

Synthesis and Optoelectronic Investigations of Triarylamines based on naphtho[2,3-*f*]quinoxaline-7,12-dione core as Donor-Acceptors for n-type materials

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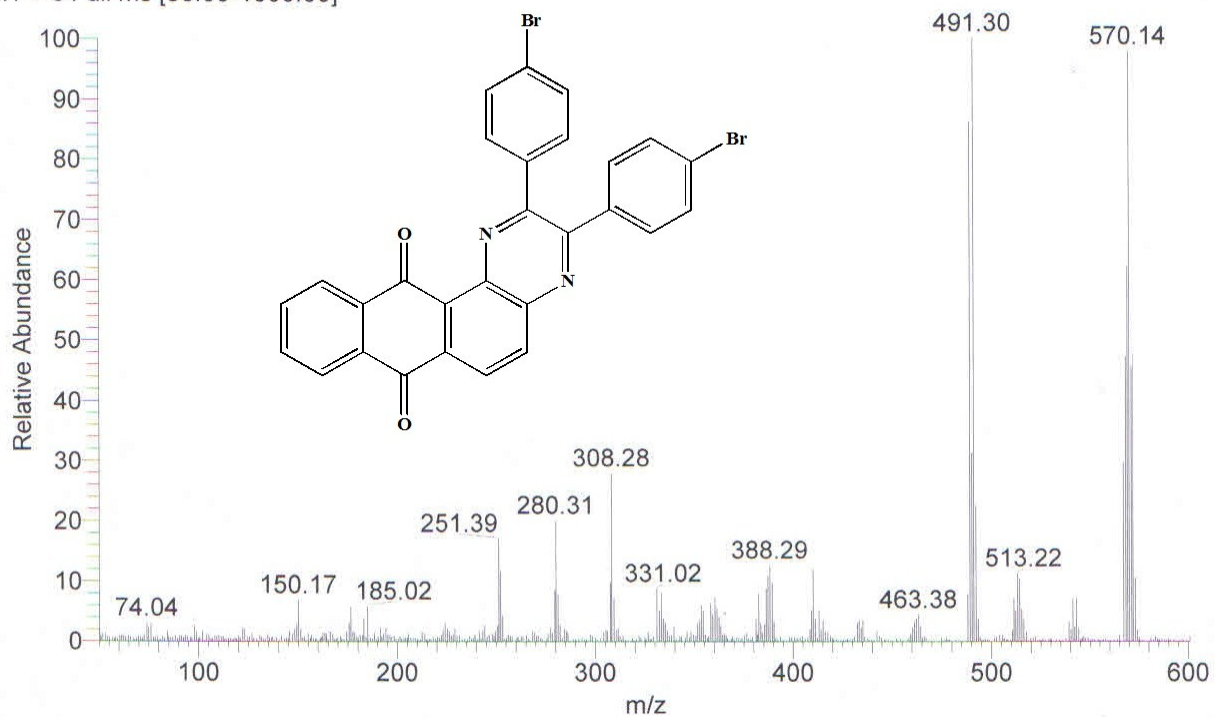
*Email: kamblerm@chem.mu.ac.in

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1. Mass spectra of compound 1

AZ-500 #207 RT: 2.90 AV: 1 NL: 2.96E5
T: + c Full ms [50.00-1000.00]



2. HRMS spectrum of compounds 2 7.

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Analysis Info

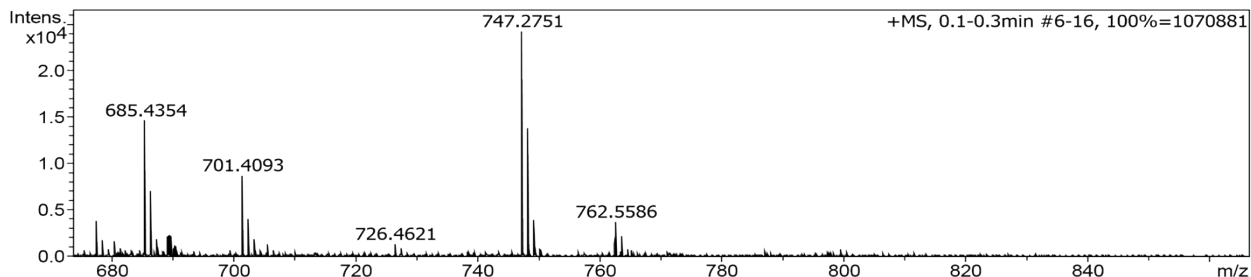
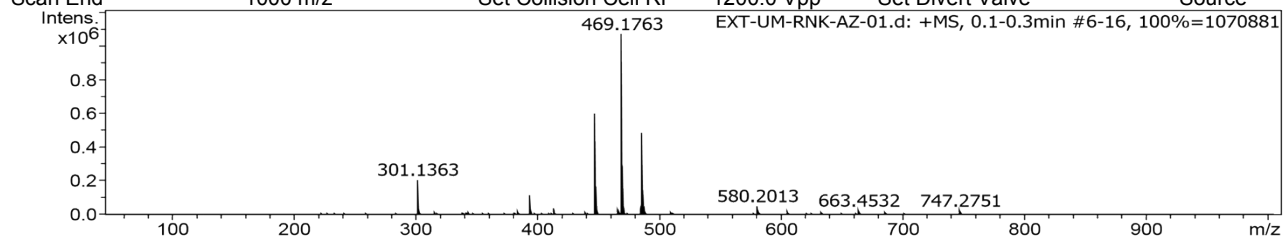
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Sample Name EXT-UM-RNK-AZ-01
Comment C52H34N4O2

Acquisition Date 12/15/2015 11:14:28 A

Operator MR OUT
Instrument maXis impact 282001.000t

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
Scan End 1000 m/z Set Collision Cell RF 1200.0 Vpp Set Divert Valve I/min Source



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747.2751	1	C52H35N4O2	747.2755	-0.5	16.7	1	100.00	37.5	even	ok	

Figure S1: HRMS spectra of compound 2.

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Analysis Info

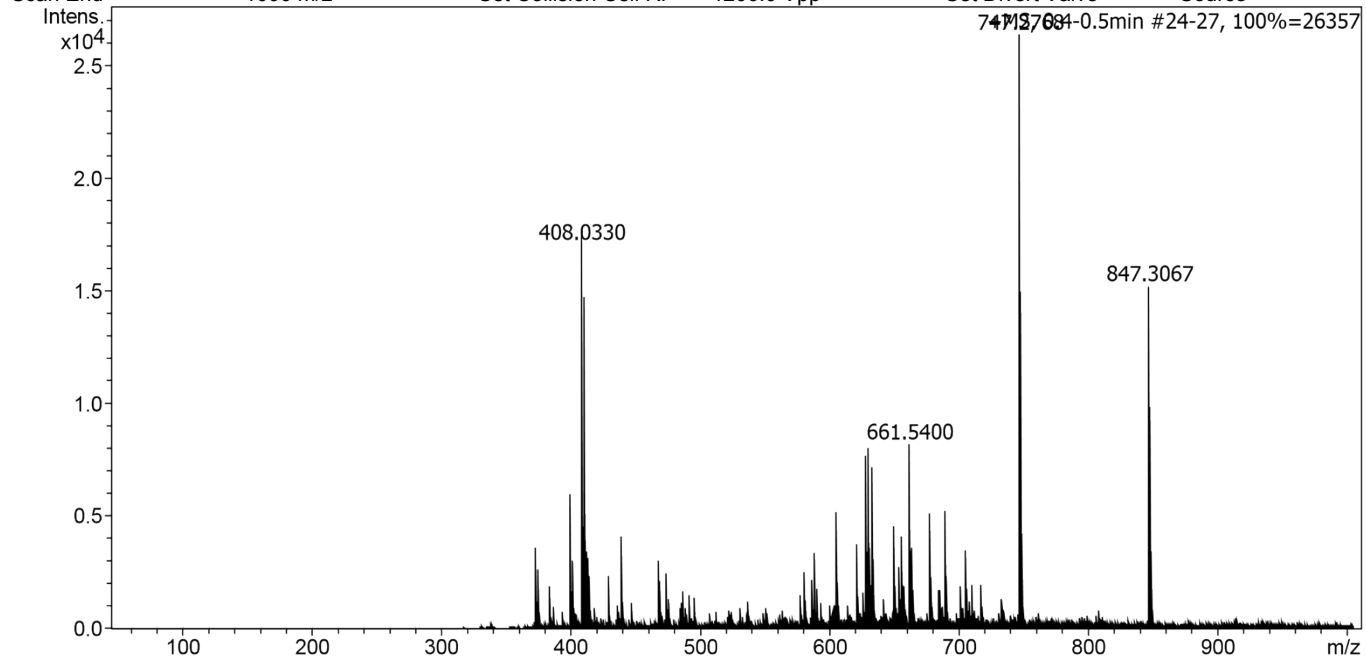
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Acquisition Date 12/15/2015 11:26:38 AM

Operator MR OUT
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Acquisition Parameter

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I/min
Scan End 1000 m/z Set Collision Cell RF 1200.0 Vpp Set Divert Valve Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
847.3067	1	C60H39N4O2	847.3068	-0.1	10.8	1	100.00	43.5	even	ok

Figure S2: HRMS spectra of compound 3.

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Analysis Info

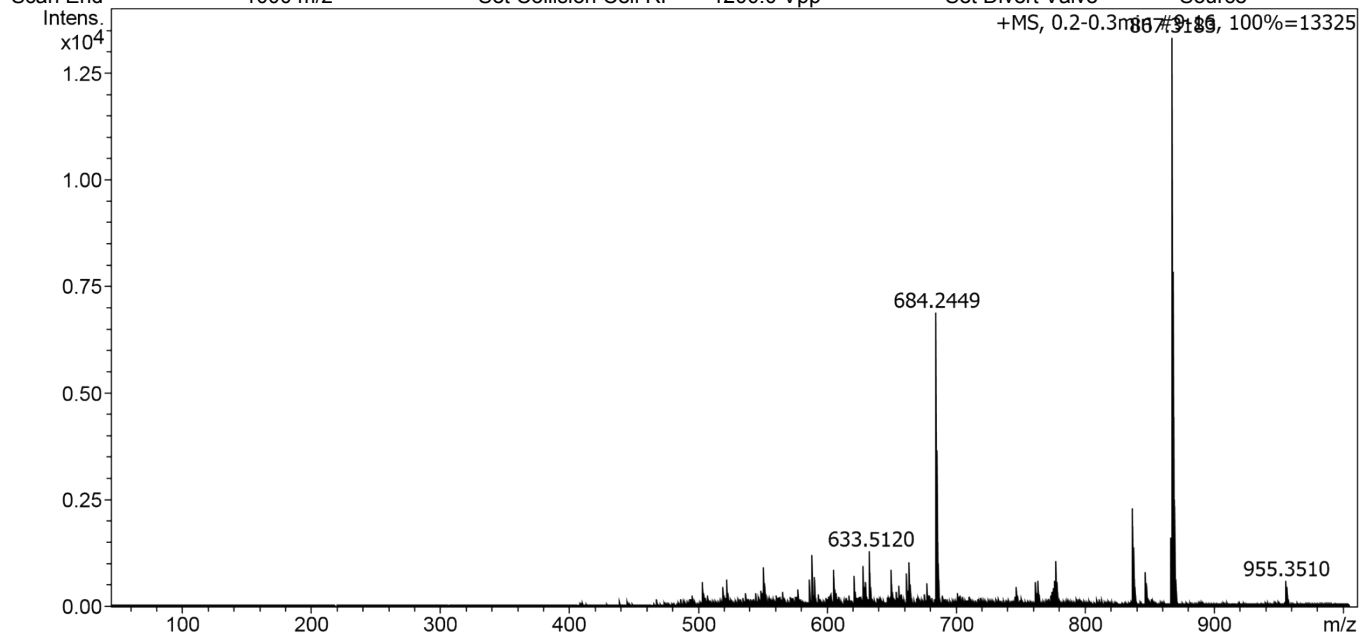
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867.3183	1	C56H43N4O6	867.3177	0.7	19.3	1	100.00	37.5	even	ok

Figure S3: HRMS spectra of compound 4.

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Analysis Info

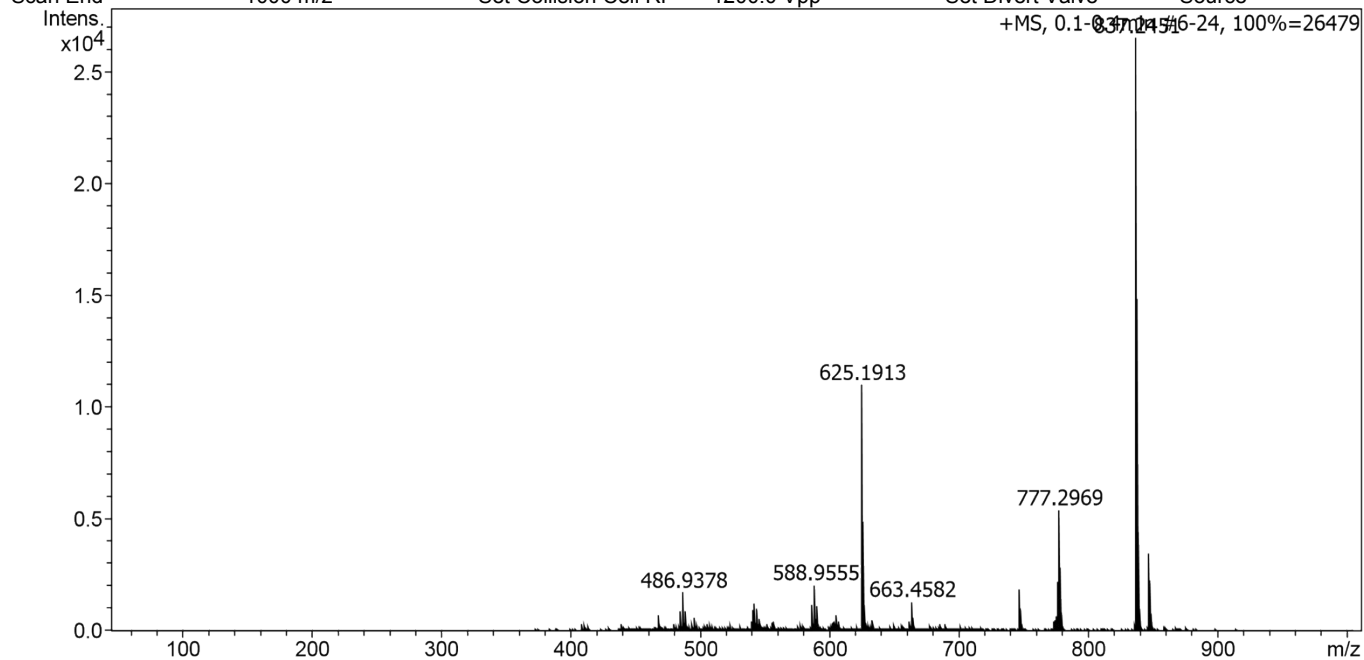
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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
837.2451	1	C52H33N6O6	837.2456	-0.6	15.7	1	100.00	39.5	even	ok

Figure S4: HRMS spectra of compound 5.

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Analysis Info

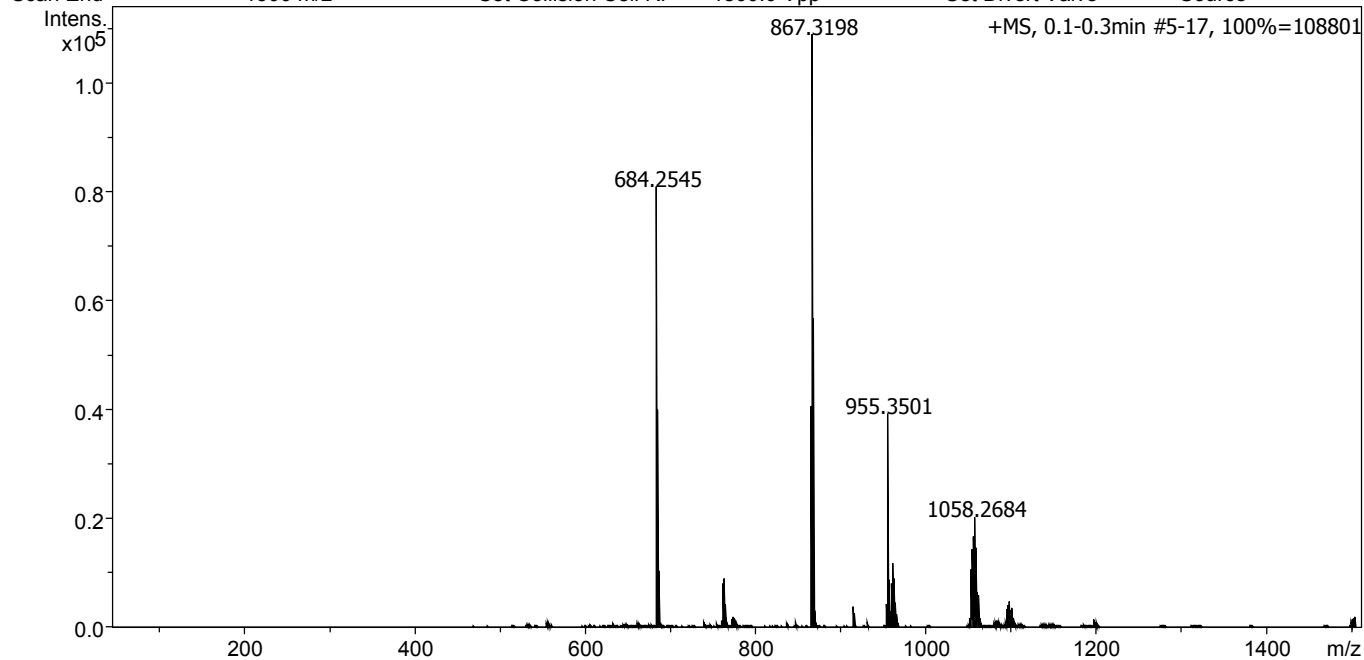
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Operator MR OUT
 Instrument maXis impact 282001.00081

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Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
955.3501	1	C64H43N8O2	955.3503	0.3	32.9	1	100.00	47.5	even	ok

Figure S5: HRMS spectra of compound **6**.

