Supporting Information

Near Infrared Absorbing Nonaromatic Core modified *m*eta-Benzicalixhexaphyrin(1.*1*.*1*.1.1.1)s

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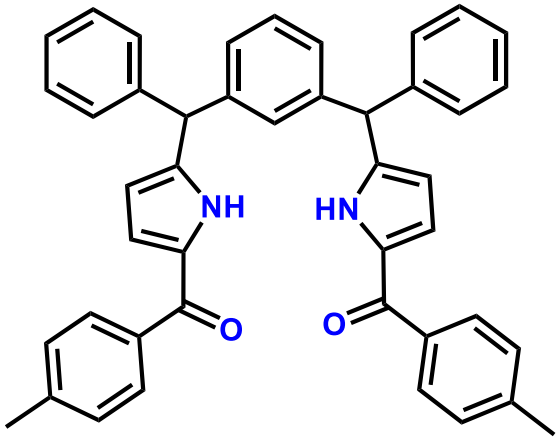
General Experimental Section:

Materials, methods and instruments

$BF_3 \cdot OEt_2$, trifluoroacetic acid (TFA), 2, 3-dichloro-5, 6-dicyano-1, 4-benzoquinone (DDQ) and other chemicals used were obtained from Aldrich. All the other chemicals used for the synthesis were reagent grade unless mentioned otherwise. Silica gel and basic alumina column chromatographic method were performed for purification. The compounds **10a-10b**[1] and **8a-8d**[2] were synthesized by the reported method. The ^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ on Bruker 400 and 500 MHz FT-NMR spectrometers using tetramethylsilane [$Si(CH_3)_4$] as the internal reference. The frequencies for ^{13}C nucleus being 100.06 and 125.77 MHz for 400 MHz and 500 MHz instruments respectively. Absorption spectra were obtained with Shimadzu UV-Vis-NIR Spectrophotometer. The stock solutions of the macrocycles (2×10^{-5} M) were prepared using HPLC-grade chloroform. Cyclic voltammetry (CV) studies were carried out with BASi C3 Cell Stand electrochemical system 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 concentrations of the samples were maintained as 0.01 M containing 0.1 M tetrabutylammonium perchlorate (TBAP) as the supporting electrolyte in dichloromethane at 25 °C under an argon atmosphere at a scan rate of 50 mV/s. The half-wave potentials measured using differential pulse voltammetry were calculated manually by taking the average of the cathodic and anodic peak potentials. All the potentials were calibrated using ferrocene as an external standard, taking $E^{1/2}$ (Fc/Fc^{+}) = 0.42 V *versus* SCE. The HR mass spectra were recorded with a Bruker maXis Impact and Q-TOF micro mass spectrometer using positive mode ESI methods in acetonitrile or methanol.

Computational Details:

All computations were performed using the Gaussian 09 program package.[3] The density functional theory (DFT) method, with hybrid functional B3LYP in conjunction with 6-31G**+LANL2DZ basis sets were implemented to optimize the geometries of macrocycles **2-5** in ground (S_0) state.[4] In order to improve the accuracy of electronic structure calculations and geometry optimization in S_0 state, dispersive interactions in the electron density of the macrocycles were studied using Grimme's dispersion correction method (GD2) over the B3LYP/6-31G**+LANL2DZ level of theory.[5] Oscillator strengths were obtained using identical basis and functional hybrid set, whereas the vertical excitation energies were obtained by the help of TD-DFT techniques for first fifty $S_0 \rightarrow S_n$ transitions.[6] All computations were performed in toluene medium using the Polarizable Continuum Model (PCM) and Self-Consistent Reaction Field (SCRF).[7] The electronic absorption spectra, and the oscillator strengths were thoroughly examined using time-dependent DFT with the PCM model based on the optimized structures in the S_0 state.



Compound **7a**

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

Analysis Info

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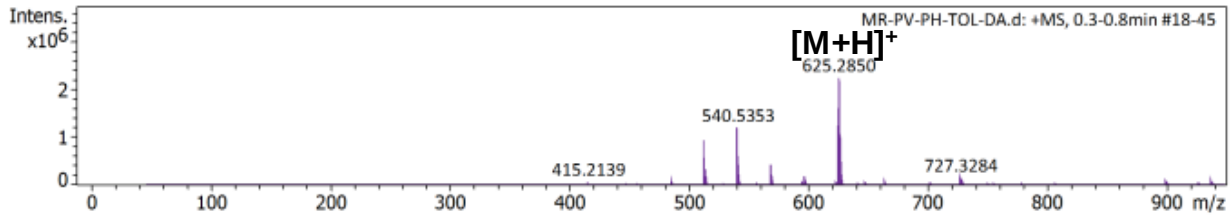
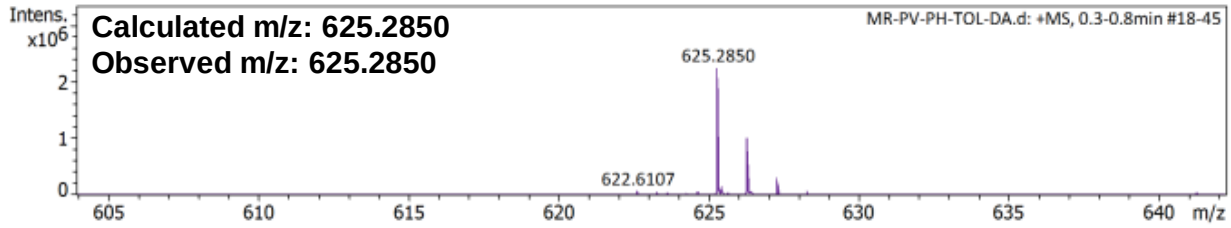
Method	Naformat_pos_1000a.m	Operator	PG-SRD-IN
Sample Name	MR-PV-PH-TOL-DA	Instrument	maXis impact 282001.00081
Comment	C44H36N2O2		

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
625.2850	1	C44H37N2O2	625.2850	-0.0	9.6	1	100.00	28.0	even	ok

Figure S1. HR mass spectrum of the compound **7a**.

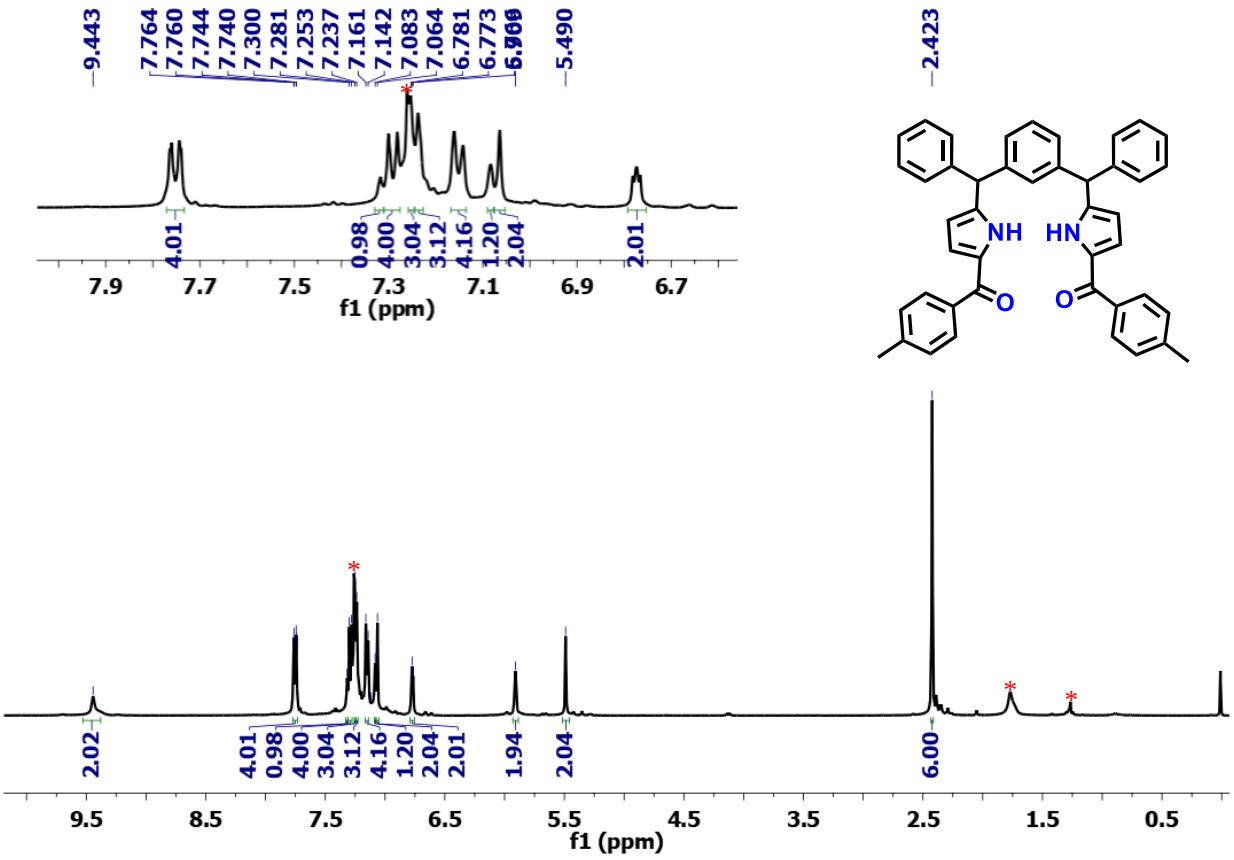


Figure S2. ^{1}H-NMR spectrum of the compound **7a** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

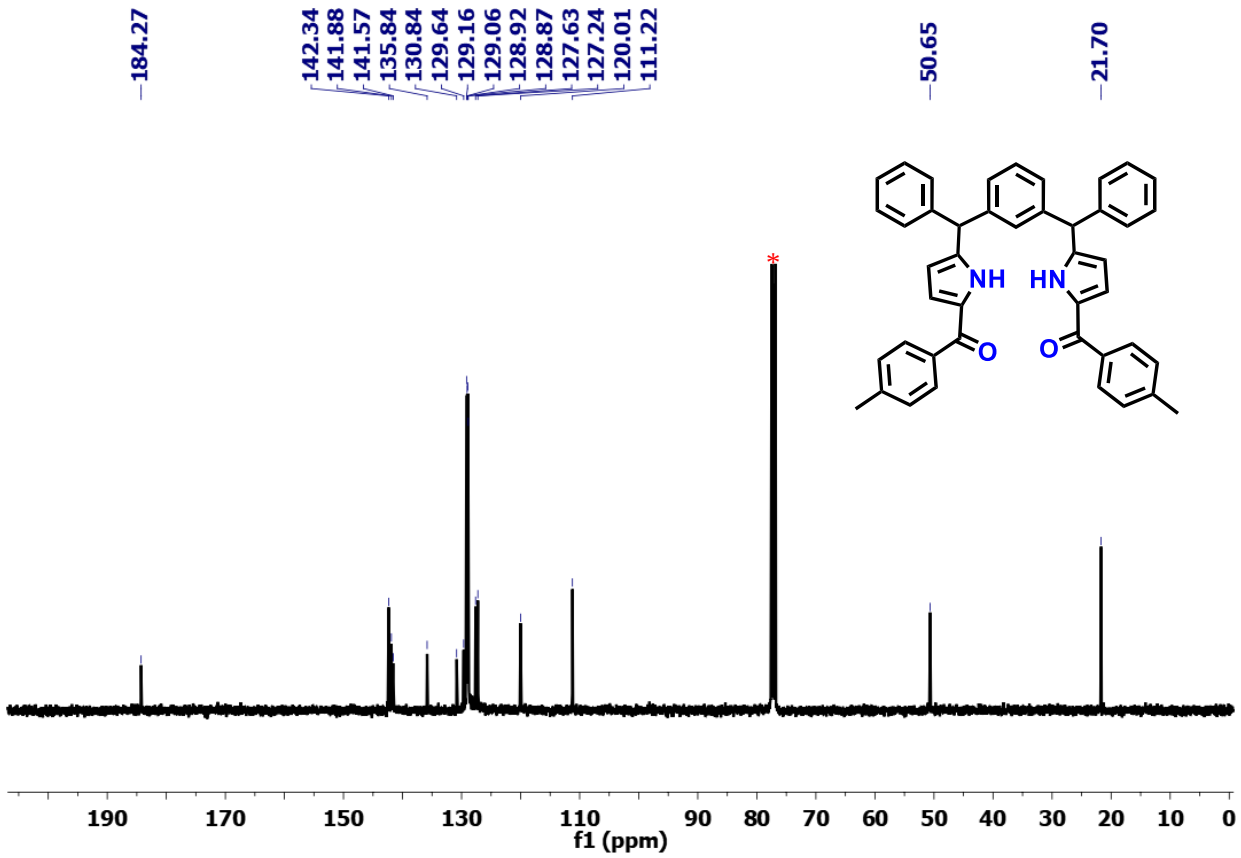
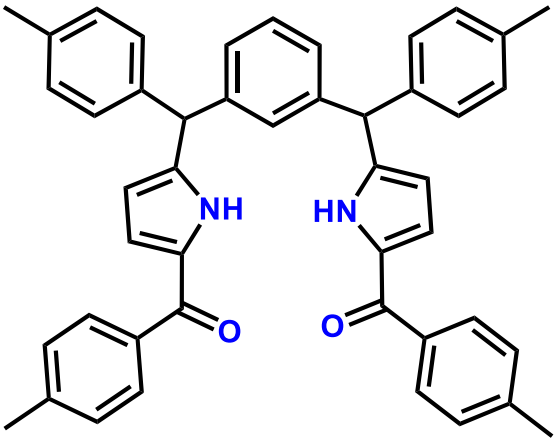


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **7a** recorded in $CDCl_3$ on 101 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **7a**

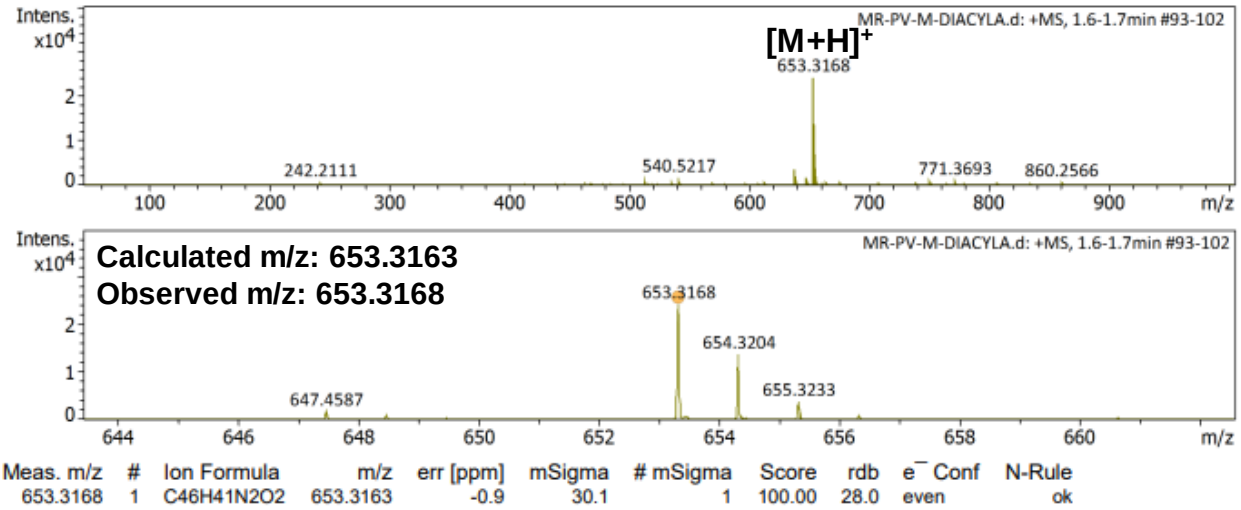
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MAY-2023\MR-PV-M-DIACYLA.d	Acquisition Date	5/15/2023 12:08:28 PM
Method	Naformat_pos_1000a.m	Operator	PG ROHAN OUT
Sample Name	MR-PV-M-DIACYLA	Instrument	maXis impact 282001.00081
Comment	C46H40N2O2		

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
653.3168	1	C46H41N2O2	653.3163	-0.9	30.1	1	100.00	28.0	even	ok

Figure S4. HR mass spectrum of the compound **7b**.

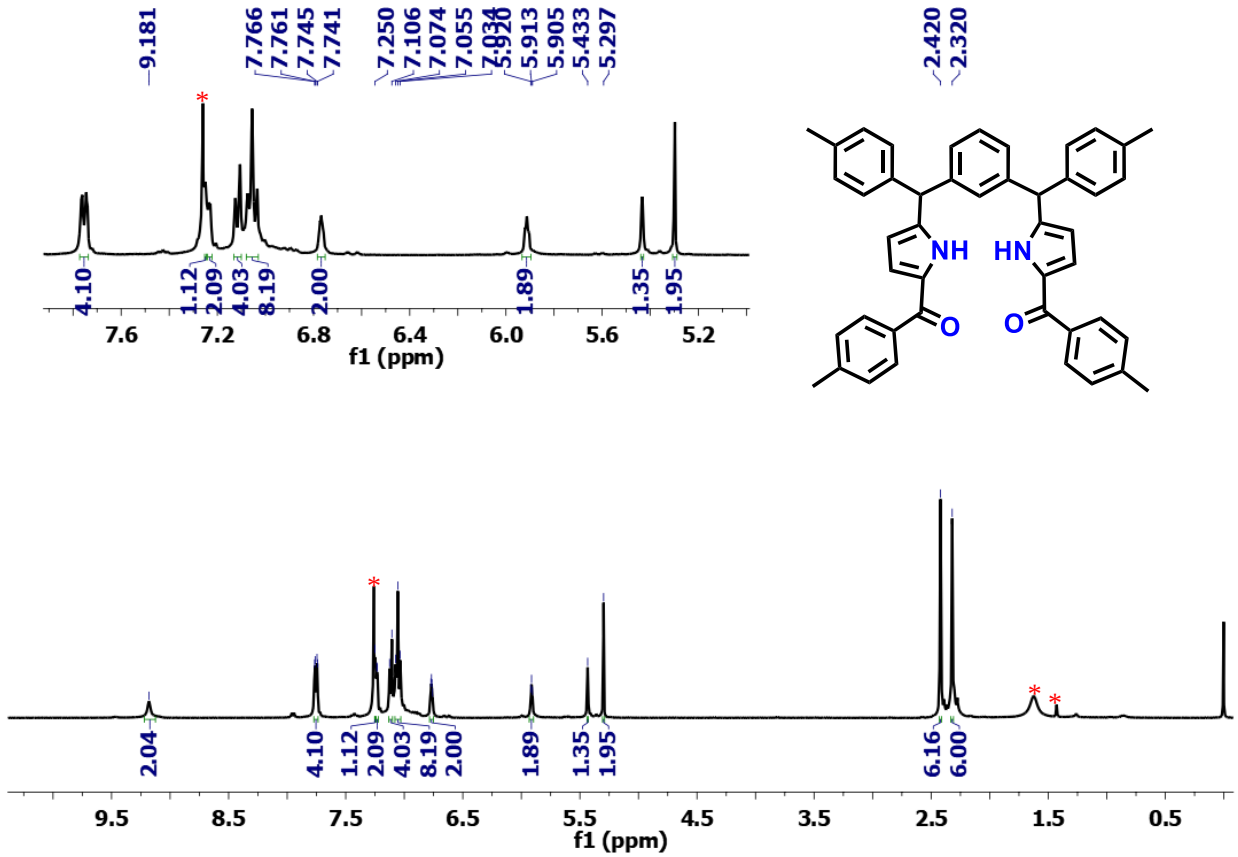


Figure S5. ^{1}H-NMR spectrum of the compound **7b** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

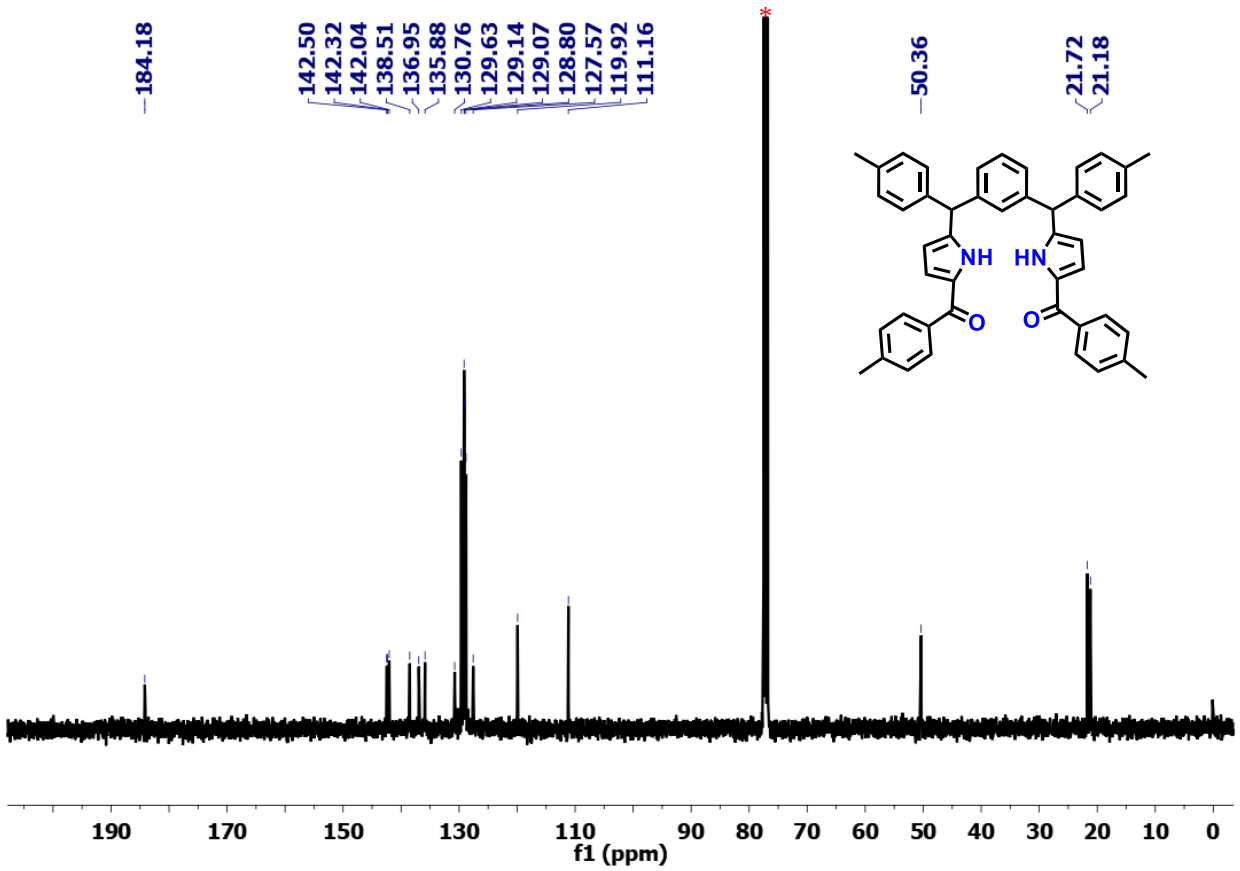
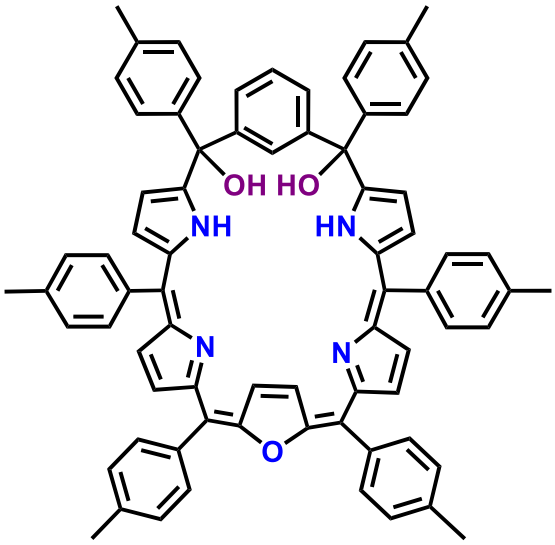


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **7b** recorded in $CDCl_3$ on 101 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **2**

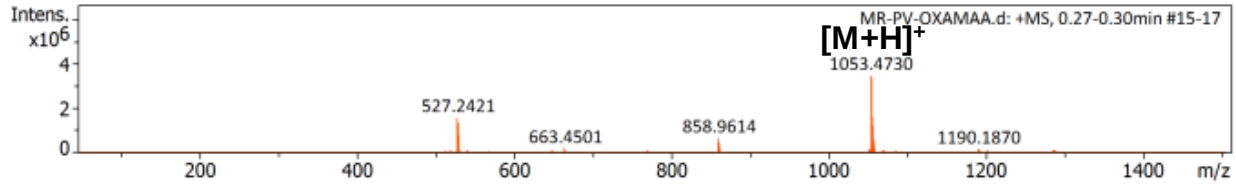
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

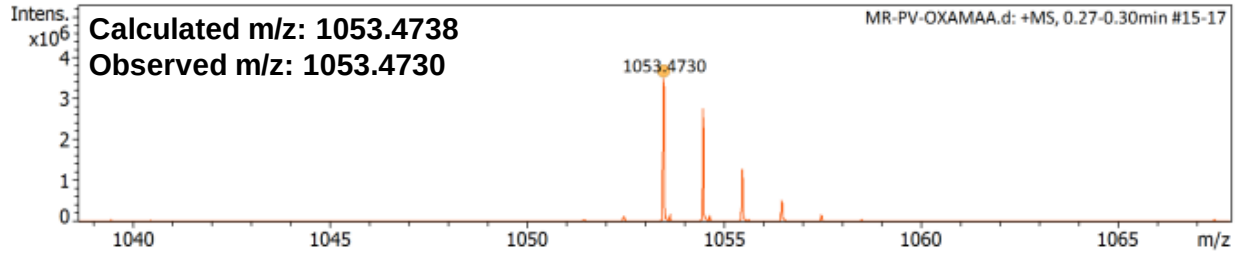
Analysis Info

Analysis Name	D:\Data\MAY-2023\MR-PV-OXAMAA.d	Acquisition Date	5/29/2023 4:06:59 PM
Method	NaICsI_pos_1500.m	Operator	GKL-LS-OUT
Sample Name	MR-PV-OXAMAA	Instrument	maXis impact 282001.00081
Comment	C74H60N4O3		

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
1053.4730	1	C74H61N4O3	1053.4738	0.8	30.5	1	100.00	47.0	even	ok

Figure S7. HR mass spectrum of the compound **2**.

