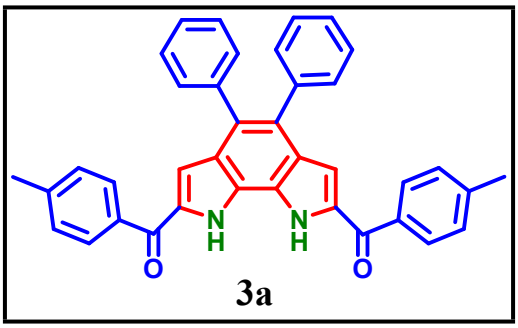
Dibenzoylbenzodipyrroles: Key Precursors for the Synthesis of Fused Meso-Aryl Sapphyrins

Prosenjit Isar and Mangalampalli Ravikanth*

Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India, E-mail: ravikanth@chem.iitb.ac.in



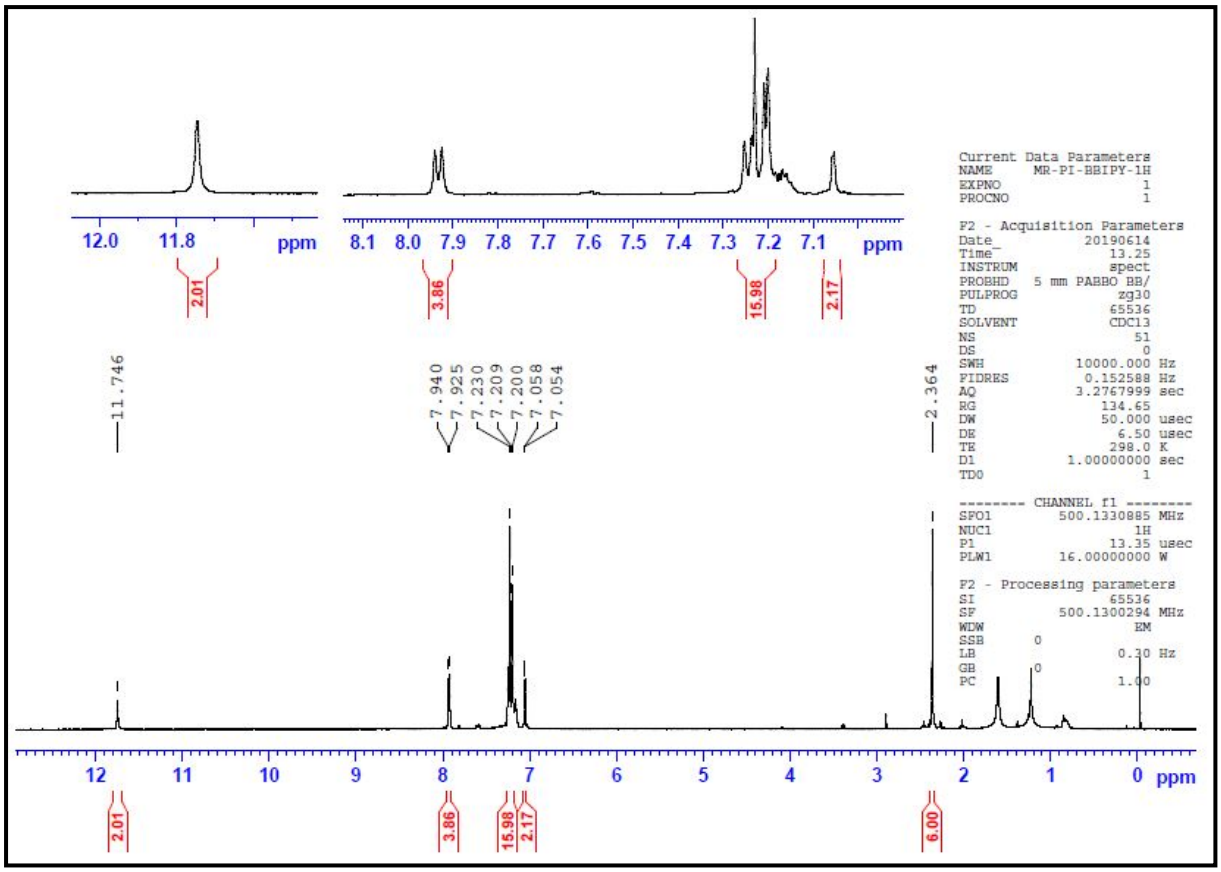
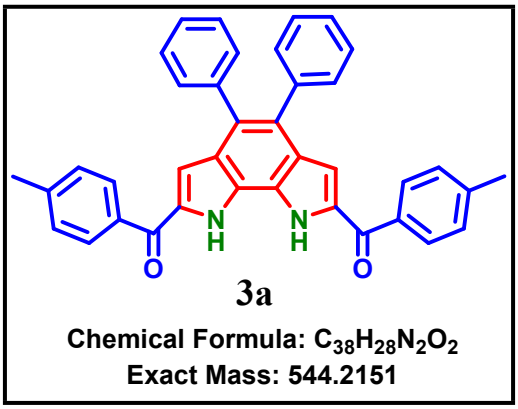


Figure S1. ^{1}H NMR of compound **3a** recorded in $CDCl_3$ at 25 °C. (500 MHz)



3a

Chemical Formula: $C_{38}H_{28}N_2O_2$
Exact Mass: 544.2151

Observed Mass= 545.2227 $[M+H]^+$

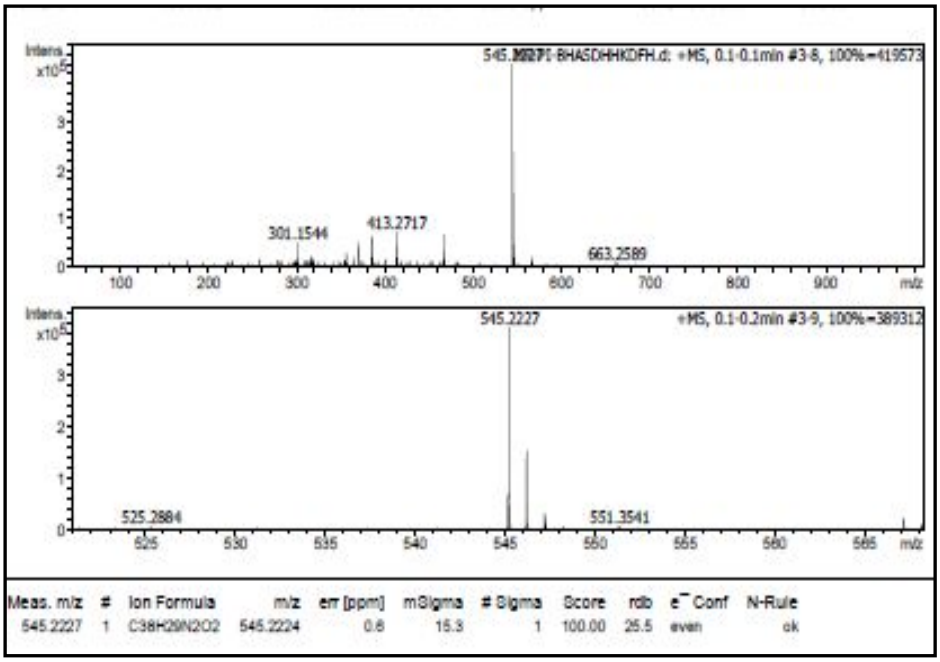
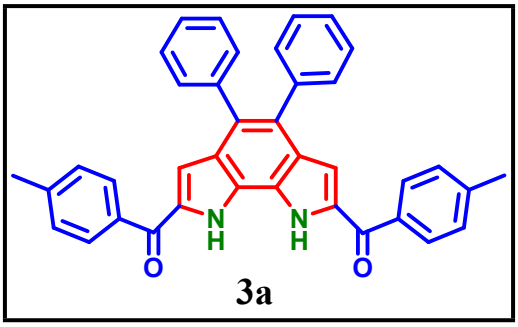


Figure S2. HRMS spectrum of compound **3a.**



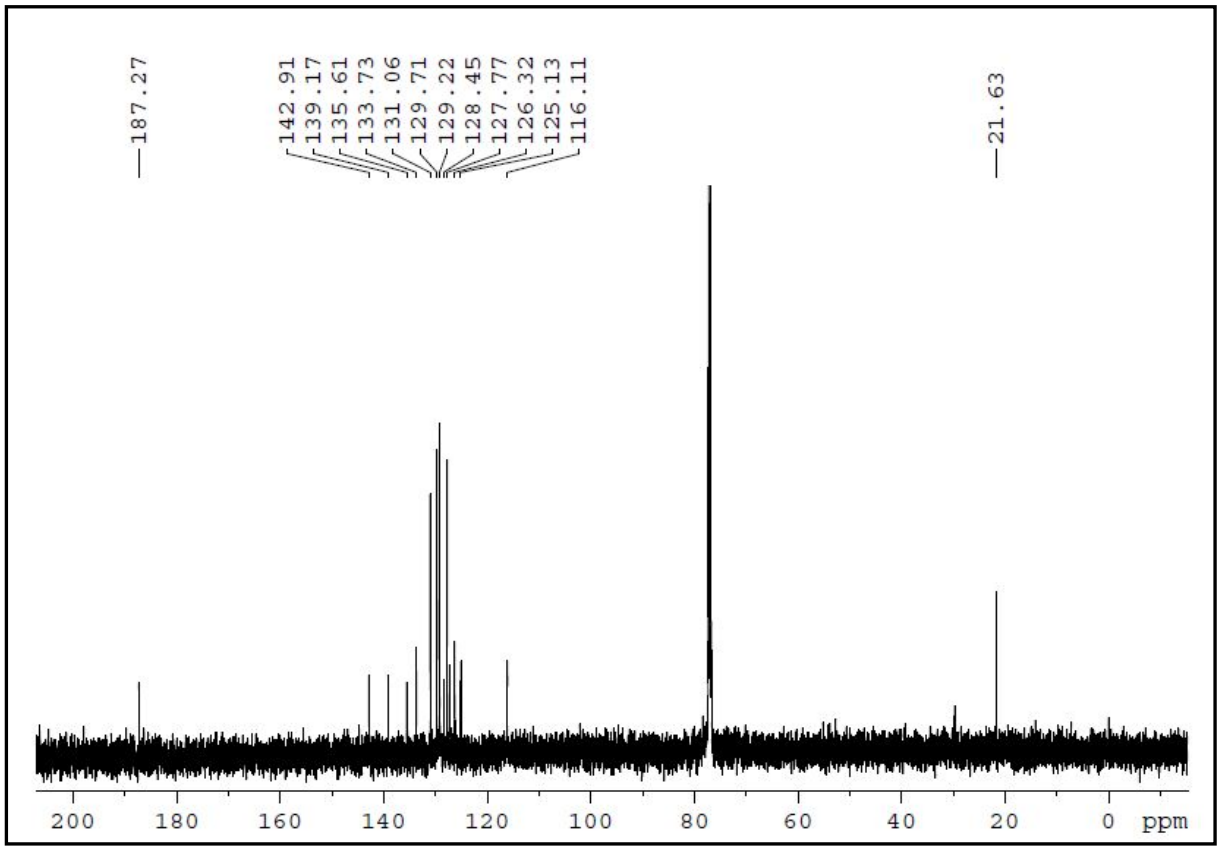
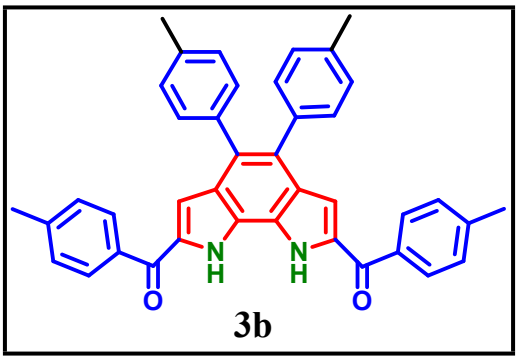


Figure S3. $^{13}C\{1H\}$ NMR of compound **3a** recorded in $CDCl_3$ at 25 °C (125 MHz) .



3b

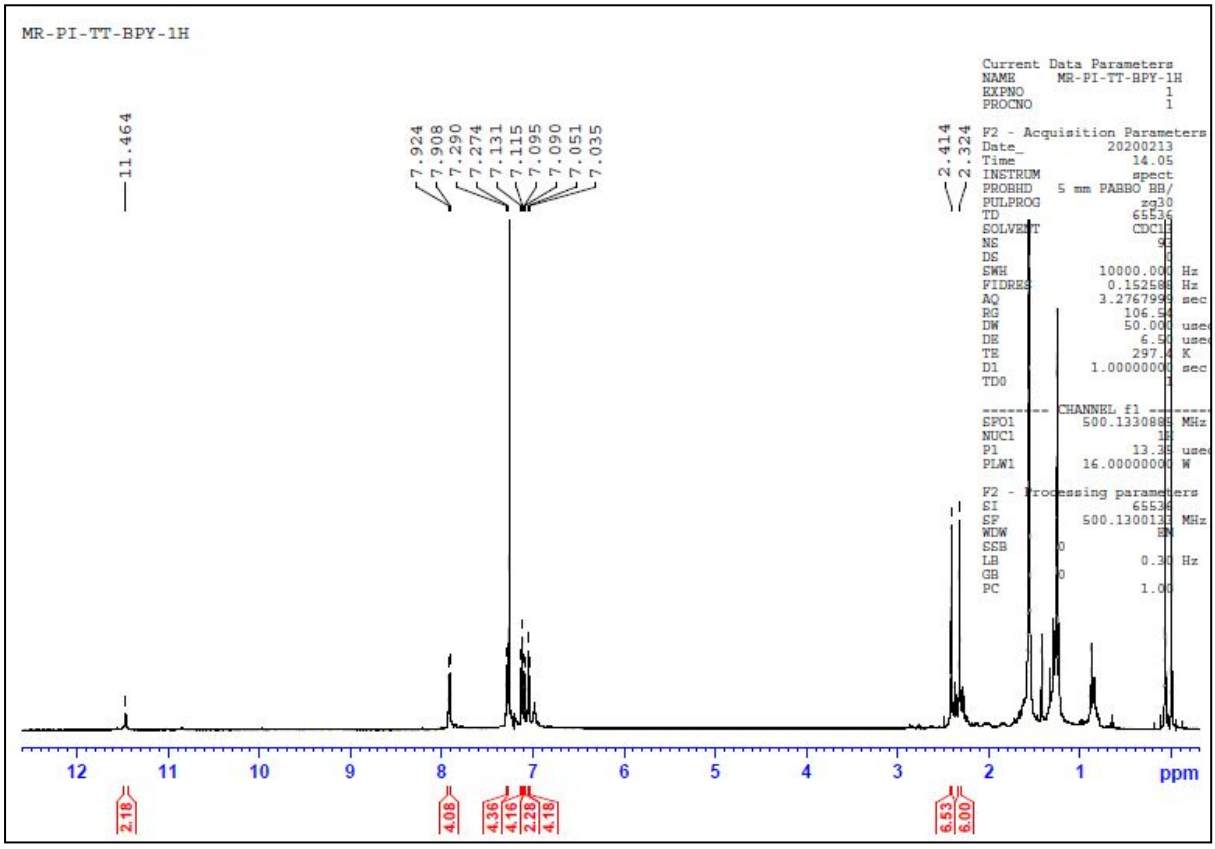
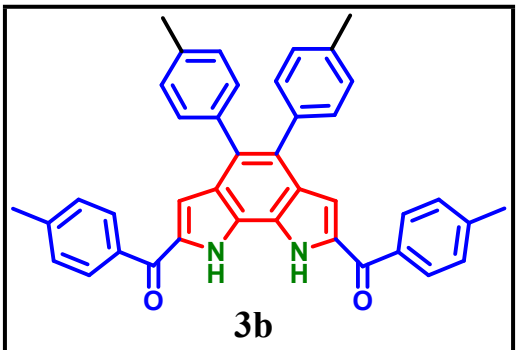


Figure S4. ^{1}H NMR of compound **3b** recorded in $CDCl_3$ at 25 °C. (500 MHz).



3b

Chemical Formula: $C_{40}H_{32}N_2O_2$
Exact Mass: 572.2464

Observed Mass= 573.2543 $[M+H]^+$

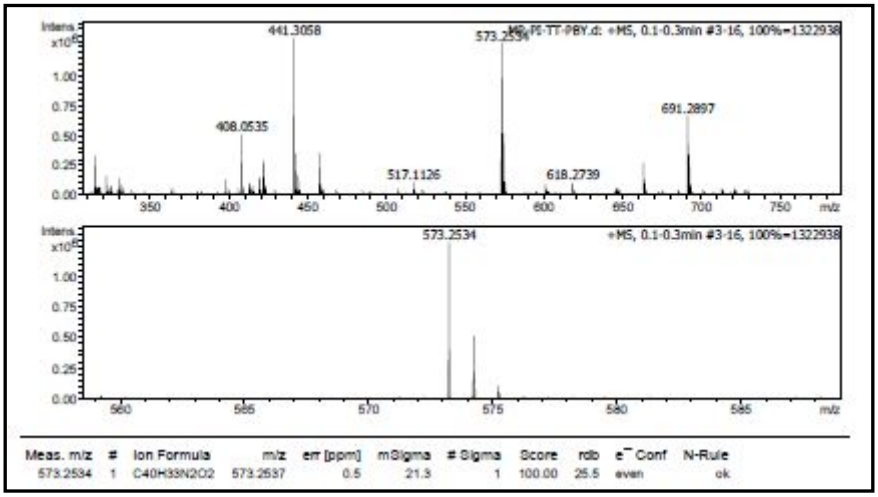
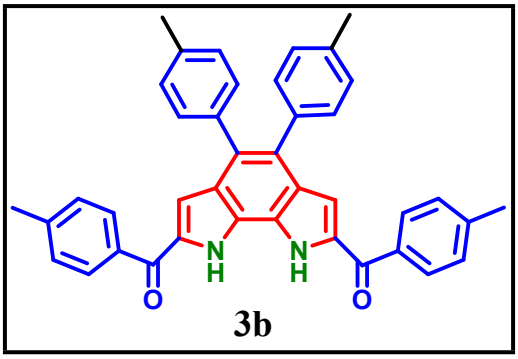


