

Supporting Information

Doubly Fused Fluorene Embedded Heterosapphyrins

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Experimental Section

General Experiment: The chemicals such as $\text{BF}_3 \cdot \text{OEt}_2$ and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) were used as obtained from Aldrich. All other chemicals used for the synthesis were reagent grade unless otherwise specified. Column chromatography was performed on silica (60–120 and 100–200 mesh), neutral alumina, and basic alumina. ^1H , ^2D , and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded in CDCl_3 on Bruker 400 and 500 MHz instruments. Tetramethylsilane [$\text{Si}(\text{CH}_3)_4$] was used as an internal standard for ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR. Absorption spectra were obtained with a Cary Series UV–Vis–NIR and UV 3600 Shimadzu spectrophotometer. Cyclic voltammetric studies were carried out with a BAS electrochemical system utilizing the three-electrode configuration consisting of glassy carbon (working electrode), platinum wire (auxiliary electrode) and saturated calomel (reference electrode) electrodes. The experiments were done in dry CH_2Cl_2 using 0.1 M tetrabutylammonium perchlorate (TBAP) as a supporting electrolyte. Half-wave potentials were measured using differential pulse voltammetry (DPV) and also calculated manually by taking the average of the cathodic and anodic peak potentials. All potentials were calibrated versus a saturated calomel electrode by the addition of ferrocene as an internal standard, taking $E_{1/2}(\text{Fc}/\text{Fc}^+) = 0.42 \text{ V}$ versus SCE. All the solutions were purged prior to electrochemical and spectral measurements with argon gas. The high-resolution mass spectra (HRMS) were recorded with a Bruker maXis Impact and QT of micro mass spectrometer using positive mode ESI methods for acetonitrile/methanol solutions. For UV–vis spectroscopy, the stock solution of all compounds ($5 \times 10^{-4} \text{ M}$) was prepared by using HPLC-grade chloroform solvent.

Computational details: Full geometry of compound **1-5** were optimization by using Gaussian 09 quantum chemical software.² For compound **1-5**, the density functional theory (DFT)³ method with the B3LYP/6-31G(d,p)¹ basis set was used for all atoms for optimization in S_0 state. The frequency calculations were done on S_0 optimized geometries to substantiate genuine global minimum energy structures and found that the sum of imaginary frequencies was zero for all the metal complexes. The optimized geometries were used to gain frontier molecular orbitals (FMOs) and were also subjected to single point TD-DFT calculations for the first 50 $S_0 \rightarrow S_n$ transitions to understand absorption properties of macrocycle **3-5**.⁴⁻¹⁰ The integral equation formalism for the polarizable continuum model (PCM) within the self-consistent reaction field (SCRF) theory was used in the TD-DFT calculations to describe the solvation of **3-5** in chloroform.

General procedure for the synthesis of doubly fused fluorene embedded heterosapphyrins

1-5: In a 250 mL one-necked round-bottom flask fitted with a nitrogen bubbler, samples of fluorene based tripyrrane **8** (0.24 mmol) and appropriate bithiophene diols **9a-e** (0.24 mmol) were dissolved in dichloromethane (150 ml) and N_2 gas was purged for 10 min. The condensation was initiated by adding $BF_3 \cdot OEt_2$ (0.12 mmol) and the reaction mixture was stirred for 45 minutes at room temperature under inert atmosphere. The oxidizing agent, DDQ (0.59 mmol) was then added and the reaction mixture was stirred for additional 1 h in open air at room temperature. The solvent was removed on rotary evaporator under reduced pressure and the crude mixture was subjected to basic alumina column chromatography. The more polar major spot of the desired macrocycle was collected using petroleum ether/dichloromethane (75:25) and the doubly fused fluorene embedded heterosapphyrins **1-5** were obtained as brown colored solids in 5-7% yields.

Compound 1: Compound **1** was synthesized from **8** (120 mg, 0.24 mmol) and **9a** (90 mg, 0.24 mmol) by following the general procedure described above. Yield 7% (15 mg); ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.86 (d, $J = 7.8$ Hz, 2H), 7.59 (d, $J = 7.5$ Hz, 4H), 7.55 (s, 2H), 7.48 (d, $J = 7.8$ Hz, 2H), 7.39 (dd, $J = 12.0, 5.5$ Hz, 8H), 7.23 (d, $J = 8.1$ Hz, 6H), 6.99 (d, $J = 5.8$ Hz, 2H), 6.61 (d, $J = 5.9$ Hz, 2H), 4.11 (d, $J = 21.7$ Hz, 1H), 3.88 – 3.71 (m, 3H), 2.42 (s, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 146.94, 142.80, 142.66, 138.78, 138.68, 138.52, 138.12, 138.01, 137.86, 137.70, 137.57, 137.37, 135.44, 135.23, 134.38, 133.87, 132.94, 131.52, 131.41, 131.21, 129.81, 129.06, 128.92, 128.83, 128.27, 128.02, 127.64, 127.17, 126.68, 126.35, 126.19, 126.07, 125.42, 122.26, 122.21, 29.72, 21.33. UV-vis (in CHCl_3 , $\lambda_{\text{max}}/\text{nm}$) 443, 566. HR ESI-MS (positive): m/z calcd for $[\text{C}_{59}\text{H}_{38}\text{N}_2\text{S}_2]^+$: 838.2476 $[\text{M}]^+$; found: 838.2475.

Compound 2: Compound **2** was synthesized from **8** (120 mg, 0.24 mmol) and **9b** (97 mg, 0.24 mmol) by following the general procedure described above. Yield 6% (14 mg); ^1H NMR (500 MHz, CDCl_3) δ (ppm): 7.85 (d, $J = 7.8$ Hz, 2H), 7.54 (s, 2H), 7.49 (t, $J = 9.9$ Hz, 6H), 7.38 (d, $J = 8.0$ Hz, 4H), 7.22 (t, $J = 7.1$ Hz, 8H), 6.97 (d, $J = 5.9$ Hz, 2H), 6.59 (d, $J = 5.9$ Hz, 2H), 4.11 (d, $J = 21.7$ Hz, 1H), 3.86 – 3.71 (m, 3H), 2.42 (s, 6H), 2.37 (s, 6H). ^{13}C NMR (126 MHz, CDCl_3) δ 146.90, 142.73, 138.57, 134.18, 131.51, 130.19, 129.62, 129.22, 129.04, 128.49, 128.29, 127.30, 126.39, 126.33, 126.11, 125.10, 122.25, 121.39, 110.17, 21.33, 21.25. UV-vis (in CHCl_3 , $\lambda_{\text{max}}/\text{nm}$) 447, 564. HR ESI-MS (positive): m/z calcd for $[\text{C}_{61}\text{H}_{42}\text{N}_2\text{S}_2]^+$: 866.2789 $[\text{M}]^+$; found: 866.2786.

Compound 3. Compound **3** was synthesized from **8** (120 mg, 0.24 mmol) and **9c** (105 mg, 0.24 mmol) by following the general procedure described above. Yield 7% (14 mg) ; ^1H NMR (500

MHz, CDCl₃) δ (ppm): 7.85 (d, J = 7.8 Hz, 2H), 7.53 (d, J = 6.3 Hz, 6H), 7.47 (d, J = 7.6 Hz, 2H), 7.38 (d, J = 7.8 Hz, 4H), 7.23 (d, J = 7.8 Hz, 4H), 6.95 (d, J = 8.6 Hz, 6H), 6.58 (d, J = 5.5 Hz, 2H), 4.10 (d, J = 21.6 Hz, 1H), 3.86 – 3.71 (m, 9H), 2.39 (s, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 158.07, 146.93, 142.73, 141.93, 138.59, 137.83, 137.81, 137.28, 135.17, 131.47, 131.20, 129.02, 128.27, 127.37, 126.89, 126.47, 126.22, 122.22, 122.14, 114.42, 110.42, 110.18, 55.35, 29.71, 21.30. UV-vis (in CHCl₃, λ_{\max} /nm) 454, 565. HR ESI-MS (positive): m/z calcd for [C₆₁H₄₂N₂O₂S₂]⁺: 898.2688 [M]⁺; found: 898.2679.

