Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Synthesis and Properties of *p*-Benzithiahexaphyrin(1.1.1.1.1.1)s

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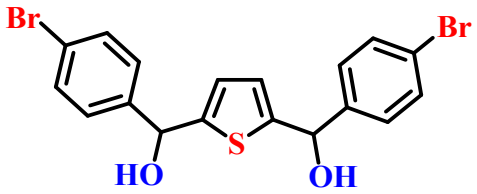


Compound **14b**

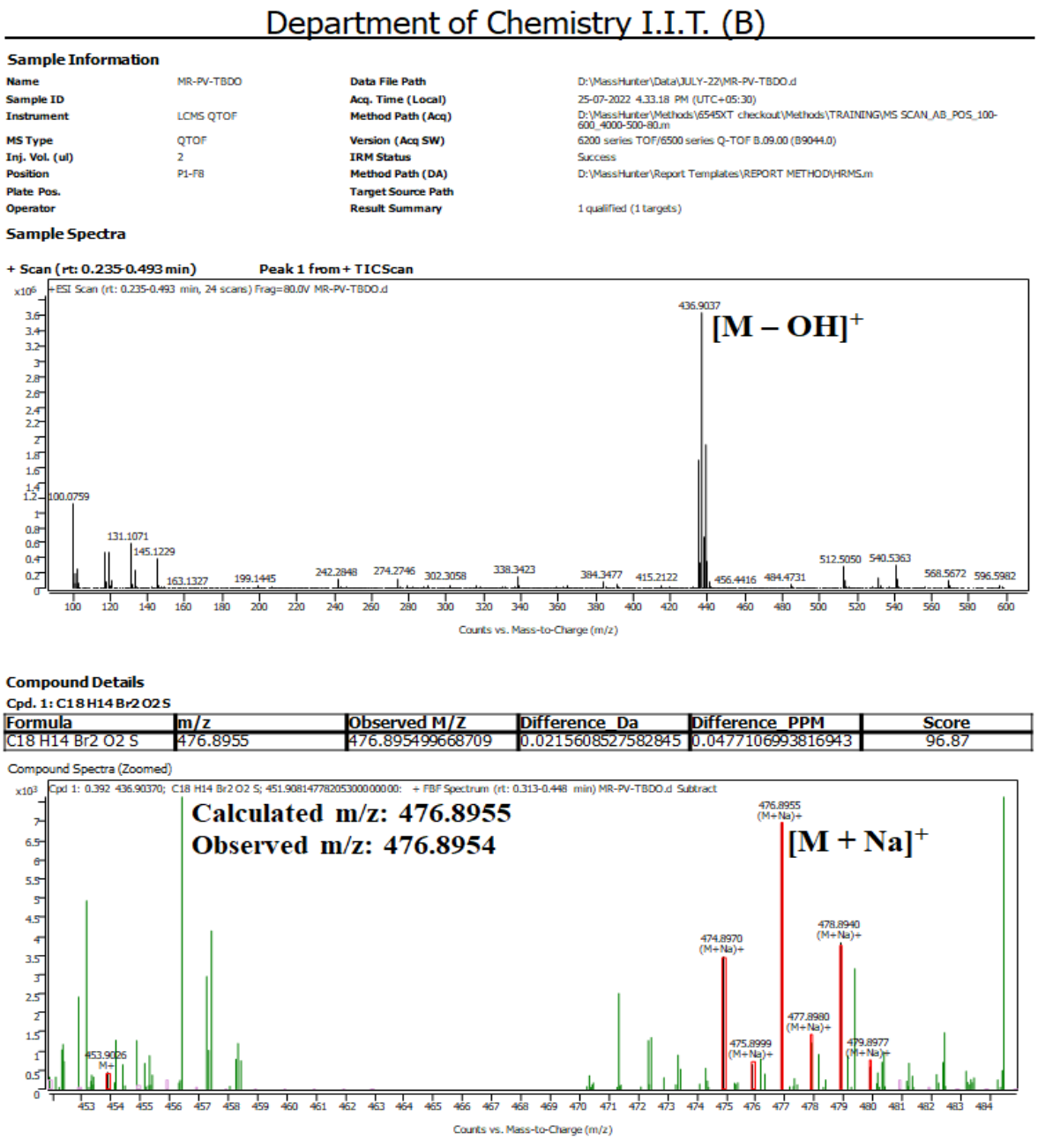


Figure S1. HR mass spectrum of the compound **14b**.

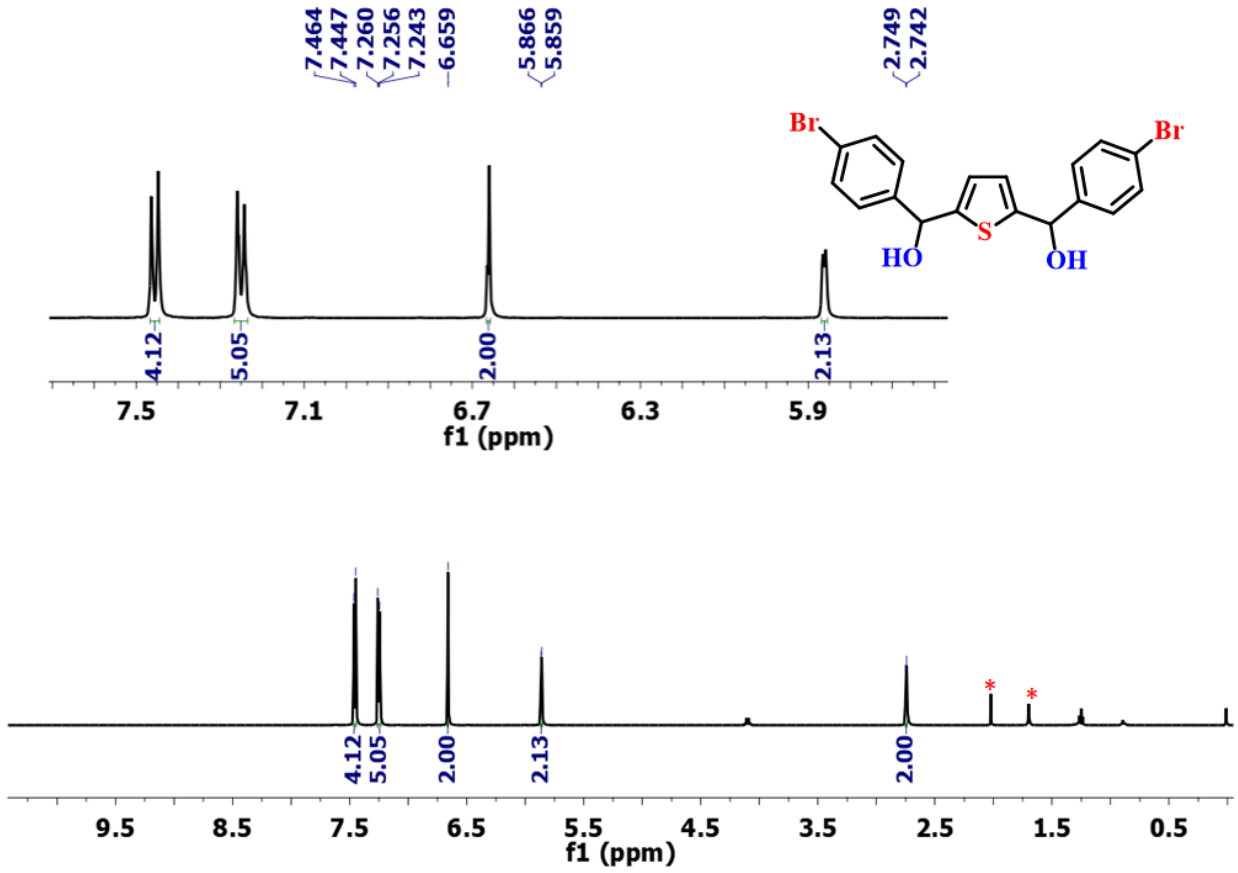


Figure S2. ^{1}H NMR spectrum of the compound **14b** recorded in $CDCl_3$ on 500 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

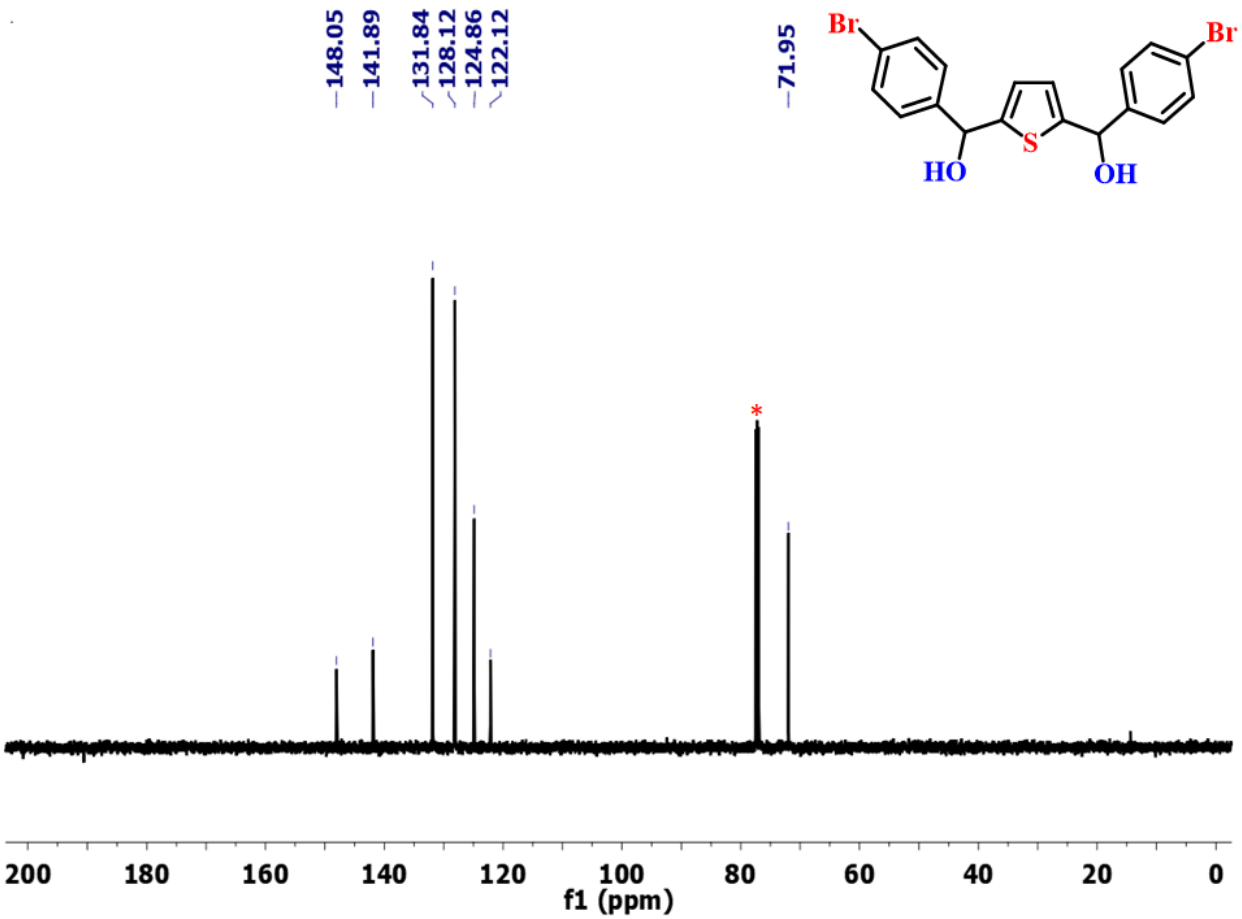
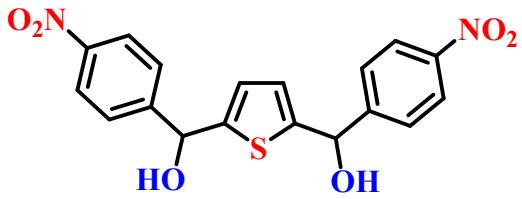


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **14b** recorded in $CDCl_3$ on 500 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **14d**

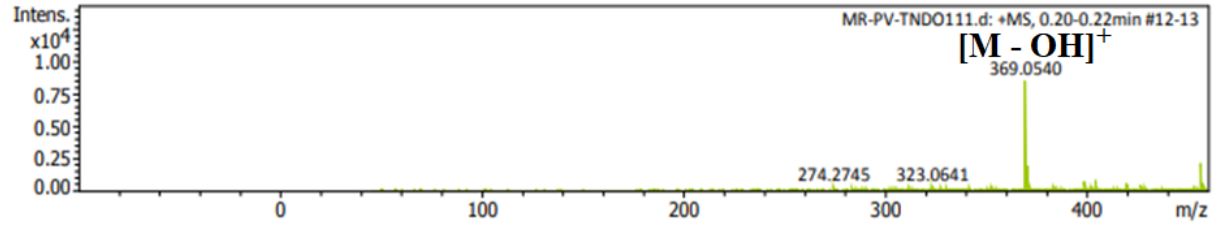
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

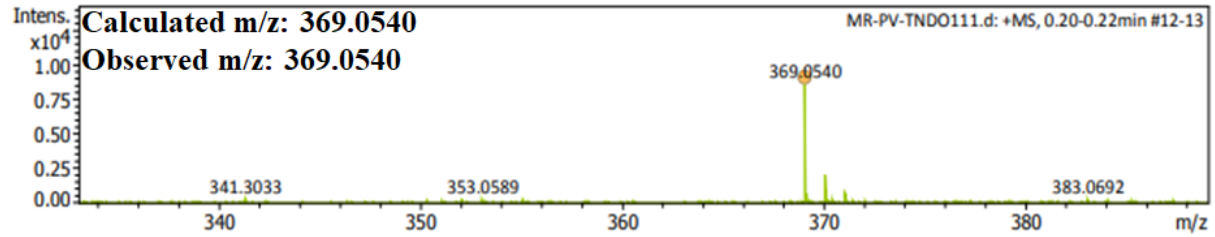
Analysis Info

Analysis Name	D:\Data\SEP-2022\MR-PV-TNDO111.d	Acquisition Date	9/9/2022 12:21:35 PM
Method	Naformat_pos_50-600.m	Operator	sjg-out
Sample Name	MR-PV-TNDO111	Instrument	maXis impact 282001.00081
Comment	C18H14N2O6S		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
369.0540	1	C18H13N2O5S	369.0540	-0.1	14.2	1	100.00	16.0	even	ok

Figure S4. HR mass spectrum of the compound **14d**.

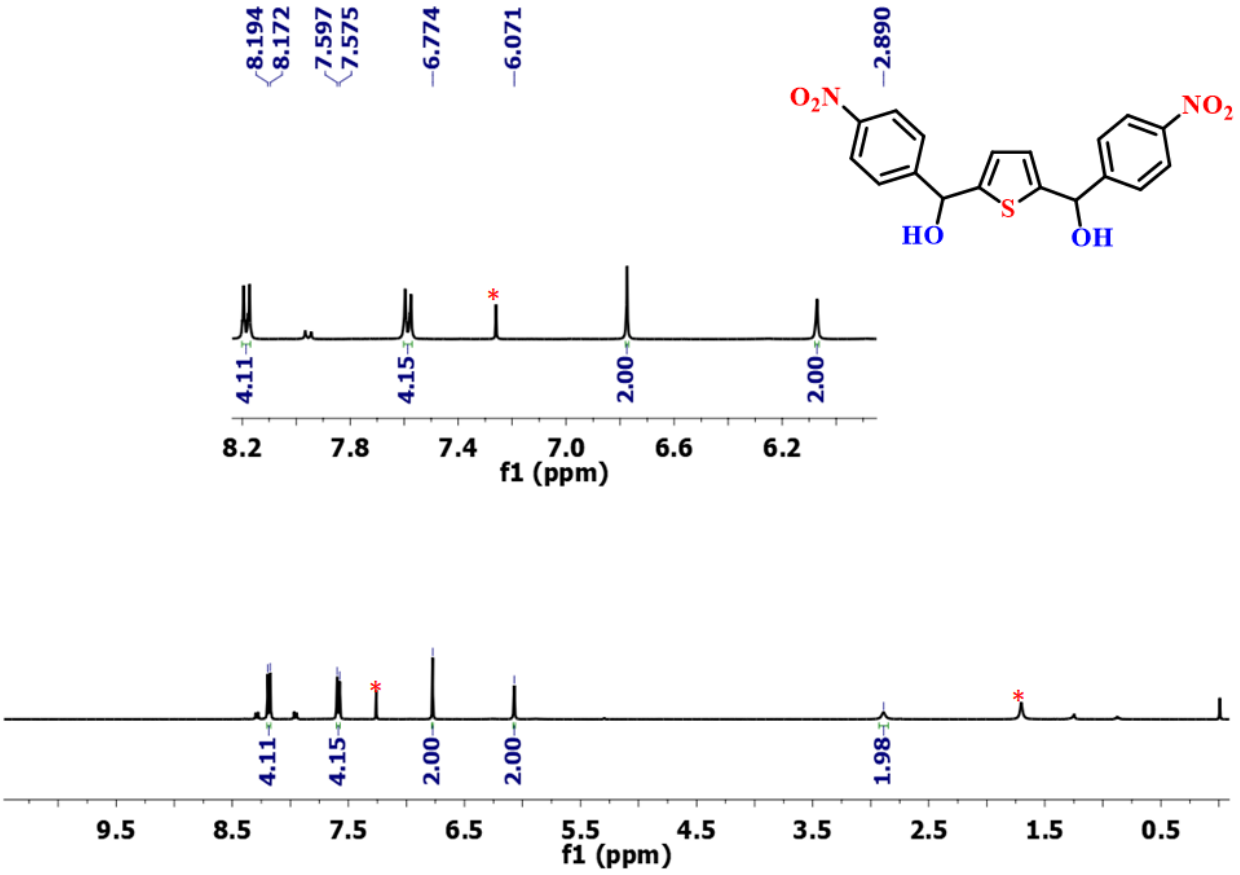


Figure S5. ^{1}H NMR spectrum of the compound **14d** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