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Analysis Info

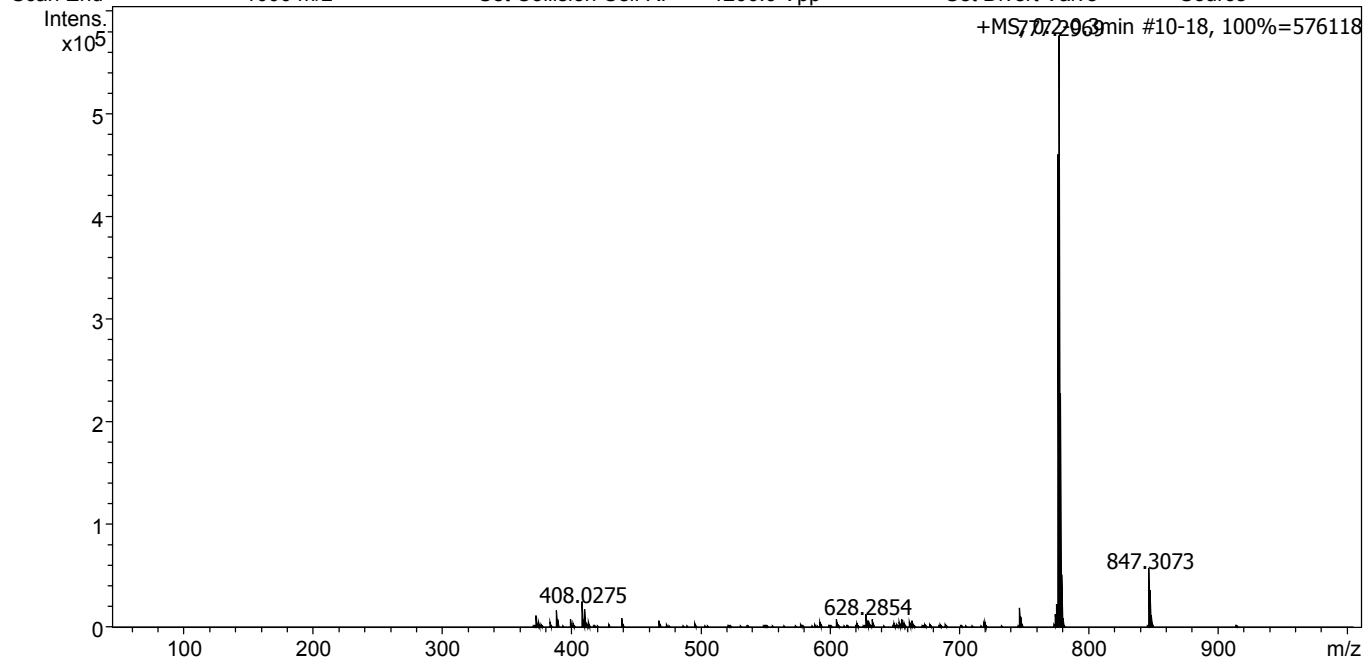
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Method Tune_pos_NAICSI-1000a.m
Sample Name EXT-UM-RNK-AZ-06
Comment C52H36N6O2

Acquisition Date 12/15/2015 11:33:26 AM

Operator MR OUT
Instrument maXis impact 282001.00081

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
777.2969	1	C52H37N6O2	777.2973	0.4	95.5	1	100.00	37.5	even	ok

Figure S6: HRMS spectra of compound 7.

3. FTIR spectrum of compounds 1 7.

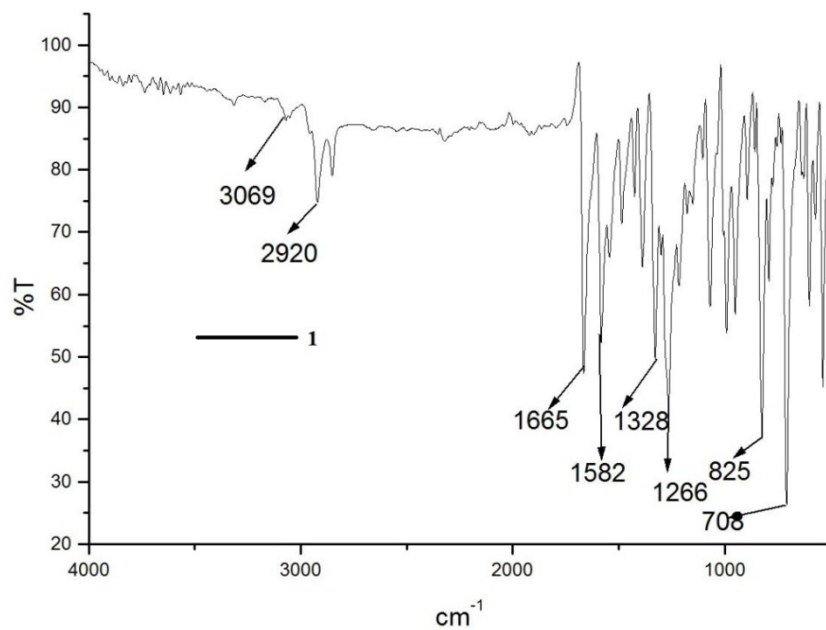


Figure S7: FTIR spectra of compound 1.

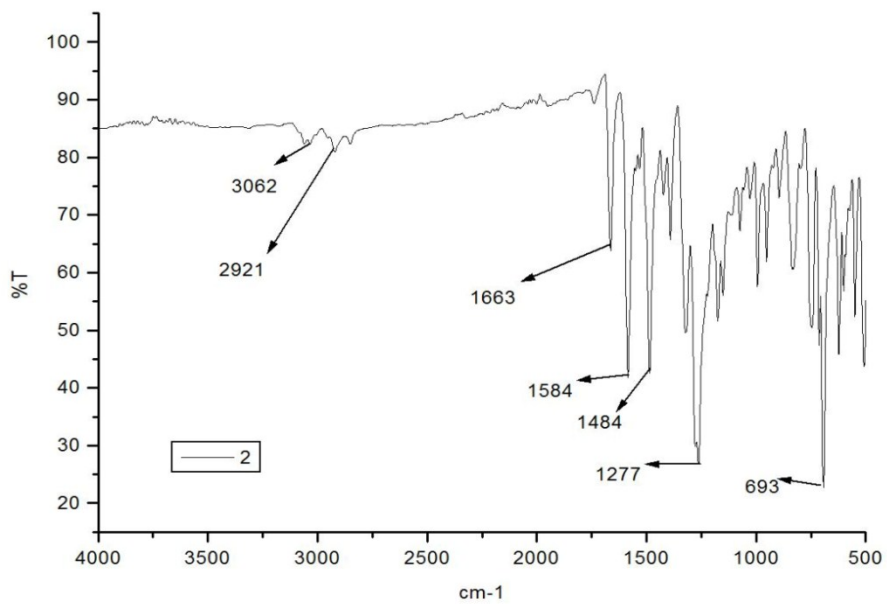


Figure S8: FTIR spectra of compound 2.

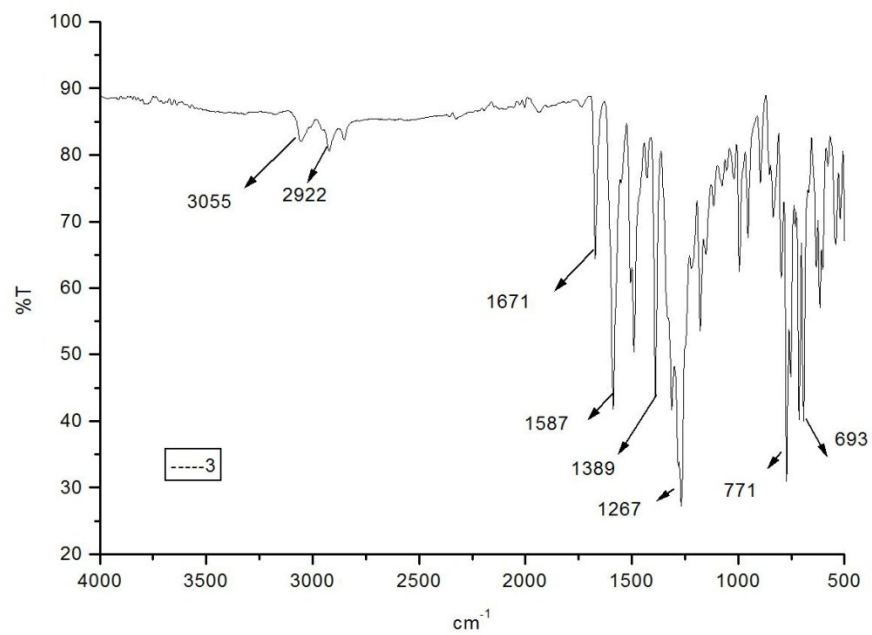


Figure S9: FTIR spectra of compound 3.

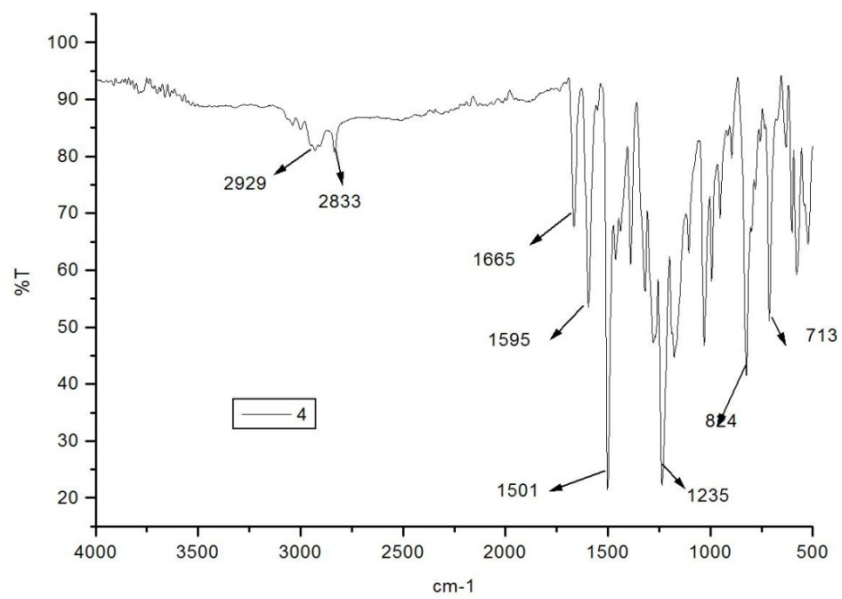


Figure S10: FTIR spectra of compound 4.

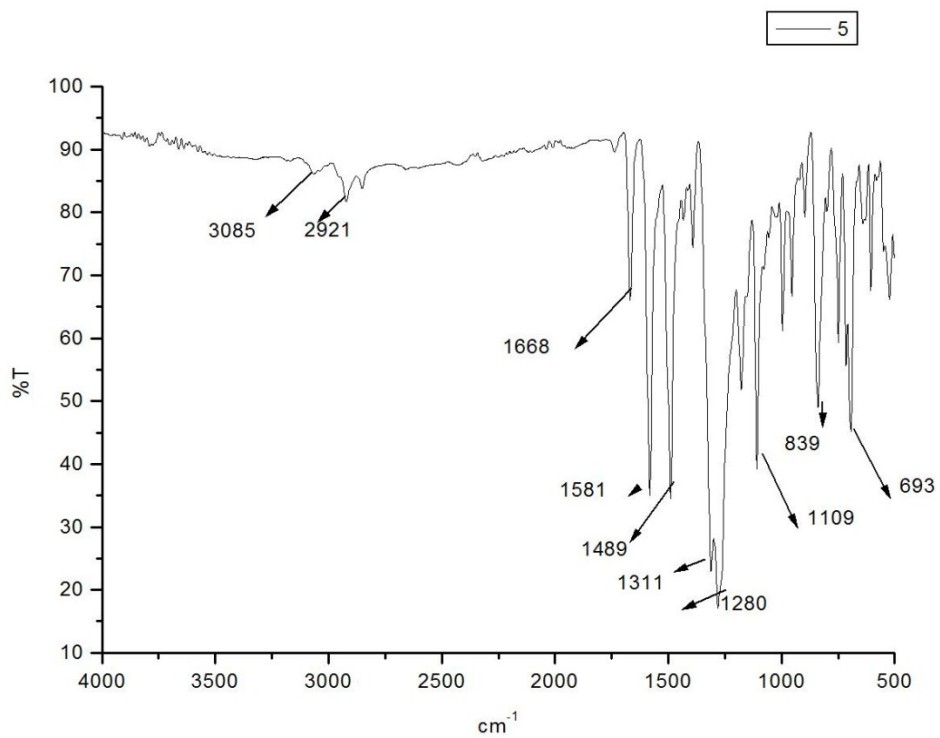


Figure S11: FTIR spectra of compound **5**

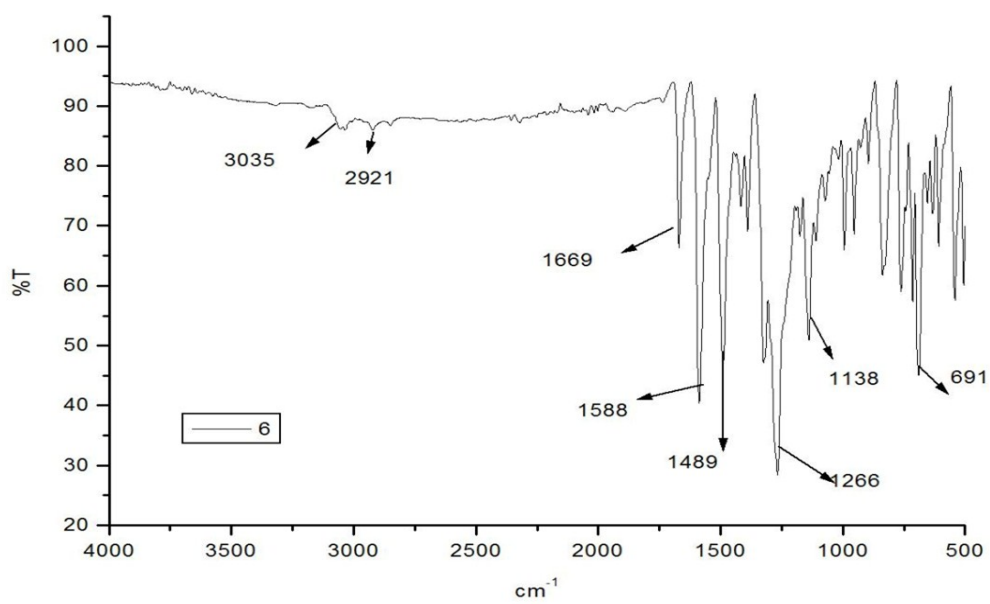


Figure S12: FTIR spectra of compound **6**.

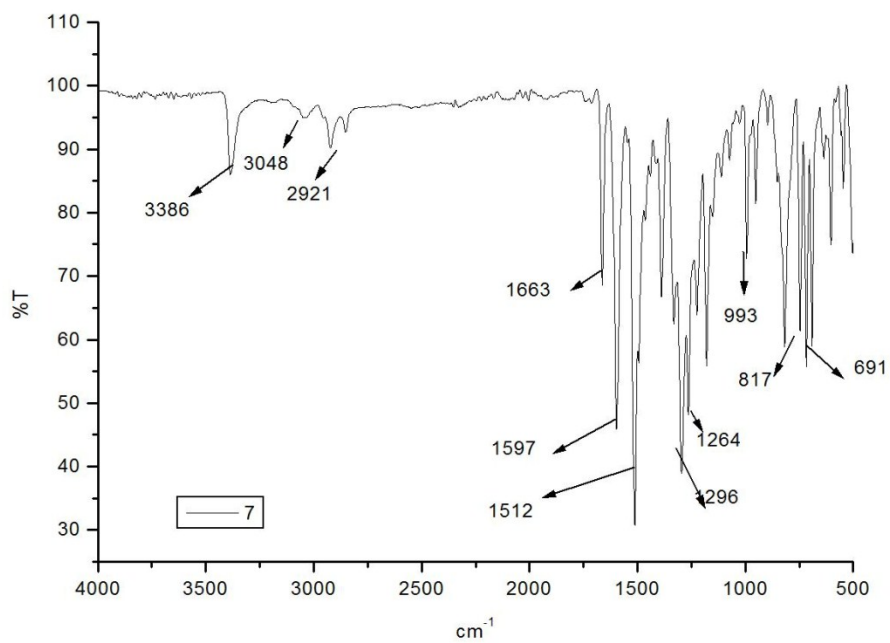


Figure S13: FTIR spectra of compound 7.

4. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectrum of compounds 1-7.

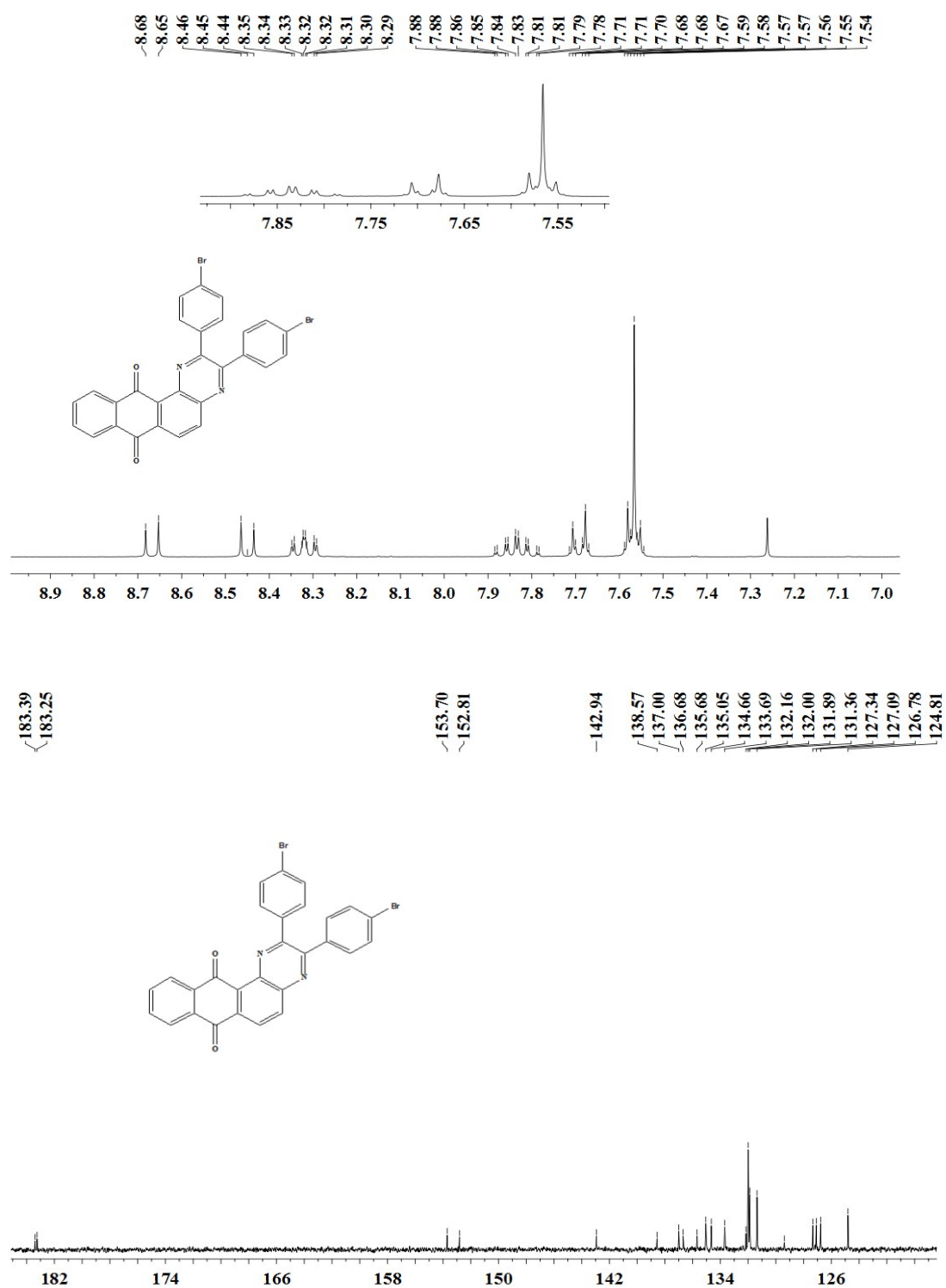


Figure S14: $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra of compound 1 in CDCl_3 .