Compound 4: Compound **4** was synthesized from **8** (120 mg, 0.24 mmol) and **9d** (127 mg, 0.24 mmol) by following the general procedure described above. Yield 4% (10 mg) ; ¹H NMR (500 MHz, CDCl₃) δ 7.86 (d, J = 7.8 Hz, 2H), 7.55 (s, 2H), 7.50 (t, J = 8.5 Hz, 4H), 7.46 (t, J = 7.1 Hz, 6H), 7.38 (d, J = 8.0 Hz, 4H), 7.24 (d, J = 8.0 Hz, 4H), 6.94 (d, J = 5.9 Hz, 2H), 6.63 (d, J = 5.9 Hz, 2H), 4.12 (d, J = 21.7 Hz, 1H), 3.88 – 3.71 (m, 3H), 2.42 (s, 6H). ¹³C NMR (126 MHz, CDCl₃) δ 146.9, 144.9, 144.42, 143.0, 140.4, 138.8, 138.3, 138.1, 137.4, 137.1, 135.0, 131.7, 131.2, 130.8, 129.2, 128.4, 128.2, 125.7, 124.5, 122.3, 110.6, 108.3, 29.7. UV-vis (in CHCl₃, λ_{\max} /nm) 444, 568. HR ESI-MS (positive): m/z calcd for [C₅₉H₃₆Br₂N₂S₂]⁺: 996.0687 [M]⁺; found: 996.0664.

Compound 5: Compound **5** was synthesized from **8** (120 mg, 0.24 mmol) and **9e** (111 mg, 0.24 mmol) by following the general procedure described above. Yield 6% (13 mg) . ¹H NMR (400 MHz, CDCl₃) δ (ppm): 8.23 (d, J = 8.8 Hz, 4H), 7.84 (t, J = 17.7 Hz, 2H), 7.66 (d, J = 8.8 Hz, 4H), 7.55 (s, 2H), 7.46 (d, J = 7.8 Hz, 2H), 7.40 (d, J = 8.0 Hz, 4H), 7.27 (d, J = 2.0 Hz, 4H), 7.02 (d, J = 5.9 Hz, 2H), 6.73 (d, J = 5.9 Hz, 2H), 4.14 (d, J = 21.5 Hz, 1H), 3.82 – 3.75 (m, 3H), 2.44 (s, 6H). ¹³C NMR δ (126 MHz, CDCl₃) 146.9, 142.8, 142.75, 138.6, 138.4, 138.2, 137.5,

137.3, 135.0, 132.7, 131.9, 131.5, 131.1, 129.1, 128.3, 128.2, 127.54, 127.0, 122.2, 121.8, 119.4, 110.3, 109.3, 21.3. UV-vis (in CHCl₃, λ_{max}/nm) 472, 587. HR ESI-MS (positive): m/z calcd for [C₅₉H₃₆N₄O₄S₂]⁺ : 928.2178 [M]⁺ ; found: 928.2172.

General procedure for the synthesis of mono-fused fluorene embedded heterosapphyrins

11-13: Samples of fluorene based tripyrrane **8** (0.24 mmol) and appropriate bithiophene diols **9a-c** (0.24 mmol) were dissolved in dichloromethane (150 ml) in a 250 mL one-necked round-bottom flask fitted with a nitrogen bubbler and purged nitrogen for 10 min.. BF₃.OEt₂ (0.12 mmol) was added to initiate the reaction and stirred for 45 min at room temperature under inert atmosphere. One equivalent of the oxidizing agent, DDQ (0.24 mmol) was then added and the reaction mixture was stirred for additional 10 minutes in open air at room temperature. The solvent was removed on rotary evaporator under reduced pressure and the crude mixture was subjected to basic alumina column chromatography. The desired less polar major spot was collected using petroleum ether/dichloromethane (85:15) and afforded the pure pink colored solids of mono fused fluorene embedded heterosapphyrins **11-13** in 6-8% yields.

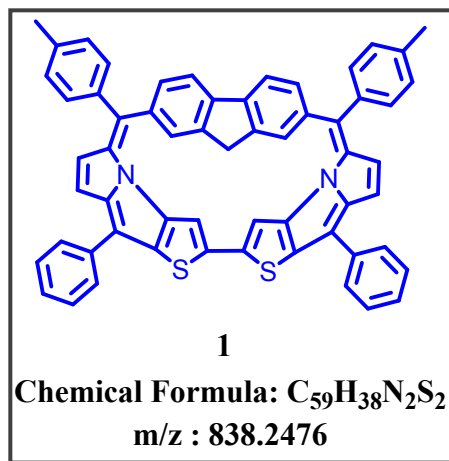
Compound 11: Compound **11** was synthesized from **8** (120 mg, 0.24 mmol) and **9a** (90 mg, 0.24 mmol) by following the general procedure described above. Yield 7% (14 mg); ¹H NMR (500 MHz, CDCl₃) δ 7.91 (d, *J* = 7.9 Hz, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.78 (s, 1H), 7.64 (d, *J* = 7.5 Hz, 2H), 7.45 (t, *J* = 6.9 Hz, 3H), 7.38 – 7.29 (m, 7H), 7.28 – 7.18 (m, 8H), 7.04 (s, 1H), 6.98 (d, *J* = 5.8 Hz, 1H), 6.80 (s, 1H), 6.52 (d, *J* = 5.8 Hz, 1H), 6.38 (d, *J* = 3.6 Hz, 1H), 6.25 (d, *J* = 3.6 Hz, 1H), 5.99 (s, 1H), 5.80 (s, 1H), 5.63 (s, 1H), 5.46 (s, 1H), 4.50 (s, 1H), 3.75 (d, *J* = 22.1 Hz, 1H), 3.47 (d, *J* = 22.1 Hz, 1H), 2.45 (s, 3H), 2.39 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 144.72, 142.96, 141.83, 141.48, 139.83, 139.56, 138.37, 138.09, 137.16, 136.63, 133.91, 131.72, 128.25, 128.03, 126.67, 126.02, 124.13, 122.79, 121.95, 120.42, 119.89, 111.77, 107.31, 106.46,

49.66, 45.19, 37.34, 29.48, 21.35, 21.08. UV-vis (in CHCl₃, λ_{max}/nm) 446, 529. HR ESI-MS (positive): m/z calcd for [C₅₉H₄₂N₂S₂]⁺ : 842.2789 [M]⁺ ; found: 842.2790.

Compound 12: Compound **12** was synthesized from **8** (120 mg, 0.24 mmol) and **9b** (97 mg, 0.24 mmol) by following the general procedure described above. Yield 8% (15 mg); ¹H NMR (500 MHz, CDCl₃) δ 7.90 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.77 (s, 1H), 7.53 (d, *J* = 7.8 Hz, 2H), 7.45 (d, *J* = 7.7 Hz, 1H), 7.31 (dd, *J* = 13.4, 7.6 Hz, 3H), 7.25 (d, *J* = 10.7 Hz, 5H), 7.21 (dd, *J* = 14.2, 7.9 Hz, 4H), 7.11 – 7.06 (m, 3H), 7.04 (s, 1H), 6.95 (d, *J* = 5.7 Hz, 1H), 6.80 (s, 1H), 6.49 (d, *J* = 5.7 Hz, 1H), 6.37 (d, *J* = 3.4 Hz, 1H), 6.24 (d, *J* = 3.4 Hz, 1H), 5.98 (s, 1H), 5.80 (s, 1H), 5.63 (s, 1H), 5.42 (s, 1H), 4.49 (s, 1H), 3.74 (d, *J* = 22.0 Hz, 1H), 3.46 (d, *J* = 22.2 Hz, 1H), 2.44 (s, 3H), 2.41 (s, 3H), 2.39 (s, 3H), 2.33 (s, 3H). ¹³C NMR (126 MHz, CDCl₃) δ 144.96, 144.71, 142.80, 141.53, 141.35, 139.91, 139.58, 138.56, 138.37, 137.95, 137.36, 136.79, 136.40, 136.28, 136.02, 135.85, 133.01, 131.75, 131.68, 131.01, 130.89, 129.66, 129.07, 128.93, 128.64, 127.88, 127.39, 126.84, 126.19, 125.95, 124.22, 122.87, 122.08, 120.48, 119.82, 111.64, 111.06, 107.14, 106.51, 44.92, 37.07, 34.07, 29.72, 22.36, 21.31, 21.25, 21.09, 21.04. UV-vis (in CHCl₃, λ_{max}/nm) 444, 531. HR ESI-MS (positive): m/z calcd for [C₆₁H₄₆N₂S₂]⁺ : 870.3102 [M]⁺ ; found: 870.3097.