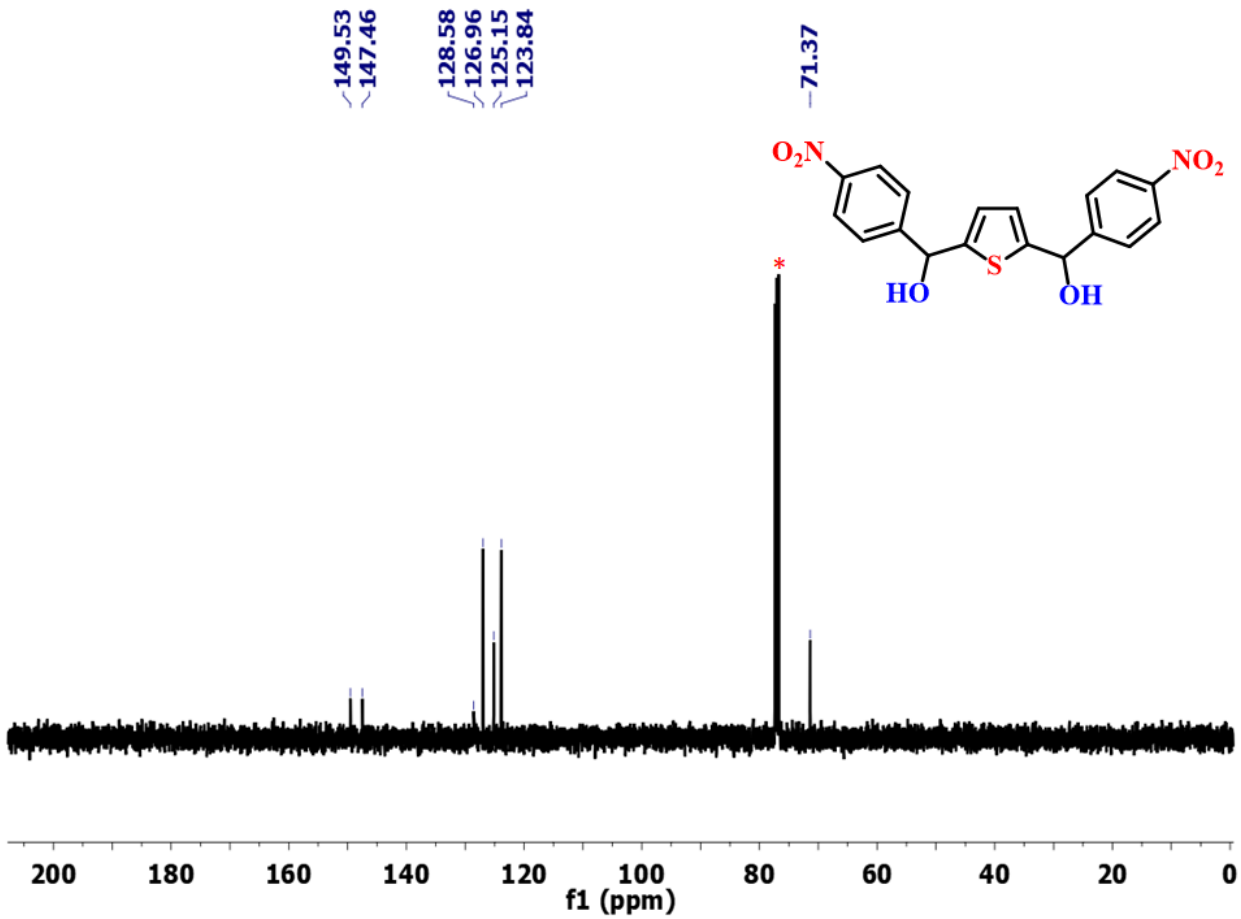
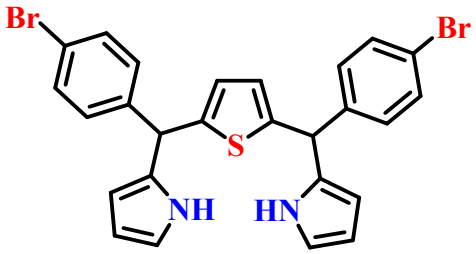


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **14d** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **13b**

Department of Chemistry I.I.T. (B)

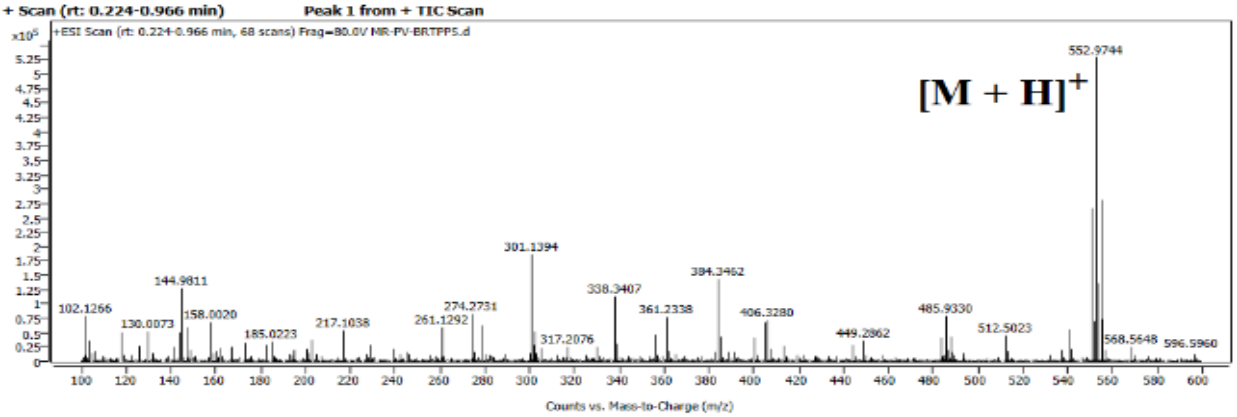
Agilent

Sample Information

Name	MR-PV-BRTPPS	**Data File Path**	D:\MassHunter\Data\AUG-22\MR-PV-BRTPPS.d
Sample ID		**Acq. Time (Local)**	16-08-2022 3.22.43 PM (UTC+05:30)
Instrument	LCMS QTOF	**Method Path (Acq)**	D:\MassHunter\Methods\6545XT checkout\Methods\TRAINING\MS SCAN_AC_POS_100-600_4000-100-80.m
MS Type	QTOF	**Version (Acq SW)**	6200 series TOF/6500 series Q-TOF B.09.00 (B9044.0)
Inj. Vol. (ul)	1	**IRM Status**	Success
Position	P1-E1	**Method Path (DA)**	D:\MassHunter\Report Templates\REPORT METHOD\HRMS.m
Plate Pos.		**Target Source Path**	
Operator		**Result Summary**	1 qualified (1 targets)

Sample Spectra

+ Scan (rt: 0.224-0.966 min) **Peak 1 from + TIC Scan**



Compound Details

Cpd. 1: C26 H20 Br2 N2 S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C26 H20 Br2 N2 S	552.9744	552.974408213666	-1.8578824637824	-3.37814381011709	92.83

Compound Spectra (Zoomed)

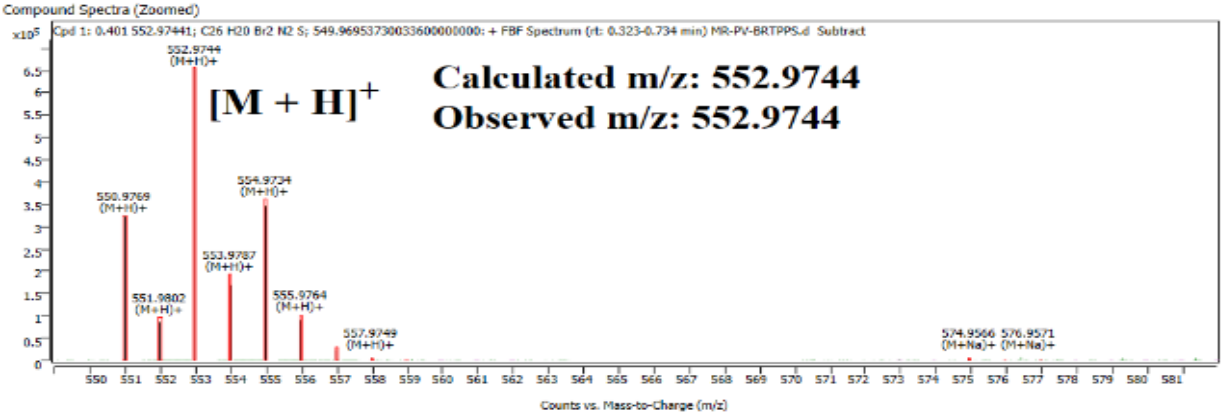


Figure S7. HR mass spectrum of the compound **13b**

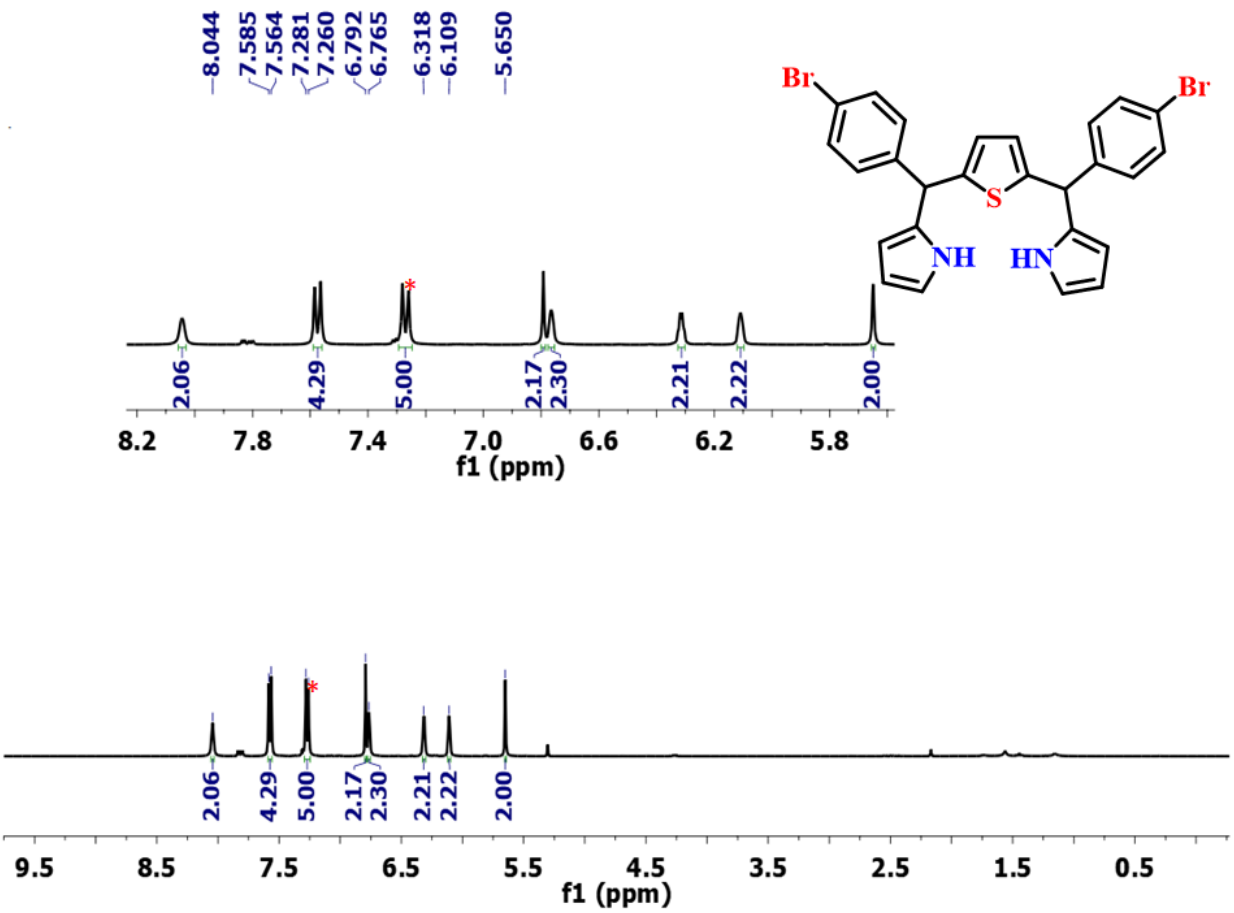


Figure S8. ^{1}H NMR spectrum of the compound **13b** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

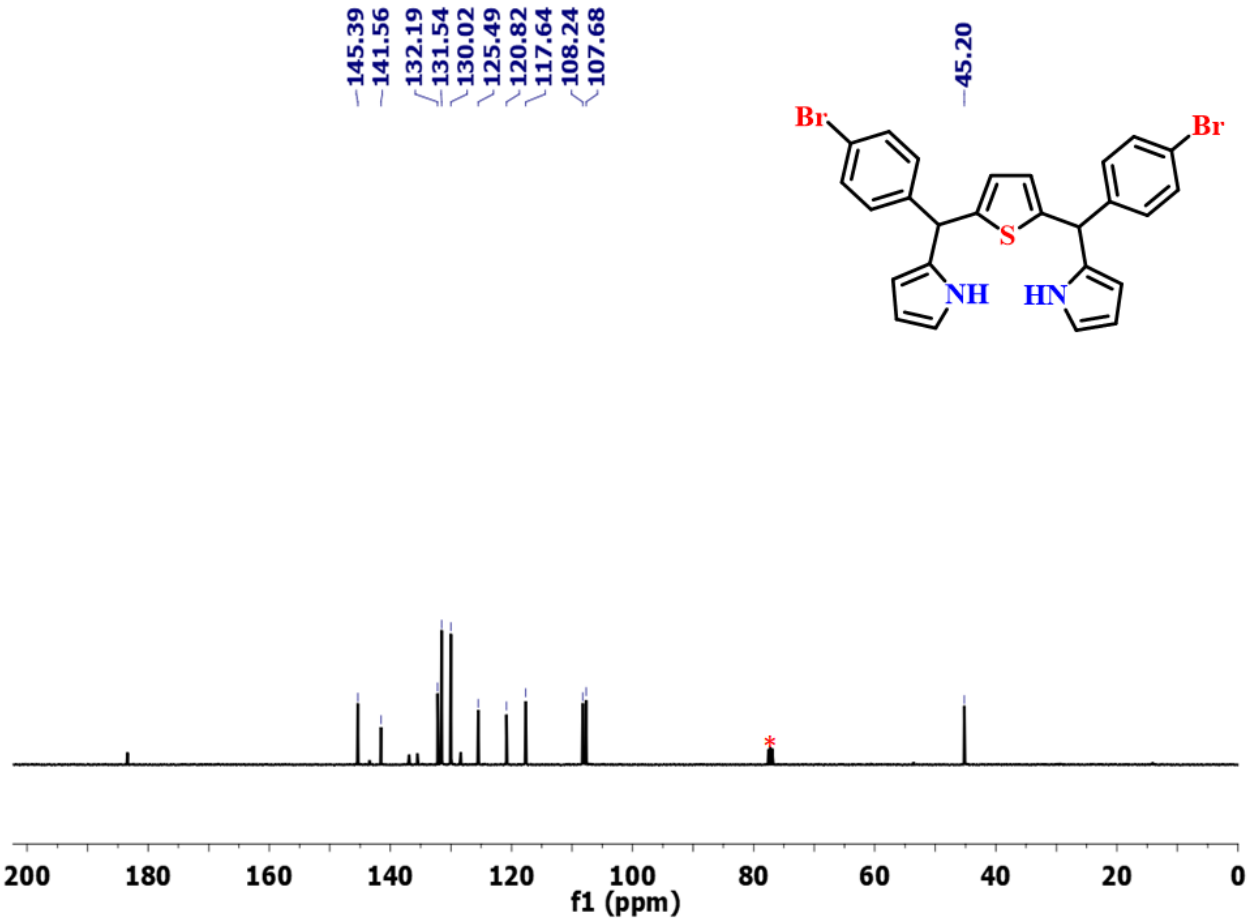
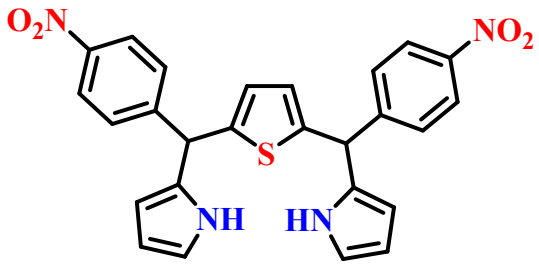


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **13b** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **12d**

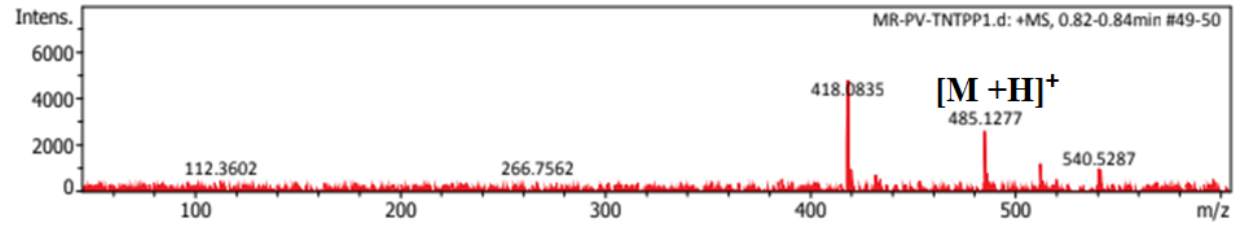
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

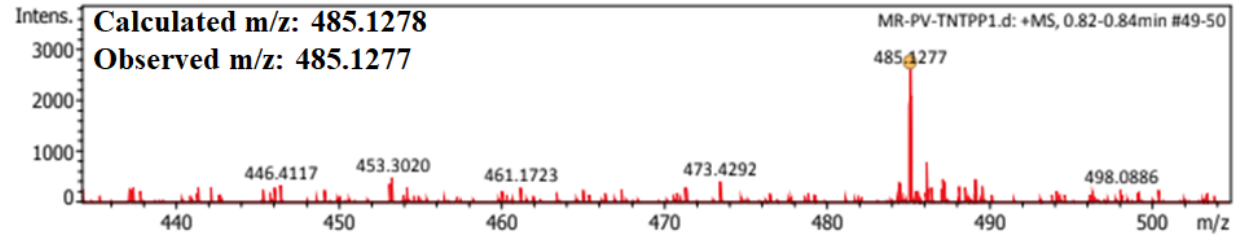
Analysis Info

Analysis Name	D:\Data\SEP-2022\MR-PV-TNTPP1.d	Acquisition Date	9/7/2022 3:24:31 PM
Method	Naformat_pos_50-600.m	Operator	PG RD IN
Sample Name	MR-PV-TNTPP1	Instrument	maXis impact 282001.00081
Comment	LRMS		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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	600 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
485.1277	1	C26H21N4O4S	485.1278	0.2	63.9	1	100.00	21.0	even	ok

Figure S10. HR mass spectrum of the compound **13d**

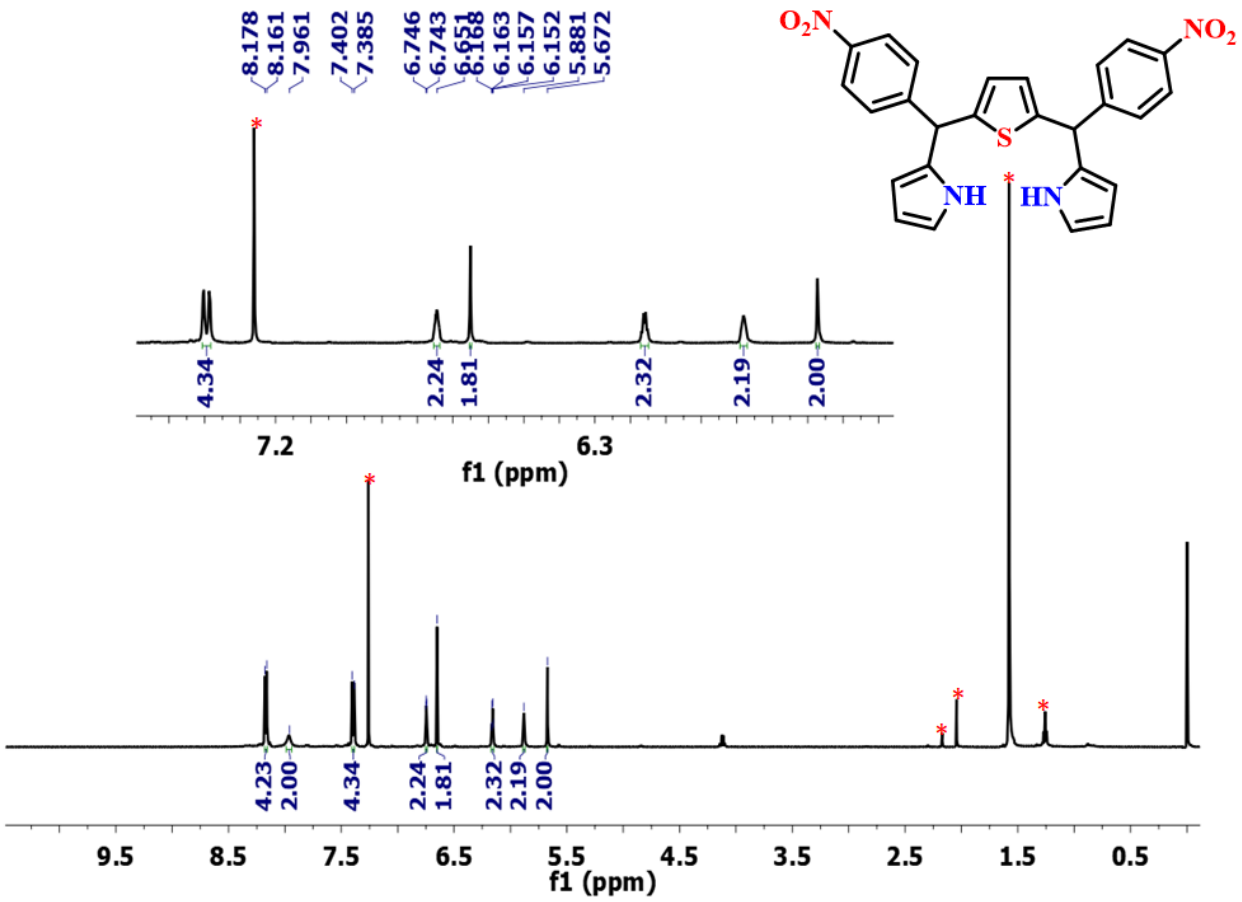


Figure S11. ^{1}H NMR spectrum of the compound **13d** recorded in $CDCl_3$ on 500 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