Figure S5. HRMS spectrum of compound **3b.**



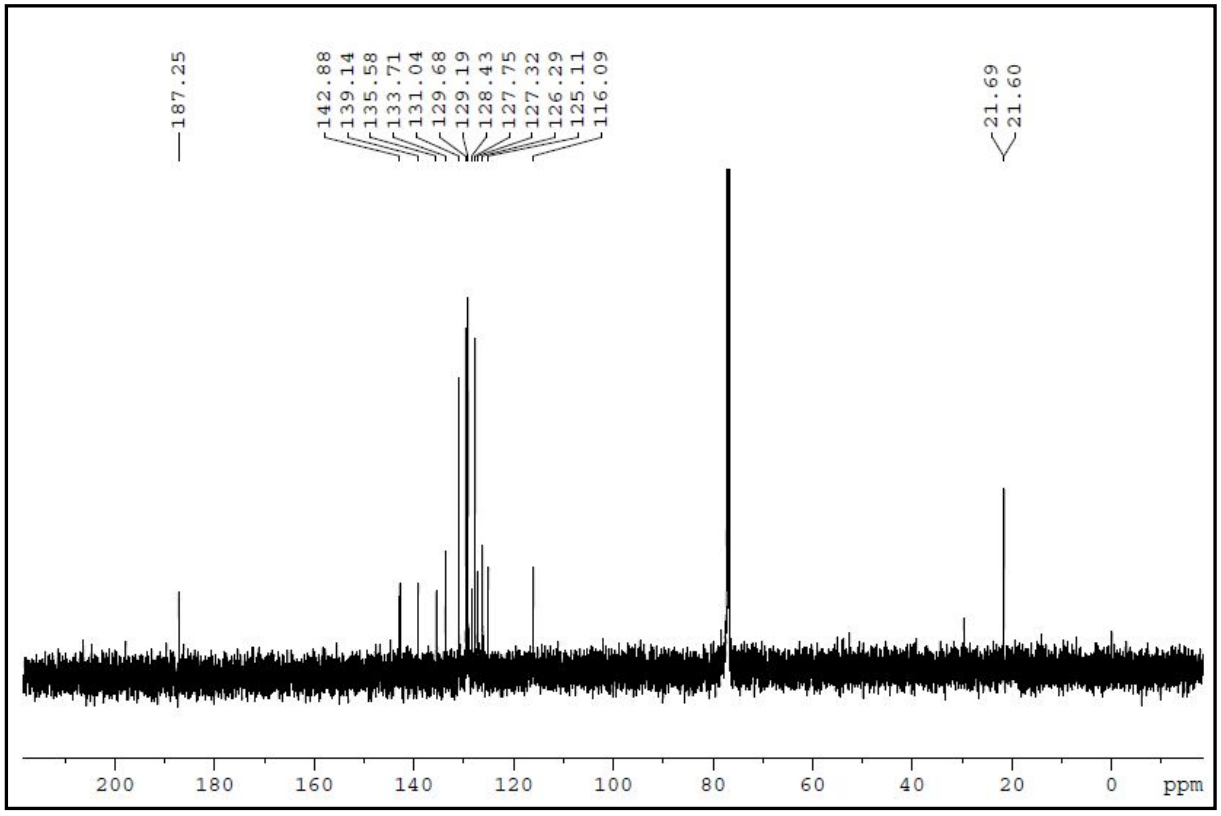
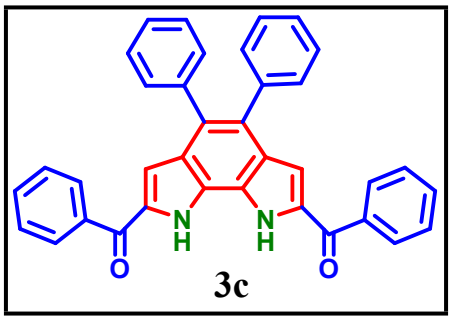


Figure S6. $^{13}C\{^{1}H\}$NMR of compound **3b** recorded in $CDCl_3$ at 25 °C (125 MHz).



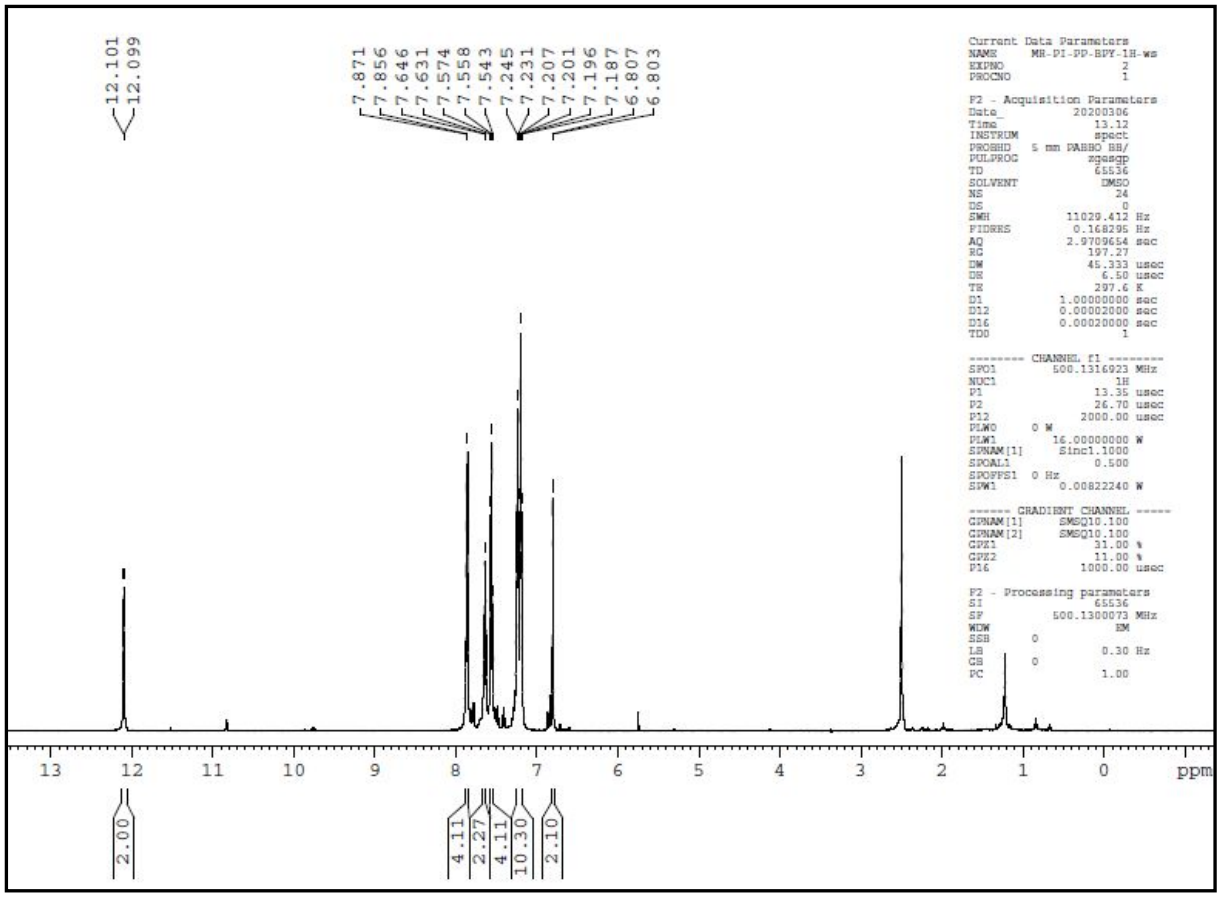
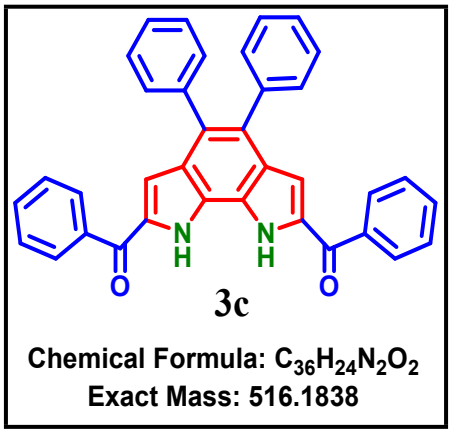


Figure S7. ^{1}H NMR of compound **3c** recorded in DMSO-d_6 at 25 °C (500 MHz).



3c

Chemical Formula: $C_{36}H_{24}N_2O_2$
Exact Mass: 516.1838

Observed Mass= 517.1918 $[M+H]^+$

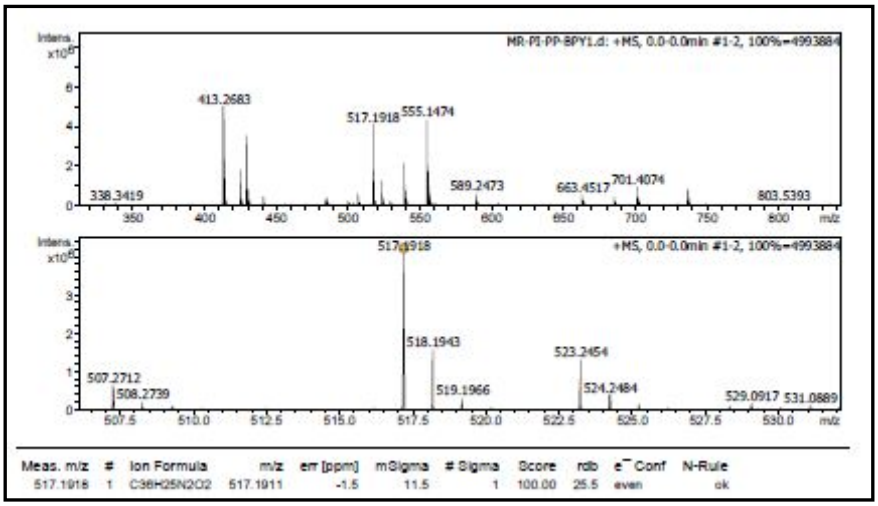
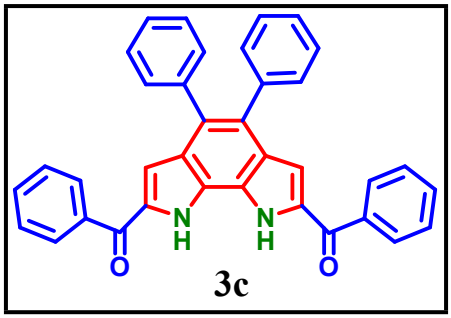


Figure S8. HRMS spectrum of compound **3c.**



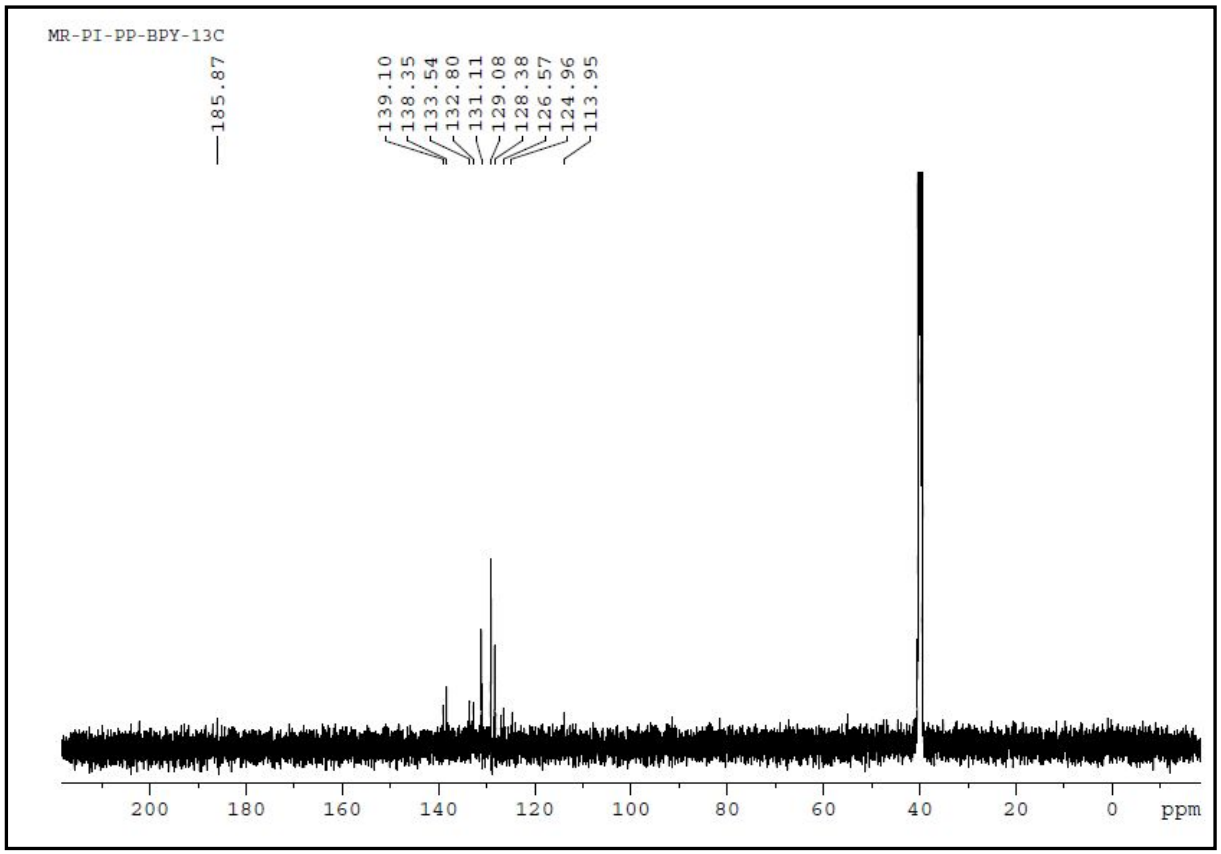
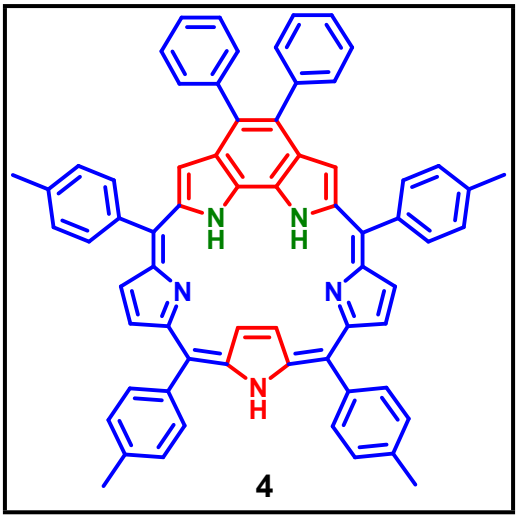


Figure S9. $^{13}C\{^{1}H\}$ NMR of compound **3c** recorded in DMSO-d_6 at 25 °C (125 MHz)..



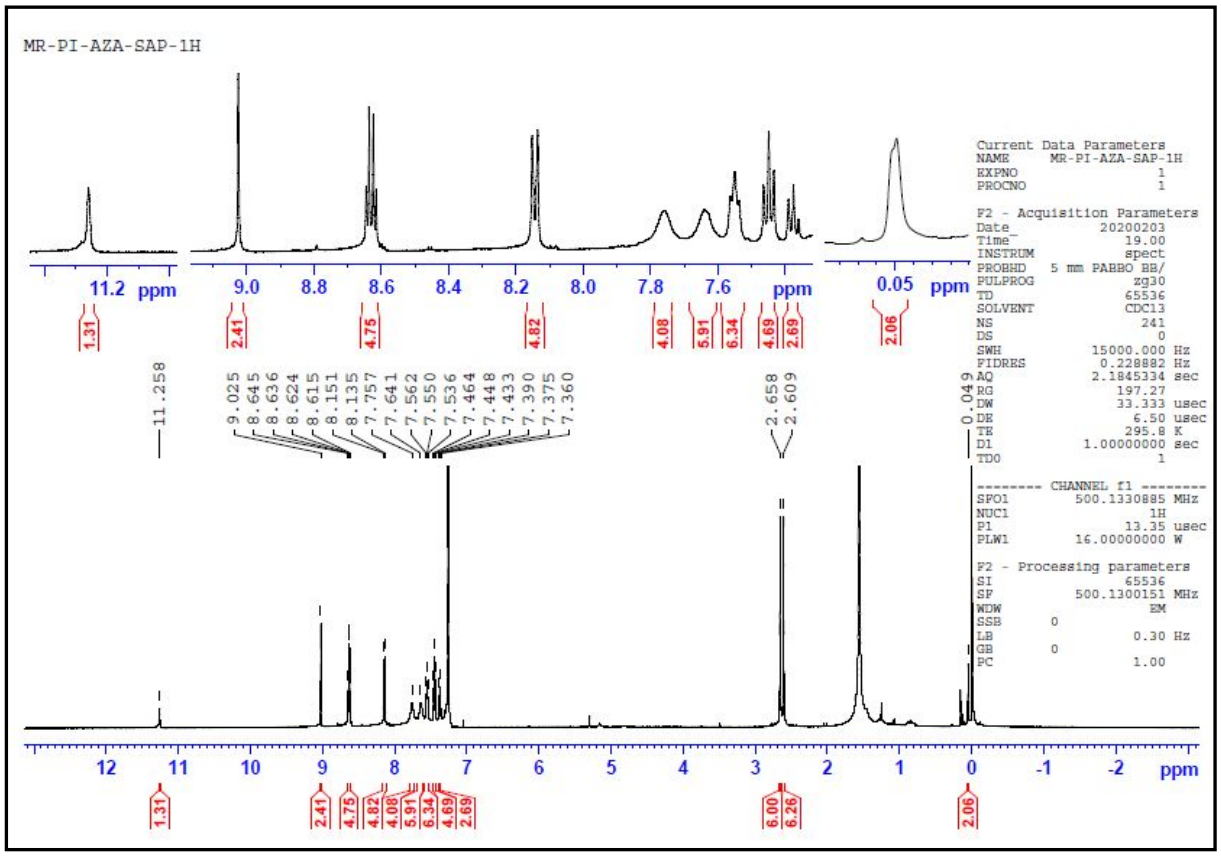
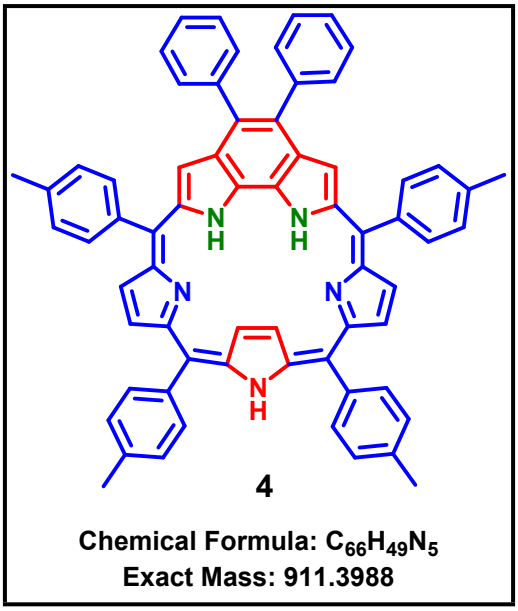


Figure S10. ^{1}H NMR of compound **4** recorded in $CDCl_3$ at 25 °C (500 MHz).



