Supporting Information

Structural Isomers of Di-*P*-Benzidithiaoctaphyrins

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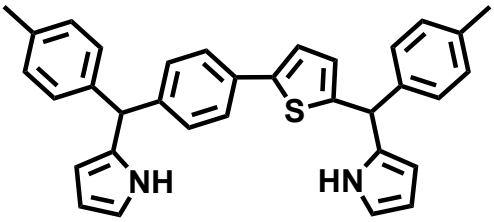
General Experimental section
Materials, methods, instrumentation and computational details.

Reagent-grade chemicals were employed during synthesis. For column chromatography purification purpose, silica (60−120 and 100−200 mesh) and basic alumina was used. Bruker 400 and 500 MHz instruments assisted us in recording 1D, 2D and ^{13}C using $CDCl_3$ as solvent. 100.06 and 125.77 MHz is the frequency for the ^{13}C nucleus for 400 and 500 MHz respectively. For ^{1}H and $^{13}C\{1H\}$ NMR the internal standard used was Tetramethylsilane [$Si(CH_3)_4$]. Structural assignments were made with additional information from gCOSY and gNOESY experiments for compounds **3a/3b** and **4.** Cary series UV−vis−NIR and UV 3600 Shimadzu spectrophotometer helped us to record the absorption spectra of the compounds. For UV−Vis stock solution of compound **3-4** (10^{-5} M) was prepared by using a HPLC grade Toluene solvent. Cyclic voltammetry (CV) studies were carried out with BASi C3 Cell Stand electrochemical system (Manufacturer: Bioanalytical Systems. Inc.) utilizing the three-electrode configuration consisting of a glassy carbon (working electrode), platinum wire (auxiliary electrode) and saturated calomel as reference electrode (the electrode is composed of Hg/Hg_2Cl_2/Saturated KCl solution). The experiments were done in dry dichloromethane using 0.1 M tetrabutylammonium perchlorate as supporting electrolyte. The initial and final potential was at 0 V, first switching potential at -2.0 V and second switching potential at 2.0 V. Glassy carbon-disk working electrodes (3 mm diameter, part # CHI 104) were purchased from CH Instruments, HRMS was recorded on a Bruker maXis Impact and LC-MS Q-Tof micro mass spectrometer using positive mode ESI methods for acetonitrile/methanol solutions.

Computational details: For all the calculations Gaussian 09 program package was used.[1] The density functional theory (DFT)[2] method, hybrid functional B3LYP in conjunction with basis set 6-31G(d,p)[3] helped to optimize the structure of compounds **3-4** in the ground (S_0) states. To obtain the oscillator strengths, identical basis and functional hybrid set were used whereas the

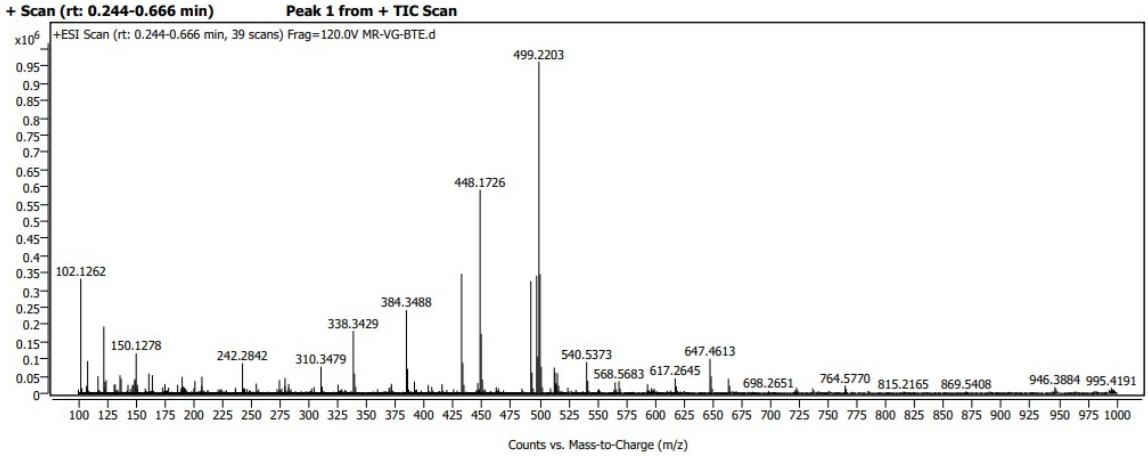
vertical excitation energies were obtained with the help of TD-DFT techniques for $S_0 \rightarrow S_n$ transitions.[4] Under the Polarisable Continuum Model (PCM) in the toluene media all the computations were done using the Self-Consistent Reaction Field (SCRF). The electronic absorption spectra as well as the oscillator strengths were thoroughly examined using TD-DFT with PCM model[5] on the basis of the optimized structures in the S_0 state.



Compound 8a

Sample Spectra

+ Scan (rt: 0.244-0.666 min) **Peak 1 from + TIC Scan**

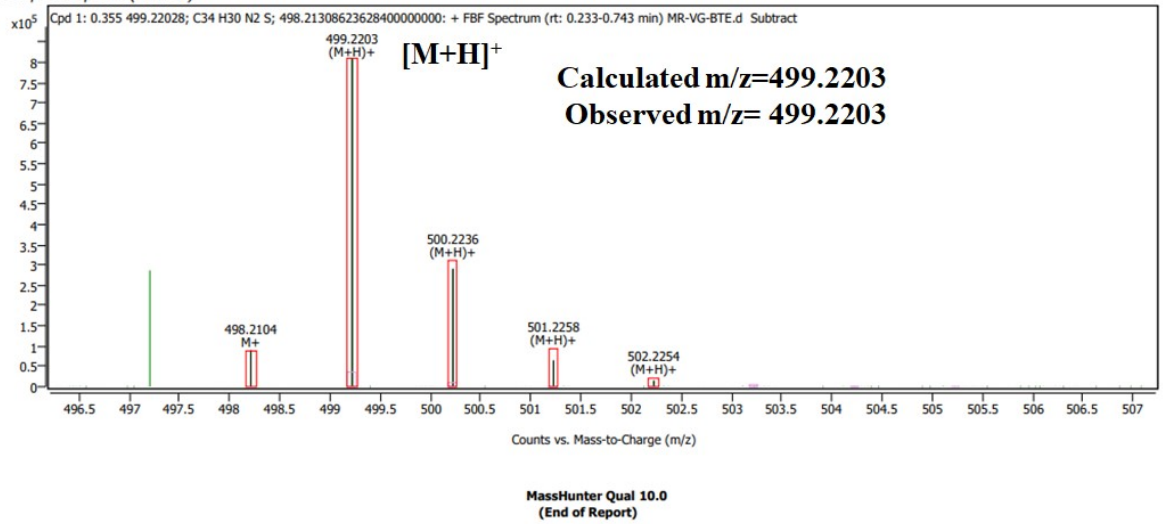


Compound Details

Cpd. 1: C34 H30 N2 S

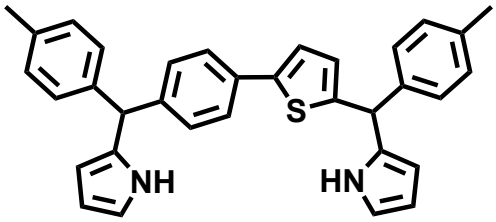
Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C34 H30 N2 S	499.2203	499.220277062171	0.116534483993291	0.233904958481996	95.15

Compound Spectra (Zoomed)



MassHunter Qual 10.0
(End of Report)

Figure S1. High resolution mass spectrum of compound **8a.**



Compound 8a

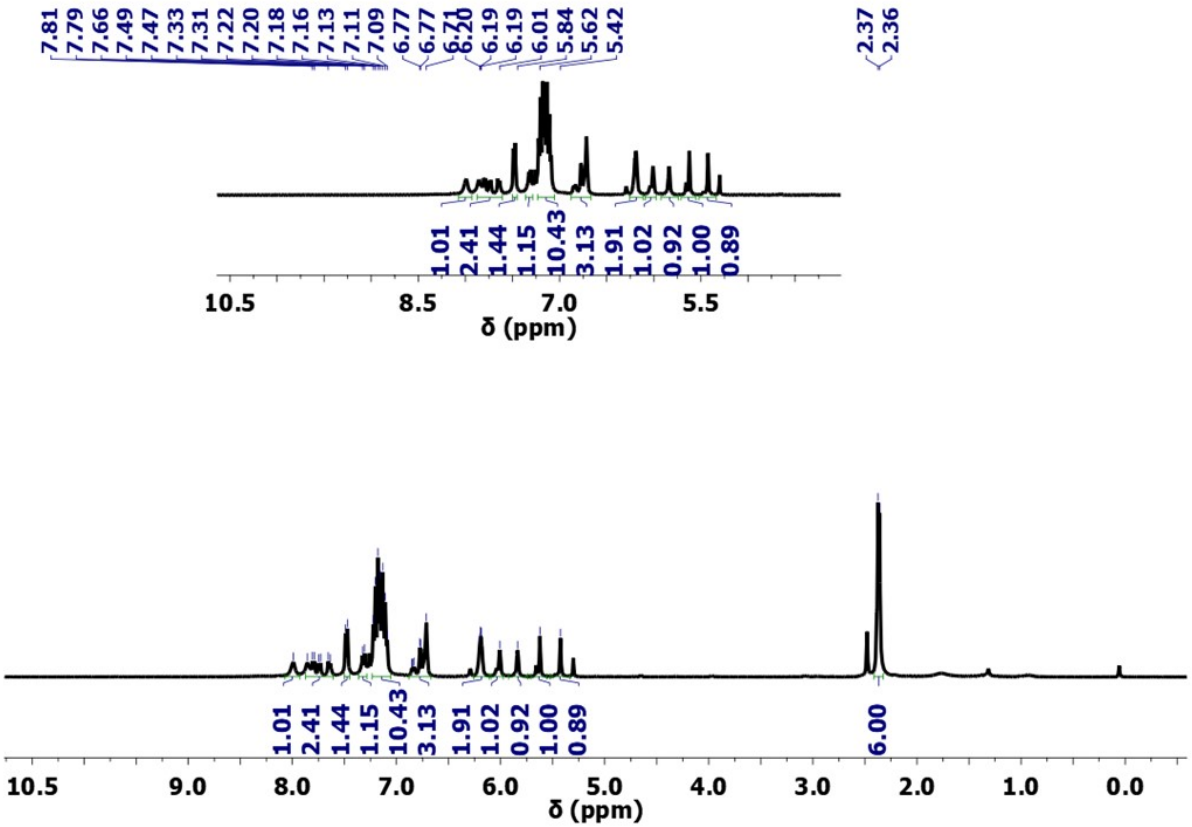
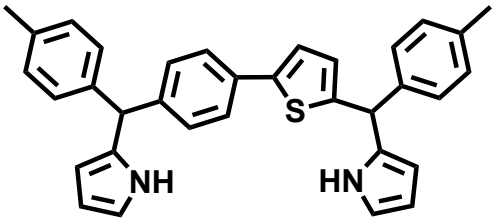


Figure S2. ^{1}H-NMR spectrum of compound **8a** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 8a

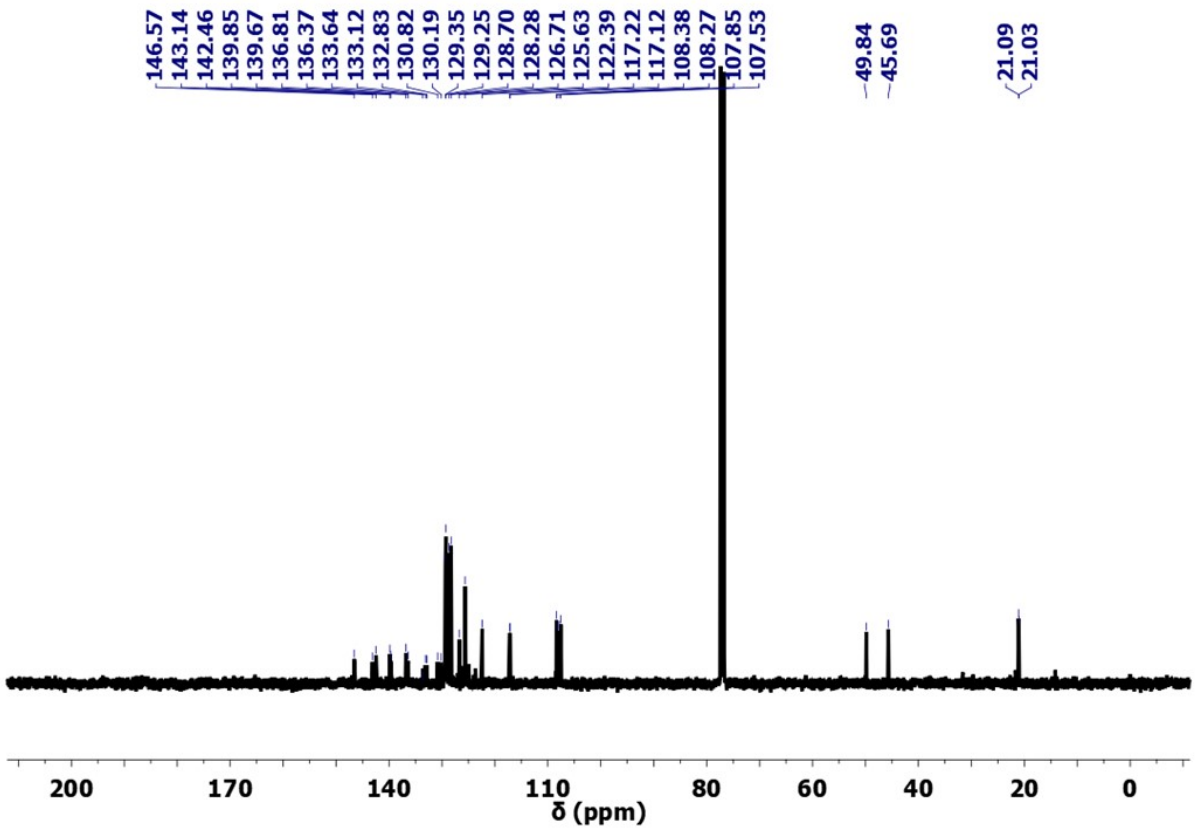
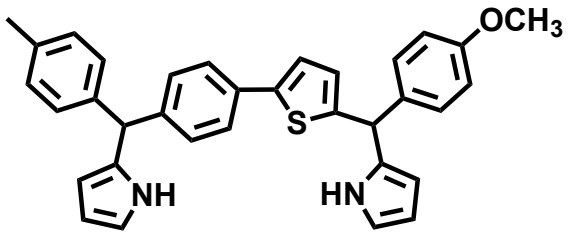
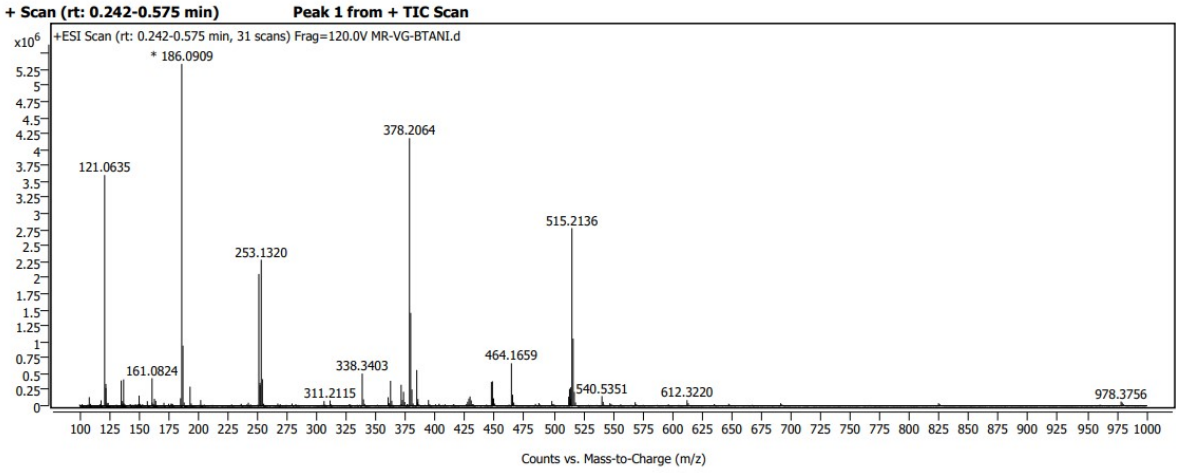