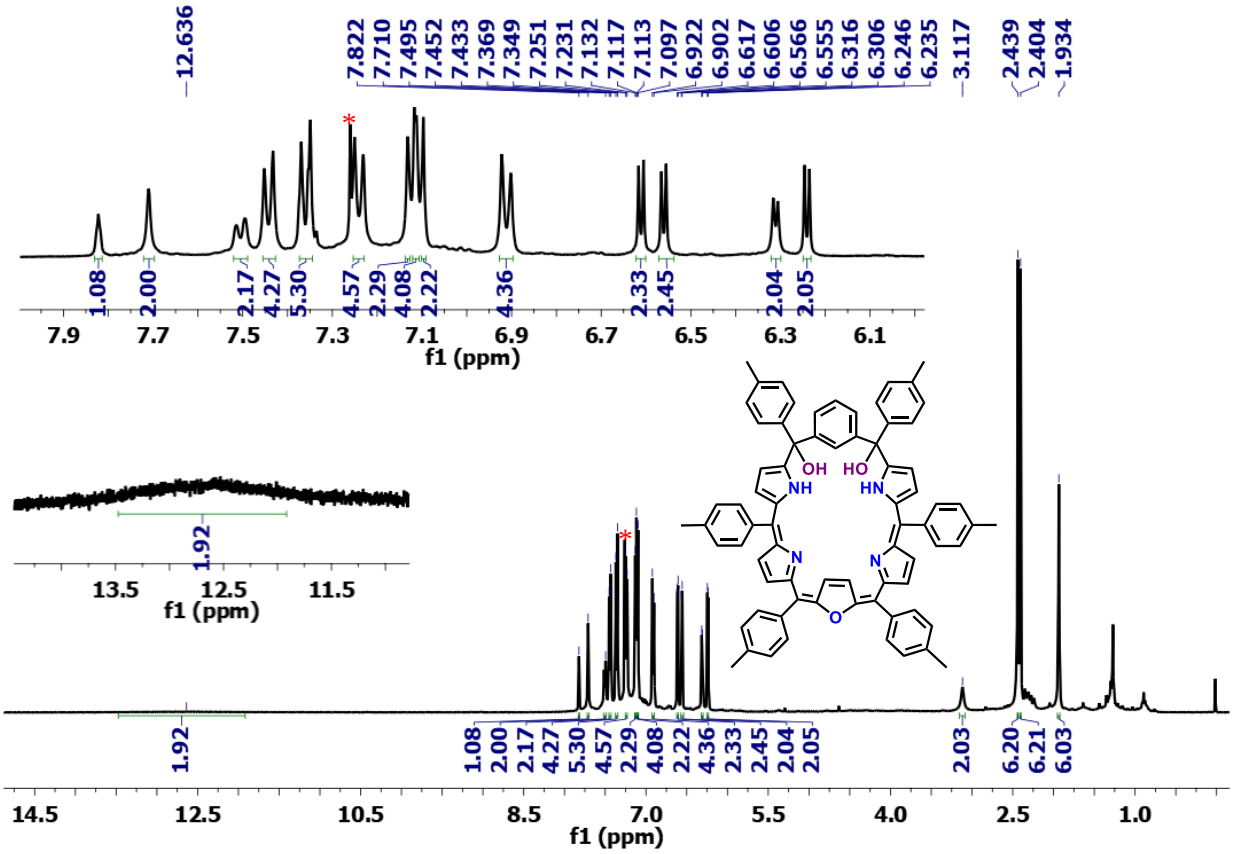


Figure S8. ^{1}H-NMR spectrum of the compound **2** recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

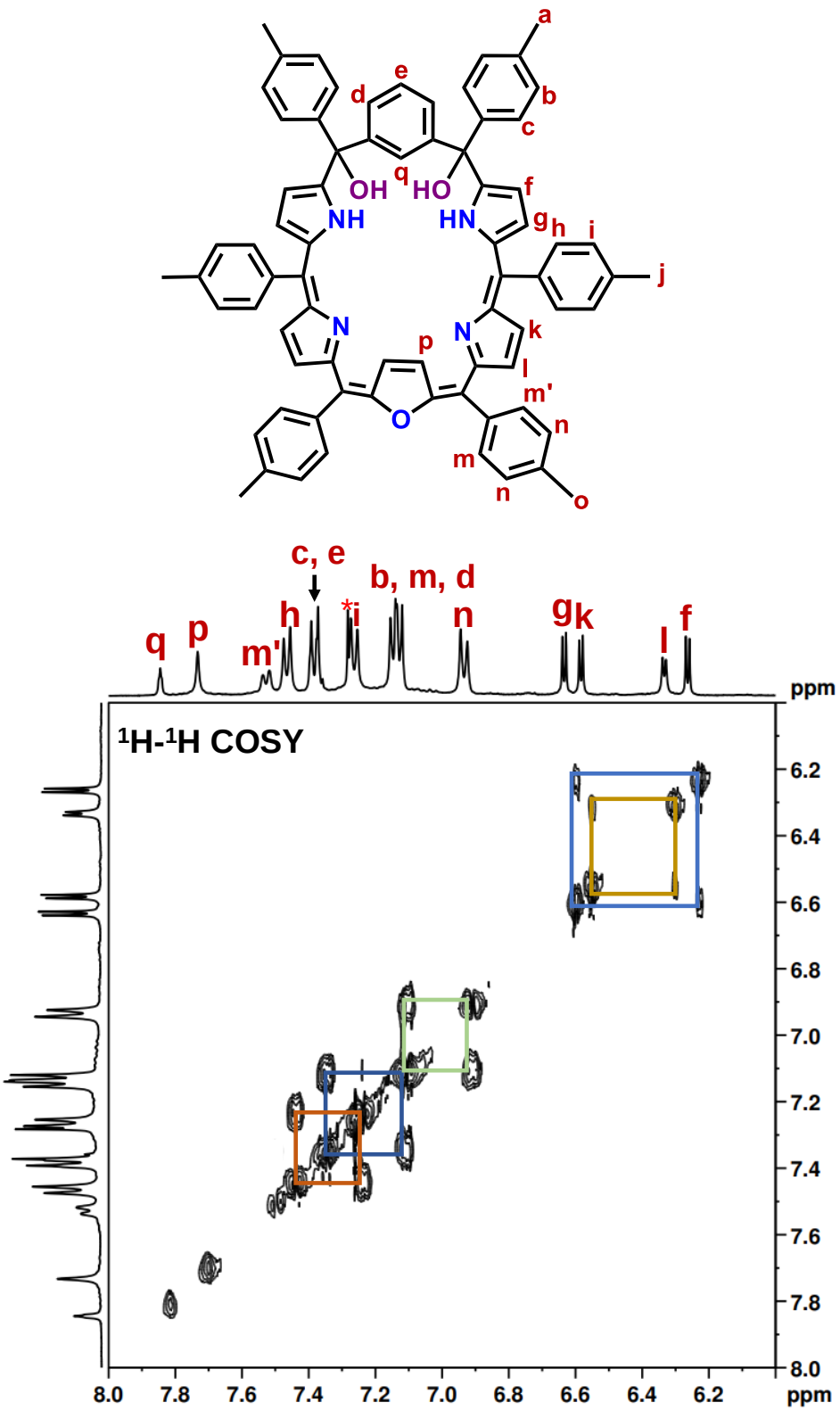


Figure S9. ^{1}H–^{1}H COSY of compound **2** recorded in $CDCl_3$ at 25 °C.

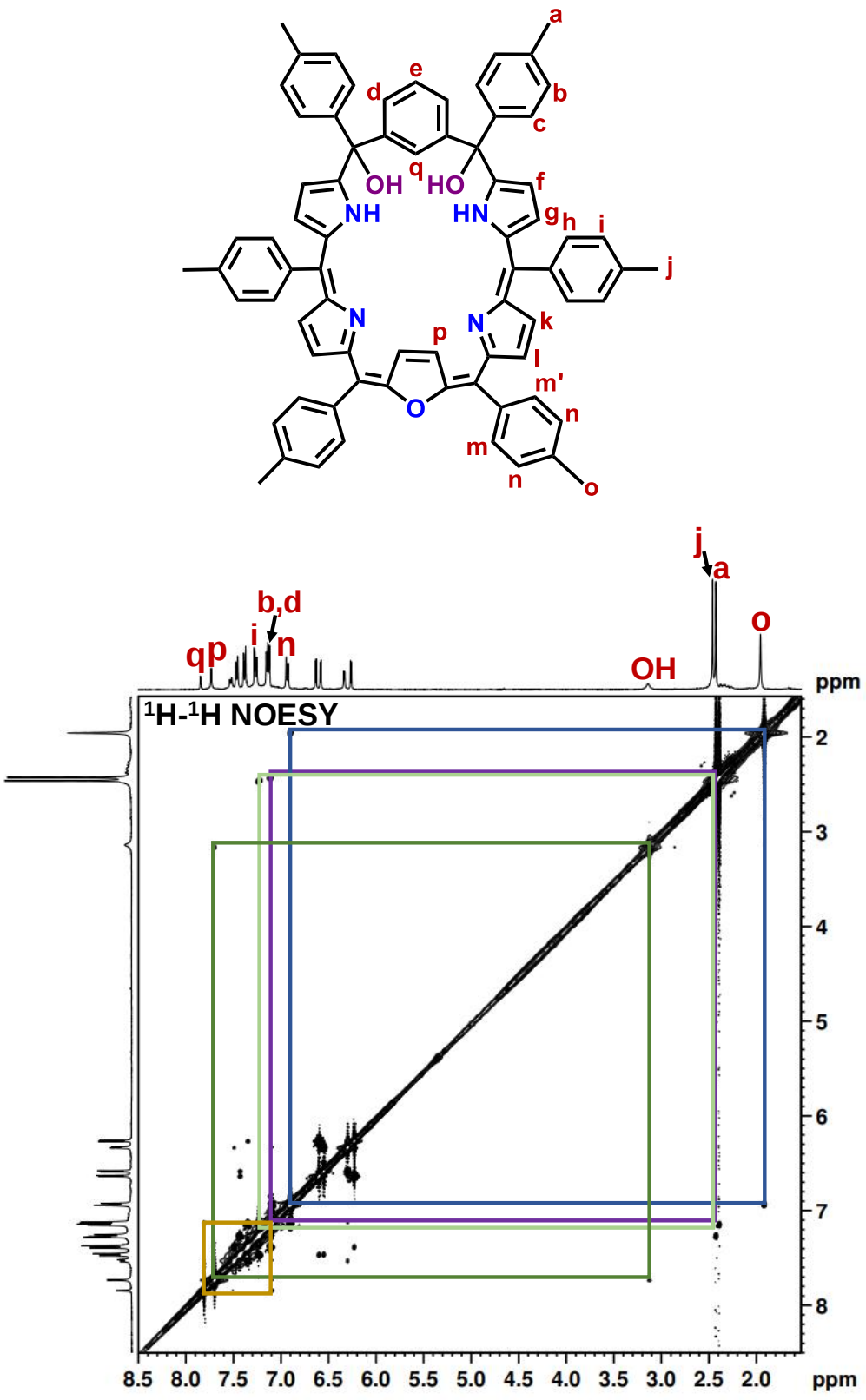


Figure S10. ^{1}H–^{1}H NOESY of compound **2** recorded in $CDCl_3$ at 25 °C.

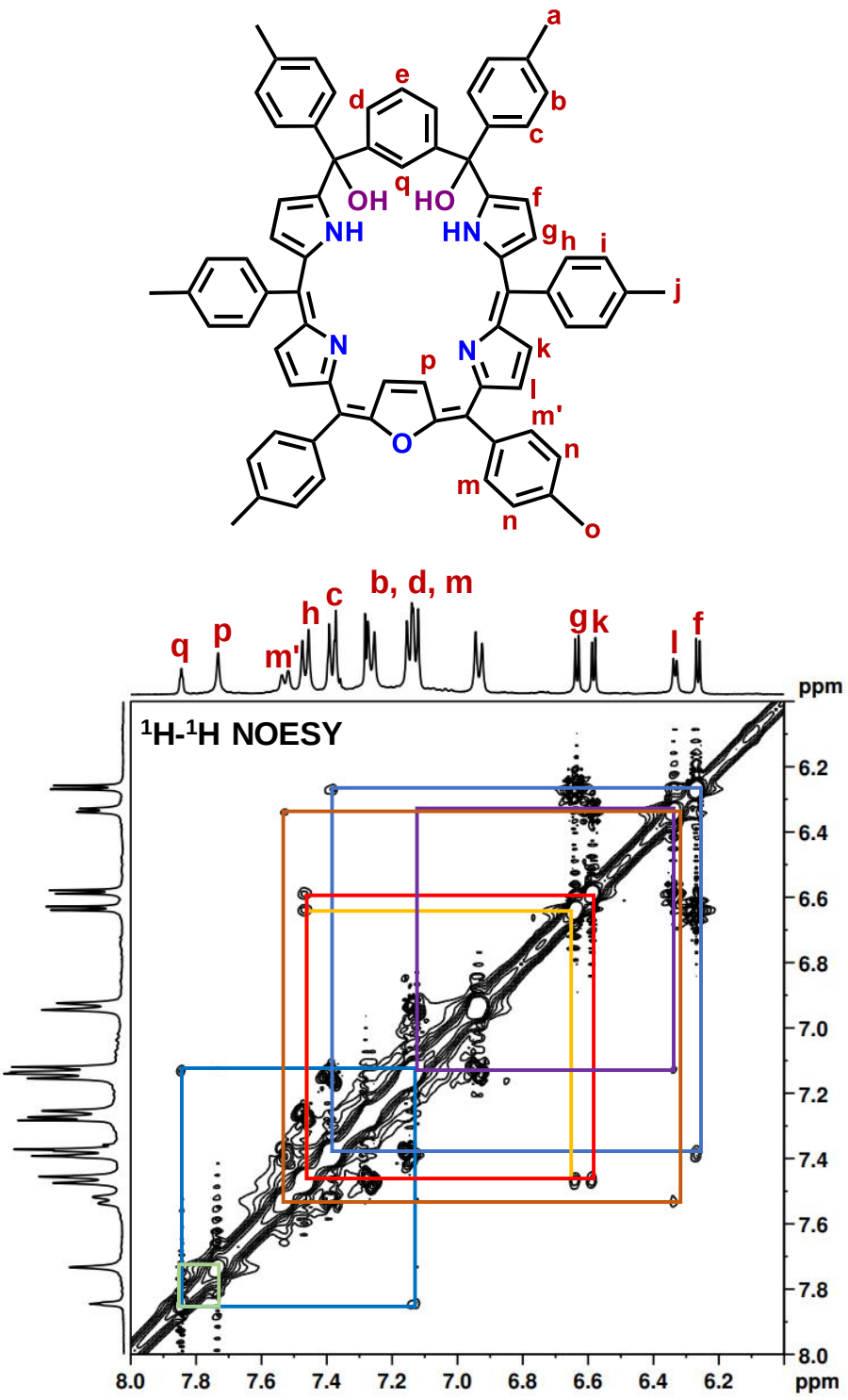


Figure S11. Expanded ^{1}H–^{1}H NOESY of compound **2** recorded in $CDCl_3$ at 25 °C.

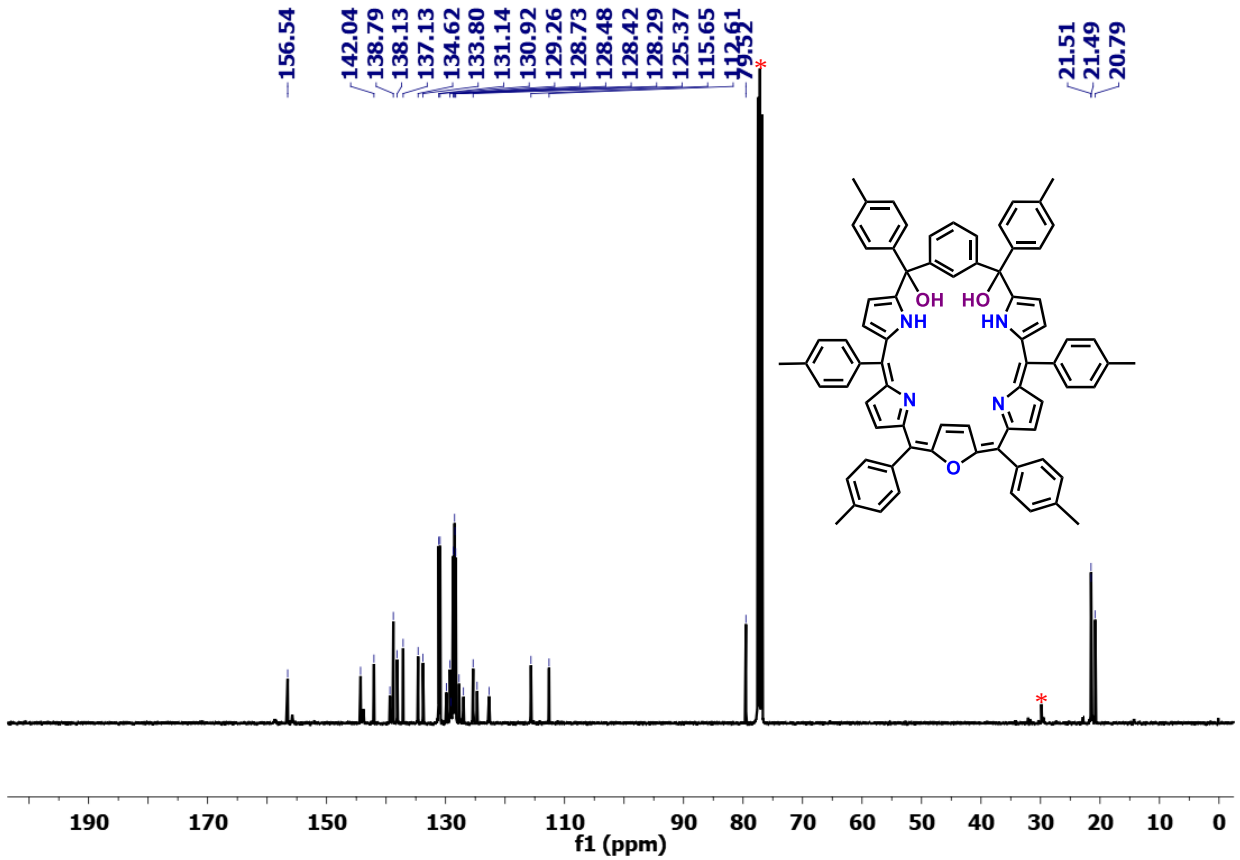
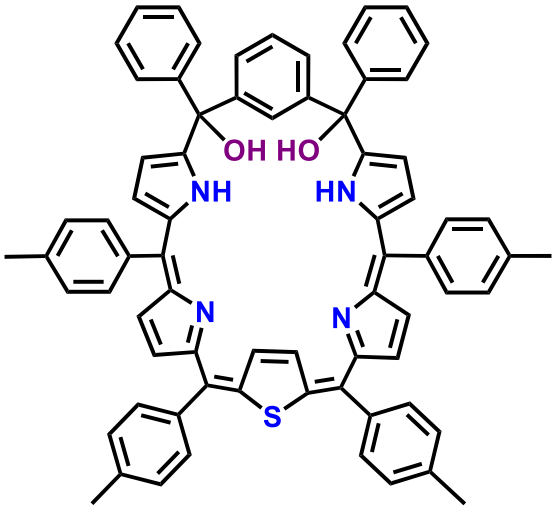


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **2** recorded in $CDCl_3$ on 101 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **3a**

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

Analysis Info

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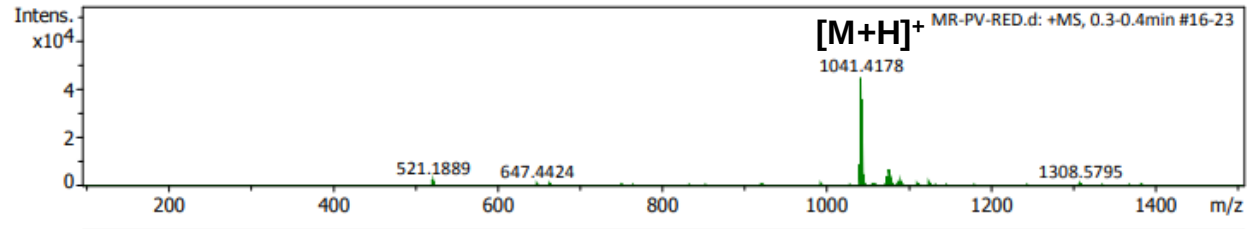
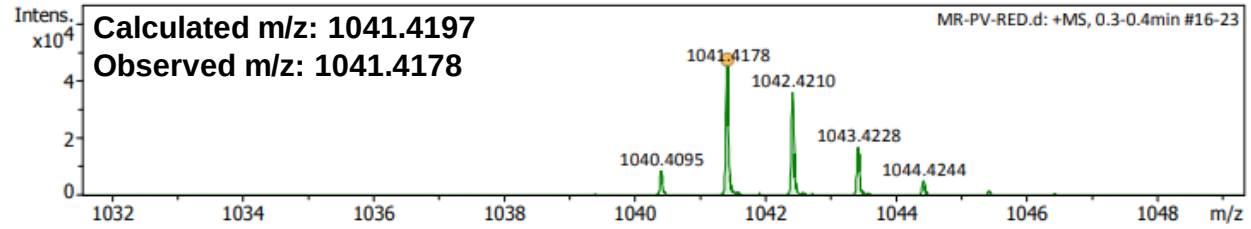
Method	Naformat_pos_1500.m	Operator	PG SRD IN
Sample Name	MR-PV-RED	Instrument	maXis impact 282001.00081
Comment	C72H56N4O2S		

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
1041.4178	1	C72H57N4O2S	1041.4197	1.8	5.6	1	100.00	49.0	even	ok

Figure S13. HR mass spectrum of the compound **3a**.

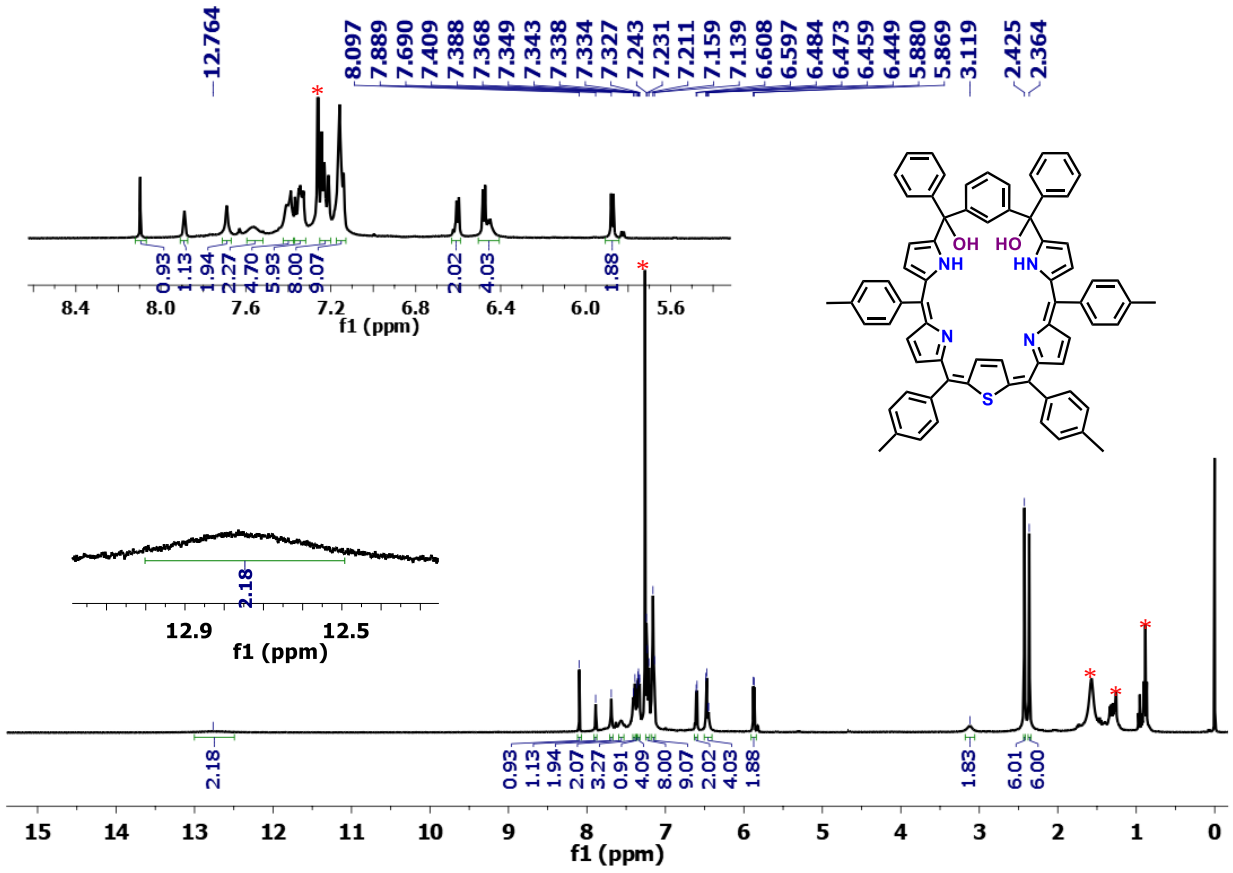


Figure S14. ^{1}H-NMR spectrum of the compound **3a** recorded in $CDCl_3$ at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

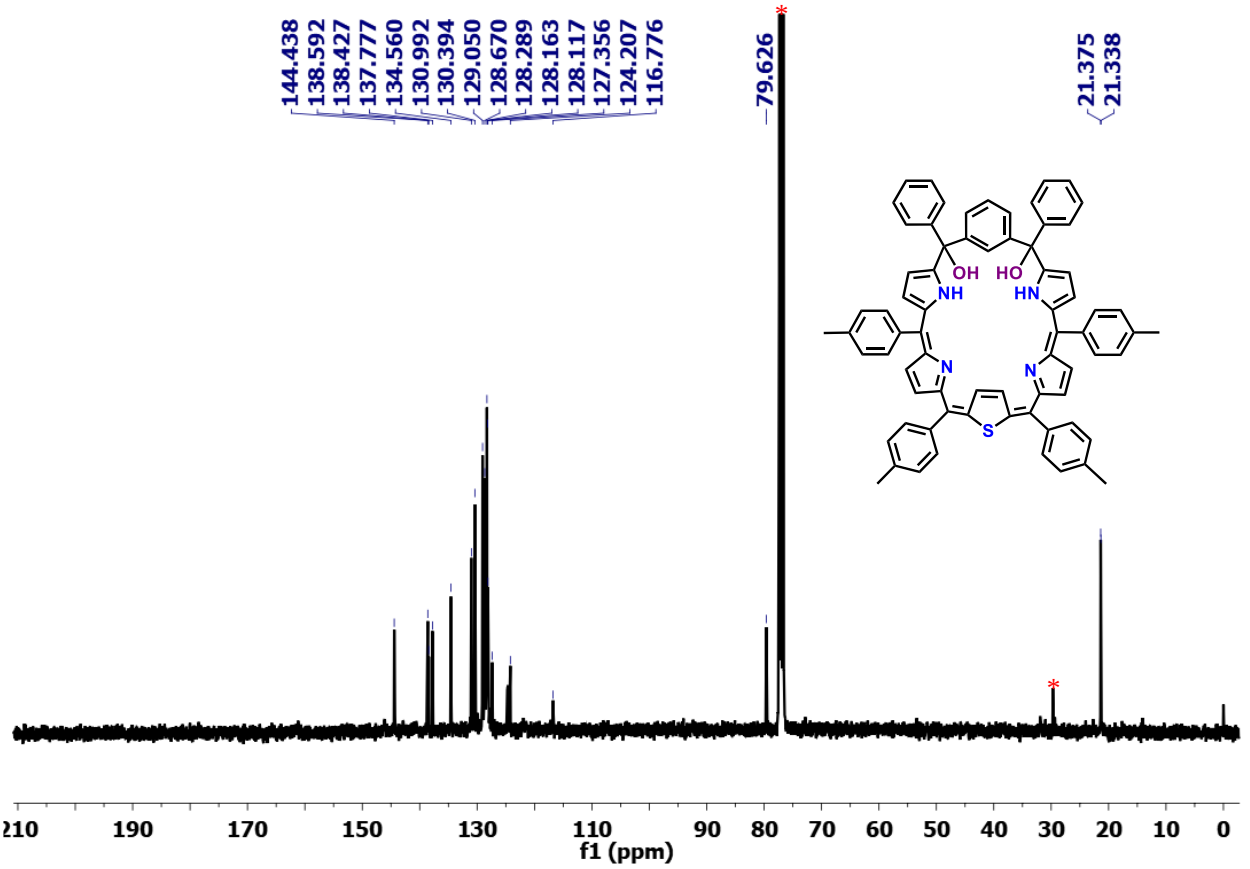
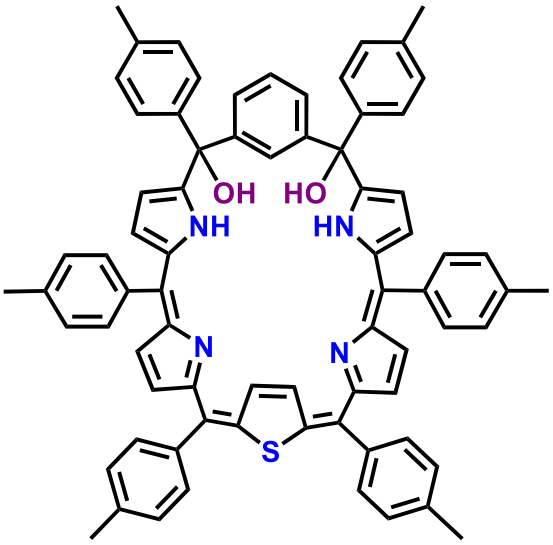


Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3a** recorded in $CDCl_3$ on 101 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **3b**

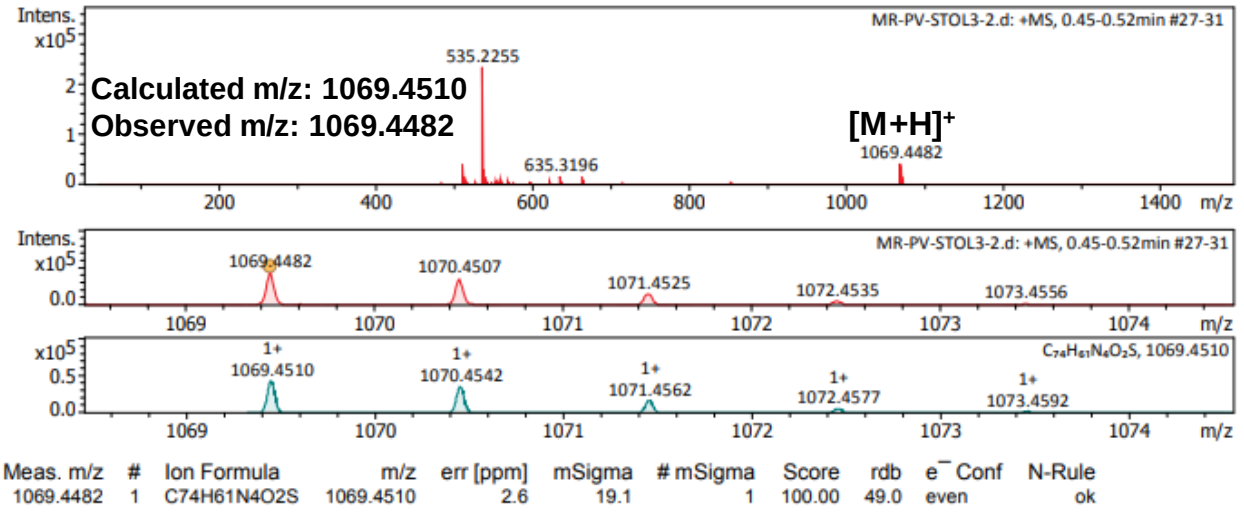
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\JULY-2023\MR-PV-STOL3-2.d	Acquisition Date	7/20/2023 4:57:20 PM
Method	NaICsI_pos_1500.m	Operator	PG ROHAN OUT
Sample Name	MR-PV-STOL3-2	Instrument	maXis impact 282001.00081
Comment	C74H60N4O2S		

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
1069.4482	1	C74H61N4O2S	1069.4510	2.6	19.1	1	100.00	49.0	even	ok

Figure S16. HR mass spectrum of the compound **3b**.