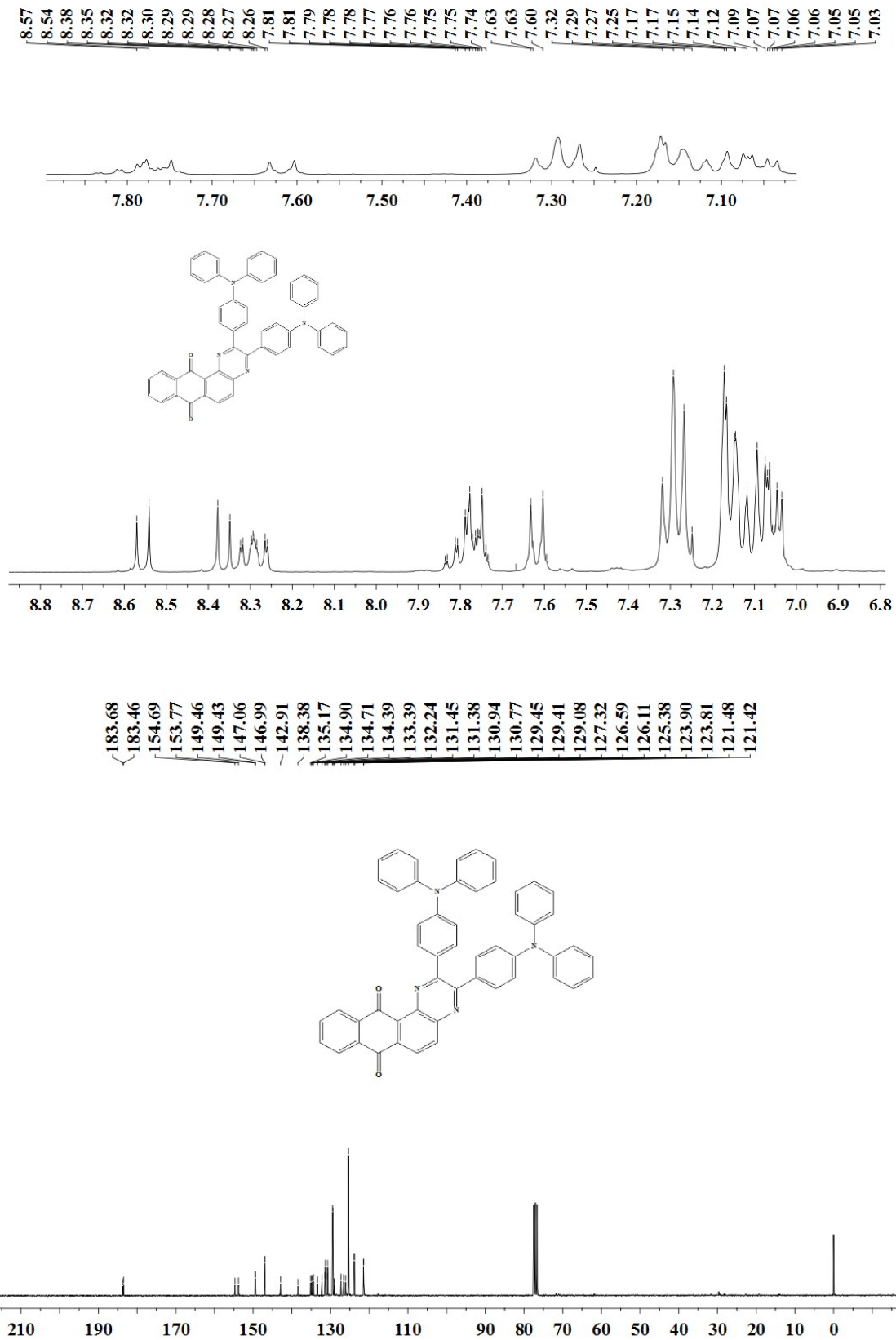


Figure S15: ¹H-NMR and ¹³C-NMR spectra of compound 2 in CDCl₃.

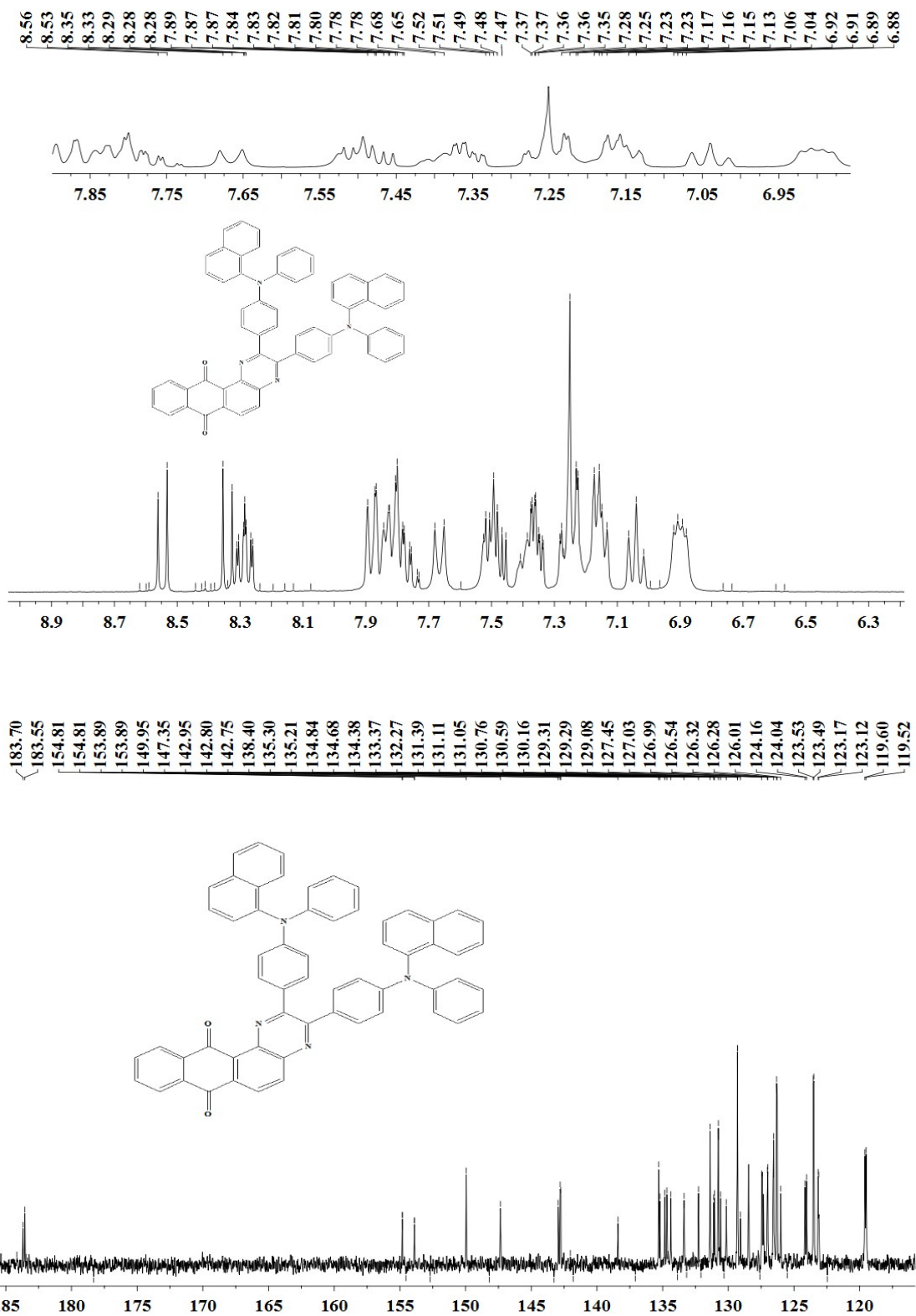


Figure S16: ¹H-NMR and ¹³C-NMR spectra of compound 3 in CDCl₃.

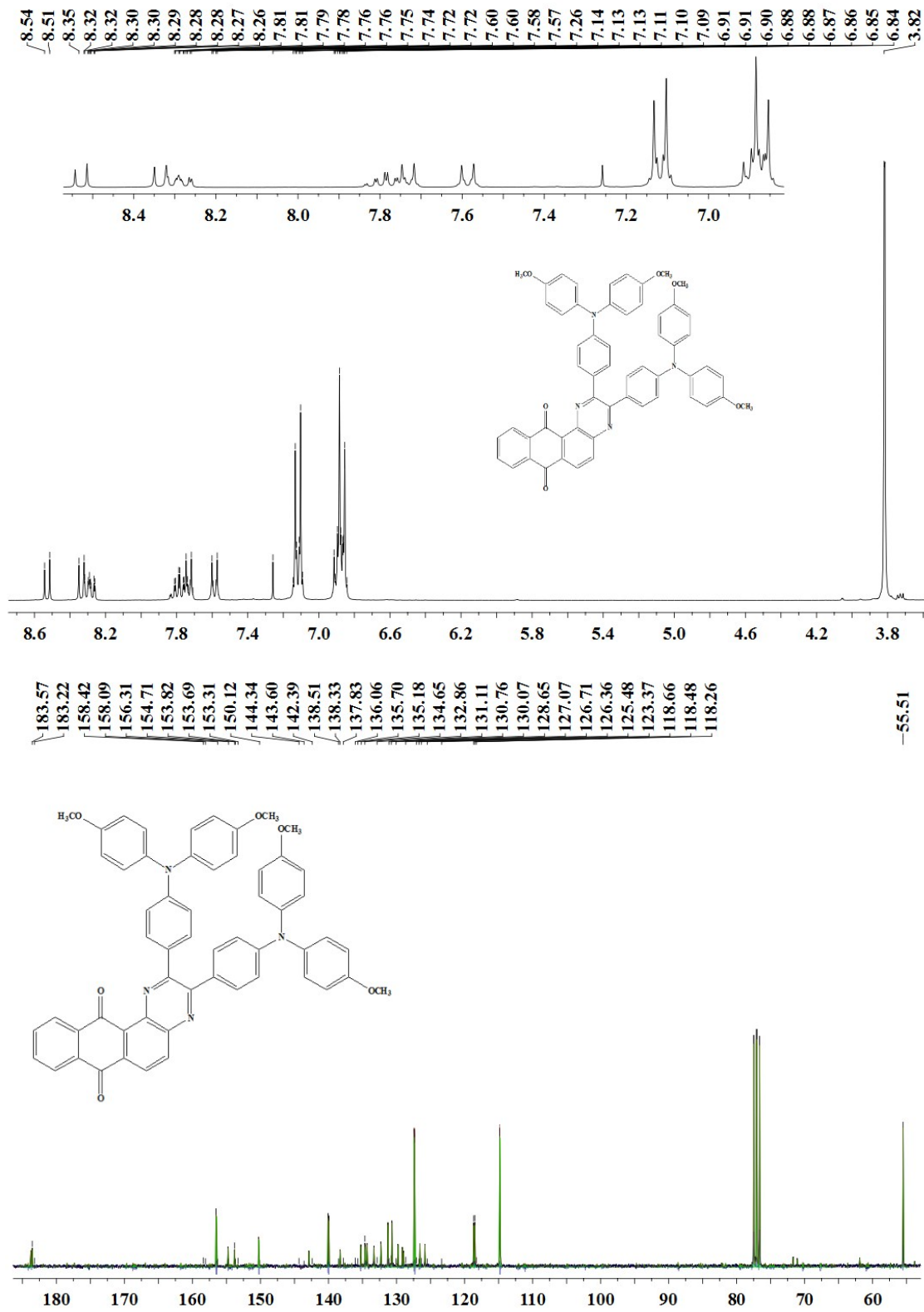


Figure S17: $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectra of compound 4 in CDCl_3 .

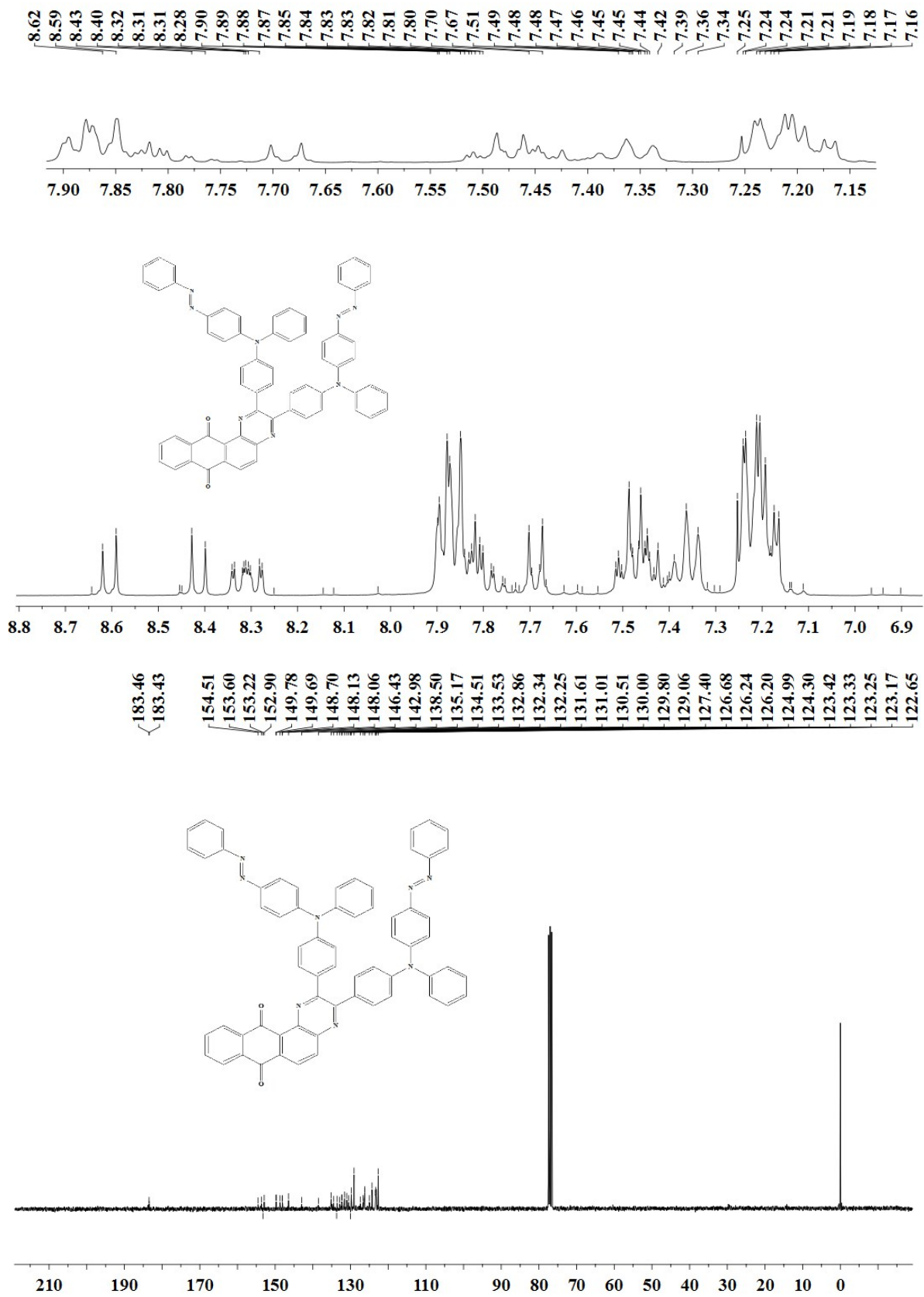


Figure S19: ¹H-NMR and ¹³C-NMR spectra of compound 6 in CDCl₃.

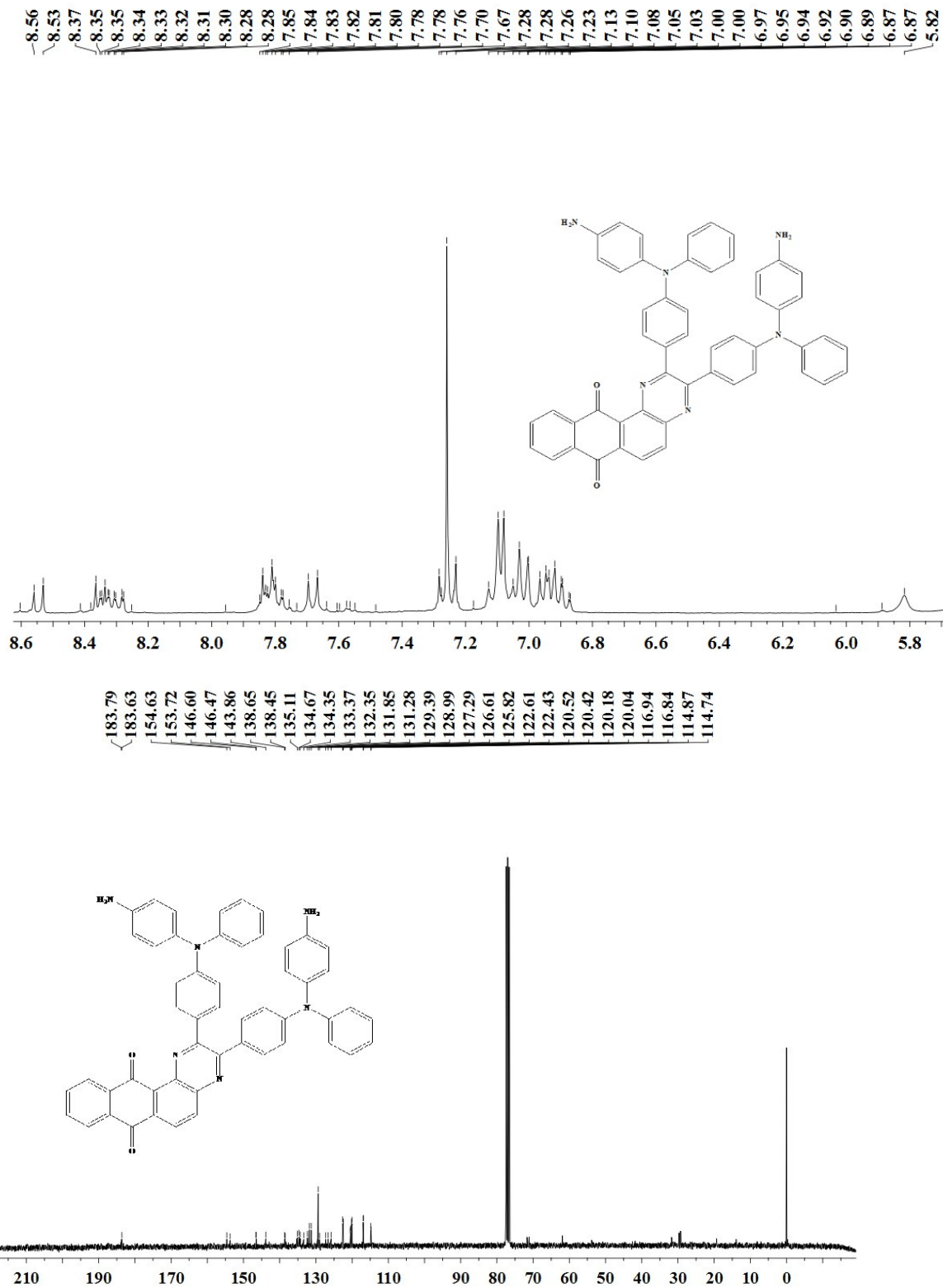


Figure S20: ¹H-NMR and ¹³C-NMR spectra of compound 7 in CDCl₃.

5. Photophysical data of compounds 2-7 in various solvents:

i) Photophysical data of compounds 2-7 in Dichloromethane.