Compound 13: Compound **13** was synthesized from **8** (120 mg, 0.24 mmol) and **9c** (105 mg, 0.24 mmol) by following the general procedure described above. Yield 7% (14 mg); ¹H NMR (500 MHz, CDCl₃) δ 7.87 (d, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 7.8 Hz, 1H), 7.74 (s, 1H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 7.8 Hz, 1H), 7.30 (d, *J* = 7.8 Hz, 4H), 7.23 (d, *J* = 7.4 Hz, 2H), 7.22 – 7.13 (m, 4H), 7.07 (d, *J* = 8.4 Hz, 2H), 7.03 – 6.95 (m, 2H), 6.90 (d, *J* = 5.7 Hz, 1H), 6.80 (d, *J* = 8.4 Hz, 2H), 6.76 (s, 1H), 6.46 (d, *J* = 5.8 Hz, 1H), 6.34 (d, *J* = 3.4 Hz, 1H), 6.20 (d, *J* = 3.4 Hz, 1H), 5.95 (s, 1H), 5.77 (s, 1H), 5.59 (s, 1H), 5.38 (s, 1H), 4.46 (s, 1H), 3.85 (s, 1H), 3.77 (s, 3H),

3.71 (d, $J = 22.0$ Hz, 4H), 3.43 (d, $J = 22.0$ Hz, 1H), 2.41 (s, 3H), 2.36 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 158.06, 145.14, 144.71, 141.30, 141.09, 139.96, 139.56, 138.61, 138.40, 137.90, 136.78, 136.29, 136.03, 133.06, 132.82, 131.87, 131.72, 130.90, 129.07, 129.02, 128.93, 128.63, 127.20, 127.06, 126.68, 126.61, 126.15, 124.18, 122.83, 121.99, 120.49, 119.83, 114.48, 113.70, 111.67, 107.12, 106.46, 55.38, 55.27, 49.96, 44.52, 37.06, 21.32, 21.10. UV-vis (in CHCl_3 , $\lambda_{\text{max}}/\text{nm}$) 449, 539. HR ESI-MS (positive): m/z calcd for $[\text{C}_{61}\text{H}_{46}\text{N}_2\text{O}_2\text{S}_2]^+$: 902.3001 $[\text{M}]^+$; found: 902.3011.



Observed Mass: 838.2475 [M⁺]

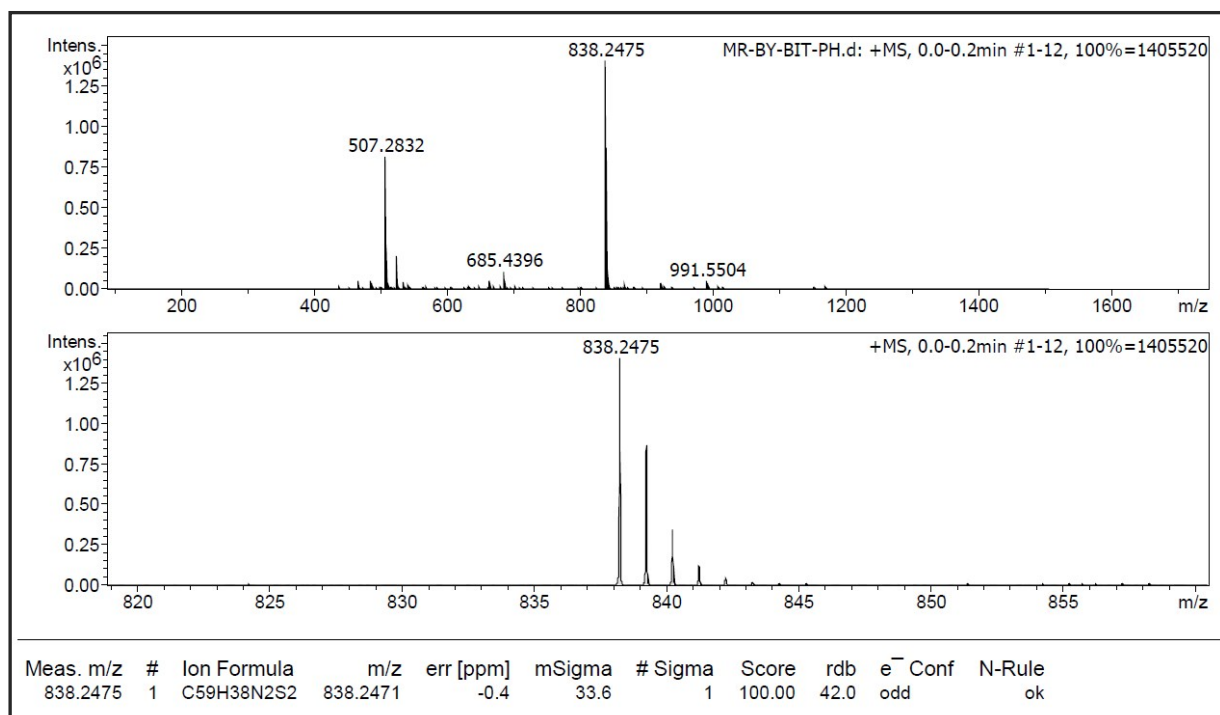


Figure S1. HRMS spectrum of compound **1**.

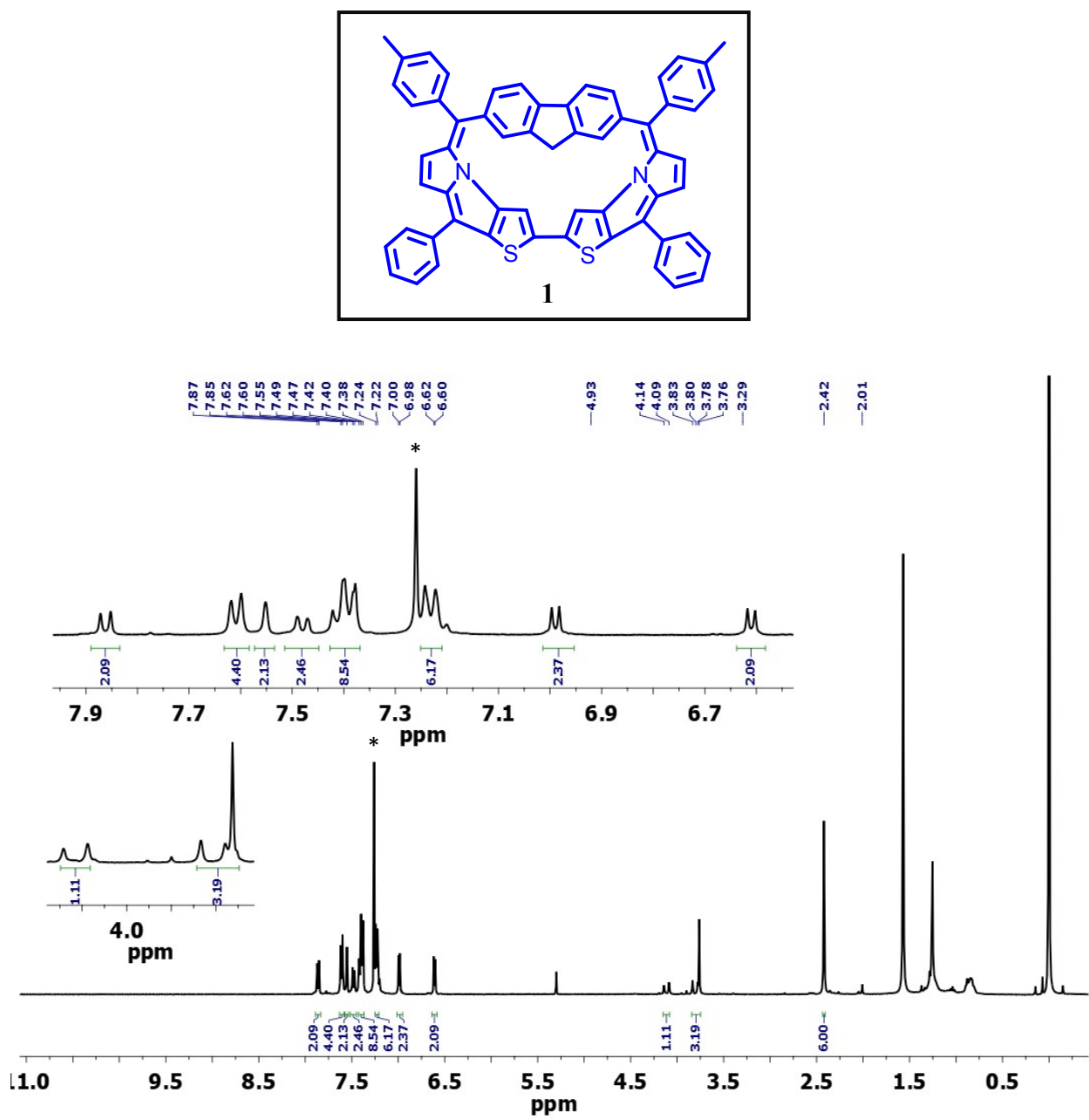


Figure S2. $^1\text{H NMR}$ of compound **1** recorded in CDCl_3 .