Figure S3. ^{13}C NMR spectrum of compound **8a** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 8b



Compound Details

Cpd. 1: C34 H30 N2 O S

Formula	m/z	Observed M/Z	Difference_Da	Difference_PPM	Score
C34 H30 N2 O S	515.2138	515.213769909942	-1.41212507571709	-2.74621435953525	91.16

Compound Spectra (Zoomed)

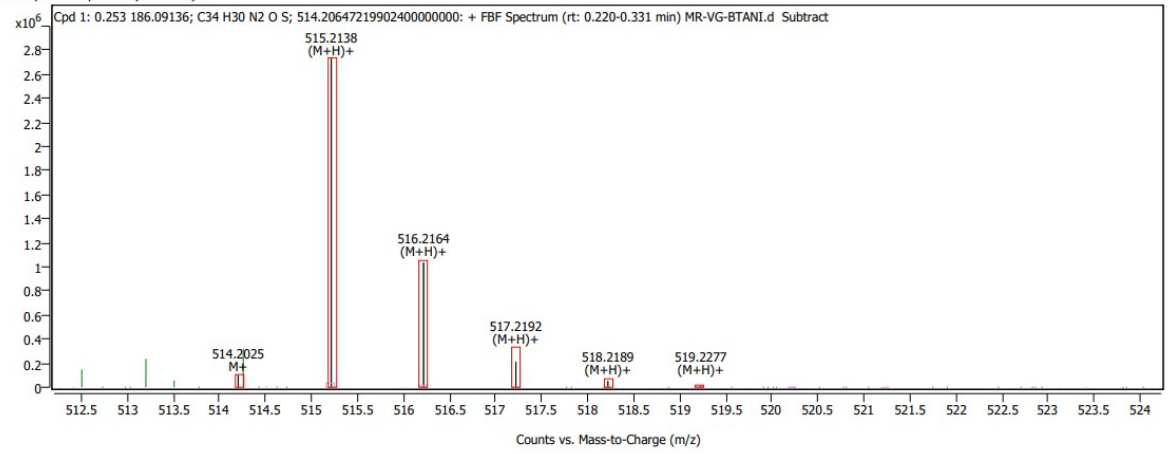
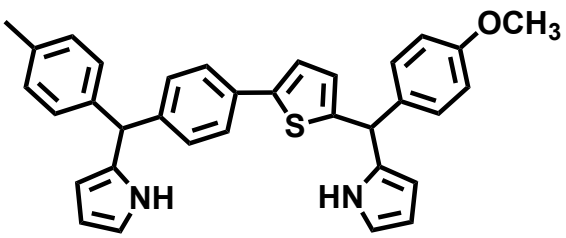


Figure S4. High resolution mass spectrum of compound **8b.**



Compound 8b

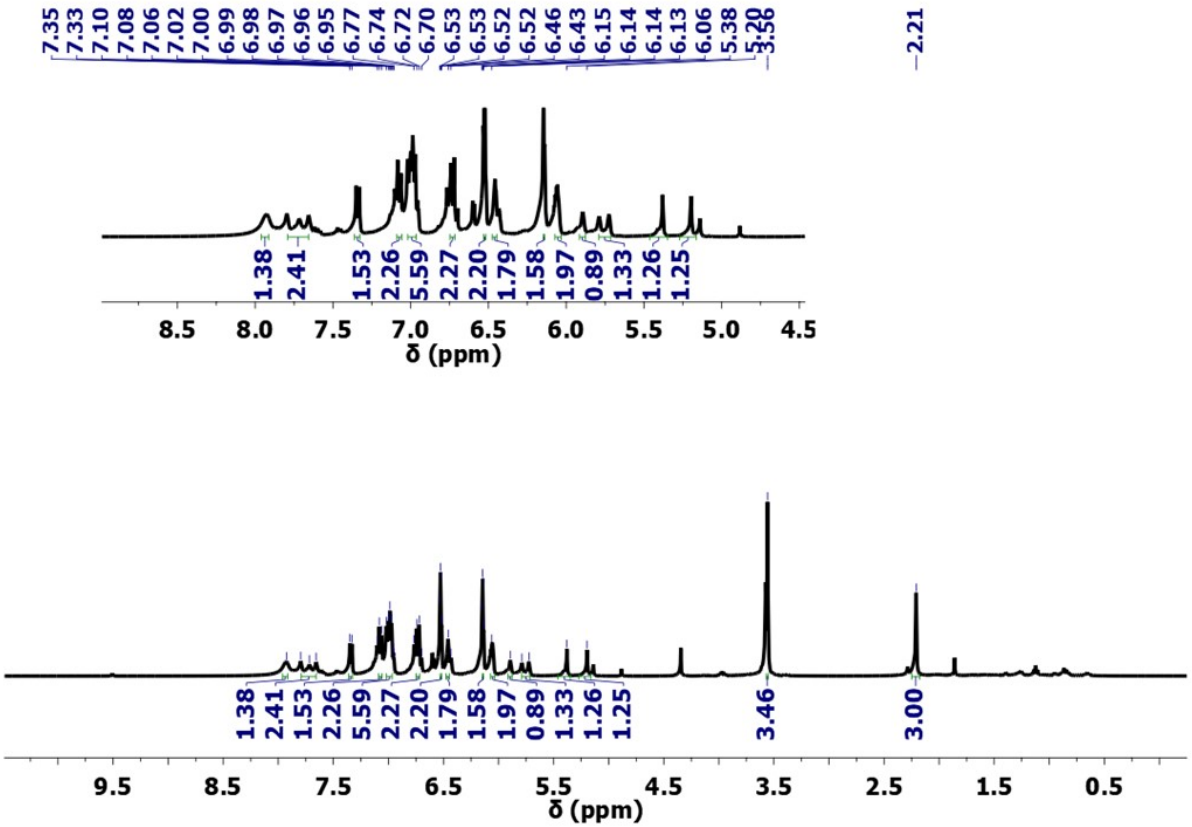
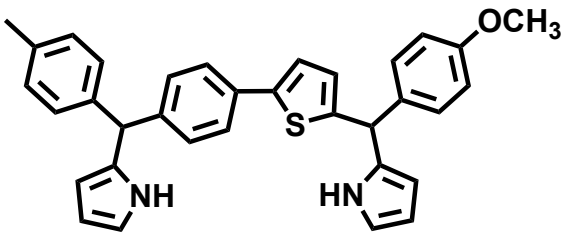


Figure S5. ^{1}H-NMR spectrum of compound **8b** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 8b

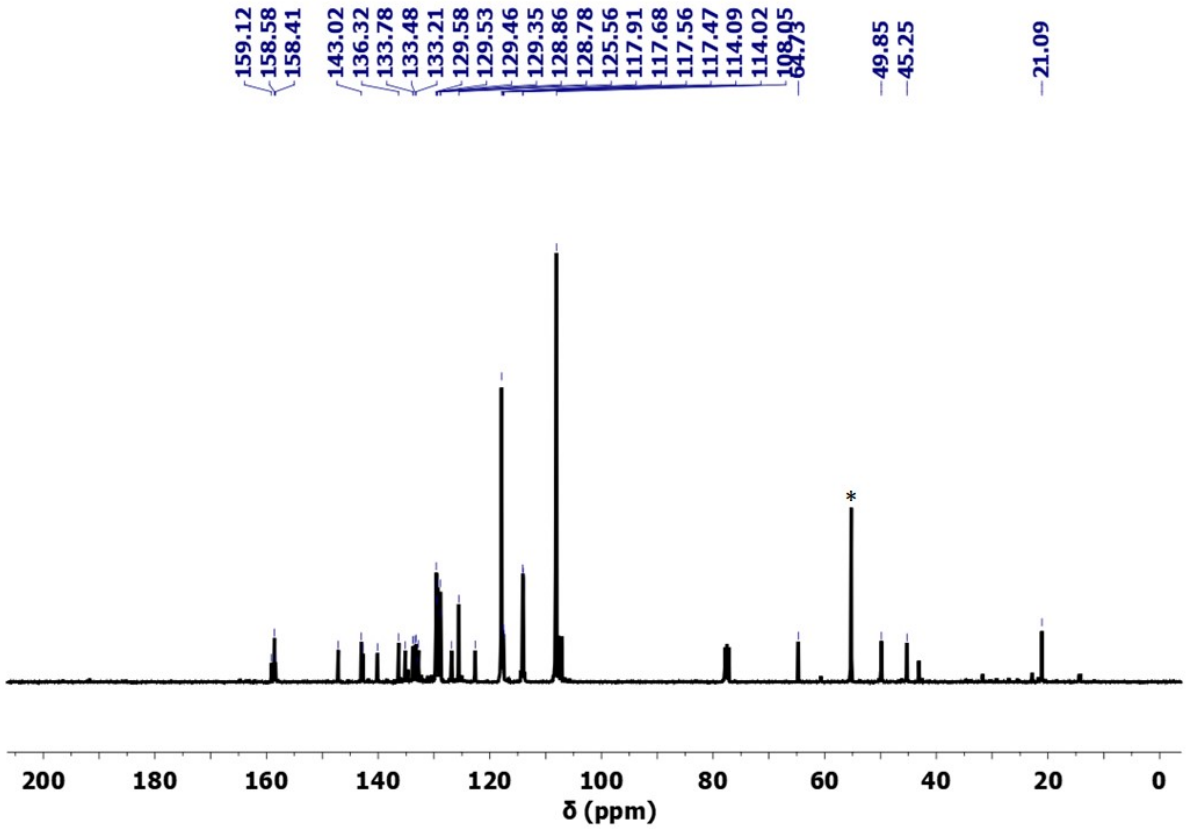
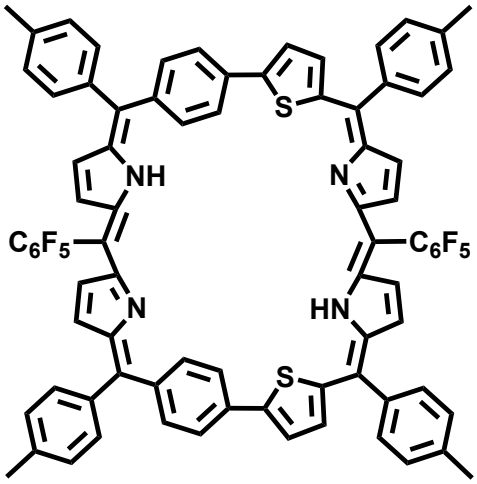


Figure S6. ^{13}C NMR spectrum of compound **8b** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 3a

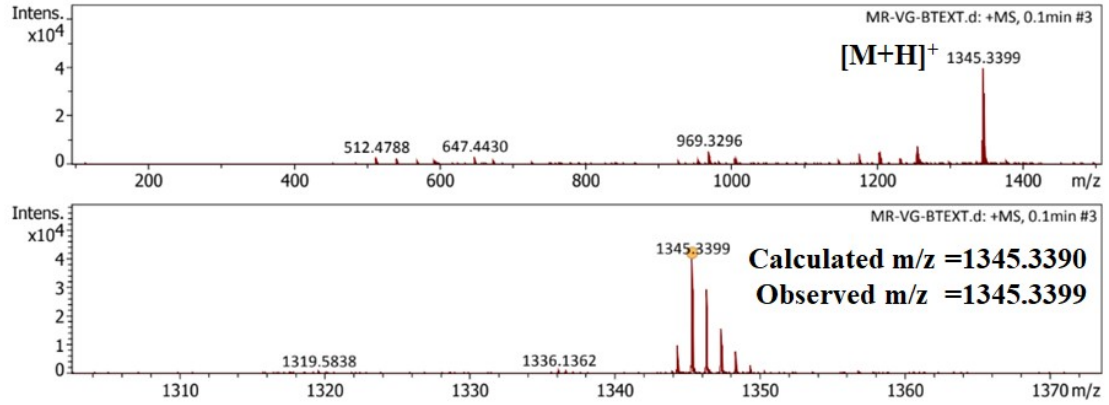
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\APR-2023\MR-VG-BTEXT.d	Acquisition Date	4/24/2023 11:53:39 AM
Method	Naformat_pos_1500.m	Operator	sjg-out
Sample Name	MR-VG-BTEXT	Instrument	maXis impact 282001.00081
Comment	C82H50F10N4S2		