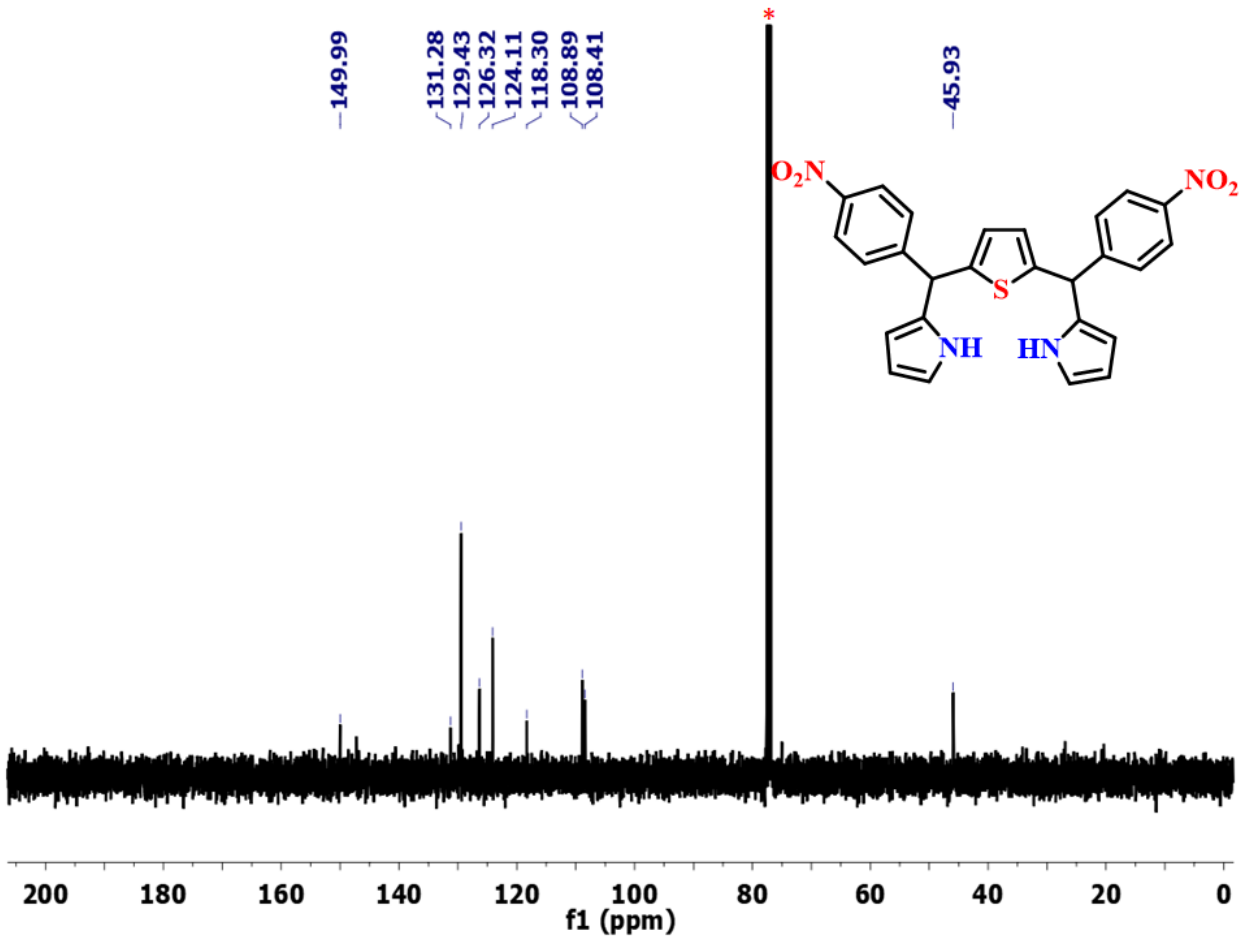
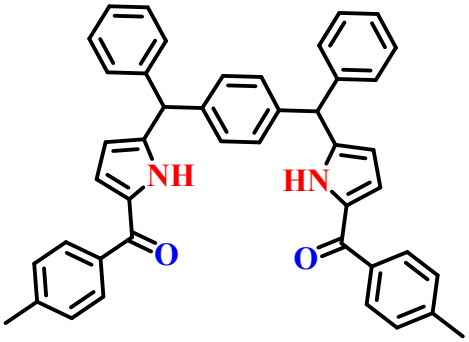


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **13d** recorded in $CDCl_3$ on 500 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **10**

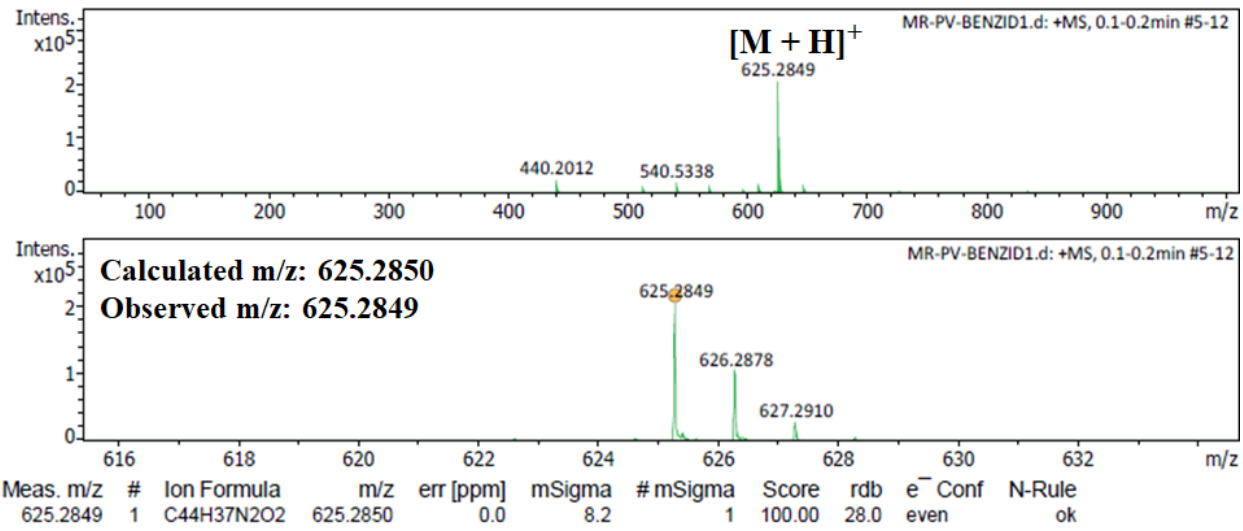
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\AUG-2022\MR-PV-BENZID1.d	Acquisition Date	8/25/2022 2:48:30 PM
Method	NaICsI_pos_1000-a.m	Operator	GKL-LS-out
Sample Name	MR-PV-BENZID1	Instrument	maXis impact 282001.00081
Comment	C44H36N2O2		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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	1000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
625.2849	1	C44H37N2O2	625.2850	0.0	8.2	1	100.00	28.0	even	ok

Figure S13. HR mass spectrum of the compound **10**.

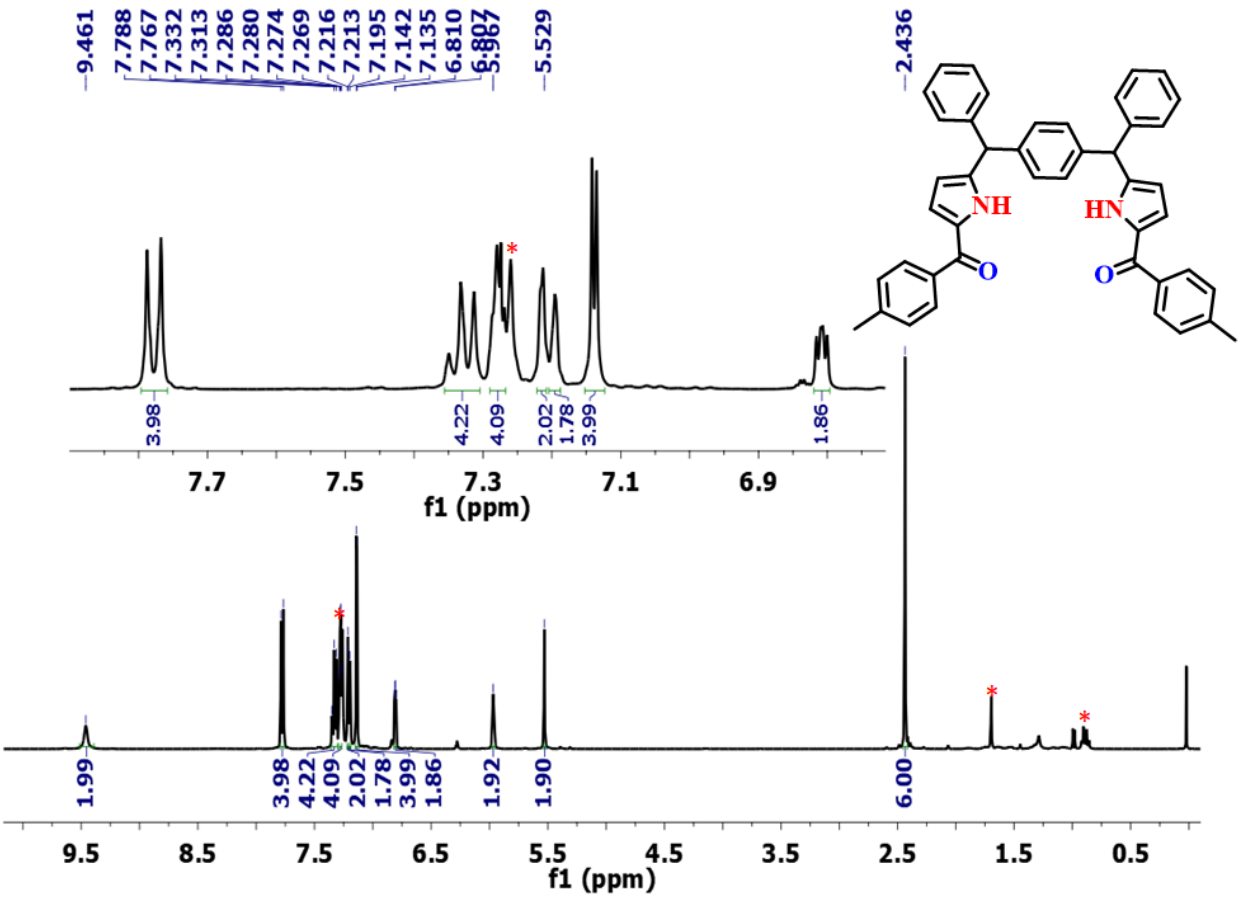


Figure S14. ^{1}H NMR spectrum of the compound **10** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

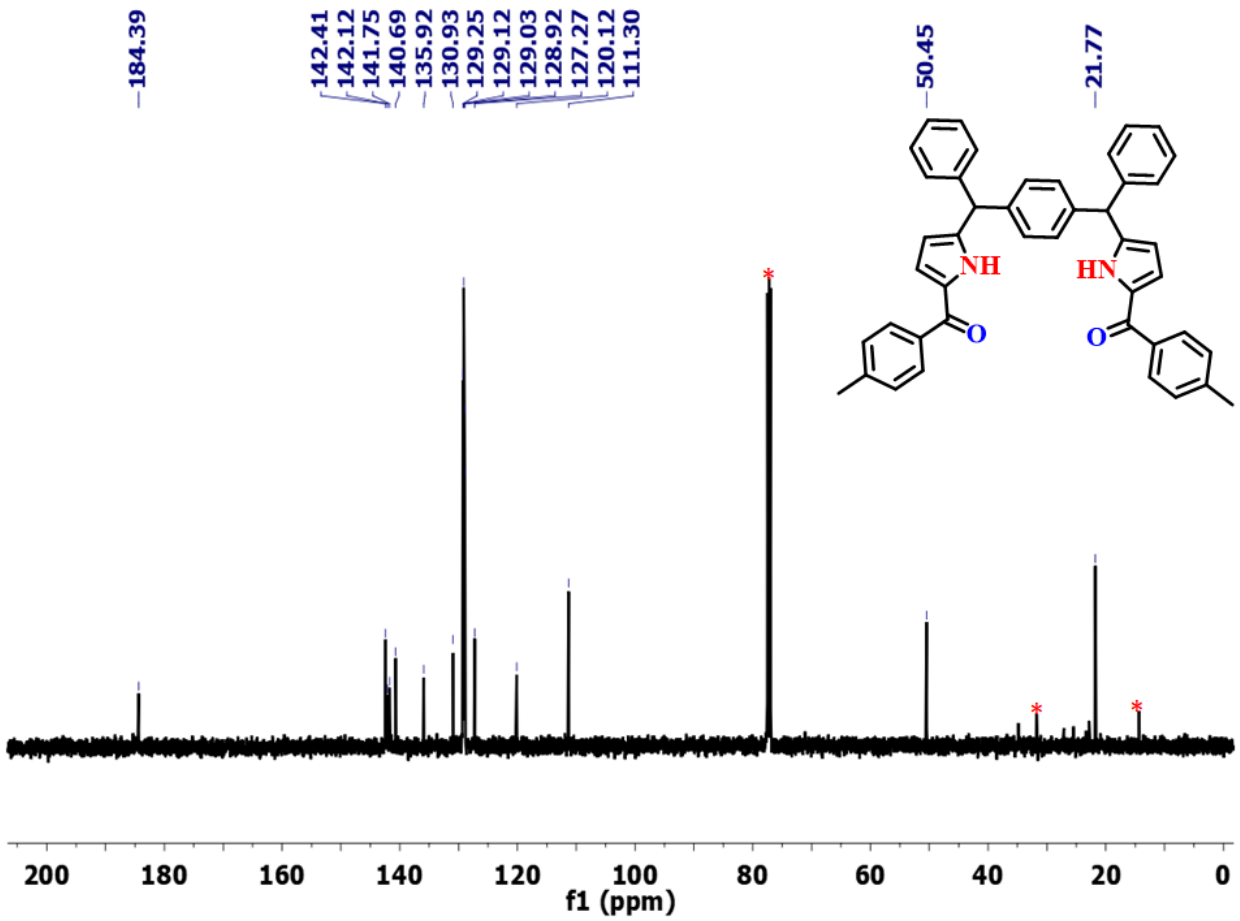
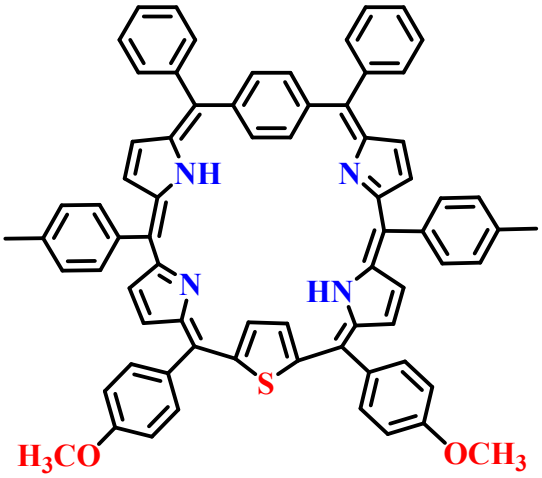


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **10** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **5**

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

Analysis Info

Analysis Name	D:\Data\DEC-2021\MR-POOJA-BLUE.d	Acquisition Date	12/23/2021 6:30:33 PM
Method	NaICsI_pos_1500a.m	Operator	ppi OUT
Sample Name	MR-POOJA-BLUE	Instrument	maXis impact 282001.00081
Comment	C72H56N4SO2		

Acquisition Parameter

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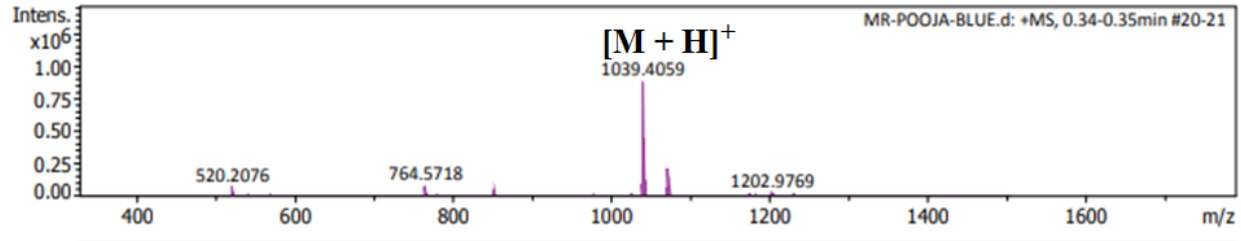
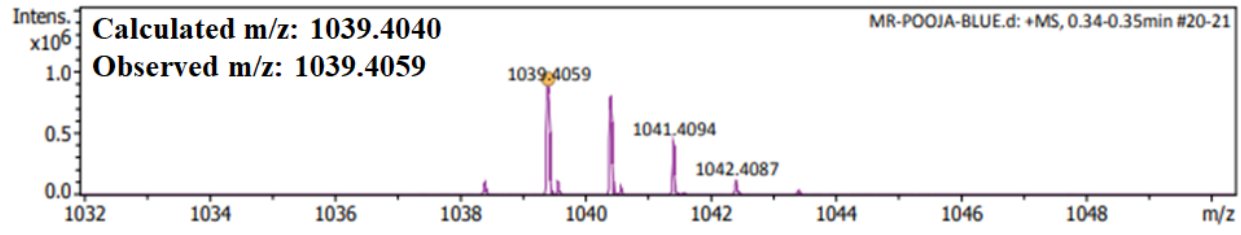
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1039.4059	1	C72H55N4O2S	1039.4040	-1.8	72.9	1	100.00	50.0	even	ok