Observed Mass= 912.4061 $[M+H]^+$

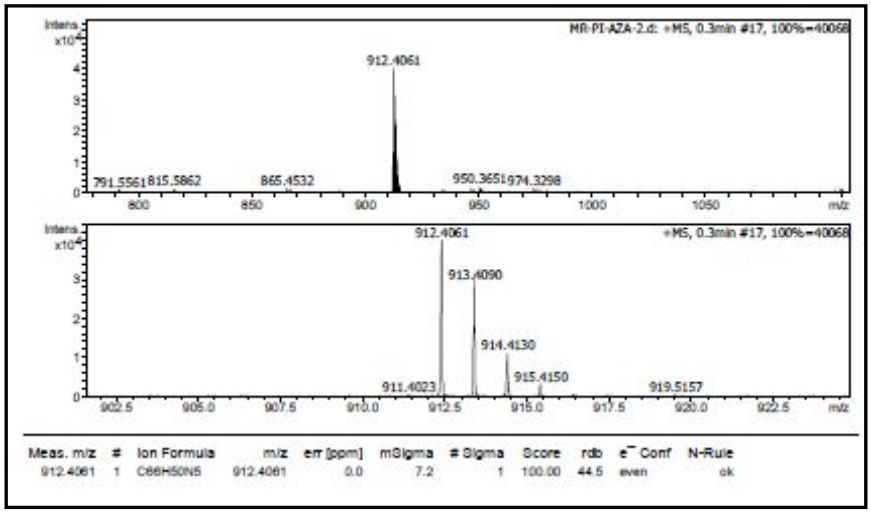
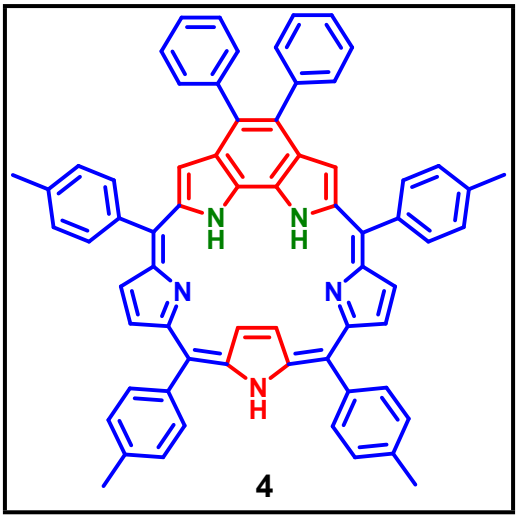


Figure S11. HRMS spectrum of compound **4.**



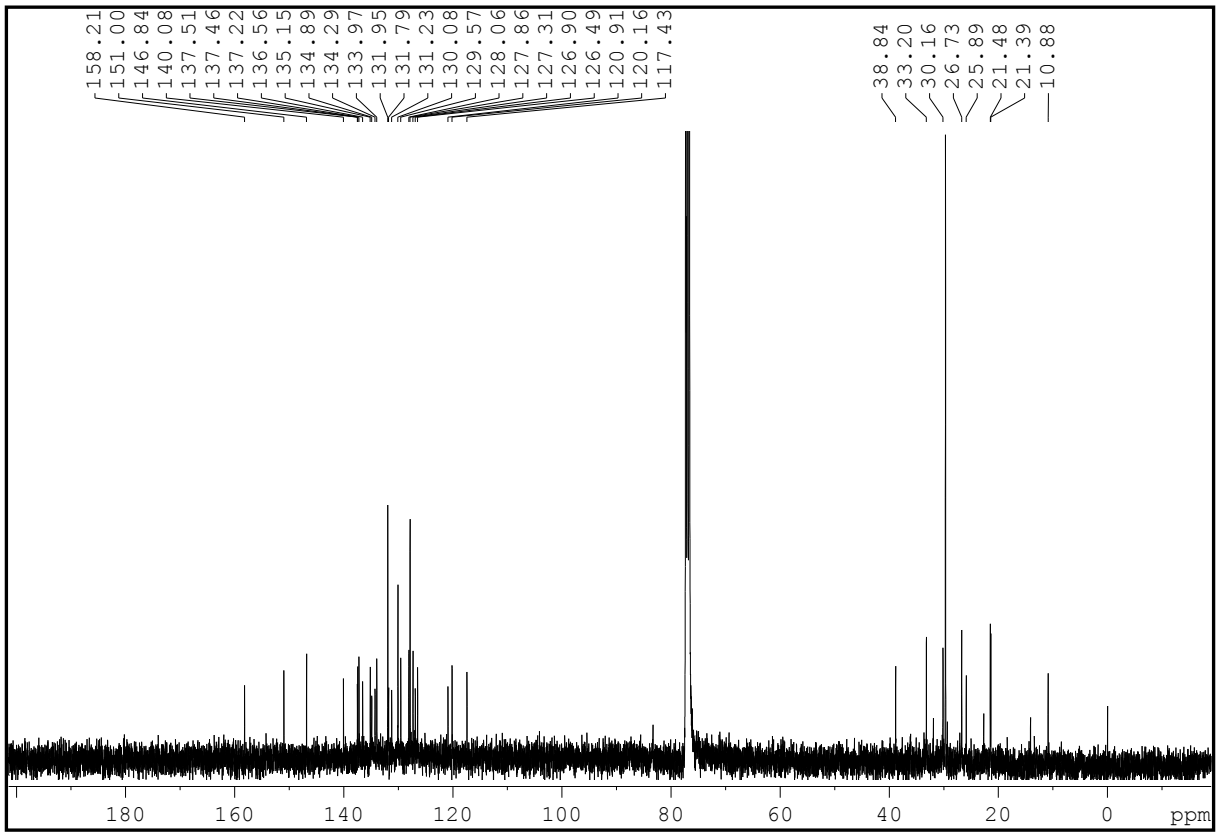
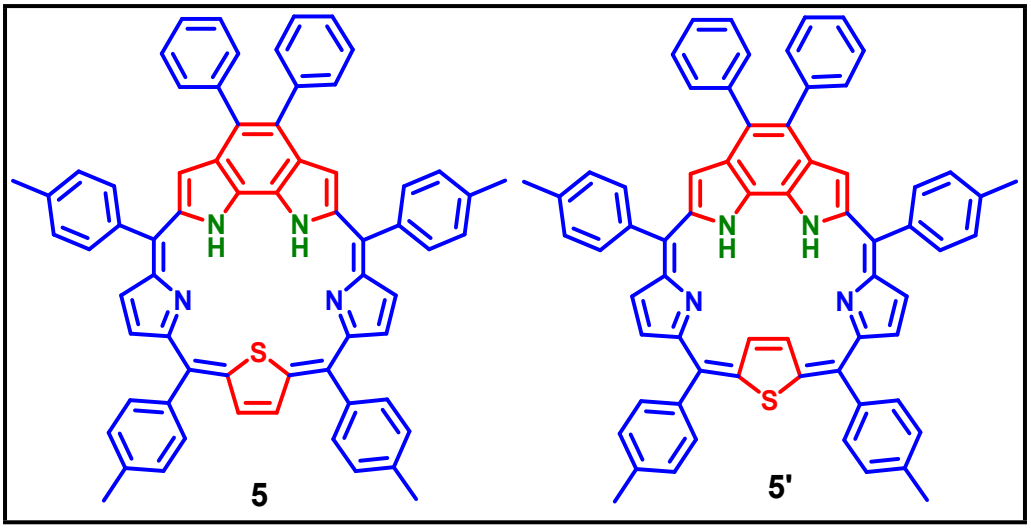


Figure S12. $^{13}C\{^{1}H\}$NMR of compound **4** recorded in $CDCl_3$ at 25 °C (125 MHz)..



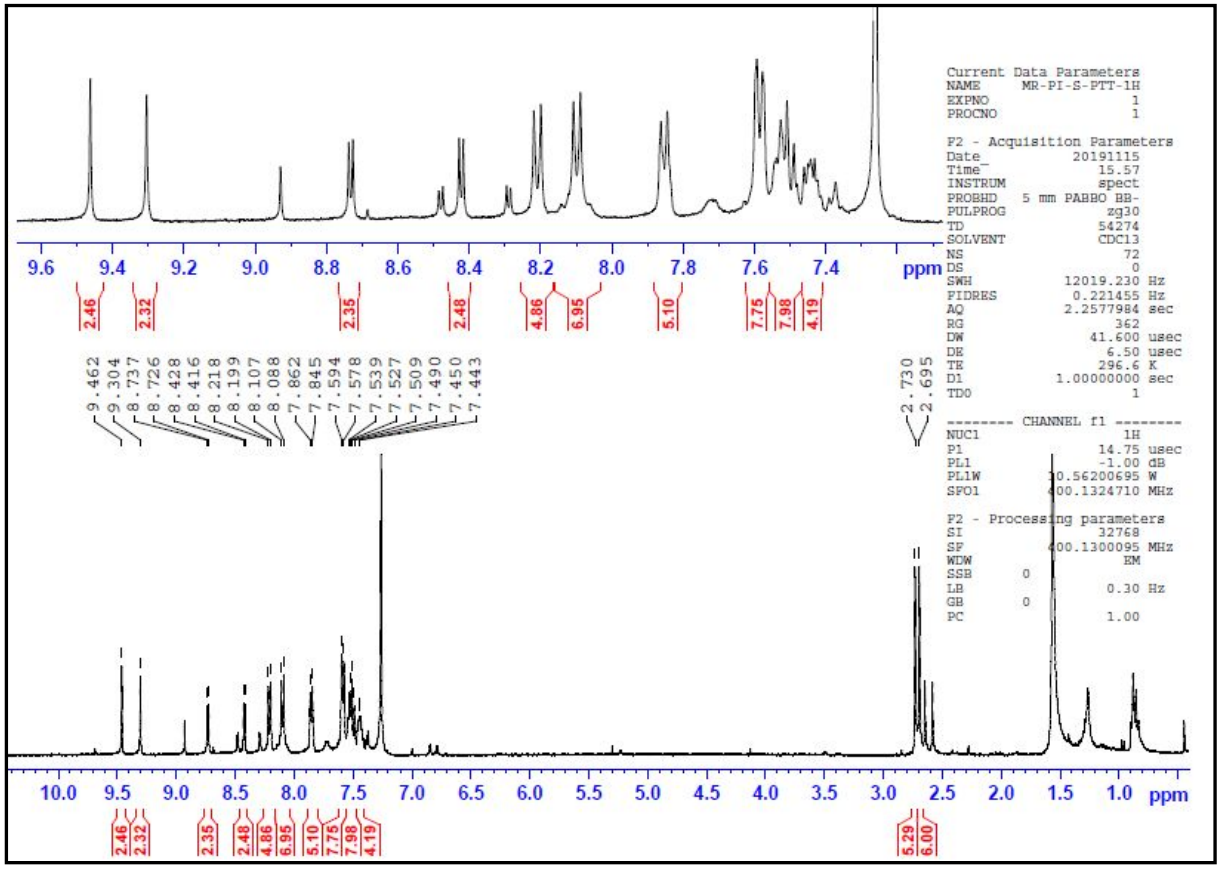
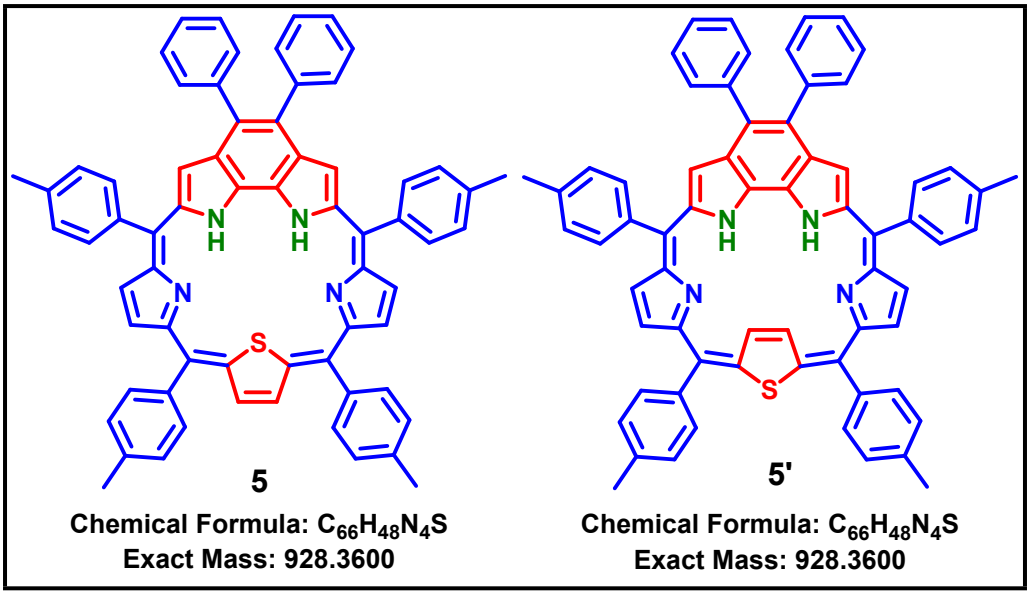


Figure S13. ^{1}H NMR of compound **5**+**5′** recorded in $CDCl_3$ at 25 °C (400 MHz).



Observed Mass= 929.3679 $[M+H]^+$

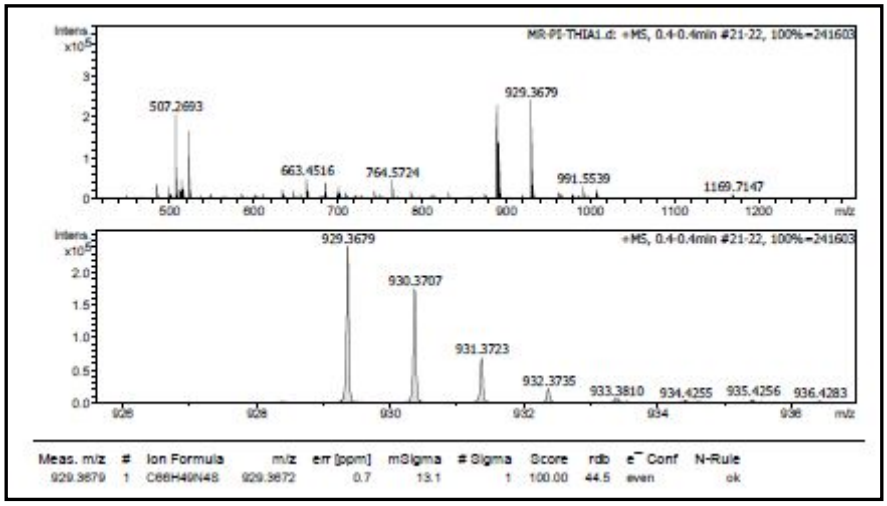
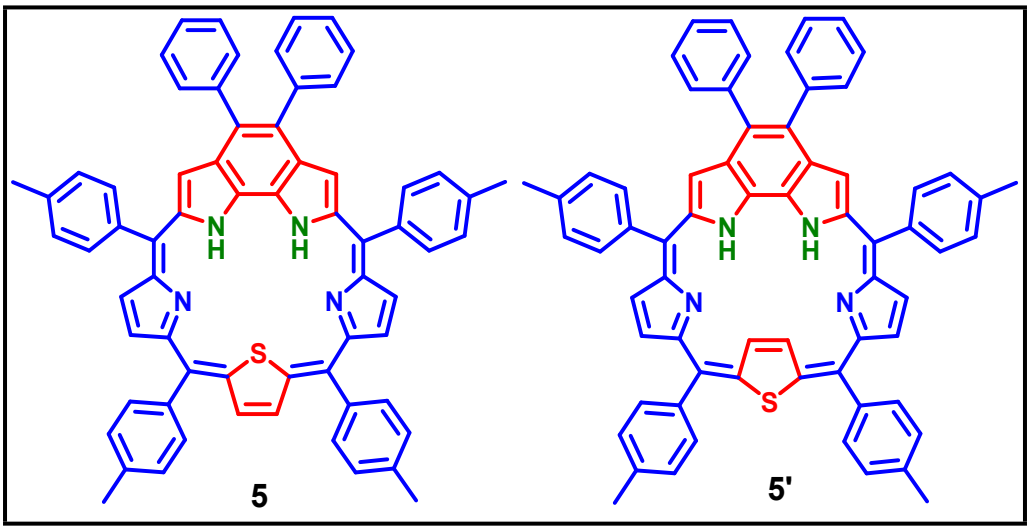


Figure S14. HRMS spectrum of compound **5+5′.**



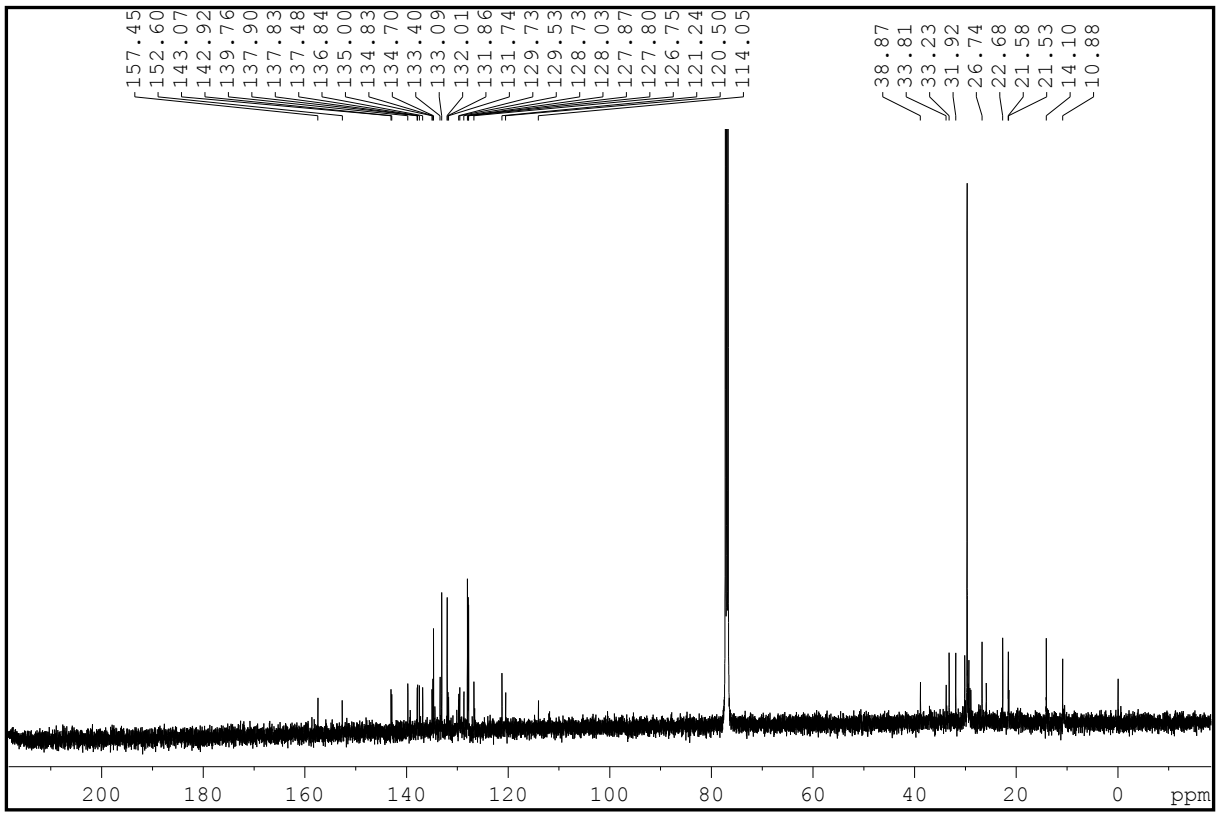
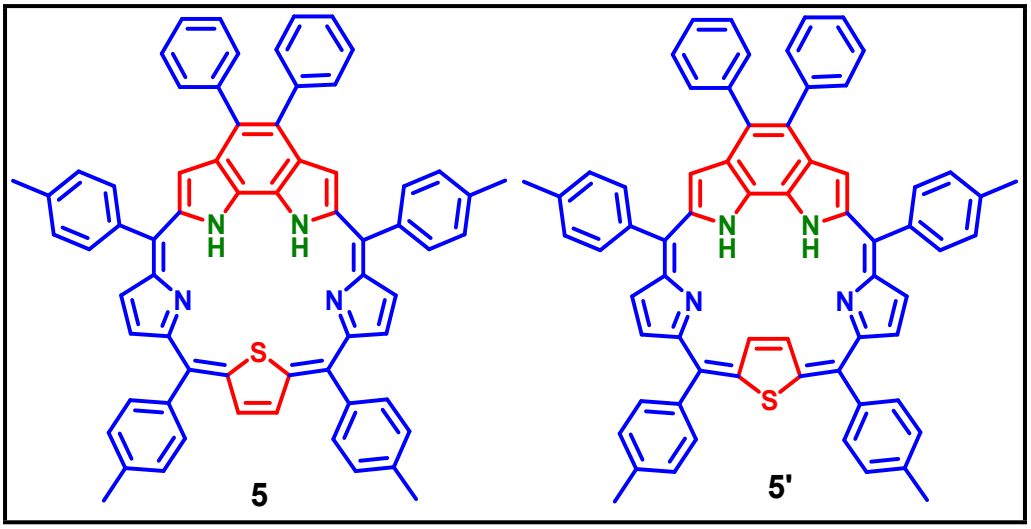


Figure S15. $^{13}C\{^{1}H\}$NMR of compound **5+5′** recorded in $CDCl_3$ at 25 °C (100 MHz).



