205731
H	0.681647	-0.302500	-9.277420
H	2.470783	-1.846034	-9.951093
H	-0.395169	-5.015378	-10.335526
H	-2.202807	-3.457642	-9.615842

H	-3.582309	5.437339	-10.366058
H	-3.301999	4.461671	-12.607917
H	-7.266856	2.827254	-12.394489
H	-7.532780	3.792138	-10.117257
H	-6.775122	7.197766	-10.238865
H	-8.850895	8.482346	-9.739126
H	-9.350882	6.240397	-6.116013
H	-7.326302	4.948209	-6.628717
H	-0.058190	1.787048	1.084129
H	0.324381	-0.542934	1.771620
H	4.563040	0.069706	1.515570
H	4.171658	2.421313	0.786944
H	2.153026	3.967693	3.107345
H	3.477326	5.718740	4.216767
H	4.451449	7.412010	0.397047
H	3.145274	5.614110	-0.726500
C	4.974045	7.836011	4.325304
C	-11.182849	8.027414	-6.538066
C	3.469464	-4.119083	-10.711837
H	5.601347	8.707975	4.477409
H	4.011911	7.985246	4.820949
H	5.467830	6.952485	4.736846
H	-11.990646	8.747211	-6.618100
H	-11.594099	7.015456	-6.514318
H	-10.613324	8.215089	-5.624686
H	3.982590	-5.020527	-11.029927
H	3.604921	-3.336050	-11.461789
H	3.874359	-3.785368	-9.753493
O	-6.606777	-0.649738	-12.154503

C	-6.566903	-0.401450	-13.588974
C	-4.046150	3.189806	-14.733439
C	1.752714	-2.628569	2.354491
H	-7.605951	-0.405197	-13.901730
H	-6.117002	0.568290	-13.807458
H	-6.027588	-1.196888	-14.109175
H	-4.248657	2.665312	-15.661527
H	-3.899706	4.252452	-14.937924
H	-3.149765	2.777081	-14.265204
H	2.257467	-3.553042	2.614403
H	1.135794	-2.299169	3.193923
H	1.124395	-2.787741	1.475093

Table S4. Cartesian coordinates of optimized structure of compound **5**

Total energy: 3452.63431309 Hartrees

Atom	x	y	z
C	-11.127738	-2.830531	0.388736
C	-11.420704	-3.612185	-0.730317
C	-10.427656	-4.352242	-1.398596
C	-9.100419	-4.308422	-0.895372
C	-8.815324	-3.517776	0.236429
C	-9.800804	-2.784667	0.868850
C	-10.736624	-5.176460	-2.583674
C	-9.705510	-5.925922	-3.210136
C	-8.345999	-5.880534	-2.691200
C	-8.042411	-5.072065	-1.542628
C	-12.032173	-5.234542	-3.130879
C	-12.325437	-6.026689	-4.241992

C	-11.293341	-6.773533	-4.848415
C	-10.010344	-6.712975	-4.339106
N	-7.388632	-6.599159	-3.299334
C	-6.121899	-6.544379	-2.804371
C	-5.813895	-5.731769	-1.665393
N	-6.796103	-5.007148	-1.050776
C	-5.079554	-7.292878	-3.414404
C	-3.801457	-7.234584	-2.919247
C	-3.490461	-6.428730	-1.775586
C	-4.492381	-5.696841	-1.160984
N	-13.651059	-6.077965	-4.770179
N	-12.154807	-2.070014	1.020730
N	-2.147602	-6.393244	-1.302220
C	-12.212060	-1.941765	2.433510
C	-13.157201	-1.434221	0.208306
C	-14.781846	-6.098722	-3.911578
C	-13.834041	-6.078480	-6.194946
C	-1.576372	-5.187763	-0.805335
C	-1.385481	-7.609374	-1.265886
C	-14.518388	-1.634510	0.479924
C	-15.487162	-1.012687	-0.309339
C	-15.109304	-0.199570	-1.381982
C	-13.752163	-0.005535	-1.657140
C	-12.777980	-0.612999	-0.863619
C	-12.666321	-0.746110	3.022364
C	-12.736368	-0.630430	4.405073
C	-12.351355	-1.693511	5.234696
C	-11.897403	-2.890367	4.650451
C	-11.832320	-3.014385	3.271642