Figure S16. HR mass spectrum of the compound **5**

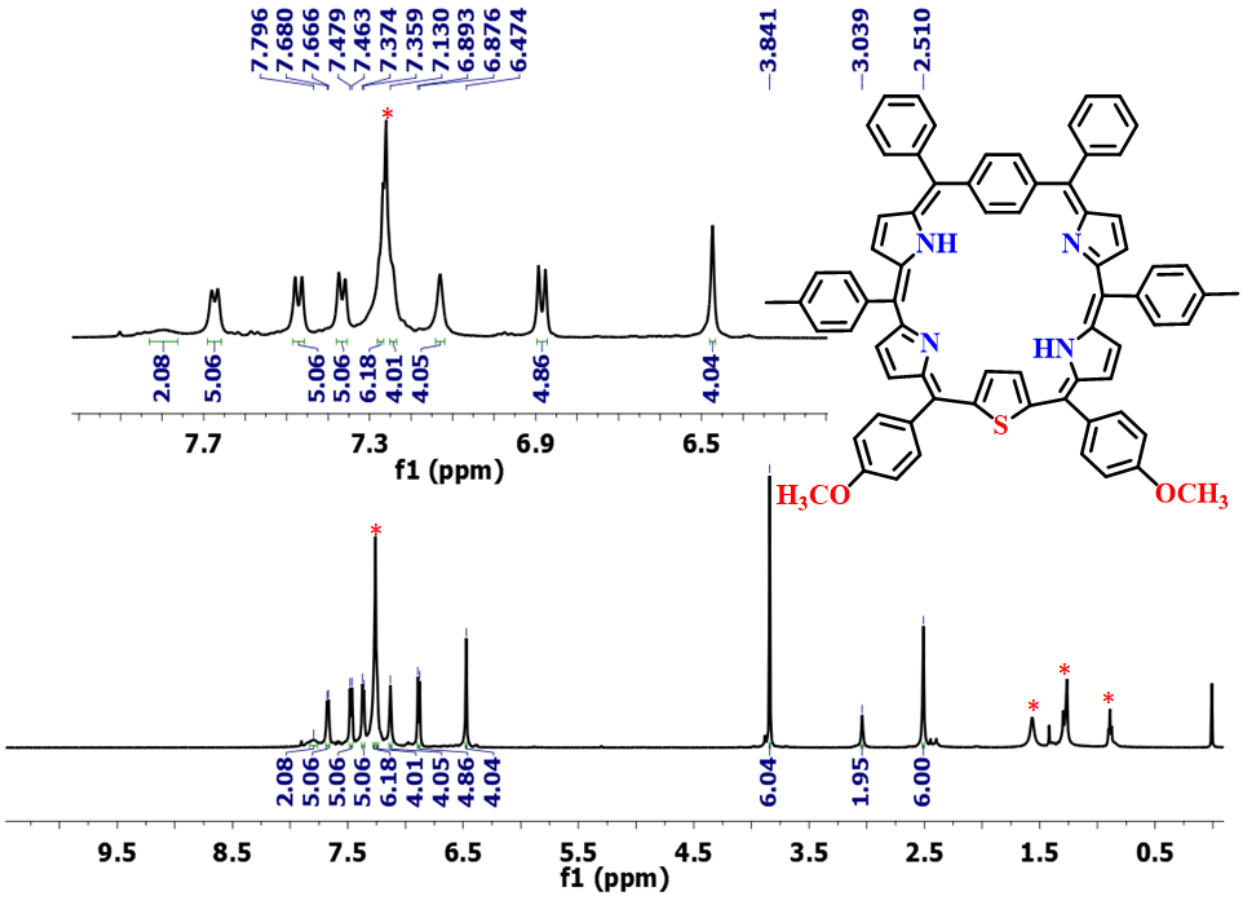


Figure S17. ^{1}H NMR spectrum of the compound **5** recorded in $CDCl_3$ at 298 K on 500 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

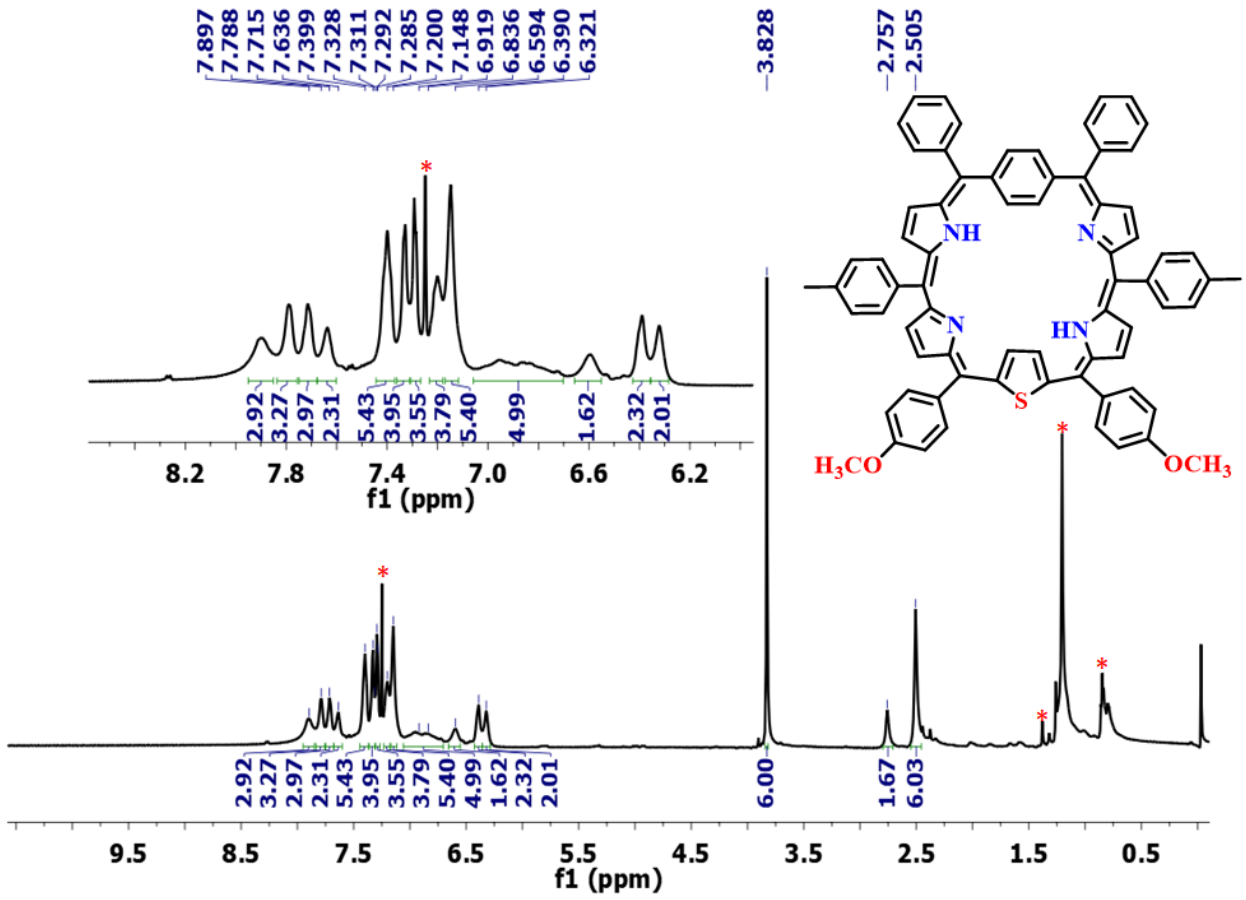


Figure S18. ^{1}H NMR spectrum of the compound **5** recorded in $CDCl_3$ at 223 K on 600 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

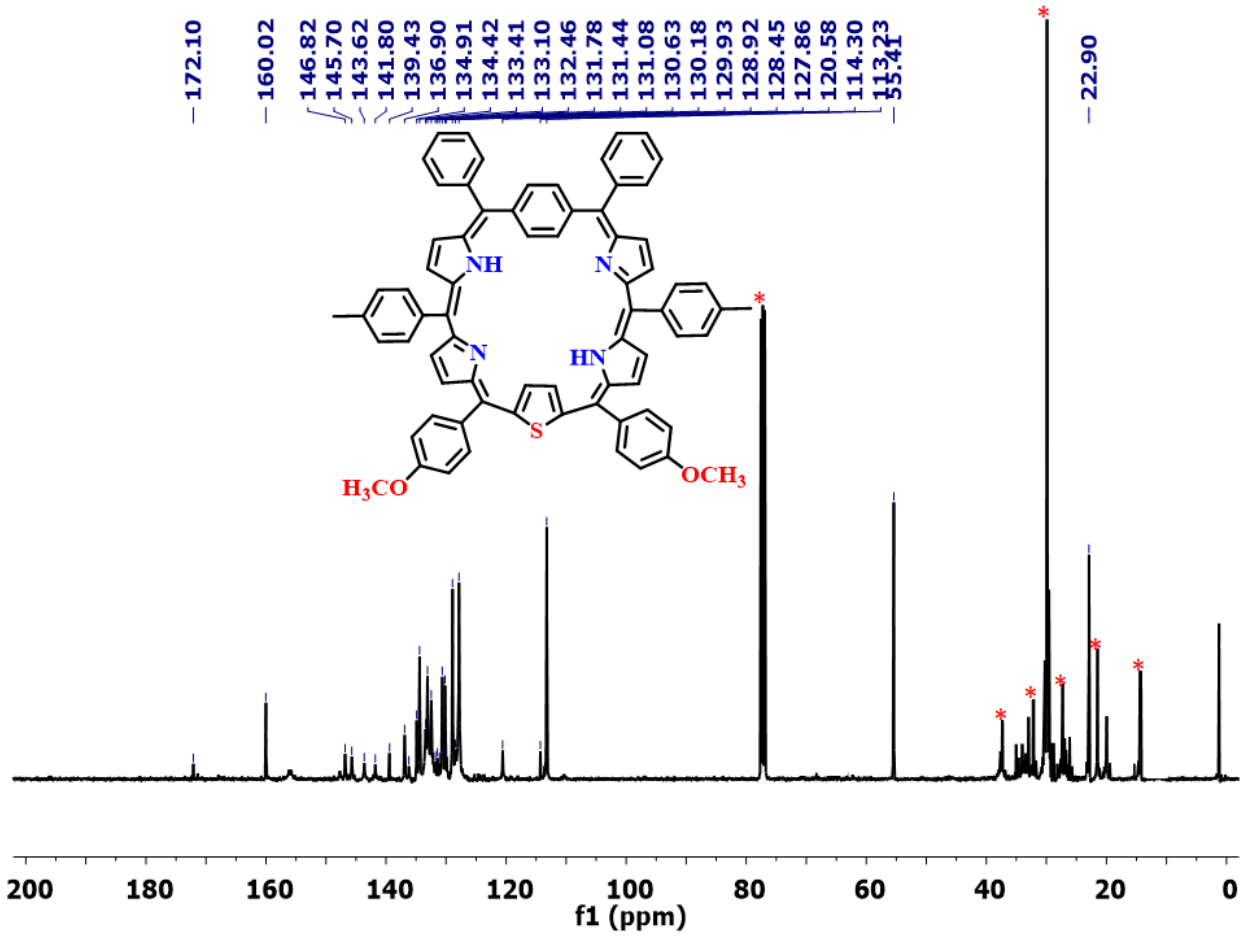
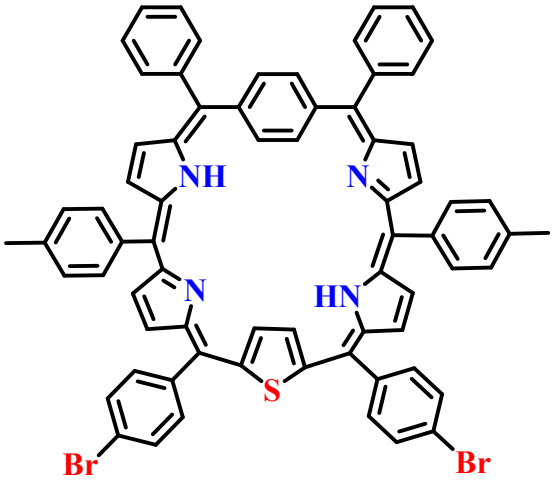


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **6**

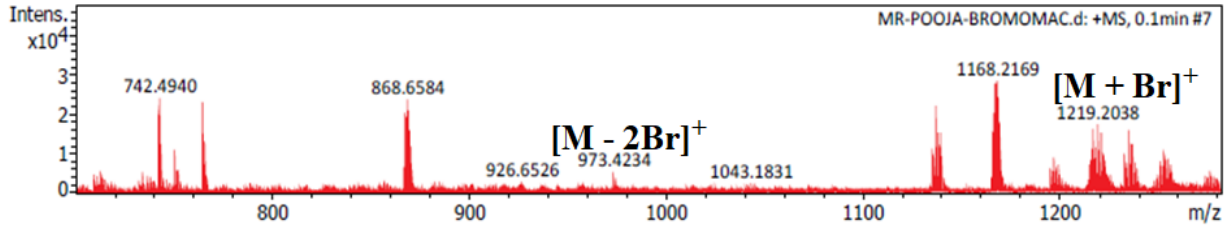
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

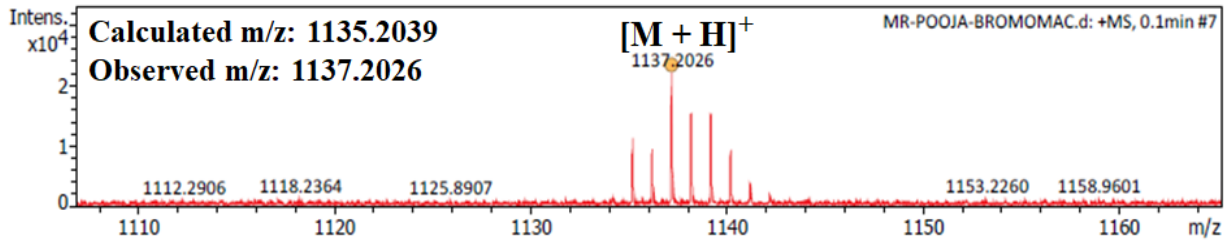
Analysis Info

Analysis Name	D:\Data\APR-2022\MR-POOJA-BROMOMAC.d	Acquisition Date	4/29/2022 11:04:57 AM
Method	NaICsI_pos_1500a.m	Operator	MR-IN
Sample Name	MR-POOJA-BROMOMAC	Instrument	maXis impact 282001.00081
Comment	C70H48Br2N4S		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.5 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1137.2026	1	C70H49Br2N4S	1135.2039	0.3	37.0	1	100.00	54.0	even	ok

Figure S20. HR mass spectrum of the compound **6**

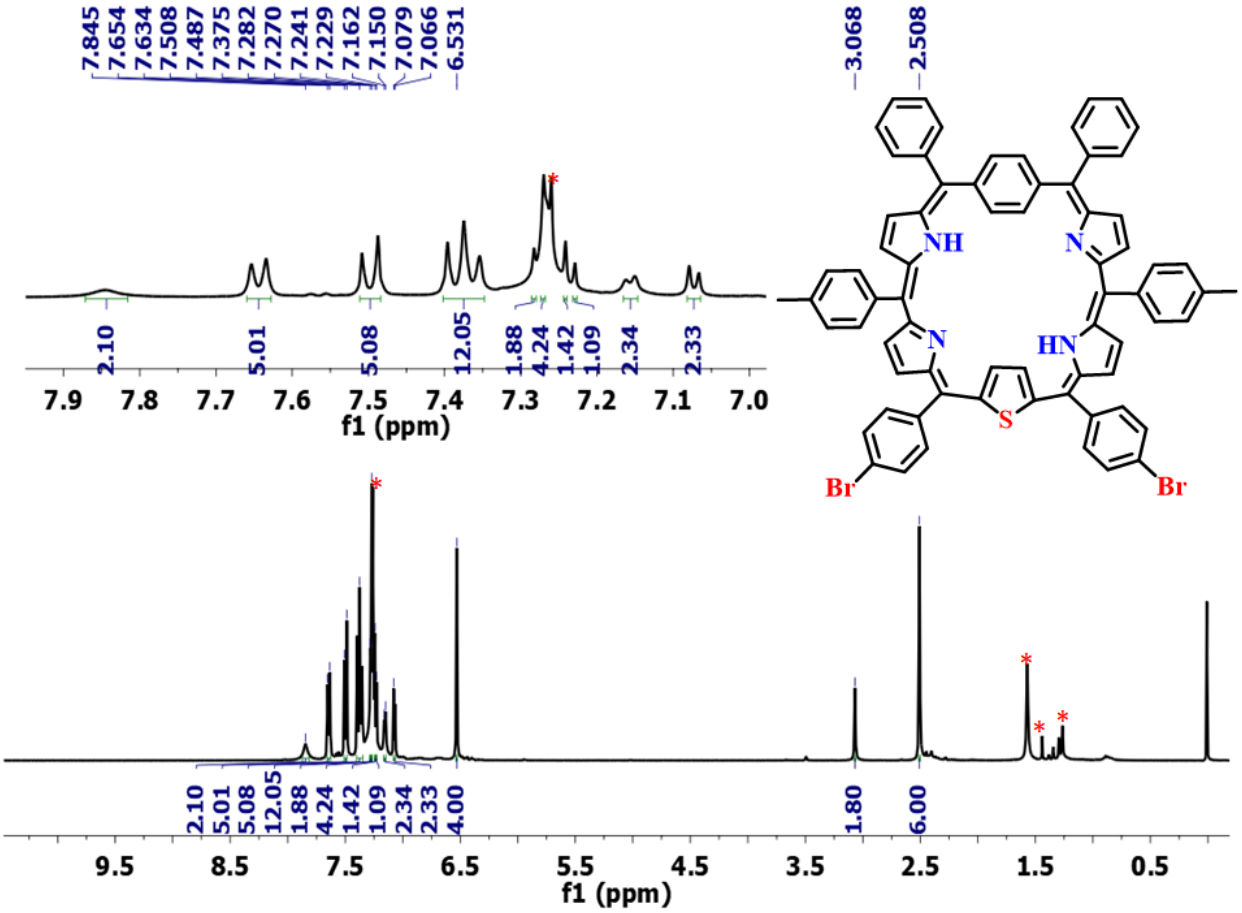


Figure S21. ^{1}H NMR spectrum of the compound **6** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