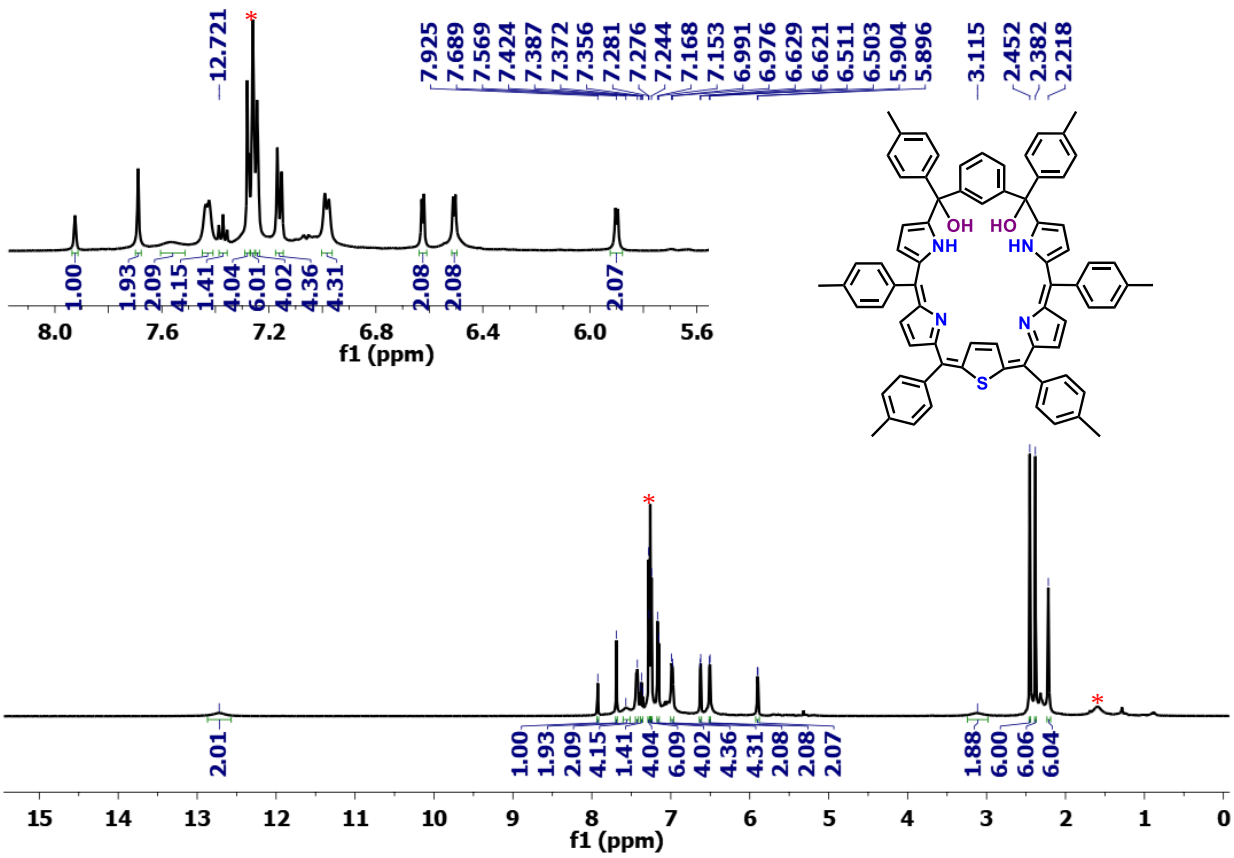


Figure S17. ^{1}H-NMR spectrum of the compound **3b** recorded in $CDCl_3$ at 25 °C on 500 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

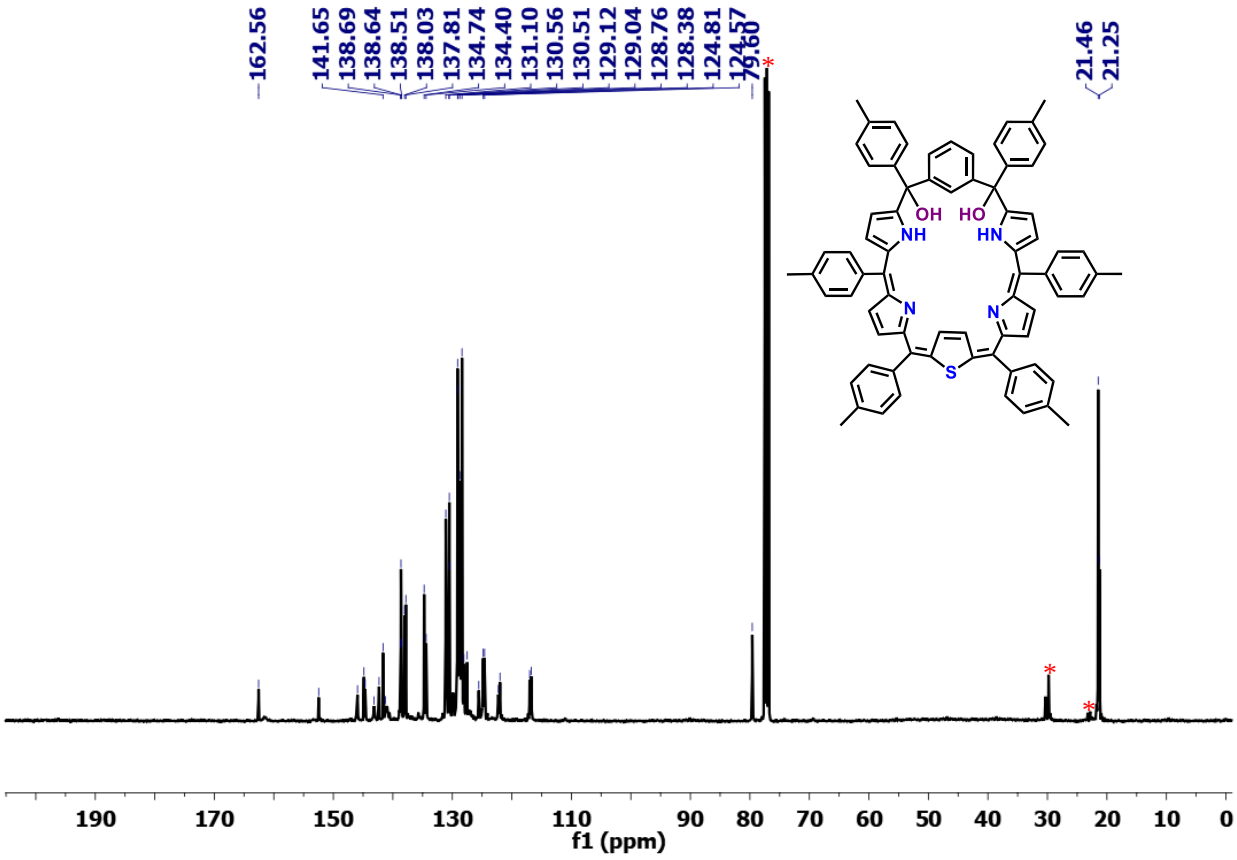
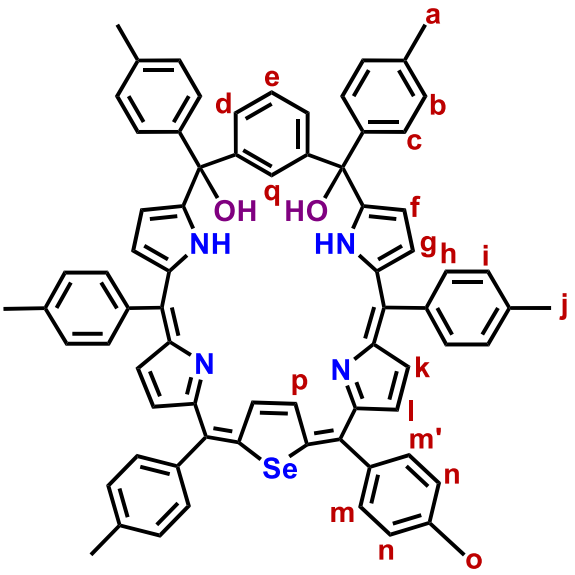


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3b** recorded in $CDCl_3$ on 101 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



Compound **4**

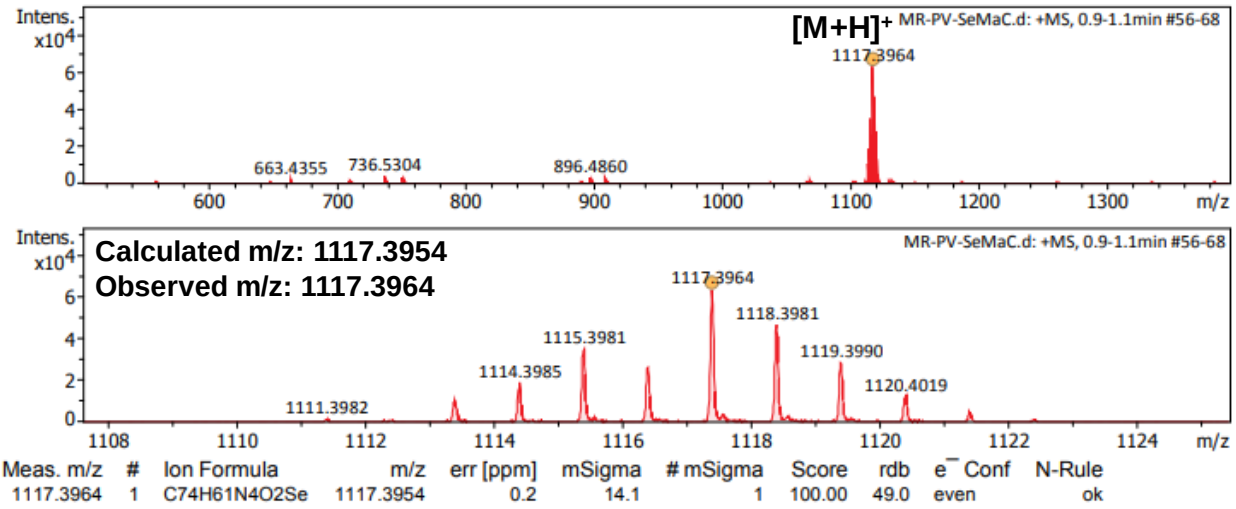
DEPARTMENT OF CHEMISTRY, I.I.T.(B)

Analysis Info

Analysis Name	D:\Data\MAY-2023\MR-PV-SeMaC.d	Acquisition Date	5/17/2023 2:36:56 PM
Method	Naformat_pos_1500.m		
Sample Name	MR-PV-SeMaC	Operator	PG ROHAN OUT
Comment	C74H60N4O2Se1	Instrument	maXis impact 282001.00081

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
1117.3964	1	C74H61N4O2Se	1117.3954	0.2	14.1	1	100.00	49.0	even	ok

Figure S19. HR mass spectrum of the compound **4**.

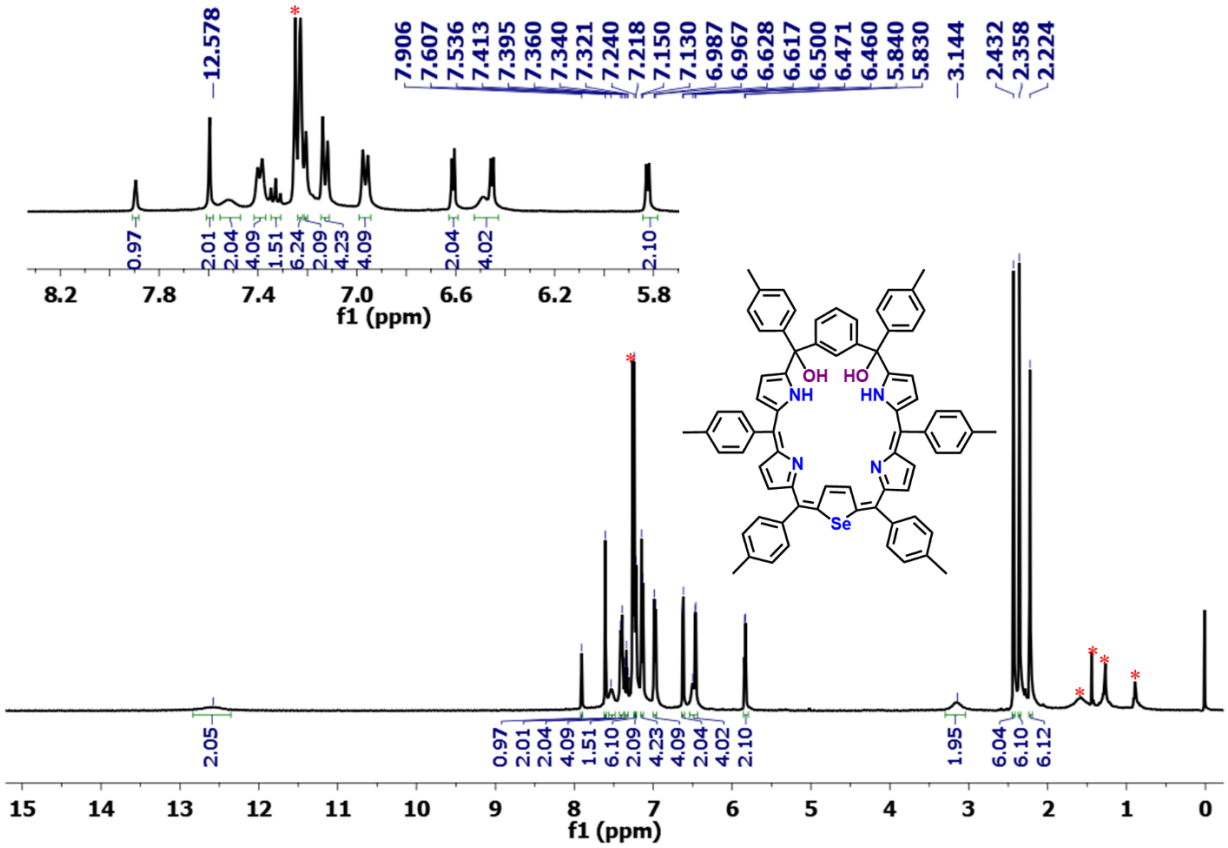


Figure S20. ^{1}H-NMR spectrum of the compound **4** recorded in $CDCl_3$ at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

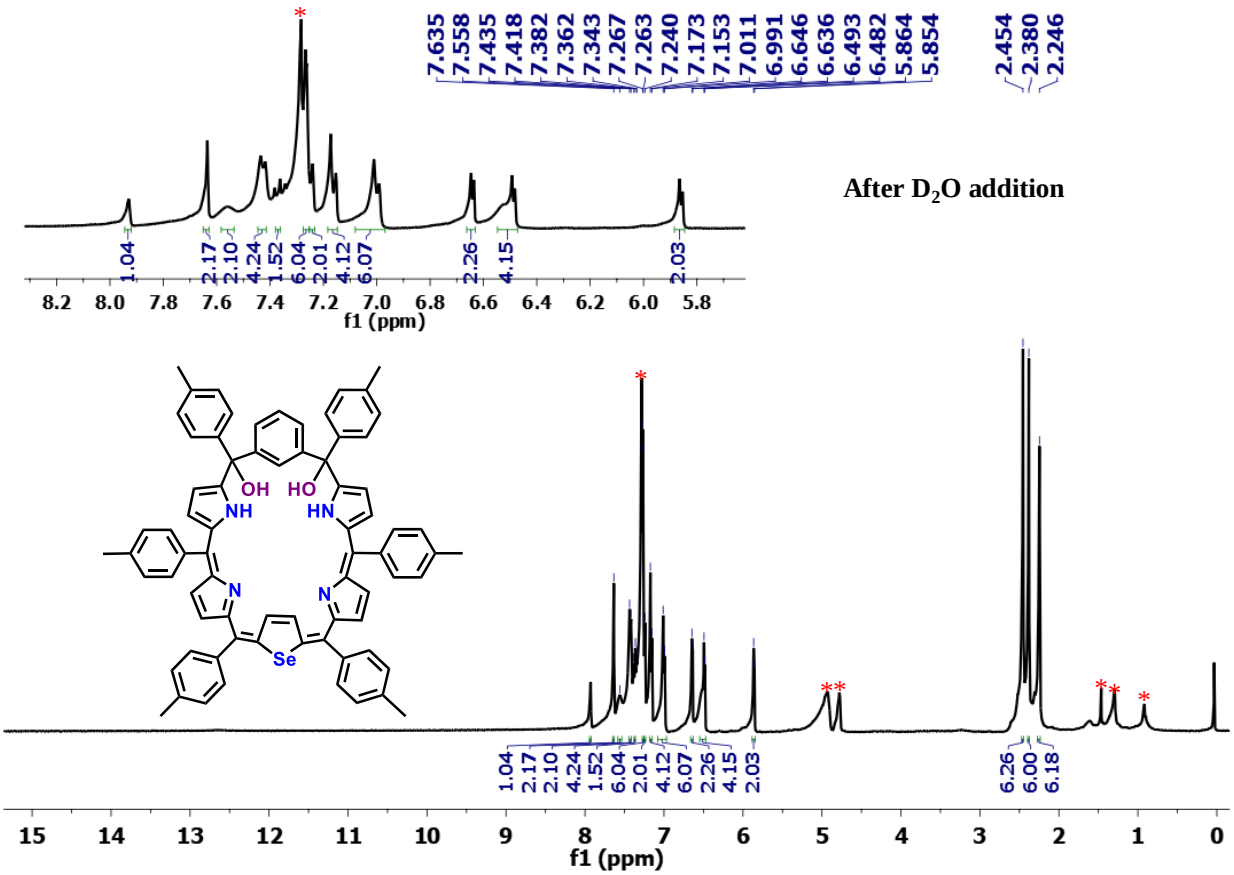
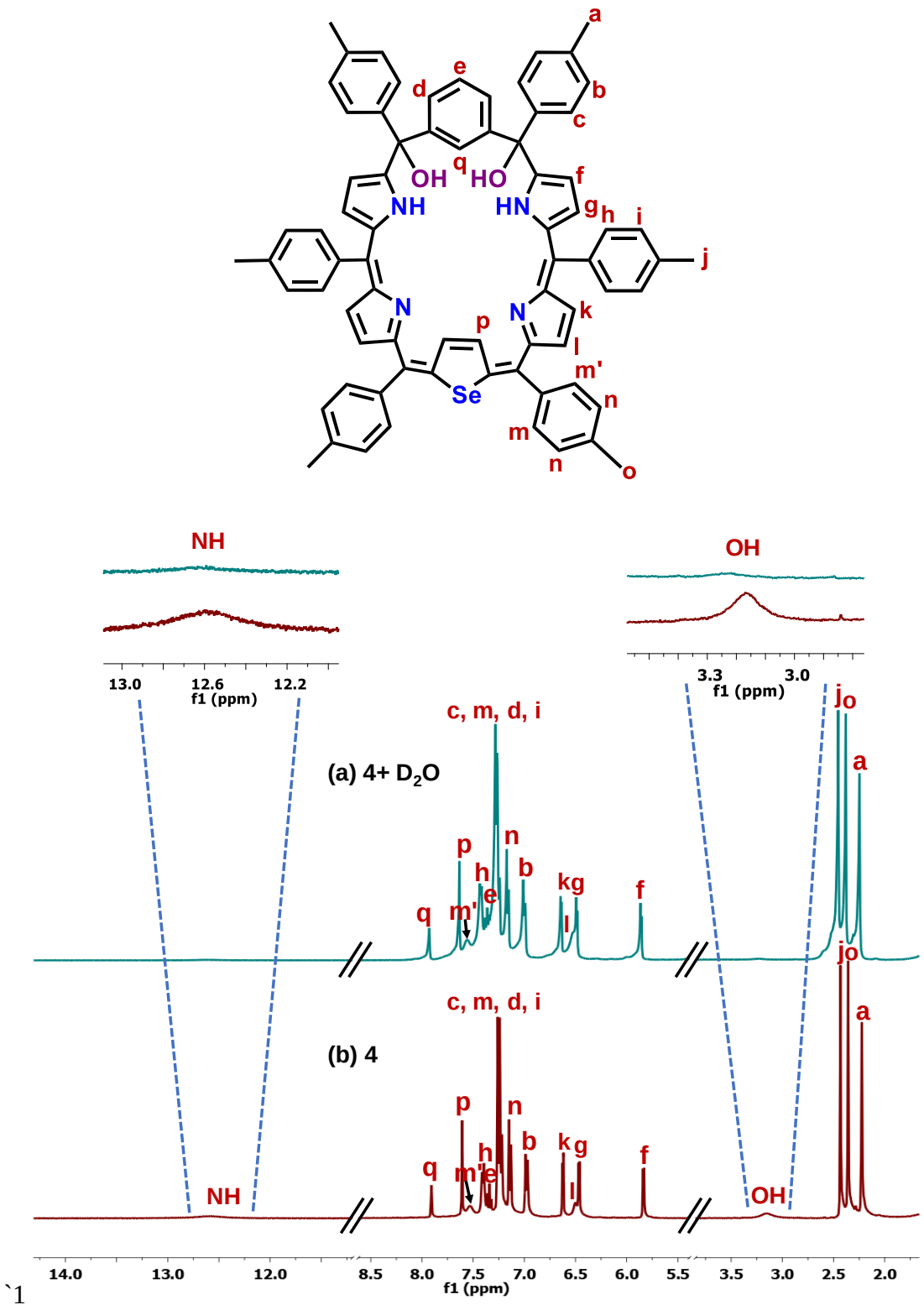


Figure S21. ^{1}H-NMR spectrum of the compound **4** recorded in $CDCl_3$ after addition of D_2O at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



`1

Figure S22. Comparison of ^{1}H-NMR spectrum of the compound **4** recorded in $CDCl_3$ at 298K (a) with D_2O and without D_2O (b) on 400 MHz NMR instrument.