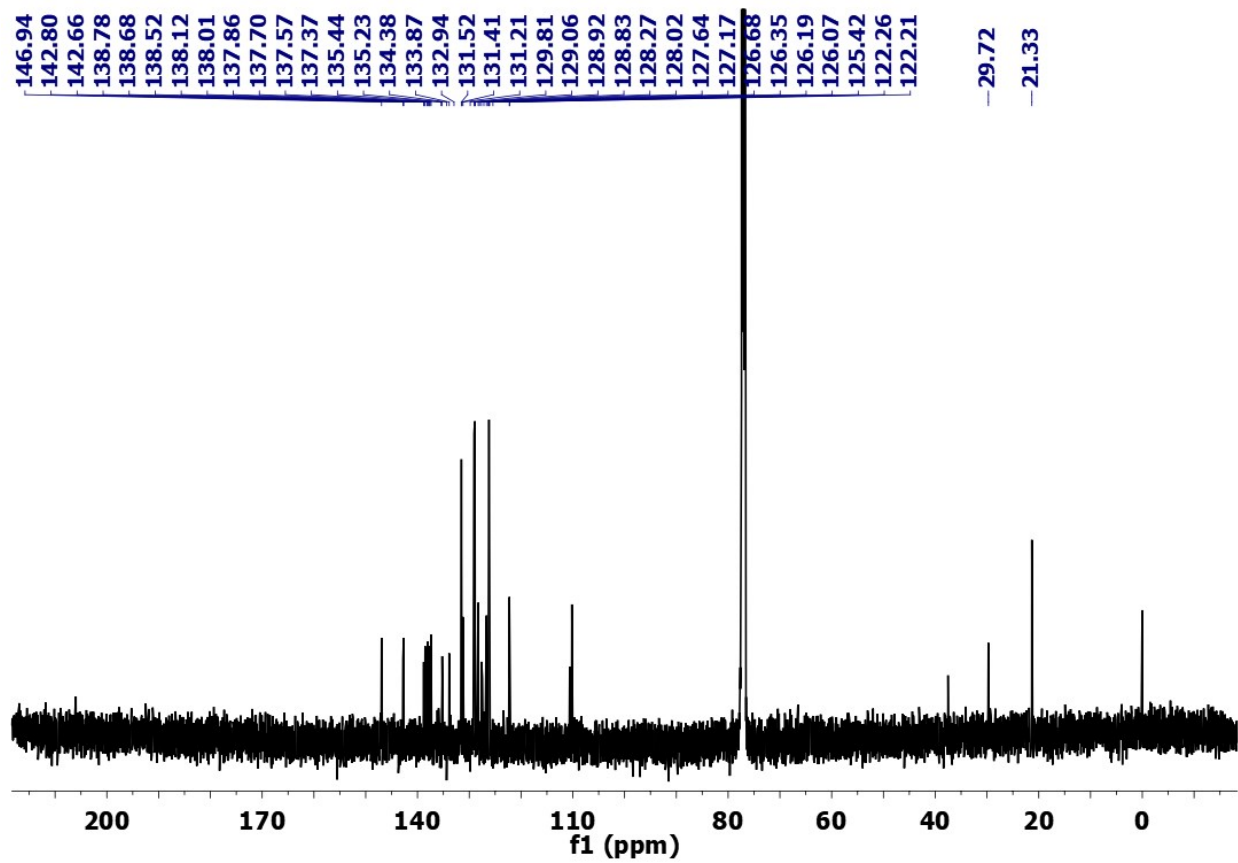
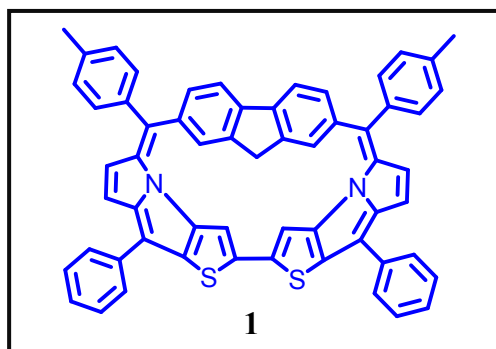
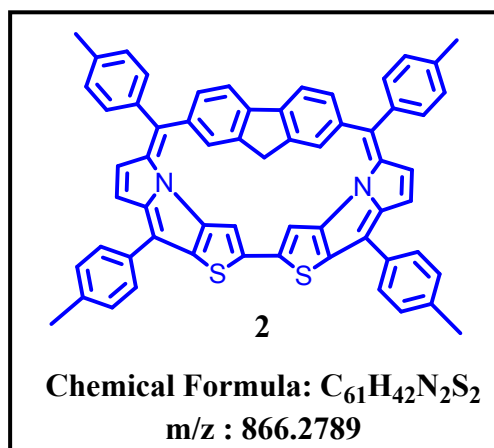


Figure S3. ^{13}C NMR of compound **1** recorded in CDCl_3 .



Observed Mass: 866.2786 [M⁺]

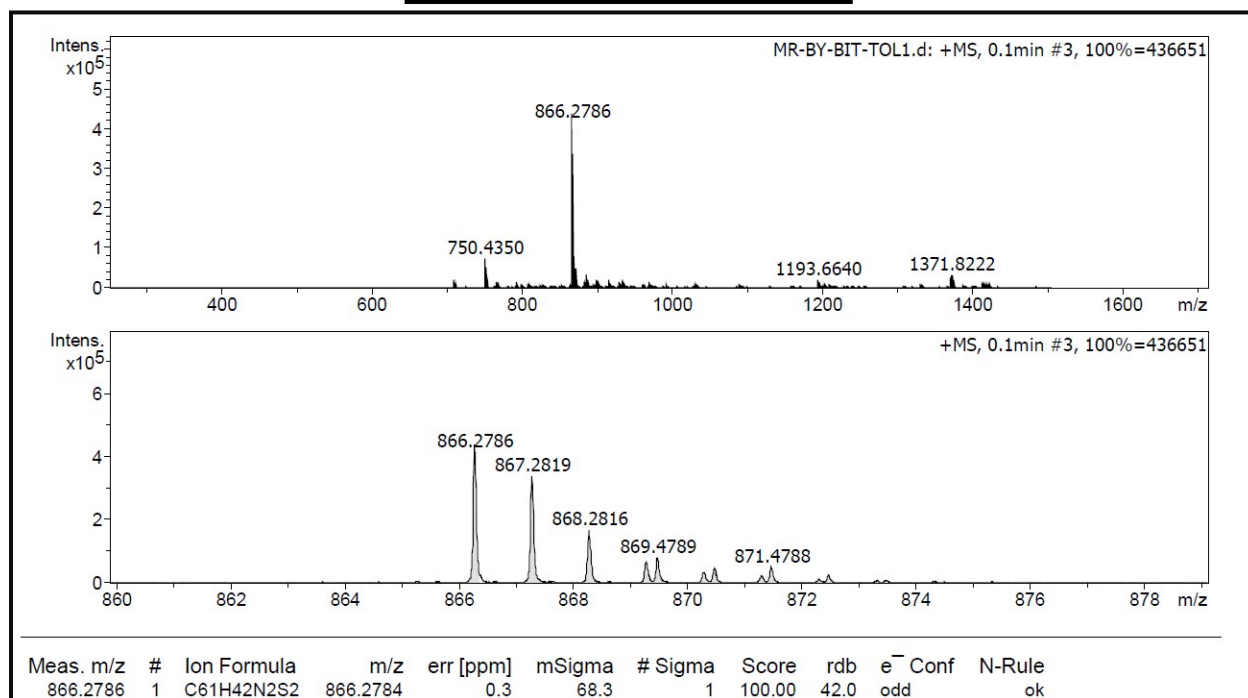


Figure S4. HRMS spectrum of compound **2**.