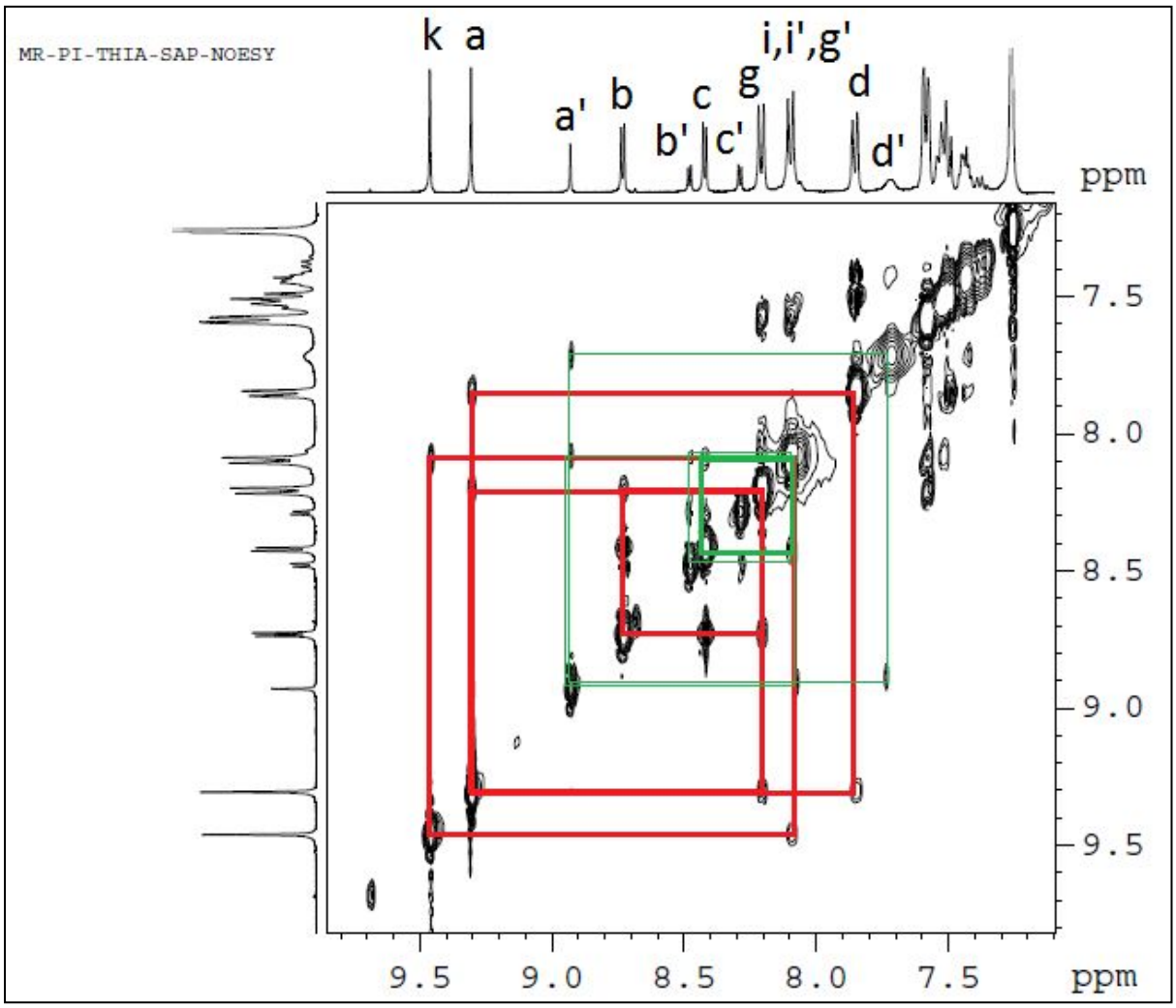


Figure S16. ^{1}H-1H NOESYspectrum of compound **5**+**5′** recorded in $CDCl_3$at 25 °C (400 MHz).

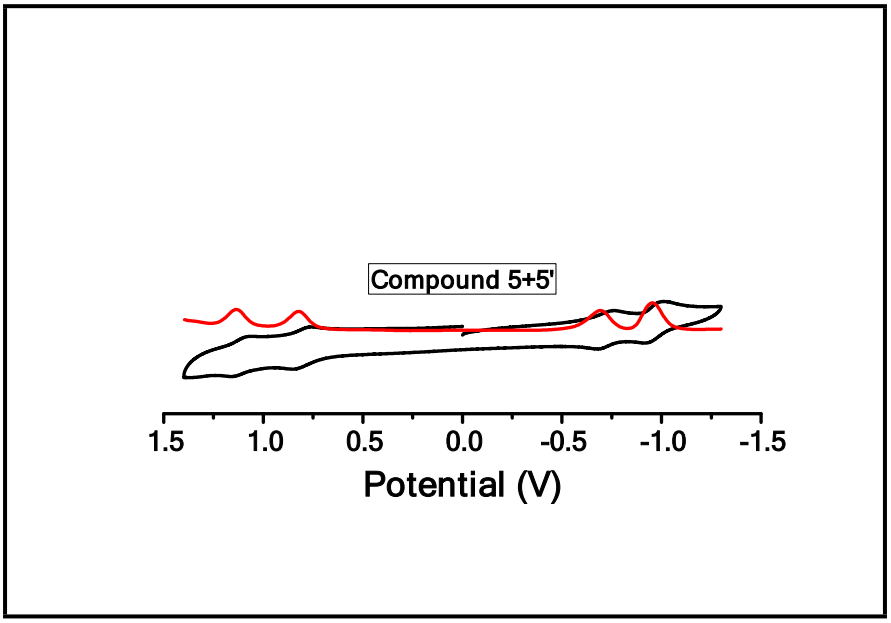


Figure S17: Cyclic voltammogram of compounds **5+5′** (black line) along with differential pulse voltammogram (red line), recorded in CH_2Cl_2 containing 0.1MTBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at scan rates of 50 mV s^{-1}.

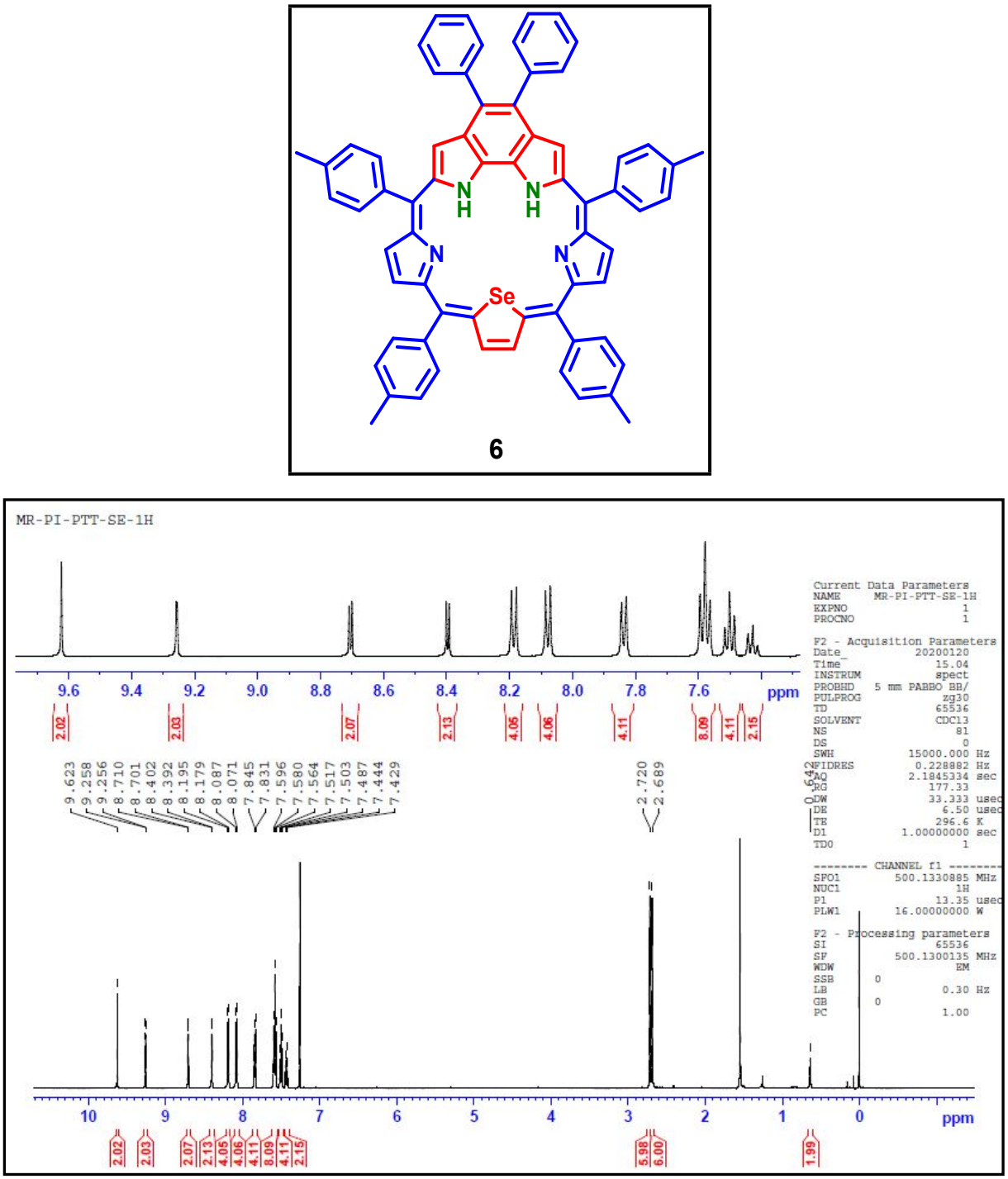
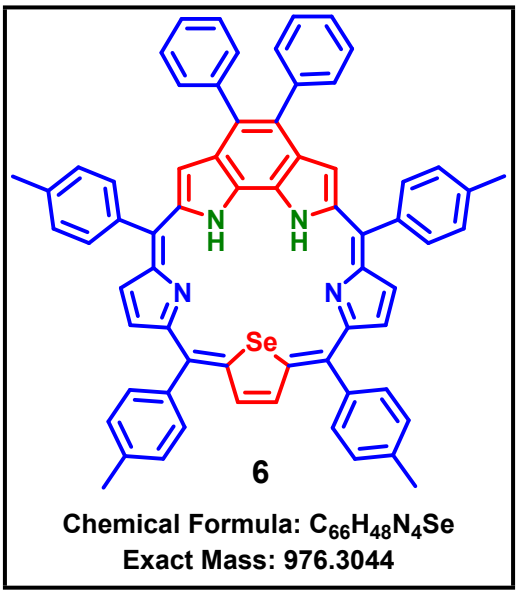


Figure S18. ^{1}H NMR of compound **6** recorded in $CDCl_3$ at 25 °C (500 MHz).



6

Chemical Formula: $C_{66}H_{48}N_4Se$
Exact Mass: 976.3044

Observed Mass= 977.3126 $[M+H]^+$

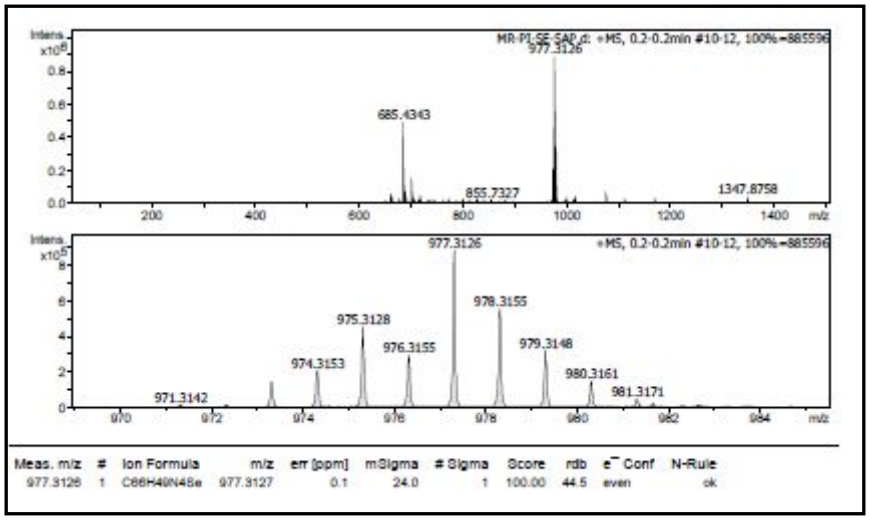
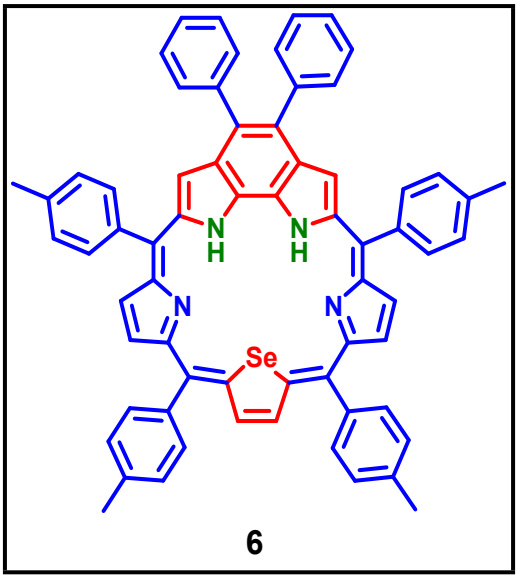


Figure S19. HRMS spectrum of compound **6.**



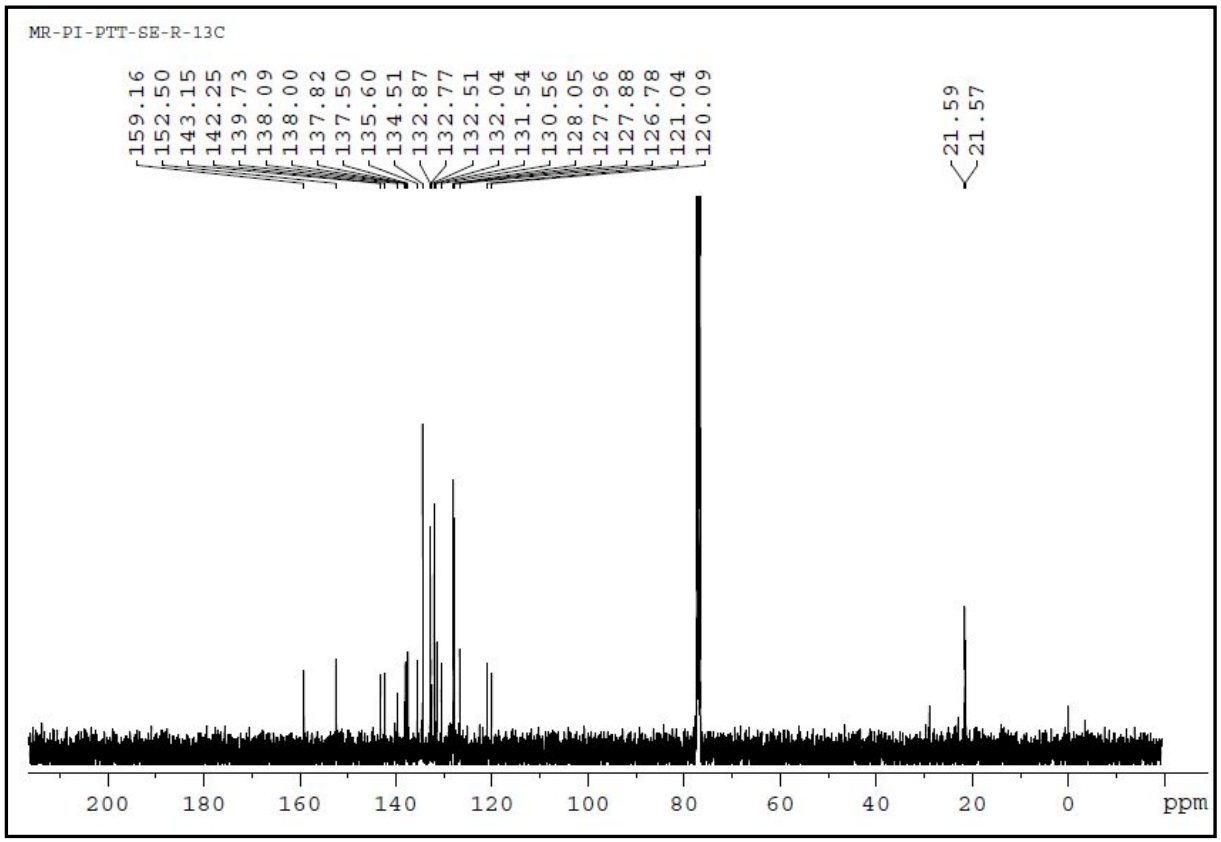


Figure S20. $^{13}C\{^{1}H\}$NMR of compound **6** recorded in $CDCl_3$ at 25 °C (125 MHz)..