Compound	λ_{abs} , nm ^a (log ϵ_{max} M ⁻¹ cm ⁻¹)	λ_{em} ^a nm	Stokes shift cm ⁻¹	ϕ_{F}
2	262 (4.80), 350 (4.63), 518(4.22)	416, 436	15232	0.100
3	263 (4.84), 350 (4.62), 519(4.12)	415, 434	14981	0.030
4	266 (4.63), 350 (4.42), 552(4.03)	417, 437	14710	0.030
5	260 (5.04), 337 (4.69), 407(4.86)	415, 433	15366	0.006
6	266 (4.64), 423 (4.49)	415, 433	14499	0.010
7	263 (4.41), 293 (4.49), 524 (3.77)	416, 434	14981	0.170

^aRecorded in 10⁻⁵ M dichloromethane.

ii) Photophysical data of compounds 2-7 in Chloroform.

Compound	λ_{abs} , nm ^a (log ϵ_{max} M ⁻¹ cm ⁻¹)	λ_{em} ^a nm	Stokes shift cm ⁻¹	ϕ_{F}
2	263 (4.85), 350(4.67), 535(4.27)	416, 435	15034	0.005
3	265 (5.04), 349 (4.83), 531(4.41)	416, 438	14904	0.003
4	266 (4.77), 361 (4.53), 561(4.13)	415, 438	14762	0.127
5	260 (5.08), 339 (4.74), 405(4.90)	415, 438	15630	0.006
6	266 (4.13), 422 (4.29)	413, 435	14605	0.090
7	293 (3.90), 545 (2.95)	415, 435	11141	0.080

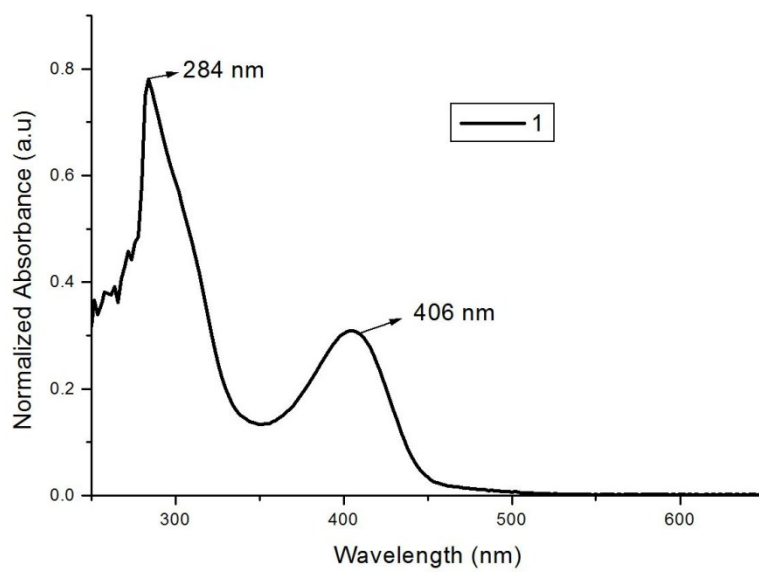
^aRecorded in 10⁻⁵ M in chloroform.

iii) Photophysical data of compounds 2-7 in n-hexane, acetonitrile and methanol.

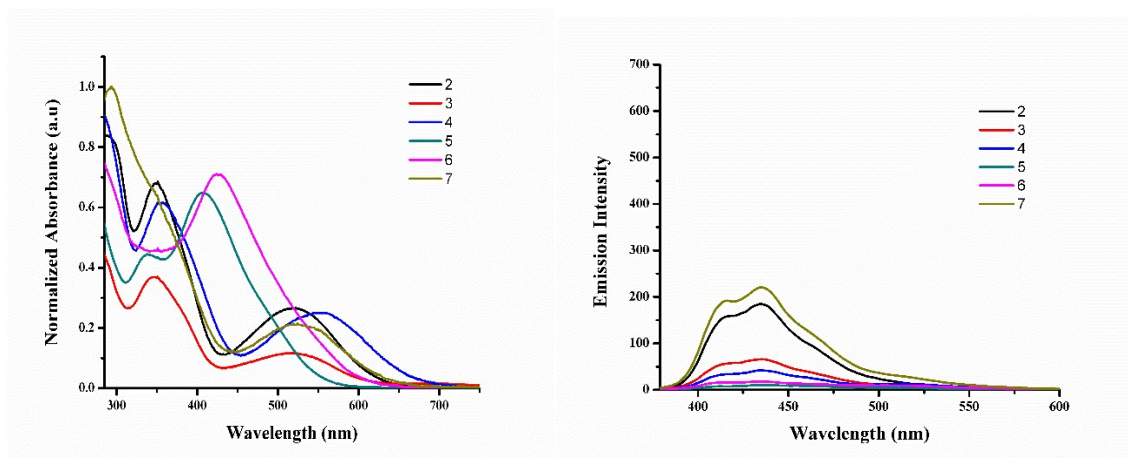
Compound	$\lambda_{\text{abs}}^{\text{a}}, \text{nm}$ ($\log \epsilon_{\text{max}} \text{M}^{-1} \text{cm}^{-1}$)	$\lambda_{\text{em}}^{\text{a}}$ nm	$\lambda_{\text{abs}}^{\text{b}}, \text{nm}$ ($\log \epsilon_{\text{max}} \text{M}^{-1} \text{cm}^{-1}$)	$\lambda_{\text{em}}^{\text{b}}$ nm	$\lambda_{\text{abs}}^{\text{c}}, \text{nm}$ ($\log \epsilon_{\text{max}} \text{M}^{-1} \text{cm}^{-1}$)	$\lambda_{\text{em}}^{\text{c}}$ nm
2	261 (4.45), 342 (4.33), 503 (3.98)		261 (4.83), 340 (4.65), 498 (4.23)		263 (4.19), 350 (4.02), 508 (3.60)	
3	261 (5.04), 341 (4.88), 504 (4.50)		261 (5.08), 339 (4.88), 497 (4.43)		261 (4.85), 341 (4.66), 507 (4.21)	
4	279 (4.89), 350 (4.76), 532(4.43)		264 (5.18) 347 (4.97), 523 (4.57)		265(4.89), 350 (4.67), 538 (4.28)	
5	256 (4.12), 381 (4.09), 458 (3.70)		259 (4.87), 335 (4.47), 404 (4.67)		258 (5.03), 405 (4.84),	
6	262(4.62), 417 (4.48)		261 (4.55), 343(4.22), 425 (4.25)		264 (4.51), 415 (4.30)	
7	261 (4.78), 334 (4.66), 528 (4.32)	415, 435	291 (4.79), 520 (4.14)		254 (4.46), 295 (4.60), 542 (3.92)	

^aRecorded in 10^{-5} M n-hexane, ^bRecorded in 10^{-5} M acetonitrile and ^cRecorded in 10^{-5} M methanol.

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



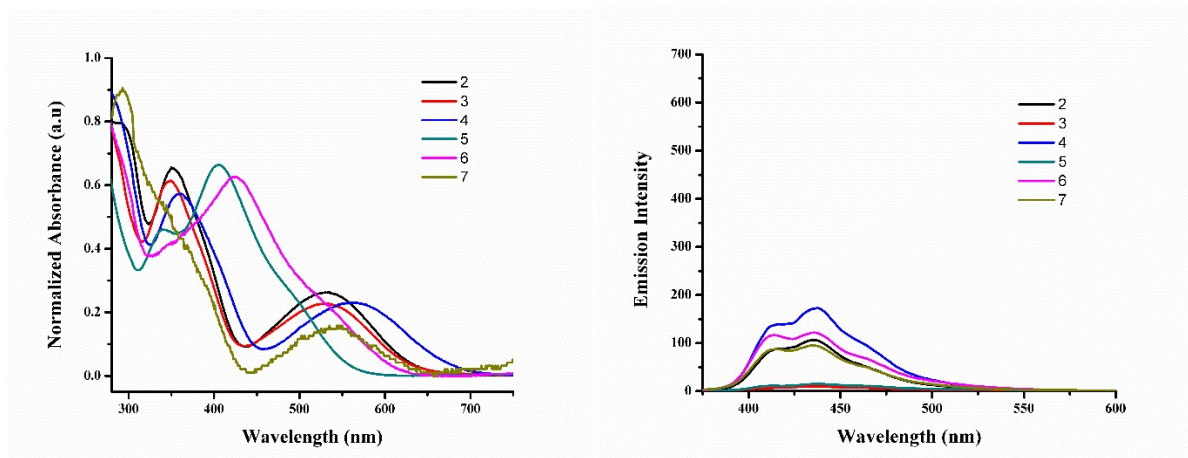
7. Absorption and Emission spectra of compounds 2-7 in various solvents:



(a)

(b)

Figure S21: Absorption spectra (a) and Emission spectra (excited at $\lambda=350$ nm) (b) of 2-7 in dichloromethane.



(a)

(b)

Figure S22: Absorption spectra (a) and Emission spectra (excited at $\lambda=350$ nm) (b) of 2-7 in chloroform.

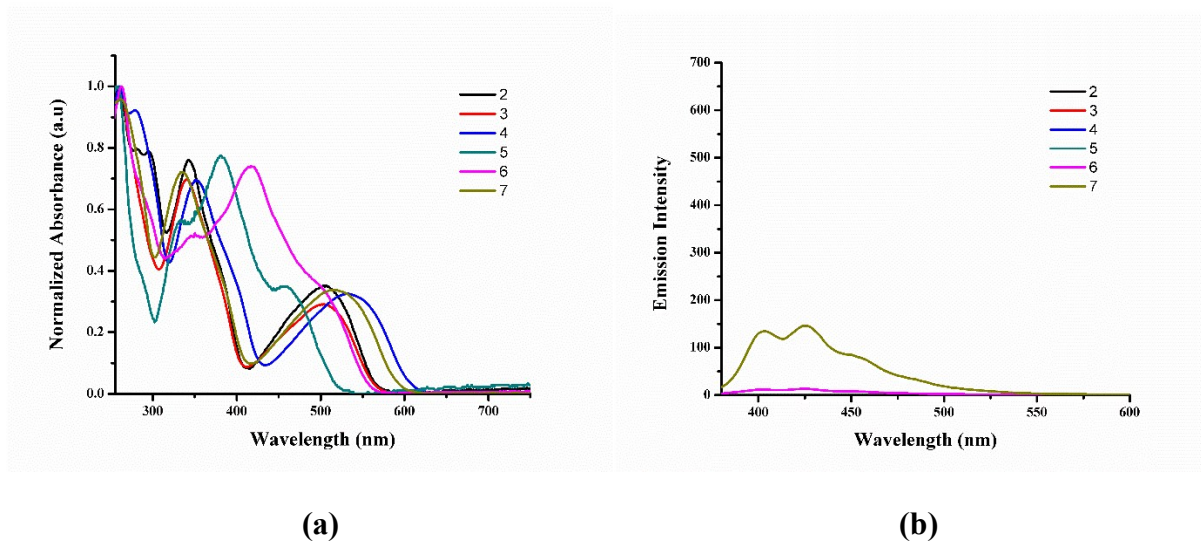


Figure S23: Absorption spectra (a) and Emission spectra (excited at $\lambda=350$ nm) (b) of 2-7 in n-hexane.

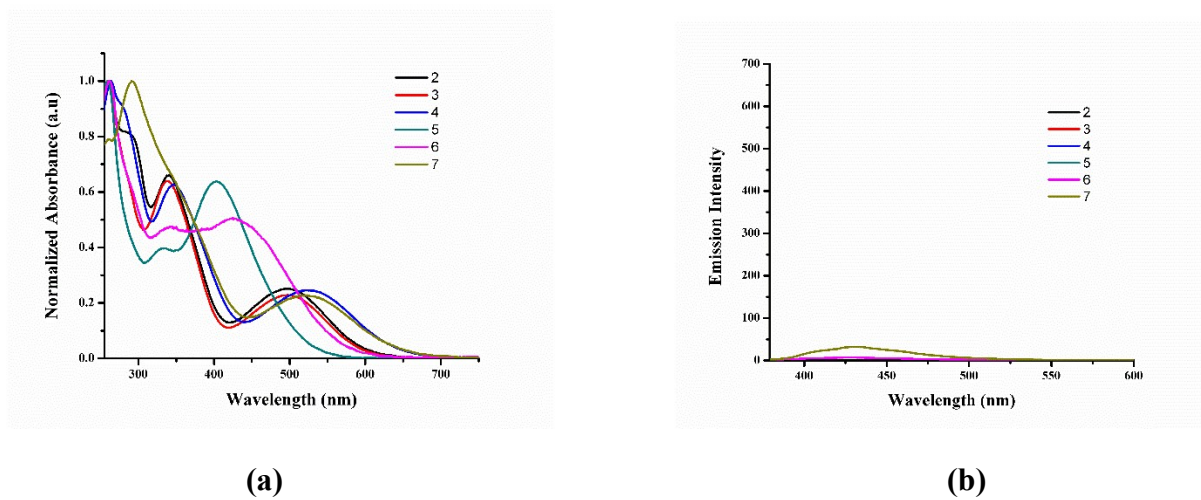
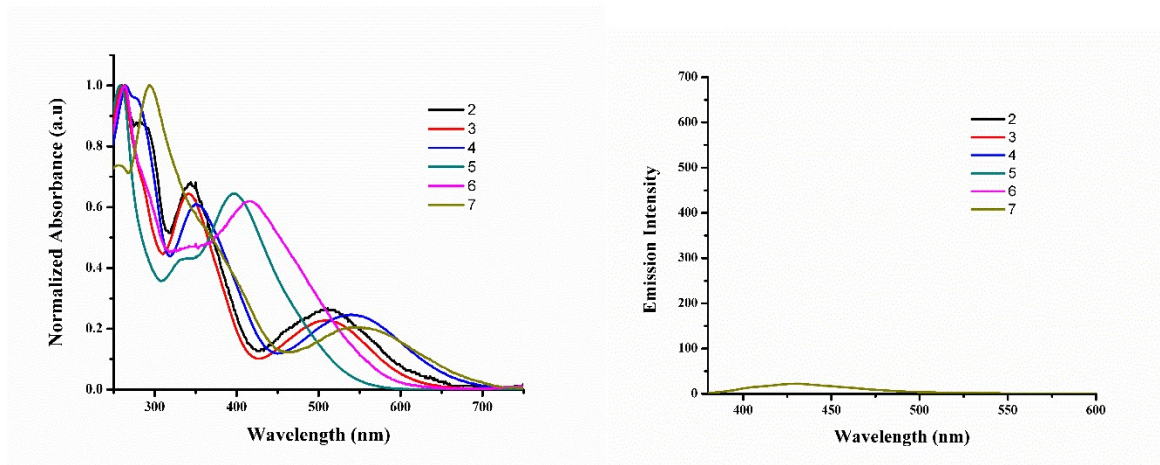


Figure S24: Absorption spectra (a) and Emission spectra (excited at $\lambda=350$ nm) (b) of 2-7 in acetonitrile.

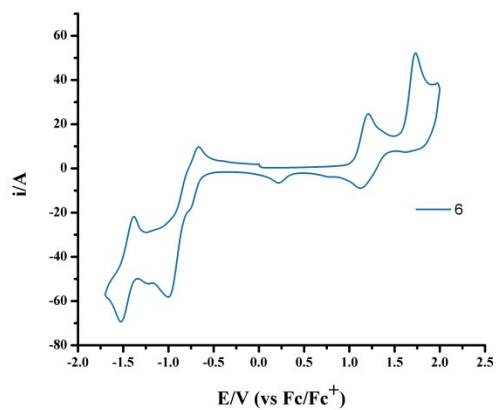
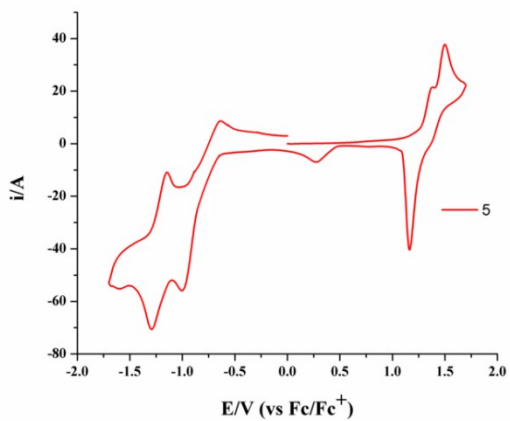
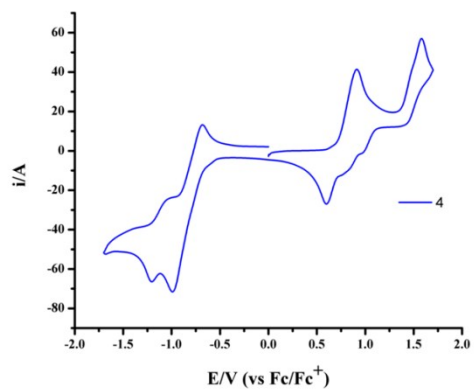
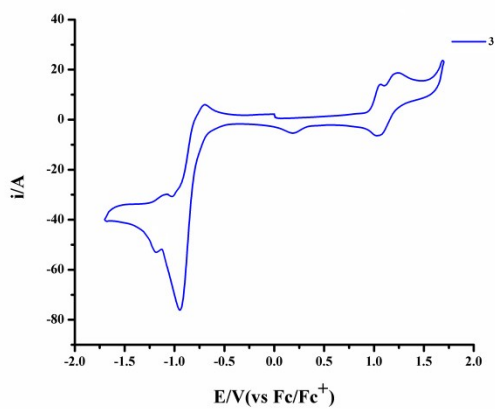
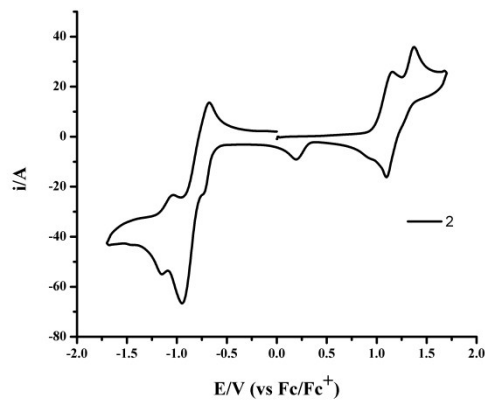
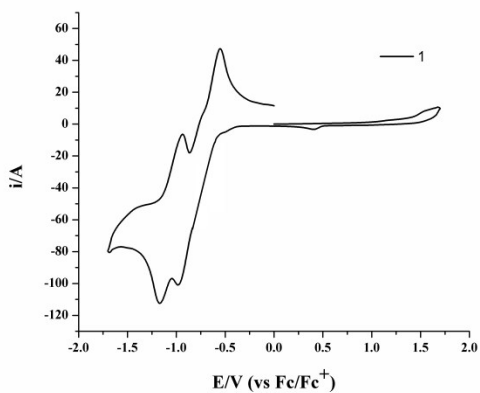


(a)

(b)

Figure S25: Absorption spectra (a) and Emission spectra (excited at $\lambda=350$ nm) (b) of **2-7** in methanol.

8. Cyclic voltammetry (CV) and Differential Pulse Voltammetry (DPV) of compounds 1-7 in anhydrous dichloromethane.



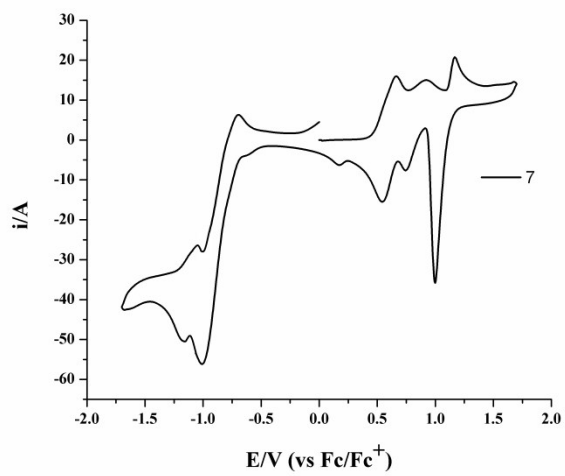


Figure S26: Full scan of compounds **1** **7** in anhydrous dichloromethane with scan rate 100mV⁻¹.