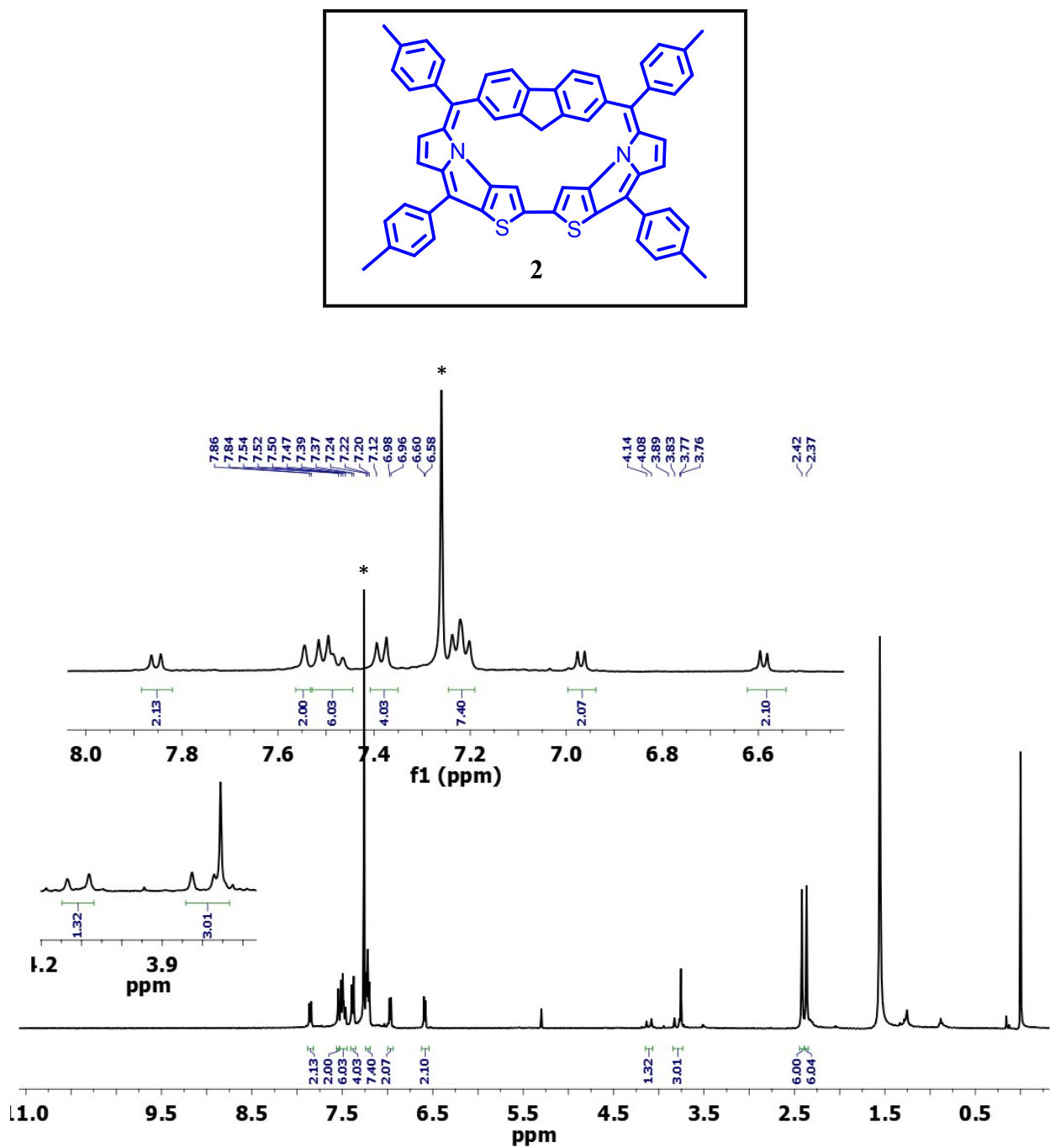


Figure S5. ^1H NMR of compound **2** recorded in CDCl_3

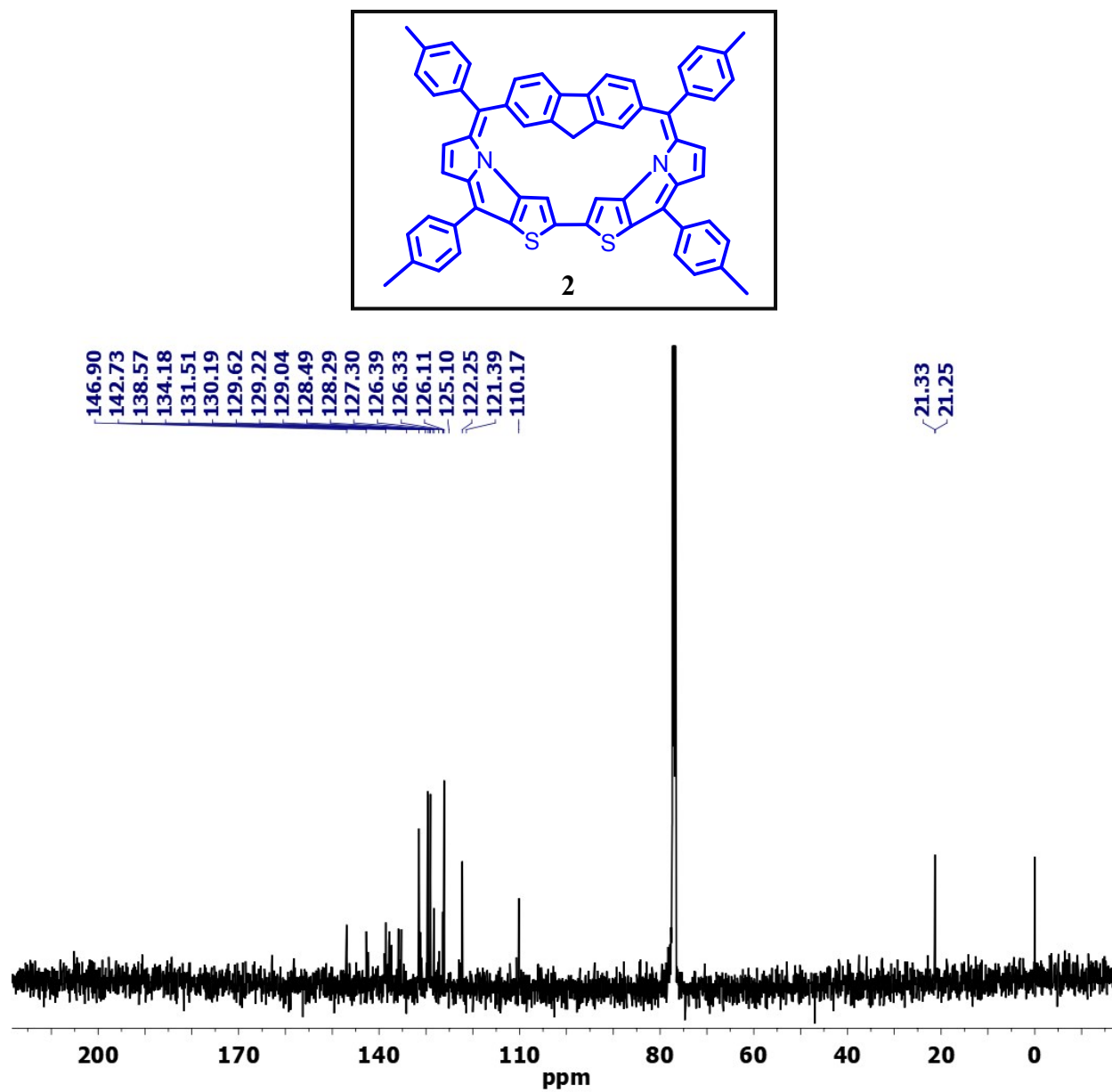
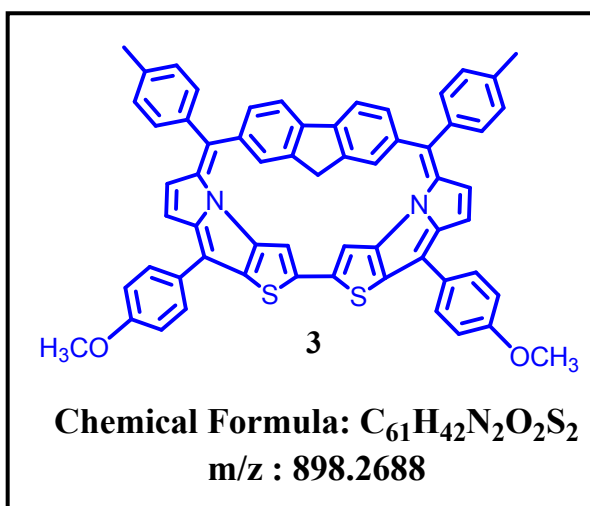


Figure S6. ^{13}C NMR of compound 2 recorded in CDCl_3 .