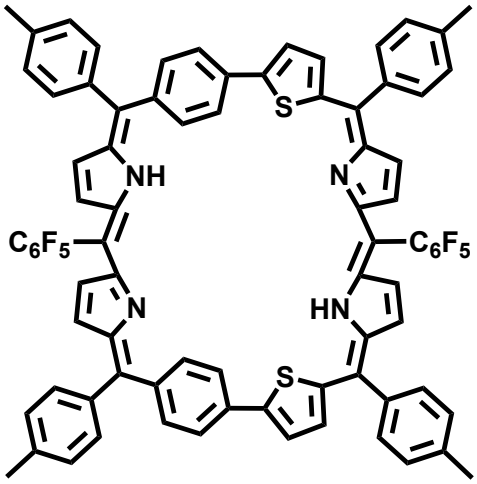
Acquisition Parameter

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	100 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
1345.3399	1	C82H51F10N4S2	1345.3390	-0.7	91.8	1	100.00	59.0	even	ok

Figure S7. High resolution mass spectrum of compound **3a.**



Compound 3a

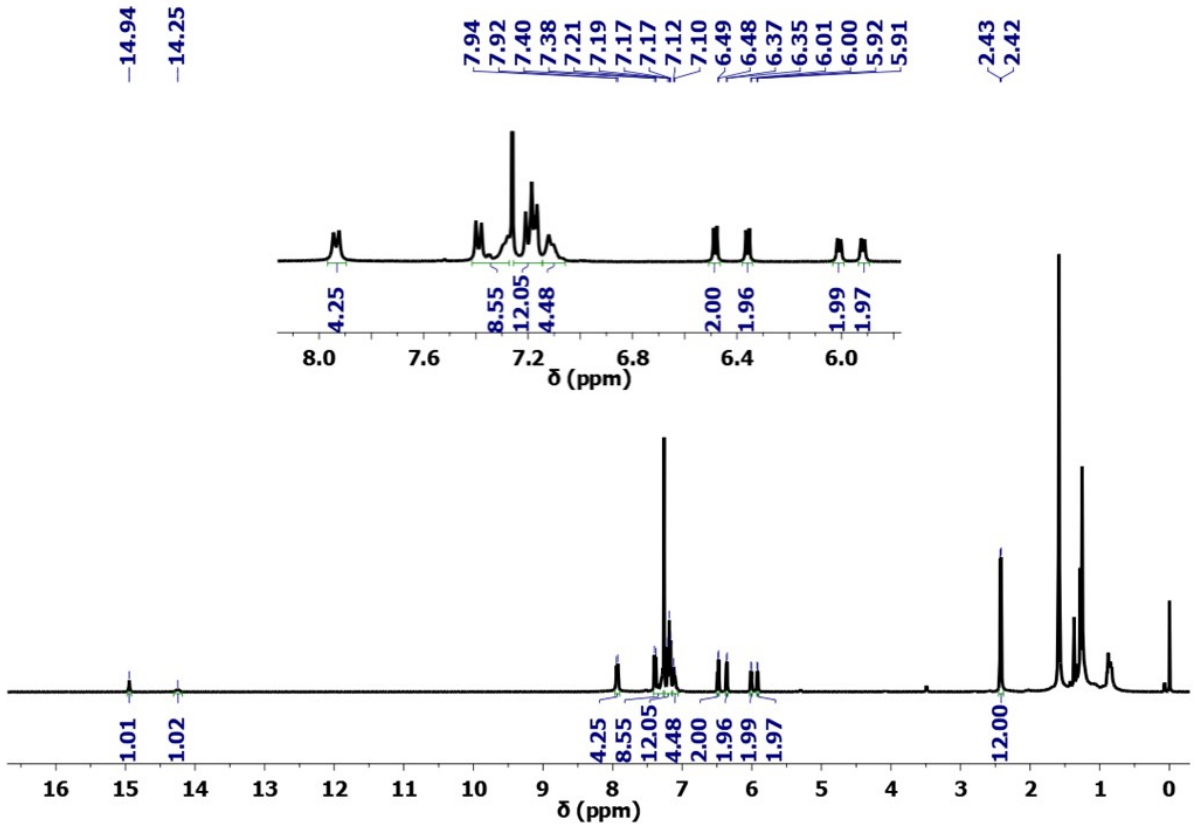


Figure S8. ^{1}H-NMR spectrum of compound **3a** in $CDCl_3$ on 400 MHz instrument at room temperature.

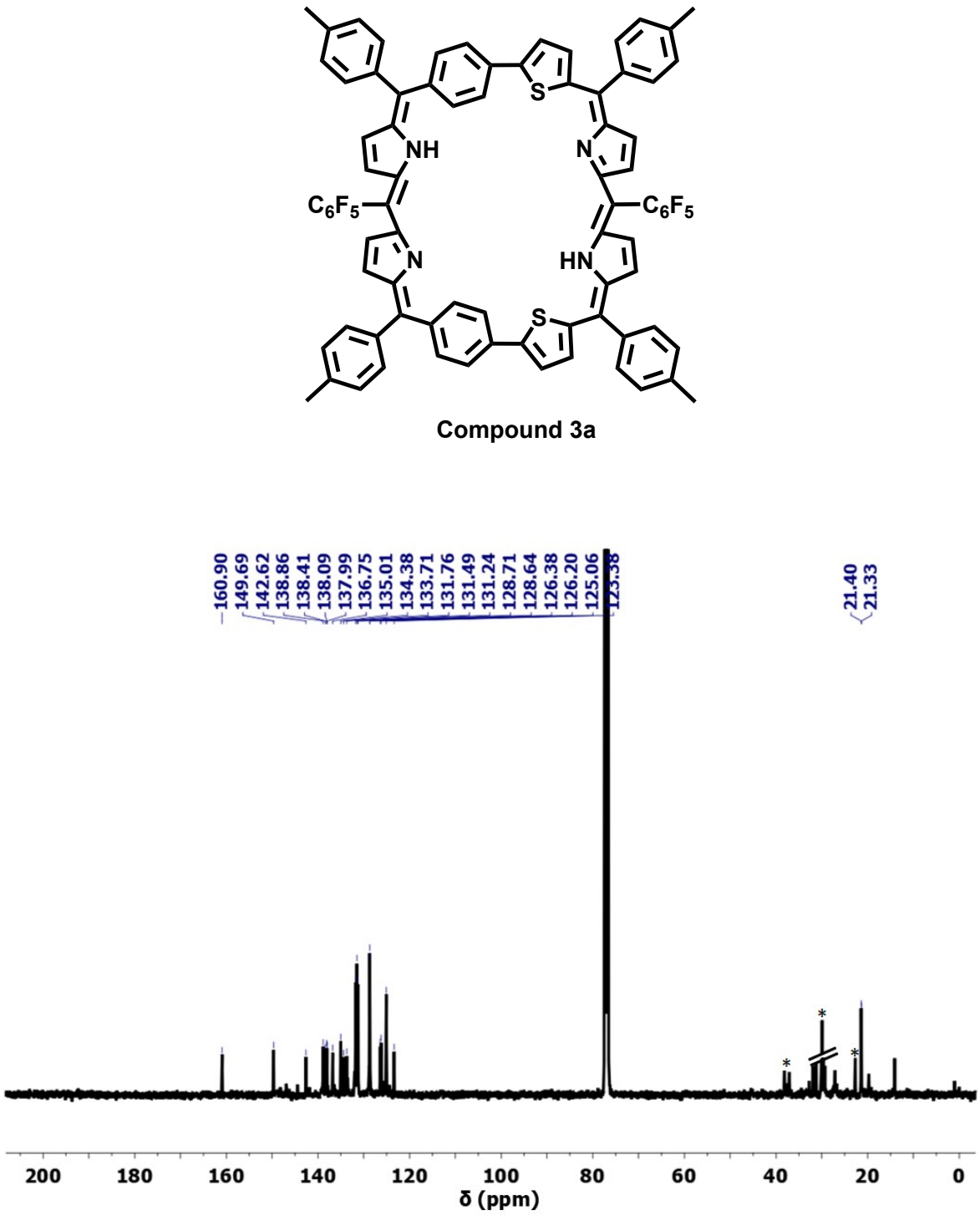
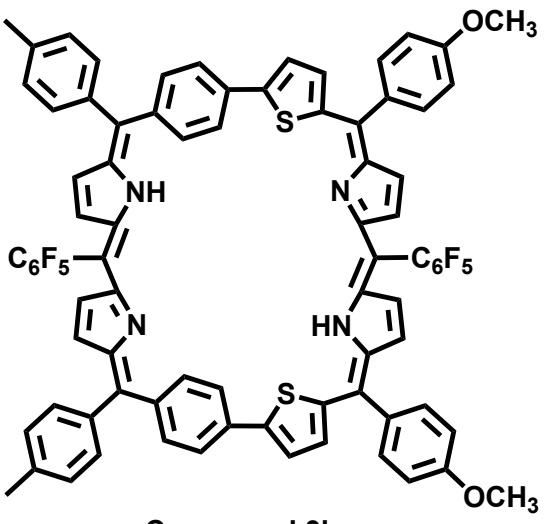


Figure S9. ^{13}C NMR spectrum of compound **3a** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 3b

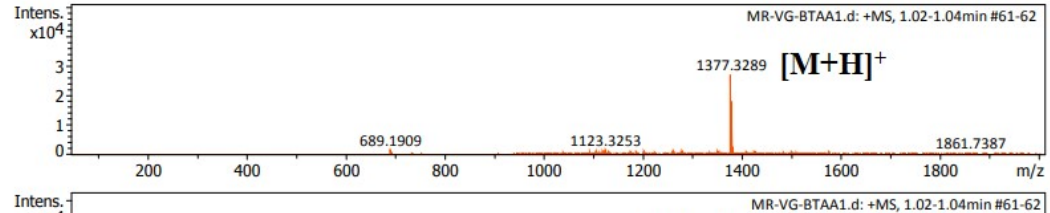
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

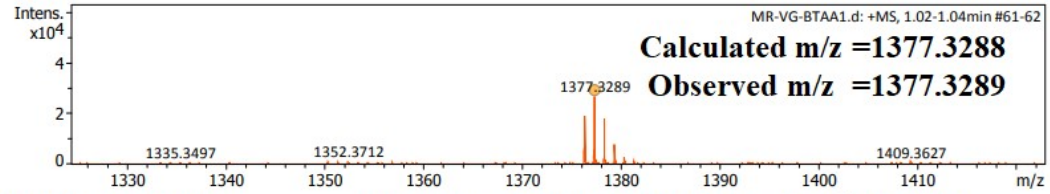
Analysis Info

Analysis Name	D:\Data\MAY-2023\MR-VG-BTAA1.d	Acquisition Date	5/29/2023 12:23:00 PM
Method	NaICsI_pos_2000.m	Operator	iitb
Sample Name	MR-VG-BTAA1	Instrument	maXis impact 282001.00081
Comment	C82H50F10N4O2S2		

Acquisition Parameter

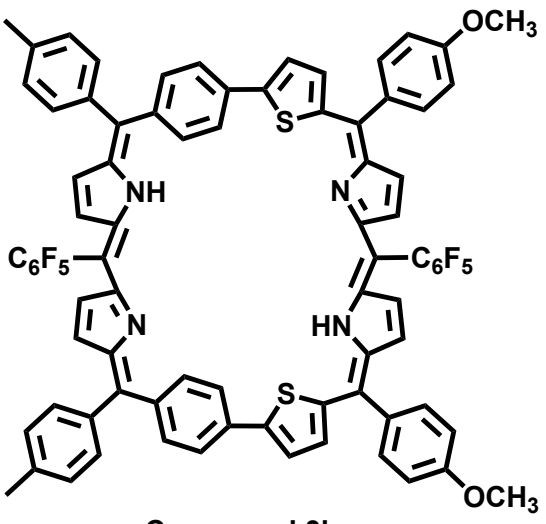
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.5 l/min
Scan End	2000 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
1377.3289	1	C82H51F10N4O2S2	1377.3288	-0.1	147.6	1	100.00	59.0	even	ok