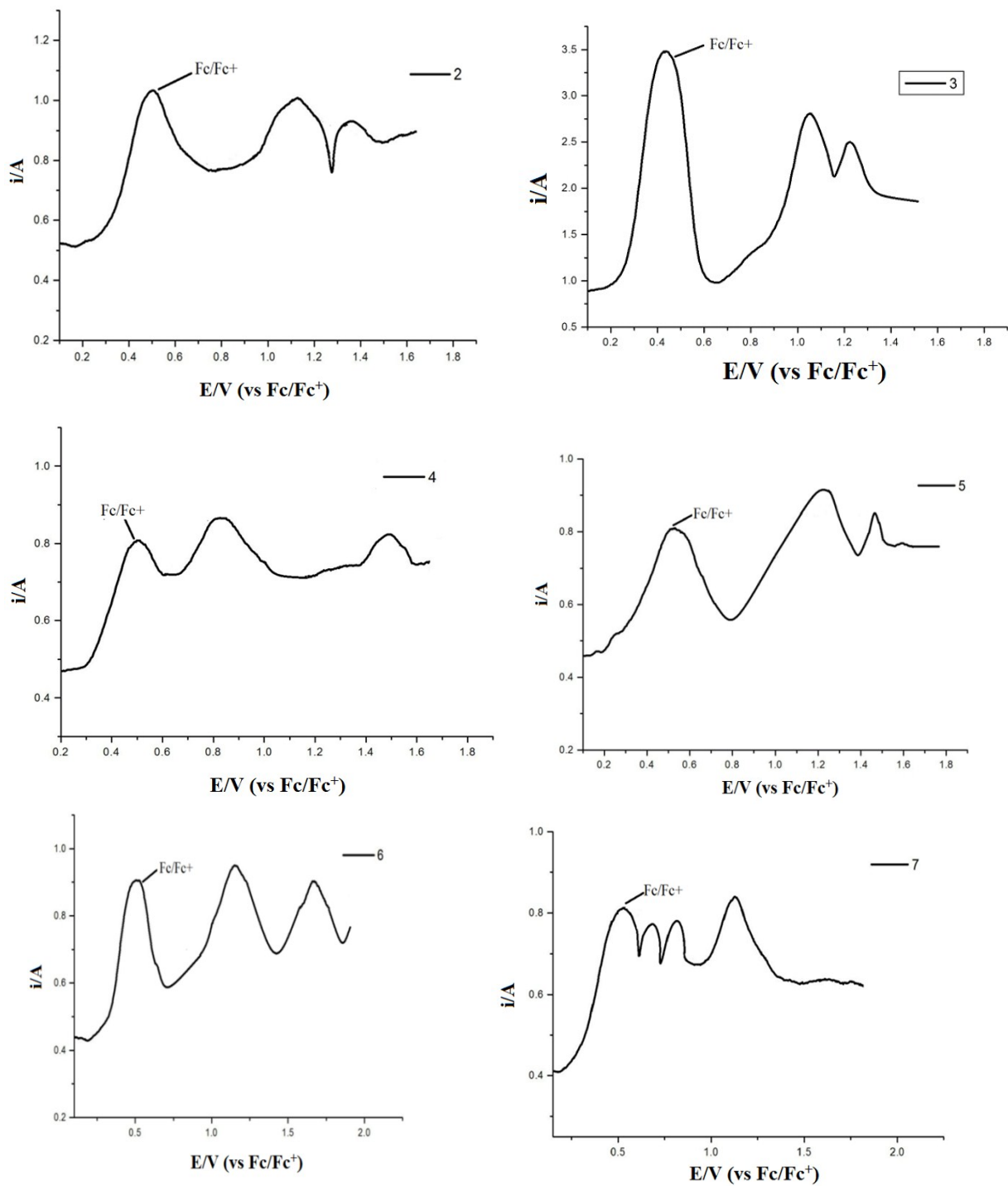


Figure S27: DPV plots (anodic sweep) of compounds 2–7.