Observed Mass: 898.2679 [M⁺]

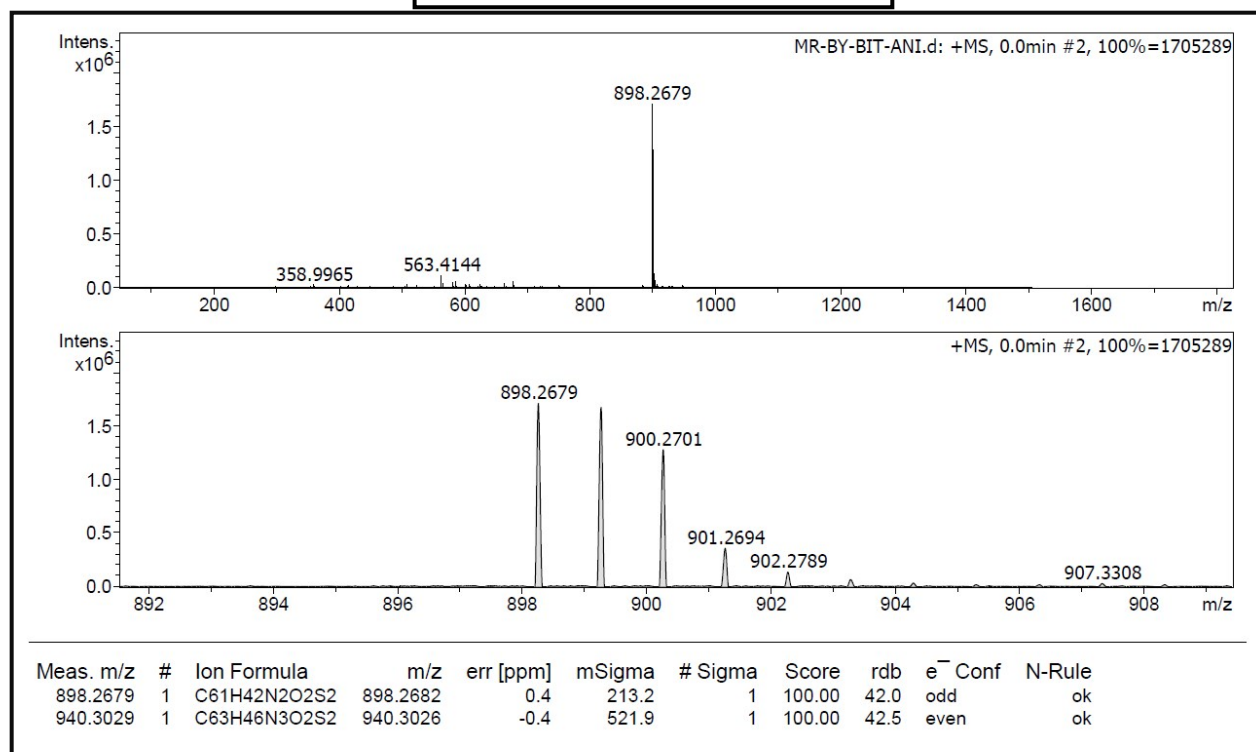


Figure S7. HRMS spectrum of compound 3.

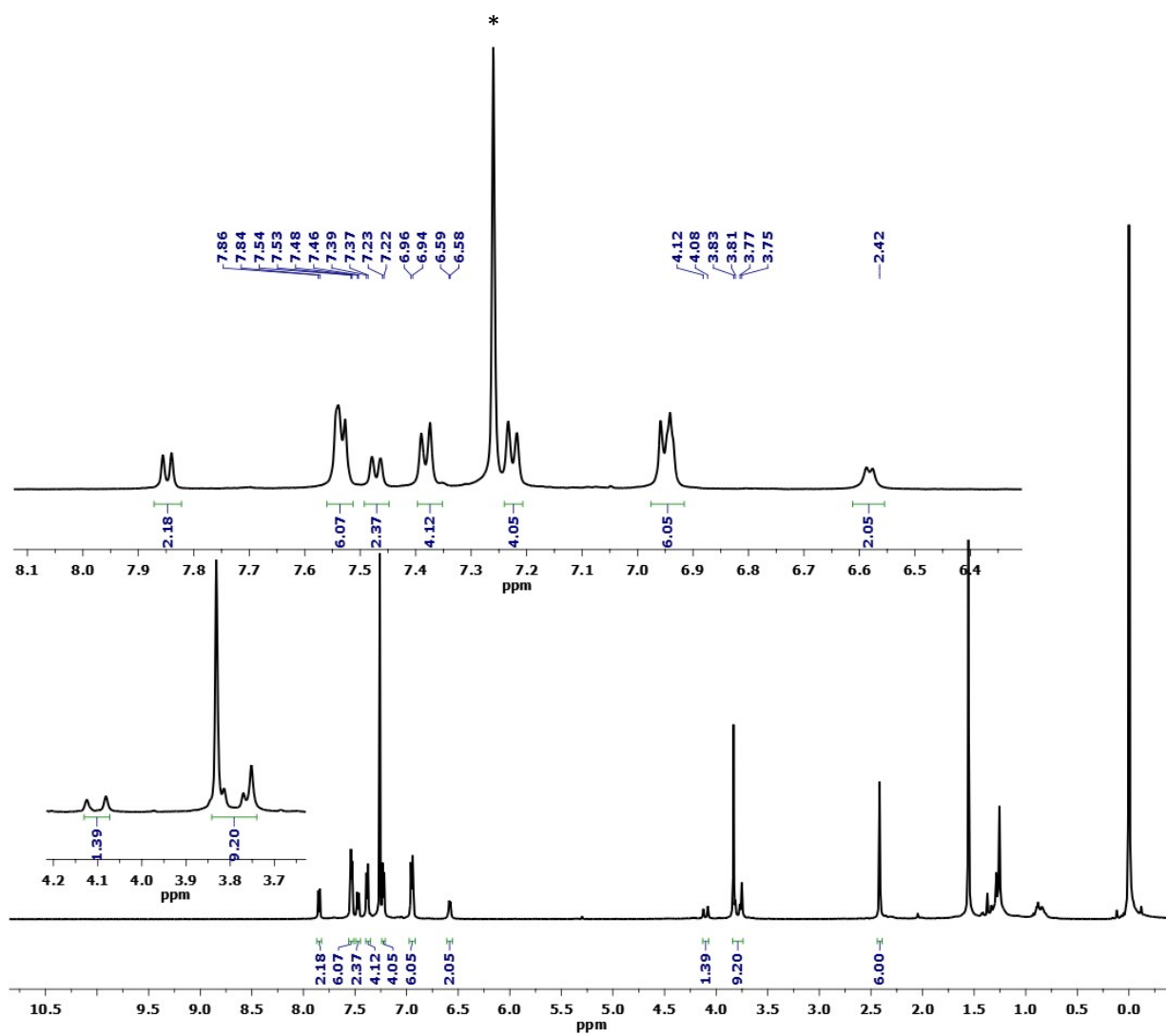
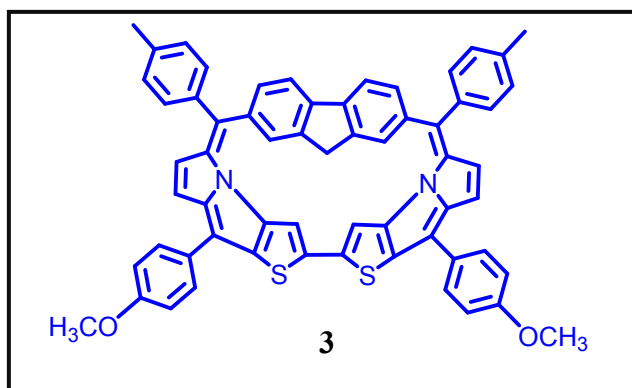


Figure S8. ^1H NMR of compound **3** recorded in CDCl_3 .