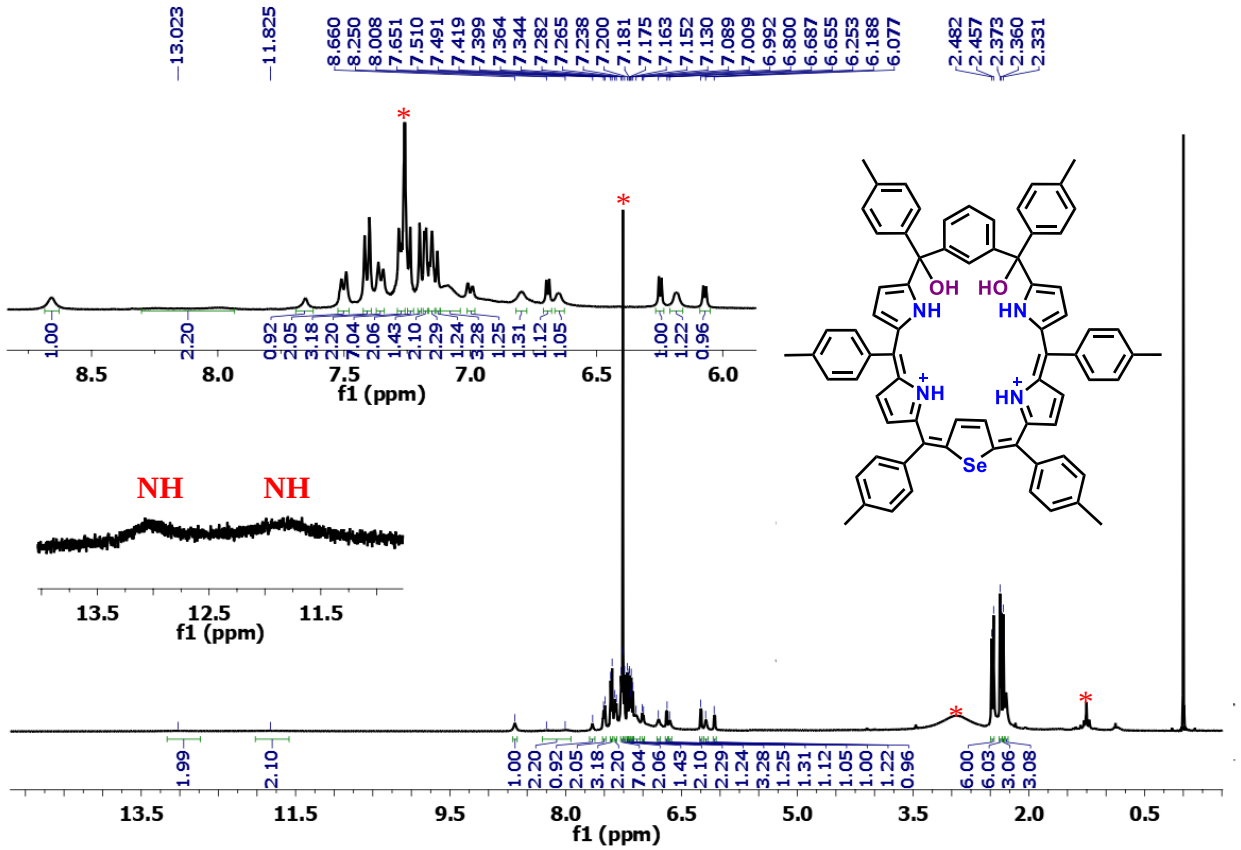


Figure S23. ^{1}H-NMR spectrum of the compound **4.2H**$^{+}$ recorded in $CDCl_3$ on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

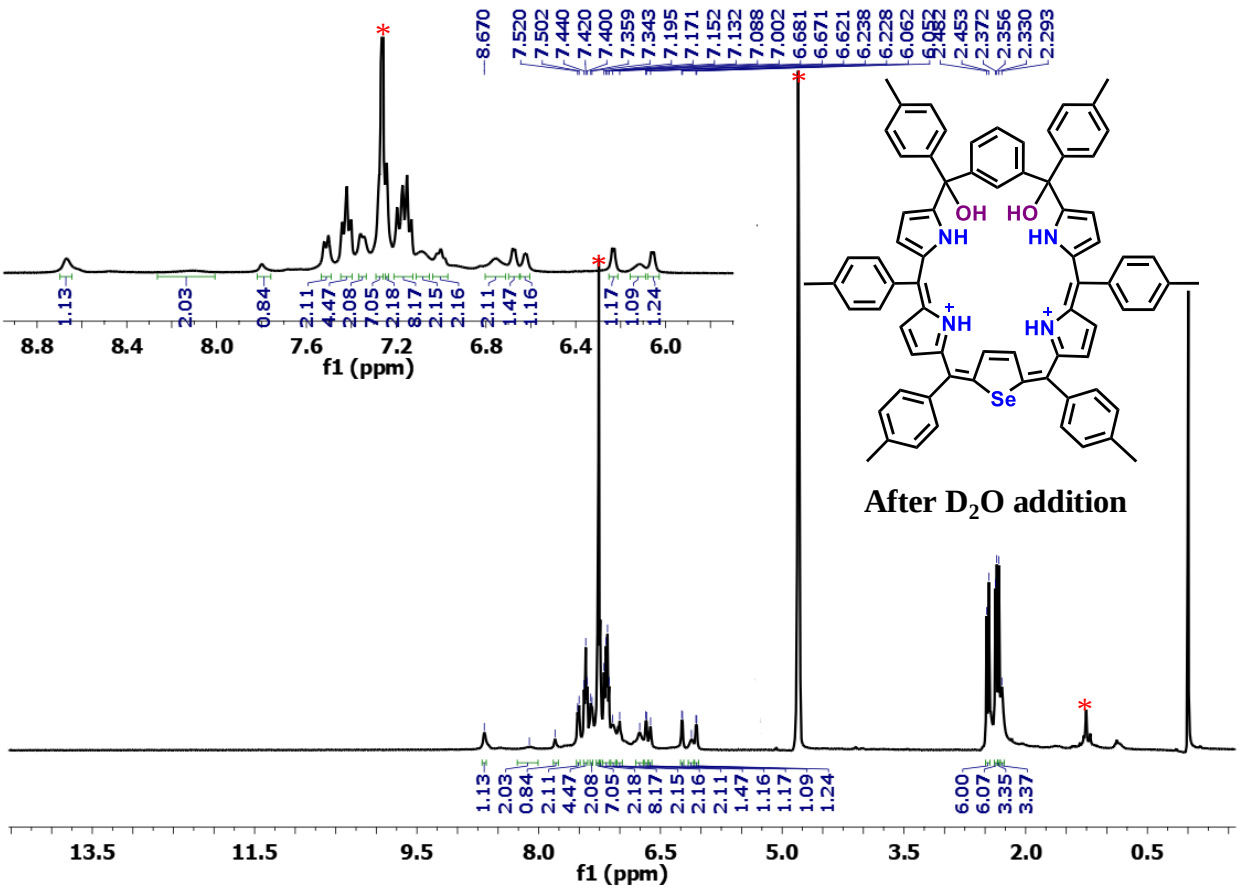


Figure S24. ^{1}H-NMR spectrum of the compound **4.2H**$^{+}$ recorded upon addition of D_2O in $CDCl_3$ at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

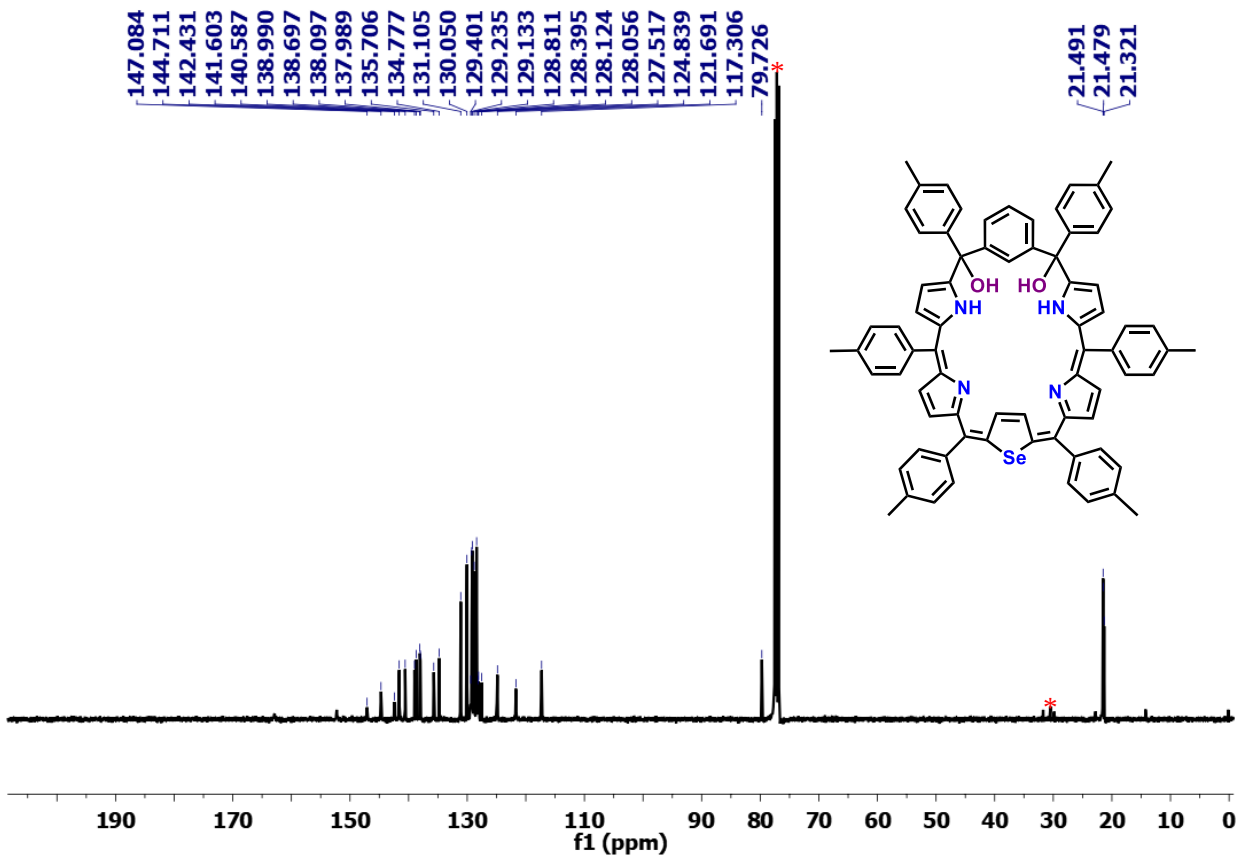


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **3** recorded in $CDCl_3$ on 101 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

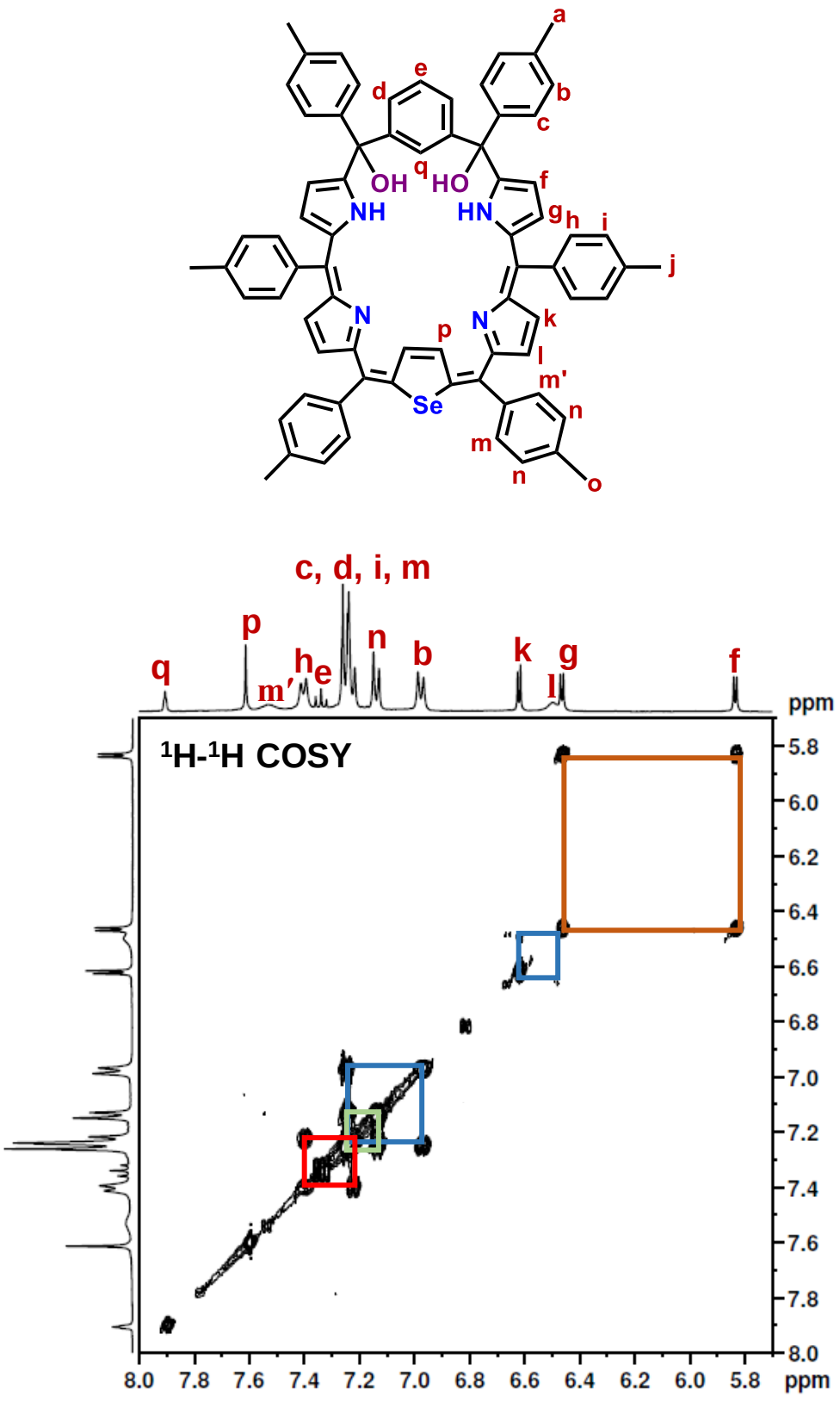


Figure S26. ^{1}H–^{1}H COSY of compound **4** recorded in $CDCl_3$ at 25 °C.

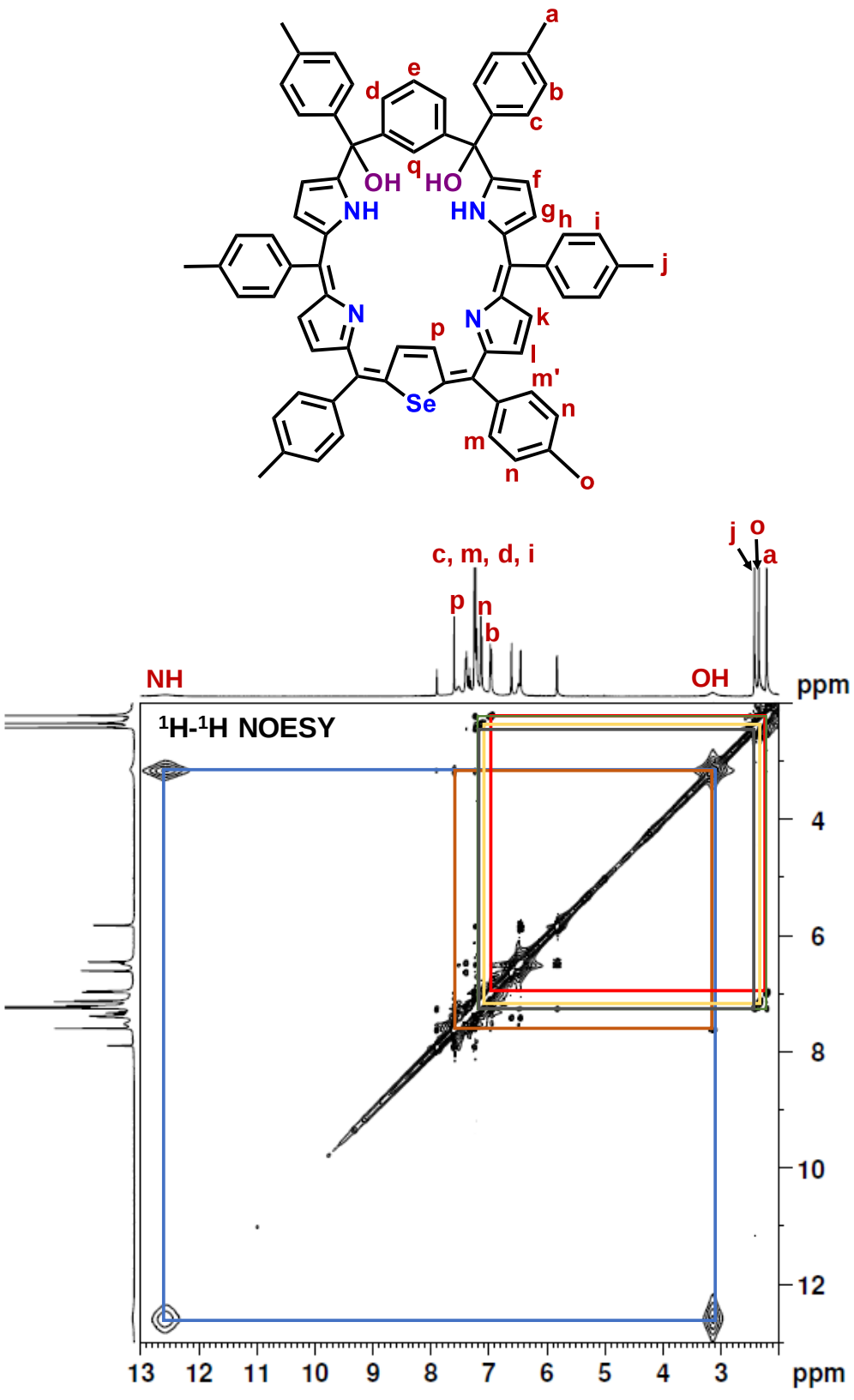


Figure S27. ^{1}H–^{1}H NOESY of compound **4** recorded in $CDCl_3$ at 25 °C.

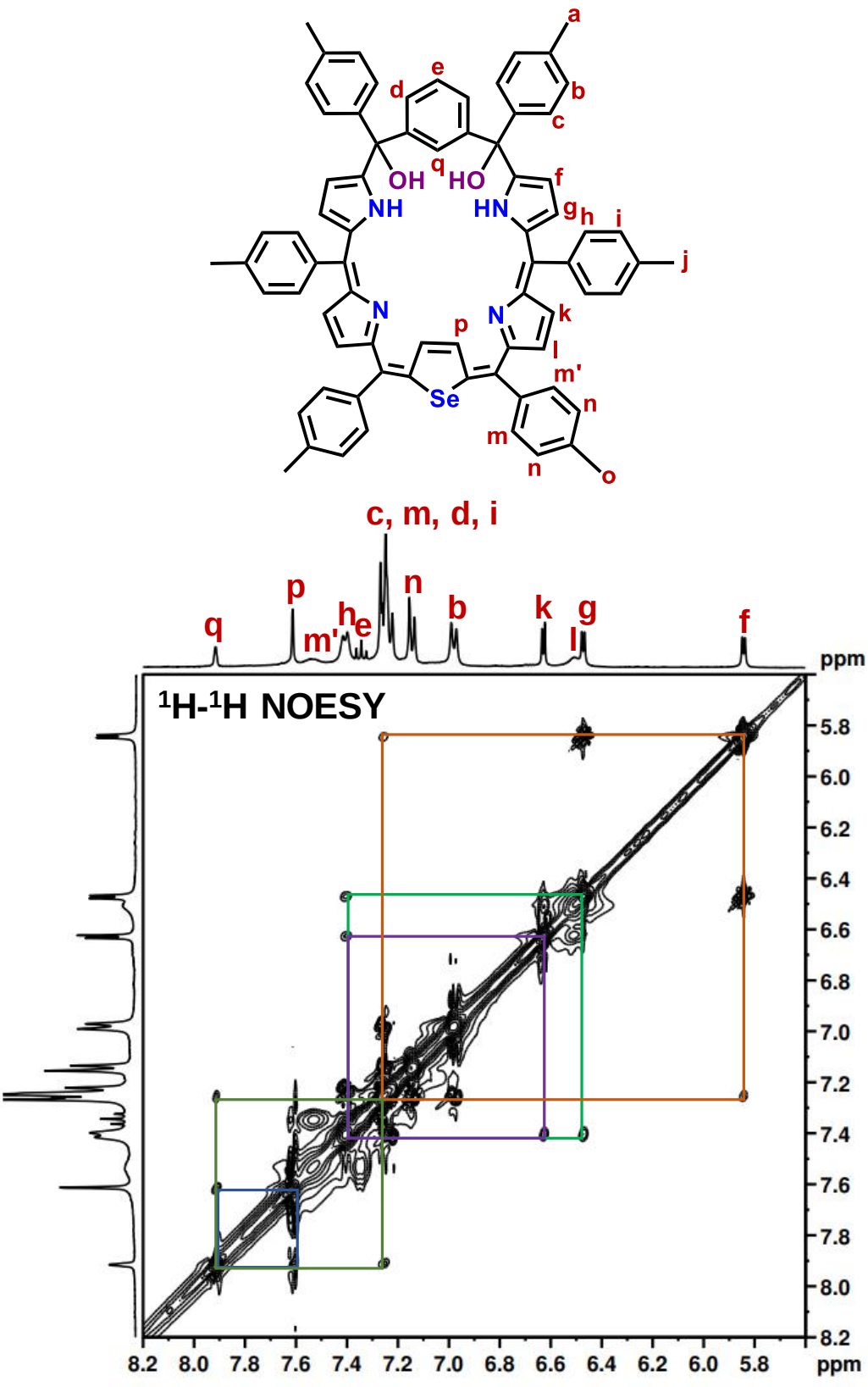


Figure S28. Expanded ^{1}H–^{1}H NOESY of compound **4** recorded in $CDCl_3$ at 25 °C.

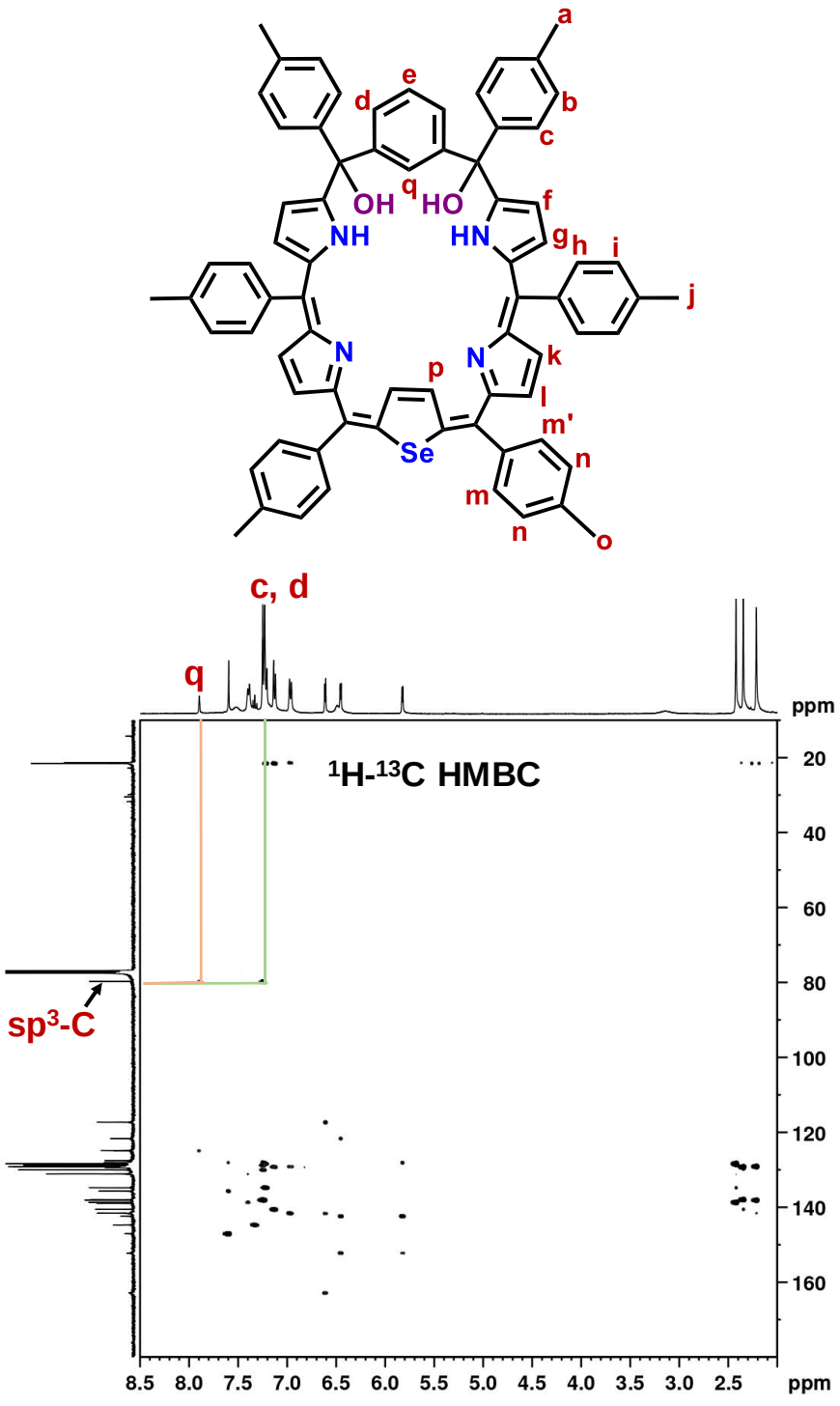
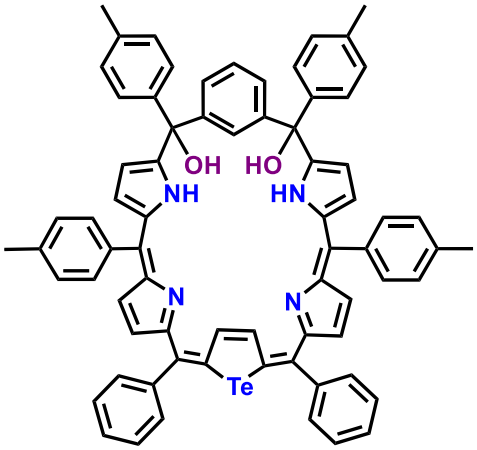


Figure S29. Partial ^{1}H NMR, partial ^{13}C NMR and partial ^{1}H-^{13}C HMBC spectra of compound **4** recorded in $CDCl_3$ at room temperature at 400 MHz NMR instrument.



Compound **5**

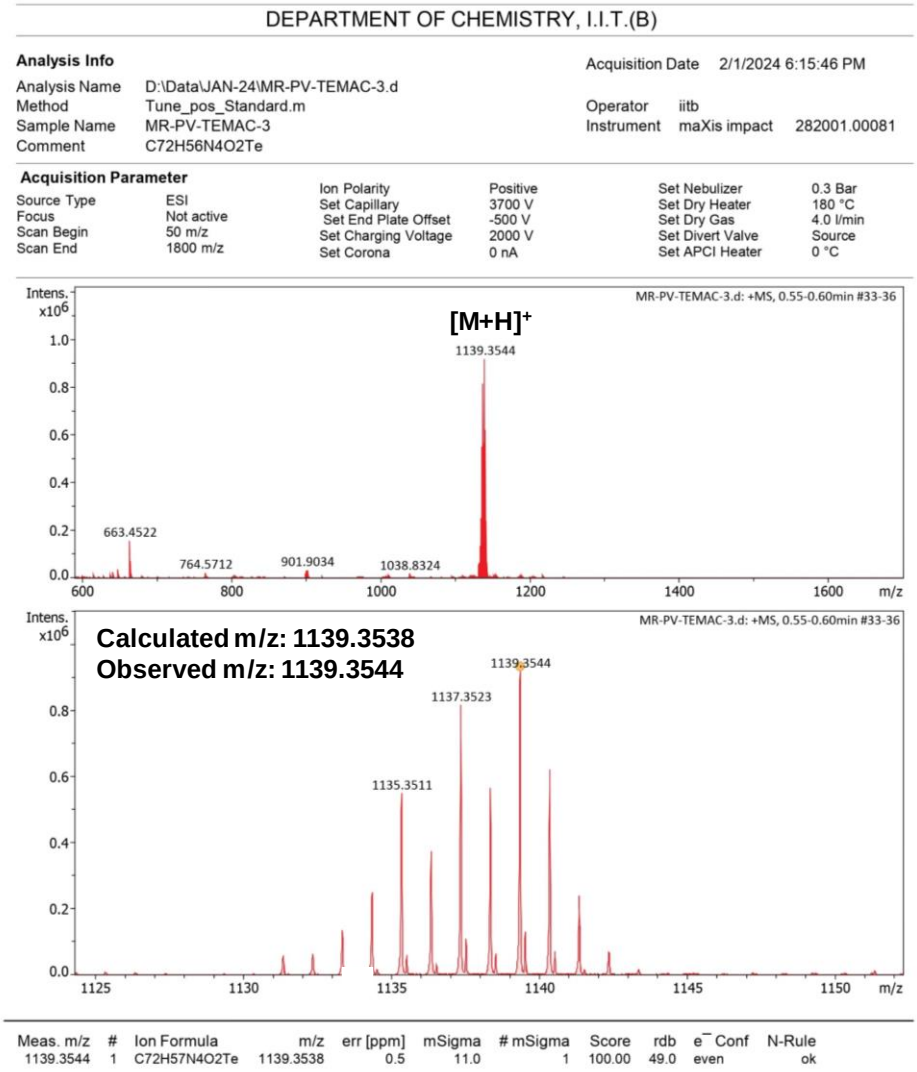


Figure S30. HR mass spectrum of the compound **5**.