Figure S10. High resolution mass spectrum of compound **3b.**



Compound 3b

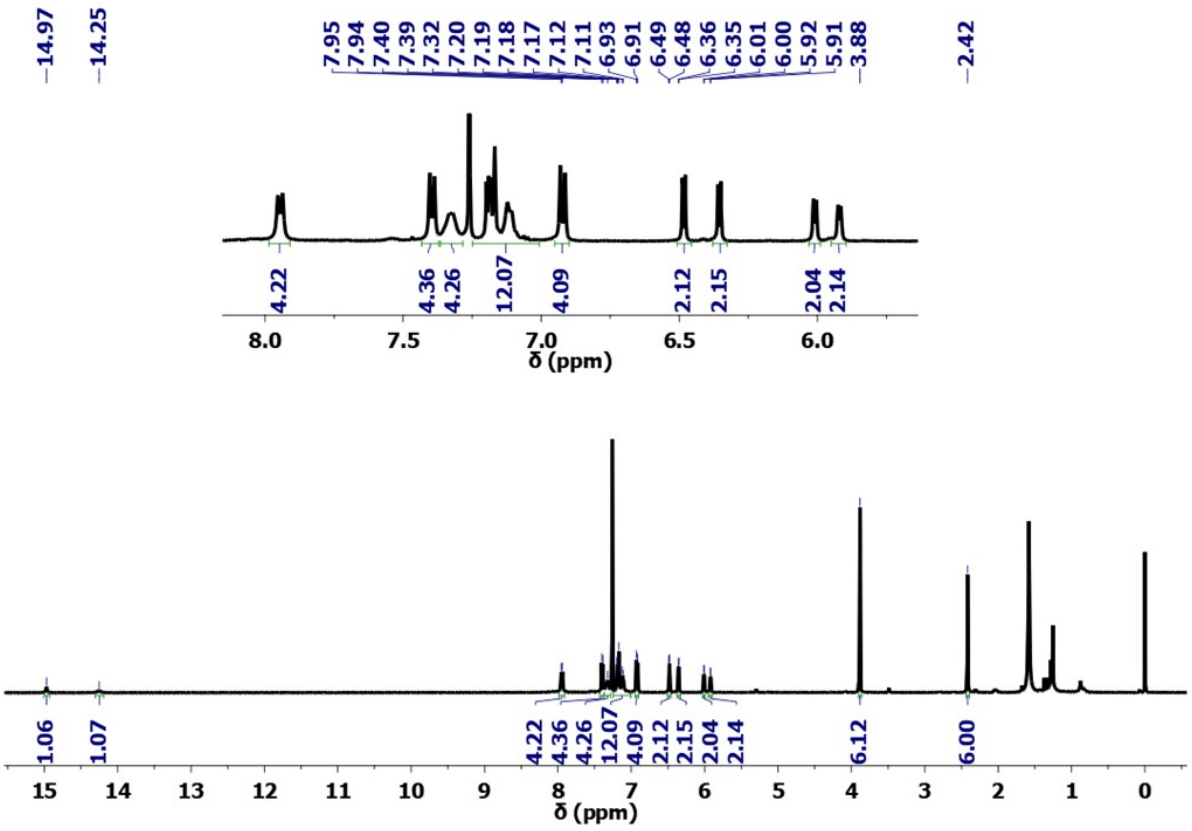
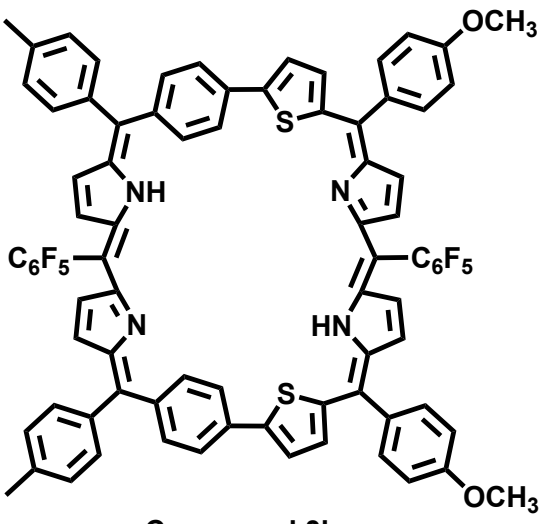


Figure S11. ^{1}H-NMR spectrum of compound **3b** in $CDCl_3$ on 500 MHz instrument at room temperature.



Compound 3b

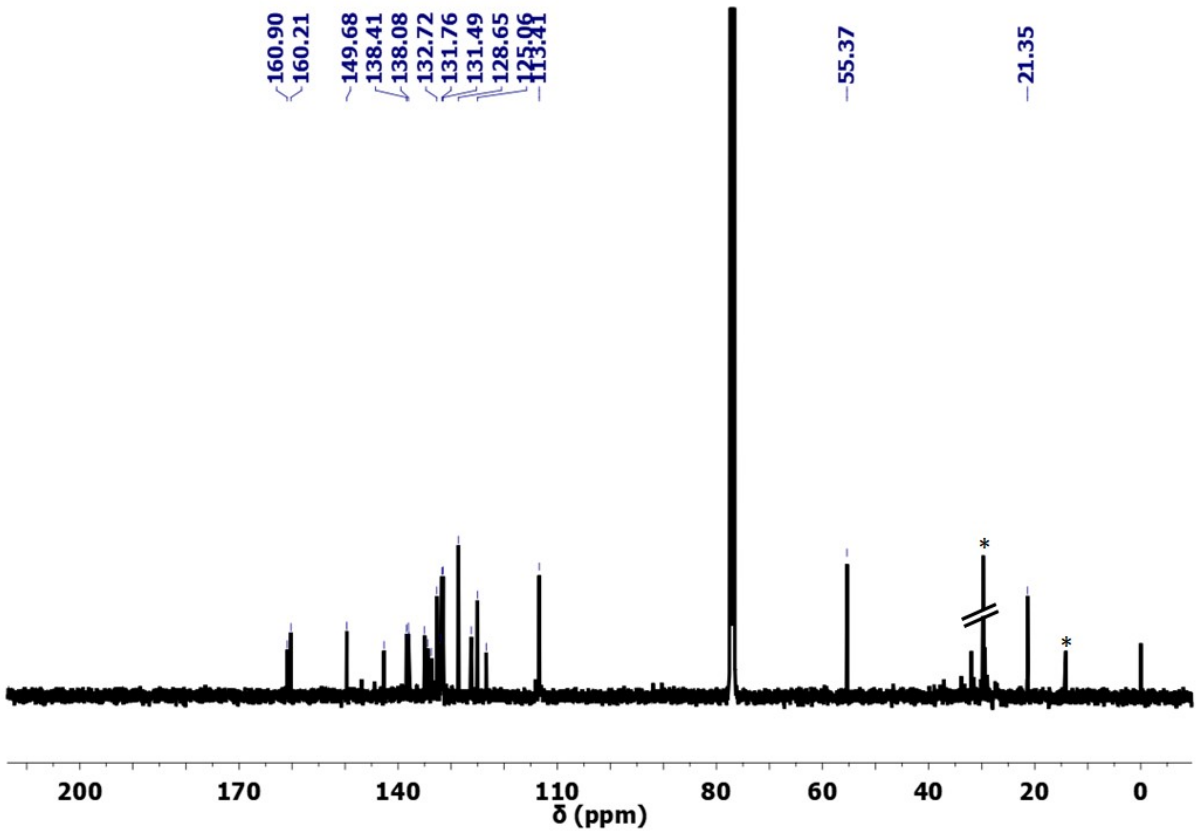
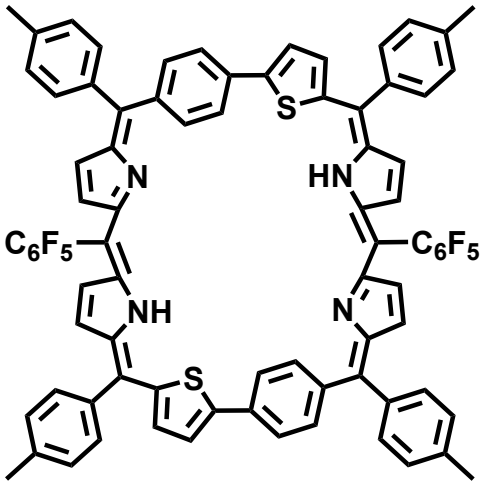


Figure S12. ^{13}C NMR spectrum of compound **3b** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 4a

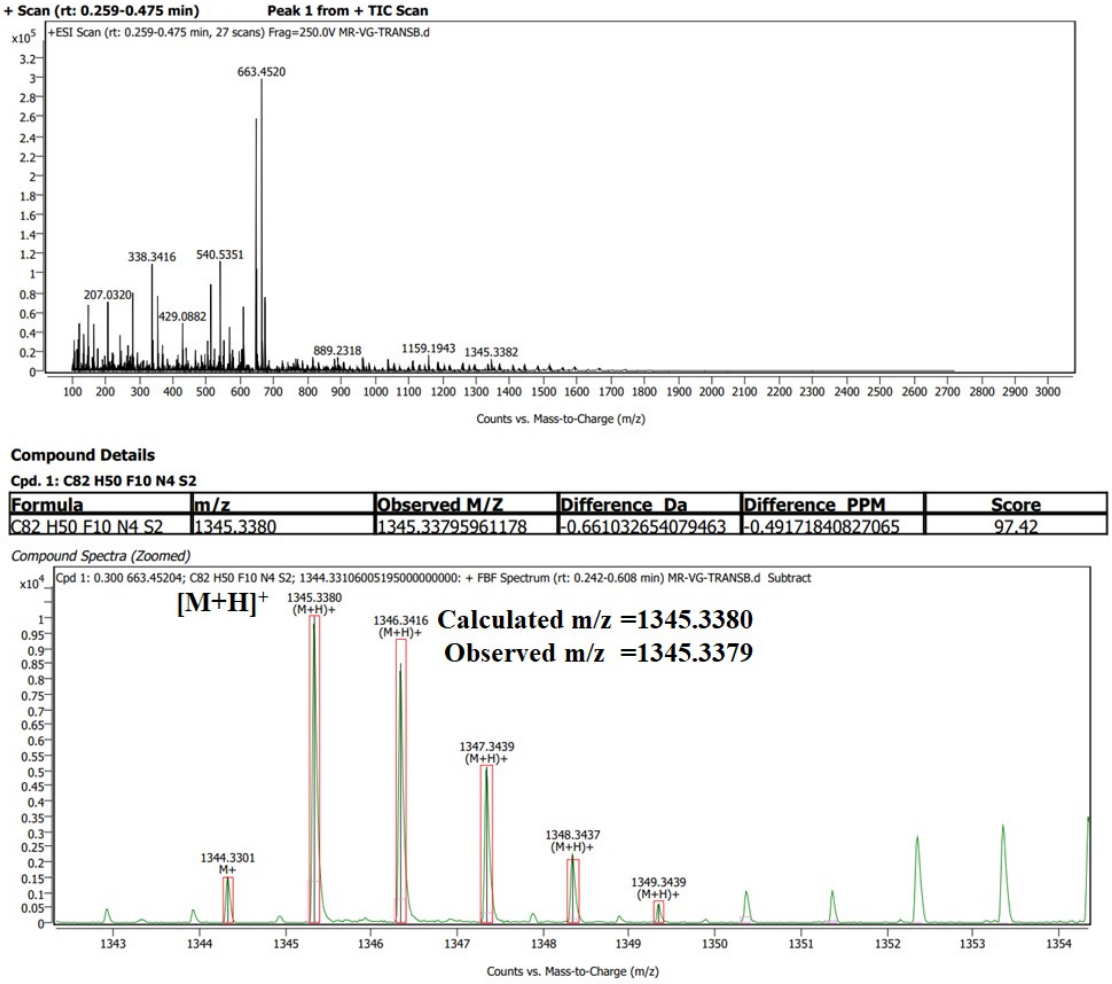
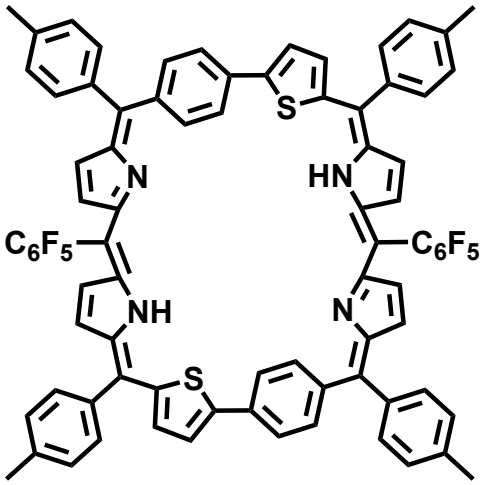


Figure S13. High resolution mass spectrum of compound **4a.**



Compound 4a

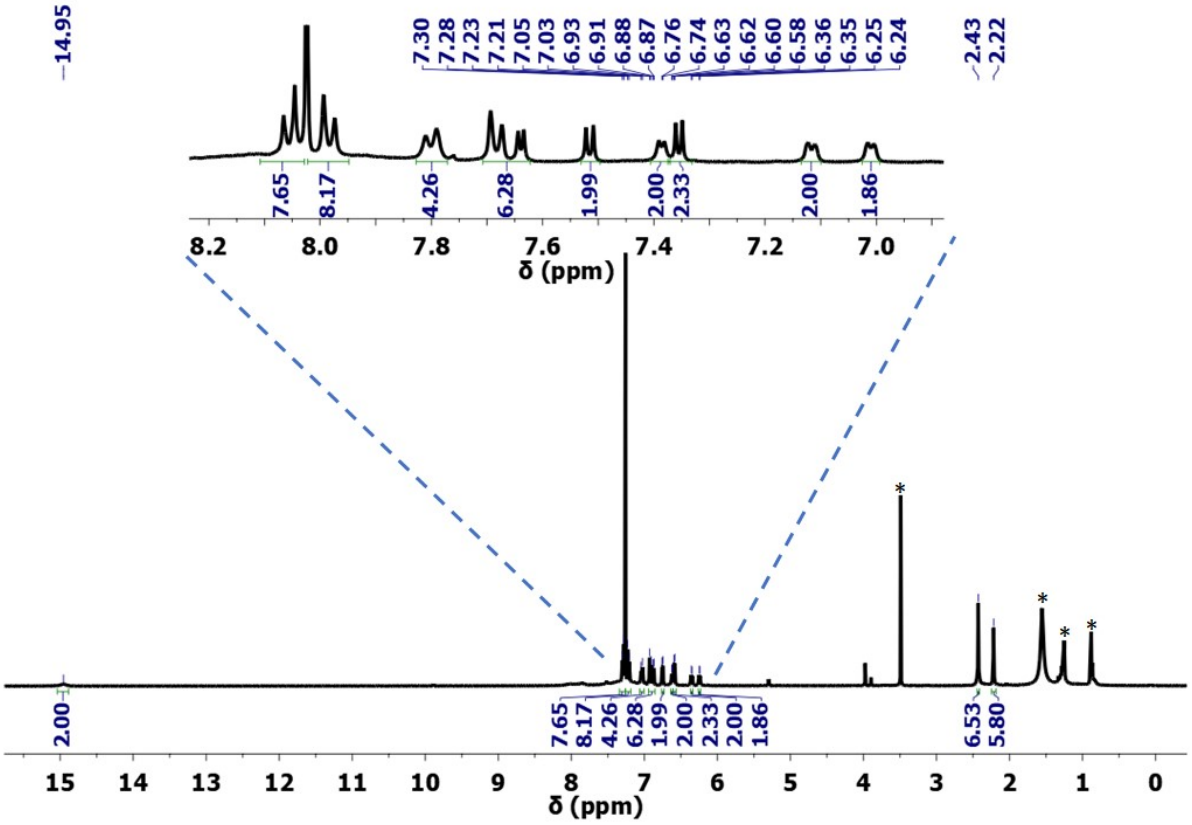


Figure S14. ^{1}H-NMR spectrum of compound **4a** in $CDCl_3$ on 400 MHz instrument at room temperature.