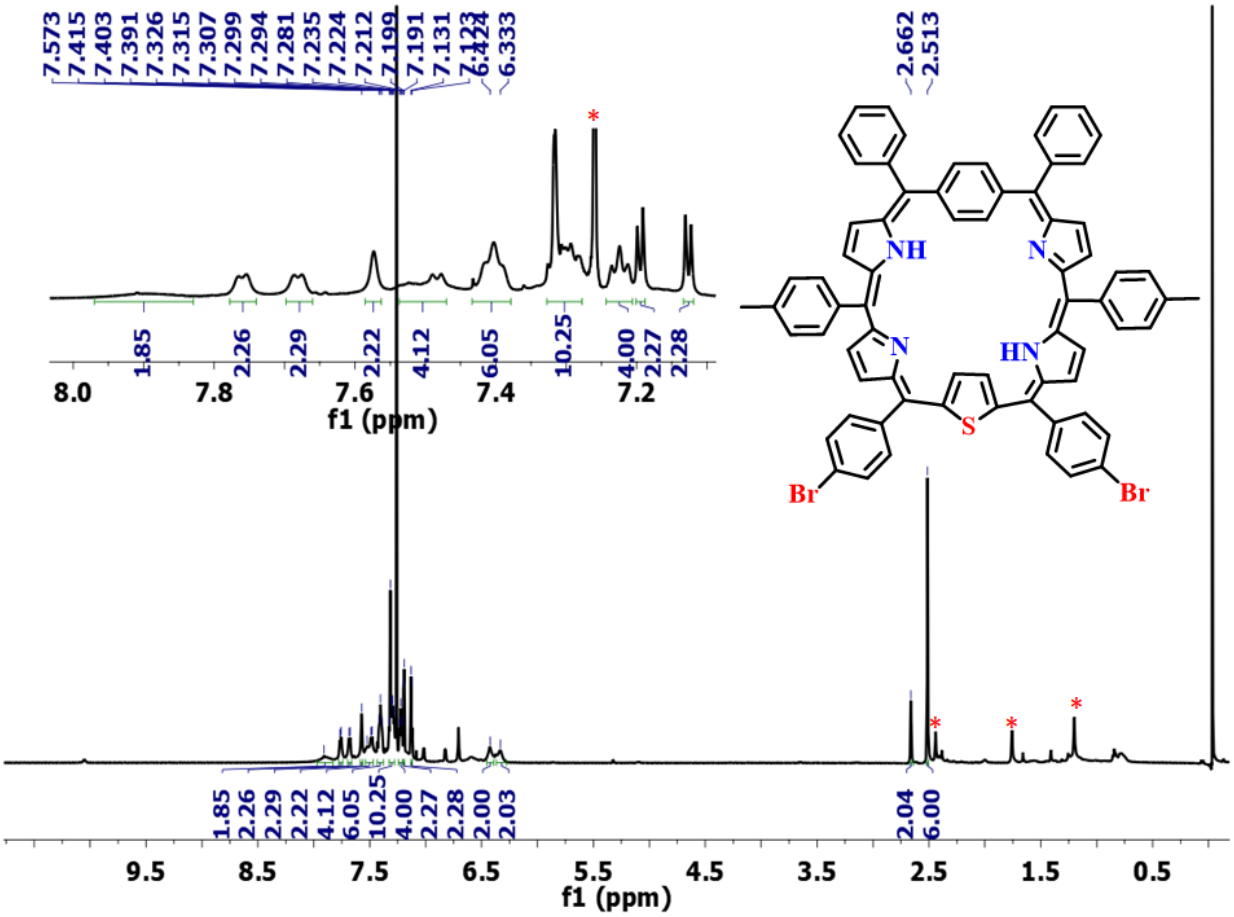


Figure S22. ^{1}H NMR spectrum of the compound **6** recorded in $CDCl_3$ at 223 K on 600 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

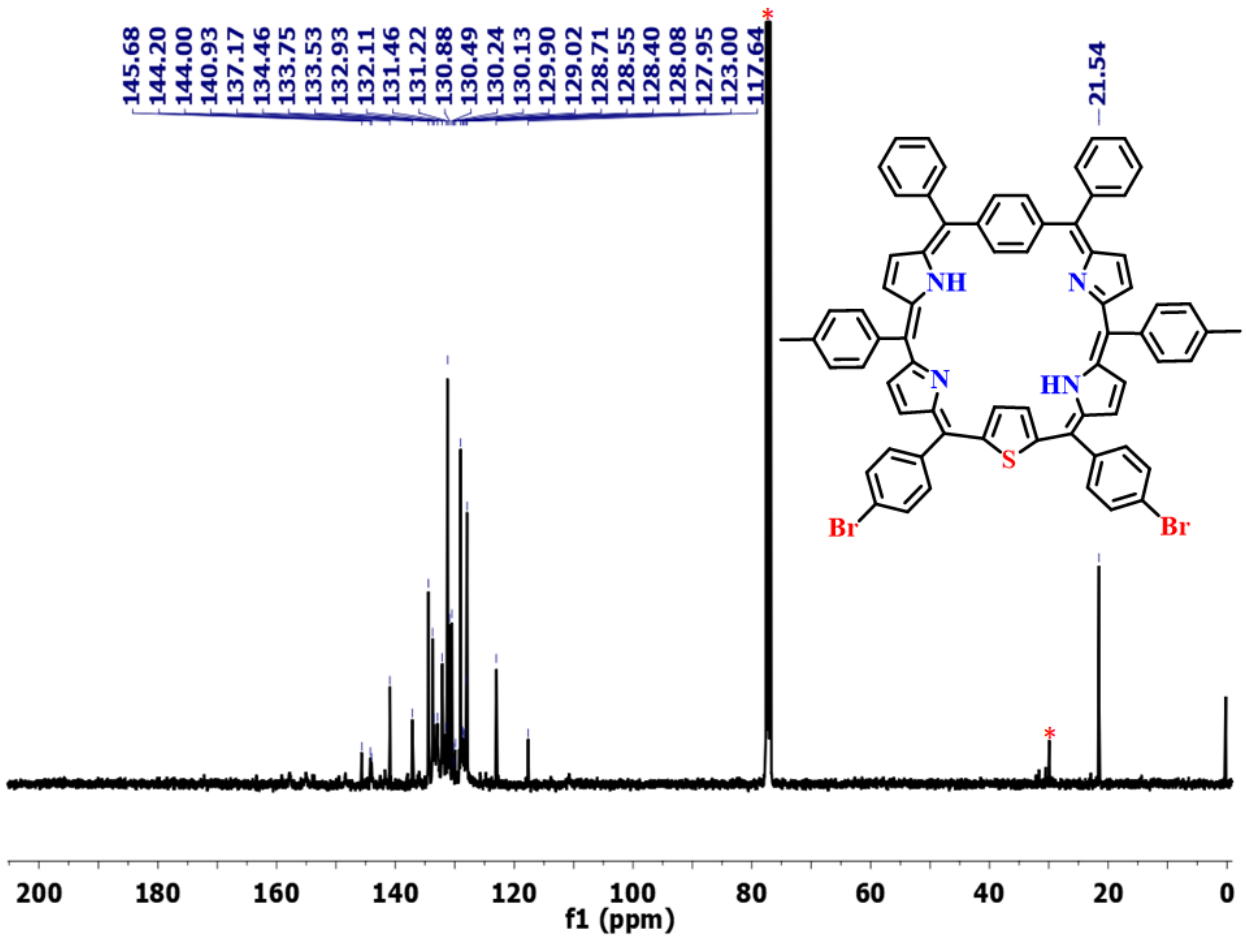
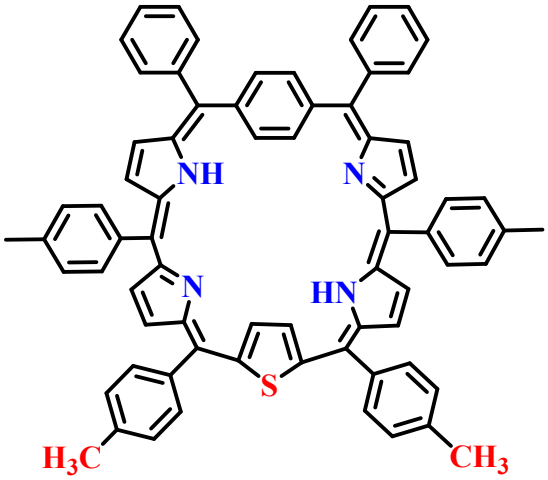


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **6** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **7**

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

Analysis Info

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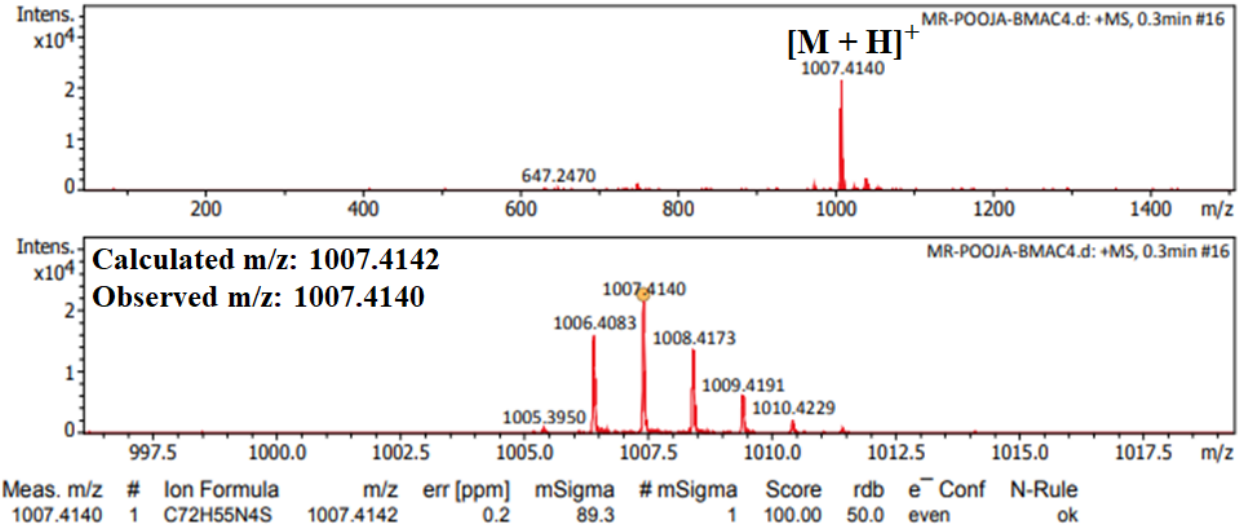
Sample Name	MR-POOJA-BMAC2	Instrument	maXis impact 282001.00081
Comment	C72H54N4S		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not 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 Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1007.4140	1	C72H55N4S	1007.4142	0.2	89.3	1	100.00	50.0	even	ok

Figure S24. HR mass spectrum of the compound **7**

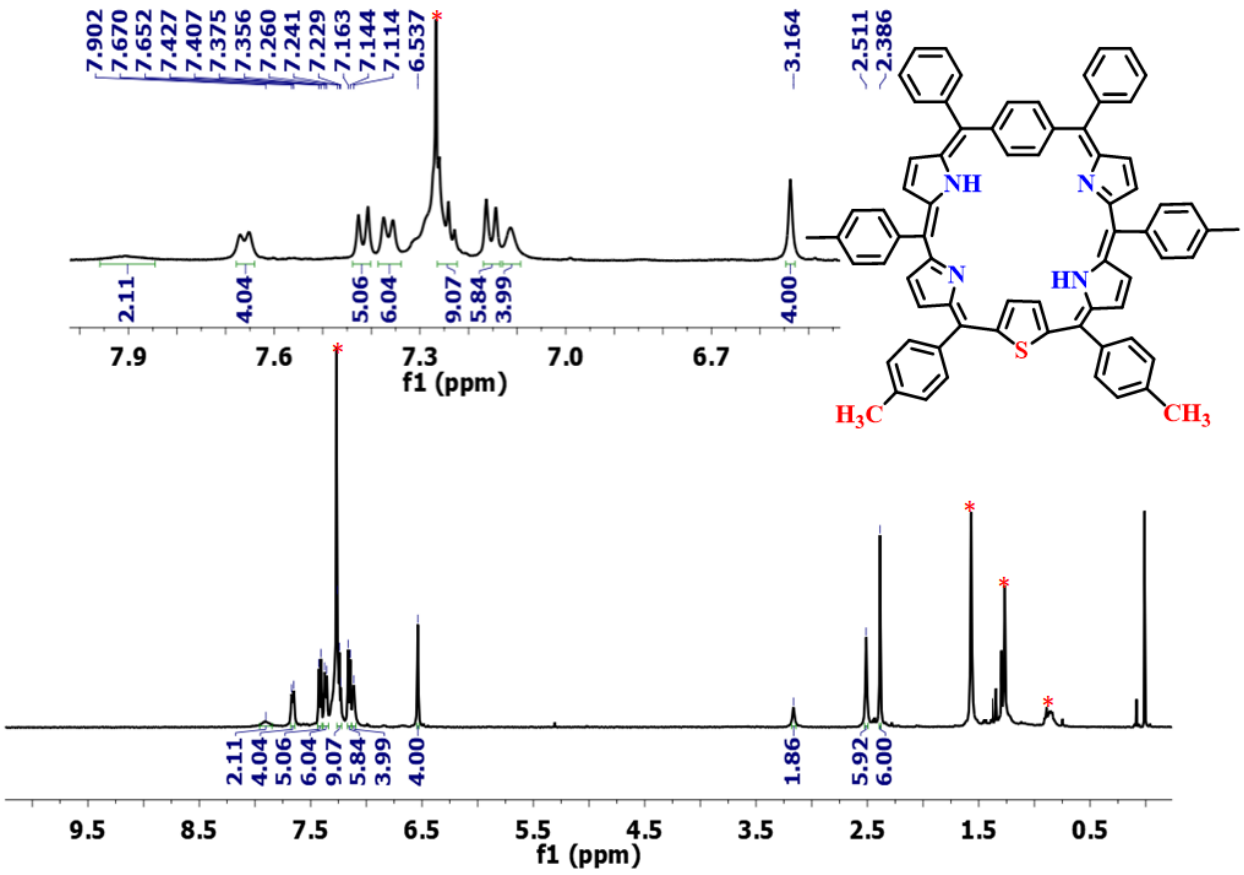


Figure S25. ^{1}H NMR spectrum of the compound **7** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

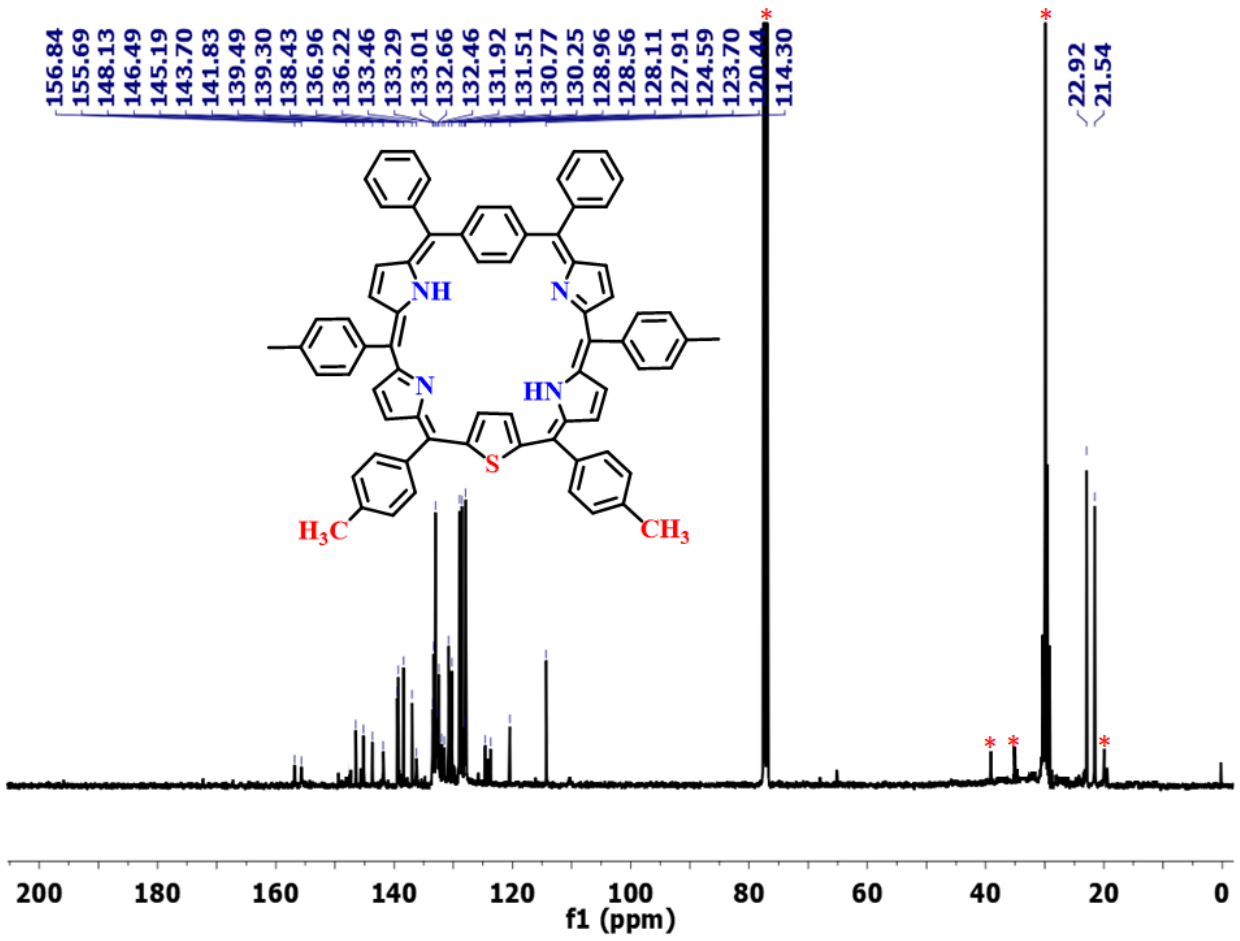
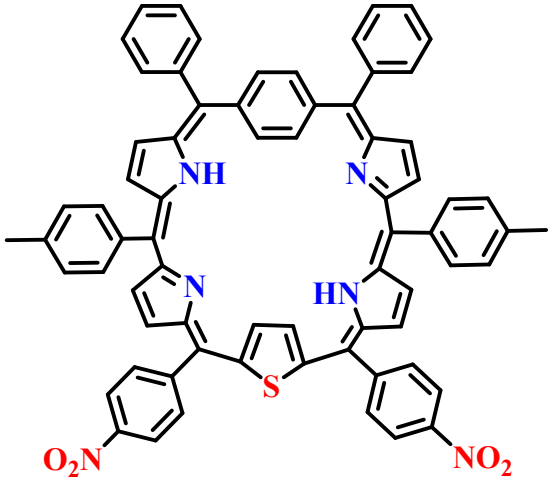


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **7** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **8**

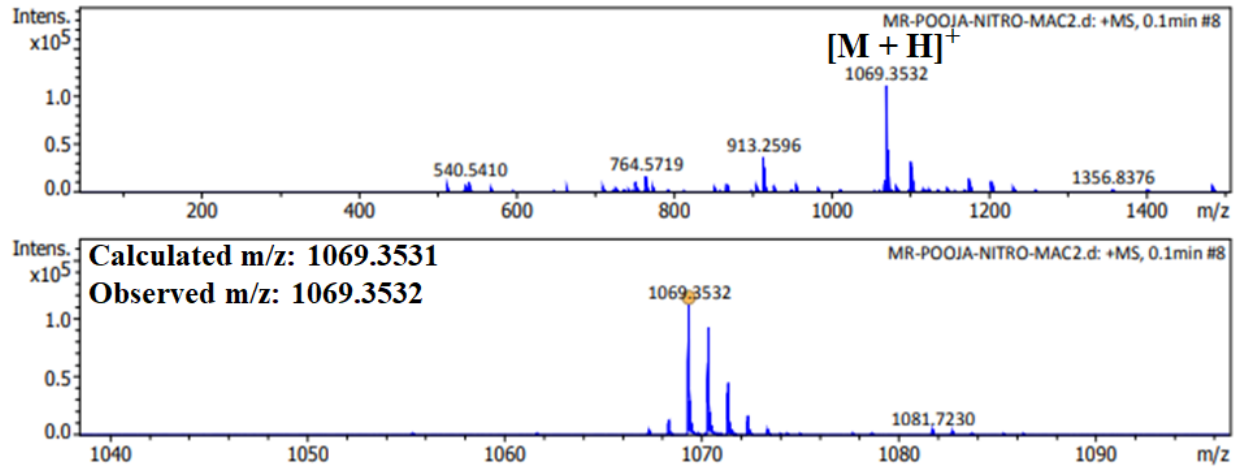
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\APR-2022\MR-POOJA-NITRO-MAC2.d	Acquisition Date	4/26/2022 2:54:29 PM
Method	NaICsI_pos_1500a.m	Operator	MR-IN
Sample Name	MR-POOJA-NITRO-MAC	Instrument	maXis impact 282001.00081
Comment	C70H48N6O4S		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.5 l/min
Scan End	1500 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1069.3532	1	C70H49N6O4S	1069.3531	-0.1	24.6	1	100.00	52.0	even	ok