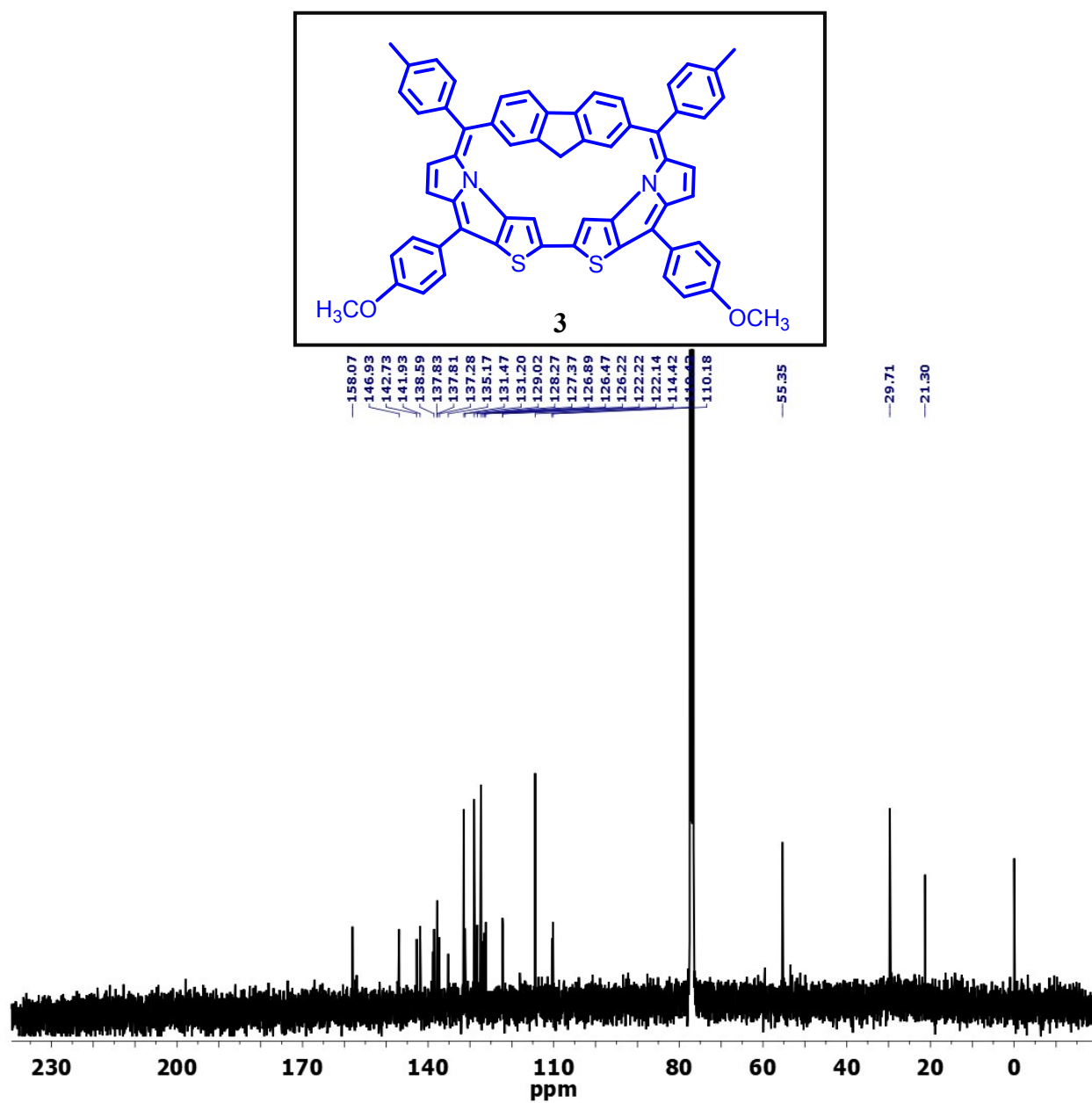


Figure S9. ^{13}C NMR of compound **3** recorded in CDCl_3 .

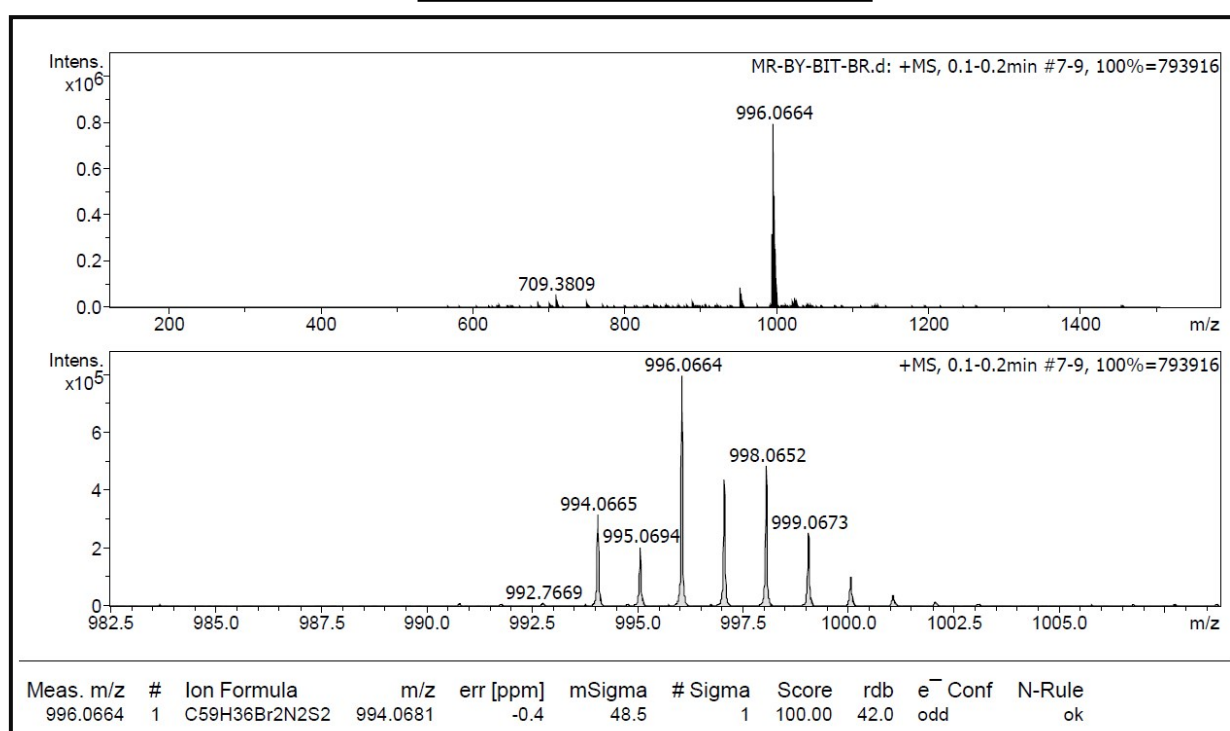
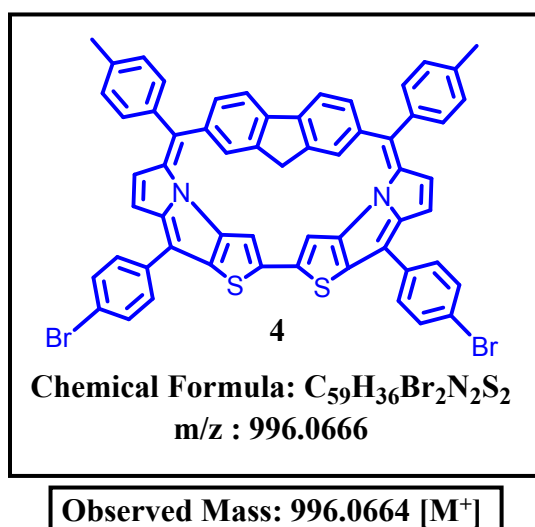


Figure S10. HRMS spectrum of compound **4**.