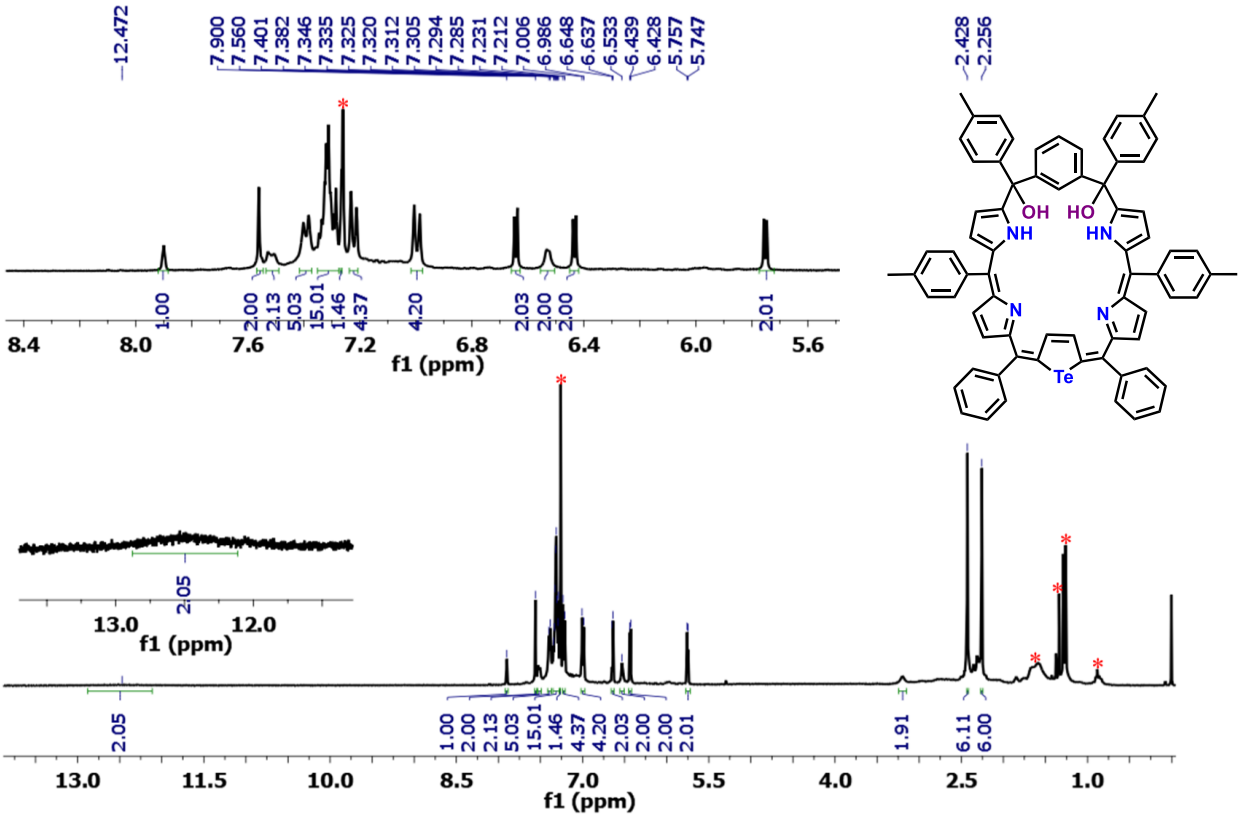


Figure S31. ^{1}H-NMR spectrum of the compound **5** recorded in $CDCl_3$ at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

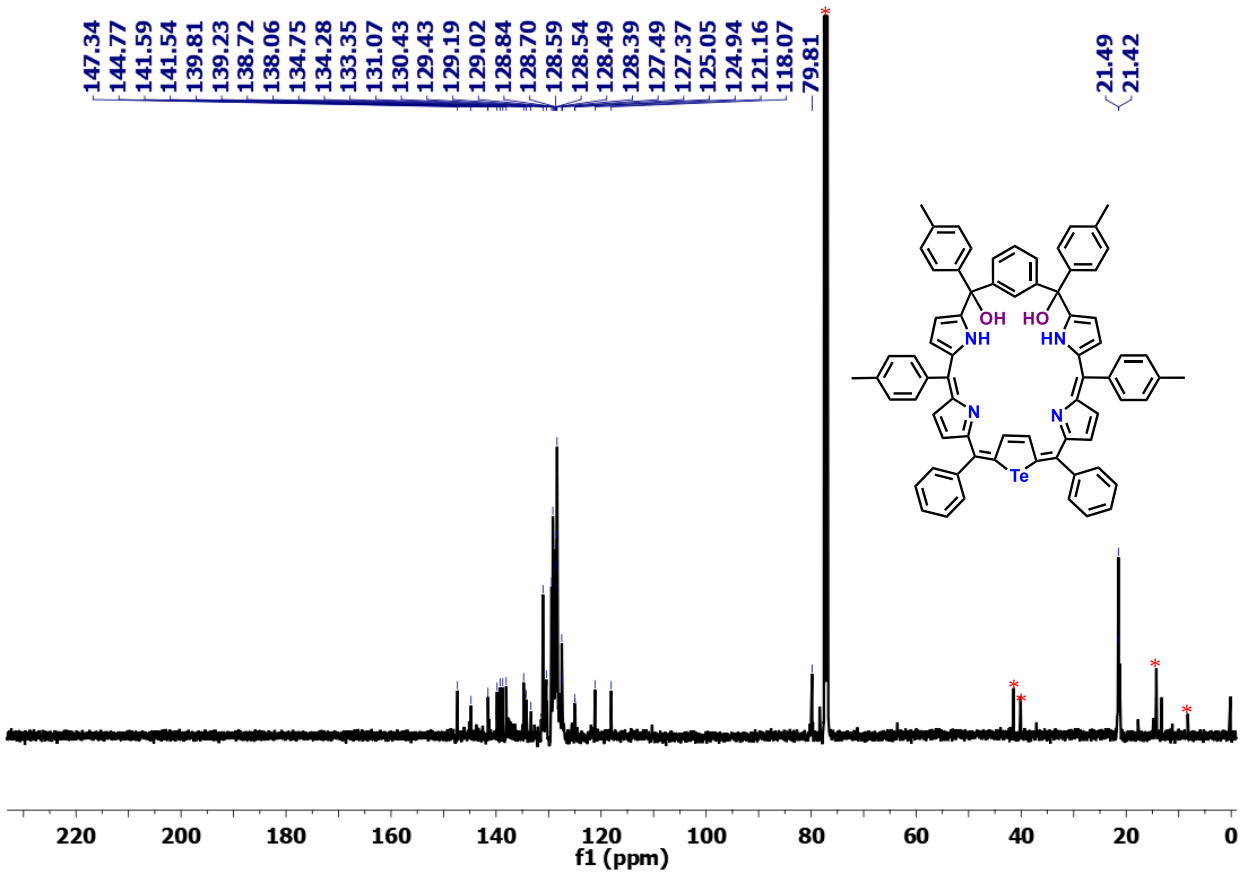
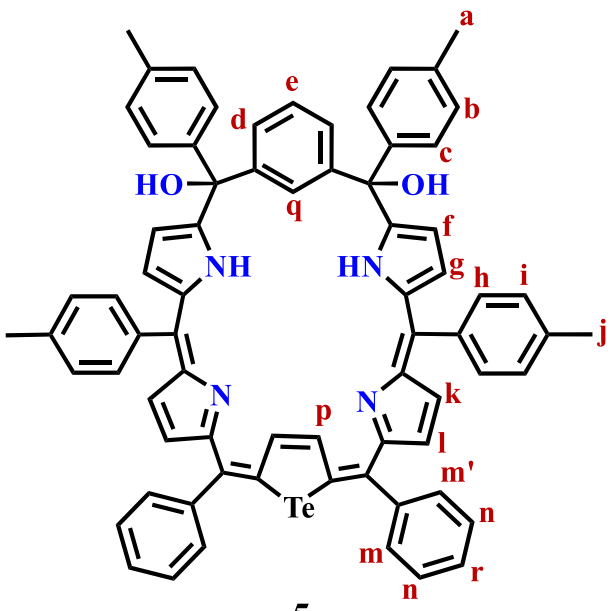


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of the compound **5** recorded in $CDCl_3$ at 25 °C on 126 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.



5

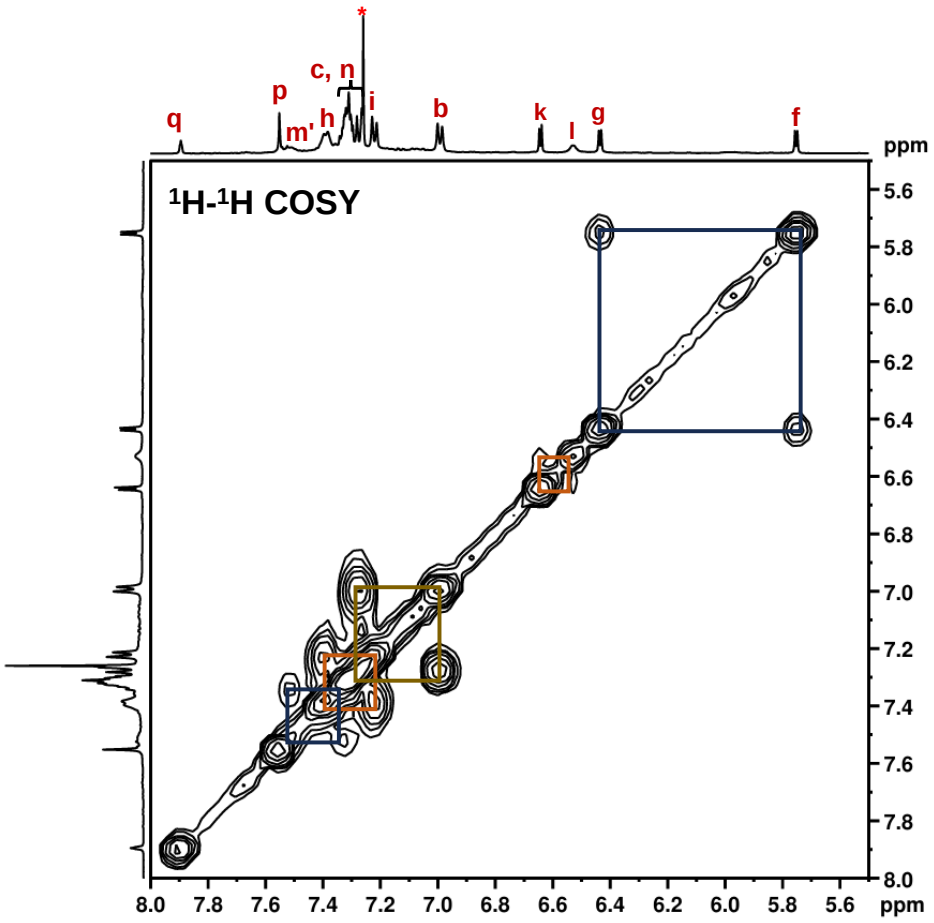
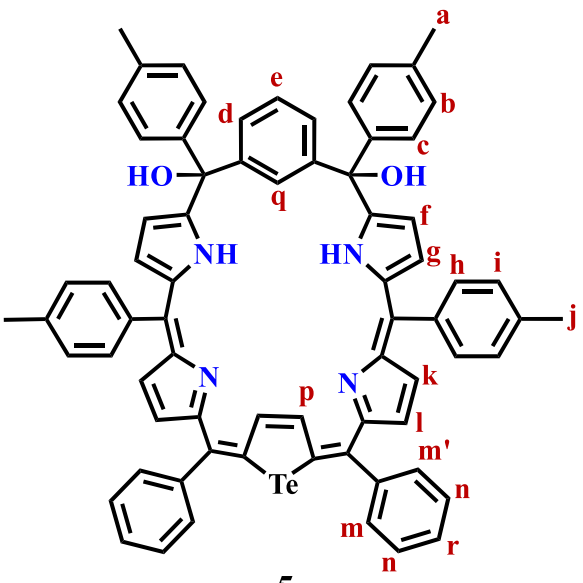


Figure S33. ^{1}H–^{1}H COSY of compound **5** recorded in $CDCl_3$ at 25 °C.



5

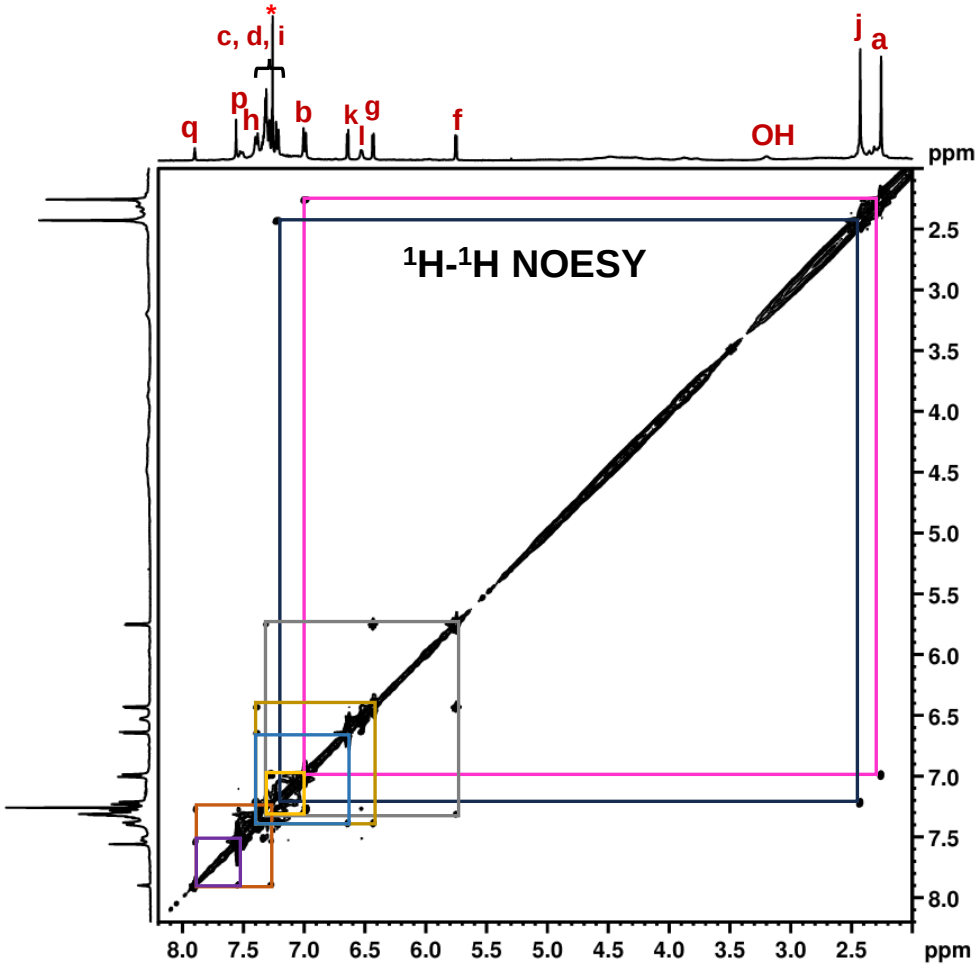
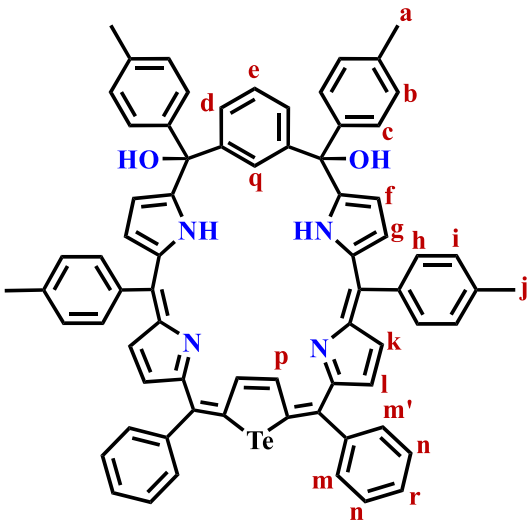


Figure S34. ^{1}H–^{1}H NOESY of compound **5** recorded in $CDCl_3$ at 25 °C.



5

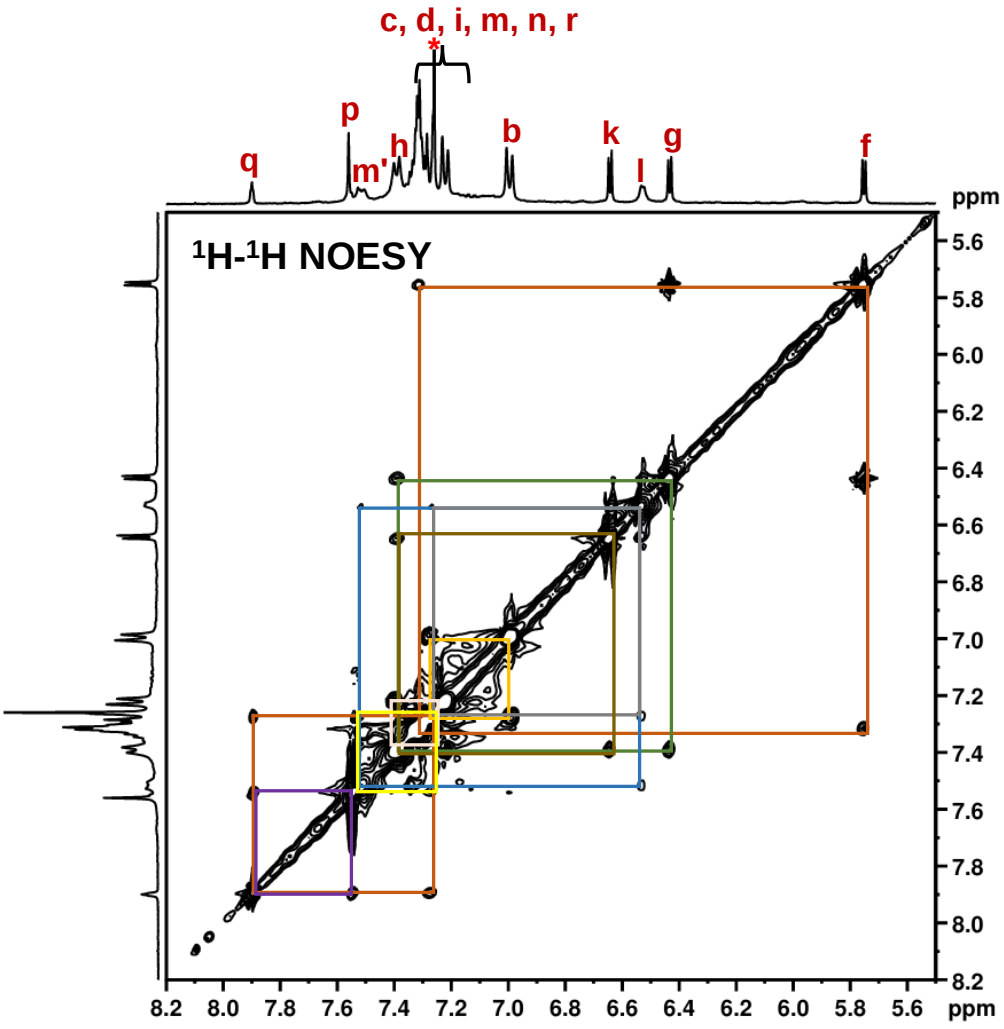


Figure S35. Expanded ^{1}H–^{1}H NOESY of compound **5** recorded in $CDCl_3$ at 25 °C.

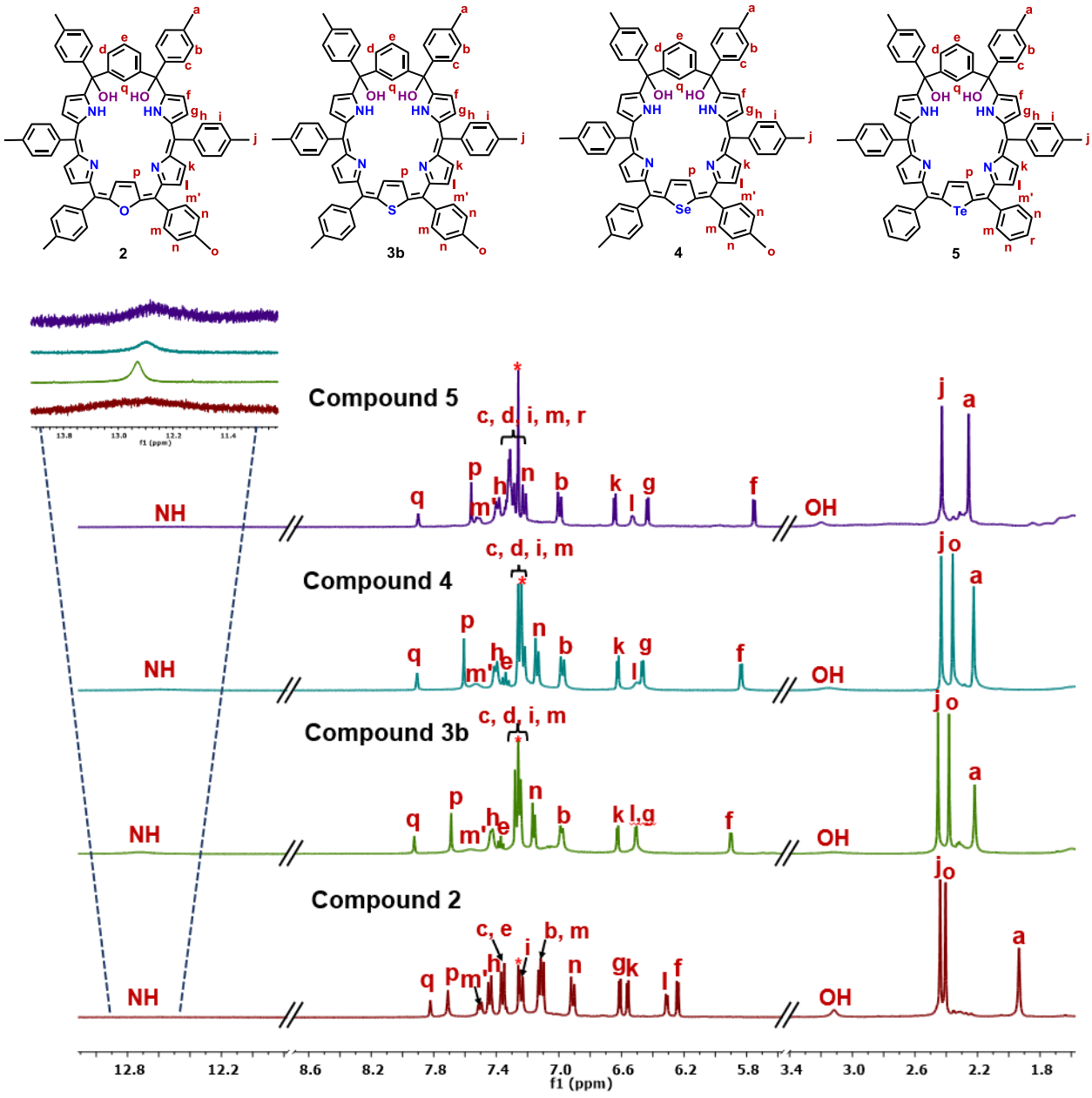


Figure S36. Comparison of partial ^{1}H-NMR spectra of the compounds **2-5** recorded in $CDCl_3$ at 25 °C on 400 MHz NMR instrument. Note: Peaks marked with asterisk (*) are due to residual solvents.

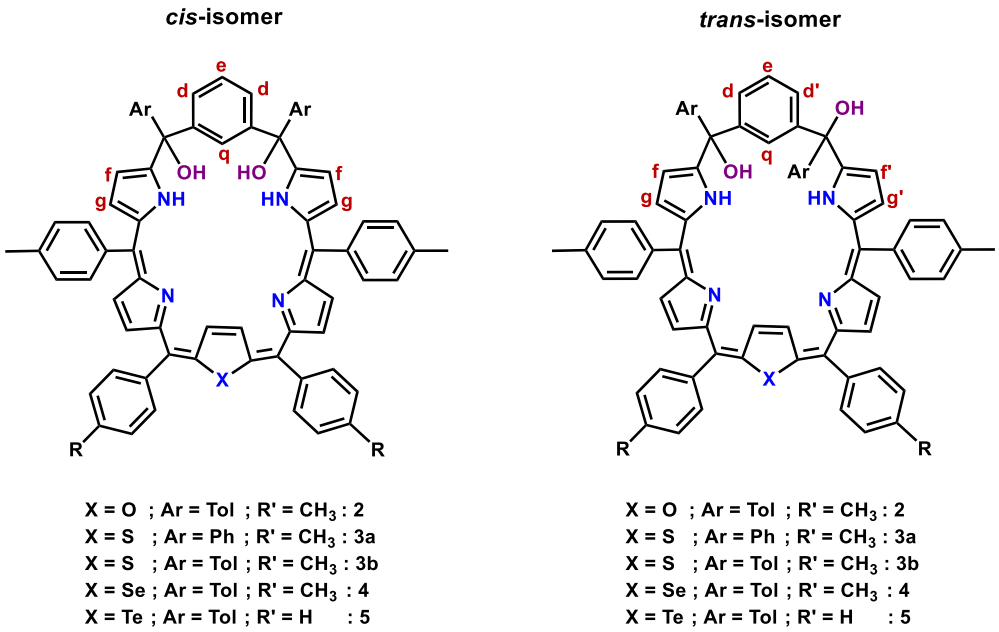


Figure S37. *Cis*- and *trans*-isomers of compounds **2-5**.

The ^{1}H-NMR spectra for compounds **2-5** are symmetrical, clearly indicating that the two hydroxy groups are in a *cis*-orientation. Moreover, the appearance of one set of *β*-pyrrole protons (*type* f), corresponding to two protons, reveals that they are in the same chemical environment. If the orientation of the two hydroxy groups were trans, the ^{1}H-NMR spectra for macrocycles **2-5** would be expected to be unsymmetrical. Additionally, in the ^{1}H-^{1}H NOESY spectrum of each of the compounds **2-5**, we would anticipate spatial correlations between the *β*-pyrrole proton and the *meso*-aryl proton (*type* c), while such correlations should be absent for the *β*-pyrrole proton that is distant from the *meso*-aryl proton (*type* c). However, we observed solely symmetrical ^{1}H-NMR spectra, conclusively indicating that the two hydroxy groups are in a *cis*-orientation in all the macrocycles **2-5**.

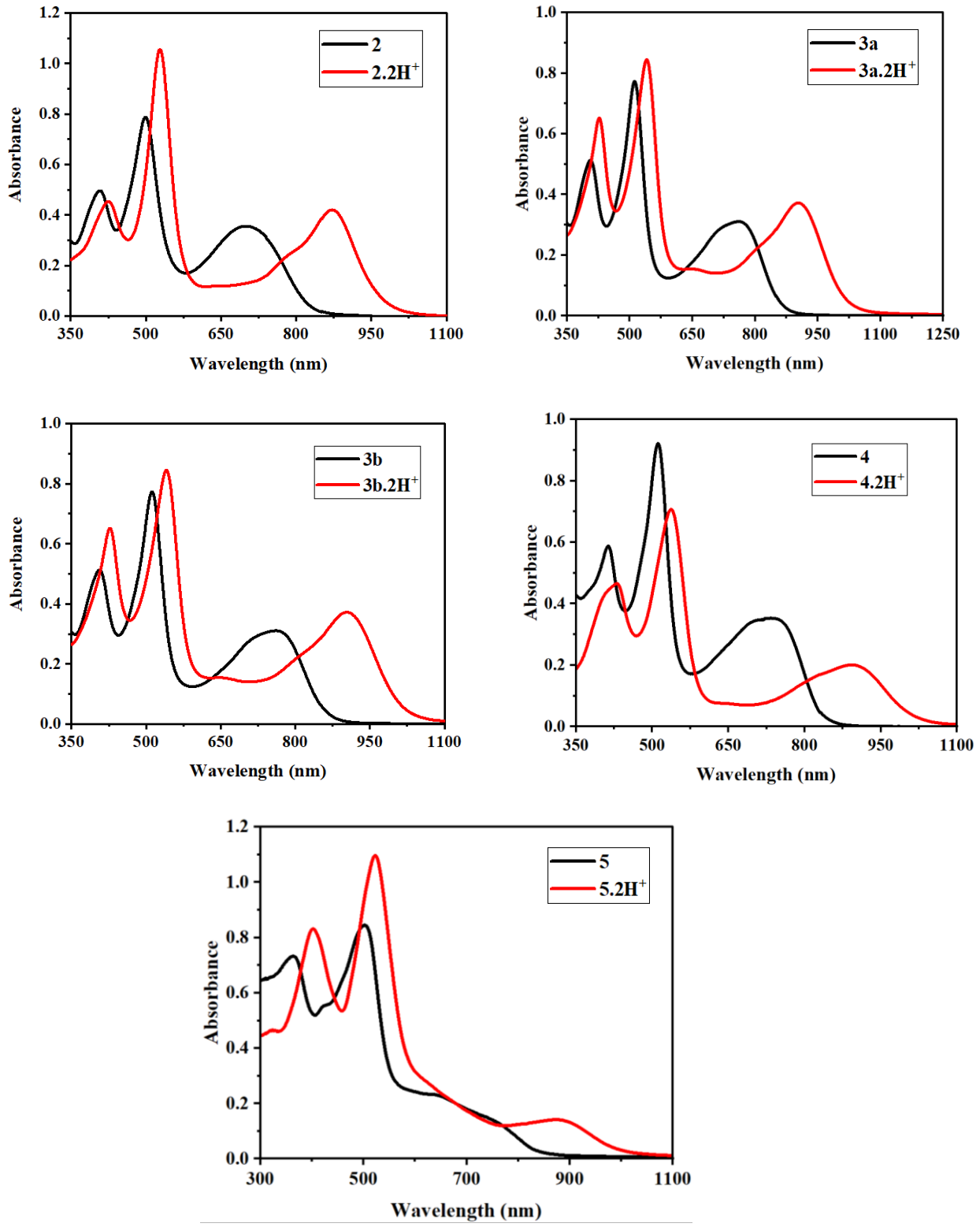


Figure S38. Comparison of absorption spectra of the compounds **2-5** (2×10^{-5} M) free base (black line) and in presence of TFA (excess) (red line) recorded in chloroform at room temperature.