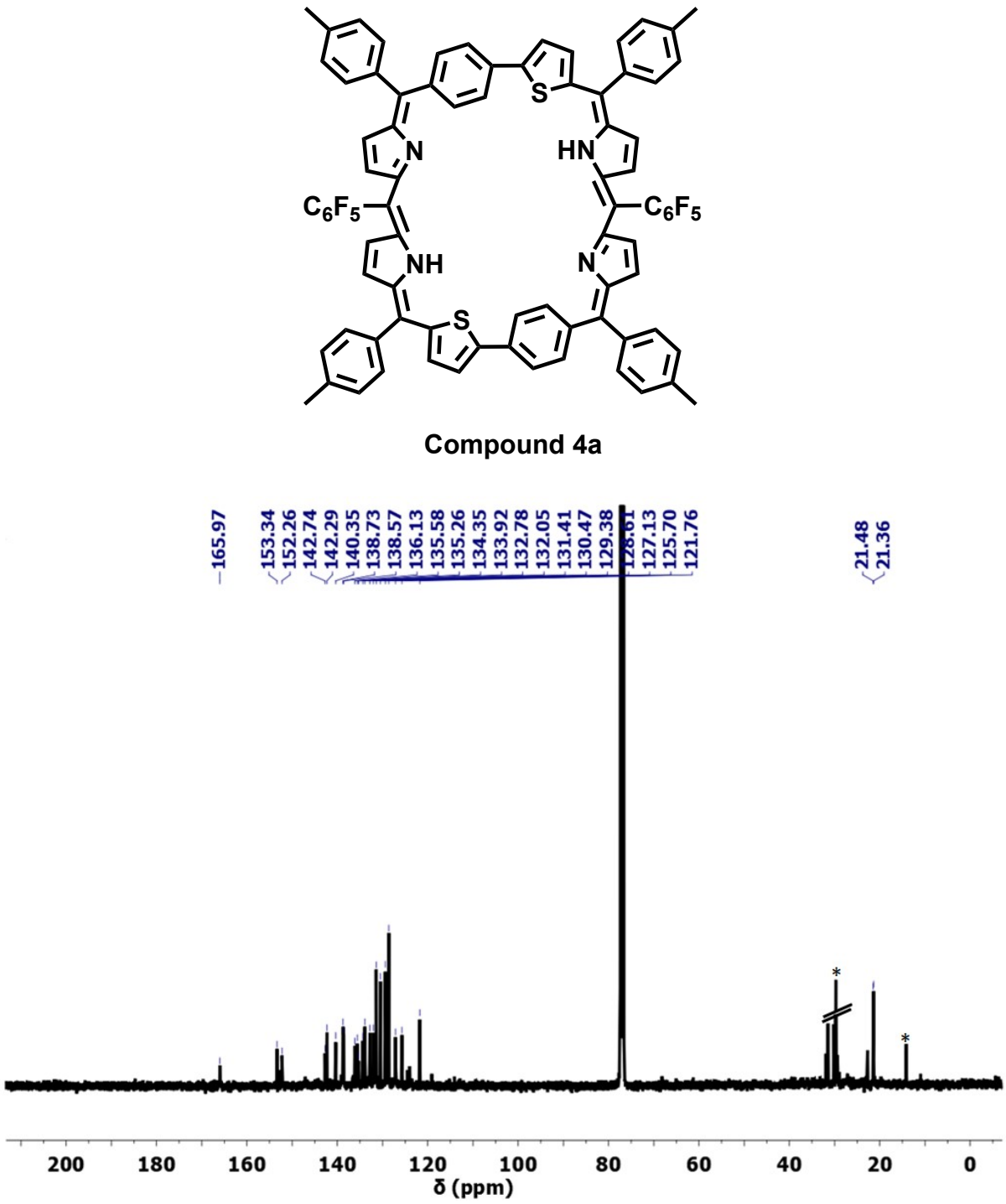
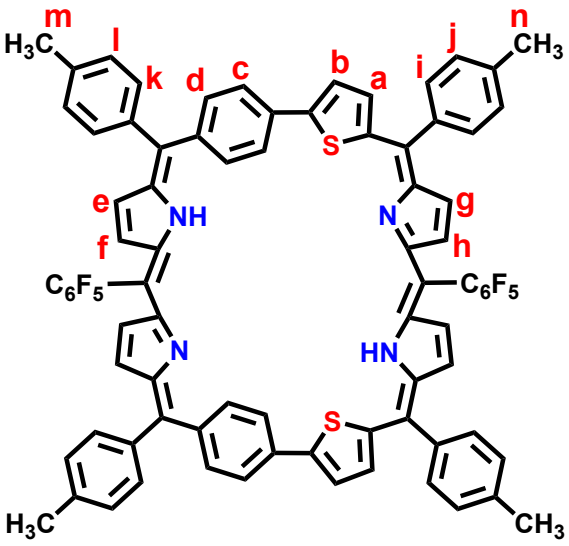


Figure S15. ^{13}C NMR spectrum of compound **4a** in $CDCl_3$ on 400 MHz instrument at room temperature.



Compound 3a

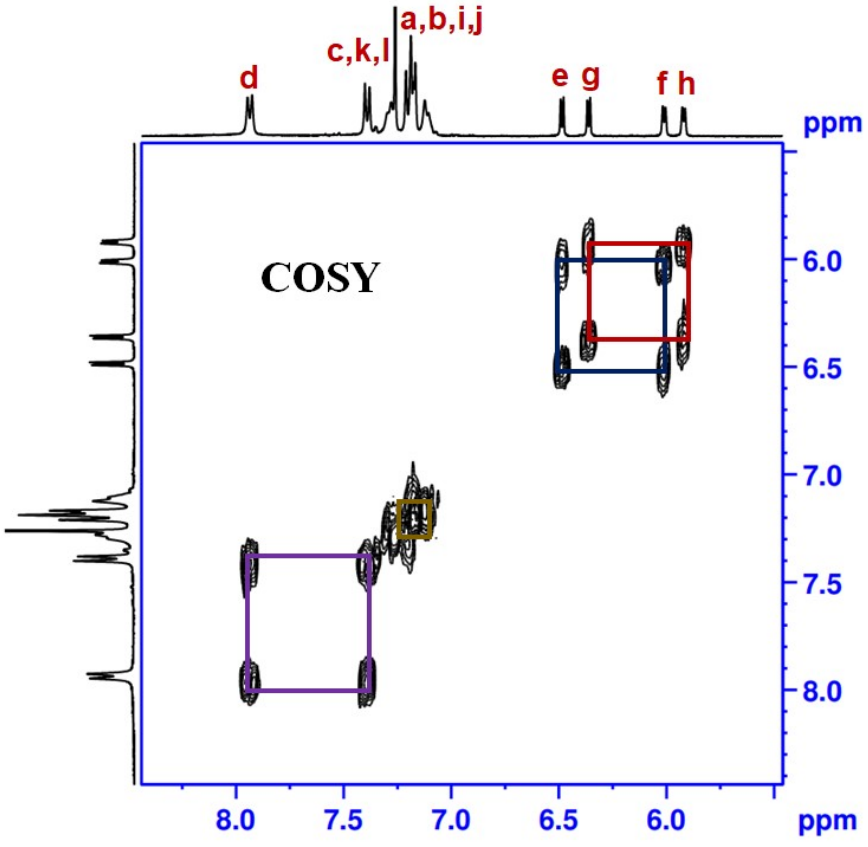
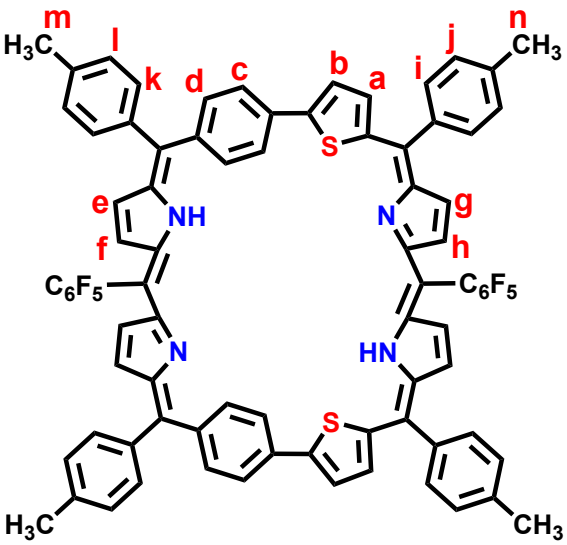


Figure S16. Partial ^{1}H-^{1}H COSY spectrum of compound **3a** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.



Compound 3a

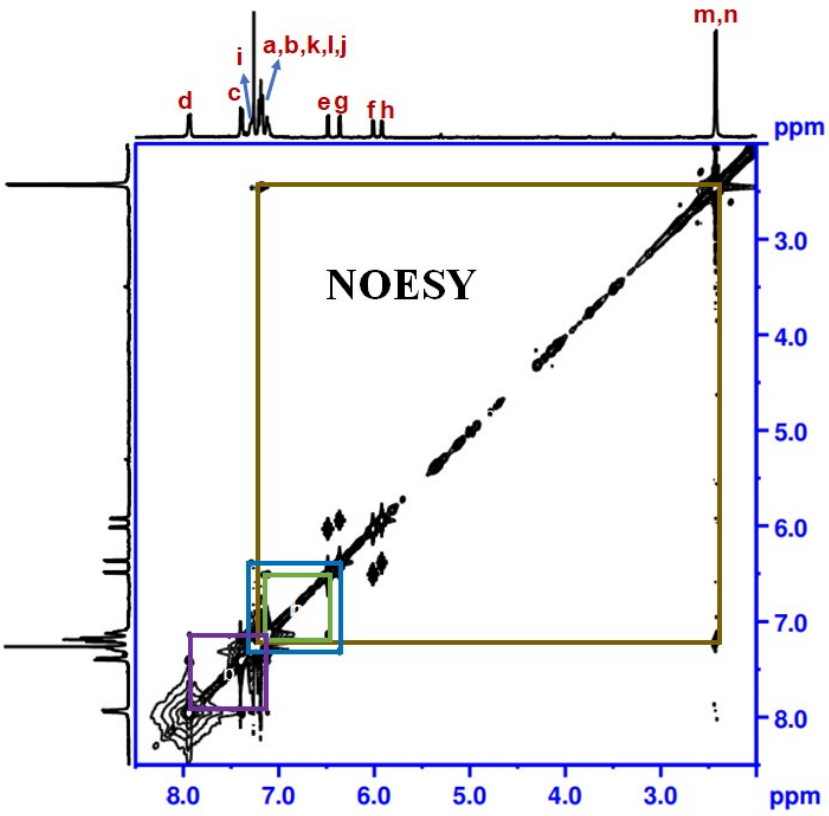
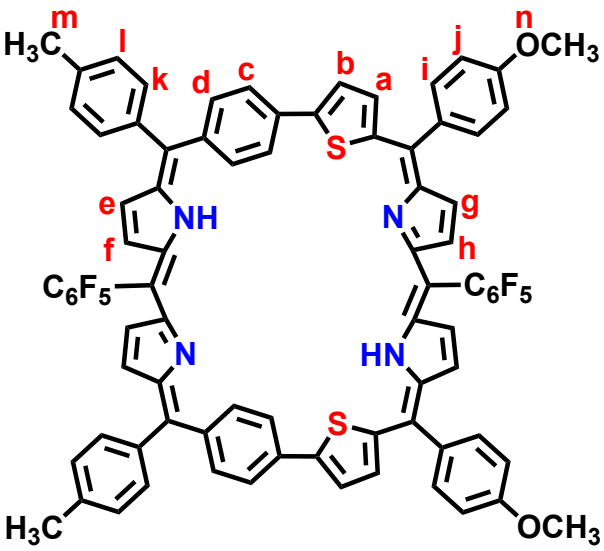


Figure S17. ^{1}H-^{1}H NOESY spectrum of compound **3a** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.