9. Optimized structure of compounds 2-7 based on DFT (B3LYP/6-311G) calculations.

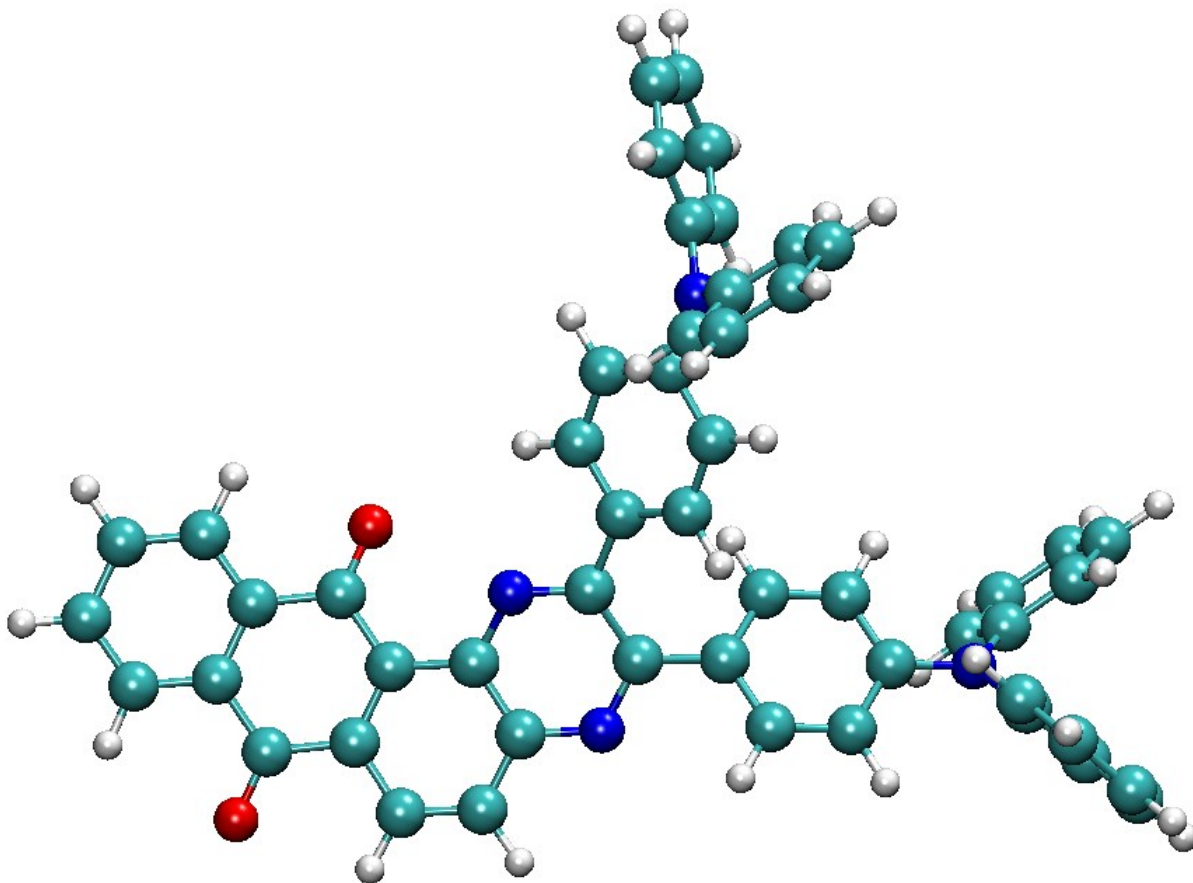


Figure S28: Optimized structure of compound 2

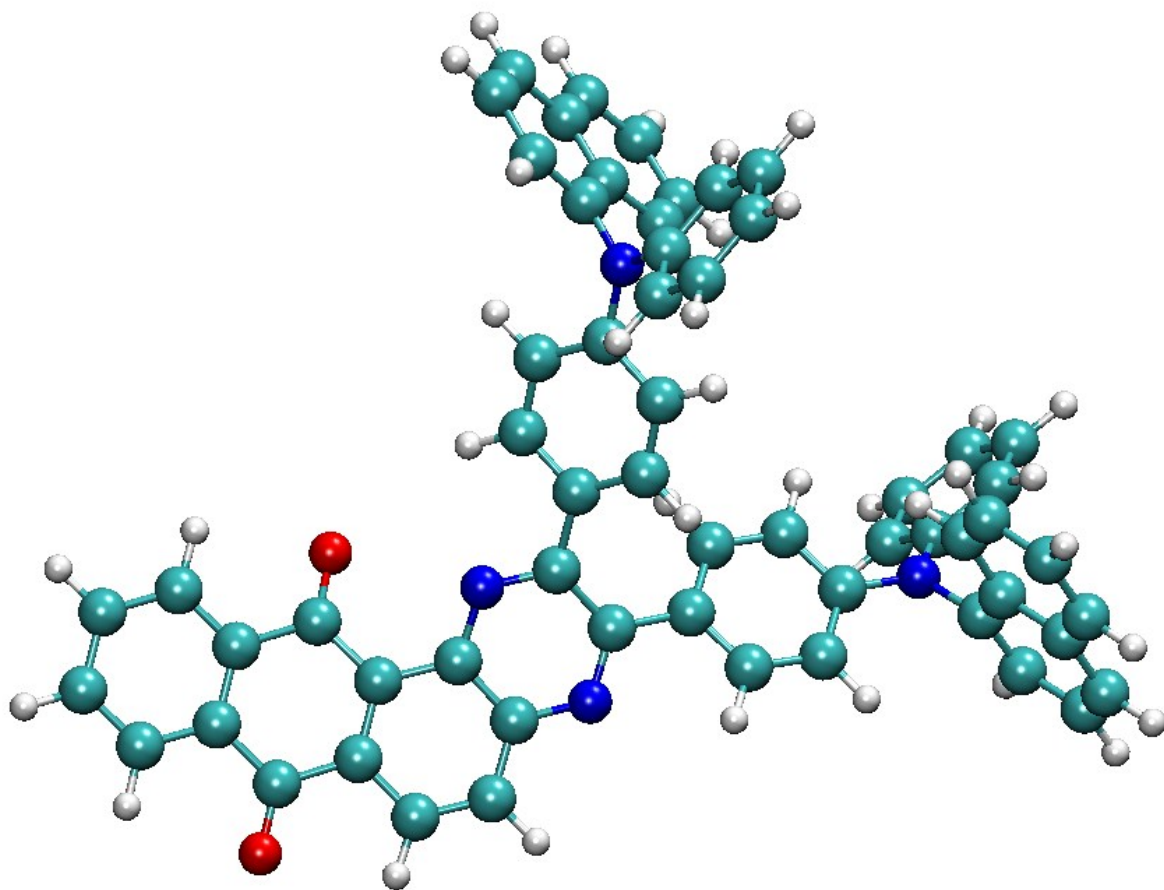


Figure S29: Optimized structure of compound 3

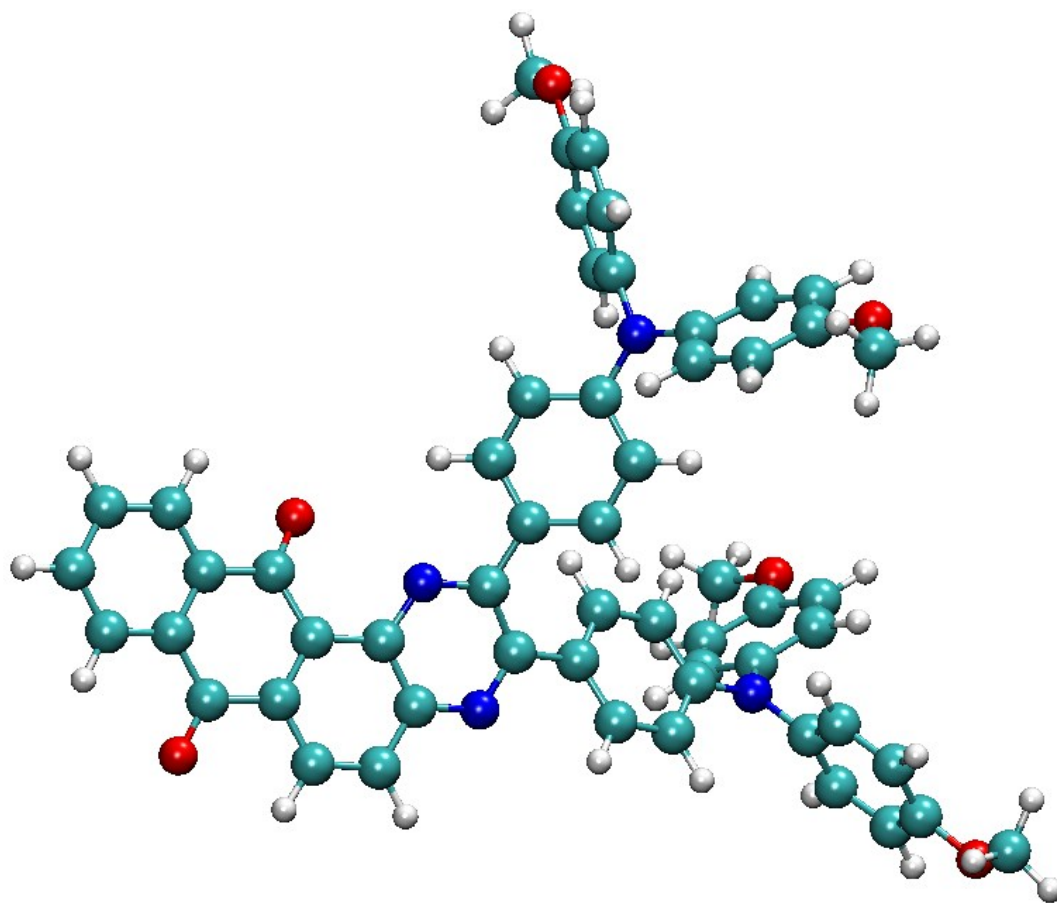


Figure S30: Optimized structure of compound 4

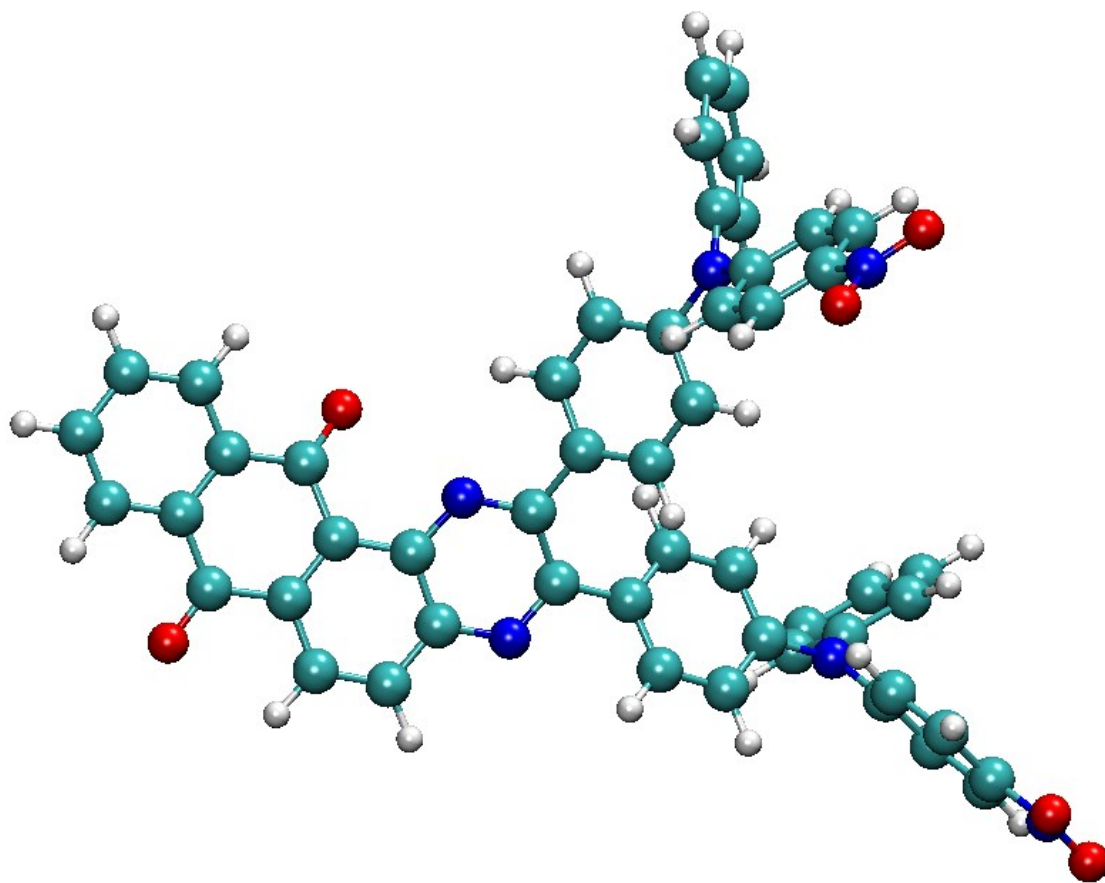


Figure S31: Optimized structure of compound **5**

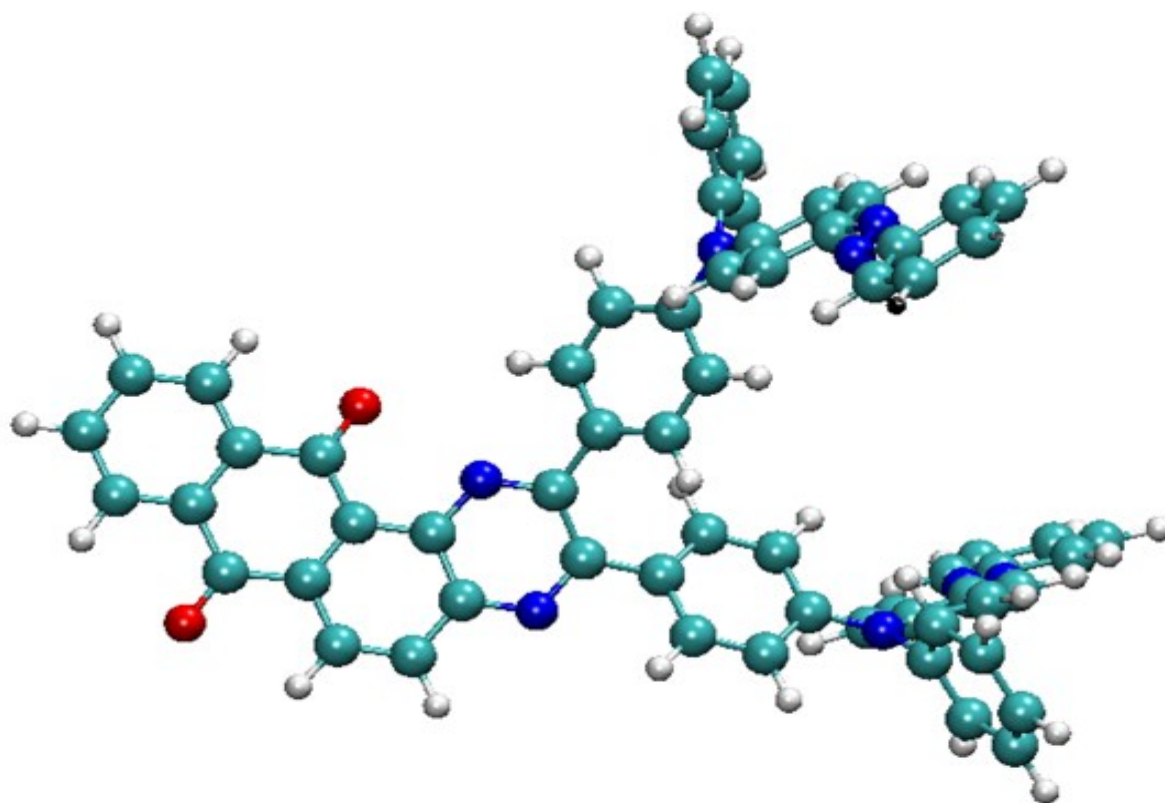


Figure S32: Optimized structure of compound 6

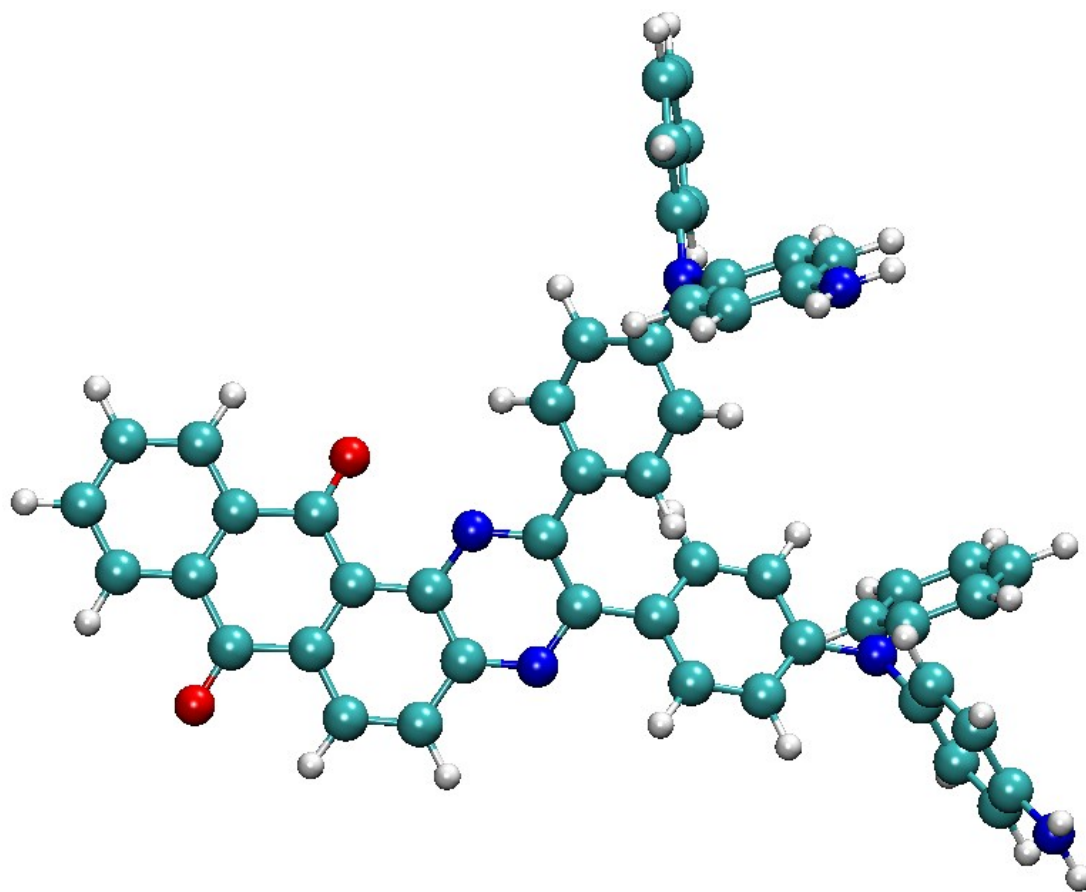


Figure S33: Optimized structure of compound 7

10. Frontier molecular orbital of compounds 4 7 based on DFT (B3LYP/6-311G) calculations.

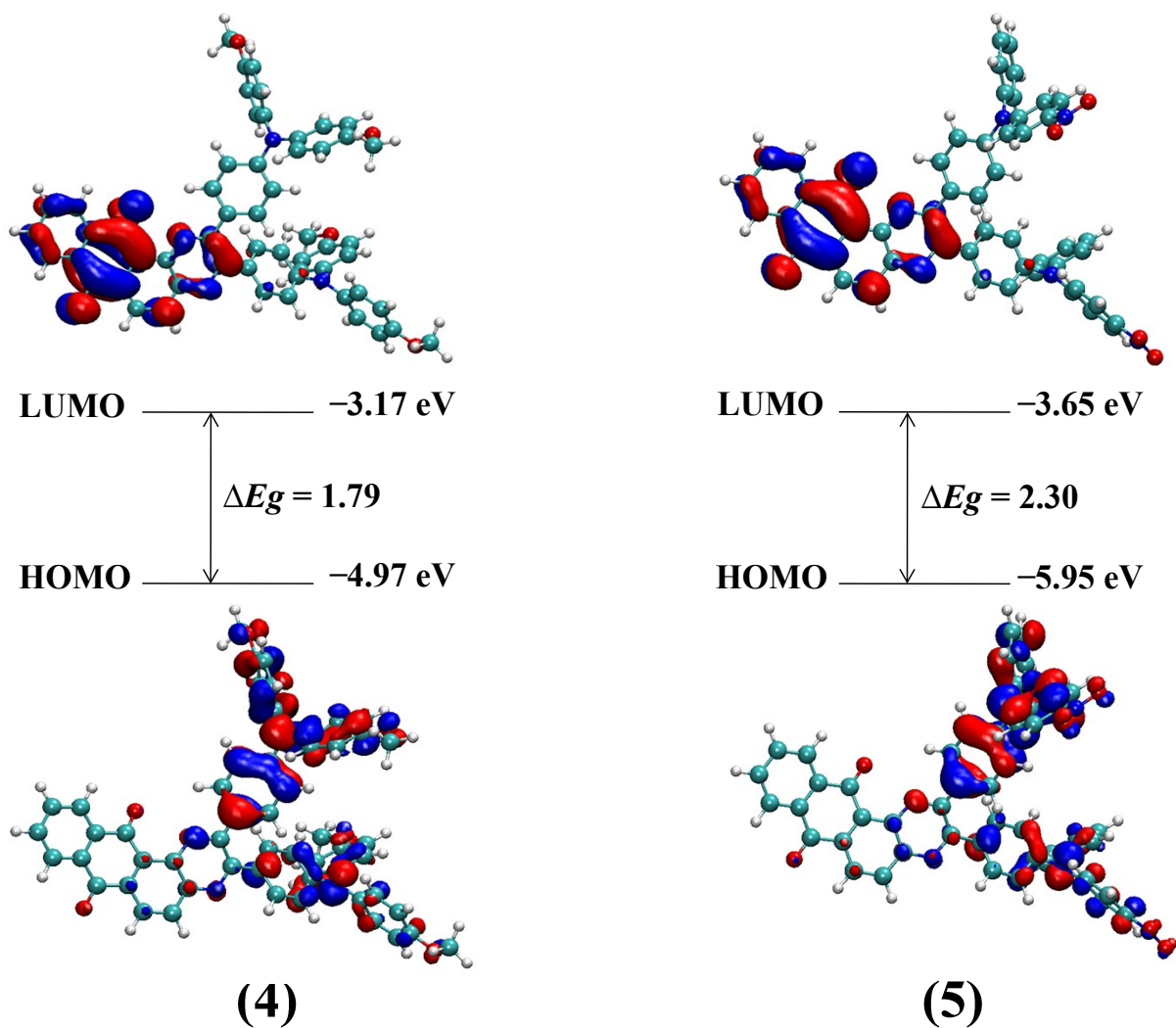
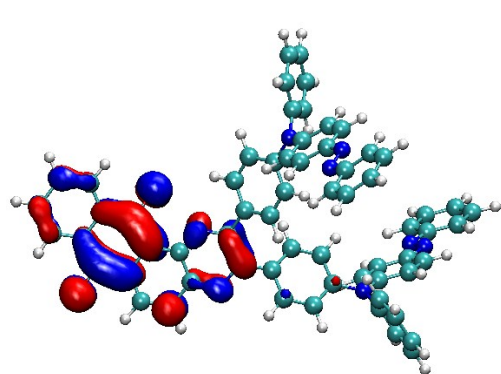
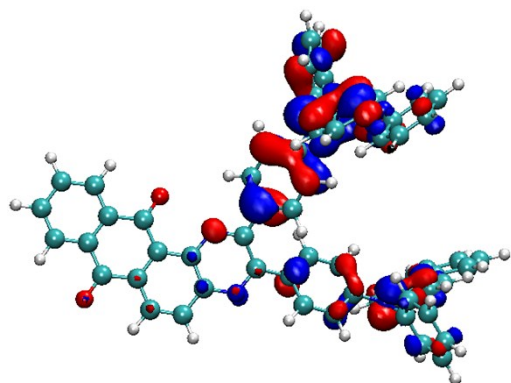


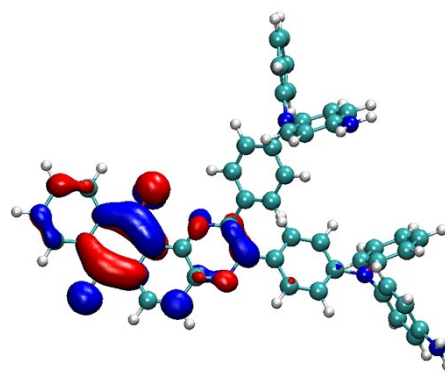
Figure S34: Frontier molecular orbital of compounds 4 and 5



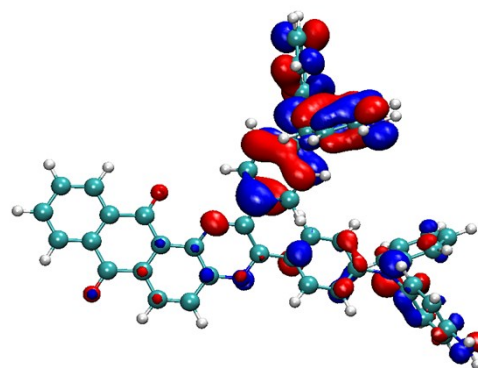
LUMO ———— -3.40 eV
↑
 $\Delta E_g = 1.99$
↓
HOMO ———— -5.39 eV



(6)



LUMO ———— -3.11
↑
 $\Delta E_g = 1.74$
↓
HOMO ———— -4.85 eV



(7)

Figure S35: Frontier molecular orbital of compounds 6 and 7

11. Differential Scanning Calorimetry (DSC) and Derivative weight loss plot of compounds 2-7.

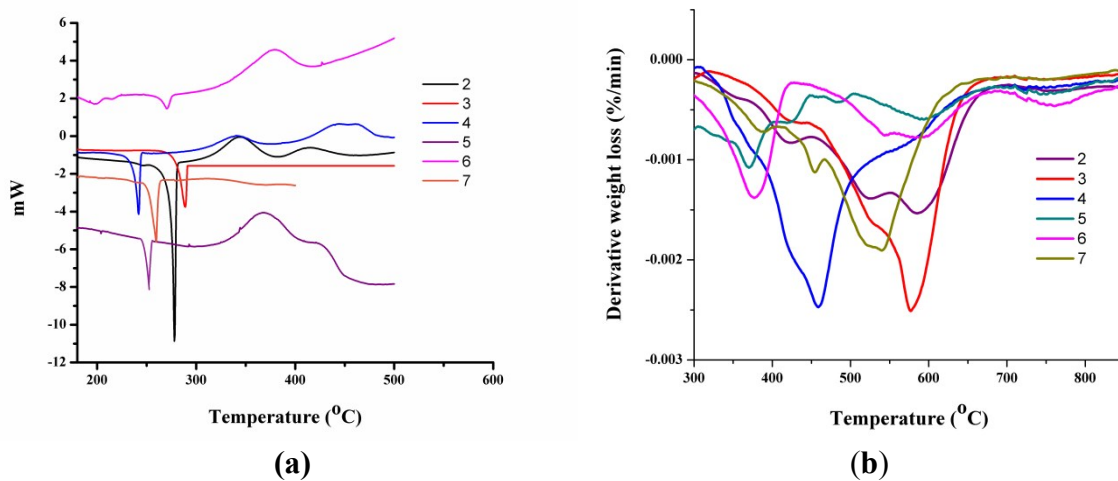


Figure S36: Differential scanning calorimetry (DSC) (a) Derivative weight loss (b) plot of compounds 2-7.

12. Glass transition temperature plots of compounds 4-6.

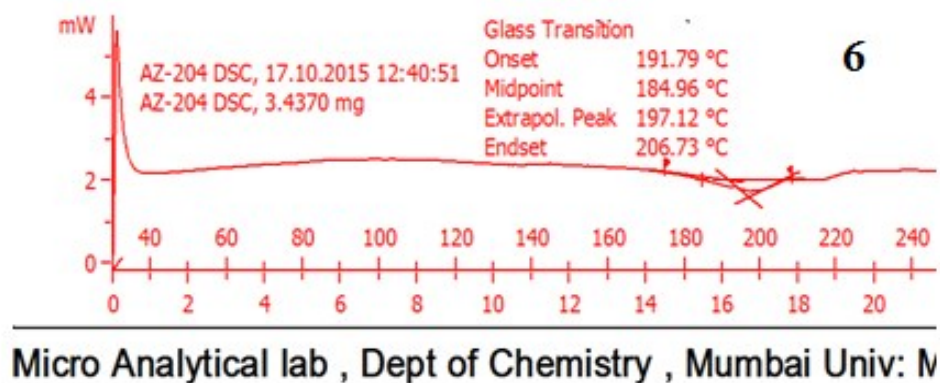
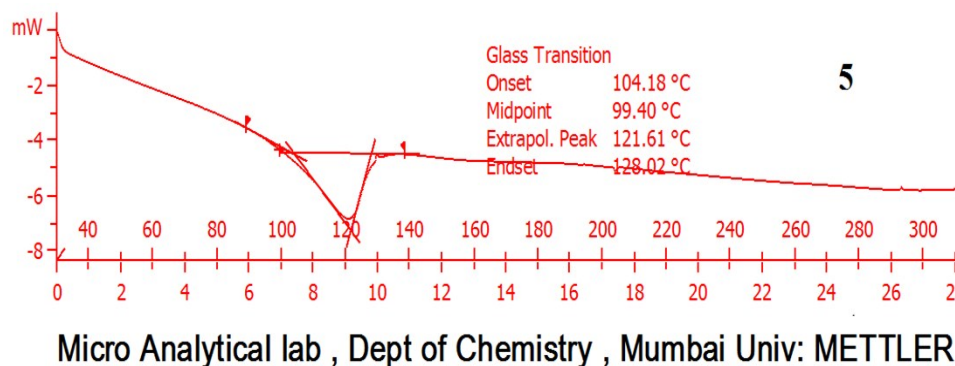
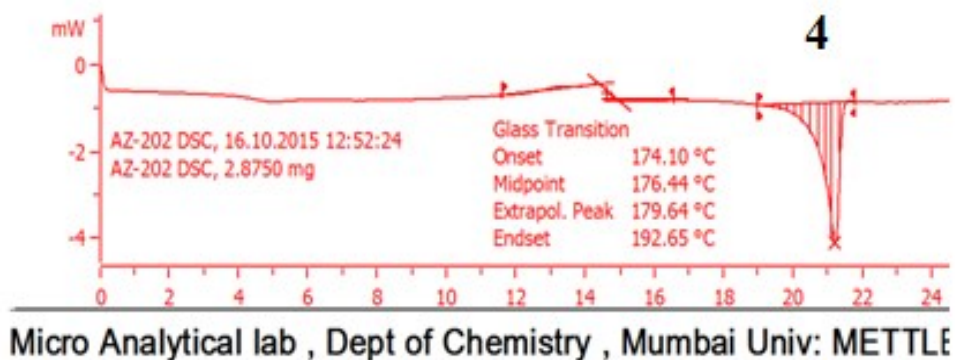


Figure: S37 Glass Transition Temperature of compounds **4**, **5** and **6**.

13. Cartesian coordinates of compounds 2-7.

a) Table S1. Cartesian coordinates for the optimized structure of compound 2.

Total energy: 2371.39951081 Hartrees

Atom	x	y	z
C	-0.27095464032447	5.34346079630652	7.57303512047607
C	-1.55790264032447	5.70894379630652	7.98958512047607
C	-2.66331764032446	5.37423879630652	7.21120812047607
C	-2.49134464032447	4.66358279630652	6.01541312047607
C	-1.19869964032447	4.29516579630652	5.59560312047607
C	-0.09186364032447	4.64682579630652	6.37913412047607
C	-3.66830264032447	4.31216779630652	5.19347612047607
C	-3.45791464032447	3.47666979630652	3.98190912047607
C	-2.17664464032447	3.06198479630652	3.59040712047607
C	-0.97985264032447	3.57793779630653	4.30639912047607
C	-4.61110764032447	3.09226479630652	3.24888312047607
C	-4.50217064032447	2.31297279630652	2.12212912047607
C	-3.22958164032447	1.85336479630652	1.71019812047607
C	-2.06828664032447	2.16629079630652	2.47923812047607
N	-3.10510464032447	1.15502479630652	0.53973612047607
C	-1.91320264032447	0.68019479630652	0.16809512047607
C	-0.80528464032447	0.74088379630652	1.11026912047607
N	-0.90022664032447	1.52470079630652	2.18536112047607
C	0.43085535967553	-0.06449220369348	1.02172812047607
C	-1.81929764032447	0.16779979630652	-1.21383987952393
C	0.46272335967553	-1.35647920369348	0.46586112047607
C	1.63146735967553	-2.10900220369348	0.46266312047607
C	2.81766235967553	-1.59397520369348	1.01920112047607
C	2.78746835967553	-0.30689920369348	1.59060912047607

C	1.61426935967553	0.43675379630652	1.59882512047607
C	-0.65886564032447	0.32689479630652	-1.99422587952393
C	-0.61869564032447	-0.09379720369348	-3.31817487952393
C	-1.74363864032447	-0.69406720369348	-3.91564287952393
C	-2.91187364032447	-0.84513720369348	-3.14297187952393
C	-2.94680064032447	-0.41423620369348	-1.82306287952393
N	4.01628235967553	-2.35743720369348	1.01162612047607
C	5.28523435967553	-1.71319920369348	0.84389712047607
C	3.97190135967553	-3.78093520369348	1.17103812047607
N	-1.70362864032447	-1.13006520369348	-5.26560287952393
C	-0.93209964032447	-0.41174320369348	-6.23751387952393
C	-2.42994464032447	-2.29479320369348	-5.67779487952393
O	0.17937335967553	3.46815179630652	3.85386412047607
O	-4.82008164032447	4.68243279630652	5.52114412047607
C	6.37127835967553	-2.06406720369348	1.66152512047607
C	7.60992335967553	-1.44607020369348	1.48683612047607
C	7.77982435967553	-0.46181620369348	0.50860912047607
C	6.69769335967553	-0.10649520369348	-0.30271387952393
C	5.46037235967553	-0.73192120369348	-0.14539587952393
C	4.74696135967553	-4.61040020369348	0.34418812047607
C	4.71386735967553	-5.99546120369348	0.51013212047607
C	3.90045535967553	-6.57298820369348	1.48928812047607
C	3.12406035967553	-5.74922920369348	2.31006612047607
C	3.16305035967553	-4.36248620369348	2.16124712047607
C	-0.09666164032447	-1.10310520369348	-7.12866387952393
C	0.64121235967553	-0.40370020369348	-8.08437287952393
C	0.56803235967553	0.99038279630652	-8.15533687952393
C	-0.25914364032447	1.68132779630652	-7.26466187952393
C	-1.01266964032447	0.98800879630652	-6.31657887952393