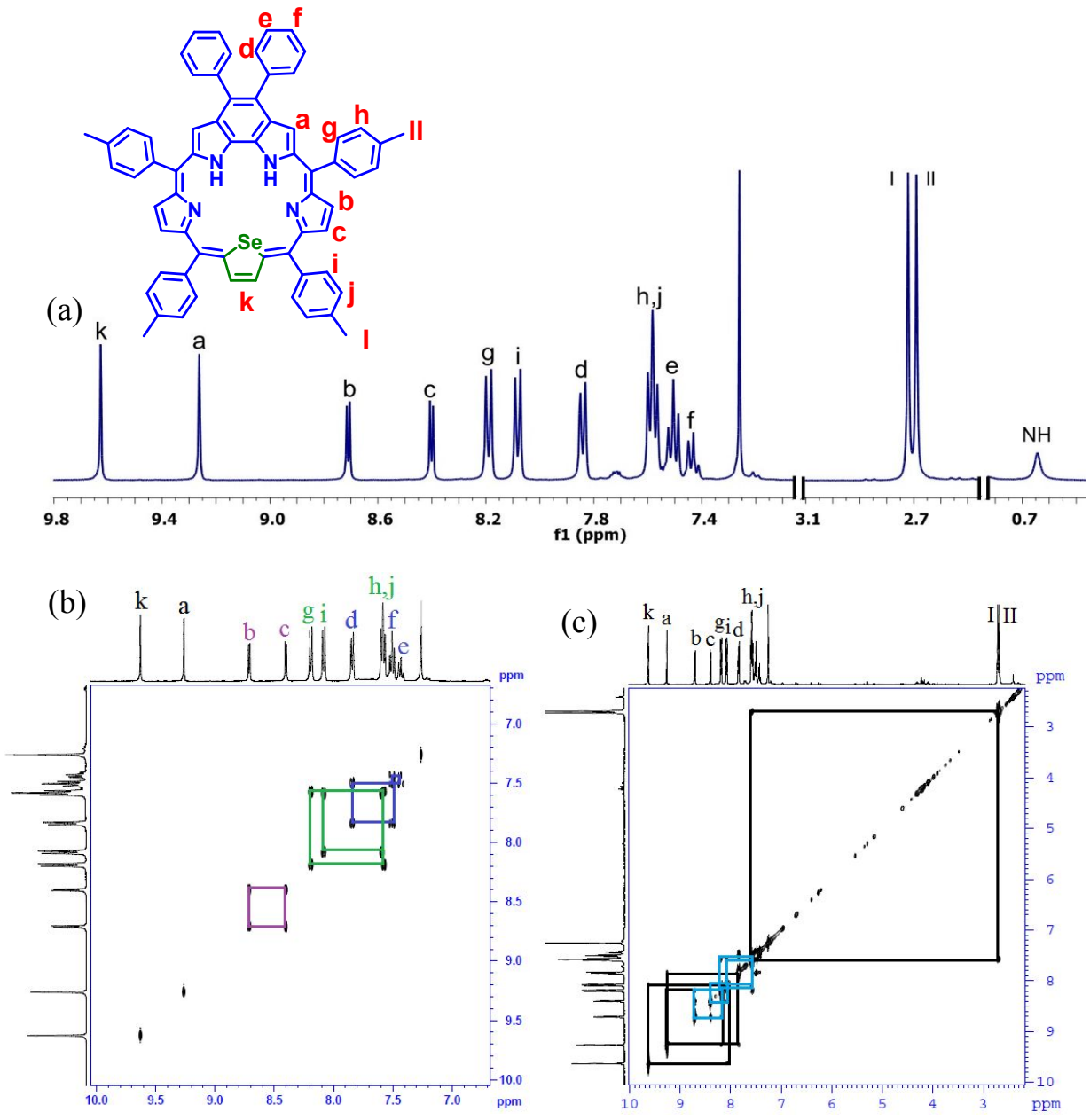
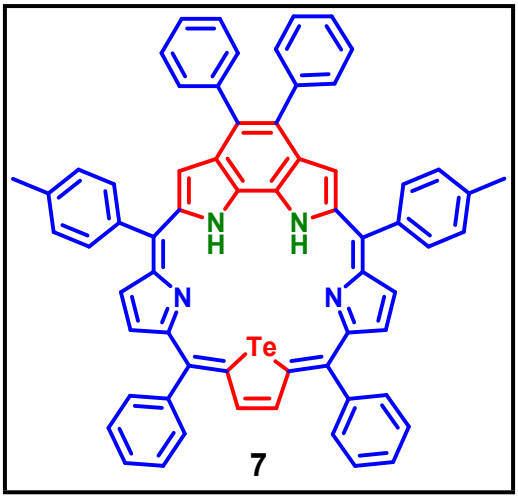


Figure S21:(a) Partial ^{1}H NMR, (b)^{1}H-^{1}H COSY and (c) ^{1}H-^{1}H NOESY NMRspectraof macrocycle **6** recorded in $CDCl_3$ at 25° C (500 MHz).



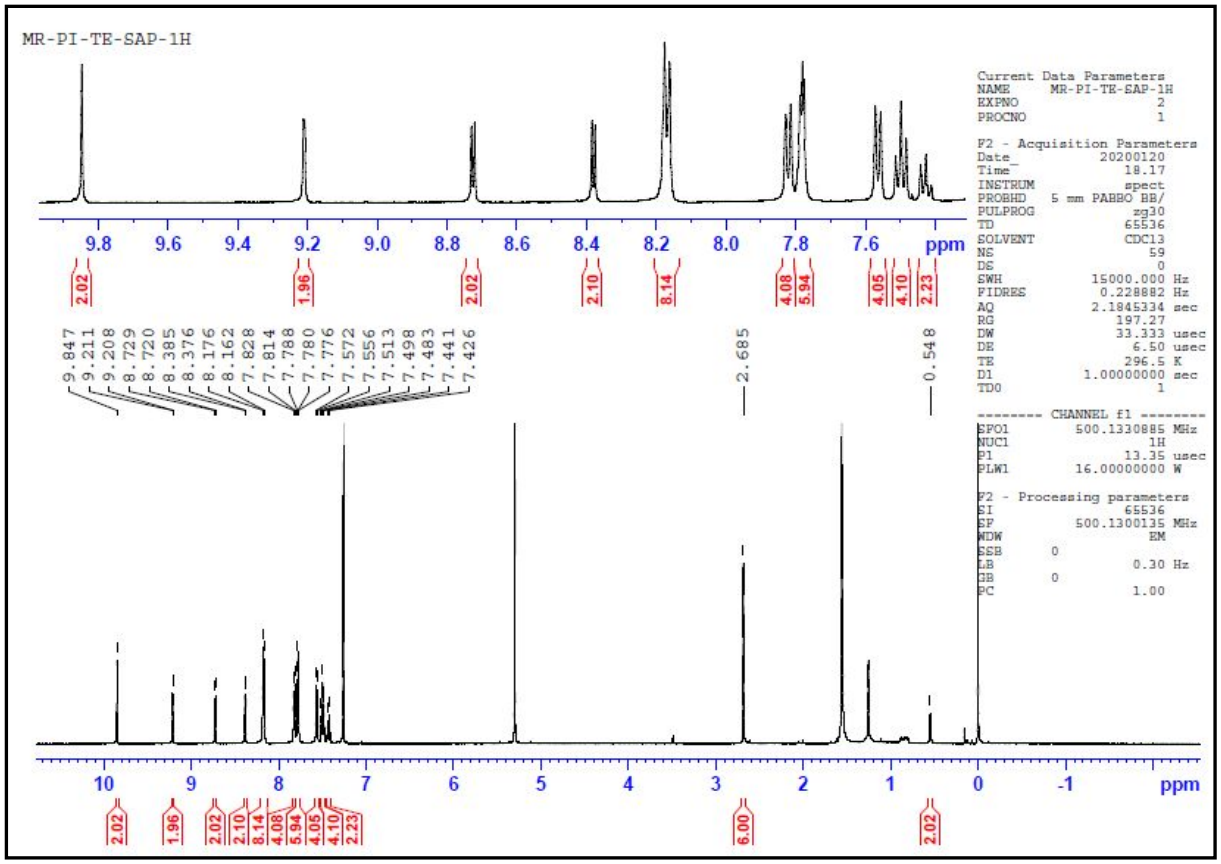
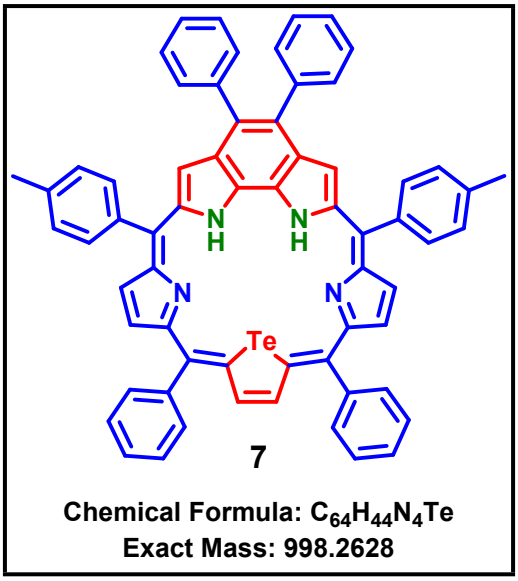


Figure S22. ^{1}H NMR of compound **7** recorded in $CDCl_3$at 25 °C (500 MHz).



7

Chemical Formula: $C_{64}H_{44}N_4Te$
Exact Mass: 998.2628

Observed Mass= 999.2708 $[M+H]^+$

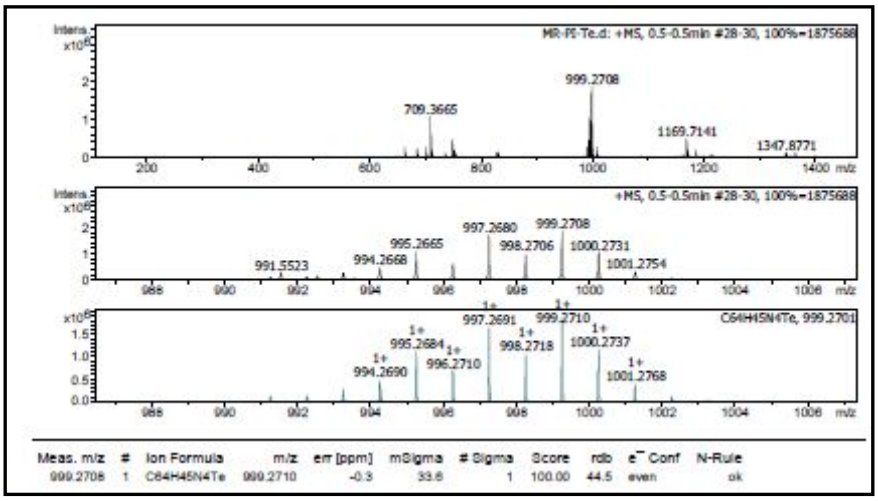
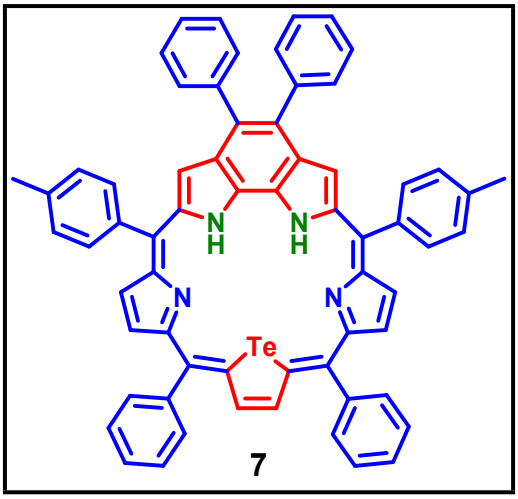


Figure S23. HRMS spectrum of compound **7.**



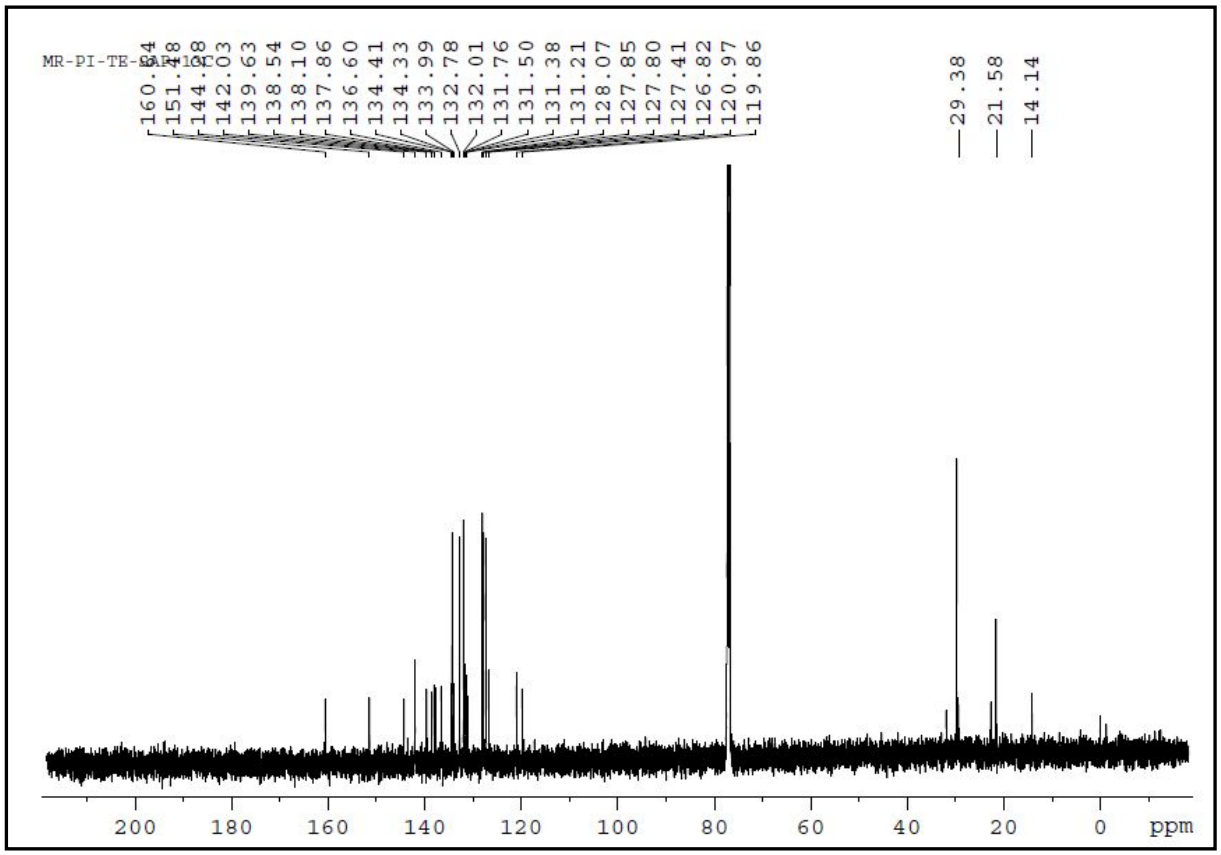


Figure S24. $^{13}C\{^{1}H\}$ NMR of compound **7** recorded in $CDCl_3$at 25 °C (125 MHz)..

Table S1. Table of free thermal energy in normal and inverted conformation of **2a** and **4-7**.

Compounds	Free Thermal Energy (a. u.)	Free Thermal Energy difference (Inverted-Normal) (a. u.)	Free Thermal Energy difference (Inverted-Normal) (kcal/mol)
Normal Benzosapphyrin	-2817.530400	-0.016162	-10.14181028
InvertedBenzosapphyrin	**-2817.546562**		
Normal Oxabenzosapphyrin	-2837.386498	-0.021581	-13.54228485
InvertedOxabenzosapphyrin	**-2837.408079**		
Normal Thiabenzosaphyrin	-3160.389176	0.000922	0.5785638586
Inverted Thiabenzosaphyrin	-3160.308314		
Normal Selenabenzosapphyrin	**-5161.592034**	0.007067	4.4346104
InvertedSelenabenzosapphyrin	-5161.584967		
Normal Tellurabenzosapphyrin	**-2691.595374**	0.013304	8.348387825
InvertedTellurabenzosapphyrin	-2691.582070		

Figure S25: Cartesian coordinates of the S0 optimized structures of the compounds inverted benzosaphyrin (**4**). # Sum of imaginary frequencies= 0;

Thermal free Energy (hartree) = **-2817.546562.**

Atoms	X	Y	Z
N	-0.82782200	1.64534900	-0.15040600
H	0.18816400	1.53921200	-0.18949900
N	1.53374800	2.98596100	-0.29269600
N	-0.85440300	-1.64743900	-0.11239700
H	0.16163900	-1.55936000	-0.18230300
N	1.46942400	-3.02446400	-0.39129900
C	-1.35019600	5.41953700	-0.10290600
C	0.78676900	4.13682700	-0.26153400
C	2.82549500	3.35967400	-0.40526500
C	5.26487300	2.74982400	-0.09805000
C	3.56391500	1.11106300	-0.94189000
C	2.41502500	-0.69573200	-1.71223100
H	1.71216400	-1.34356800	-2.21123700
C	1.66345100	5.29742900	-0.36482000
H	1.34871700	6.33133400	-0.40234600
C	7.92042600	3.41234000	0.69979500
C	-0.61303900	4.12635800	-0.15839200
C	5.51030200	3.58379100	1.01035300
H	4.66994300	3.96637300	1.58118300
C	2.42771200	0.67257800	-1.69817100
H	1.73840200	1.34247500	-2.18732800
C	-1.37580400	2.92068400	-0.10258100
C	-1.82476300	0.70703200	-0.05105000
C	5.20635200	-2.82674100	-0.10009800
C	6.38589100	2.25533600	-0.79592100
H	6.23321900	1.63342000	-1.67353600
C	6.80890000	3.90902900	1.39313500
H	6.96240700	4.55451000	2.25537700
C	-3.07342900	1.40485500	0.06192600
C	1.58456600	-5.33235200	-0.24672200
H	1.26631100	-6.36164300	-0.15505600
C	0.71362500	-4.16333600	-0.27887000
C	-1.08519200	6.35836100	0.90641200
H	-0.34937700	6.12258700	1.66966000
C	2.93553000	4.81353100	-0.42863900
H	3.85270300	5.37670600	-0.54053700
C	-2.32579500	5.74487500	-1.06151900
H	-2.54253700	5.04057800	-1.85935400
C	6.33593200	-2.38509800	-0.81782200
H	6.19407400	-1.80157300	-1.72328200
C	-1.83787100	-0.69189300	-0.05914800
C	3.89016400	2.40778500	-0.51533200
C	5.43550600	-3.60984000	1.04804700
H	4.58801200	-3.94963200	1.63523700
C	7.68058900	2.58088500	-0.40346300
H	8.52258900	2.19331500	-0.97324900
C	-2.77243500	2.77364600	0.03182000
H	-3.47766100	3.58690600	0.09953900
C	3.83896400	-2.47402800	-0.53942600
C	-5.61058800	-1.46791600	0.19846200