Compound 3b

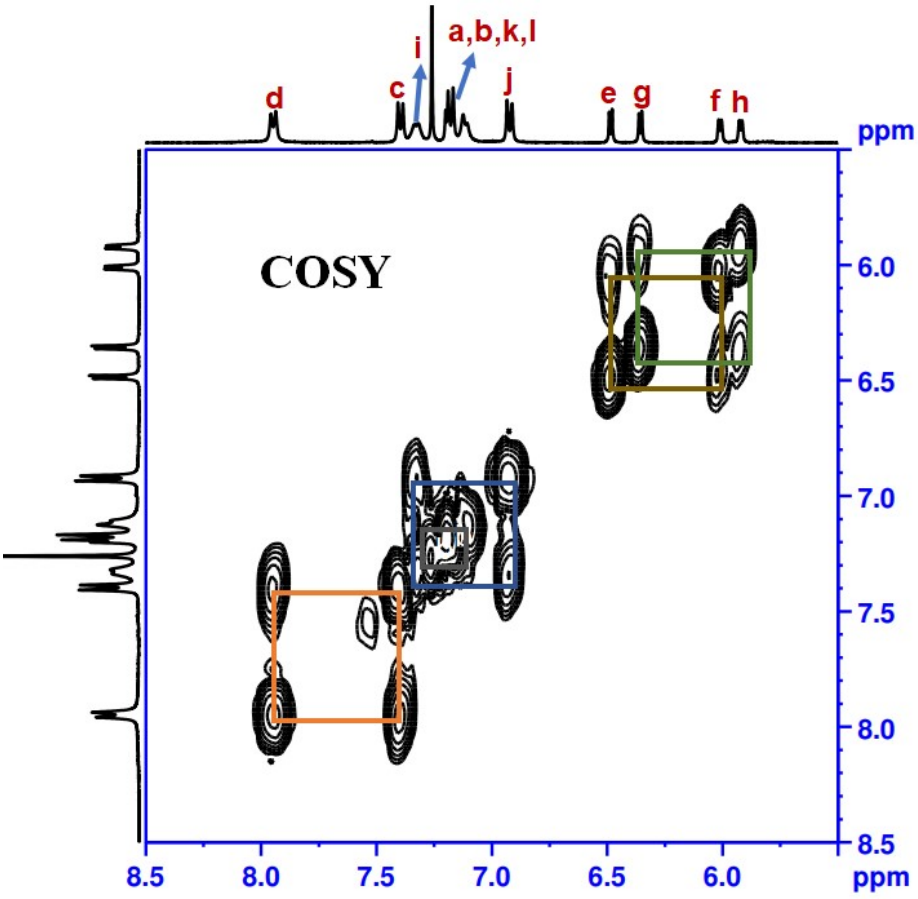
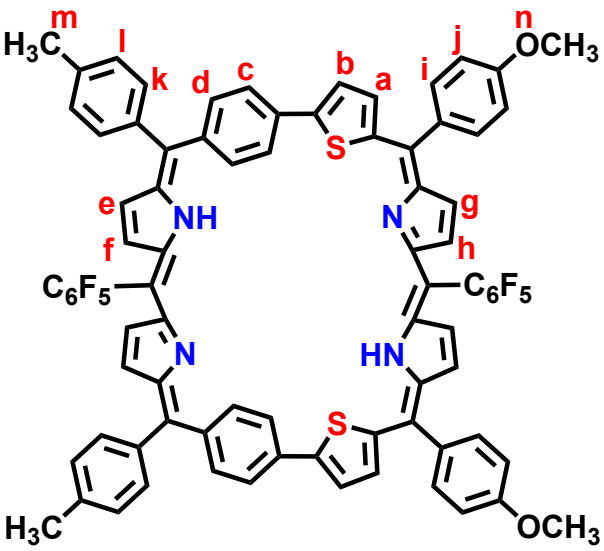


Figure S18. Partial ^{1}H-^{1}H COSY spectrum of compound **3b** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.



Compound 3b

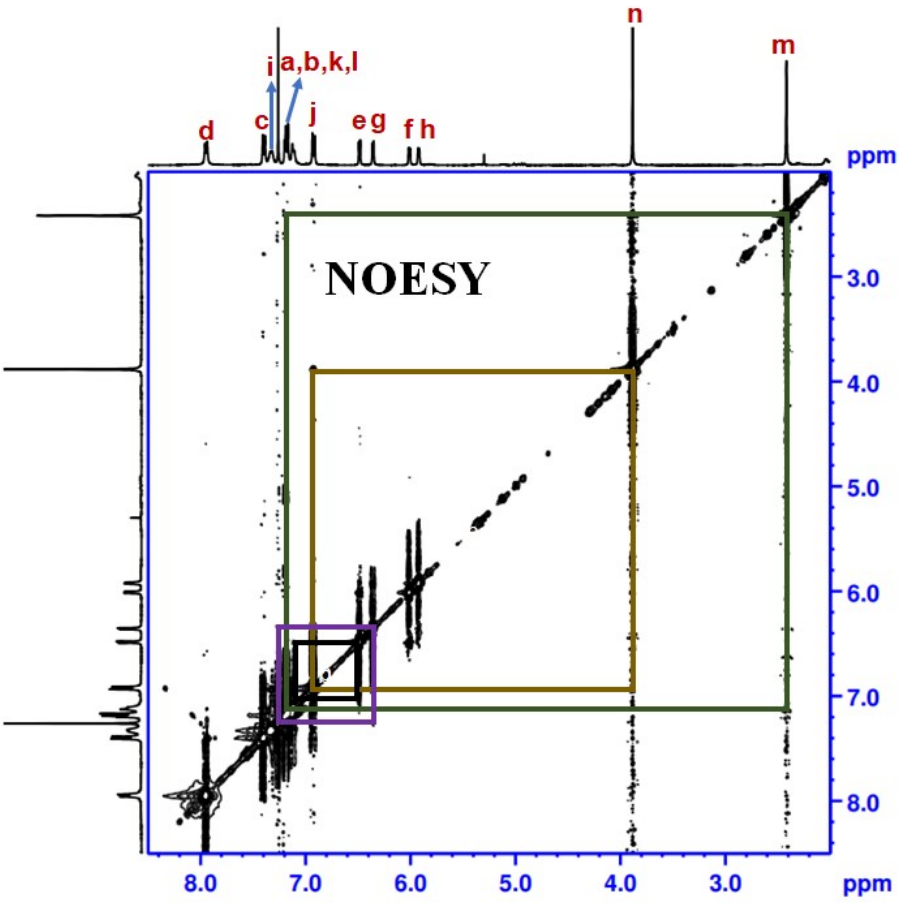


Figure S19. ^{1}H-^{1}H NOESY spectrum of compound **3b** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.

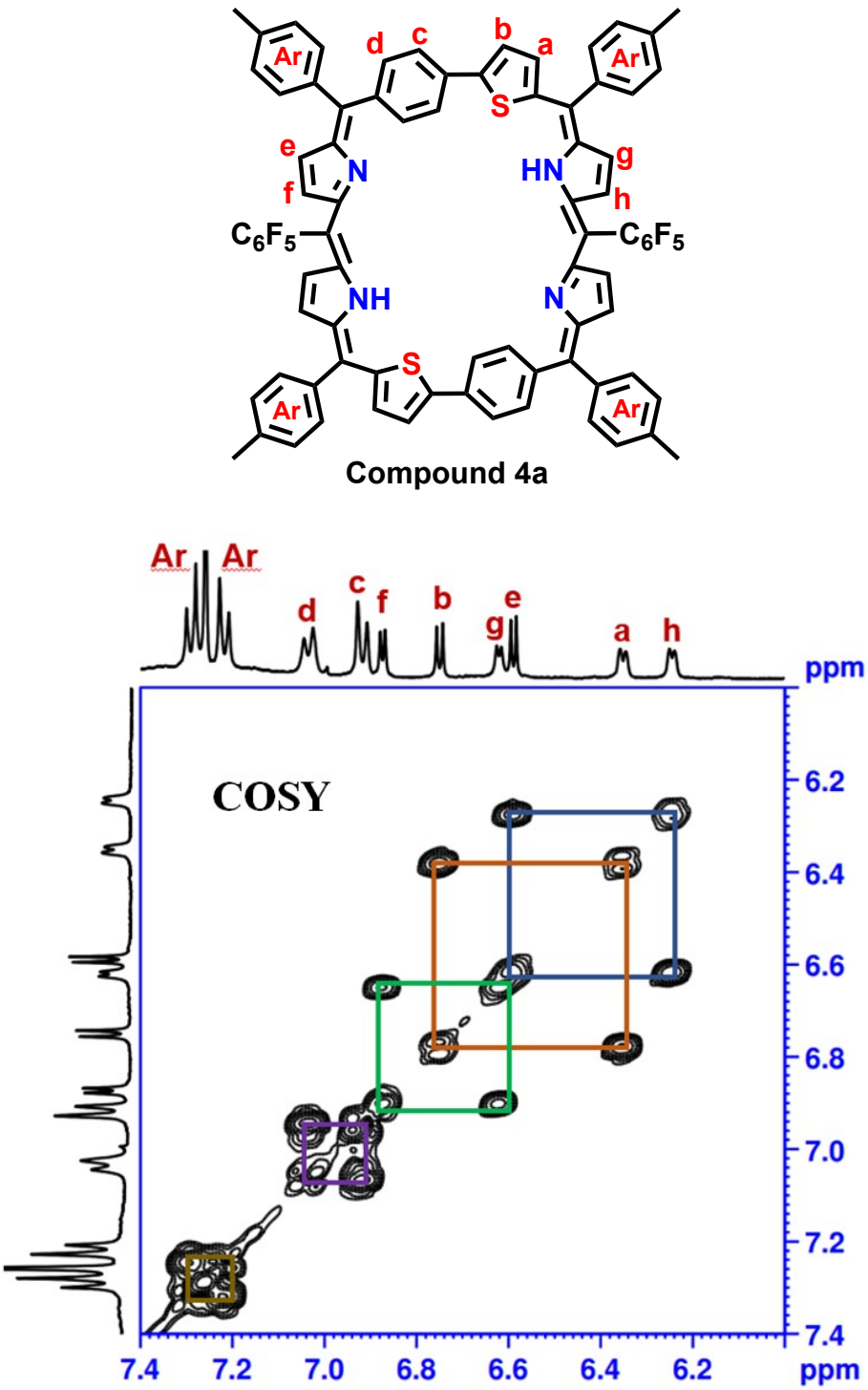


Figure S20. Partial ^{1}H-^{1}H COSY spectrum of compound **4a** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.

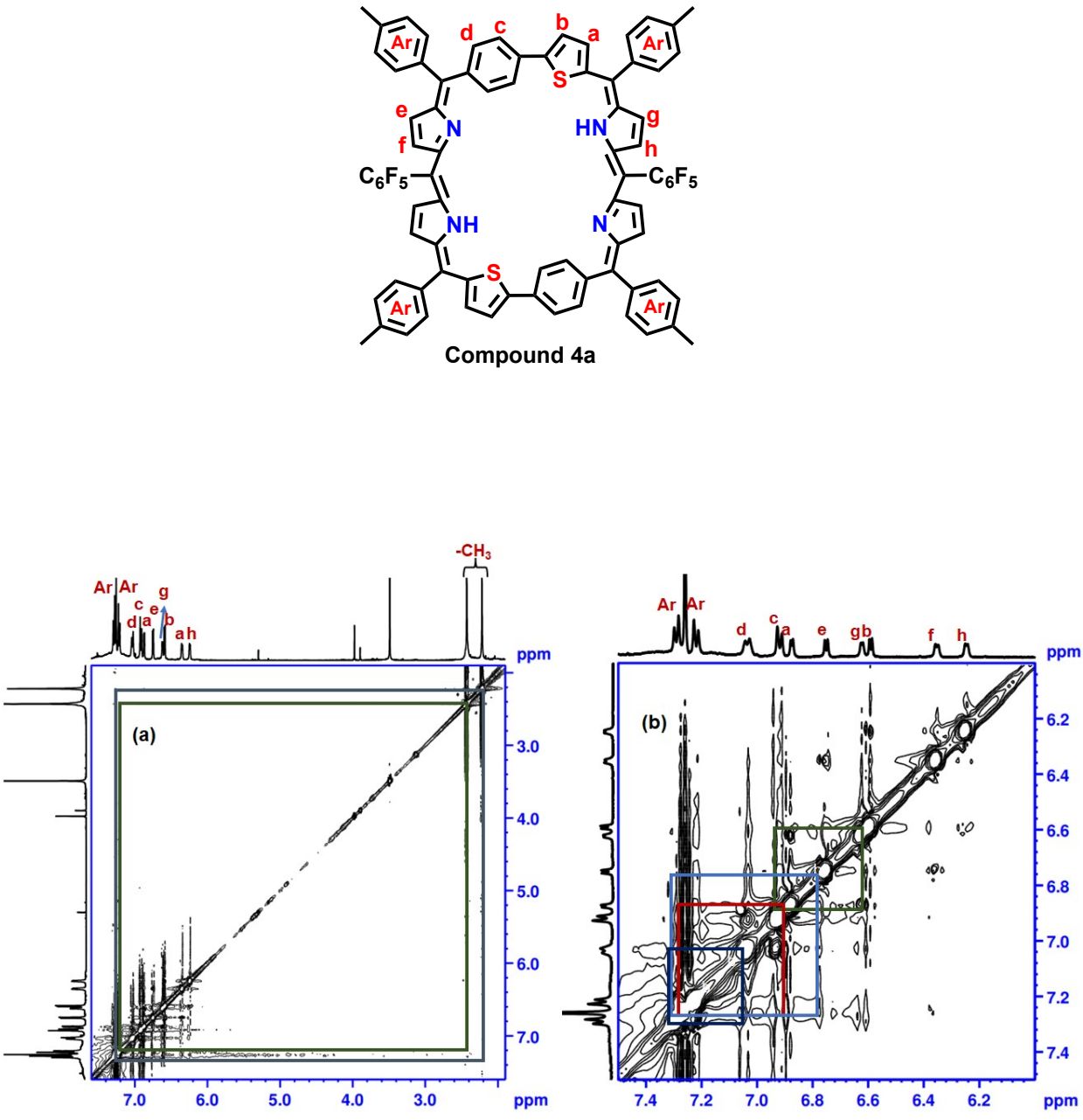


Figure S21. (a) ^{1}H-^{1}H NOESY spectrum and (b) partial ^{1}H-^{1}H NOESY spectrum of compound **4a** recorded in $CDCl_3$ at room temperature on 400 MHz instrument.