C	-15.969826	-5.436395	-4.275642
C	-17.076171	-5.471421	-3.435360
C	-17.026337	-6.152566	-2.210795
C	-15.841871	-6.818785	-1.844288
C	-14.739372	-6.796738	-2.682971
C	-14.689035	-7.013726	-6.797778
C	-14.865439	-7.009669	-8.181805
C	-14.181202	-6.087275	-8.979708
C	-13.322255	-5.161456	-8.380452
C	-13.152574	-5.149331	-6.995106
C	-0.066290	-7.631207	-1.745082
C	0.671969	-8.814001	-1.707192
C	0.101325	-9.989520	-1.208100
C	-1.214758	-9.970295	-0.738387
C	-1.954769	-8.786698	-0.757649
C	-0.720361	-5.210492	0.310539
C	-0.145575	-4.032499	0.774372
C	-0.414329	-2.808787	0.146172
C	-1.272984	-2.781873	-0.968580
C	-1.842472	-3.954004	-1.439234
N	-18.207528	-6.116914	-1.428875
N	-18.146608	-6.702236	-0.290110
C	-19.340403	-6.672157	0.488181
C	-20.548002	-6.086835	0.070426
C	-21.655016	-6.116473	0.913532
C	-21.570275	-6.725730	2.173765
C	-20.369027	-7.308268	2.588621
C	-19.256701	-7.282625	1.747092
N	-12.462416	-1.466210	6.629041

N	-12.108104	-2.435693	7.388599
C	-12.224528	-2.199814	8.789743
C	-12.676468	-0.996858	9.358827
C	-12.749442	-0.875248	10.743393
C	-12.375639	-1.944695	11.569795
C	-11.926132	-3.141090	11.003210
C	-11.850130	-3.268130	9.616005
N	0.224868	-1.670824	0.700634
N	-0.024256	-0.551670	0.128768
C	0.623179	0.588717	0.687719
C	1.480395	0.550178	1.800718
C	2.060198	1.727738	2.263489
C	1.793647	2.947643	1.625316
C	0.940521	2.985413	0.518481
C	0.356123	1.808184	0.050723
H	-12.443037	-3.641776	-1.071040
H	-7.794964	-3.489930	0.587671
H	-9.560735	-2.169073	1.723165
H	-12.831672	-4.655464	-2.697389
H	-11.514039	-7.393203	-5.705145
H	-9.209760	-7.280570	-4.788714
H	-5.326099	-7.890197	-4.280499
H	-3.006380	-7.789902	-3.394643
H	-4.297849	-5.087084	-0.291950
H	-14.808351	-2.274480	1.301270
H	-16.534622	-1.175853	-0.094553
H	-15.862354	0.275402	-1.995821
H	-13.450708	0.626439	-2.481841
H	-11.727942	-0.456079	-1.066960

H	-12.954949	0.082343	2.392784
H	-13.076808	0.282980	4.871708
H	-11.618810	-3.709024	5.296209
H	-11.501514	-3.942518	2.828877
H	-16.014503	-4.894824	-5.208701
H	-17.992487	-4.962667	-3.699079
H	-15.818363	-7.356593	-0.908845
H	-13.839461	-7.325436	-2.404729
H	-15.205961	-7.735618	-6.181494
H	-15.526631	-7.734977	-8.636897
H	-14.314886	-6.091017	-10.052814
H	-12.791787	-4.441010	-8.988640
H	-12.497403	-4.426590	-6.529696
H	0.369763	-6.725931	-2.143122
H	1.687870	-8.819867	-2.078960
H	0.674367	-10.906292	-1.185917
H	-1.663516	-10.872439	-0.344606
H	-2.966755	-8.768180	-0.378440
H	-0.515778	-6.146943	0.807880
H	0.509271	-4.031908	1.634052
H	-1.463380	-1.836649	-1.453324
H	-2.489679	-3.930830	-2.303806
H	-20.590767	-5.624187	-0.903578
H	-22.586236	-5.667569	0.593904
H	-22.434760	-6.745298	2.823933
H	-20.300587	-7.778848	3.560063
H	-18.314353	-7.724598	2.037664
H	-12.959111	-0.187057	8.703989
H	-13.096534	0.050115	11.183952