Atoms	X	Y	Z
C	3.54117700	-1.16946700	-0.96243700
C	-1.76857900	7.57312300	0.95329500
H	-1.54952500	8.27680000	1.75347100
C	2.76216900	-3.41118000	-0.43294200
C	2.86059100	-4.86305300	-0.33510600
H	3.77564000	-5.43970500	-0.36122700
C	-1.43627400	-5.41109800	-0.03009500
C	-1.42487400	-2.91284000	-0.07637500
C	-0.68247900	-4.13108900	-0.13277300
C	7.62497200	-2.71460600	-0.40833400
H	8.47424200	-2.36917400	-0.99413300
C	-5.58176400	1.55073400	0.21592800
C	-2.82341900	-2.74183000	-0.00249400
H	-3.54444600	-3.54341600	0.02969800
C	-4.34318700	0.72115500	0.14387200
C	-3.00263800	6.96057700	-1.01033900
H	-3.74891700	7.18642100	-1.76915500
C	-7.72059700	2.24877800	-0.71208500
H	-8.47752500	2.15838300	-1.48701500
C	-4.35821500	-0.66156000	0.10458400
C	-2.73683900	7.89928100	-0.00345100
C	-3.10189600	-1.36789300	0.00998700
C	-6.57669500	1.45383600	-0.76992500
H	-6.44753800	0.74954200	-1.58608800
C	-5.76579700	2.47387700	1.25878400
H	-5.00725100	2.55969100	2.03214700
C	7.84873800	-3.49654800	0.73311000
C	-1.35490200	-6.37692500	-1.04655200
H	-0.75182600	-6.17144900	-1.92625900
C	6.72772300	-3.93905600	1.44829100
H	6.86889400	-4.54467000	2.34107800
C	-2.05453300	-7.57878500	-0.95163300
H	-1.98103300	-8.30286400	-1.76027900
C	9.32770300	3.73901800	1.13932900
H	9.37181700	4.70009400	1.66241700
H	10.01377800	3.78555200	0.28657500
H	9.71781500	2.97650600	1.82731900
C	-5.95032900	-2.37953600	-0.81509400
H	-5.30290400	-2.47494200	-1.68258300
C	-2.24581400	-5.69741100	1.08234500
H	-2.31911500	-4.97197500	1.88729900
C	-6.46417300	-1.35774900	1.30749400
H	-6.21339100	-0.66156800	2.10204800
C	-2.85745600	-7.86632600	0.15900300
C	-6.91152800	3.26821300	1.31852300
H	-7.03663200	3.97111900	2.13826300
C	-7.11052500	-3.14954600	-0.72689800
H	-7.35775000	-3.84367300	-1.52613300
C	-7.89325500	3.15915500	0.33235500
H	-8.78530100	3.77846100	0.37712200

Atoms	X	Y	Z
C	-2.94054100	-6.90135100	1.17194200
H	-3.55652800	-7.09606600	2.04730600
C	-7.95114900	-3.02730100	0.38063700
H	-8.85452200	-3.62747500	0.45122800
C	9.24890100	-3.82843300	1.19138000
H	9.95135300	-3.84937100	0.35136900
H	9.28781800	-4.80293200	1.68994700
H	9.62112400	-3.08335200	1.90777000
C	-7.62238500	-2.12880100	1.39758900
H	-8.26830300	-2.02839100	2.26609400

Atoms	X	Y	Z
C	-3.59205200	-9.18134400	0.27442600
H	-3.76858300	-9.62933200	-0.70904900
H	-3.01809000	-9.90784400	0.86545400
H	-4.56166200	-9.05758700	0.76916800
C	-3.45986900	9.22518900	0.03201100
H	-3.36041200	9.70968300	1.00878000
H	-3.05943000	9.91790900	-0.72024400
H	-4.52879600	9.10550800	-0.17856500
H	5.02202600	-0.05263800	0.05341900
N	4.26700800	-0.03871000	-0.61851700

Figure S26: Cartesian coordinates of the S0 optimized structures of the compounds normalbenzosaphyrin. # Sum of imaginary frequencies= 0;# Thermal Free Energy (hartree) = **-2817.530400**.

Atoms	X	Y	Z
C	-4.18834800	-1.14893600	0.25522200
C	-5.42336500	-0.68528800	0.82919400
C	-5.42146000	0.67275200	0.84740000
C	-4.18636900	1.14792900	0.28288200
C	-0.69949300	3.93627000	-0.45657300
C	-1.54361000	5.05584600	-0.83433700
C	-2.82196500	4.61889800	-0.73794700
C	-2.75903000	3.22411300	-0.30088600
N	-1.47207400	2.81748600	-0.18328000
C	-3.94996800	2.50890500	0.03614000
C	1.96727200	0.69238500	0.12733300
C	3.21172500	1.39254600	0.20935000
C	2.90104700	2.75541400	0.07686900
C	1.50502300	2.86761400	-0.10958500
N	0.96459800	1.59840200	-0.05403700
C	1.96302500	-0.69259600	0.15436800
C	3.20343200	-1.39460000	0.26621400
C	2.89565800	-2.75634900	0.11760500
C	1.50164500	-2.86835800	-0.08321200
N	0.96108300	-1.59897500	-0.03135400
C	-0.69753600	-3.93196900	-0.47480700
C	-1.53660300	-5.04491600	-0.88244400
C	-2.81568300	-4.60591600	-0.80616900
C	-2.75823900	-3.21726800	-0.34915600
N	-1.47284500	-2.81507200	-0.20257200
C	-3.95258300	-2.50512600	-0.01844000
C	0.69927000	4.00824100	-0.35633500
C	0.69927700	-4.00708300	-0.35038700
C	4.46107200	-0.69511100	0.41440700
C	4.46523400	0.69113500	0.38153100
C	1.38801100	5.31906400	-0.51610300
C	1.38834800	-5.31770800	-0.50950600
C	5.70480600	1.50589500	0.54586500
C	5.70085600	-1.51570000	0.53696200
C	-5.17190600	3.37748400	0.18724200

Atoms	X	Y	Z
C	-5.18024700	-3.37091500	0.09716100
C	-5.26675200	4.31565500	1.22669500
C	-6.39719000	5.11828100	1.36703700
C	-7.46914500	5.02547900	0.46874000
C	-7.37289900	4.09092700	-0.56968400
C	-6.24737400	3.27911700	-0.70746800
C	-6.24138800	-3.24776900	-0.81139600
C	-7.37087600	-4.05975700	-0.71126500
C	-7.48757900	-5.01602000	0.30489000
C	-6.42700500	-5.13829500	1.21329300
C	-5.29291800	-4.33536200	1.11065400
C	2.37309500	5.50550200	-1.50077400
C	3.01328400	6.73314200	-1.65024500
C	2.70508400	7.81933600	-0.82022100
C	1.72394000	7.63296600	0.16140400
C	1.07625700	6.40846800	0.31315200
C	1.05632800	-6.41429200	0.30318900
C	1.70898100	-7.63665400	0.15911100
C	2.71286100	-7.81562600	-0.80136200
C	3.04555600	-6.72112900	-1.61002700
C	2.39968900	-5.49511300	-1.46849600
C	6.76188600	-1.37492200	-0.37180100
C	7.90491700	-2.16521500	-0.26390600
C	8.01123200	-3.11457200	0.75411000
C	6.96331800	-3.26829400	1.66271400
C	5.81821500	-2.47922200	1.55279700
C	6.10329400	2.41497000	-0.44796800
C	7.24977200	3.19363000	-0.28777900
C	8.01681100	3.08277500	0.87261700
C	7.62913300	2.18627500	1.87003800
C	6.48517000	1.40644400	1.70842700
C	-8.67595000	5.92353600	0.60271300
C	-8.72468600	-5.87243400	0.43472400
C	3.42614300	9.13806000	-0.96461800
C	3.39581700	-9.15083600	-0.97686300

Atoms	X	Y	Z
H	8.90247900	-3.72976300	0.83774300
H	7.03626400	-4.00200500	2.46057100
H	8.71298800	-2.04116800	-0.97928900
H	6.68453800	-0.64153600	-1.16762600
H	5.00781600	-2.59992600	2.26556100
H	8.21741800	2.09485200	2.77866300
H	6.18741100	0.71217600	2.48752300
H	8.90849000	3.68990500	0.99905400
H	7.54458800	3.88509500	-1.07220000
H	5.51478800	2.49986400	-1.35676800
H	3.58851700	-3.58240400	0.13333800
H	3.59035300	3.58418800	0.10278900
H	2.61911900	4.68460000	-2.16704300
H	3.76044900	6.85228000	-2.43122700
H	1.46474200	8.45728900	0.82125100
H	0.32616400	6.28631700	1.08809800
H	4.37383400	9.13424000	-0.41154100
H	2.82666600	9.96680700	-0.57699100
H	-9.56040700	5.47843800	0.13771400
H	-8.91016300	6.12602700	1.65240100
H	-6.44915300	5.82780600	2.18941600
H	-4.44802300	4.40621300	1.93419300
H	-6.19663200	2.56005000	-1.51968900
H	-8.18975800	3.99654600	-1.28106300
H	-1.19703000	6.02985600	-1.14601700

Atoms	X	Y	Z
H	-3.72379100	5.17039900	-0.95504600
H	-6.19261400	1.31675600	1.23728200
H	-6.19608300	-1.33743900	1.20214100
H	-6.17306000	-2.51448500	-1.60953000
H	-4.48174700	-4.45156800	1.82307400
H	-6.48959100	-5.87367000	2.01192900
H	-8.17325600	-3.95031700	-1.43686900
H	-9.42347100	-5.45198500	1.16886300
H	-8.47808500	-6.88520900	0.76840300
H	-3.71423400	-5.15235100	-1.04827400
H	-1.18612100	-6.01581500	-1.19944400
H	2.66990800	-4.66651300	-2.11542600
H	0.29167500	-6.29644700	1.06449400
H	1.43838100	-8.46420200	0.81038400
H	3.81998100	-6.83012000	-2.36529000
H	3.43788000	-9.70618600	-0.03515000
H	-0.05243600	1.48880000	-0.06470600
H	-0.05523200	-1.48768600	-0.06435300
H	-8.50513600	6.89256100	0.11707400
H	-9.25916400	-5.95009400	-0.51639800
H	3.66420000	9.35192800	-2.01117700
H	2.85986500	-9.77838200	-1.70014200
H	4.41863600	-9.03203400	-1.34655600
N	-3.43824700	0.00198000	0.00536500
H	-2.54746300	0.00734000	-0.46674000

Figure S27: Cartesian coordinates of the S0 optimized structures of the compounds normaloxabenzosaphyrin. #Sum of imaginary frequencies= 0; #Thermal Free Energy (hartree) = **-2837.386498**.

Atoms	X	Y	Z
C	-4.19384300	-1.11690000	0.29126400
C	-5.38231700	-0.67617500	0.94781400
C	-5.37742500	0.68227000	0.96343700
C	-4.18701300	1.12932500	0.31437100
C	-0.69810400	3.91782400	-0.55195500
C	-1.55515000	4.99326500	-1.01891700
C	-2.82623400	4.53273800	-0.91812700
C	-2.73975100	3.17083100	-0.38621200
N	-1.45477100	2.80534600	-0.21785000
C	-3.92460600	2.46412800	0.01547800
C	1.94802200	0.69009900	0.13742200
C	3.19052500	1.38736200	0.24926800
C	2.88394300	2.75025600	0.09485500
C	1.49425300	2.85954800	-0.13281400
N	0.95145600	1.59138200	-0.07794000
C	1.94039600	-0.69705200	0.16303400
C	3.17534700	-1.40121000	0.30349400
C	2.86712000	-2.76141500	0.13034100
C	1.47950200	-2.86492800	-0.11182000
N	0.94141400	-1.59454500	-0.05905300
C	-0.71078700	-3.90981800	-0.57230200
C	-1.56613000	-4.97480800	-1.06585400

Atoms	X	Y	Z
C	-2.83632600	-4.50878900	-0.97891900
C	-2.75101600	-3.15448200	-0.42801800
N	-1.46682600	-2.79769900	-0.23619700
C	-3.93684800	-2.44770300	-0.02998200
C	0.69644700	3.99792500	-0.42911700
C	0.68152300	-3.99796700	-0.42889600
C	4.42921100	-0.70380600	0.49109600
C	4.43680400	0.68295800	0.45975800
C	1.38507900	5.30158800	-0.62526500
C	1.36652700	-5.30295700	-0.62786700
C	5.67170900	1.49564600	0.66466600
C	5.66288200	-1.52672100	0.65240400
C	-5.12368000	3.35757300	0.21040200
C	-5.14412800	-3.33552700	0.13703600
C	-5.13288100	4.34177300	1.21068500
C	-6.23934100	5.16941100	1.39065400
C	-7.37025800	5.05768100	0.57029800
C	-7.35825700	4.07838700	-0.43105900
C	-6.25766800	3.24050600	-0.60690000
C	-6.26731100	-3.19638800	-0.69118500
C	-7.37447500	-4.03180500	-0.54489600
C	-7.40580500	-5.02687400	0.43986800

Atoms	X	Y	Z
C	-6.28225200	-5.16561700	1.26685300
C	-5.16973200	-4.34082400	1.11634400
C	2.41876200	5.44473000	-1.56650100
C	3.05498000	6.66982900	-1.75030400
C	2.69499900	7.79596300	-0.99842100
C	1.66460500	7.65300500	-0.06036100
C	1.01979500	6.43216100	0.12440800
C	0.97986700	-6.43979800	0.10030800
C	1.62562000	-7.66135700	-0.08193500
C	2.67491900	-7.79864300	-0.99849500
C	3.06137900	-6.66351700	-1.72474800
C	2.42447100	-5.43918100	-1.54414000
C	6.75752400	-1.38141200	-0.21499800
C	7.89514400	-2.17341200	-0.06901900
C	7.96251500	-3.12934100	0.94620200
C	6.88079800	-3.28823000	1.81335800
C	5.74131300	-2.49732000	1.66538600
C	6.10358300	2.40586700	-0.31408000
C	7.24437400	3.18391800	-0.11466700
C	7.97227500	3.07132100	1.07049300
C	7.55131700	2.17345200	2.05310700
C	6.41306500	1.39439000	1.85239500
C	-8.55139100	5.98271600	0.74308900
C	-8.61836600	-5.90819800	0.62224800
C	3.41160200	9.11298000	-1.17555100
C	3.35563100	-9.12847300	-1.21739100
H	8.84967700	-3.74571900	1.05943500
H	6.92304800	-4.02719500	2.60859700
H	8.72966300	-2.04557400	-0.75268300
H	6.71079100	-0.64300100	-1.00849700
H	4.90465700	-2.62160000	2.34646900
H	8.10904000	2.08047800	2.98067100
H	6.08918800	0.69925600	2.62022800
H	8.85938300	3.67805000	1.22740900
H	7.56543500	3.87627700	-0.88794100
H	5.54599100	2.49191900	-1.24208200
H	3.55636800	-3.59031400	0.15714800
H	3.57234700	3.57938800	0.13285200

Atoms	X	Y	Z
H	2.70522400	4.59205700	-2.17384500
H	3.84045400	6.75487700	-2.49728400
H	1.36415300	8.50942100	0.53832600
H	0.23139100	6.34363600	0.86492600
H	4.28259500	9.18232000	-0.51169300
H	2.75841100	9.95911700	-0.94251300
H	-9.48185600	5.51144600	0.41288500
H	-8.67514500	6.28312600	1.78792900
H	-6.22563400	5.91447000	2.18247400
H	-4.26653700	4.44844100	1.85640400
H	-6.27136400	2.48731700	-1.38910500
H	-8.22174300	3.96964100	-1.08283800
H	-1.22278400	5.95057200	-1.39252300
H	-3.73632500	5.04642200	-1.18897800
H	-6.11536700	1.33413600	1.40163800
H	-6.12472100	-1.33275400	1.37120300
H	-6.26464800	-2.43323600	-1.46381500
H	-4.30800000	-4.47078500	1.76393000
H	-6.27802500	-5.93209200	2.03816900
H	-8.22651700	-3.91049600	-1.20938600
H	-9.27353800	-5.52281600	1.41363900
H	-8.33498200	-6.92644300	0.90624600
H	-3.74479200	-5.01416300	-1.27020500
H	-1.23297700	-5.92901000	-1.44659200
H	2.73537200	-4.57906500	-2.12833400
H	0.17894900	-6.35513200	0.82773700
H	1.31238700	-8.52161700	0.50440000
H	3.87134100	-6.74010000	-2.44607200
H	3.17639400	-9.81201200	-0.38275200
H	-0.06699700	1.47586000	-0.11333800
H	-0.07539800	-1.47336600	-0.11342200
H	-8.42533400	6.90040500	0.15485000
H	-9.21329800	-5.96517100	-0.29384200
H	3.77484300	9.23658200	-2.20018100
H	2.98605400	-9.61757500	-2.12729300
H	4.43783500	-9.01043700	-1.33276900
O	-3.43803900	0.00730100	-0.02862800

Figure S28: Cartesian coordinates of the S0 optimized structures of the compounds invertedselenabenzosaphyrin. #Sum of imaginary frequencies= 0; #Thermal free Energy (hartree) =**-5161.584967**.