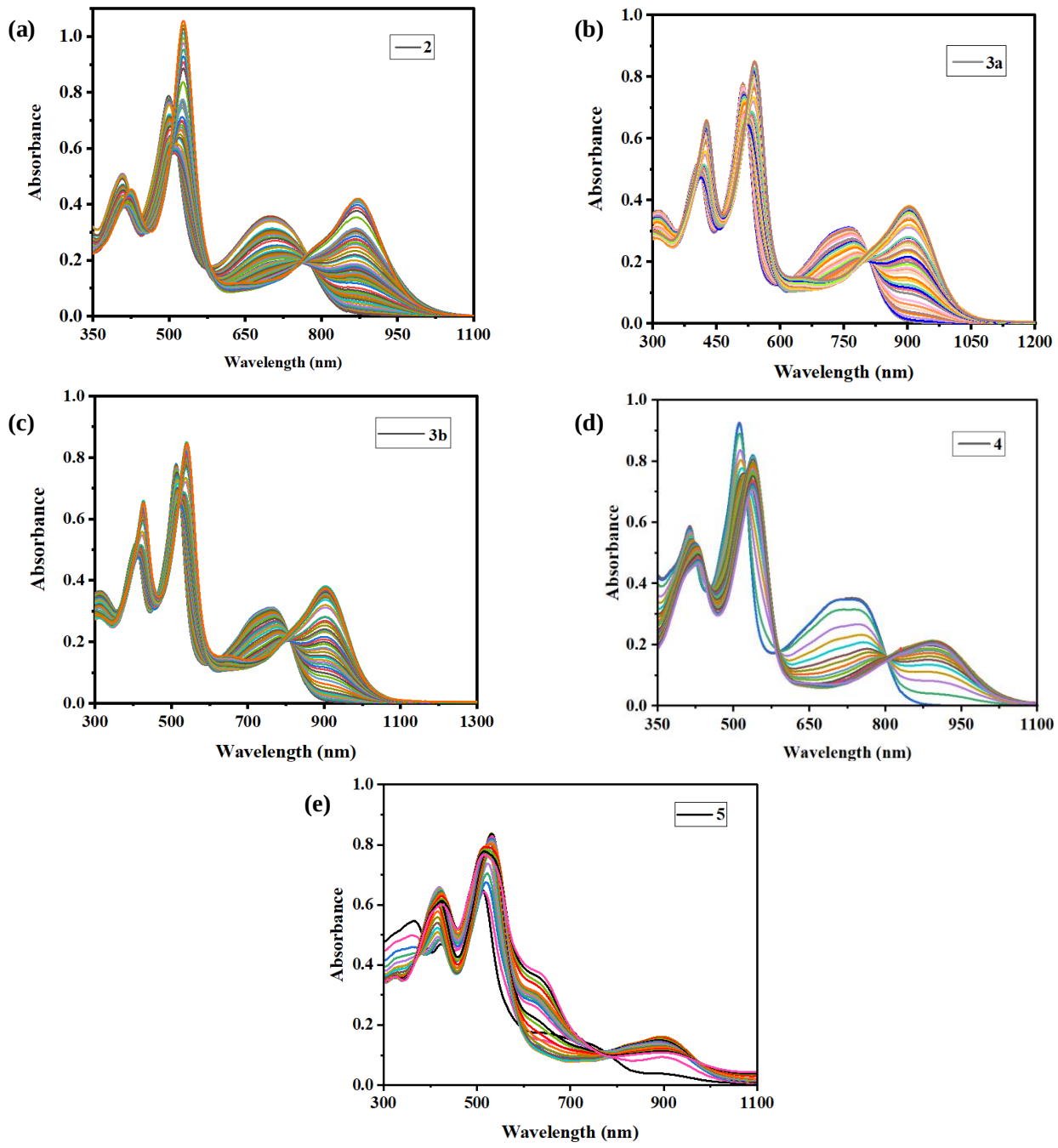


Figure S39. (a-d) Systematic titrations of $CHCl_3$ solutions of compounds **2-4** (2×10^{-5} M) with increasing addition of TFA (0-2 equiv.) recorded at room temperature; (e) Systematic titration of $CHCl_3$ solution of compound **5** (2×10^{-5} M) with increasing addition of $HClO_4$ (0-2.5 equiv.) recorded at room temperature.

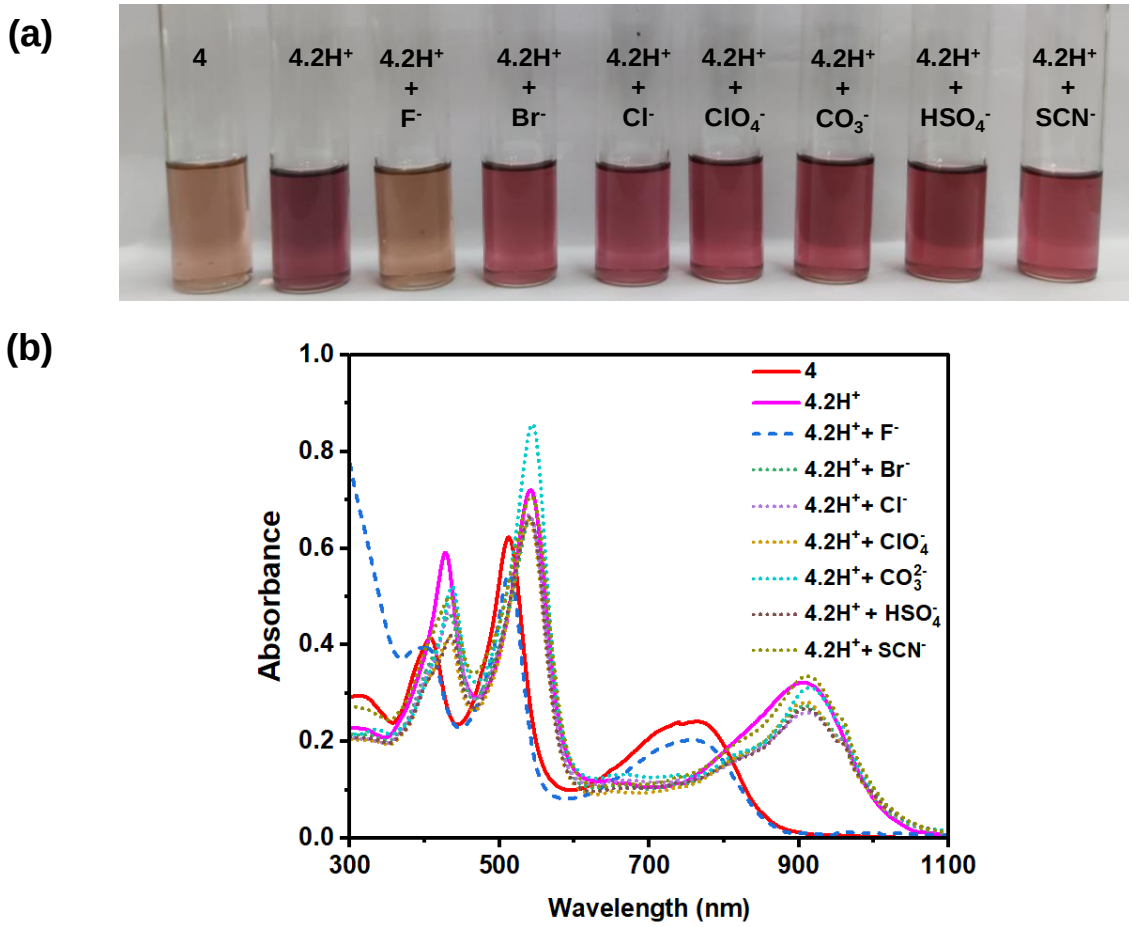


Figure S40. (a) Visual representation of solutions of **4** (2×10^{-5} M), **4.2H**$^{+}$ and **4.2H**$^{+}$ upon addition of various anions (excess) as their tetrabutylammonium salts in $CHCl_3$. (b) Absorption spectra of **4** (2×10^{-5} M), **4.2H**$^{+}$ and response of **4.2H**$^{+}$ to various anions (excess) as their tetrabutylammonium salts in $CHCl_3$.

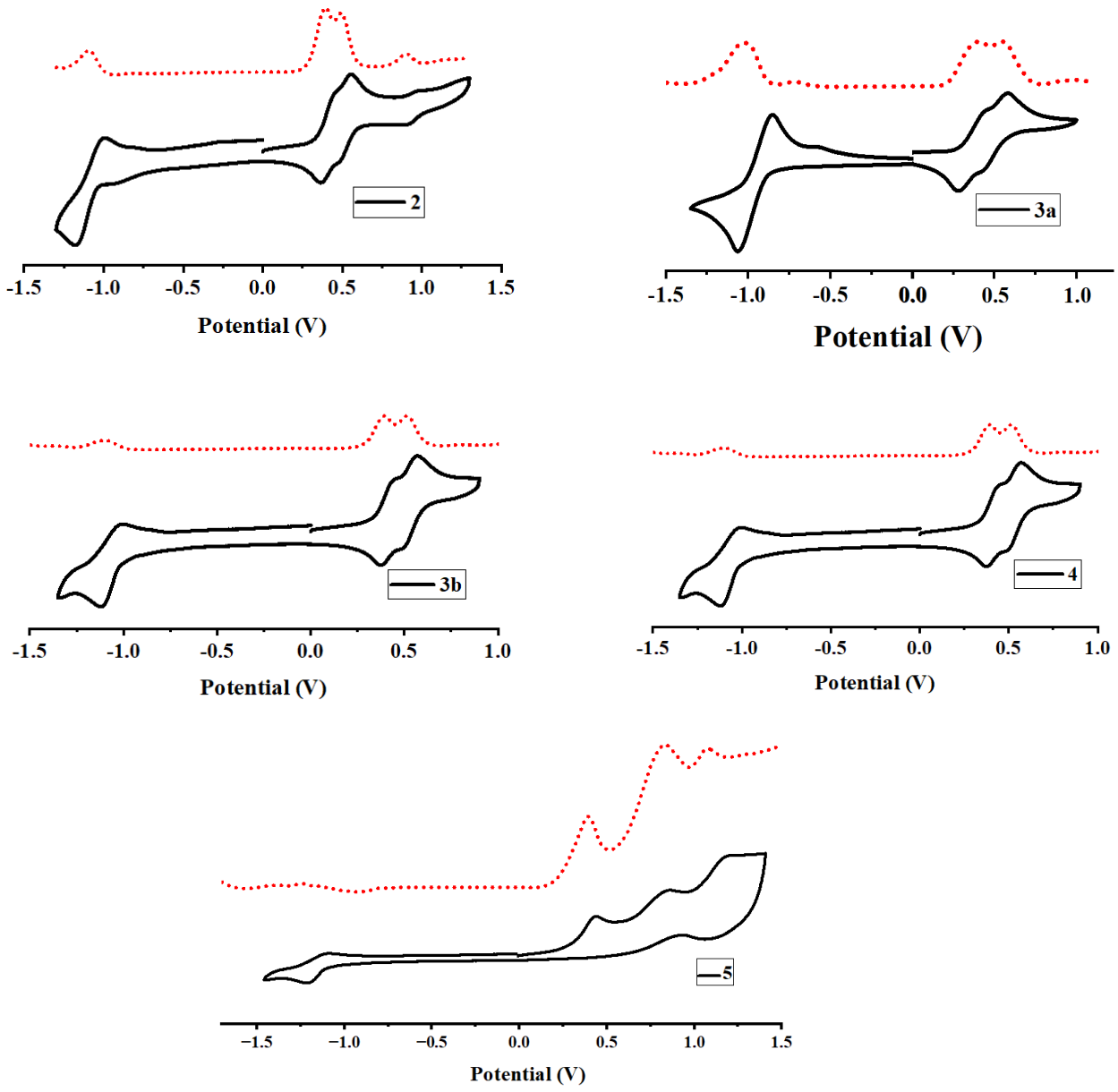


Figure S41. Comparison of cyclic voltammograms (black solid lines) along with differential pulse voltammograms (red dotted lines) of the compounds **2-5** recorded in CH_2Cl_2 containing 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at scan rates of 50 mV s^{-1}.

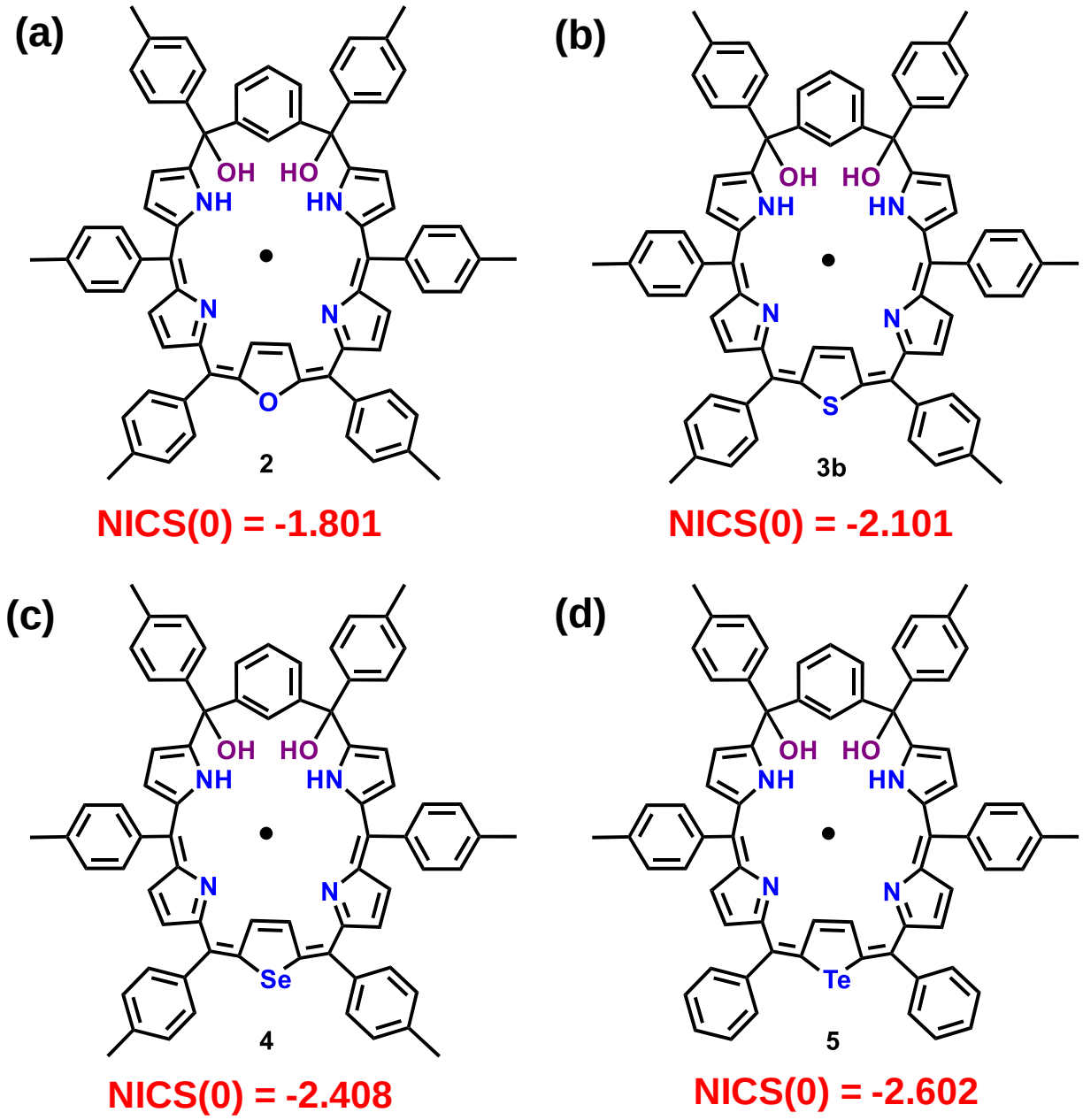


Figure S42. NICS(0) values of macrocycles **2**-**5**.

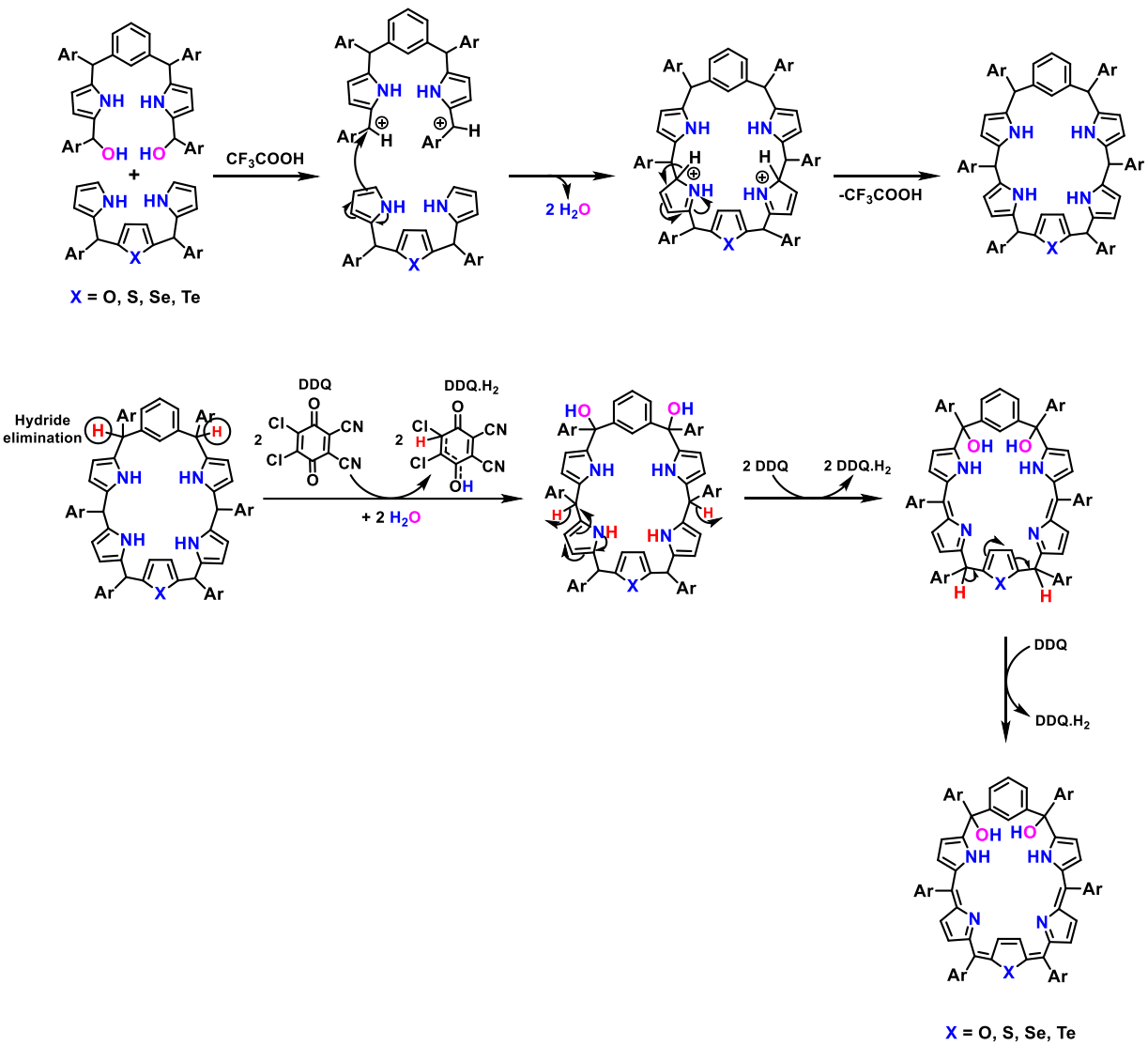


Figure S43. Probable mechanism for the formation of *m*-benziheterocalixhexaphyrin(1.*1*.*1*.1.1.1)s **2**-**5**. Note: All the different aryl groups are denoted as Ar in the molecular structures for simplicity.

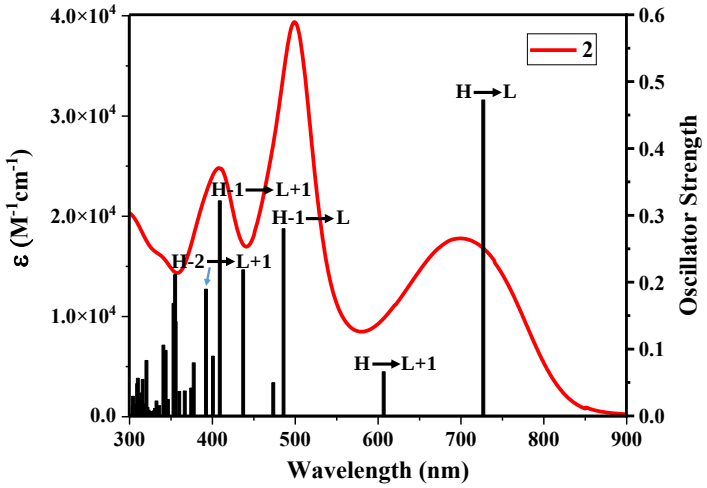


Figure S44. Calculated excitations (black vertical lines) and experimental absorption spectra (red line) for macrocycle **2**.

Table S1. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **2**.

Wavelength (nm)	Oscillator Strength	Major contributions
727.265	0.4725	HOMO->LUMO (99%)
607.022	0.066	HOMO->L+1 (91%)
486.232	0.2799	H-1->LUMO (89%)
473.873	0.0497	H-2->LUMO (46%), HOMO->L+2 (48%)
437.504	0.2185	H-2->LUMO (29%), H-1->L+1 (52%), HOMO->L+2 (15%)
409.297	0.3217	H-2->LUMO (16%), H-1->L+1 (38%), HOMO->L+2 (31%)
401.010	0.0894	H-3->LUMO (57%), H-2->L+1 (29%)
392.628	0.1895	H-3->LUMO (30%), H-2->L+1 (55%)
377.805	0.0794	H-4->LUMO (69%)
374.846	0.0417	H-6->LUMO (72%), H-4->LUMO (10%)
367.002	0.0374	H-5->LUMO (97%)
360.388	0.0367	H-3->L+1 (68%), H-1->L+2 (10%)
355.918	0.1412	H-9->LUMO (30%), H-7->LUMO (42%)
355.368	0.2112	H-9->LUMO (10%), H-7->LUMO (43%), H-1->L+2 (22%)
353.402	0.1683	H-9->LUMO (25%), H-1->L+2 (51%)
346.605	0.0246	H-10->LUMO (23%), H-8->LUMO (49%)
343.932	0.098	H-10->LUMO (33%), H-8->LUMO (20%), H-4->L+1 (15%)
341.253	0.1058	H-11->LUMO (14%), H-10->LUMO (35%), H-4->L+1 (32%)
336.237	0.0152	H-11->LUMO (63%), H-4->L+1 (28%)

334.785	0.0055	HOMO->L+3 (97%)
332.888	0.0224	H-6->L+1 (24%), H-2->L+2 (58%)
331.101	0.0112	H-13->LUMO (19%), H-12->LUMO (36%), H-5->L+1 (13%)
329.684	0.0077	H-13->LUMO (36%), H-12->LUMO (17%), H-5->L+1 (17%)
327.299	0.006	H-6->L+1 (28%), H-5->L+1 (11%), H-2->L+2 (23%)
327.135	0.0064	H-22->LUMO (30%), H-21->LUMO (27%), H-5->L+1 (10%)
326.532	0.0015	H-12->LUMO (18%), H-6->L+1 (21%), H-5->L+1 (39%)
323.381	0.0086	HOMO->L+4 (88%)
322.079	0.0127	H-21->LUMO (10%), H-14->LUMO (39%), H-13->LUMO (10%)
320.804	0.083	H-7->L+1 (60%)
320.116	0.0116	HOMO->L+5 (73%)
319.144	0.0082	H-15->LUMO (23%), H-14->LUMO (12%), HOMO->L+5 (10%)
317.257	0.0178	H-18->LUMO (10%), H-15->LUMO (19%), HOMO->L+6 (15%)
316.214	0.0546	H-15->LUMO (12%), HOMO->L+6 (37%)
315.473	0.0165	HOMO->L+7 (51%), HOMO->L+9 (10%)
314.976	0.0344	H-10->L+1 (14%), H-8->L+1 (21%), HOMO->L+6 (20%)
313.995	0.0054	H-8->L+1 (13%), HOMO->L+8 (40%)
312.925	0.0171	H-19->LUMO (10%), H-17->LUMO (12%), H-8->L+1 (12%), HOMO->L+8 (29%)
312.091	0.0331	H-19->LUMO (10%), H-10->L+1 (30%), HOMO->L+7 (11%)
311.510	0.0064	H-19->LUMO (25%), H-18->LUMO (12%), H-10->L+1 (15%), HOMO->L+8 (17%)
310.411	0.0564	HOMO->L+9 (50%), HOMO->L+10 (17%), HOMO->L+11 (10%)
309.581	0.0482	H-9->L+1 (63%)
308.066	0.0002	H-17->LUMO (35%), H-16->LUMO (45%)
307.676	0.0179	HOMO->L+7 (12%), HOMO->L+9 (25%), HOMO->L+10 (42%)
306.793	0.0036	H-20->LUMO (61%), H-20->L+1 (14%)
305.696	0.0074	H-11->L+1 (58%), H-10->L+1 (16%)
304.607	0.0293	H-19->LUMO (11%), H-16->LUMO (10%), HOMO->L+10 (13%), HOMO->L+11 (28%)
304.256	0.0149	H-19->LUMO (15%), H-18->LUMO (19%), H-16->LUMO (13%), HOMO->L+11 (10%)
300.699	0.0025	H-3->L+2 (13%), HOMO->L+12 (30%), HOMO->L+13 (23%)
298.613	0.0081	H-12->L+1 (79%)

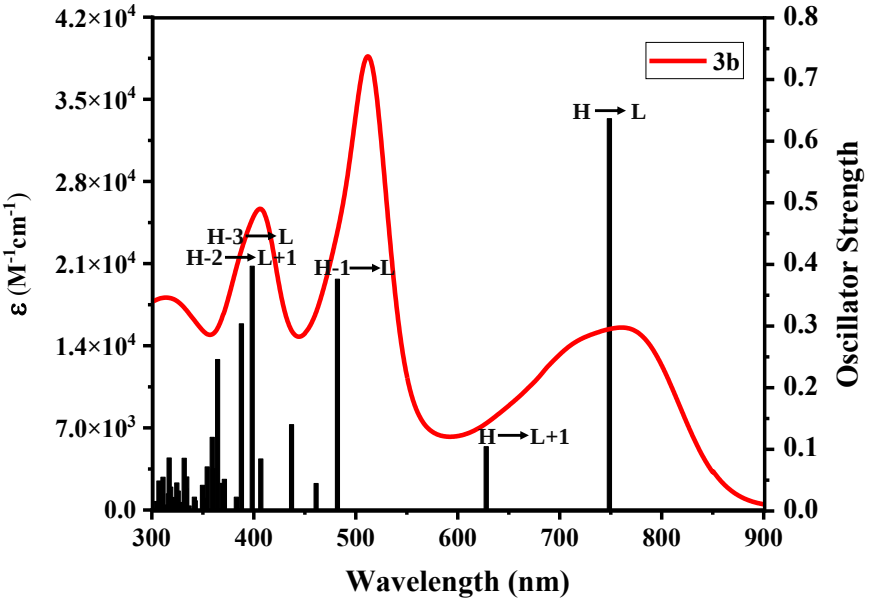


Figure S45. Calculated excitations (black vertical lines) and experimental absorption spectra (red line) for macrocycle **3b**.