Figure S27. HR mass spectrum of the compound **8**

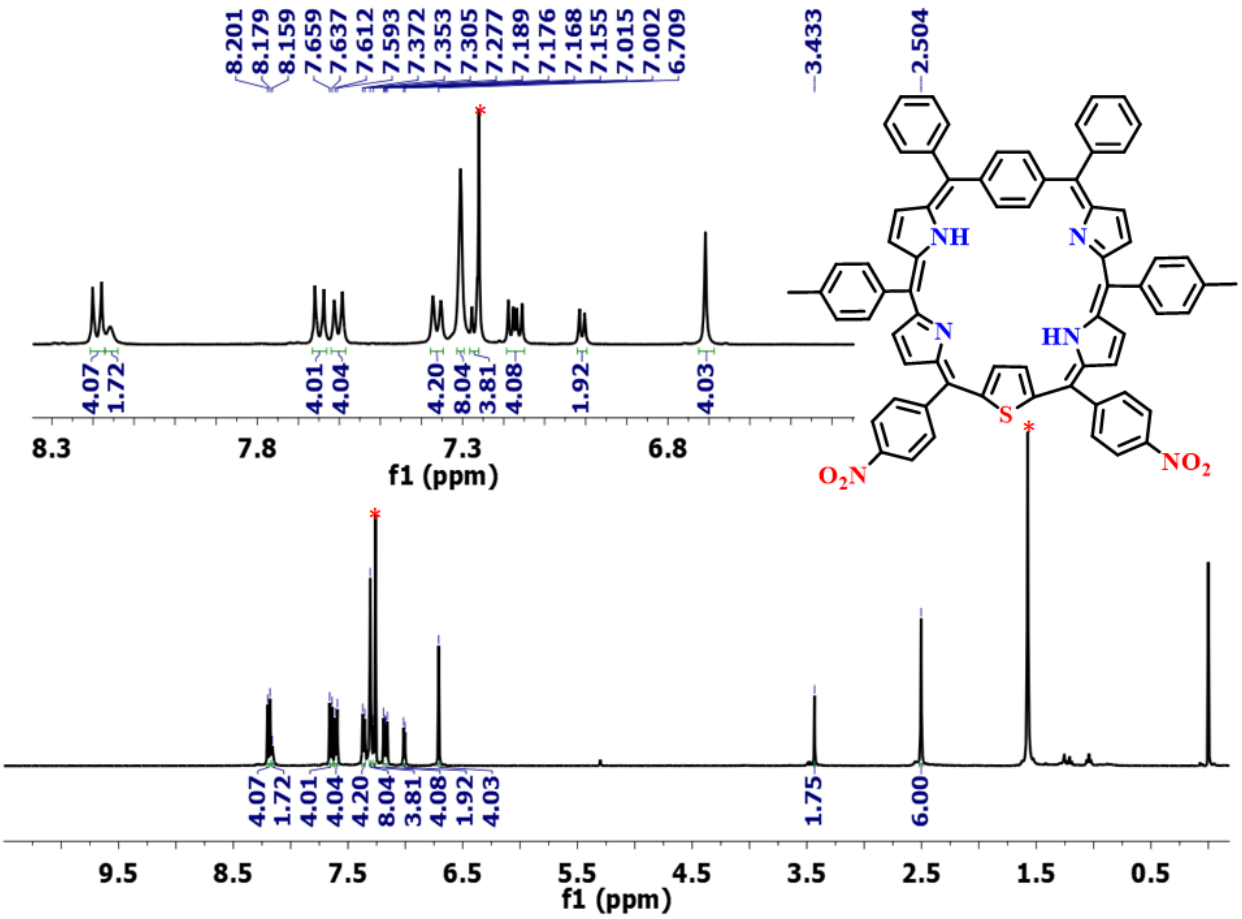


Figure S28. ^{1}H NMR spectrum of the compound **8** recorded in $CDCl_3$ at 298 K on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

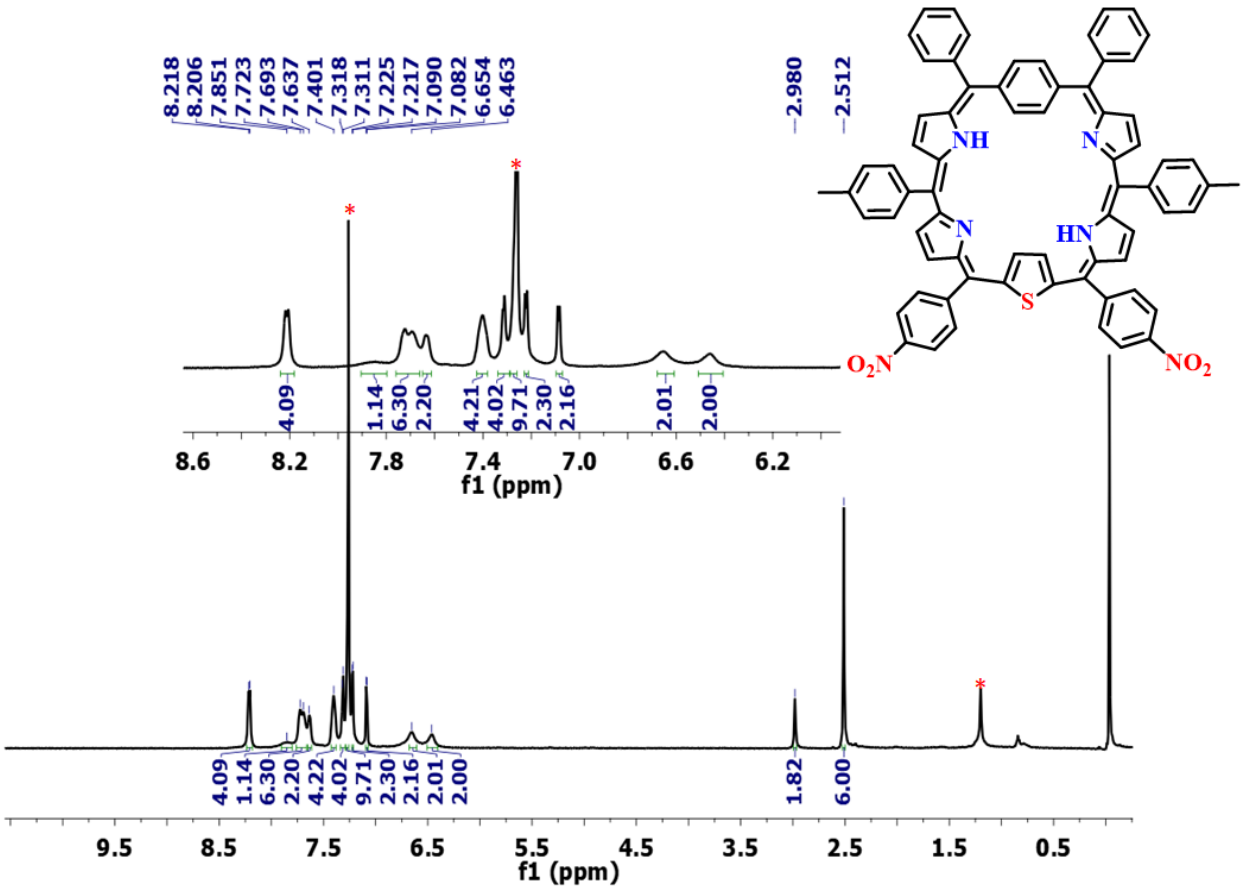


Figure S29. ^{1}H NMR spectrum of the compound **8** recorded in $CDCl_3$ at 223 K on 600 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

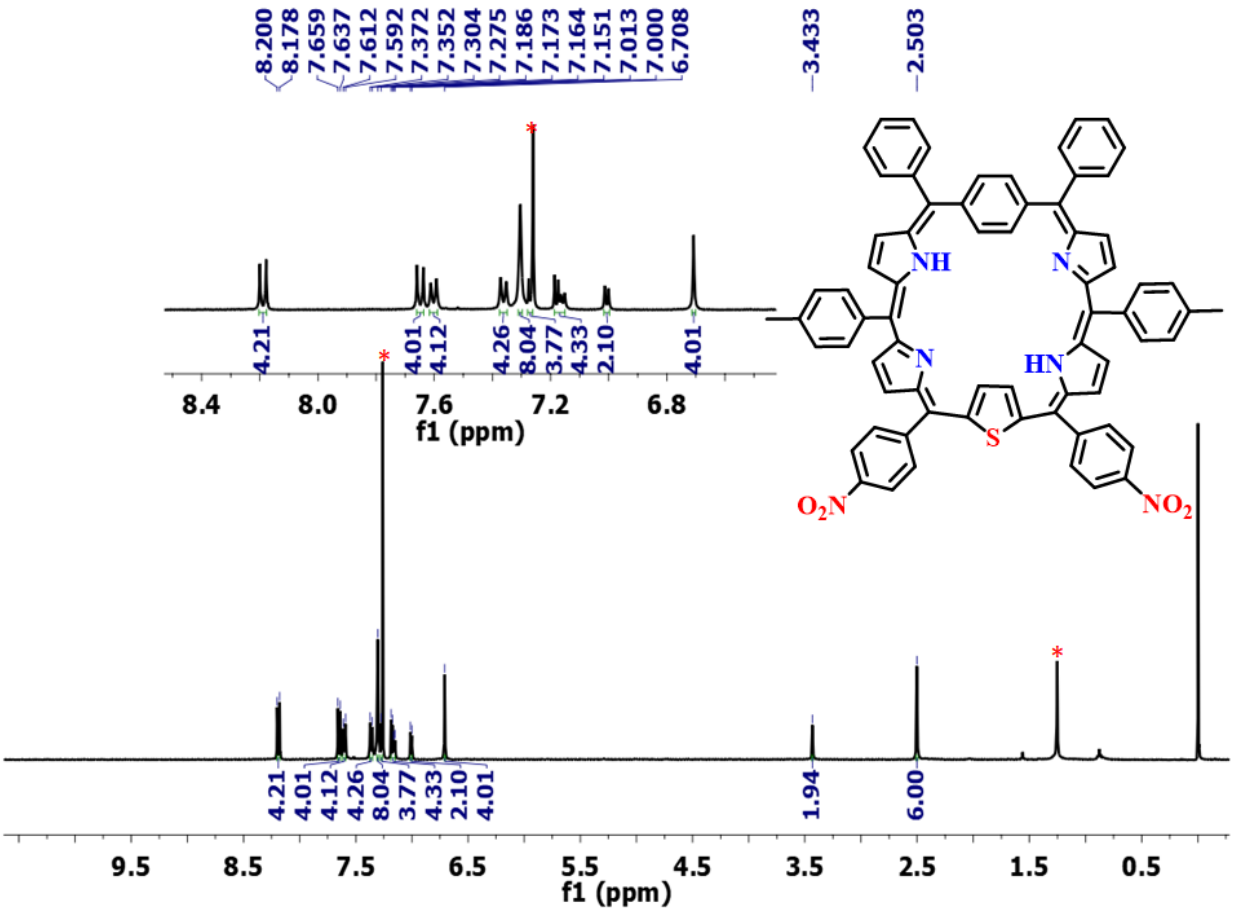


Figure S30. ^{1}H NMR spectrum of the compound **8** recorded upon addition of D_2O in $CDCl_3$ at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

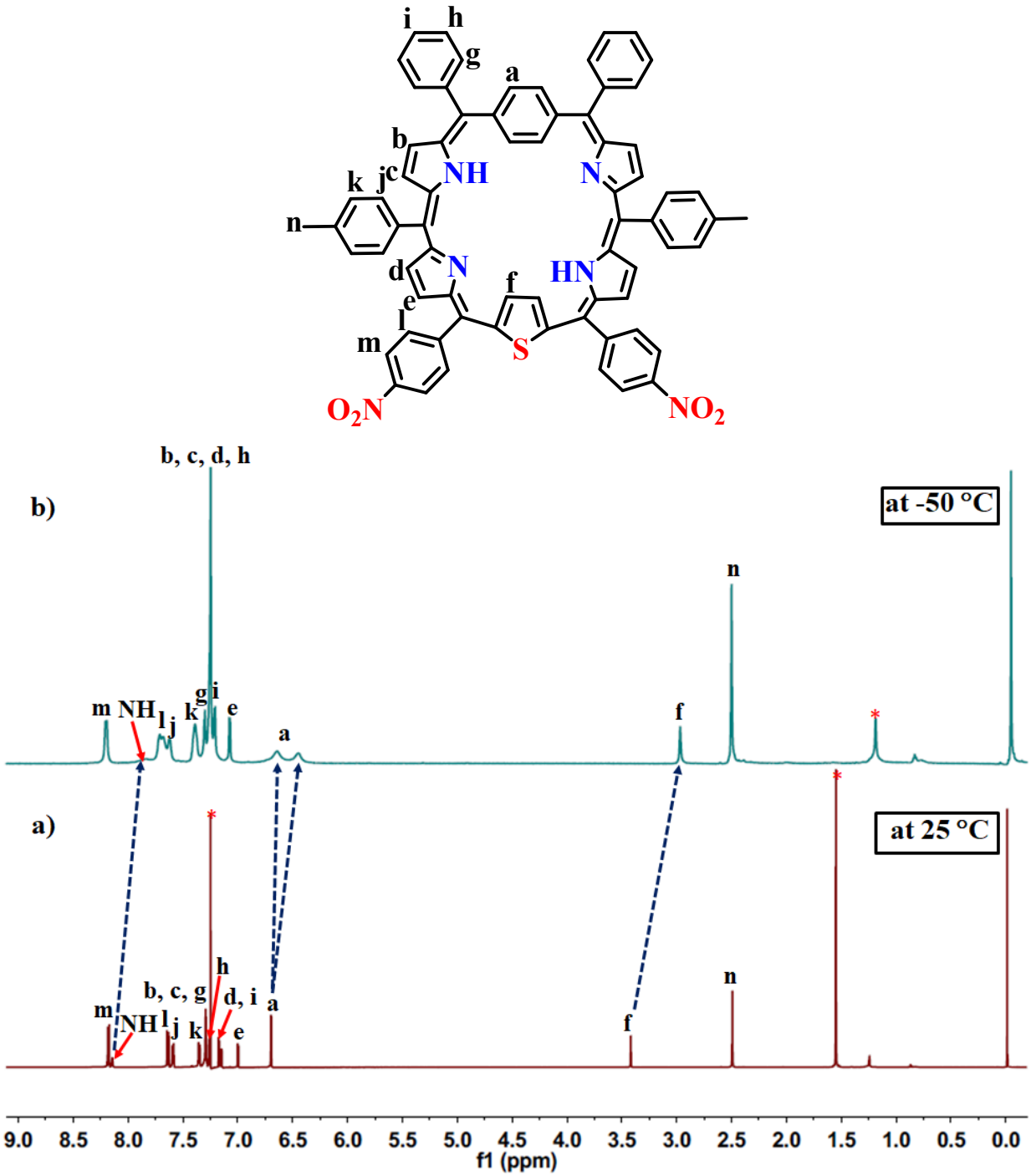


Figure S31. Comparison of ^{1}H NMR spectrum of the compound **8** recorded in $CDCl_3$ at 298K (a) and 223 K (b) on 600 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

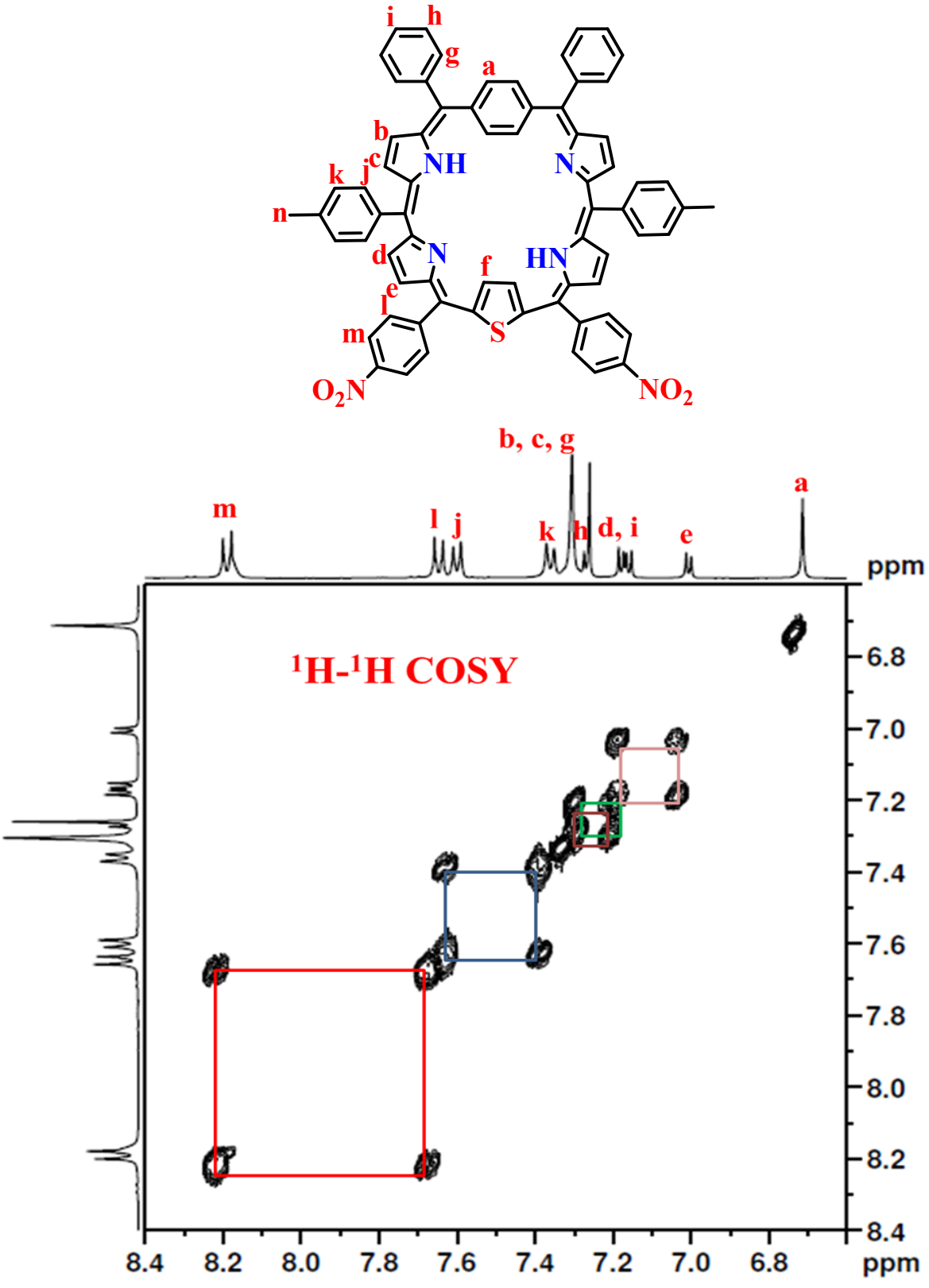


Figure S32. ^{1}H–^{1}H COSY of compound **8** recorded in $CDCl_3$ at 25 °C.