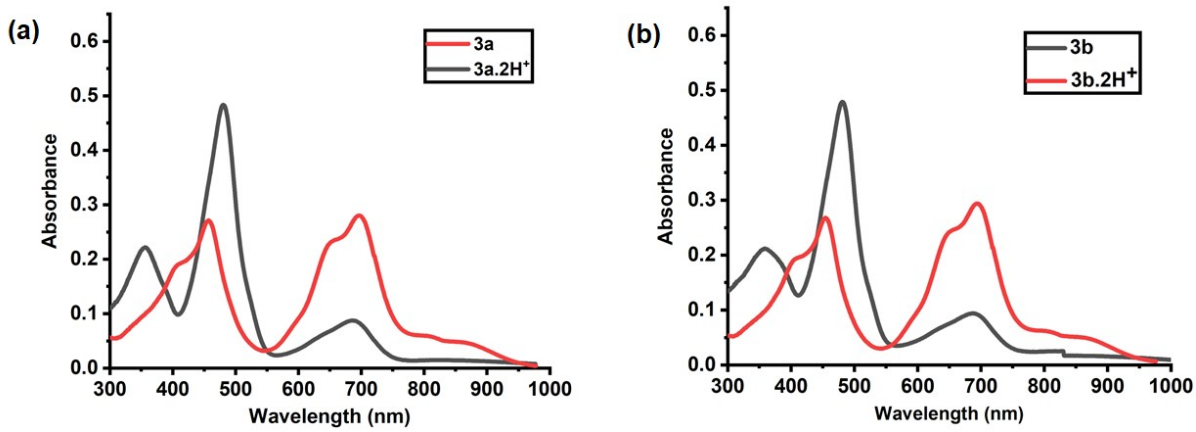


Figure S22. Comparison of UV-Vis absorption spectra of Macrocycles **3a-3b** ($3X10^{-5}$ M) free base (red color line) and in presence of TFA (excess) (black color line) recorded in toluene at 25°C.

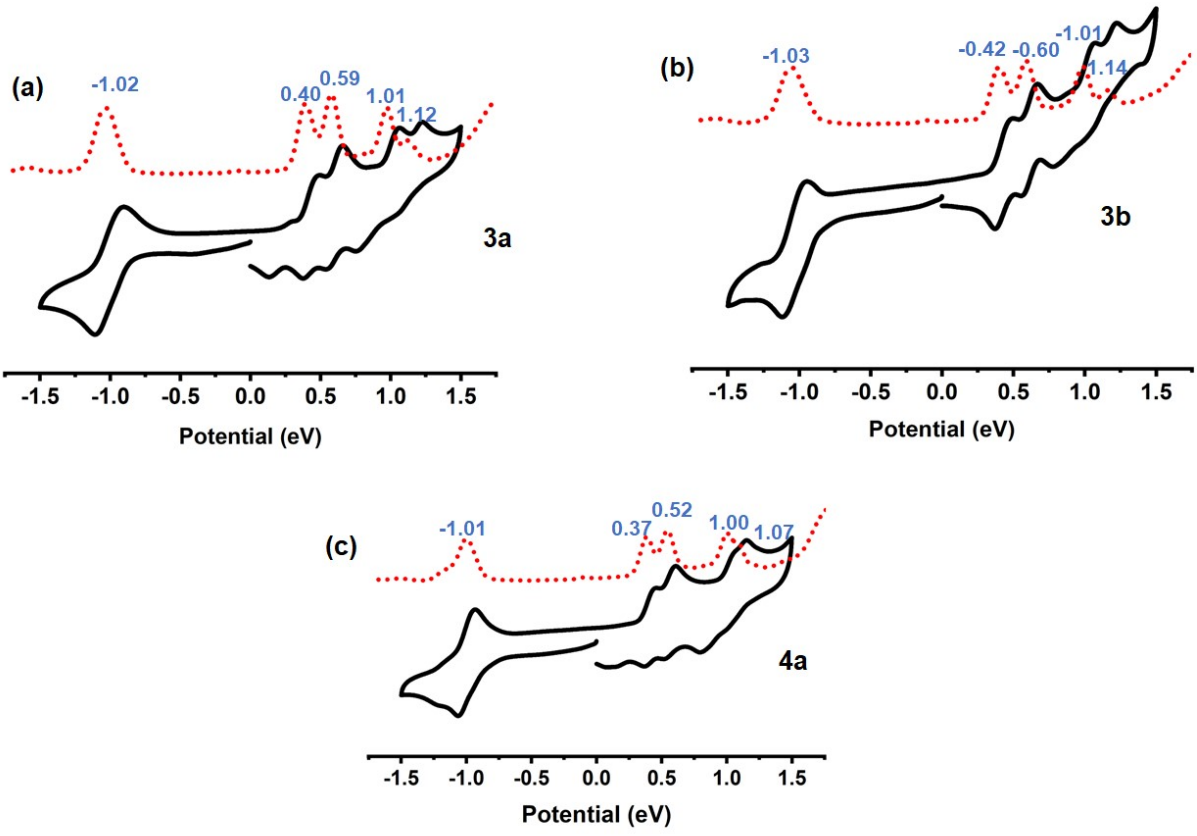


Figure S23: Cyclic voltammograms (black lines) along with differential pulse voltammograms (red dotted lines) of macrocycles **3-4** recorded in CH_2Cl_2 containing 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at scan rates of 50 mVs^{-1}.

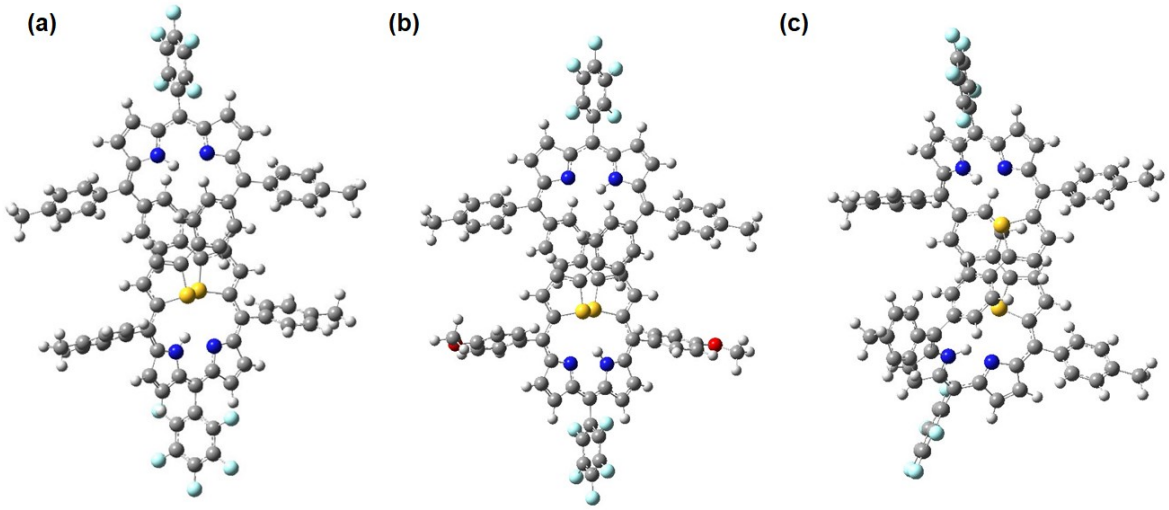


Figure S24: Ground state optimized structures all macrocycles **3-4.**

Table S1. Comparison of Bond Angles

Deviation of the pyrrole rings from the mean plane	**Compound 3a (deg)**	**Compound 3b (deg)**	**Compound 4a (deg)**
ring A	19.57	19.07	52.22
ring B	8.56	7.38	26.12
ring C	21.37	20.68	38.51
ring D	14.68	13.74	22.10
ring E	4.11	3.56	31.11
ring F	14.82	14.02	10.55
ring G	29.37	39.07	13.13
ring H	22.64	21.74	13.12

Table S2: Cartesian coordinates of the S_0 optimized structures of the compound **3a**.

Sum of imaginary frequencies = 0;

Total Free Energy (hartree) with = -5168.492823

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.74327	-0.18177	2.025713	C	7.059922	-0.00662	-0.05414
C	-2.07456	-0.51236	2.362263	C	-7.47758	-0.07514	-0.09361
C	-3.09459	0.416157	2.265149	C	8.552552	-0.06388	-0.16057
C	-2.84062	1.740427	1.847202	C	-8.96174	-0.1089	-0.07074
C	-1.49851	2.092594	1.598619	C	-9.67958	-0.08117	1.134209
C	-0.47547	1.154799	1.675136	C	-11.0709	-0.09068	1.176476
C	-3.93335	2.715334	1.69368	C	-11.7964	-0.14334	-0.01111
C	-3.6659	4.128446	2.042314	C	-11.1207	-0.17841	-1.22774
C	-5.1893	2.330817	1.247341	C	-9.72844	-0.15157	-1.24418
C	-6.43087	3.093698	1.384667	C	9.186715	-0.76658	-1.19066
C	-7.43075	2.289936	0.945136	C	10.57421	-0.82858	-1.30314
C	-6.79721	1.047967	0.496744	C	11.36885	-0.16735	-0.37054
N	-5.47311	1.090526	0.681832	C	10.77131	0.545666	0.665896
N	5.097239	-1.32054	0.734107	C	9.382079	0.584817	0.760366
C	6.445846	-1.11858	0.502412	F	-9.02309	-0.04934	2.303065
C	7.12291	-2.3023	0.981272	F	-11.7151	-0.06848	2.350354
C	6.193634	-3.17086	1.448499	F	-13.1328	-0.16192	0.017554
C	4.878545	-2.58062	1.302402	F	-11.812	-0.21904	-2.37429
C	3.799176	-4.64298	2.089744	F	-9.12448	-0.16595	-2.44273
C	3.704656	-3.1984	1.701196	F	8.842797	1.279997	1.771232
C	2.380315	-2.63385	1.779813	F	11.53415	1.179418	1.565681
C	1.202763	-3.37271	1.840942	F	12.70091	-0.21773	-0.46843
C	0.039833	-2.59465	1.954405	F	11.14693	-1.51477	-2.30031
C	0.269504	-1.2305	1.989982	F	8.4563	-1.41724	-2.10668
S	1.997354	-0.91704	1.897203	H	-2.31008	-1.51387	2.706905
C	-0.59374	0.257158	-1.88741	H	-4.10773	0.127023	2.51433
C	-1.90205	0.567445	-2.3165	H	-1.26036	3.106055	1.292408
C	-2.90748	-0.3829	-2.30988	H	0.53486	1.455733	1.41356
C	-2.66333	-1.70721	-1.88765	H	-6.52163	4.077206	1.824026
C	-1.33862	-2.0357	-1.5351	H	-8.48934	2.512469	0.917453
C	-0.33075	-1.07875	-1.52883	H	4.407334	-0.64338	0.42263
C	-3.74576	-2.70863	-1.84907	H	8.194375	-2.43663	0.972575
C	-3.43953	-4.09997	-2.24978	H	6.371625	-4.1352	1.898922
C	-5.03151	-2.36957	-1.46833	H	1.195478	-4.45335	1.778032
C	-6.26196	-3.10808	-1.69336	H	-0.95562	-3.02185	1.963495
C	-7.30889	-2.36333	-1.24843	H	-2.13062	1.567874	-2.66834
C	-6.78999	-1.13088	-0.68782	H	-3.89853	-0.10519	-2.65308
N	-5.42695	-1.18232	-0.85281	H	-1.10652	-3.04885	-1.22288
N	5.092973	1.38932	-0.60853	H	0.663185	-1.36453	-1.19703
C	6.418468	1.187045	-0.51831	H	-6.31035	-4.06304	-2.19602
C	7.176936	2.367053	-0.93596	H	-8.35683	-2.62231	-1.29726
C	6.263235	3.313028	-1.24686	H	-4.84237	-0.4661	-0.41818
C	4.9509	2.698102	-1.05692	H	8.253633	2.451292	-0.98272
C	3.832152	4.82347	-1.63371	H	6.444272	4.311729	-1.61631
C	3.765429	3.352712	-1.36631	H	1.232106	4.558164	-1.47929
C	2.45788	2.763264	-1.4704	H	-0.87859	3.083951	-1.76433
C	1.264978	3.479124	-1.55658	H	4.457784	-5.31804	0.153609
C	0.125887	2.680346	-1.72485	H	4.614614	-7.69525	0.798754

C	0.398226	1.322207	-1.77782	H	3.299479	-6.70222	4.764569
S	2.121729	1.039835	-1.60271	H	3.131299	-4.32999	4.115617
C	4.212105	-5.61741	1.168657	H	-2.57953	3.671493	3.852003
C	4.298575	-6.96061	1.536141	H	-2.14441	6.01702	4.448742
C	3.978772	-7.37944	2.832915	H	-4.20547	7.305631	0.908464
C	3.55647	-6.40541	3.749968	H	-4.63739	4.95495	0.304847
C	3.462448	-5.06473	3.387107	H	-4.51388	-5.03357	-0.62964
C	-2.93876	4.464365	3.202801	H	-4.02208	-7.34084	-1.33613
C	-2.69618	5.790766	3.53875	H	-1.72715	-5.83984	-4.64048
C	-3.1505	6.84293	2.727747	H	-2.23357	-3.53558	-3.94984
C	-3.85674	6.512242	1.565742	H	3.084849	4.692175	-3.65308
C	-4.11033	5.184192	1.225885	H	3.233753	7.112086	-4.09352
C	-3.9254	-5.20421	-1.52629	H	4.723343	7.746566	-0.11585
C	-3.63639	-6.50962	-1.92229	H	4.591664	5.318995	0.31846
C	-2.84564	-6.76992	-3.04679	H	-3.23236	8.96936	2.328972
C	-2.34563	-5.66967	-3.7616	H	-3.38013	8.548465	4.04145
C	-2.62882	-4.36611	-3.3726	H	-1.80721	8.460614	3.24951
C	3.441464	5.359559	-2.87371	H	-1.44988	-8.35005	-3.54698
C	3.526722	6.726364	-3.1192	H	-2.94293	-8.91645	-2.78135
C	3.988257	7.614981	-2.13552	H	-2.94976	-8.39639	-4.47275
C	4.366893	7.081364	-0.89906	H	3.313138	-9.11725	3.943033
C	4.294293	5.709992	-0.65017	H	4.047352	-9.49546	2.374618
C	-2.87917	8.280329	3.102444	H	5.063119	-9.01985	3.739163
C	-2.53189	-8.18184	-3.48083	H	4.483032	9.642015	-1.55669
C	4.103141	-8.82847	3.241072	H	4.696984	9.31053	-3.28256
C	4.066507	9.098323	-2.41028	H	3.075304	9.518899	-2.62214

Table S3: Cartesian coordinates of the S_0 optimized structures of compound **3b**.