Table S2. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **3b**.

Wavelength (nm)	Oscillator Strength	Major contributions
747.929	0.6364	HOMO->LUMO (99%)
627.196	0.1042	HOMO->L+1 (92%)
481.286	0.376	H-1->LUMO (88%)
460.377	0.0445	H-2->LUMO (65%), HOMO->L+2 (29%)
436.288	0.14	H-2->LUMO (13%), H-1->L+1 (74%)
406.186	0.0843	H-3->LUMO (20%), H-2->L+1 (36%), HOMO->L+2 (19%)
397.717	0.397	H-3->LUMO (30%), H-1->L+1 (10%), HOMO->L+2 (30%)
387.172	0.3036	H-3->LUMO (42%), H-2->L+1 (48%)
382.219	0.0225	H-5->LUMO (15%), H-4->LUMO (64%)
370.489	0.0513	H-8->LUMO (16%), H-7->LUMO (21%), H-6->LUMO (18%), H-4->LUMO (11%)
368.288	0.0449	H-5->LUMO (62%), H-4->LUMO (14%)
363.803	0.2457	H-8->LUMO (10%), H-7->LUMO (17%), H-6->LUMO (47%)
359.281	0.0685	H-9->LUMO (35%), H-7->LUMO (10%), H-6->LUMO (16%)
358.553	0.1194	H-9->LUMO (12%), H-8->LUMO (38%), H-7->LUMO (29%)
353.574	0.0714	H-11->LUMO (29%), H-9->LUMO (11%), H-3->L+1 (41%)

350.327	0.0207	H-12->LUMO (13%), H-11->LUMO (22%), H-10->LUMO (27%), H-3->L+1 (15%)
348.986	0.0417	H-11->LUMO (21%), H-10->LUMO (31%), H-3->L+1 (14%)
341.884	0.0165	H-4->L+1 (45%), HOMO->L+3 (11%)
341.000	0.0224	HOMO->L+3 (79%)
337.804	0.0001	H-12->LUMO (63%), H-10->LUMO (16%)
335.828	0.0081	H-16->LUMO (14%), H-1->L+2 (22%)
333.569	0.0553	H-15->LUMO (31%)
332.951	0.0361	H-16->LUMO (11%), H-13->LUMO (19%), H-1->L+2 (24%), HOMO->L+4 (11%)
332.290	0.0033	H-13->LUMO (19%), HOMO->L+4 (54%)
331.713	0.0295	H-5->L+1 (37%), H-4->L+1 (13%), HOMO->L+4 (14%)
331.013	0.0855	H-13->LUMO (19%), H-5->L+1 (18%), H-1->L+2 (22%), HOMO->L+4 (12%)
328.748	0.0137	H-16->LUMO (17%), H-14->LUMO (49%)
327.040	0.0046	H-7->L+1 (14%), H-6->L+1 (61%)
325.213	0.0324	H-15->LUMO (16%), H-7->L+1 (25%)
323.803	0.0454	H-9->L+1 (19%), H-7->L+1 (27%), H-6->L+1 (13%)
323.094	0.007	H-22->LUMO (27%), H-9->L+1 (22%)
320.588	0.0161	H-23->LUMO (23%), H-19->LUMO (15%), H-18->LUMO (11%), H-16->LUMO (12%)
319.341	0.022	H-11->L+1 (11%), H-9->L+1 (12%), H-8->L+1 (32%)
318.742	0.0192	H-18->LUMO (20%), HOMO->L+7 (11%), HOMO->L+11 (13%)
317.851	0.0388	HOMO->L+7 (15%), HOMO->L+11 (11%)
317.436	0.0025	H-20->LUMO (26%), HOMO->L+6 (33%)
316.642	0.0006	H-19->LUMO (12%), HOMO->L+8 (35%)
316.335	0.086	HOMO->L+5 (16%), HOMO->L+7 (11%), HOMO->L+11 (22%), HOMO->L+12 (10%)
315.940	0.009	H-10->L+1 (19%), HOMO->L+5 (48%)
315.465	0.0279	H-10->L+1 (31%), HOMO->L+5 (11%)
313.717	0.0059	H-18->LUMO (11%), H-17->LUMO (22%), HOMO->L+7 (21%), HOMO->L+8 (16%)
313.384	0.0097	H-20->LUMO (11%), H-19->LUMO (13%), H-17->LUMO (10%), H-11->L+1 (12%), HOMO->L+6 (19%), HOMO->L+7 (12%)
312.807	0.0035	H-20->LUMO (17%), H-17->LUMO (28%), HOMO->L+6 (18%)
312.366	0.0068	H-11->L+1 (38%), H-8->L+1 (11%), H-2->L+2 (12%)
310.302	0.0547	H-2->L+2 (17%), HOMO->L+8 (23%), HOMO->L+13 (16%)

308.495	0.0192	H-2->L+2 (35%), HOMO->L+10 (26%), HOMO->L+11 (12%)
307.104	0.0258	H-12->L+1 (59%)
306.315	0.0486	H-12->L+1 (13%), H-2->L+2 (20%), HOMO->L+9 (27%), HOMO->L+10 (14%)
304.607	0.0022	H-21->LUMO (81%)

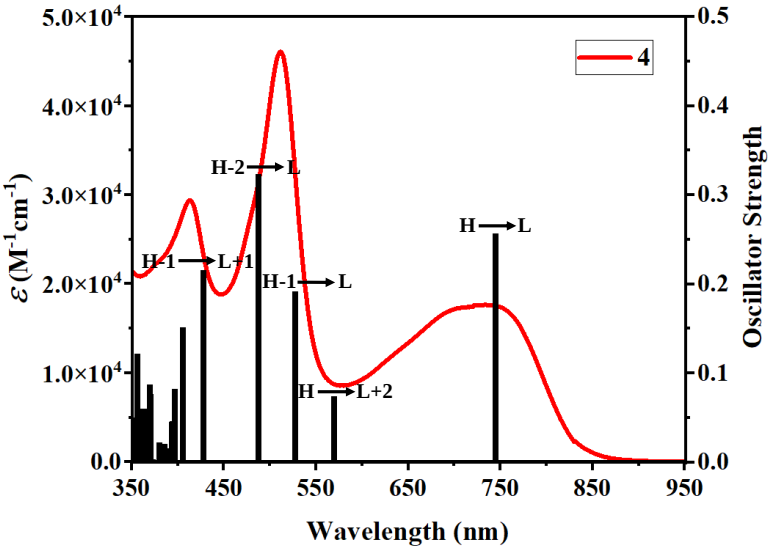


Figure S46. Calculated excitations (black vertical lines) and experimental absorption spectra (red line) for macrocycle **4**.

Table S3. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **4**.

Wavelength (nm)	Oscillator Strength	Major contributions
1026.359	0.3500	HOMO->LUMO (95%)
743.578	0.2568	HOMO->L+1 (89%)
568.396	0.0738	H-2->LUMO (20%), HOMO->L+2 (77%)
526.293	0.1916	H-1->LUMO (85%)
486.441	0.3231	H-2->LUMO (74%), HOMO->L+2 (16%)
426.943	0.2151	H-1->L+1 (90%)
404.516	0.1515	H-2->L+1 (86%)
395.446	0.0821	H-3->LUMO (87%)
393.002	0.0456	H-7->LUMO (10%), H-6->LUMO (23%), H-5->LUMO (45%), H-4->LUMO (11%)
386.015	0.0156	H-6->LUMO (15%), HOMO->L+3 (72%)

384.602	0.02	H-6->LUMO (39%), H-4->LUMO (17%), HOMO->L+3 (25%)
378.797	0.0223	H-5->LUMO (30%), H-4->LUMO (57%)
372.113	0.0027	HOMO->L+4 (90%)
369.661	0.0759	H-7->LUMO (51%), H-1->L+2 (19%)
368.990	0.0018	HOMO->L+5 (81%), HOMO->L+6 (12%)
368.474	0.0872	H-8->LUMO (13%), H-7->LUMO (26%), H-1->L+2 (41%)
366.156	0.0582	H-8->LUMO (44%), H-1->L+2 (28%)
364.188	0.0538	H-8->LUMO (18%), HOMO->L+6 (32%), HOMO->L+10 (18%)
361.807	0.0601	HOMO->L+6 (21%), HOMO->L+10 (40%)
358.315	0.0061	H-10->LUMO (43%), H-9->LUMO (33%)
356.000	0.0198	HOMO->L+7 (83%), HOMO->L+8 (11%)
355.276	0.1217	H-10->LUMO (22%), H-9->LUMO (38%), HOMO->L+6 (10%)
352.930	0.004	H-12->LUMO (19%), H-2->L+2 (11%), HOMO->L+7 (10%), HOMO->L+8 (42%)
352.158	0.0038	HOMO->L+9 (70%)
352.058	0.0288	H-11->LUMO (14%), H-2->L+2 (29%), HOMO->L+9 (24%)
351.280	0.0407	H-12->LUMO (14%), H-11->LUMO (20%), H-2->L+2 (22%), HOMO->L+8 (19%)
350.287	0.0504	H-12->LUMO (28%), H-11->LUMO (13%), H-10->LUMO (11%)
344.362	0.047	HOMO->L+11 (25%), HOMO->L+12 (11%), HOMO->L+13 (22%), HOMO->L+14 (16%)
343.000	0.0245	H-13->LUMO (12%), H-11->LUMO (25%), HOMO->L+14 (26%)
341.799	0.0657	H-5->L+1 (14%), H-3->L+1 (11%), HOMO->L+10 (11%), HOMO->L+11 (29%), HOMO->L+14 (14%)
340.953	0.0092	H-13->LUMO (10%), HOMO->L+12 (36%)
339.394	0.0112	H-13->LUMO (33%), HOMO->L+11 (10%), HOMO->L+14 (10%)
337.280	0.0109	H-14->LUMO (70%)
334.803	0.065	H-19->LUMO (40%), HOMO->L+16 (12%)
334.207	0.0402	H-5->L+1 (12%), H-3->L+1 (48%)
332.192	0.0021	HOMO->L+12 (20%), HOMO->L+13 (53%)
330.572	0.0147	H-15->LUMO (66%)
329.587	0.0017	H-6->L+1 (23%), HOMO->L+16 (34%)
328.470	0.007	HOMO->L+14 (16%), HOMO->L+15 (63%)
325.743	0.0565	H-22->LUMO (26%), H-16->LUMO (25%)

324.770	0.1184	H-16->LUMO (14%), H-4->L+1 (35%), HOMO->L+16 (12%)
322.850	0.0709	H-23->LUMO (12%), H-22->LUMO (15%), H-16->LUMO (28%), H-6->L+1 (18%)
321.069	0.0766	H-6->L+1 (14%), H-5->L+1 (26%), H-4->L+1 (28%)
320.621	0.0026	H-18->LUMO (59%), H-17->LUMO (22%)
317.063	0.0081	H-18->LUMO (22%), H-17->LUMO (45%), H-15->LUMO (11%)
316.302	0.0654	H-7->L+1 (42%)
314.633	0.0364	H-21->LUMO (66%), H-7->L+1 (12%)
313.250	0.0056	H-20->LUMO (45%), H-8->L+1 (19%), H-7->L+1 (11%)
312.649	0.0051	H-20->LUMO (31%), H-8->L+1 (24%)
310.147	0.0198	H-23->LUMO (29%), H-8->L+1 (26%)

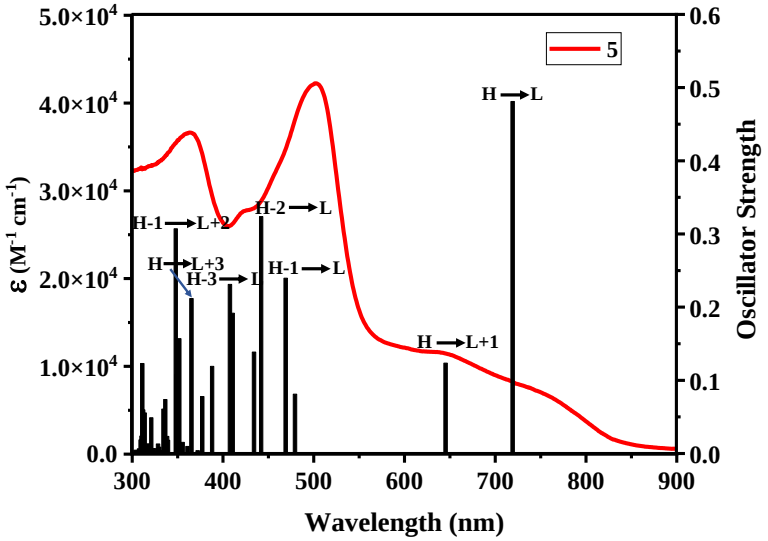


Figure S47. Calculated excitations (black vertical lines) and experimental absorption spectra (red line) for macrocycle **5**.

Table S4. Selected TD-DFT calculated oscillator strengths and compositions of the major electronic transitions of **5**.

Wavelength (nm)	Oscillator Strength	Major contributions
719.75	0.481	HOMO->LUMO (95%)
645.886	0.1236	HOMO->L+1 (92%)
480.057	0.0811	H-1->LUMO (44%), H-1->L+1 (10%), HOMO->L+2 (40%)

469.779	0.2396	H-2->LUMO (27%), H-1->LUMO (40%), HOMO->L+2 (31%)
442.785	0.3238	H-3->LUMO (12%), H-2->LUMO (54%), H-1->LUMO (11%)
434.864	0.1387	H-1->L+1 (77%)
411.443	0.1918	H-3->LUMO (16%), H-2->L+1 (74%)
408.38	0.2311	H-3->LUMO (53%), H-2->L+1 (15%)
388.775	0.1192	H-4->LUMO (16%), H-3->L+1 (67%)
377.874	0.0779	H-6->LUMO (27%), H-4->LUMO (42%), H-3->L+1 (14%)
372.896	0.0039	H-6->LUMO (41%), H-4->LUMO (23%), HOMO->L+3 (17%)
366.037	0.2118	HOMO->L+3 (65%)
361.607	0.0097	H-7->LUMO (44%), H-7->L+1 (11%), H-4->L+1 (18%), H-1->L+2 (10%)
356.358	0.0153	H-5->LUMO (90%)
352.608	0.1569	H-7->LUMO (19%), H-1->L+2 (58%)
351.121	0.0757	H-4->L+1 (51%), H-1->L+2 (19%)
349.497	0.1079	H-10->LUMO (54%), H-9->LUMO (17%), H-8->LUMO (10%)
348.701	0.3072	H-8->LUMO (50%), H-8->L+1 (20%), H-4->L+1 (12%)
340.186	0.0182	H-12->LUMO (12%), H-10->LUMO (12%), H-9->LUMO (54%)
339.19	0.0234	H-11->LUMO (35%), H-7->LUMO (13%), H-7->L+1 (19%)
337.216	0.0738	H-11->LUMO (21%), H-2->L+2 (45%)
335.246	0.0608	H-11->LUMO (28%), H-7->L+1 (22%), H-2->L+2 (22%)
333.425	0.0002	H-5->L+1 (77%)
331.269	0.0041	HOMO->L+4 (57%)
330.563	0.0087	H-23->LUMO (14%), H-16->LUMO (11%), H-7->L+1 (10%), HOMO->L+4 (26%)
329.246	0.0131	H-6->L+1 (49%)
329.071	0.0072	H-12->LUMO (26%), H-6->L+1 (18%)
326.687	0.0015	H-22->LUMO (12%), H-22->L+1 (10%), H-12->LUMO (20%)
324.422	0.0068	HOMO->L+6 (40%), HOMO->L+9 (20%)
323.55	0.0036	H-22->LUMO (10%), H-22->L+1 (14%), H-13->LUMO (11%), H-12->LUMO (17%), H-8->L+1 (14%)
321.753	0.0489	H-18->LUMO (10%), H-13->LUMO (28%), H-8->LUMO (10%), H-8->L+1 (19%)
321.552	0.0015	HOMO->L+5 (80%)
321.219	0.0099	H-14->LUMO (47%), H-9->L+1 (11%)
319.654	0.0079	H-14->LUMO (19%), H-11->L+1 (20%), H-9->L+1 (19%)
318.128	0.0133	H-11->L+1 (45%)
317.257	0.0094	H-15->LUMO (22%), H-11->L+1 (14%), H-9->L+1 (14%)

316.682	0.0014	H-18->LUMO (18%), H-16->LUMO (31%)
314.489	0.0555	HOMO->L+7 (64%), HOMO->L+8 (14%)
313.701	0.003	H-18->LUMO (18%), HOMO->L+7 (12%)
312.823	0.0597	H-3->L+2 (24%), HOMO->L+6 (17%), HOMO->L+8 (13%)
312.673	0.0112	H-21->LUMO (11%), HOMO->L+9 (18%), HOMO->L+10 (35%)
311.8	0.123	H-16->LUMO (11%), H-3->L+2 (30%), HOMO->L+8 (12%)
311.041	0.0239	H-20->LUMO (18%), H-20->L+1 (12%), HOMO->L+6 (12%), HOMO->L+9 (12%)
310.675	0.0182	H-21->LUMO (12%), H-18->LUMO (10%), H-12->L+1 (16%), HOMO->L+10 (18%)
310.131	0.0187	H-12->L+1 (10%), H-10->L+1 (56%), H-9->L+1 (14%)
309.226	0.0029	H-20->LUMO (10%), HOMO->L+8 (39%), HOMO->L+9 (12%)
308.288	0.0065	H-21->LUMO (36%), H-12->L+1 (28%)
307.439	0.001	H-17->LUMO (65%), H-15->LUMO (12%)
305.523	0.0036	HOMO->L+9 (10%), HOMO->L+11 (56%), HOMO->L+15 (18%)
304.338	0.0045	HOMO->L+12 (79%)

Table S5. S_0 optimized geometry of the compound **2** at B3LYP/6-31G (d,p) level of theory and Empirical Dispersion GD2.

Charge = 0

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3300.746290

Atom	X	Y	Z	Atom	X	Y	Z
C	1.65374	1.44485	-2.02306	C	2.45239	6.58242	0.96435
C	1.28173	1.99566	-0.79770	C	2.08491	5.71967	2.00075
C	-0.05669	2.35356	-0.57404	C	2.04144	4.33522	1.80948
C	-1.01892	2.15512	-1.56149	C	-4.18254	4.10804	-2.47312
C	-0.63783	1.59671	-2.79006	C	-4.53107	5.27968	-3.14565
C	0.68853	1.24637	-3.01761	C	-3.55259	6.18923	-3.56428
C	2.29397	2.27141	0.32684	C	-2.21379	5.89396	-3.27483
C	-2.47774	2.58532	-1.35041	C	-1.86073	4.72477	-2.60315
O	-2.59614	2.93049	0.04102	C	2.51490	8.07618	1.17241
C	-3.37542	1.39415	-1.62905	C	-3.92564	7.43837	-4.32486
O	1.76777	1.57489	1.47157	H	2.68673	1.16944	-2.20633
C	3.65668	1.68721	0.02298	H	-0.34289	2.79003	0.37389

C	2.36638	3.78136	0.57079	H	-1.38853	1.43721	-3.55783
C	-2.84066	3.80807	-2.20110	H	0.97860	0.81320	-3.97036
C	4.83709	2.21021	-0.51390	H	-3.49566	3.25682	0.18004
C	5.72328	1.13329	-0.70030	H	2.42938	1.61960	2.17654
C	5.07709	-0.03675	-0.25533	H	5.01439	3.25004	-0.74364
N	3.82749	0.35294	0.17824	H	6.71975	1.17599	-1.11433
N	-3.51069	0.45624	-0.66916	H	3.16171	-0.35381	0.51583
C	-4.26041	-0.60842	-1.12319	H	-3.17782	0.47358	0.30348
C	-4.61495	-0.30676	-2.45235	H	-5.22038	-0.93185	-3.09255
C	-4.05682	0.94527	-2.76799	H	-4.13296	1.48170	-3.70264
C	1.04123	-2.37483	2.29273	H	2.82696	-1.22563	2.96829
C	1.75281	-1.32483	2.97638	H	1.00830	0.37464	4.15619
C	0.83280	-0.51641	3.57128	H	5.69691	-4.39083	-0.30800
C	-0.47249	-1.02339	3.24695	H	3.40581	-5.49704	0.54784
O	-0.29297	-2.22589	2.58426	H	-2.68928	-3.32469	3.62335
C	-1.73023	-0.49041	3.29665	H	-4.32245	-4.01100	1.59533
C	1.44338	-3.38670	1.45559	H	-3.84563	0.55703	4.59916
C	2.79148	-3.34455	0.90943	H	-4.31435	2.94398	5.05719
C	0.45568	-4.37389	0.93725	H	-0.68532	4.03922	3.03908
C	-2.80022	-1.27978	2.67339	H	-0.22671	1.67131	2.56991
C	-1.96870	0.92945	3.60999	H	1.54844	-6.14004	1.52238
N	3.38862	-2.17595	0.68938	H	-0.10304	-7.72531	0.60494
C	4.63370	-2.44320	0.14032	H	-2.56883	-4.44110	-0.64468
C	4.81272	-3.88243	0.04985	H	-0.91381	-2.85585	0.25457
C	3.64689	-4.44523	0.48951	H	-2.67635	-7.98303	0.04160
C	-3.10315	-2.68578	2.85551	H	-3.41327	-6.65805	-0.88921
C	-3.93467	-3.03069	1.83026	H	-2.10755	-7.62806	-1.59133
C	-4.10924	-1.83018	1.02735	H	-3.87373	5.31587	4.45825
N	-3.44798	-0.76792	1.63717	H	-2.35866	5.42589	5.36140
C	-3.14009	1.31946	4.28218	H	-2.36821	5.76616	3.62646
C	-3.40348	2.66335	4.53357	H	7.87119	-0.36558	0.40066
C	-2.51762	3.66670	4.11332	H	10.09190	-0.88705	-0.55656
C	-1.36391	3.27879	3.41937	H	8.27034	-3.67626	-3.26208
C	-1.09072	1.93636	3.16741	H	6.04863	-3.14989	-2.30766
C	0.66161	-5.76033	1.02446	H	-6.53098	-3.32435	0.62064
C	-0.27912	-6.65577	0.51415	H	-7.37000	-5.44081	-0.35698
C	-1.45514	-6.20120	-0.09967	H	-4.61817	-5.01794	-3.62403
C	-1.66074	-4.81918	-0.18321	H	-3.78535	-2.90249	-2.64809
C	-0.72415	-3.92062	0.32172	H	11.37782	-1.80636	-2.49339
C	-2.47058	-7.16799	-0.66244	H	11.17389	-3.47934	-1.96123
C	-2.79724	5.12151	4.40117	H	10.63012	-3.00305	-3.57462

C	5.47380	-1.41924	-0.29451	H	-7.51151	-6.96746	-2.25789
C	-4.52036	-1.75890	-0.30367	H	-6.53606	-6.68426	-3.71732
C	-5.09517	-2.96451	-0.93983	H	-5.83233	-7.52078	-2.32958
C	6.80057	-1.73329	-0.87280	H	2.93117	4.22419	-1.45851
C	7.95867	-1.09110	-0.40142	H	3.03691	6.67063	-1.10918
C	9.20771	-1.38927	-0.94105	H	1.82160	6.13478	2.97049
C	9.34596	-2.32920	-1.97184	H	1.72628	3.69009	2.62223
C	8.18913	-2.95821	-2.44999	H	-4.95920	3.41623	-2.16264
C	6.93667	-2.66937	-1.91137	H	-5.57808	5.49123	-3.34859
C	-6.11258	-3.69846	-0.30798	H	-1.43777	6.59244	-3.57838
C	-6.57958	-4.88948	-0.85966	H	-0.81776	4.52420	-2.38319
C	-6.04598	-5.39178	-2.05458	H	2.02992	8.61112	0.34777
C	-5.04489	-4.64803	-2.69524	H	2.02381	8.36617	2.10671
C	-4.57857	-3.45253	-2.15382	H	3.55475	8.42531	1.21798
C	10.70423	-2.66888	-2.53452	H	-4.93192	7.77886	-4.05888
C	-6.51218	-6.70955	-2.62253	H	-3.21910	8.25053	-4.12312
C	2.71816	4.64165	-0.47917	H	-3.91562	7.25670	-5.40788
C	2.76605	6.01858	-0.28225				

Table S6. S_0 optimized geometry of the compound **3b** at B3LYP/6-31G (d,p) level of theory and Empirical Dispersion GD2.