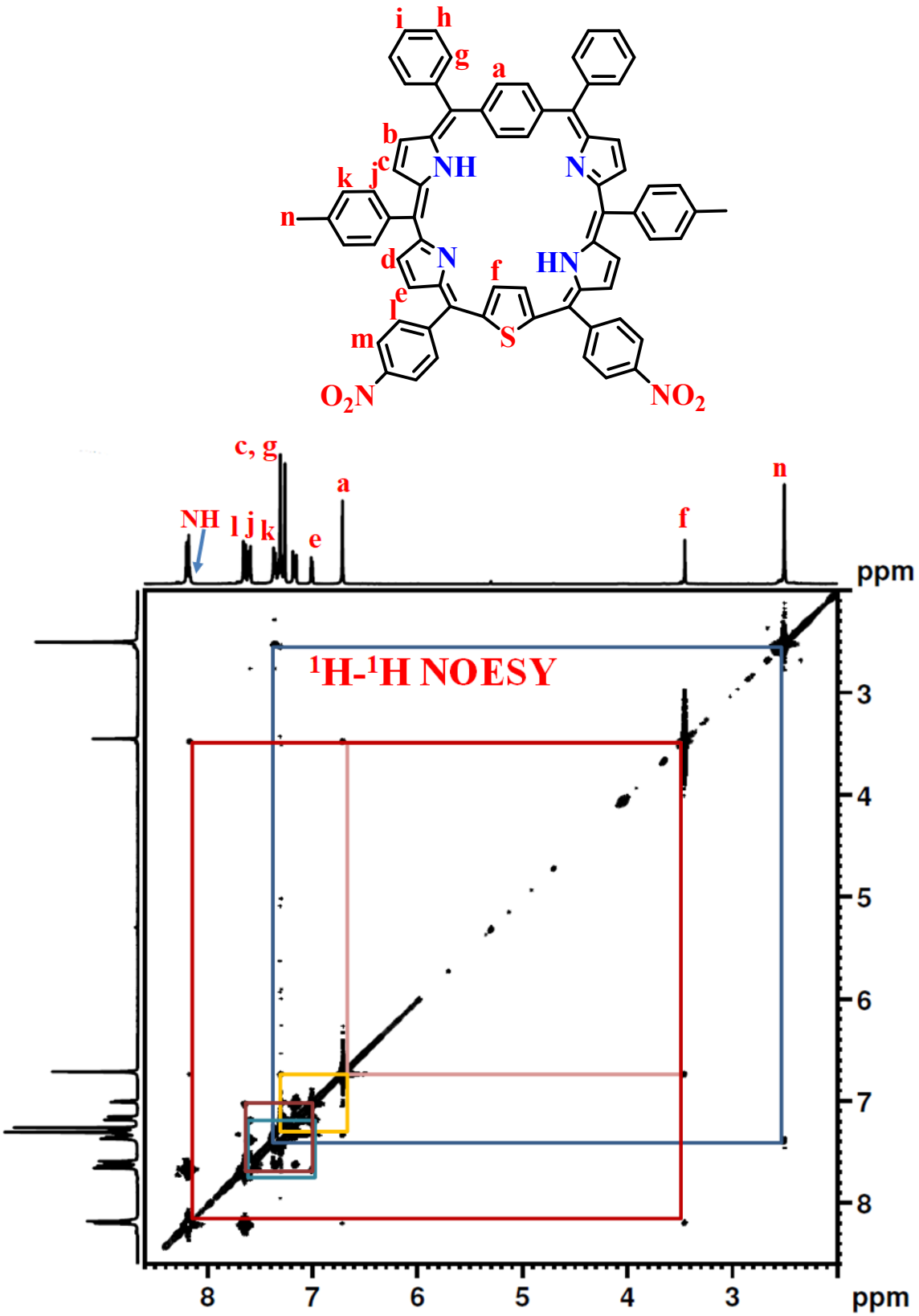


Figure S33. ^{1}H–^{1}H NOESY of compound **8** recorded in $CDCl_3$ at 25 °C.

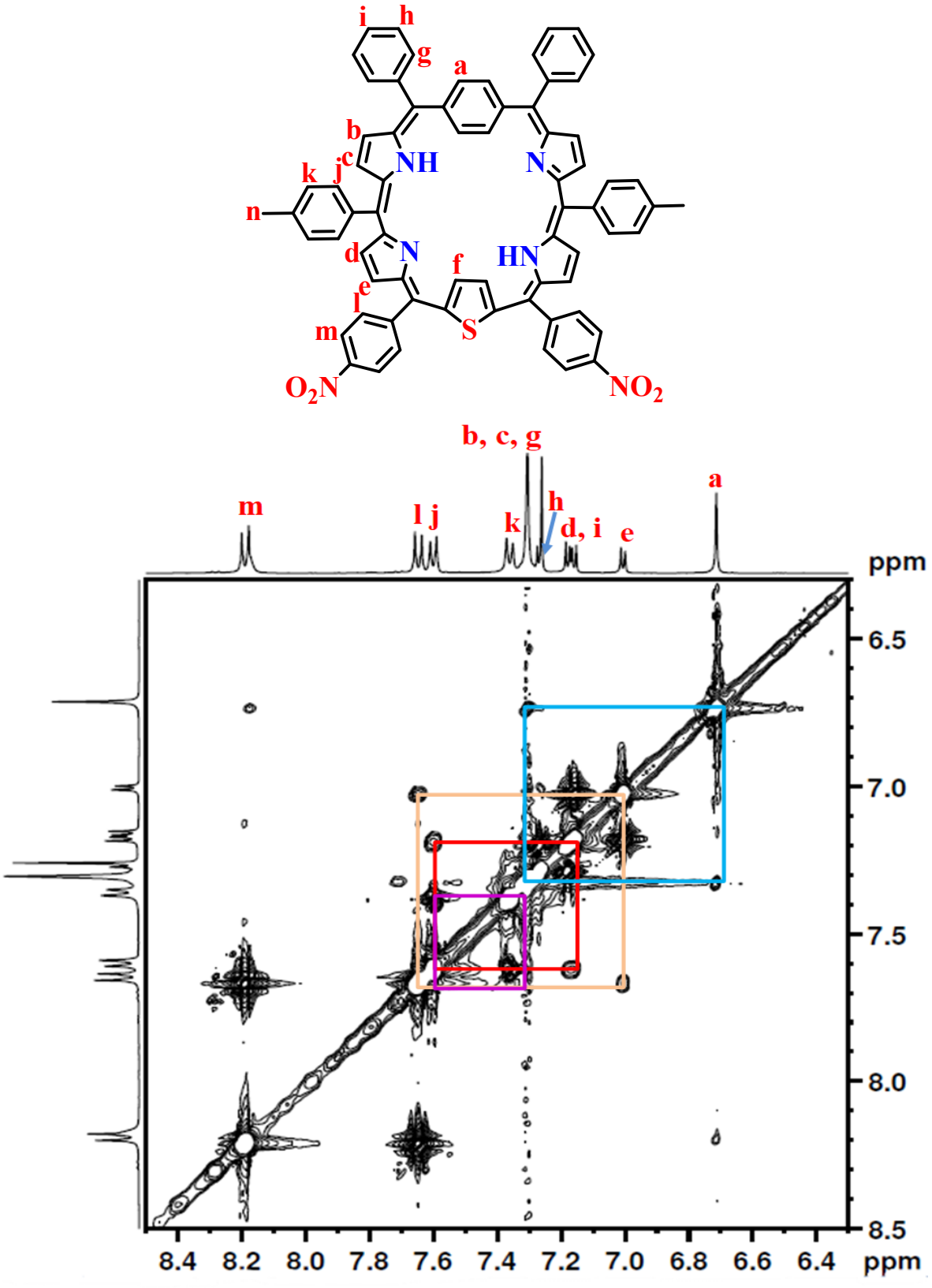


Figure S34. Expanded ^{1}H–^{1}H NOESY of compound **8** recorded in $CDCl_3$ at 25 °C.

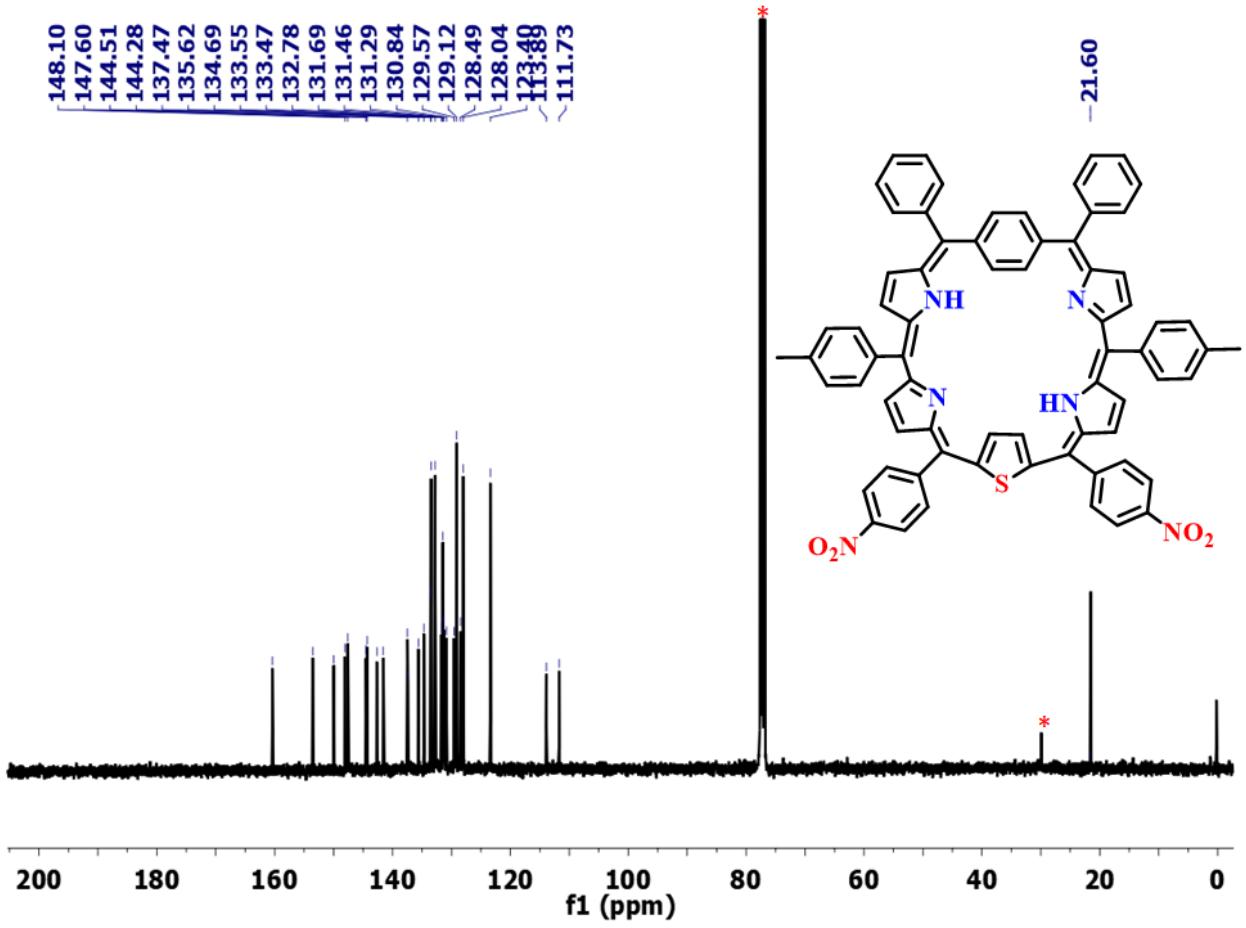


Figure S35. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **8** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

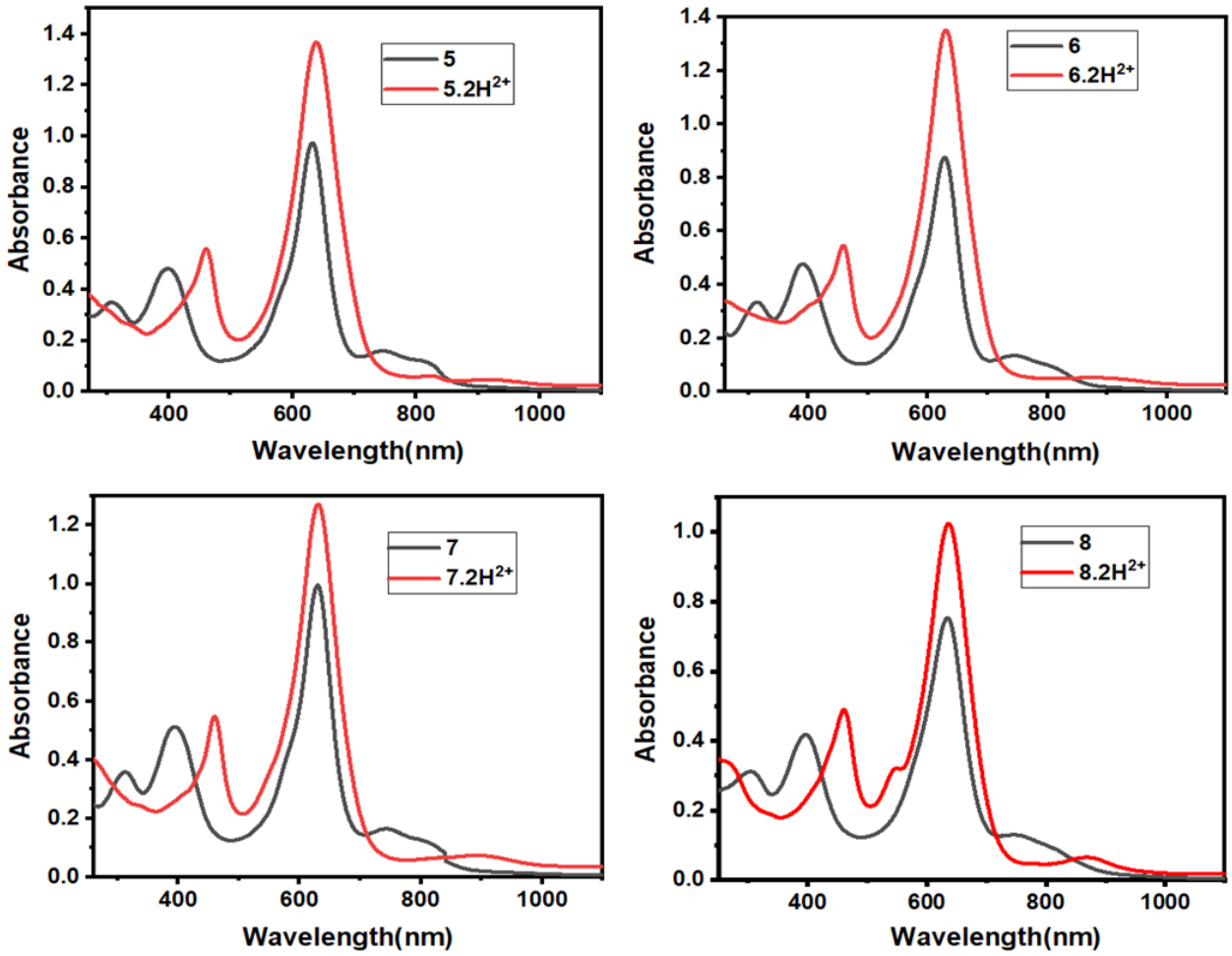


Figure S36. Comparison of absorption spectra of the compounds **5-8** ($8 \cdot 10^{-6}$ M) free base (black line) and in presence of TFA (excess) (red line) recorded in chloroform at room temperature.

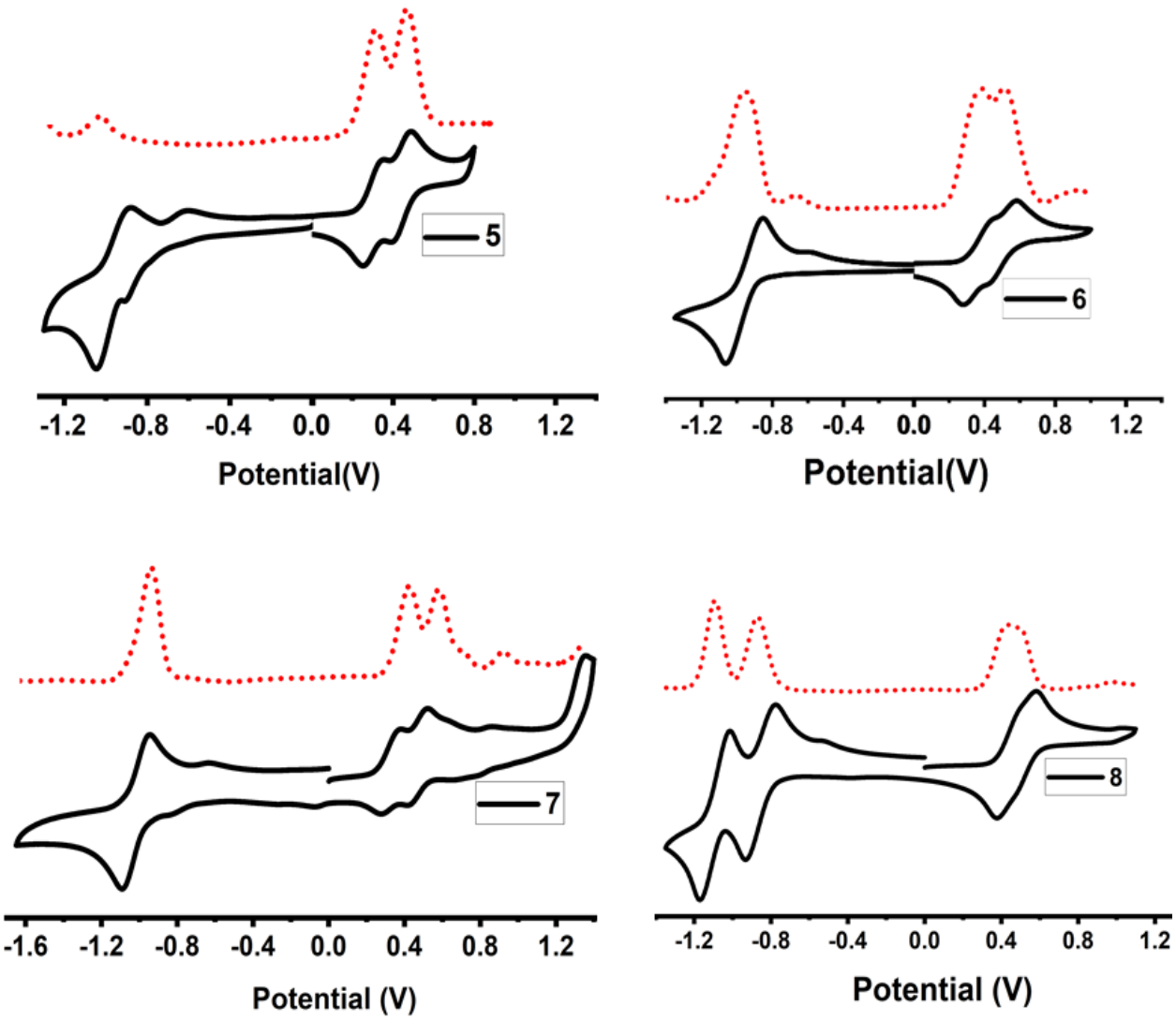


Figure S37. Comparison of cyclic voltammograms (black solid lines) along with differential pulse voltammograms (red dotted lines) of the compounds **5-8** recorded in CH_2Cl_2 containing 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at scan rates of 50 mV s^{-1}.