Sum of imaginary frequencies = 0;

Total Free Energy (hartree) with = -5318.902322

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	0.666489	0.349124	1.872103	C	9.031863	-0.09079	0.061375
C	1.976754	0.683378	2.27723	C	-9.27862	-0.08052	-1.0498
C	2.984486	-0.26369	2.312278	C	-10.6695	-0.10091	-0.97332
C	2.741032	-1.60845	1.960569	C	-11.2895	-0.07103	0.272893
C	1.414974	-1.95766	1.634753	C	-10.5139	-0.02768	1.428765
C	0.404814	-1.00413	1.584626	C	-9.12521	-0.01898	1.325359
C	3.827512	-2.60642	1.970123	C	9.812204	0.849561	0.746812
C	3.534981	-3.97111	2.460814	C	11.20414	0.827086	0.720946
C	5.108908	-2.28441	1.559653	C	11.86297	-0.17069	0.007179
C	6.3464	-2.98933	1.846521	C	11.12243	-1.12934	-0.67867
C	7.388482	-2.26073	1.365354	C	9.730915	-1.07467	-0.65041
C	6.859133	-1.0792	0.711989	F	9.21839	1.818791	1.459511
N	5.494671	-1.14099	0.861136	F	11.91192	1.745455	1.391285
N	-5.00749	1.409612	0.502363	F	13.19902	-0.20838	-0.01787

C	-6.33061	1.214118	0.377319	F	11.75108	-2.08768	-1.37171
C	-7.0867	2.439278	0.639474	F	9.058928	-2.01198	-1.33627
C	-6.17274	3.398109	0.907249	F	-8.41488	0.017358	2.460868
C	-4.86354	2.753256	0.83419	F	-11.1079	-0.00616	2.628797
C	-3.74015	4.907403	1.284294	F	-12.6233	-0.08631	0.360497
C	-3.68108	3.42108	1.126161	F	-11.4118	-0.13808	-2.0876
C	-2.37948	2.833061	1.299364	F	-8.7229	-0.10256	-2.2699
C	-1.18587	3.550319	1.363003	O	-3.98268	9.071945	1.623226
C	-0.05066	2.760107	1.586624	C	-3.65146	9.736174	2.833082
C	-0.32568	1.406929	1.706697	O	-3.83549	-8.8956	-2.50391
S	-2.04882	1.118631	1.529459	C	-4.24644	-9.82577	-1.51364
C	0.827143	-0.28221	-2.01331	H	2.206129	1.701007	2.574725
C	2.160037	-0.62457	-2.33137	H	3.977476	0.03388	2.632618
C	3.175192	0.313042	-2.28539	H	1.183084	-2.98606	1.376779
C	2.914384	1.657428	-1.94321	H	-0.59004	-1.30887	1.273053
C	1.570927	2.016596	-1.71421	H	6.401163	-3.90389	2.41888
C	0.55254	1.070494	-1.73756	H	8.440337	-2.48914	1.46211
C	4.005179	2.643147	-1.85691	H	4.907776	-0.44004	0.405111
C	3.740813	4.025281	-2.3115	H	-8.16201	2.545528	0.605435
C	5.261139	2.28859	-1.38474	H	-6.35498	4.430331	1.167875
C	6.508824	3.018268	-1.61418	H	-1.14916	4.623115	1.225911
C	7.508259	2.239695	-1.13068	H	0.953826	3.164628	1.614142
C	6.868576	1.054245	-0.55522	H	2.400318	-1.64251	-2.61993
N	5.540138	1.100225	-0.71651	H	4.189799	0.015767	-2.51903
N	-5.00424	-1.36975	-0.67722	H	1.327798	3.044706	-1.46595
C	-6.35446	-1.16406	-0.45783	H	-0.45916	1.380325	-1.49233
C	-7.01695	-2.39742	-0.81542	H	6.602744	3.95503	-2.14557
C	-6.07829	-3.2926	-1.20817	H	8.570538	2.440406	-1.16746
C	-4.77098	-2.67467	-1.12613	H	-4.32123	-0.66512	-0.41478
C	-3.66441	-4.78946	-1.71188	H	-8.08438	-2.55299	-0.76953
C	-3.58969	-3.31397	-1.46659	H	-6.2456	-4.29775	-1.56326
C	-2.27269	-2.74216	-1.59757	H	-1.06724	-4.54357	-1.4666
C	-1.08691	-3.47079	-1.60905	H	1.066957	-3.10683	-1.76134
C	0.067003	-2.69066	-1.78217	H	-4.4309	5.275863	-0.72519
C	-0.17721	-1.33488	-1.91313	H	-4.545	7.745702	-0.45728
S	-1.90825	-1.03439	-1.84147	H	-3.19108	7.349468	3.60648
C	-4.16092	5.731038	0.223112	H	-3.06071	4.915732	3.326869
C	-4.22769	7.110818	0.364094	H	2.31474	-3.31208	4.115438
C	-3.87976	7.713082	1.582127	H	1.834688	-5.57293	4.954112
C	-3.45796	6.912	2.651186	H	4.155641	-7.25776	1.758315
C	-3.3855	5.527537	2.490144	H	4.620842	-4.99661	0.90415
C	2.724215	-4.17316	3.595886	H	4.761907	4.978269	-0.66886
C	2.455822	-5.45277	4.069027	H	4.344688	7.2768	-1.45263
C	2.973117	-6.59042	3.431204	H	2.194067	5.732973	-4.83418
C	3.761438	-6.39477	2.290619	H	2.616361	3.437662	-4.05857
C	4.035326	-5.1155	1.811004	H	-3.00298	-4.67384	-3.76392
C	4.214898	5.13893	-1.59272	H	-3.14117	-7.12129	-4.16625
C	3.969518	6.437468	-2.03408	H	-4.44777	-7.70229	-0.10935

C	3.239044	6.682194	-3.20327	H	-4.31887	-5.28002	0.276945
C	2.758526	5.574027	-3.91784	H	3.40477	-8.23847	4.766938
C	2.993583	4.275684	-3.48035	H	1.691263	-8.05082	4.389646
C	-3.32061	-5.33634	-2.9639	H	2.797086	-8.73512	3.184757
C	-3.39266	-6.70141	-3.19726	H	1.928627	8.39449	-3.40019
C	-3.80229	-7.57319	-2.17502	H	3.636063	8.810876	-3.21309
C	-4.13806	-7.05306	-0.92028	H	3.035863	8.177846	-4.75622
C	-4.06489	-5.67425	-0.70298	H	-3.80758	10.79942	2.642493
C	2.699266	-7.97532	3.967132	H	-4.30022	9.416784	3.659168
C	2.949364	8.089441	-3.66738	H	-2.60293	9.567914	3.112063
C	-6.97472	-0.01084	0.001734	H	-4.20143	-10.8073	-1.98867
C	7.544686	-0.04332	0.08324	H	-3.57573	-9.81236	-0.64441
C	-8.46621	-0.04435	0.089894	H	-5.274	-9.63136	-1.17929

Table S4: Cartesian coordinates of the S_0 optimized structures of the compound **4a**.

Sum of imaginary frequencies = 0;

Total Free Energy (hartree) with = -5168.502815

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	-0.79693	1.149692	-1.8725	C	-1.66805	-4.63166	4.488204
C	-0.96493	2.519624	-1.58491	C	-2.15856	-3.43836	3.969432
C	-2.2282	3.084813	-1.49466	C	5.194085	8.435071	3.560349
C	-3.39837	2.313963	-1.66711	C	-1.28	-7.13358	4.366859
C	-3.228	0.94099	-1.94488	C	9.997261	-0.08445	-0.91645
C	-1.9642	0.378944	-2.04974	C	11.35068	-0.41112	-0.90103
C	-4.72843	2.944459	-1.62636	C	11.77486	-1.55515	-0.22992
C	-4.84226	4.34193	-2.10992	C	10.84187	-2.35461	0.424518
C	-5.867	2.281106	-1.19465	C	9.495886	-1.99678	0.407945
C	-7.24524	2.68556	-1.48027	C	-9.99723	-0.08428	0.916452
C	-8.04586	1.701966	-1.004	C	-11.3506	-0.41095	0.901089
C	-7.16219	0.714681	-0.38127	C	-11.7748	-1.55507	0.23015
N	-5.8753	1.070339	-0.51019	C	-10.8419	-2.3546	-0.42424
N	5.351757	-1.09041	-1.07473	C	-9.49588	-1.99677	-0.40773
C	6.697266	-1.33287	-0.93479	F	-9.63055	1.017219	1.588616
C	6.957802	-2.5792	-1.62445	F	-12.2426	0.355881	1.541282
C	5.780688	-3.04778	-2.12065	F	-13.0703	-1.88459	0.21589
C	4.729373	-2.10311	-1.79678	F	-11.2449	-3.45338	-1.07551
C	2.861224	-3.41355	-2.74896	F	-8.63449	-2.7917	-1.06081
C	3.405114	-2.14349	-2.2022	F	8.634452	-2.7917	1.060963
C	2.541822	-0.98053	-2.1305	F	11.24484	-3.45334	1.075885
C	2.867087	0.368311	-2.18043	F	9.630596	1.016982	-1.58874
C	1.752852	1.227608	-2.09981	F	12.24268	0.35564	-1.54131
C	0.539729	0.570956	-1.98137	F	13.07033	-1.88467	-0.21561
S	0.798259	-1.15948	-1.96709	H	-0.09432	3.143762	-1.41183
C	2.158438	-3.43879	-3.96888	H	-2.31822	4.143332	-1.27188

C	1.667884	-4.63217	-4.48743	H	-4.10403	0.323017	-2.09943
C	1.843986	-5.84826	-3.80993	H	-1.87974	-0.67576	-2.29729
C	2.537146	-5.82357	-2.59419	H	-7.54116	3.564576	-2.03515
C	3.034711	-4.63163	-2.06973	H	-9.12344	1.64169	-1.07426
C	-5.57007	5.307619	-1.3922	H	4.93348	-0.29491	-0.58859
C	-5.68138	6.617602	-1.85752	H	7.933779	-3.03112	-1.72873
C	-5.07341	7.018104	-3.05221	H	5.631218	-3.93777	-2.7143
C	-4.33845	6.057971	-3.76628	H	3.881766	0.725432	-2.31043
C	-4.21649	4.75295	-3.30462	H	1.839334	2.306545	-2.15511
C	-5.19415	8.434462	-3.56193	H	2.019137	-2.51482	-4.52213
C	1.279683	-7.13405	-4.36557	H	1.142964	-4.62222	-5.44025
C	7.587999	-0.48852	-0.27672	H	2.682752	-6.7495	-2.04228
C	-7.58796	-0.48845	0.276766	H	3.550339	-4.63681	-1.11388
C	9.029358	-0.85743	-0.26116	H	-6.03259	5.029209	-0.45027
C	-9.02933	-0.85736	0.261264	H	-6.24371	7.34342	-1.27444
C	0.797014	1.149755	1.872453	H	-3.85718	6.339661	-4.70058
C	0.964997	2.519605	1.58446	H	-3.64678	4.030125	-3.8809
C	2.228249	3.08484	1.494177	H	-5.70279	8.466416	-4.53383
C	3.398429	2.314094	1.666962	H	-4.20839	8.895138	-3.70209
C	3.228078	0.941209	1.945191	H	-5.76157	9.062796	-2.86848
C	1.964304	0.379122	2.050085	H	1.751862	-8.00973	-3.90878
C	4.728484	2.944606	1.62608	H	0.200057	-7.20792	-4.17852
C	4.84228	4.342192	2.109292	H	1.422625	-7.19891	-5.45017
C	5.867058	2.281193	1.194453	H	0.094369	3.143631	1.411036
C	7.245306	2.685716	1.479909	H	2.318233	4.14329	1.271052
C	8.045913	1.702065	1.003733	H	4.104123	0.323337	2.100045
C	7.16223	0.714679	0.381198	H	1.879927	-0.67551	2.29795
N	5.875347	1.070327	0.510163	H	7.541254	3.564828	2.034627
N	-5.35172	-1.09031	1.07485	H	9.123505	1.641809	1.073892
C	-6.69724	-1.33272	0.934965	H	-4.93341	-0.29491	0.588567
C	-6.95783	-2.5789	1.624881	H	-7.93382	-3.03075	1.729281
C	-5.78073	-3.04748	2.121123	H	-5.6313	-3.93736	2.714939
C	-4.72937	-2.10294	1.797038	H	-3.8817	0.725619	2.310241
C	-2.86128	-3.4133	2.749461	H	-1.83922	2.306667	2.154825
C	-3.40511	-2.14331	2.202469	H	3.646659	4.030819	3.880252
C	-2.54179	-0.98038	2.130572	H	3.856983	6.340561	4.699382
C	-2.86703	0.368465	2.180293	H	6.243771	7.343484	1.273173
C	-1.75277	1.227722	2.099623	H	6.032708	5.029073	0.449551
C	-0.53966	0.571025	1.981304	H	-3.5503	-4.63681	1.114538
S	-0.79824	-1.15941	1.967187	H	-2.68282	-6.74937	2.043347
C	4.216419	4.753505	3.30384	H	-1.14317	-4.62156	5.441048
C	4.33833	6.05864	3.76519	H	-2.01926	-2.5143	4.522533
C	5.073353	7.018598	3.050941	H	5.761173	9.063348	2.866567
C	5.681414	6.617804	1.856398	H	4.208313	8.895639	3.700788
C	5.570138	5.307708	1.391388	H	5.703079	8.467279	4.532051
C	-3.03475	-4.63149	2.070427	H	-1.42432	-7.19884	5.451265
C	-2.53723	-5.82335	2.595112	H	-1.75122	-8.00931	3.909202
C	-1.84415	-5.84786	3.810897	H	-0.2001	-7.20692	4.181214

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