Atoms	X	Y	Z
N	-1.06331200	1.65796400	-0.08564800
H	-0.04792400	1.56129000	-0.09895200
N	1.29977200	3.08484800	-0.22655800
N	-1.09243500	-1.65688600	-0.05330100
H	-0.07610100	-1.57829200	-0.09093200
N	1.23334200	-3.11652400	-0.32382800
C	-1.67083600	5.42102300	-0.16053200
C	0.50150400	4.20439500	-0.26039300

Atoms	X	Y	Z
C	2.56966100	3.51721700	-0.35388100
C	5.04537100	3.19185200	-0.02193800
C	3.55536100	1.29196500	-0.67391100
C	2.41899000	-0.69794000	-1.30908400
H	1.62437200	-1.27944900	-1.75566100
C	1.31965000	5.39750100	-0.42966200
H	0.95451300	6.41002600	-0.52339100
C	7.60318100	4.24238500	0.64292200

Atoms	X	Y	Z
C	-0.89412100	4.14850900	-0.16186800
C	5.21476700	4.05262100	1.07653900
H	4.35519900	4.30886900	1.68742300
C	2.43426800	0.66999000	-1.29601700
H	1.65306100	1.27557800	-1.73448300
C	-1.62721600	2.92787700	-0.06607900
C	-2.05522500	0.71059700	0.01685100
C	4.98157900	-3.26577900	-0.02844300
C	6.18492000	2.87133400	-0.78297900
H	6.07951800	2.21960100	-1.64481100
C	6.46909900	4.56495300	1.39906500
H	6.56980500	5.22353600	2.25830600
C	-3.30957700	1.40230500	0.11149600
C	1.23496800	-5.43729000	-0.30191400
H	0.86486400	-6.45154900	-0.26519300
C	0.42465100	-4.22727500	-0.27289000
C	-1.45609400	6.39304700	0.82840800
H	-0.72976700	6.20068400	1.61184600
C	2.61121800	4.97070000	-0.46839800
H	3.50193700	5.56667200	-0.60810500
C	-2.63195800	5.69045100	-1.14985000
H	-2.80981800	4.95874400	-1.93166900
C	6.11921300	-3.00033100	-0.81252800
H	6.01627100	-2.38912900	-1.70395700
C	-2.06935700	-0.69112300	0.00543700
C	3.71219200	2.64258700	-0.37699500
C	5.14690300	-4.07017400	1.11204700
H	4.28856100	-4.28138800	1.74163600
C	7.43464000	3.38835700	-0.45567300
H	8.29405500	3.13295900	-1.07077400
C	-3.02009900	2.77198100	0.06295200
H	-3.73270000	3.57901800	0.10954000
C	3.65516500	-2.70792000	-0.40314900
C	-5.85003700	-1.46314700	0.21938500
C	3.52520200	-1.35378600	-0.69602100
C	-2.17673900	7.58668300	0.82759500
H	-1.99708000	8.31696900	1.61264200
C	2.50249800	-3.56737800	-0.37851000
C	2.53044400	-5.02609700	-0.36537800
H	3.41753200	-5.64110700	-0.41601600
C	-1.76334100	-5.40831200	-0.08411200
C	-1.67926800	-2.91589000	-0.04681100
C	-0.96680700	-4.14925200	-0.13608100
C	7.36413800	-3.51921700	-0.46879500
H	8.22251600	-3.30780900	-1.10178700
C	-5.81805000	1.55598600	0.25128900
C	-3.07361500	-2.73427400	0.01925100
H	-3.80163700	-3.52881500	0.02924200
C	-4.58080500	0.72419400	0.18508000
C	-3.34488600	6.88617600	-1.14709500
H	-4.07843300	7.06939500	-1.92849700
C	-7.95046800	2.25792900	-0.68655500

Atoms	X	Y	Z
H	-8.70290500	2.17054400	-1.46523400
C	-4.59648800	-0.65699300	0.14054300
C	-3.13148600	7.85788200	-0.15936700
C	-3.33947800	-1.35930800	0.05261700
C	-6.80730600	1.46213500	-0.74031200
H	-6.67439100	0.75984300	-1.55678500
C	-6.00661300	2.47633400	1.29558400
H	-5.25254400	2.55936100	2.07275200
C	7.52860500	-4.31848300	0.67056500
C	-1.73859900	-6.31941900	-1.15164100
H	-1.14733900	-6.08851200	-2.03229800
C	6.39626000	-4.58432500	1.45107600
H	6.49456100	-5.19926800	2.34233700
C	-2.47787200	-7.50003500	-1.10214200
H	-2.44848500	-8.18224700	-1.94821200
C	8.96666300	4.77366600	1.01371700
H	8.89521600	5.73143200	1.53747400
H	9.59502800	4.91585200	0.12920000
H	9.49497800	4.07797000	1.67789200
C	-6.18914700	-2.36004300	-0.80710900
H	-5.53997700	-2.44586400	-1.67353100
C	-2.55577000	-5.72423400	1.03191500
H	-2.58553800	-5.03953600	1.87374600
C	-6.70653500	-1.36370000	1.32689900
H	-6.45620400	-0.67812900	2.13001200
C	-3.26394000	-7.81857500	0.01192800
C	-7.15171600	3.27140600	1.35080900
H	-7.28094800	3.97193600	2.17102700
C	-7.35175300	-3.12737500	-0.73201600
H	-7.59886200	-3.81001900	-1.54019200
C	-8.12778700	3.16559500	0.35909500
H	-9.01894700	3.78518600	0.40052200
C	-3.28969400	-6.90693300	1.07600900
H	-3.89137200	-7.12689100	1.95450900
C	-8.19516000	-3.01639700	0.37422700
H	-9.10006200	-3.61414600	0.43430200
C	8.88690600	-4.85141700	1.05816600
H	9.50814700	-5.04236500	0.17784700
H	8.80516600	-5.78335200	1.62528400
H	9.42842000	-4.13388900	1.68754400
C	-7.86723200	-2.13198700	1.40333000
H	-8.51557900	-2.04064900	2.27016700
C	-4.04066700	-9.11185700	0.07751300
H	-4.24617500	-9.50635400	-0.92173500
H	-3.48257700	-9.88211800	0.62451500
H	-4.99681000	-8.97917900	0.59313900
C	-3.89337000	9.16146800	-0.17663000
H	-3.84448200	9.66645800	0.79215900
H	-3.48467100	9.84976800	-0.92685700
H	-4.94824000	9.00540900	-0.42455000
Se	4.81679000	-0.04946800	-0.17886500

Figure S29: Cartesian coordinates of the S0 optimized structures of the compounds normalselenabenzosaphyrin**6**. #Sum of imaginary frequencies= 0; #Thermal Free Energy (hartree) = **-5161.592034**.

Atoms	X	Y	Z
C	3.96792100	1.32965500	0.07390600
C	5.22497400	0.67694800	0.26440300
C	5.22343600	-0.68500800	0.27377800
C	3.96494800	-1.33737300	0.09145300
C	0.55679900	-4.11626500	-0.17126100
C	1.35325600	-5.32448800	-0.31793700
C	2.64976000	-4.93329500	-0.26386900
C	2.63792900	-3.48343800	-0.09147800
N	1.37603100	-3.00690900	-0.05553700
C	3.83996700	-2.71872700	0.02774300
C	-2.04530500	-0.69500700	-0.03961100
C	-3.30083000	-1.38244300	0.02708800
C	-3.00288800	-2.75107900	0.00063200
C	-1.60419900	-2.89420900	-0.10157400
N	-1.04692000	-1.62751400	-0.12149200
C	-2.04186500	0.69713800	-0.01685300
C	-3.29365300	1.38759500	0.07775700
C	-2.99479800	2.75520200	0.02641200
C	-1.59717400	2.89543600	-0.09196500
N	-1.04240800	1.62760800	-0.11020900
C	0.56467600	4.11274100	-0.20051900
C	1.36250200	5.31698000	-0.37081100
C	2.65861600	4.92356100	-0.32287000
C	2.64508100	3.47623800	-0.13059900
N	1.38254900	3.00311400	-0.07807000
C	3.84605300	2.71036600	-0.00753900
C	-0.84252000	-4.09094700	-0.16015400
C	-0.83456300	4.09050100	-0.17312200
C	-4.55860500	0.69589800	0.16210200
C	-4.56247300	-0.68730500	0.12968400
C	-1.59927500	-5.37554900	-0.20119900
C	-1.58891600	5.37621700	-0.22135000
C	-5.80712800	-1.50377600	0.23371000
C	-5.80219800	1.51763600	0.23055100
C	5.11398800	-3.51809800	0.09229000
C	5.12233800	3.50705000	0.04172300
C	5.47675300	-4.19948500	1.26271600
C	6.65238300	-4.94658500	1.31912800
C	7.50283100	-5.04592800	0.20993100
C	7.13825700	-4.36317600	-0.95711800
C	5.96496800	-3.61131000	-1.01722500
C	5.96942400	3.58302100	-1.07299500
C	7.14035400	4.33845200	-1.03052700
C	7.51018300	5.03855500	0.12545500
C	6.66116700	4.96181200	1.23658600
C	5.48659100	4.21073700	1.19760800
C	-2.49269600	-5.65779800	-1.24698000
C	-3.19508100	-6.86044900	-1.28270500
C	-3.04231600	-7.82122500	-0.27475100

Atoms	X	Y	Z
C	-2.15071900	-7.53827800	0.76793700
C	-1.44113700	-6.33994500	0.80683800
C	-1.41335500	6.35400600	0.77076800
C	-2.12548900	7.55090800	0.72964600
C	-3.03365800	7.82084800	-0.30205300
C	-3.20964900	6.84333800	-1.29008100
C	-2.50459800	5.64243900	-1.25229500
C	-6.80215300	1.40148500	-0.74792500
C	-7.95020800	2.19005800	-0.69322000
C	-8.12203400	3.11262900	0.34027600
C	-7.13547500	3.24052100	1.31888800
C	-5.98534800	2.45287200	1.26260600
C	-6.14581800	-2.42213600	-0.77374600
C	-7.29923800	-3.20045400	-0.67460600
C	-8.13312700	-3.08008300	0.43778400
C	-7.80502300	-2.17491200	1.44864200
C	-6.65402600	-1.39511900	1.34780700
C	8.75836400	-5.88382900	0.26503000
C	8.79572400	5.82977400	0.17775900
C	-3.83289800	-9.10742900	-0.29699500
C	-3.77948900	9.13243100	-0.36150300
H	-9.01700800	3.72663000	0.38238500
H	-7.26037600	3.95262400	2.12975300
H	-8.71078000	2.08549900	-1.46180600
H	-6.67339600	0.68796700	-1.55527800
H	-5.22333900	2.55295000	2.02992300
H	-8.44544800	-2.07667300	2.32055000
H	-6.40310400	-0.69411400	2.13720300
H	-9.03055200	-3.68676600	0.51695900
H	-7.54708400	-3.89904000	-1.46887100
H	-5.50404700	-2.51501700	-1.64494300
H	-3.69730000	3.57136800	0.07099400
H	-3.70497100	-3.56682700	0.05994200
H	-2.62064000	-4.93437000	-2.04629000
H	-3.86968500	-7.05837300	-2.11207800
H	-2.01156500	-8.26489600	1.56470900
H	-0.76244200	-6.13992800	1.63002700
H	-4.77944000	-8.99953500	0.24747800
H	-3.28024700	-9.92594600	0.17383400
H	9.50200900	-5.53939300	-0.45949000
H	9.21534300	-5.85597100	1.25900800
H	6.91481300	-5.45893700	2.24165600
H	4.83325100	-4.13641200	2.13538100
H	5.70304700	-3.08975800	-1.93323900
H	7.78070900	-4.42001300	-1.83249200
H	0.96622800	-6.32243100	-0.46024700
H	3.53091900	-5.55117000	-0.34799200
H	6.12650600	-1.26395600	0.41365200
H	6.12930600	1.25577500	0.39646800

Atoms	X	Y	Z
H	5.70089200	3.05149000	-1.98132700
H	4.84165200	4.16935600	2.07048900
H	6.92134300	5.49814000	2.14592200
H	7.77544100	4.38791500	-1.91184700
H	9.64606200	5.18853200	0.44186100
H	8.74505800	6.62676300	0.92526000
H	3.54033200	5.53825200	-0.42305500
H	0.97658300	6.31386900	-0.52309500
H	-2.65541300	4.90409300	-2.03363900
H	-0.72458300	6.16257400	1.58763500
H	-1.97740300	8.28517900	1.51772400
H	-3.90791300	7.02442700	-2.10346200
H	-3.94527400	9.54442900	0.63834400
H	-0.03461400	-1.51048400	-0.11740500
H	-0.03046200	1.50840500	-0.12171800
H	8.54396600	-6.93547900	0.03693600
H	9.02449200	6.28660400	-0.79001500
H	-4.07939700	-9.40836900	-1.31949700
H	-3.21754200	9.88208600	-0.93275000
H	-4.75312100	9.01794700	-0.84714000
Se	2.60025100	-0.00325200	-0.05342600

Figure S30: Cartesian coordinates of the S0 optimized structures of the compounds invertedtellurabenzosaphyrin. #Sum of imaginary frequencies= 0; #Thermal free Energy (hartree) = **-2691.582070**.

Atoms	X	Y	Z
N	-0.98318300	1.65805100	-0.06682900
H	0.03242900	1.56589300	-0.06358400
N	1.38182600	3.11182400	-0.17627300
N	-1.00008200	-1.66008700	-0.03191400
H	0.01613100	-1.57778400	-0.04893800
N	1.34264300	-3.13238500	-0.25961500
C	-1.61841100	5.41649100	-0.14002100
C	0.56595500	4.22278600	-0.20827000
C	2.64392600	3.56763100	-0.26980500
C	5.11907300	3.35793500	0.08942700
C	3.75178300	1.37384300	-0.56373300
C	2.63278500	-0.69202000	-1.14291900
H	1.80930300	-1.25364200	-1.56671600
C	1.36759800	5.43080900	-0.34275000
H	0.98795300	6.43899800	-0.42506000
C	7.58079400	4.52874200	0.80257000
C	-0.82826800	4.15142800	-0.13527500
C	5.25122100	4.08589500	1.28536800
H	4.39227100	4.18448000	1.94185200
C	2.64244900	0.67642900	-1.13395500
H	1.82676000	1.25332400	-1.55259600
C	-1.55485100	2.92484200	-0.05753500
C	-1.97294300	0.70592700	0.01424000
C	5.08329400	-3.39440000	0.08484500
C	6.24382200	3.23688500	-0.74614600
H	6.15016800	2.70308900	-1.68701500
C	6.47060600	4.66214200	1.63930500
H	6.55485500	5.21213500	2.57236800
C	-3.23219900	1.39125800	0.08386900
C	1.32094500	-5.45562800	-0.19367100
H	0.94011100	-6.46529100	-0.14204700
C	0.52214600	-4.23835000	-0.20437300
C	-1.44560400	6.37578600	0.87076300
H	-0.74141100	6.17942000	1.67346500
C	2.66565200	5.02402200	-0.36085700
H	3.55071800	5.63538800	-0.46640900
C	-2.55151200	5.68901100	-1.15388000
H	-2.69832400	4.96644500	-1.95077700
C	6.19547300	-3.32090000	-0.77228800
H	6.09151000	-2.82610800	-1.73327100
C	-1.98136300	-0.69701500	0.00355700
C	3.81941500	2.72883600	-0.28346000
C	5.22850400	-4.06631700	1.31141400
H	4.37951100	-4.12693700	1.98529000
C	7.46254700	3.81680200	-0.39259600
H	8.31694200	3.71966700	-1.05646700
C	-2.94803000	2.76325500	0.04272200
H	-3.66501400	3.56715900	0.07550800
C	3.78491200	-2.76584800	-0.30001900
C	-5.76290600	-1.48357200	0.13827700
C	3.73201300	-1.40995600	-0.57946300
C	-2.18020500	7.56031400	0.86592700
H	-2.03417300	8.28012700	1.66782800
C	2.60535200	-3.59730300	-0.27965000
C	2.62057800	-5.05641300	-0.23753900
H	3.50373300	-5.67908200	-0.25170800
C	-1.67012900	-5.41180500	-0.05430600
C	-1.58479700	-2.92041600	-0.03406100
C	-0.86956400	-4.15450600	-0.09862700
C	7.41486700	-3.89575200	-0.41195900
H	8.25959800	-3.83594400	-1.09241400
C	-5.74323700	1.53658500	0.17379500
C	-2.97943700	-2.74361900	0.00074100
H	-3.70527500	-3.54028500	-0.00238100
C	-4.50198300	0.70941200	0.13129500
C	-3.27906200	6.87742700	-1.15513700
H	-3.99117200	7.06395400	-1.95535600
C	-7.86133100	2.23012100	-0.80326500

Atoms	X	Y	Z
H	-8.59916900	2.13966300	-1.59566400
C	-4.51146000	-0.67221300	0.08597400
C	-3.10763100	7.83587200	-0.14736700
C	-3.25016500	-1.36846400	0.02486300
C	-6.71401100	1.43851700	-0.83595700
H	-6.56357500	0.73634500	-1.64972700
C	-5.95460700	2.45642500	1.21462900
H	-5.21523400	2.54244600	2.00570600
C	7.54585000	-4.55395200	0.81217600
C	-1.62920600	-6.32723400	-1.11793800
H	-1.02154000	-6.10168400	-1.98895400
C	6.44846300	-4.63753400	1.67199100
H	6.54308600	-5.14449700	2.62814800
C	-2.37303400	-7.50570400	-1.07645600
H	-2.33115900	-8.19155700	-1.91921900
C	-6.07456200	-2.38472600	-0.89365600
H	-5.40533900	-2.46978200	-1.74498400
C	-2.48254600	-5.72041500	1.04956500
H	-2.52554600	-5.03162400	1.88769100
C	-6.64522200	-1.38496400	1.22589000
H	-6.41654000	-0.69610500	2.03285900
C	-3.17887400	-7.81752900	0.02577400
C	-7.10381800	3.24736400	1.24871300

Atoms	X	Y	Z
H	-7.25082500	3.94757600	2.06641400
C	-7.23539000	-3.15743900	-0.84309300
H	-7.46097400	-3.84328700	-1.65505100
C	-8.06138800	3.13754300	0.23902400
H	-8.95570500	3.75373000	0.26392400
C	-3.22026600	-6.90147400	1.08602000
H	-3.83747100	-7.11640800	1.95509500
C	-8.10460600	-3.04736200	0.24357300
H	-9.00812300	-3.64909100	0.28456900
C	-7.80423400	-2.15846500	1.27774500
H	-8.47280200	-2.06784200	2.12936800
C	-3.96018100	-9.10875500	0.08320300
H	-4.15799200	-9.50185400	-0.91830000
H	-3.40893900	-9.88121200	0.63426100
H	-4.92047600	-8.97381800	0.59064600
C	-3.87825500	9.13459300	-0.16707700
H	-4.05640300	9.51007100	0.84516300
H	-3.32798100	9.91353000	-0.71002500
H	-4.84739100	9.01785400	-0.66124000
Te	5.26656700	-0.03167500	-0.05716100
H	8.49522000	-5.00063900	1.09330900
H	8.52994700	4.97920600	1.07834300

Figure S31: Cartesian coordinates of the S0 optimized structures of the compounds normaltellurabenzosaphyrin**7**. #Sum of imaginary frequencies= 0; #Thermal free Energy (hartree) = **-2691.595374.**