C	-3.18245864032447	-2.27574020369348	-6.86281987952393
C	-3.87538864032446	-3.41548420369348	-7.27283787952393
C	-3.84034064032446	-4.58190820369348	-6.50328687952393
C	-3.09615664032447	-4.60104320369348	-5.31993887952393
C	-2.38725864032446	-3.47092820369348	-4.91147087952393
H	0.58742735967553	5.60437379630652	8.17716212047607
H	-1.69328364032447	6.25370379630652	8.91386612047607
H	-3.66566364032447	5.65152579630652	7.50348912047607
H	0.89166735967553	4.36836179630652	6.02997812047607
H	-5.56683064032446	3.45223679630652	3.59909212047607
H	-5.35901864032447	2.04560079630652	1.52052412047607
H	-0.43141864032447	-1.78250520369348	0.03467512047607
H	1.63154535967553	-3.09826220369348	0.02911312047607
H	3.68308835967553	0.09772579630652	2.03927812047607
H	1.58373135967553	1.40602679630652	2.07535212047607
H	0.22030535967553	0.78544679630652	-1.56558287952393
H	0.28450135967553	0.03904479630652	-3.89501487952393
H	-3.79037964032447	-1.28884220369348	-3.58803887952393
H	-3.85677264032446	-0.50388920369348	-1.24827887952393
H	6.23836235967553	-2.81527720369348	2.42706912047607
H	8.43838635967554	-1.72505120369348	2.12433412047607
H	8.73920535967553	0.02055079630652	0.37994612047607
H	6.81896335967553	0.64872779630652	-1.06819287952393
H	4.62958035967553	-0.46631820369348	-0.78365187952393
H	5.36828335967553	-4.16587620369348	-0.42035387952393
H	5.31560235967553	-6.62282520369348	-0.13401987952393
H	3.87273635967553	-7.64701920369348	1.61211012047607
H	2.49704435967553	-6.18412520369348	3.07719712047607
H	2.57375935967553	-3.72654320369348	2.80656512047607

H	-0.03089264032447	-2.18000020369348	-7.06715387952393
H	1.28168635967553	-0.94818020369348	-8.76537487952393
H	1.14550535967553	1.52999379630652	-8.89339387952393
H	-0.33014264032447	2.75979979630652	-7.31514087952393
H	-1.66302264032447	1.52198479630652	-5.63809387952393
H	-3.22089464032446	-1.37106920369348	-7.45276087952393
H	-4.45206164032447	-3.38662920369348	-8.18787087952393
H	-4.38318164032447	-5.46154420369348	-6.82098787952393
H	-3.05444764032447	-5.50051520369348	-4.71998687952393
H	-1.79991264032447	-3.49325120369348	-4.00445187952393

b) Table S2. Cartesian coordinates for the optimized structure of compound **3**.

Total energy: 2678.67077603 Hartrees

Atom	x	y	z
C	3.72842859150736	8.97922662424571	0.50647943350124
C	4.49704459150736	9.38979062424571	-0.59088956649876
C	4.79562259150736	8.48729362424571	-1.60892756649876
C	4.31987359150736	7.17048162424571	-1.54209056649876
C	3.54693259150736	6.75693062424571	-0.44048256649876
C	3.26214059150736	7.66811062424571	0.58449343350124
C	4.64101759150736	6.21740762424571	-2.62503356649876
C	4.04016459150736	4.85896562424571	-2.56974756649876
C	3.22382859150736	4.46127662424571	-1.50027856649876
C	3.06347459150736	5.35139162424571	-0.32029156649876
C	4.30358959150736	3.98629062424571	-3.65744956649876
C	3.77651859150736	2.71730562424571	-3.68616956649876
C	2.92731059150736	2.28906662424571	-2.63967756649876
C	2.59029759150736	3.17981862424571	-1.57628556649876

N	2.47492659150736	0.99718862424571	-2.61697556649876
C	1.63789959150736	0.59882162424571	-1.65538356649876
C	1.06338159150736	1.59638262424571	-0.76369556649876
N	1.59874659150736	2.81654562424571	-0.71142356649876
C	-0.14086640849264	1.39666862424571	0.06832343350124
C	1.40405459150736	-0.85543237575429	-1.55720756649876
C	-0.28310040849264	2.14135862424571	1.25437043350124
C	-1.42119540849264	2.02837862424571	2.04318343350124
C	-2.47779040849264	1.17894262424571	1.66231243350124
C	-2.34914340849264	0.44573862424571	0.46525143350124
C	-1.20324840849264	0.55536162424571	-0.31290856649876
C	1.45824059150736	-1.65352037575429	-2.71401356649876
C	1.30878459150736	-3.03314337575429	-2.64877556649876
C	1.11862159150736	-3.67659037575429	-1.41034056649876
C	1.07796859150736	-2.88384937575429	-0.24491856649876
C	1.21847459150736	-1.50393237575429	-0.32099656649876
N	-3.62902940849264	1.04548862424571	2.47963343350124
C	-4.92306340849264	0.78835962424571	1.92160943350124
C	-3.54238340849264	1.31965162424571	3.89276543350124
N	0.94258059150736	-5.08076837575429	-1.34660756649876
C	0.46421559150736	-5.79800637575429	-2.50318956649876
C	1.36884759150736	-5.84442637575429	-0.21101056649876
O	2.58181659150736	4.95885062424571	0.76359543350124
O	5.37637559150736	6.55157662424571	-3.58339656649876
C	-5.33946140849264	1.41687262424571	0.73600843350124
C	-6.61009340849264	1.16523962424571	0.21694043350124
C	-7.48958440849264	0.30204862424571	0.87731343350124
C	-7.08222940849264	-0.31307937575429	2.06475243350124
C	-5.80801240849264	-0.07933837575429	2.58256543350124

C	-2.77823540849264	0.45979962424571	4.74890643350124
C	-2.70921540849264	0.77690062424571	6.14939743350124
C	-3.41638640849264	1.90643562424571	6.64651543350124
C	-4.16405440849264	2.69454562424571	5.80068843350124
C	-4.22083340849264	2.40291162424571	4.41834143350124
C	-0.88112440849264	-5.61040037575429	-2.96240456649876
C	-1.31090840849264	-6.33239737575429	-4.12887356649876
C	-0.40872140849264	-7.22538737575429	-4.77065056649876
C	0.86708159150736	-7.40414237575429	-4.28483256649876
C	1.30595759150736	-6.68186537575429	-3.15121556649876
C	2.58812759150736	-5.57083237575429	0.43075243350124
C	2.99233359150736	-6.33708637575429	1.52477443350124
C	2.20128659150736	-7.39509937575429	1.98236343350124
C	0.99483859150736	-7.67800837575429	1.33539443350124
C	0.57553059150736	-6.90700537575429	0.25085943350124
C	-2.10465940849264	-0.70229537575429	4.27876343350124
C	-1.38453640849264	-1.49951737575429	5.14190543350124
C	-1.29753940849264	-1.17564037575429	6.51862543350124
C	-1.94815740849264	-0.06552537575429	7.00811343350124
C	-1.81335140849264	-4.76002837575429	-2.30452156649876
C	-3.09725640849264	-4.61411337575429	-2.78366856649876
C	-3.51521740849264	-5.30791137575429	-3.94633656649876
C	-2.64191440849264	-6.14852337575429	-4.59898556649876
H	3.49788859150736	9.68023062424571	1.29730643350124
H	4.86128959150736	10.40661662424571	-0.64663956649876
H	5.39377659150736	8.77403862424571	-2.46166456649876
H	2.68118059150736	7.32499462424571	1.42796543350124
H	4.94641559150736	4.35102562424571	-4.44441356649876
H	3.99931959150736	2.01778962424571	-4.47899256649876

H	0.50755259150736	2.82370162424571	1.53132043350124
H	-1.50175940849264	2.60488962424571	2.95281143350124
H	-3.14751340849264	-0.21001837575429	0.15110743350124
H	-1.13875940849264	-0.01802737575429	-1.22618056649876
H	1.63391059150736	-1.17375737575429	-3.66544456649876
H	1.34768859150736	-3.62074137575429	-3.55397756649876
H	0.93333559150736	-3.35286337575429	0.71683543350124
H	1.18583259150736	-0.92636437575429	0.59140243350124
H	-4.67148440849264	2.09985362424571	0.23130843350124
H	-6.91729140849264	1.65786362424571	-0.69624156649876
H	-8.47599640849264	0.11490462424571	0.47542143350124
H	-7.75272040849264	-0.98380437575429	2.58572143350124
H	-5.49324340849264	-0.56287837575429	3.49643043350124
H	-3.36066940849264	2.13250662424571	7.70382243350124
H	-4.70308640849264	3.55031162424571	6.18418343350124
H	-4.79725740849264	3.03316362424571	3.75558843350124
H	-0.74549540849264	-7.76734137575429	-5.64528856649876
H	1.54780759150736	-8.08792637575429	-4.77364856649876
H	2.31359459150736	-6.81390937575429	-2.78244956649876
H	3.21306659150736	-4.76654637575429	0.06993943350124
H	3.93440759150736	-6.11563837575429	2.00883543350124
H	2.52151159150736	-7.99067237575429	2.82629643350124
H	0.37307659150736	-8.49379537575429	1.67977843350124
H	-0.36188740849264	-7.12272237575429	-0.24182056649876
H	-2.16775640849264	-0.95568737575429	3.23128043350124
H	-0.88155940849264	-2.38151237575429	4.76830943350124
H	-0.72297040849264	-1.80755337575429	7.18264143350124
H	-1.89403440849264	0.18231862424571	8.06088043350124
H	-1.50208040849264	-4.23068337575429	-1.41660856649876

H	-3.79443740849264	-3.96666037575429	-2.26877956649876
H	-4.52443240849264	-5.17853237575429	-4.31381256649876
H	-2.95818640849264	-6.68979037575429	-5.48196956649876

c) Table S3. Cartesian coordinates for the optimized structure of compound **4**.

Total energy = 2829.45513666 Hartrees

Atom	x	y	z
C	5.47222270943047	-3.18340805972063	7.61137025892681
C	4.94118470943047	-2.98410605972063	8.89273725892681
C	3.77302870943047	-2.24310305972063	9.05502225892681
C	3.12144970943047	-1.70491105972063	7.93672025892681
C	3.65285570943047	-1.90601905972063	6.64868325892681
C	4.83548270943047	-2.64103505972063	6.49650425892681
C	1.88209770943047	-0.91953905972063	8.11562425892681
C	1.16194770943047	-0.45418205972063	6.90213225892681
C	1.65919470943047	-0.70299105972063	5.61334925892681
C	3.00389270943047	-1.31275105972063	5.44405125892681
C	-0.06702829056953	0.22793294027937	7.09577425892681
C	-0.80130329056953	0.67577594027937	6.02329325892681
C	-0.34799229056953	0.41890094027937	4.70885325892681
C	0.84910670943047	-0.32876205972063	4.49419125892681
N	-1.02684829056953	0.94031394027937	3.64067425892681
C	-0.62729529056953	0.66788394027937	2.39498425892681
C	0.40274370943047	-0.34256805972063	2.19053525892681
N	1.13742270943047	-0.74735305972063	3.22808125892681
C	0.67430170943047	-1.03736705972063	0.91625825892681
C	-1.25117029056953	1.46898494027937	1.32455425892681
C	-0.31585629056953	-1.28091705972063	-0.05432674107319

C	-0.03373229056953	-2.00575105972063	-1.20590474107319
C	1.25907770943047	-2.51905705972063	-1.43593074107319
C	2.25115570943047	-2.28846605972063	-0.45991774107319
C	1.95918670943047	-1.57262505972063	0.69257625892681
C	-2.56729629056953	1.94397194027937	1.48185725892681
C	-3.16190429056953	2.75833894027937	0.52786425892681
C	-2.45098129056953	3.15348194027937	-0.62468574107319
C	-1.12539329056953	2.69769994027937	-0.77757374107319
C	-0.54304029056953	1.87251594027937	0.17643825892681
N	1.55094970943047	-3.25191205972063	-2.61078674107319
C	2.86877570943047	-3.23937805972063	-3.17954774107319
C	0.53607070943047	-4.03097405972063	-3.26174074107319
N	-3.04801129056953	3.99033394027937	-1.59633274107319
C	-4.46542729056953	3.96217894027937	-1.82266074107319
C	-2.25185229056953	4.90083594027937	-2.37031774107319
O	3.61638570943047	-1.31353005972063	4.35481025892681
O	1.42984670943047	-0.67813705972063	9.25965925892681
C	3.49330470943047	-4.44412505972063	-3.54865374107319
C	4.75850170943047	-4.43807705972063	-4.12254474107319
C	5.43404670943047	-3.22746105972063	-4.32340574107319
C	4.82782370943047	-2.02210505972063	-3.95617774107319
C	3.54591470943047	-2.03407805972063	-3.39806074107319
C	0.32901870943047	-3.91171905972063	-4.64752774107319
C	-0.63565929056953	-4.68022005972063	-5.28721374107319
C	-1.42522429056953	-5.57298305972063	-4.55102874107319
C	-1.23423029056953	-5.69824705972063	-3.17139774107319
C	-0.24817729056953	-4.93619605972063	-2.53743374107319
C	-5.20066929056953	5.15992094027937	-1.87125474107319
C	-6.56887429056953	5.14040594027937	-2.11170974107319

C	-7.23434229056953	3.92105194027937	-2.29259774107319
C	-6.51712129056953	2.72173994027937	-2.24175274107319
C	-5.13686929056953	2.75003294027937	-2.01964474107319
C	-2.39176529056953	4.95501294027937	-3.76841874107319
C	-1.64192729056953	5.85187794027937	-4.51937774107319
C	-0.72404929056953	6.70205794027937	-3.88915374107319
C	-0.57000729056953	6.65473094027937	-2.50003274107319
C	-1.34246529056953	5.76398594027937	-1.74853274107319
O	-2.37018929056953	-6.28723705972063	-5.28628874107319
C	-3.22007029056953	-7.24226405972063	-4.59899574107319
O	6.70100470943047	-3.33344705972063	-4.89510674107319
O	-8.60661929056953	4.01325094027937	-2.51756374107319
O	-0.01680029056953	7.55498194027937	-4.73447074107319
C	7.46899070943047	-2.12466105972063	-5.13109574107319
C	-9.36925129056953	2.79598394027937	-2.72619674107319
C	0.94278570943047	8.47988494027937	-4.15899874107319
H	6.38033870943047	-3.75754305972063	7.48609225892681
H	5.43955970943047	-3.40278505972063	9.75649625892681
H	3.34655270943047	-2.06560005972063	10.03163925892681
H	5.23448670943047	-2.76871905972063	5.50091725892681
H	-0.38905629056953	0.39549794027937	8.11255225892681
H	-1.71662629056953	1.23697694027937	6.14519825892681
H	-1.31841029056953	-0.90544705972063	0.08946925892681
H	-0.81240129056953	-2.17621705972063	-1.93437274107319
H	3.24424770943047	-2.68721805972063	-0.60501374107319
H	2.71220370943047	-1.43496605972063	1.45508925892681
H	-3.10846429056953	1.67710494027937	2.37759825892681
H	-4.17355929056953	3.10630594027937	0.67496625892681
H	-0.55787029056953	2.99195894027937	-1.64773174107319

H	0.47491870943047	1.54262694027937	0.02784925892681
H	2.97894370943047	-5.38025105972063	-3.38414574107319
H	5.24970270943047	-5.35575205972063	-4.41141274107319
H	5.32669270943047	-1.07678505972063	-4.10806074107319
H	3.07220070943047	-1.10085705972063	-3.12797074107319
H	0.93124070943047	-3.21700505972063	-5.21569874107319
H	-0.80455729056953	-4.60028505972063	-6.35115874107319
H	-1.82549029056953	-6.38604205972063	-2.58572574107319
H	-0.09005529056953	-5.04405005972063	-1.47358074107319
H	-4.69162629056953	6.10144394027937	-1.72189574107319
H	-7.14592129056953	6.05263594027937	-2.15272374107319
H	-7.00788829056953	1.77098794027937	-2.38599974107319
H	-4.58032729056953	1.82368894027937	-1.99622074107319
H	-3.09293329056953	4.29357794027937	-4.25735874107319
H	-1.73987529056953	5.90600994027937	-5.59377374107319
H	0.12590870943047	7.30575494027937	-1.99262374107319
H	-1.23460629056953	5.73849194027937	-0.67331574107319
H	-3.85802229056953	-7.66014605972063	-5.37055474107319
H	-2.63086829056953	-8.03882905972063	-4.13877574107319
H	-3.83459229056953	-6.75244205972063	-3.83993574107319
H	8.40316270943047	-2.46321805972063	-5.56653174107319
H	6.95770670943047	-1.45979805972063	-5.83120674107319
H	7.67001270943047	-1.59382105972063	-4.19761574107319
H	-10.39184929056953	3.12510594027937	-2.87720174107319
H	-9.02255629056953	2.25739894027937	-3.61122474107319
H	-9.31973929056953	2.14158894027937	-1.85267374107319
H	1.35205670943047	9.02452394027937	-5.00320674107319
H	0.45843470943047	9.17763794027937	-3.47201974107319
H	1.74491470943047	7.94888294027937	-3.64110474107319

d) Table S4. Cartesian coordinates for the optimized structure of compound **5**.