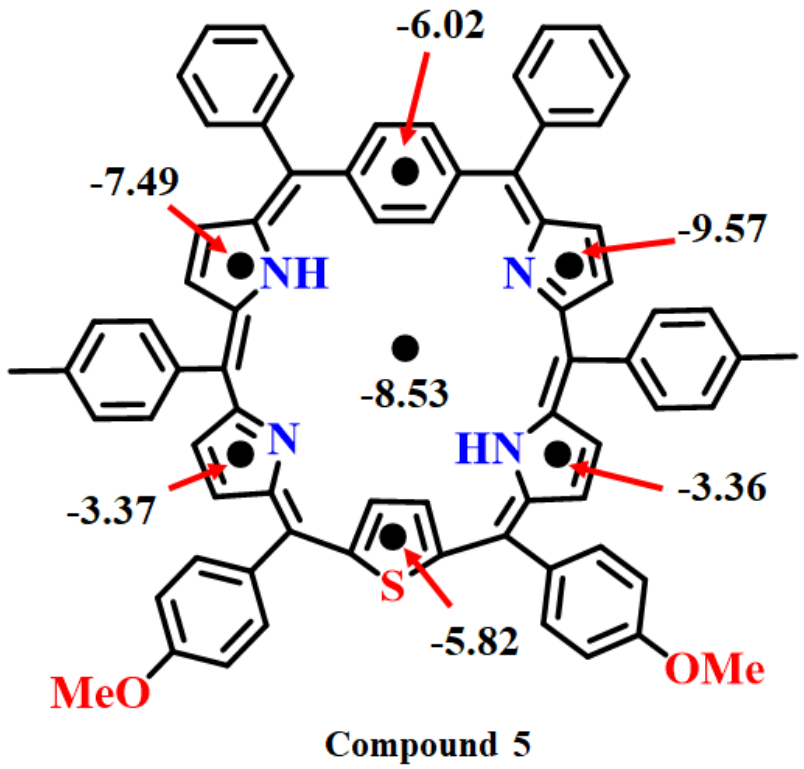


Figure S38. NICS(0) values of compound **5** on the optimized structures (B3LYP/6-31G (d, p) (black dots represent the Bq atoms).

Figure S39. NICS(0) values of compounds (a) **6** (b) **7** and (c) **8** on the optimized structures (B3LYP/6-31G (d, p) at the centre of the macrocycle (black dots represent the Bq atoms).

Table S1. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **5**.

Wavelength (nm)	Osc. Strength	Major Contributions	Minor Contributions
1161.436	0.0741	H-1->L+1 (10%), HOMO->LUMO (84%)	HOMO->L+1 (3%)
1038.126	0.1463	H-1->LUMO (50%), HOMO->L+1 (43%)	HOMO->LUMO (4%)
1025.249	0.0787	H-1->LUMO (44%), HOMO->L+1 (52%)	
909.4355	0.4652	H-1->L+1 (83%), HOMO->LUMO (10%)	HOMO->L+3 (4%)
815.8409	0.0194	H-1->L+2 (32%), HOMO->L+3 (60%)	H-1->L+1 (4%)
795.2238	0.0714	H-1->L+3 (27%), HOMO->L+2 (67%)	H-1->LUMO (2%)
654.6111	0.9761	H-1->L+2 (15%), H-1->L+3 (53%), HOMO->L+2 (19%)	HOMO->L+1 (2%), HOMO->L+3 (9%)
640.0131	0.5563	H-1->L+2 (50%), H-1->L+3 (15%), HOMO->L+3 (23%)	HOMO->L+2 (9%)
514.2616	0.007	H-2->LUMO (92%)	HOMO->L+4 (3%)
497.2261	0.0164	H-14->L+1 (15%), H-2->L+1 (20%)	H-24->L+1 (4%), H-19->LUMO (2%), H-17->LUMO (2%)
493.3089	0.0293	H-2->L+1 (52%), HOMO->L+4 (11%)	H-16->L+1 (2%), H-14->LUMO (6%), H-14->L+1 (8%)
478.6817	0.0463	H-3->LUMO (33%), H-2->L+1 (14%)	H-24->LUMO (5%), H-20->LUMO (2%)
475.214	0.109	HOMO->L+4 (30%)	H-24->LUMO (5%), H-24->L+1 (4%)
469.9721	0.0365	H-1->L+4 (21%), HOMO->L+5 (64%)	HOMO->L+4 (7%)
465.5078	0.2371	H-3->LUMO (46%), HOMO->L+4 (15%)	H-24->L+1 (2%), H-19->LUMO (3%), H-14->L+1 (2%)
459.0785	0.0276	H-4->LUMO (12%), H-3->L+1 (55%), H-1->L+4 (14%)	H-3->L+2 (2%), H-1->L+5 (2%), HOMO->L+4 (2%)
449.5733	0.0067	H-4->LUMO (33%), H-1->L+4 (21%)	H-6->LUMO (6%), H-5->LUMO (6%), H-4->L+1 (7%)
444.0505	0.0074	H-4->LUMO (14%), H-3->L+1 (26%), H-2->L+3 (14%), H-1->L+4 (24%)	HOMO->L+5 (9%)
435.2431	0.2087	H-1->L+5 (66%)	H-6->LUMO (3%), H-5->LUMO (2%), H-4->LUMO (3%)

431.0515	0.0057	H-6->LUMO (45%), H-5->LUMO (24%)	H-6->L+1 (3%), H-6->L+3 (5%), H-5->L+3 (2%)
424.0486	0.0279	H-5->LUMO (39%), H-4->LUMO (20%), H-4->L+1 (14%)	H-6->LUMO (6%), H-5->L+1 (3%), H-2->L+2 (2%)
420.6961	0.0399	H-4->L+1 (53%)	H-7->LUMO (5%), H-6->LUMO (4%), H-5->LUMO (9%)
418.2268	0.1484	H-6->LUMO (12%), H-2->L+2 (28%)	H-7->LUMO (2%), H-6->L+1 (3%), H-5->LUMO (9%)
413.6363	0.392	H-7->LUMO (17%), H-2->L+2 (20%), H-2->L+3 (26%)	H-6->LUMO (9%), H-5->L+1 (3%), H-3->L+2 (6%)
409.3886	0.1291	H-6->L+1 (37%), H-5->L+1 (37%)	H-6->LUMO (4%), H-2->L+2 (8%), H-2->L+3 (5%)
406.6094	0.0933	H-7->LUMO (38%), H-6->L+1 (27%)	H-5->LUMO (3%), H-5->L+1 (7%), H-3->L+2 (4%)
403.6573	0.2589	H-7->LUMO (21%), H-6->L+1 (15%), H-5->L+1 (39%)	H-4->L+1 (9%), H-2->L+2 (2%)
395.5821	0.0216	H-7->L+1 (68%)	H-10->LUMO (4%), H-6->L+1 (4%), H-3->L+2 (8%)

Table S2. S_0 optimized geometry of the compound **5** at B3LYP/TZVP level of theory and Empirical Dispersion GD2.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3544.989570

Atom	X	Y	Z	Atom	X	Y	Z
C	1.021171	-2.98043	1.126557	C	1.180113	3.883352	-2.99709
C	1.384727	-2.99798	-0.24024	C	-4.67143	1.754248	2.064264
C	0.437895	-3.08218	-1.23582	C	-5.64477	0.922047	1.622955
C	-0.94463	-3.12049	-0.94828	C	-5.03687	0.09325	0.592762
C	-1.30906	-3.0585	0.41764	N	-3.73132	0.390965	0.448122
C	-0.36117	-3.00992	1.415141	N	3.73205	0.456344	-0.64159
C	-1.92656	-3.31594	-1.99967	C	5.07673	0.172143	-0.69621
C	2.015206	-3.03598	2.181325	C	5.648974	1.105945	-1.62734
C	-1.55747	-4.0788	-3.2066	C	4.657936	1.929547	-2.0664
C	-3.23174	-2.86148	-1.87781	O	-2.28556	7.20245	3.908845
C	3.303679	-2.53802	2.008088	C	-1.23765	7.562315	4.80069
C	1.682379	-3.7142	3.447527	O	2.083268	7.338225	-3.90656
C	-0.76648	-5.23552	-3.1161	C	1.056477	7.666164	-4.83426
C	-0.43633	-5.96579	-4.24929	H	2.43142	-2.97207	-0.501
C	-0.88445	-5.55678	-5.50464	H	0.759077	-3.13267	-2.26777
C	-1.66347	-4.40803	-5.61307	H	-2.35354	-3.09595	0.691796
C	-1.99288	-3.67557	-4.47835	H	-0.6828	-3.00046	2.448068

C	2.10593	-3.18203	4.675068	H	-0.42165	-5.5601	-2.14294
C	1.818365	-3.82895	5.871213	H	0.16767	-6.8602	-4.15384
C	1.099812	-5.0215	5.867253	H	-0.62357	-6.12518	-6.38901
C	0.667143	-5.56033	4.656284	H	-2.00477	-4.07315	-6.58538
C	0.950559	-4.91254	3.461958	H	-2.57824	-2.76952	-4.56796
C	4.501369	-3.01481	2.689295	H	2.649586	-2.24637	4.677593
C	5.556016	-2.45431	2.048371	H	2.147483	-3.39632	6.808418
C	4.996828	-1.57273	1.030267	H	0.873916	-5.52529	6.799226
N	3.65334	-1.64181	1.034791	H	0.112144	-6.49073	4.644192
N	-3.65697	-1.9059	-0.98274	H	0.621156	-5.338	2.522977
C	-5.0226	-1.77518	-1.00135	H	4.51798	-3.74616	3.481336
C	-5.49973	-2.70861	-1.98652	H	6.605385	-2.62388	2.227299
C	-4.42229	-3.34086	-2.53301	H	-3.09777	-1.20407	-0.49837
C	5.720482	-0.75896	0.116615	H	-6.53866	-2.85862	-2.2275
C	-5.72103	-0.87963	-0.19652	H	-4.42675	-4.11919	-3.27775
C	-7.19837	-0.92702	-0.18063	H	7.53322	-0.33502	2.091983
C	7.197648	-0.86684	0.040454	H	9.987435	-0.51338	1.957197
C	8.001722	-0.62048	1.158461	H	9.682516	-1.56704	-2.17813
C	9.385663	-0.71831	1.078322	H	7.225961	-1.41049	-2.03441
C	10.01757	-1.06184	-0.11851	H	-7.31614	-3.04394	0.154425
C	9.215998	-1.29942	-1.23622	H	-9.77757	-3.12553	0.156644
C	7.83098	-1.20798	-1.15913	H	-9.91562	1.102364	-0.48574
C	-7.88421	-2.13496	0.00181	H	-7.45289	1.178384	-0.50796
C	-9.27253	-2.17708	0.008567	H	11.88322	-0.97819	-1.198
C	-10.0307	-1.01645	-0.15882	H	12.01008	-0.52753	0.51147
C	-9.34932	0.188841	-0.34027	H	11.82653	-2.22147	0.052961
C	-7.96116	0.235563	-0.35114	H	-11.972	-0.24805	-0.69913
C	11.51592	-1.2003	-0.19339	H	-11.9166	-2.00811	-0.49653
C	-11.5357	-1.05917	-0.11165	H	-11.8969	-0.95263	0.91707
C	1.059604	1.831083	-0.71536	H	1.102395	-0.35084	-0.71748
C	0.596848	0.55141	-0.40544	H	-1.10653	-0.37003	0.612811
C	-0.60943	0.535114	0.301245	H	-0.45817	3.102652	3.049766
C	-1.11109	1.797169	0.606836	H	-0.40351	5.251114	4.224398
S	-0.041	3.037082	-0.05161	H	-4.03187	6.417312	2.253286
C	2.23272	2.264327	-1.41028	H	-4.08576	4.229487	1.086311
C	-2.29675	2.184801	1.304862	H	3.905519	4.395713	-1.06641
C	-3.47552	1.440628	1.293533	H	3.792803	6.602438	-2.19051
C	-2.28298	3.495238	1.994452	H	0.318921	5.302123	-4.34629
C	-1.24692	3.823079	2.874464	H	0.436925	3.128667	-3.2217
C	-1.21386	5.041949	3.541026	H	-4.73807	2.498072	2.841124
C	-2.22726	5.977902	3.317829	H	-6.666	0.85324	1.961268
C	-3.26395	5.674915	2.429284	H	3.139296	-0.07166	-0.00127
C	-3.28824	4.452816	1.7823	H	6.691702	1.131893	-1.89515

C	3.429819	1.56428	-1.40465	H	4.745351	2.740443	-2.76909
C	2.189801	3.589105	-2.07729	H	-1.47252	8.566225	5.149429
C	3.130246	4.591966	-1.79562	H	-1.19228	6.87658	5.653788
C	3.073104	5.826432	-2.41792	H	-0.26879	7.565576	4.289602
C	2.062479	6.097749	-3.34552	H	1.25414	8.688466	-5.15126
C	1.110392	5.11697	-3.63441	H	1.081079	6.999309	-5.70311
				H	0.068308	7.609168	-4.36492

Table S3. S_0 optimized geometry of the compound **5** at B3LYP/6-31G (d, p) level of theory and Empirical Dispersion GD2.

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3543.865656

Atom	X	Y	Z	Atom	X	Y	Z
C	0.9616	-3.102	1.1601	C	1.1692	3.6738	-3.0048
C	1.3712	-3.1228	-0.1985	C	-4.6944	1.587	1.9893
C	0.4529	-3.211	-1.2275	C	-5.669	0.7688	1.5185
C	-0.9411	-3.2598	-0.9799	C	-5.0461	-0.0577	0.4879
C	-1.3518	-3.2051	0.3779	N	-3.7289	0.227	0.3706
C	-0.4327	-3.1423	1.4084	N	3.7506	0.2905	-0.5817
C	-1.8928	-3.4556	-2.0653	C	5.097	-0.0115	-0.6047
C	1.9254	-3.1503	2.2496	C	5.6999	0.8992	-1.5453
C	-1.4896	-4.212	-3.2671	C	4.7246	1.726	-2.0216
C	-3.2052	-2.9992	-1.9742	H	2.4281	-3.092	-0.4257
C	3.2256	-2.6583	2.1072	H	0.8053	-3.2571	-2.2521
C	1.555	-3.8155	3.5149	H	-2.4066	-3.2561	0.619
C	-0.6627	-5.3489	-3.164	H	-0.7862	-3.1318	2.4333
C	-0.3007	-6.0747	-4.296	H	-0.3183	-5.6625	-2.1841
C	-0.754	-5.6821	-5.5598	H	0.33	-6.9527	-4.1923
C	-1.5695	-4.554	-5.6804	H	-0.469	-6.2474	-6.4422
C	-1.9292	-3.824	-4.5483	H	-1.9147	-4.2329	-6.6588
C	1.973	-3.2827	4.7503	H	-2.5401	-2.9326	-4.646
C	1.6513	-3.9182	5.9487	H	2.5383	-2.3568	4.7558
C	0.9028	-5.0981	5.9387	H	1.9764	-3.4867	6.8908
C	0.476	-5.6375	4.7207	H	0.6497	-5.5919	6.8723
C	0.7951	-5.0027	3.523	H	-0.1004	-6.5578	4.7049
C	4.4009	-3.1413	2.8273	H	0.474	-5.4297	2.5787
C	5.4815	-2.6009	2.2028	H	4.3871	-3.8657	3.6293
C	4.9555	-1.7255	1.1592	H	6.5266	-2.7802	2.4099
N	3.6083	-1.7743	1.1283	H	-3.0982	-1.3475	-0.575

N	-3.648	-2.0456	-1.0807	H	-6.5107	-2.9793	-2.4007
C	-5.0124	-1.9105	-1.1309	H	-4.3727	-4.2481	-3.4126
C	-5.4741	-2.8354	-2.1357	H	7.4931	-0.598	2.275
C	-4.3833	-3.4716	-2.6621	H	9.9538	-0.82	2.1865
C	5.7145	-0.9347	0.2416	H	9.7212	-1.7481	-1.9965
C	-5.7268	-1.0163	-0.3234	H	7.2565	-1.5545	-1.901
C	-7.2061	-1.0605	-0.3316	H	-7.3321	-3.1985	-0.1001
C	7.1925	-1.0674	0.1947	H	-9.8018	-3.2739	-0.1411
C	7.9781	-0.8672	1.3419	H	-9.9249	0.9936	-0.5745
C	9.3656	-0.9883	1.2878	H	-7.454	1.0659	-0.5655
C	10.0193	-1.3087	0.0903	H	11.9135	-1.216	-0.9476
C	9.2364	-1.4999	-1.0556	H	12.0097	-0.8299	0.7847
C	7.8477	-1.3868	-1.0059	H	11.8109	-2.5052	0.2573
C	-7.8982	-2.2798	-0.2171	H	-11.983	-0.3546	-0.9013
C	-9.2906	-2.3188	-0.2338	H	-11.931	-2.1254	-0.7551
C	-10.047	-1.145	-0.3537	H	-11.936	-1.1139	0.6942
C	-9.3596	0.0712	-0.4663	H	1.1184	-0.5349	-0.7829
C	-7.9672	0.1157	-0.4574	H	-1.1077	-0.5676	0.5534
C	11.5193	-1.4685	0.0424	H	-0.4267	2.8095	3.0627
C	-11.555	-1.1874	-0.3333	H	-0.3634	4.9552	4.3332
C	1.0834	1.6487	-0.7323	H	-3.9852	6.2106	2.4032
C	0.614	0.3632	-0.4493	H	-4.0567	4.0616	1.1347
C	-0.601	0.3406	0.2578	H	4.0108	4.1877	-1.2032
C	-1.0907	1.6042	0.5887	H	3.905	6.3632	-2.4158
S	-0.0069	2.8438	-0.0405	H	0.3002	5.103	-4.3738
C	2.2729	2.086	-1.4155	H	0.4028	2.9238	-3.1669
C	-2.2874	1.991	1.2847	H	-4.7708	2.3238	2.7758
C	-3.4832	1.2687	1.2316	H	-6.7008	0.7076	1.8338
C	-2.2585	3.2766	2.025	H	3.1387	-0.2147	0.0623
C	-1.2044	3.5516	2.9199	H	6.7498	0.9068	-1.7959
C	-1.1597	4.7432	3.6313	H	4.837	2.5178	-2.7464
C	-2.1758	5.6808	3.4331	O	-2.1349	6.9436	4.1769
C	-3.2257	5.452	2.5433	O	2.0422	7.1132	-4.1691
C	-3.2592	4.2512	1.8434	C	2.99257	7.97634	-3.9566
C	3.4781	1.3892	-1.3676	H	3.93172	7.55022	-4.2417
C	2.2293	3.3897	-2.1191	H	2.81018	8.85746	-4.5356
C	3.2121	4.3778	-1.9106	H	3.01726	8.23104	-2.9176
C	3.1588	5.5959	-2.5781	C	-3.094	7.80059	3.97938
C	2.104	5.8331	-3.4603	H	-4.0295	7.35791	4.25121
C	1.1023	4.8846	-3.6805	H	-2.9238	8.67075	4.57833
				H	-3.1175	8.07779	2.94617