H	-12.434766	-1.843049	12.645278
H	-11.636733	-3.967686	11.637973
H	-11.506222	-4.178871	9.146821
H	1.671348	-0.399482	2.276303
H	2.720053	1.701189	3.120607
H	2.247914	3.859083	1.990501
H	0.732621	3.924972	0.024665
H	-0.308002	1.803186	-0.801770

Table S5. Cartesian coordinates of optimized structure of compound **6**

Total energy: 1738.59276454 Hartrees

Atom	x	y	z
C	-5.002911	3.490685	7.451179
C	-6.149905	3.228579	6.686530
C	-6.087318	2.720666	5.378457
C	-4.808774	2.471854	4.809551
C	-3.659051	2.745469	5.571972
C	-3.740783	3.238871	6.861316
C	-7.306221	2.455817	4.582844
C	-7.182785	1.934187	3.267426
C	-5.871781	1.665614	2.694659
C	-4.685534	1.935307	3.460867
C	-8.593682	2.692782	5.093325
C	-9.758326	2.444572	4.350624
C	-9.608720	1.932246	3.038787
C	-8.349911	1.681834	2.524223
N	-5.786727	1.166586	1.451985
C	-4.551207	0.921876	0.934423

C	-3.366581	1.184164	1.693933
N	-3.464613	1.697186	2.960415
C	-4.407366	0.390658	-0.371437
C	-3.163057	0.136923	-0.894245
C	-1.961768	0.409922	-0.150369
C	-2.096138	0.926502	1.137730
N	-11.031824	2.678771	4.908978
N	-5.117848	4.007769	8.758843
N	-0.701625	0.162815	-0.718257
C	-3.933850	4.538866	9.452289
C	-4.364250	5.553828	10.510620
O	-5.327096	4.972490	11.439410
C	-6.513057	4.503274	10.730308
C	-6.129908	3.461413	9.685857
C	-12.243964	2.182089	4.240055
C	-13.349452	1.953101	5.270392
O	-13.606955	3.160422	6.047631
C	-12.399660	3.597993	6.740710
C	-11.283073	3.872939	5.739736
C	-0.545731	-0.212858	-2.132140
C	0.788742	0.305372	-2.670133
O	1.903894	-0.153860	-1.852266
C	1.750581	0.298380	-0.472926
C	0.448674	-0.231200	0.117768
H	-7.110589	3.463790	7.114713
H	-2.698934	2.540406	5.122382
H	-2.831898	3.401875	7.420236
H	-8.699993	3.043632	6.106637
H	-10.472934	1.755225	2.416968

H	-8.234174	1.297006	1.521904
H	-5.306307	0.176394	-0.932293
H	-3.096451	-0.302403	-1.877219
H	-1.245741	1.176679	1.752062
H	-3.290104	5.039868	8.730756
H	-3.354121	3.735802	9.931043
H	-4.807638	6.430189	10.024854
H	-3.518568	5.865316	11.119142
H	-7.014860	5.352103	10.251915
H	-7.162485	4.077664	11.491751
H	-7.012818	3.153007	9.132672
H	-5.728366	2.573540	10.195639
H	-12.023809	1.233991	3.752141
H	-12.597939	2.888381	3.474677
H	-13.063120	1.138357	5.944724
H	-14.291162	1.708657	4.784622
H	-12.085888	2.827509	7.454134
H	-12.679430	4.501228	7.277997
H	-10.377336	4.157711	6.267916
H	-11.576283	4.717985	5.099987
H	-1.344215	0.233330	-2.720938
H	-0.591883	-1.303719	-2.259497
H	0.778032	1.400928	-2.692865
H	0.977777	-0.076353	-3.670737
H	1.763239	1.393555	-0.441632
H	2.612551	-0.091378	0.063262
H	0.325322	0.149696	1.126617
H	0.502387	-1.327258	0.177376