Total energy = 2780.36899014 Hartrees

Atom	x	y	z
C	8.79653517647612	2.57649485852145	3.73189451819118
C	9.43890117647612	3.62176285852145	3.05531451819118
C	8.93315217647612	4.08105685852145	1.84129151819118
C	7.77526717647612	3.50562985852145	1.30038451819118
C	7.12715117647612	2.45643285852145	1.98074451819118
C	7.65094817647612	1.99236285852145	3.19400651819118
C	7.24645217647612	3.99485085852145	0.01086151819118
C	5.96147717647612	3.42970085852145	-0.48517848180882
C	5.28313317647612	2.42905885852145	0.22167351819118
C	5.91772217647612	1.79928385852145	1.41152851819118
C	5.43592917647612	3.96565685852145	-1.69112048180882
C	4.24966917647612	3.50514285852145	-2.20868848180882
C	3.52035517647612	2.51565785852145	-1.50798248180882
C	3.99633117647612	2.02238985852145	-0.25646348180882
N	2.38166117647612	1.99138085852145	-2.05771448180882
C	1.66384217647612	1.09390585852145	-1.37858048180882
C	1.99720417647612	0.82810785852145	0.00942551819118
N	3.16591617647612	1.24407385852145	0.49617851819118
C	1.10273917647612	0.17712885852145	0.99416451819118
C	0.60190517647612	0.40229585852145	-2.14249248180882
C	-0.29664882352388	0.31265685852145	0.95692851819118
C	-1.09644682352388	-0.25413114147855	1.94471751819118
C	-0.51571282352388	-0.96888914147855	3.00509951819118
C	0.88133317647612	-1.10299814147855	3.05254651819118
C	1.67724017647612	-0.53086114147855	2.06667251819118

C	-0.06190182352388	1.07833885852145	-3.18250848180882
C	-1.01069682352388	0.43340785852145	-3.96727748180882
C	-1.32115782352388	-0.91843114147855	-3.73966048180882
C	-0.64895482352388	-1.60631814147855	-2.71660748180882
C	0.29730817647612	-0.95446214147855	-1.93214948180882
N	-1.33136482352388	-1.56961414147855	4.01731251819118
C	-1.01804882352388	-2.91029014147855	4.44143651819118
C	-2.40623682352388	-0.87151414147855	4.60508551819118
N	-2.27414182352388	-1.60126014147855	-4.55875448180882
C	-3.48744582352388	-0.99295314147855	-4.94466548180882
C	-1.96528782352388	-2.93845014147855	-5.00008648180882
O	5.49821617647612	0.73499685852145	1.91316451819118
O	7.84108817647612	4.88373485852145	-0.64043648180882
C	-0.88173982352388	-3.93132414147855	3.49124151819118
C	-0.55745982352388	-5.22603714147855	3.89978951819118
C	-0.37987182352388	-5.51449514147855	5.25603951819118
C	-0.52077882352388	-4.49637414147855	6.20388051819118
C	-0.83046782352388	-3.19648814147855	5.80119451819118
C	-2.38056282352388	0.53726485852145	4.71743751819118
C	-3.43762682352388	1.21949585852145	5.30044851819118
C	-4.53616682352388	0.50402585852145	5.78604651819118
C	-4.58333582352388	-0.88984114147855	5.69187851819118
C	-3.52779182352388	-1.57141514147855	5.10501051819118
C	-4.11932982352388	-0.04239314147855	-4.11146548180882
C	-5.31366682352388	0.54996685852145	-4.49357148180882
C	-5.89870282352388	0.19652485852145	-5.71286448180882
C	-5.29744982352388	-0.74579414147855	-6.55175148180882
C	-4.10061882352388	-1.33432414147855	-6.17099448180882
C	-0.74817082352388	-3.20002514147855	-5.64362548180882

C	-0.44211482352388	-4.49831814147855	-6.05483348180882
C	-1.35027082352388	-5.53924414147855	-5.83975648180882
C	-2.56648282352388	-5.27621414147855	-5.20217148180882
C	-2.87286682352388	-3.98305214147855	-4.77529848180882
N	-5.64061182352388	1.21789485852145	6.39896151819118
O	-5.58663982352388	2.48711985852145	6.44793851819118
O	-6.61428382352388	0.54331485852145	6.86063151819118
N	-7.14953182352388	0.81559085852145	-6.11201648180882
H	9.19110817647612	2.21940685852145	4.67340351819118
H	10.32939217647612	4.07071485852145	3.47341651819118
H	9.41444417647612	4.87840385852145	1.29391451819118
H	7.14841117647612	1.17595085852145	3.69157351819118
H	6.01329617647612	4.72942485852145	-2.18991548180882
H	3.85177817647612	3.86313685852145	-3.14715248180882
H	-0.76715282352388	0.86662585852145	0.15784651819118
H	-2.17024782352388	-0.14329314147855	1.89768451819118
H	1.33735017647612	-1.64438914147855	3.86884051819118
H	2.75408717647612	-0.59533114147855	2.12420151819118
H	0.19733917647612	2.10759685852145	-3.38053848180882
H	-1.50181982352388	0.96821685852145	-4.76736148180882
H	-0.86576782352388	-2.65044414147855	-2.54420648180882
H	0.80681617647612	-1.50836714147855	-1.15723648180882
H	-1.02957782352388	-3.70605014147855	2.44443251819118
H	-0.45320382352388	-6.00898214147855	3.16080651819118
H	-0.13323282352388	-6.51921514147855	5.57043751819118
H	-0.37712982352388	-4.70949714147855	7.25447251819118
H	-0.92454482352388	-2.40457414147855	6.53092051819118
H	-1.52324782352388	1.08655585852145	4.36041051819118
H	-3.42145882352388	2.29319185852145	5.40122551819118

H	-5.44792182352388	-1.41466814147855	6.06641651819118
H	-3.56762482352388	-2.64631614147855	5.01983751819118
H	-3.67587882352388	0.21558185852145	-3.16220748180882
H	-5.80922282352388	1.26850985852145	-3.86004248180882
H	-5.76687982352388	-0.99188614147855	-7.49105248180882
H	-3.62687682352388	-2.05158414147855	-6.82318248180882
H	-0.05324982352388	-2.39053114147855	-5.81719048180882
H	0.49873317647612	-4.69320714147855	-6.55140848180882
H	-1.11326782352388	-6.54291814147855	-6.16475848180882
H	-3.27156782352388	-6.07741314147855	-5.02681748180882
H	-3.80658682352388	-3.77893914147855	-4.27014348180882
O	-7.66137982352388	1.69078685852145	-5.34552648180882
O	-7.67781582352388	0.45551085852145	-7.21050348180882

e) **Table S5.** Cartesian coordinates for the optimized structure of compound **6**.

Total energy = 3052.37826672 Hartrees

Atom	x	y	z
C	-6.17754158572630	-0.60005901954972	8.40096258866334
C	-7.27678258572630	-1.46680101954972	8.34060358866333
C	-7.59850958572630	-2.10160801954972	7.14319758866333
C	-6.81738858572630	-1.88225701954972	6.00021458866334
C	-5.71102758572630	-1.01332501954972	6.06012658866333
C	-5.40327958572630	-0.36918001954972	7.26520358866334
C	-7.16557258572630	-2.55623401954972	4.73241458866333
C	-6.25912058572630	-2.37798301954972	3.56646658866334
C	-5.12217858572630	-1.56163301954972	3.64149558866333
C	-4.88477758572630	-0.73061001954972	4.85218458866334
C	-6.57545758572630	-3.09228001954972	2.38095458866333

C	-5.77991758572630	-2.99287601954972	1.26509058866333
C	-4.60712058572630	-2.20353301954972	1.31172458866333
C	-4.23504958572630	-1.53792801954972	2.51802258866334
N	-3.85589358572630	-2.03425501954972	0.17986058866334
C	-2.72326358572630	-1.32897901954972	0.22906558866334
C	-2.20652258572630	-0.91149301954972	1.52251058866333
N	-2.99549358572630	-0.97263601954972	2.59563158866333
C	-0.81756358572630	-0.47569401954972	1.78578058866333
C	-2.11013758572630	-0.99617301954972	-1.07432341133666
C	0.28646641427370	-0.96247301954972	1.06222858866334
C	1.58315041427370	-0.58065101954972	1.38957158866334
C	1.81964141427370	0.30011898045028	2.45999358866333
C	0.72104541427370	0.78181098045028	3.19451858866333
C	-0.57201258572630	0.39353298045028	2.86668858866333
C	-1.47699158572630	0.23855698045028	-1.30779141133667
C	-0.96927958572630	0.55879098045028	-2.56212841133667
C	-1.07996058572630	-0.34922801954972	-3.63043341133667
C	-1.72070958572630	-1.58115801954972	-3.40628141133667
C	-2.23251158572630	-1.89162401954972	-2.15241041133666
N	3.14531341427370	0.70541798045028	2.79281258866333
C	3.38598441427370	2.06605298045028	3.18791158866333
C	4.22977141427370	-0.21005001954972	2.72781558866333
N	-0.54598958572630	-0.03822501954972	-4.91447641133666
C	-0.63998258572630	1.27376298045028	-5.45216241133667
C	0.09944041427370	-1.07407801954972	-5.67420241133667
O	-4.05746858572630	0.20503998045028	4.87736458866333
O	-8.18029058572630	-3.28561201954972	4.64332158866333
C	2.87985441427370	3.12514598045028	2.42004658866334
C	3.10853741427370	4.44505798045028	2.81152858866333

C	3.85446441427370	4.72250898045028	3.96088158866333
C	4.36486441427370	3.66709398045028	4.72281858866333
C	4.12720841427370	2.34476598045028	4.34597758866334
C	5.50354441427370	0.21866198045028	2.30830858866334
C	6.56225941427370	-0.68008101954972	2.25808958866333
C	6.37990641427370	-2.02443301954972	2.61267058866333
C	5.10925441427370	-2.45637001954972	3.03621658866333
C	4.05210441427370	-1.56253001954972	3.09735758866333
C	0.39875541427370	1.79576898045028	-6.24609541133666
C	0.29183141427370	3.07162498045028	-6.78651341133667
C	-0.84068258572630	3.86154098045028	-6.54275041133667
C	-1.88089358572630	3.34387398045028	-5.74899241133667
C	-1.78447958572630	2.06818698045028	-5.21603041133667
C	1.08290241427370	-1.87703001954972	-5.07820641133666
C	1.70111741427370	-2.88879701954972	-5.81434941133667
C	1.35683041427370	-3.10001501954972	-7.15275541133667
C	0.38153141427370	-2.29498801954972	-7.74927541133667
C	-0.25172758572630	-1.29144901954972	-7.01484941133667
N	7.52476541427370	-2.85444301954972	2.51721258866333
N	-0.84378158572630	5.14672298045028	-7.14084641133666
N	7.35231141427370	-4.08836301954972	2.81748658866333
N	-1.86553858572630	5.87973298045028	-6.89426141133666
C	-1.86715158572630	7.16762598045028	-7.50525241133666
C	8.50796741427370	-4.91752201954972	2.72230058866333
C	9.78085941427370	-4.46642801954972	2.33296458866333
C	10.84099141427370	-5.36624001954972	2.27279258866333
C	10.64467541427370	-6.71613601954972	2.59800958866334
C	9.37846941427370	-7.16418201954972	2.98577458866334
C	8.31226941427370	-6.26666601954972	3.04769358866333

C	-0.84832858572630	7.65084498045028	-8.34417441133666
C	-0.95387058572630	8.92688798045028	-8.88974141133667
C	-2.06864658572630	9.72913698045028	-8.60643941133667
C	-3.08176558572630	9.24791498045028	-7.77191241133666
C	-2.98130858572630	7.96950598045028	-7.22256341133667
H	-5.92934458572630	-0.10619501954972	9.33063358866334
H	-7.87792258572630	-1.64094601954972	9.22255058866333
H	-8.44626658572630	-2.76677301954972	7.06579158866333
H	-4.56023358572630	0.30573398045028	7.28512458866334
H	-7.47042958572630	-3.69605301954972	2.38703358866333
H	-6.02308058572630	-3.48924901954972	0.33672858866333
H	0.13736741427370	-1.64656701954972	0.23982458866333
H	2.41622641427370	-0.96280801954972	0.81806558866333
H	0.88850541427370	1.44931498045028	4.02728558866333
H	-1.41178758572630	0.73170698045028	3.45622358866333
H	-1.38093958572630	0.95548898045028	-0.50533441133667
H	-0.48363158572630	1.51083098045028	-2.71827741133666
H	-1.82200958572630	-2.28378101954972	-4.22049641133666
H	-2.75140558572630	-2.82527301954972	-1.99395541133667
H	2.31406841427370	2.90946098045028	1.52472258866333
H	2.71340341427370	5.25476098045028	2.21276358866333
H	4.03452141427370	5.74624398045028	4.25905758866333
H	4.93721941427370	3.87143898045028	5.61777358866334
H	4.50997641427370	1.52807398045028	4.94154758866334
H	5.65206141427370	1.24872598045028	2.02026058866334
H	7.54394541427370	-0.36743401954972	1.93170958866333
H	4.98276641427370	-3.48839801954972	3.32567458866334
H	3.08337341427370	-1.89471601954972	3.44117858866333
H	1.28099841427370	1.20091298045028	-6.43007541133666

H	1.08275241427370	3.48770398045028	-7.39415141133667
H	-2.75622858572630	3.95245898045028	-5.58082641133667
H	-2.59495758572630	1.66801798045028	-4.62453141133667
H	1.35738641427370	-1.70374101954972	-4.04727341133666
H	2.45892441427370	-3.50236001954972	-5.34583941133666
H	1.84147641427370	-3.88067601954972	-7.72289141133666
H	0.10393141427370	-2.45510901954972	-8.78250241133667
H	-1.01497658572630	-0.67683401954972	-7.47087541133667
H	9.90916841427370	-3.42360001954972	2.08684358866333
H	11.82200941427370	-5.02159001954972	1.97340658866333
H	11.47339541427370	-7.40986301954972	2.54900158866333
H	9.22403741427370	-8.20459701954972	3.23787958866334
H	7.32153041427370	-6.58111001954972	3.34335658866333
H	0.00011641427370	7.01621198045028	-8.54885141133667
H	-0.17119958572630	9.30130598045028	-9.53628941133666
H	-2.14401358572630	10.72000098045028	-9.03416341133666
H	-3.94283658572630	9.86433298045028	-7.55184741133666
H	-3.74719858572630	7.56803998045028	-6.57444041133667

f) Table S6. Cartesian coordinates for the optimized structure of compound 7.

Total energy = 2482.10837061 Hartrees

Atom	x	y	z
C	-5.82802070086417	0.45447921586014	7.50571025777396
C	-5.27299170086417	-0.01128478413986	8.70513225777396
C	-4.02368870086417	-0.62717978413986	8.70151825777396
C	-3.31581970086417	-0.77308078413986	7.50042325777396
C	-3.87177870086417	-0.30464978413986	6.29502625777396
C	-5.13432970086417	0.30201021586014	6.30656125777396

C	-1.99073370086417	-1.42840478413986	7.50307125777396
C	-1.22763670086417	-1.47934778413986	6.22939025777396
C	-1.75622370086417	-0.96300978413986	5.03584825777396
C	-3.16174770086417	-0.48259178413986	4.99552425777396
C	0.07174629913583	-2.04771778413986	6.27076425777396
C	0.84521329913583	-2.12230878413986	5.13654225777396
C	0.35827029913583	-1.58897878413986	3.92105325777396
C	-0.91498670086417	-0.94427078413986	3.87808525777396
N	1.08243929913583	-1.74522378413986	2.76972225777396
C	0.64688929913583	-1.20671178413986	1.62715225777396
C	-0.48401070086417	-0.28816078413986	1.66746725777396
N	-1.25294970086417	-0.24437978413986	2.75656425777396
C	-0.82815970086417	0.68310321586014	0.61027225777396
C	1.33909029913583	-1.63862478413986	0.39824925777396
C	0.13274729913583	1.27460021586014	-0.23107574222604
C	-0.22352870086417	2.24257421586014	-1.16255074222604
C	-1.56427870086417	2.65608921586014	-1.29539374222604
C	-2.52777470086417	2.07903121586014	-0.44161774222604
C	-2.16298370086417	1.12159121586014	0.49437925777396
C	2.69948329913583	-1.99761178413986	0.44742025777396
C	3.36328629913583	-2.47168878413986	-0.67606774222604
C	2.68209329913583	-2.63161878413986	-1.90047174222604
C	1.31504629913583	-2.28957378413986	-1.95125474222604
C	0.66244129913583	-1.80311378413986	-0.82564474222604
N	-1.92229870086417	3.64691521586014	-2.24189974222604
C	-3.20992570086417	3.65867721586014	-2.86308174222604
C	-0.97784270086417	4.67556121586014	-2.59305574222604
N	3.36293829913583	-3.10657278413986	-3.04676674222604
C	4.76566129913583	-2.82488778413986	-3.21333874222604

C	2.69293629913583	-3.86575078413986	-4.05684674222604
O	-3.77341470086417	-0.26213878413986	3.92835425777396
O	-1.50729370086417	-1.90310478413986	8.55800725777396
C	-3.80845870086417	2.46426921586014	-3.30101474222604
C	-5.05946770086417	2.48861921586014	-3.91727574222604
C	-5.72641770086417	3.70004121586014	-4.12481474222604
C	-5.12729370086417	4.89058421586014	-3.70335974222604
C	-3.88268270086417	4.87436821586014	-3.07297974222604
C	-0.40630670086417	5.49104721586014	-1.60638474222604
C	0.50885229913583	6.48381721586014	-1.94278374222604
C	0.86698529913583	6.70872021586014	-3.28789974222604
C	0.28082829913583	5.89295921586014	-4.27712374222604
C	-0.61803470086417	4.88854621586014	-3.93061074222604
C	5.23566029913583	-1.50444878413986	-3.21325174222604
C	6.59050929913583	-1.22871778413986	-3.37063774222604
C	7.52160129913583	-2.27153378413986	-3.55502274222604
C	7.04154229913583	-3.59721678413986	-3.56604174222604
C	5.68762429913583	-3.86552078413986	-3.38871474222604
C	1.77247029913583	-4.87019978413986	-3.71006274222604
C	1.13554029913583	-5.61400578413986	-4.70335474222604
C	1.41647829913583	-5.38450578413986	-6.05390474222604
C	2.34264929913583	-4.39673478413986	-6.40089274222604
C	2.97391129913583	-3.63819978413986	-5.41451174222604
N	1.76926229913583	7.70357021586014	-3.62742574222604
N	8.86951429913583	-2.00131978413986	-3.72178874222604
H	-6.79899870086417	0.93115921586014	7.50879025777396
H	-5.81556070086417	0.10422221586014	9.63360925777396
H	-3.57578270086417	-1.00414278413986	9.60951425777396
H	-5.54906470086417	0.63897121586014	5.36786525777396

H	0.41652129913583	-2.43448678413986	7.21795625777396
H	1.81797429913583	-2.59281778413986	5.13195825777396
H	1.17026529913583	0.98346221586014	-0.15584574222604
H	0.53377129913583	2.68419021586014	-1.79295874222604
H	-3.55732370086417	2.39850921586014	-0.50605074222604
H	-2.89800570086417	0.71313321586014	1.17290525777396
H	3.22252129913583	-1.91257378413986	1.38855825777396
H	4.40922929913583	-2.73302078413986	-0.61306374222604
H	0.77011729913583	-2.40179678413986	-2.87660074222604
H	-0.38557270086417	-1.55153178413986	-0.89970074222604
H	-3.29061270086417	1.52666221586014	-3.15870274222604
H	-5.50643870086417	1.56013921586014	-4.24774674222604
H	-6.69391670086417	3.71563321586014	-4.60783674222604
H	-5.63317870086417	5.83514421586014	-3.85524774222604
H	-3.42641570086417	5.79608121586014	-2.74160074222604
H	-0.67900470086417	5.33974821586014	-0.57089674222604
H	0.94127529913583	7.10043421586014	-1.16434774222604
H	0.54169329913583	6.04369021586014	-5.31753174222604
H	-1.05118670086417	4.26531321586014	-4.70096274222604
H	4.53295329913583	-0.69250278413986	-3.08445774222604
H	6.93340829913583	-0.20131378413986	-3.36345574222604
H	7.73705929913583	-4.41606478413986	-3.70319874222604
H	5.33772429913583	-4.88878478413986	-3.38983974222604
H	1.56515029913583	-5.06483078413986	-2.66759874222604
H	0.43019329913583	-6.38408278413986	-4.41964574222604
H	0.92521729913583	-5.96741278413986	-6.82101774222604
H	2.56908029913583	-4.20794378413986	-7.44215474222604
H	3.68492329913583	-2.87153578413986	-5.68693174222604
H	2.18201629913583	8.28836121586014	-2.92602474222604

H	2.02014629913583	7.86995921586014	-4.58327374222604
H	9.53318229913583	-2.74118078413986	-3.85024474222604
H	9.21449729913583	-1.06055178413986	-3.70518774222604