Charge = 0

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3623.724133

Atom	X	Y	Z	Atom	X	Y	Z
C	-1.10371	-1.03076	-1.51122	C	-1.28419	-5.75369	2.27556
C	-0.84073	-1.91404	-0.46119	C	-1.49730	-4.38713	2.06475
C	0.47056	-2.36964	-0.26595	C	4.37880	-4.45893	-1.67960
C	1.51128	-1.95991	-1.10028	C	4.59387	-5.67570	-2.32134
C	1.23401	-1.08178	-2.15403	C	3.55846	-6.31388	-3.01933
C	-0.06543	-0.61839	-2.35174	C	2.30483	-5.69432	-3.04358
C	-1.92903	-2.40107	0.51567	C	2.08496	-4.47441	-2.39962
C	2.91633	-2.54512	-0.90835	C	-1.07957	-8.13702	1.43731
O	3.01745	-2.83853	0.50122	C	3.80100	-7.61732	-3.74077
C	3.96988	-1.50838	-1.24787	H	-2.10897	-0.66224	-1.67958
O	-1.71815	-1.62033	1.70864	H	0.68605	-3.06067	0.53776
C	-3.34085	-2.13013	0.03745	H	2.03684	-0.76317	-2.81201

C	-1.73785	-3.89836	0.78149	H	-0.27558	0.06830	-3.16629
C	3.12029	-3.83716	-1.70990	H	3.87485	-3.26113	0.64720
C	-4.32957	-2.95496	-0.50550	H	-2.44252	-1.82127	2.31938
C	-5.44988	-2.14980	-0.77119	H	-4.23323	-4.01658	-0.67383
C	-5.13947	-0.83680	-0.37247	H	-6.38746	-2.46097	-1.20697
N	-3.84950	-0.87170	0.11918	H	-3.38729	-0.00308	0.40605
N	4.03650	-0.39470	-0.49006	H	3.52564	-0.16248	0.37323
C	5.01787	0.45882	-0.94940	H	6.41865	0.21824	-2.65188
C	5.60255	-0.17626	-2.06509	H	5.12207	-2.13473	-3.02541
C	4.93706	-1.39984	-2.25607	H	-2.89782	1.31319	2.37935
C	-1.66669	2.92273	1.53000	H	-0.81361	0.33747	3.53824
C	-1.90302	1.72775	2.30101	H	-7.03636	3.10428	-0.55952
C	-0.80436	1.21964	2.91322	H	-5.16084	4.92481	0.09178
C	0.43044	1.89862	2.60185	H	2.76854	4.28041	2.63311
C	1.69842	1.41091	2.78570	H	4.83235	4.40008	0.90056
C	-2.58847	3.65683	0.81950	H	3.54239	0.70837	4.62439
C	-3.87077	3.09742	0.43587	H	4.00511	-1.54418	5.53686
C	-2.26189	5.02717	0.32690	H	0.93601	-3.18601	3.01980
C	2.86177	2.06373	2.18126	H	0.47157	-0.95056	2.12347
C	1.93748	0.05493	3.34192	H	-3.59670	6.02212	1.69268
N	-4.07063	1.78533	0.29413	H	-3.06675	8.29737	0.87272
C	-5.37284	1.62481	-0.15501	H	-0.29615	6.63378	-1.95103
C	-6.01234	2.92575	-0.26384	H	-0.84223	4.35574	-1.14467
C	-5.06489	3.84827	0.07171	H	-1.33976	9.74934	-0.30382
C	3.23946	3.46215	2.10427	H	-0.37041	9.04982	-1.61845
C	4.29840	3.52169	1.23564	H	-2.10026	9.34341	-1.84569
C	4.52420	2.16330	0.77547	H	3.83681	-4.05935	5.08429
N	3.65459	1.30885	1.43083	H	2.27269	-4.03825	5.90258
C	2.95573	-0.14299	4.29151	H	2.39191	-4.68484	4.25904
C	3.21695	-1.41191	4.79913	H	-7.87084	-1.25992	0.40007
C	2.48594	-2.52964	4.36565	H	-10.18524	-1.44484	-0.45331
C	1.49229	-2.33365	3.40119	H	-9.33657	1.55580	-3.40204
C	1.22273	-1.06441	2.89245	H	-7.02054	1.73828	-2.54816
C	-2.88300	6.15501	0.88485	H	7.13100	3.22541	0.87114
C	-2.58067	7.43488	0.42293	H	8.73637	4.80243	-0.16477
C	-1.64854	7.63048	-0.60589	H	7.10134	3.91796	-4.03341
C	-1.02566	6.50374	-1.15548	H	5.49408	2.34989	-2.99716
C	-1.32966	5.21908	-0.70230	H	-11.73202	-1.06915	-2.41863
C	-1.34416	9.01735	-1.11899	H	-12.02378	0.58948	-1.88489
C	2.76329	-3.90230	4.92906	H	-11.43137	0.28990	-3.52435
C	-5.89955	0.37679	-0.48175	H	9.90767	5.55402	-2.21423
C	5.24569	1.74292	-0.34735	H	9.25938	5.15583	-3.82140
C	6.19954	2.67119	-0.98740	H	8.53765	6.45880	-2.86981

C	-7.28254	0.26549	-1.00141	H	-1.89466	-4.42701	-1.29934
C	-8.19285	-0.64219	-0.43178	H	-1.54046	-6.84443	-0.92230
C	-9.49533	-0.74219	-0.91399	H	-1.08882	-6.11623	3.28164
C	-9.93469	0.05089	-1.98360	H	-1.44171	-3.69935	2.90110
C	-9.02297	0.94476	-2.55945	H	5.20058	-3.97726	-1.15633
C	-7.71922	1.05411	-2.07867	H	5.57695	-6.13845	-2.28246
C	7.12018	3.38721	-0.20166	H	1.48509	-6.17457	-3.57221
C	8.02285	4.27036	-0.78872	H	1.09990	-4.02328	-2.42905
C	8.03383	4.47810	-2.17472	H	-0.31360	-8.52702	0.75672
C	7.11343	3.76643	-2.95705	H	-0.75940	-8.33681	2.46474
C	6.21193	2.87695	-2.37854	H	-1.99788	-8.70939	1.25335
C	-11.3550	-0.04281	-2.48413	H	4.46948	-8.26929	-3.16772
C	8.99025	5.46032	-2.80451	H	2.86250	-8.15260	-3.91769
C	-1.74522	-4.80191	-0.29140	H	4.27311	-7.44419	-4.71693
C	-1.53773	-6.16050	-0.07708	S	0.05075	3.37975	1.66621
C	-1.30462	-6.66140	1.21375				

Table S7. S_0 optimized geometry of the compound **4** at B3LYP/6-31G (d,p) level of theory and Empirical Dispersion GD2.

Charge = 0

Sum of imaginary frequencies = 0

Total Energy (hartree) = -5624.917655

Atom	**X**	**Y**	**Z**	**Atom**	**X**	**Y**	**Z**
C	1.11587	1.01574	-1.41750	C	1.36668	5.79528	2.34068
C	0.87392	1.96474	-0.41987	C	1.56729	4.42850	2.11929
C	-0.42299	2.47353	-0.26739	C	-4.21652	4.66833	-1.75223
C	-1.46867	2.05580	-1.09292	C	-4.37313	5.87583	-2.42724
C	-1.21052	1.11494	-2.09524	C	-3.31167	6.43826	-3.15101
C	0.07418	0.59557	-2.24868	C	-2.09314	5.75229	-3.16731
C	1.96816	2.44897	0.55354	C	-1.93211	4.54119	-2.48998
C	-2.85380	2.69796	-0.94257	C	1.16758	8.18471	1.51869
O	-2.96911	3.02122	0.46012	C	-3.49171	7.73220	-3.90699
C	-3.94352	1.69947	-1.28324	H	2.10762	0.60088	-1.55336
O	1.76314	1.66086	1.74288	H	-0.62662	3.21100	0.49692
C	3.37824	2.17978	0.06788	H	-2.01521	0.79006	-2.74767
C	1.78672	3.94523	0.83027	H	0.26977	-0.14125	-3.02195
C	-2.99267	3.98040	-1.77300	H	-3.81226	3.47846	0.58288

C	4.36986	3.01068	-0.46075	H	2.49352	1.85401	2.34904
C	5.49005	2.20793	-0.73362	H	4.27534	4.07470	-0.61424
C	5.17627	0.88998	-0.35472	H	6.42935	2.52327	-1.16273
N	3.88610	0.92024	0.13623	H	3.41894	0.04786	0.40215
N	-4.05184	0.58944	-0.52529	H	-3.54718	0.33523	0.33579
C	-5.06876	-0.22409	-0.98011	H	-6.46589	0.07302	-2.67701
C	-5.63247	0.43436	-2.09322	H	-5.07681	2.37118	-3.05651
C	-4.91892	1.63000	-2.28723	H	2.83367	-1.31812	2.25808
C	1.63866	-2.92088	1.36942	H	0.79845	-0.33826	3.41283
C	1.84083	-1.73631	2.16380	H	7.05578	-3.05249	-0.62309
C	0.75019	-1.21785	2.78449	H	5.16213	-4.88113	-0.05987
C	-0.52005	-1.83769	2.49827	H	-2.93794	-4.12608	2.58671
C	-1.75838	-1.30146	2.72282	H	-5.02073	-4.17070	0.86850
C	2.57876	-3.62307	0.65607	H	-3.54451	-0.56262	4.60308
C	3.87366	-3.05882	0.31867	H	-3.91645	1.69258	5.55018
C	2.25337	-4.97370	0.11073	H	-0.84077	3.26339	2.99609
C	-2.95419	-1.90851	2.13137	H	-0.46417	1.02387	2.06799
C	-1.94167	0.05376	3.29959	H	3.61485	-6.02966	1.40254
N	4.08226	-1.74434	0.22065	H	3.06964	-8.26417	0.48947
C	5.39297	-1.57753	-0.20258	H	0.24053	-6.47740	-2.19751
C	6.02790	-2.87732	-0.33914	H	0.79766	-4.23769	-1.29228
C	5.07054	-3.80435	-0.04699	H	1.34806	-9.66806	-0.72499
C	-3.38420	-3.29241	2.05965	H	0.31420	-8.91281	-1.95722
C	-4.45160	-3.31278	1.19867	H	2.03465	-9.17294	-2.27568
C	-4.63067	-1.94726	0.74044	H	-3.67608	4.21686	5.09745
N	-3.72456	-1.12579	1.38939	H	-2.11977	4.11516	5.92424
C	-2.93646	0.27331	4.26927	H	-2.20067	4.79248	4.29033
C	-3.14658	1.54363	4.79647	H	7.89713	1.28449	0.45143
C	-2.38731	2.64200	4.36182	H	10.22013	1.48440	-0.37625
C	-1.41811	2.42537	3.37730	H	9.39124	-1.44034	-3.40568
C	-1.19891	1.15403	2.84984	H	7.06735	-1.63873	-2.57688
C	2.88622	-6.12498	0.60292	H	-7.27220	-2.90732	0.85899
C	2.57471	-7.38265	0.08902	H	-8.94770	-4.42018	-0.16121
C	1.62225	-7.53279	-0.92873	H	-7.31871	-3.59690	-4.04589
C	0.98668	-6.38317	-1.41243	H	-5.64124	-2.09341	-3.02541
C	1.29976	-5.12042	-0.90770	H	11.79156	1.14756	-2.31334
C	1.30885	-8.89464	-1.49986	H	12.06254	-0.53787	-1.85741
C	-2.60925	4.01620	4.94575	H	11.48553	-0.15442	-3.48454
C	5.93077	-0.32417	-0.48792	H	-10.16272	-5.13417	-2.19247
C	-5.34345	-1.49865	-0.37705	H	-9.53025	-4.74347	-3.80778
C	-6.33858	-2.38831	-1.00874	H	-8.83553	-6.07811	-2.88052
C	7.31900	-0.20561	-0.99145	H	1.92139	4.48498	-1.24916
C	8.22581	0.68595	-0.39176	H	1.58777	6.90234	-0.85420

C	9.53286	0.79459	-0.85968	H	1.18774	6.15335	3.35141
C	9.97997	0.02707	-1.94447	H	1.51841	3.73675	2.95269
C	9.07151	-0.85017	-2.55058	H	-5.05865	4.24593	-1.21031
C	7.76348	-0.96851	-2.08412	H	-5.33010	6.39086	-2.39446
C	-7.27830	-3.06860	-0.21391	H	-1.25432	6.17277	-3.71654
C	-8.22045	-3.91565	-0.79212	H	-0.97341	4.03636	-2.51592
C	-8.25350	-4.12177	-2.17795	H	0.39643	8.58433	0.84964
C	-7.31412	-3.44579	-2.96941	H	0.86135	8.38071	2.55108
C	-6.37294	-2.59241	-2.39979	H	2.08781	8.75144	1.32702
C	11.40487	0.12953	-2.43021	H	-4.11380	8.43681	-3.34402
C	-9.25339	-5.06582	-2.79847	H	-2.52754	8.20842	-4.11235
C	1.78711	4.85502	-0.23735	H	-3.98786	7.55838	-4.87101
C	1.59172	6.21374	-0.01282	Se	-0.20351	-3.44055	1.47733
C	1.37911	6.70885	1.28379				

Table S8. S_0 optimized geometry of the compound **4.2H$^+$** at B3LYP/6-31G (d,p) level of theory and Empirical Dispersion GD2.

Charge = 2

Sum of imaginary frequencies = 1

Total Energy (hartree) = -5625.785978

Atom	X	Y	Z	Atom	X	Y	Z
C	-0.79826	-1.00648	-1.15859	C	-1.22403	-4.39471	2.43434
C	-0.54891	-2.01215	-0.21852	C	4.35949	-4.78258	-1.42143
C	0.75682	-2.49309	-0.07468	C	4.61032	-5.82032	-2.31735
C	1.80531	-2.01383	-0.86307	C	3.93731	-5.89419	-3.54410
C	1.53346	-1.02009	-1.81366	C	2.99716	-4.89809	-3.83784
C	0.23960	-0.51250	-1.94960	C	2.73869	-3.85772	-2.94561
C	-1.66065	-2.55384	0.70684	C	-0.54651	-8.14463	2.12105
C	3.19945	-2.64925	-0.71474	C	4.23238	-6.99908	-4.52717
O	3.37029	-3.13314	0.63042	H	-1.80265	-0.62252	-1.29512
C	4.31878	-1.62754	-0.85124	H	0.95965	-3.25347	0.66603
O	-1.65913	-1.66830	1.84255	H	2.32726	-0.65250	-2.45674
C	-3.03224	-2.43734	0.05435	H	0.03770	0.25791	-2.68695

C	-1.37992	-4.00796	1.10188	H	3.03428	-4.04093	0.65764
C	3.41827	-3.78673	-1.72433	H	-2.24848	-2.04200	2.51550
C	-3.75626	-3.27284	-0.80047	H	-3.43547	-4.23799	-1.15816
C	-4.96146	-2.62908	-1.09325	H	-5.74284	-2.97729	-1.75216
C	-4.98074	-1.38983	-0.42053	H	-3.50318	-0.63606	0.96496
N	-3.76455	-1.30851	0.25719	H	3.25257	0.06389	-0.27354
N	4.15687	-0.34447	-0.46029	H	7.35176	-0.35788	-1.20215
C	5.35494	0.36291	-0.57734	H	6.09808	-2.72833	-1.55024
C	6.30484	-0.57332	-1.04798	H	-3.13688	1.42458	2.21152
C	5.66296	-1.79939	-1.21563	H	-0.94016	0.75199	3.26530
C	-2.16665	3.01943	1.04858	H	-7.66108	1.98409	0.03764
C	-2.19577	1.89440	1.95129	H	-6.20658	4.20425	0.47353
C	-1.02061	1.54830	2.53738	H	2.24619	4.67607	1.36365
C	0.15152	2.27023	2.11239	H	4.51766	4.51515	-0.07002
C	1.44429	1.88386	2.37262	H	3.15596	1.50746	4.45590
C	-3.24643	3.59746	0.41754	H	3.77388	-0.63468	5.52658
C	-4.47107	2.84017	0.27328	H	1.07048	-2.72162	2.92181
C	-3.18611	4.95357	-0.18901	H	0.45877	-0.59424	1.85186
C	2.58222	2.50747	1.72828	H	-4.71707	5.78872	1.08368
C	1.74476	0.61239	3.08630	H	-4.61831	8.03393	0.06610
N	-4.41907	1.49518	0.02774	H	-1.51713	6.70970	-2.58745
C	-5.69659	0.97786	-0.16091	H	-1.63268	4.44590	-1.59907
C	-6.58452	2.06806	0.03660	H	-3.26864	9.68271	-1.24249
C	-5.83430	3.21113	0.27535	H	-2.03211	9.11652	-2.38814
C	2.85372	3.79568	1.21100	H	-3.74854	8.97745	-2.78966
C	4.04601	3.72439	0.49460	H	3.74516	-3.57081	4.35665
C	4.50816	2.38704	0.54068	H	3.20786	-3.02408	5.95000
N	3.60940	1.69950	1.33375	H	2.08298	-3.88287	4.87172
C	2.69818	0.58130	4.12037	H	-7.39431	-2.56315	0.19028
C	3.04593	-0.62682	4.72014	H	-9.66051	-3.17433	-0.57671
C	2.47269	-1.83723	4.29904	H	-9.81653	0.38288	-2.97781

C	1.52737	-1.79906	3.26695	H	-7.54886	0.99873	-2.22360
C	1.17387	-0.59636	2.66202	H	6.78039	3.74563	1.00439
C	-4.03261	5.97768	0.26278	H	8.67144	5.08110	0.14591
C	-3.96727	7.24748	-0.30543	H	8.64034	2.80025	-3.49453
C	-3.06517	7.53455	-1.34051	H	6.72979	1.48054	-2.66000
C	-2.22224	6.50868	-1.78557	H	-11.4240	-2.87909	-2.33814
C	-2.28159	5.23296	-1.22518	H	-12.0364	-1.43376	-1.52764
C	-3.02126	8.90380	-1.97070	H	-11.5464	-1.33901	-3.22438
C	2.89493	-3.14930	4.90887	H	10.55331	5.24972	-1.45754
C	-5.96638	-0.36606	-0.48396	H	10.54743	4.29591	-2.96213
C	5.49351	1.73595	-0.24808	H	9.53634	5.73858	-2.81806
C	6.61594	2.51070	-0.76188	H	-1.26889	-4.68680	-0.94314
C	-7.30990	-0.72808	-0.94691	H	-0.82148	-7.03540	-0.36133
C	-7.92030	-1.92304	-0.50927	H	-0.83132	-6.00649	3.80347
C	-9.19794	-2.25978	-0.93619	H	-1.28067	-3.66631	3.23627
C	-9.90839	-1.43298	-1.82183	H	4.89521	-4.74137	-0.47860
C	-9.29302	-0.25388	-2.27091	H	5.33789	-6.58545	-2.06055
C	-8.02077	0.10113	-1.83975	H	2.45394	-4.94114	-4.77802
C	7.17124	3.55546	0.01081	H	1.99699	-3.11098	-3.20400
C	8.24089	4.29739	-0.47023	H	0.19786	-8.58325	1.44779
C	8.78949	4.03964	-1.73770	H	-0.18647	-8.24064	3.14965
C	8.23415	3.00396	-2.50809	H	-1.46082	-8.74436	2.02907
C	7.16897	2.25028	-2.03562	H	4.55843	-7.90952	-4.01469
C	-11.3022	-1.79421	-2.26009	H	3.35316	-7.23505	-5.13500
C	9.92540	4.87058	-2.26936	H	5.03626	-6.70205	-5.21321
C	-1.21839	-4.97823	0.10088	Se	-0.38738	3.69814	0.94824
C	-0.94725	-6.30190	0.43031	H	3.73597	0.76023	1.68685
C	-0.81732	-6.70356	1.769625	H	-3.57296	1.052712	-0.29912
C	-0.95004	-5.72690	2.760412				

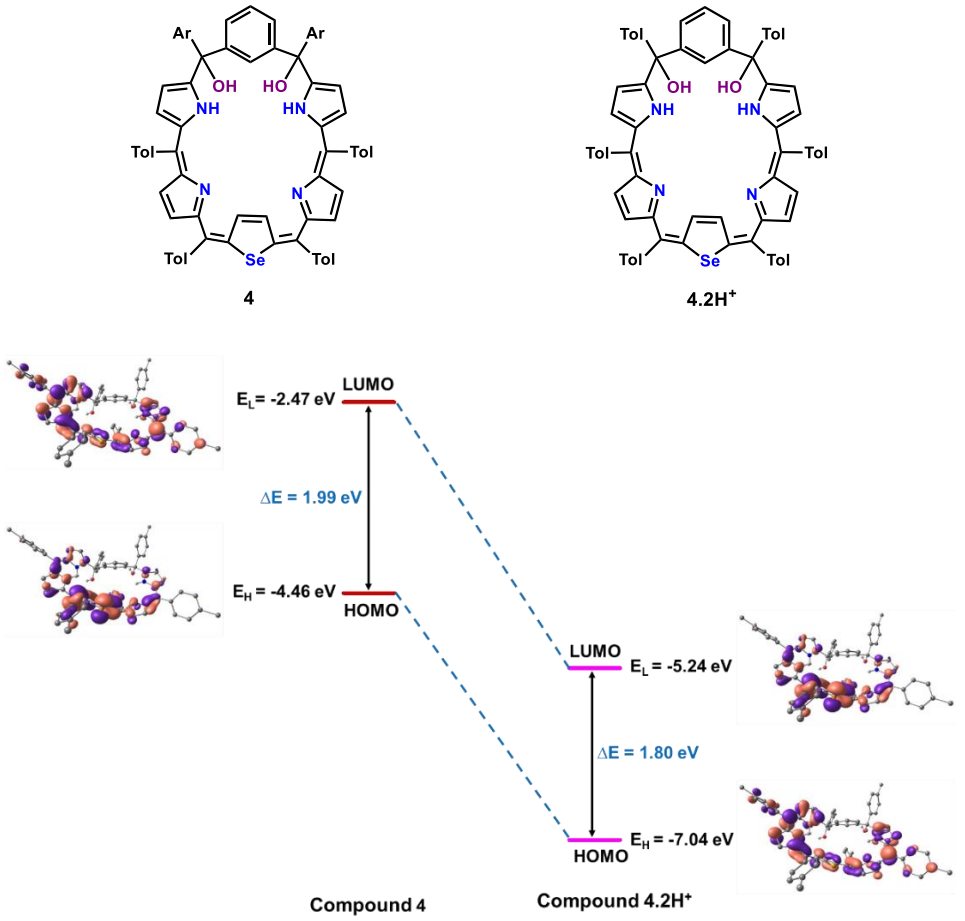


Figure S48. Energy-level diagram (selected FMOs) of compound **4** and its protonated derivative **4.2H**$^{+}$.

Table S9. S_0 optimized geometry of the compound **5** at B3LYP/6-31G (d,p) + LANL2DZ level of theory and Empirical Dispersion GD2.

Charge = 0

Sum of imaginary frequencies= 0

Total Energy (hartree) = -3233.447628

Atom	X	Y	Z	Atom	X	Y	Z
C	1.036886	1.773424	-2.08677	C	1.61407	5.929444	2.301107
C	0.744744	2.374165	-0.86198	C	1.68705	4.581407	1.941639
C	-0.58983	2.67374	-0.54856	C	-4.81788	4.560779	-1.54445
C	-1.62827	2.376223	-1.43283	C	-5.22733	5.79308	-2.04686

C	-1.32129	1.766005	-2.65705	C	-4.34468	6.610424	-2.76684
C	0.001665	1.471207	-2.97806	C	-3.0384	6.147255	-2.95322
C	1.819569	2.716299	0.187757	C	-2.62296	4.914181	-2.44643
C	-3.07376	2.770383	-1.07669	C	1.445591	8.393239	1.720062
O	-3.07253	2.935608	0.354705	C	-4.79971	7.931513	-3.34037
C	-4.0456	1.64779	-1.41366	H	2.06251	1.537187	-2.35038
O	1.527676	1.843118	1.296157	H	-0.8267	3.146743	0.395147
C	3.248262	2.435704	-0.25182	H	-2.11761	1.521222	-3.35397
C	1.701016	4.198267	0.598877	H	0.232542	0.997438	-3.92786
C	-3.5059	4.09568	-1.73558	H	-3.93958	3.275282	0.612268
C	4.245008	3.285758	-0.74041	H	2.273271	1.887338	1.911638
C	5.405922	2.519511	-0.92032	H	4.133545	4.343901	-0.91994
C	5.118095	1.201484	-0.52315	H	6.359072	2.866256	-1.29011
N	3.791027	1.188985	-0.13059	H	3.340793	0.30967	0.137787
N	-4.07022	0.53929	-0.63868	H	-3.53764	0.328564	0.216091
C	-5.02922	-0.35069	-1.08185	H	-6.44081	-0.17755	-2.78648
C	-5.63281	0.245626	-2.20853	H	-5.2348	2.202485	-3.19601
C	-5.01054	1.486472	-2.41931	H	2.921591	-1.45072	2.398668
C	1.83036	-2.98626	1.301131	H	0.889223	-0.53842	3.50571
C	1.938189	-1.86568	2.204237	H	7.337286	-2.55876	-0.35519
C	0.825017	-1.36537	2.806015	H	5.582098	-4.52718	0.174838
C	-0.47668	-1.89796	2.469904	H	-3.0374	-4.09004	2.795133
C	-1.69527	-1.34941	2.750686	H	-5.05053	-4.1949	1.013783
C	2.839655	-3.53405	0.547968	H	-3.44834	-0.8906	4.736072
C	4.09346	-2.82553	0.29167	H	-3.82202	1.186477	6.007336
C	2.681861	-4.84983	-0.13097	H	-0.81754	3.157902	3.655009
C	-2.90683	-1.92571	2.130497	H	-0.43847	1.093575	2.389329
C	-1.8821	-0.07582	3.496252	H	2.006971	-5.903	1.625171
N	4.179434	-1.50361	0.13714	H	1.729931	-8.071	0.487967
C	5.507844	-1.2341	-0.1858	H	3.082067	-6.3152	-3.18953
C	6.274667	-2.46971	-0.18015	H	3.346832	-4.14291	-2.05581
C	5.387016	-3.46682	0.090458	H	1.474344	-9.31082	-1.66366
C	-3.40491	-3.29065	2.165086	H	2.010543	-8.58119	-3.18598
C	-4.44527	-3.33772	1.27332	H	3.191057	-9.26674	-2.06862
C	-4.54858	-2.01043	0.696478	H	-3.60224	3.729824	5.997106
N	-3.60759	-1.17705	1.294221	H	-1.98483	3.576809	6.681188
C	-2.85622	-0.00836	4.509276	H	-2.21899	4.475593	5.179793
C	-3.0677	1.166273	5.223767	H	7.814286	1.663281	0.639661
C	-2.32924	2.326337	4.946088	H	10.17275	1.976036	-0.00743
C	-1.38039	2.265318	3.918953	H	9.65873	-0.81103	-3.23239
C	-1.15522	1.089139	3.203002	H	7.299539	-1.12774	-2.58128

C	2.227455	-5.98375	0.565215	H	-7.36062	-2.78738	0.811976
C	2.079645	-7.21118	-0.07874	H	-9.03744	-4.32258	-0.15027
C	2.384889	-7.35941	-1.43789	H	-7.10868	-4.0282	-3.97489
C	2.845081	-6.23138	-2.13138	H	-5.43171	-2.49935	-3.01323
C	2.997347	-5.0031	-1.49311	H	11.9054	1.782433	-1.82104
C	2.254185	-8.69775	-2.12547	H	12.18902	0.074396	-1.4839
C	-2.54698	3.593814	5.738387	H	11.71317	0.578664	-3.10643
C	5.960445	0.038965	-0.51699	H	-10.1076	-5.31658	-2.1031
C	-5.26586	-1.61037	-0.43313	H	-9.50899	-4.9508	-3.72953
C	-6.27062	-2.52867	-1.02709	H	-8.79181	-6.26588	-2.79971
C	7.38279	0.234229	-0.91559	H	1.614525	4.931381	-1.42669
C	8.215312	1.119156	-0.20984	H	1.507783	7.306437	-0.79047
C	9.547904	1.292124	-0.57694	H	1.60258	6.198591	3.354664
C	10.09818	0.599861	-1.66452	H	1.715386	3.827609	2.721354
C	9.263253	-0.27193	-2.37486	H	-5.53738	3.947131	-1.0081
C	7.93113	-0.45661	-2.00796	H	-6.24965	6.124317	-1.87976
C	-7.29752	-3.06758	-0.23477	H	-2.32783	6.76119	-3.50165
C	-8.24514	-3.9303	-0.7831	H	-1.59981	4.593512	-2.60386
C	-8.19952	-4.29475	-2.13439	H	0.419591	8.762228	1.598451
C	-7.17198	-3.75782	-2.92348	H	1.729429	8.551708	2.764409
C	-6.22652	-2.88905	-2.38553	H	2.089517	9.021699	1.095856
C	11.55047	0.771053	-2.04179	H	-5.50102	8.438978	-2.67035
C	-9.2077	-5.25351	-2.72149	H	-3.95452	8.602919	-3.51786
C	1.6284	5.204281	-0.37553	H	-5.31343	7.791906	-4.29992
C	1.562024	6.547199	-0.01356	Te	-0.20568	-3.61846	1.224247
C	1.551993	6.936879	1.333763				

Table S10. Comparison of the relative energies of *m*-benzicalixhexaphyrin(1.*1*.*1*.1.1.1)s **2-5** and *m*-benziheterohexaphyrin(1.1.1.1.1.1)s **6a**-**6d**.

Compound	**Relative Energy (hartree)**	**Compound**	**Relative Energy (hartree)**
2	-3300.8	6a	-3147.8
3b	-3623.7	6b	-3470.8
4	-5624.9	6c	-5472.0
5	-3233.4	6d	-3080.5

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