Atoms	X	Y	Z
C	4.17908700	1.38475500	0.06811700
C	5.41342000	0.67007000	0.18458800
C	5.40957000	-0.69773900	0.19445400
C	4.17125000	-1.40704000	0.08774500
C	0.76286600	-4.13806400	-0.10093100
C	1.53899000	-5.36468200	-0.20282200
C	2.84375100	-4.99759000	-0.15518200
C	2.86072000	-3.54515600	-0.03056500
N	1.60762300	-3.04209300	-0.01282900
C	4.07582800	-2.78807000	0.04899400
C	-1.84000500	-0.69344100	-0.07696400
C	-3.09688700	-1.37932400	-0.01770700
C	-2.80152400	-2.75036600	-0.01896000
C	-1.40188200	-2.89863900	-0.09719500
N	-0.84471000	-1.63272400	-0.13324600
C	-1.83484900	0.70076200	-0.05587600
C	-3.08615100	1.39350800	0.03182200
C	-2.78480900	2.76285100	0.00464200
C	-1.38561000	2.90372500	-0.09170700
N	-0.83532200	1.63476200	-0.12515400
C	0.78485600	4.13188500	-0.13758100
C	1.56690300	5.35228100	-0.26562100
C	2.87001500	4.97857400	-0.22341900
C	2.88001700	3.52824800	-0.07608600

Atoms	X	Y	Z
N	1.62437100	3.03258900	-0.04113300
C	4.09138100	2.76560400	0.00883700
C	-0.63703900	-4.09665200	-0.11218200
C	-0.61543300	4.09801900	-0.13162900
C	-4.35268600	0.70265600	0.09690200
C	-4.35835100	-0.68118500	0.06454200
C	-1.40235800	-5.37793800	-0.13004700
C	-1.37396300	5.38307900	-0.15788900
C	-5.60574900	-1.49546800	0.15029200
C	-5.59653300	1.52530700	0.14929000
C	5.35259900	-3.58361100	0.08890800
C	5.37249300	3.55461500	0.03246000
C	5.74679300	-4.24226100	1.26331300
C	6.92888900	-4.98355800	1.30136100
C	7.73408900	-5.07941400	0.16458800
C	7.35115900	-4.42845000	-1.00966000
C	6.17004800	-3.68519300	-1.04668600
C	6.19109400	3.62759800	-1.10451900
C	7.37587400	4.36561000	-1.08269700
C	7.76153300	5.03955300	0.07759100
C	6.95538000	4.97203600	1.21576200
C	5.76956900	4.23620100	1.19281200
C	-2.26448500	-5.69131400	-1.19313800
C	-2.97560000	-6.88977200	-1.20756600

Atoms	X	Y	Z
C	-2.86257500	-7.81413200	-0.16060700
C	-2.00226600	-7.49951900	0.89963800
C	-1.28403700	-6.30538300	0.91757000
C	-1.23104700	6.32763300	0.87121600
C	-1.94815700	7.52257600	0.84974700
C	-2.82852800	7.82285600	-0.19796500
C	-2.97221600	6.87784200	-1.22269400
C	-2.26206900	5.67904400	-1.20490600
C	-6.58057300	1.41409700	-0.84615300
C	-7.72909200	2.20355600	-0.80656000
C	-7.91712700	3.12180000	0.22849600
C	-6.94641400	3.24447300	1.22402300
C	-5.79581400	2.45587700	1.18295000
C	-5.92608500	-2.41872900	-0.85919200
C	-7.08218400	-3.19578700	-0.77818500
C	-7.93708400	-3.06917600	0.31793100
C	-7.62723700	-2.15914400	1.33073500
C	-6.47355700	-1.38054000	1.24797000
C	-3.66266300	-9.09498200	-0.16139800
C	-3.57924000	9.13278300	-0.23496900
H	-8.81238200	3.73635500	0.25877500
H	-7.08418300	3.95292900	2.03620000
H	-8.47726800	2.10305900	-1.58796300
H	-6.43925400	0.70371800	-1.65443900
H	-5.04648200	2.55162000	1.96344200
H	-8.28401100	-2.05626600	2.19004600
H	-6.23714300	-0.67585100	2.03876600
H	-8.83658500	-3.67473300	0.38306100
H	-7.31566600	-3.89808600	-1.57373200
H	-5.26771500	-2.51668300	-1.71757000
H	-3.48754500	3.57865400	0.05473200
H	-3.50732500	-3.56274300	0.04504800
H	-2.36125100	-4.99636000	-2.02183000

Atoms	X	Y	Z
H	-3.62537600	-7.11330900	-2.05031200
H	-1.89448200	-8.19764300	1.72635800
H	-0.62925900	-6.08035900	1.75384000
H	-4.62326400	-8.96157000	0.35211900
H	-3.13012300	-9.90089900	0.35266500
H	7.22103900	-5.48454800	2.22008300
H	5.12177000	-4.16793500	2.14852200
H	5.87195500	-3.18084300	-1.96130300
H	7.97065300	-4.49994500	-1.89934600
H	1.13365000	-6.35926900	-0.31467400
H	3.71330900	-5.63516900	-0.21352700
H	6.33690900	-1.25293900	0.28176800
H	6.34386300	1.22121700	0.26415800
H	5.89079700	3.10529400	-2.00825800
H	5.14366400	4.18400000	2.07897300
H	7.24973700	5.49101800	2.12373000
H	7.99607200	4.41506600	-1.97338900
H	3.74251500	5.61026300	-0.29920500
H	1.16629700	6.34734800	-0.38943600
H	-2.38759400	4.96607300	-2.01408500
H	-0.56359500	6.11227500	1.70000500
H	-1.82589900	8.23114000	1.66547300
H	-3.64872700	7.08298400	-2.04883500
H	-3.77014900	9.51361000	0.77284600
H	0.16482000	-1.51935700	-0.12984300
H	0.17337500	1.51595200	-0.14268400
H	-3.88285500	-9.42911400	-1.17971500
H	-3.00772100	9.90175400	-0.77011800
H	-4.54085800	9.02923800	-0.74662100
Te	2.58976100	-0.00724100	0.00761600
H	8.65343400	-5.65730800	0.19370400
H	8.68381000	5.61323900	0.09488700

Figure S32: Cartesian coordinates of the S0 optimized structures of the compounds inverted thiabenzosaphyrin**5′**. #Sum of imaginary frequencies= 0; #Thermal Free Energy (hartree) = -**3160.308314**.

Atoms	X	Y	Z
N	-0.88531400	1.65517200	-0.10936600
H	0.13036500	1.55648000	-0.13009600
N	1.47834300	3.05463900	-0.25657700
N	-0.91903900	-1.65434200	-0.07691800
H	0.09764500	-1.57674000	-0.12167100
N	1.40334900	-3.09521400	-0.35031600
C	-1.46579600	5.42190400	-0.13652300
C	0.69573300	4.18411500	-0.26140600
C	2.75537600	3.47211900	-0.37463200
C	5.22451900	3.09527800	-0.05841700

Atoms	X	Y	Z
C	3.68616100	1.23702300	-0.74833300
C	2.54269700	-0.70406100	-1.41701600
H	1.77176600	-1.30488100	-1.87721100
C	1.53043900	5.37015700	-0.40119200
H	1.17921200	6.38968900	-0.46870700
C	7.79813800	4.08777600	0.63295700
C	-0.70151100	4.14242400	-0.16015600
C	5.41123400	3.90547500	1.07560200
H	4.55839400	4.14358600	1.70308900
C	2.55853700	0.66386000	-1.40543600

Atoms	X	Y	Z
H	1.80226200	1.28856000	-1.85843600
C	-1.44373300	2.92680300	-0.07986100
C	-1.87998800	0.71128600	-0.00999300
C	5.15120000	-3.18747900	-0.04947100
C	6.35456300	2.79731800	-0.84166300
H	6.23670000	2.19576300	-1.73738300
C	6.67319200	4.38964000	1.41104000
H	6.78733300	5.00889200	2.29740900
C	-3.13226800	1.40632800	0.08979900
C	1.43136700	-5.41349900	-0.27081500
H	1.07246800	-6.43055300	-0.20830300
C	0.60729000	-4.21191100	-0.27319700
C	-1.23794100	6.37781900	0.86508400
H	-0.51032200	6.16762200	1.64270100
C	2.81640100	4.92746200	-0.45002800
H	3.71533300	5.51472600	-0.57354900
C	-2.42900700	5.71420300	-1.11751400
H	-2.61662200	4.99545300	-1.90902400
C	6.28445800	-2.95228000	-0.84855300
H	6.17545800	-2.39399200	-1.77314700
C	-1.89604800	-0.68935000	-0.02119400
C	3.88170800	2.58209000	-0.42596700
C	5.32452400	-3.93830100	1.12618800
H	4.46869600	-4.12562300	1.76670100
C	7.61209500	3.28634700	-0.50184200
H	8.46424100	3.04999600	-1.13438700
C	-2.83820000	2.77504600	0.04934600
H	-3.54749600	3.58462800	0.10306000
C	3.81863500	-2.66113700	-0.44294300
C	-5.67650000	-1.45700100	0.20102900
C	3.65529700	-1.31222800	-0.76609200
C	-1.94730000	7.57813500	0.88409000
H	-1.75741800	8.29577000	1.67833300
C	2.67892800	-3.53264100	-0.39284500
C	2.72268500	-4.99004300	-0.34094300
H	3.61679100	-5.59620800	-0.37270300
C	-1.57276100	-5.40780100	-0.06803400
C	-1.50427200	-2.91354400	-0.06179900
C	-0.78617900	-4.14403700	-0.13687300
C	7.53333700	-3.44762300	-0.48551300
H	8.38858900	-3.26122900	-1.13047700
C	-5.64071300	1.56204500	0.23240400
C	-2.89978500	-2.73227300	0.00395700
H	-3.62725700	-3.52729900	0.01965300
C	-4.40448800	0.72889400	0.16409600
C	-3.13094900	6.91610700	-1.09463700
H	-3.86627900	7.11714800	-1.86998500
C	-7.77326500	2.26714800	-0.70273400
H	-8.52658800	2.18124400	-1.48071600
C	-4.42216800	-0.65238800	0.11954900

Atoms	X	Y	Z
C	-2.90396000	7.87191900	-0.09439700
C	-3.16611400	-1.35745500	0.03059500
C	-6.63105400	1.47012300	-0.75828900
H	-6.49971700	0.76831100	-1.57543000
C	-5.82717600	2.48174500	1.27765200
H	-5.07233900	2.56317800	2.05423100
C	7.70613300	-4.19154300	0.68967900
C	-1.52886600	-6.33948200	-1.11740500
H	-0.93015200	-6.12052800	-1.99607100
C	6.57778900	-4.42885900	1.48487600
H	6.68243300	-5.00201700	2.40283300
C	-2.25907000	-7.52485800	-1.05339900
H	-2.21488300	-8.22276800	-1.88592800
C	9.17024800	4.58645700	1.01699000
H	9.11389600	5.52311300	1.57939800
H	9.79578500	4.75618700	0.13534300
H	9.69289700	3.85785900	1.64961400
C	-6.01626100	-2.35664800	-0.82286100
H	-5.36727500	-2.44524400	-1.68913300
C	-2.37502300	-5.70922100	1.04511200
H	-2.41918600	-5.00934500	1.87370000
C	-6.53260200	-1.35425700	1.30857400
H	-6.28170800	-0.66673500	2.10982100
C	-3.05507100	-7.82849100	0.05786500
C	-6.97135600	3.27802500	1.33468200
H	-7.09901600	3.97796700	2.15564500
C	-7.17920200	-3.12321900	-0.74537100
H	-7.42683400	-3.80797300	-1.55159700
C	-7.94852800	3.17413300	0.34385400
H	-8.83895900	3.79466700	0.38670400
C	-3.09987500	-6.89691100	1.10381900
H	-3.70928100	-7.10512900	1.97984000
C	-8.02222700	-3.00888800	0.36081700
H	-8.92734300	-3.60610900	0.42280500
C	9.06903300	-4.69719600	1.09724400
H	9.68307600	-4.94106800	0.22492800
H	8.99428600	-5.59247800	1.72147300
H	9.61443900	-3.94119200	1.67618300
C	-7.69357100	-2.12186400	1.38744400
H	-8.34153900	-2.02798900	2.25428900
C	-3.82175500	-9.12681700	0.13955600
H	-4.02446400	-9.53508700	-0.85475200
H	-3.25743400	-9.88611400	0.69545700
H	-4.77868800	-8.99529000	0.65390600
C	-3.65496800	9.18188200	-0.08932300
H	-3.57384500	9.68595600	0.87776100
H	-3.26294900	9.86694400	-0.85123200
H	-4.71803200	9.03477300	-0.30624900
S	4.79995000	-0.05408800	-0.26249100

Figure S33: Cartesian coordinates of the S0 optimized structures of the compounds normal thiabenzosaphyrin**5**. #Sum of imaginary frequencies= 0; #Thermal Free Energy (hartree) =**-3160.389176**.

Atoms	X	Y	Z
C	4.08592100	1.28084900	0.10030200
C	5.35465800	0.67407000	0.36009200
C	5.35237300	-0.68639000	0.37006700
C	4.08174000	-1.29261400	0.11802800
C	0.64608800	-4.09230400	-0.22624100
C	1.45569300	-5.28549300	-0.41455700
C	2.74720000	-4.87998400	-0.35440700
C	2.71988700	-3.43477500	-0.13512700
N	1.45146800	-2.97690400	-0.08289500
C	3.91979500	-2.67362500	0.02275300
C	-1.96084500	-0.69411300	-0.02294000
C	-3.21616200	-1.38176300	0.05269400
C	-2.91903100	-2.75005600	0.01000200
C	-1.52096000	-2.89097200	-0.11102900
N	-0.96383200	-1.62491300	-0.12354900
C	-1.95636700	0.69745100	-0.00004300
C	-3.20689900	1.38952000	0.10366500
C	-2.90791700	2.75631700	0.03679000
C	-1.51097600	2.89294200	-0.10022600
N	-0.95750300	1.62525100	-0.11135900
C	0.65745300	4.08694300	-0.25434400
C	1.46905300	5.27491400	-0.46585600
C	2.75983500	4.86603100	-0.41237200
C	2.72995200	3.42392200	-0.17399100
N	1.46069500	2.97081400	-0.10507800
C	3.92832100	2.66098600	-0.01297300
C	-0.75419900	-4.08216800	-0.19952300
C	-0.74252700	4.08140000	-0.21107300
C	-4.47120000	0.69788900	0.20411500
C	-4.47611900	-0.68530500	0.17171400
C	-1.50014600	-5.37148600	-0.25769900
C	-1.48492100	5.37240500	-0.27623900
C	-5.72012700	-1.50079100	0.29074600
C	-5.71340700	1.52035500	0.28657600
C	5.18487300	-3.48868800	0.10432900
C	5.19661800	3.47239500	0.05242100
C	5.50673500	-4.20279600	1.26719500
C	6.67439700	-4.96095700	1.33977600
C	7.55655300	-5.04045900	0.25394300
C	7.23230800	-4.32590500	-0.90604000
C	6.06804300	-3.56145000	-0.98133000
C	6.07406400	3.52920000	-1.03970800
C	7.23674800	4.29644900	-0.98330700
C	7.56878600	5.02643200	0.16570300
C	6.68998000	4.96796600	1.25465200
C	5.52268700	4.20650900	1.20077200
C	-2.41753100	-5.63331800	-1.28823400
C	-3.10984000	-6.84114200	-1.33996200
C	-2.92315400	-7.82809200	-0.36349400
C	-2.00802000	-7.56564600	0.66407600
C	-1.30829600	-6.36220000	0.71865900

Atoms	X	Y	Z
C	-1.27575000	6.37501800	0.68429600
C	-1.97637500	7.57798300	0.62747600
C	-2.90631900	7.82977500	-0.38936200
C	-3.11603500	6.82774400	-1.34573100
C	-2.42260900	5.62076000	-1.29200100
C	-6.72645200	1.40220500	-0.67812500
C	-7.87324700	2.19158700	-0.61026700
C	-8.03075200	3.11704100	0.42292800
C	-7.03108700	3.24703700	1.38787400
C	-5.88222000	2.45862700	1.31835900
C	-6.07483500	-2.41550400	-0.71448100
C	-7.22770700	-3.19267700	-0.60072800
C	-8.04497500	-3.07476000	0.52419100
C	-7.70087600	-2.17312000	1.53287000
C	-6.55045900	-1.39448400	1.41744700
C	8.80292100	-5.89068500	0.32501300
C	8.84556200	5.83038900	0.23477000
C	-3.70226200	-9.12084800	-0.40226600
C	-3.63970200	9.14737000	-0.46714200
H	-8.92473400	3.73169600	0.47533600
H	-7.14474200	3.96145000	2.19836200
H	-8.64402600	2.08542800	-1.36839100
H	-6.60882900	0.68659000	-1.48529100
H	-5.10986600	2.56044600	2.07502100
H	-8.32832300	-2.07667900	2.41435900
H	-6.28699100	-0.69613700	2.20512500
H	-8.94190100	-3.68059600	0.61466600
H	-7.48814800	-3.88846900	-1.39341700
H	-5.44618000	-2.50634900	-1.59539900
H	-3.60925400	3.57360200	0.08115800
H	-3.62030700	-3.56661800	0.06873800
H	-2.57158000	-4.88956200	-2.06386100
H	-3.80324500	-7.02246000	-2.15755800
H	-1.84252100	-8.31263100	1.43660500
H	-0.61136200	-6.17830900	1.53022900
H	-4.63813900	-9.03615700	0.16432500
H	-3.13232200	-9.94568900	0.03575200
H	9.57093200	-5.53447500	-0.36769500
H	9.22983500	-5.89249300	1.33265100
H	6.90511400	-5.49846900	2.25643900
H	4.83740500	-4.15658200	2.12125300
H	5.83807600	-3.01396400	-1.89076100
H	7.89980600	-4.36713900	-1.76336800
H	1.08065800	-6.28331500	-0.58690500
H	3.63428100	-5.48511300	-0.46307900
H	6.23380900	-1.28321900	0.55649500
H	6.23805100	1.27068900	0.53781500
H	5.83549300	2.97331600	-1.94180100
H	4.85343400	4.18074000	2.05572900
H	6.92040500	5.52771800	2.15788300
H	7.89532700	4.33125100	-1.84792000

Atoms	X	Y	Z
H	9.69322700	5.20415100	0.54024700
H	8.76621700	6.64595000	0.95941400
H	3.64775700	5.46688700	-0.53685400
H	1.09568700	6.27169000	-0.64753000
H	-2.59900100	4.86369300	-2.04963900
H	-0.57001800	6.19797800	1.48979900
H	-1.80199800	8.33153600	1.39160900
H	-3.83158600	6.99442500	-2.14708800
H	-3.77683100	9.58853200	0.52456200

Atoms	X	Y	Z
H	0.05165600	-1.51613700	-0.12417600
H	0.05737800	1.51310000	-0.13004000
H	8.58692800	-6.93416900	0.06340100
H	9.09880900	6.26415700	-0.73749100
H	-3.96748300	-9.39800100	-1.42682200
H	-3.08408300	9.87476500	-1.07234700
H	-4.62602100	9.03042200	-0.92586900
S	2.85973500	-0.00516700	-0.07277100