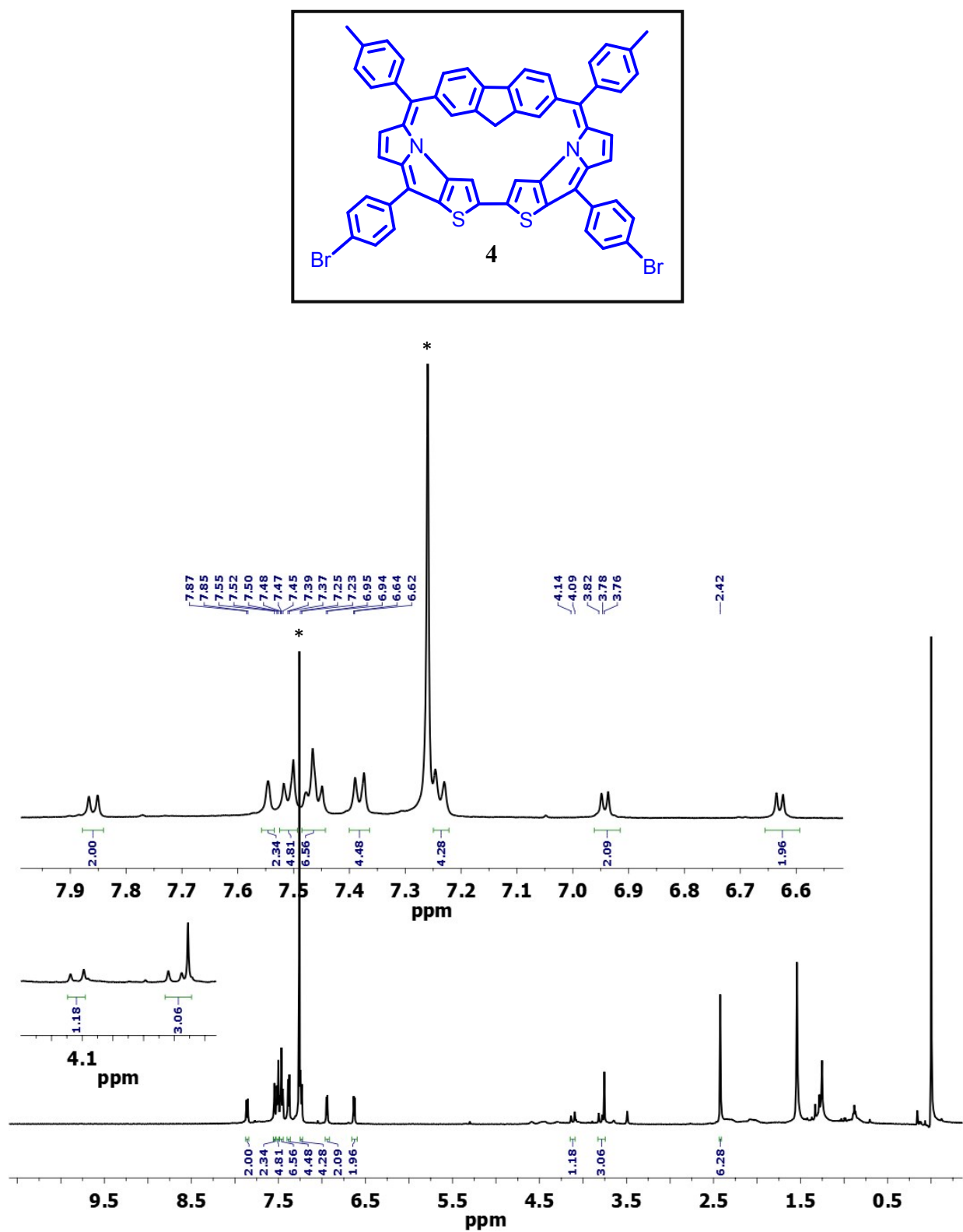


Figure S11. ^1H NMR of compound **4** recorded in CDCl_3 .

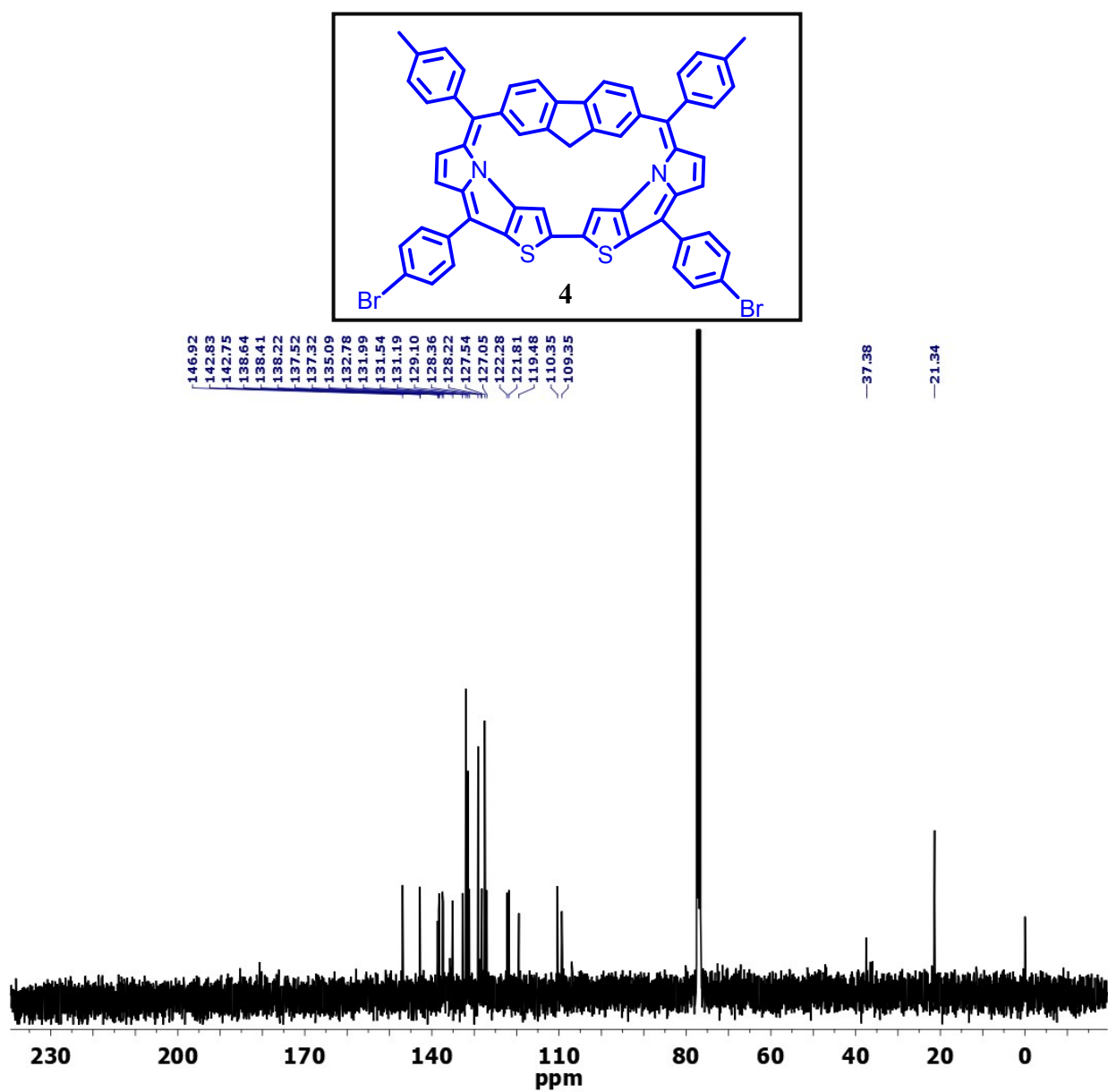
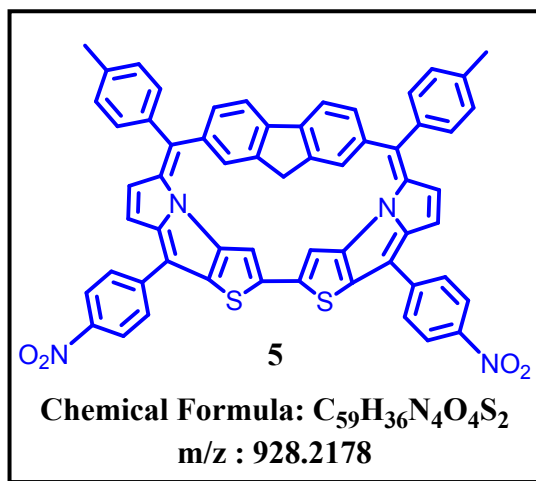
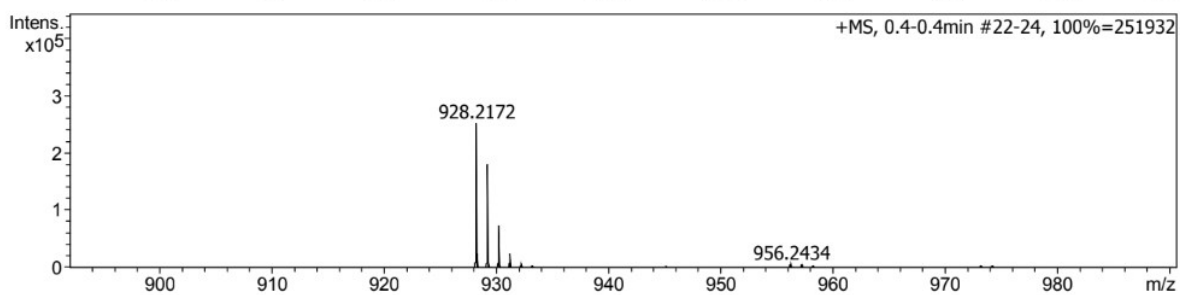
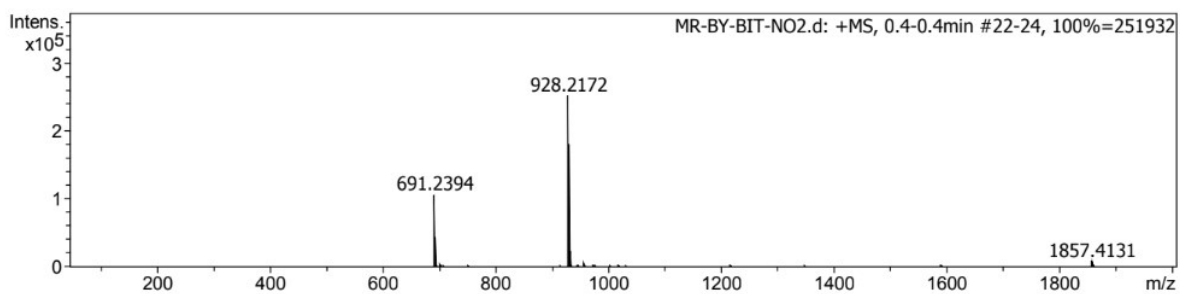


Figure S12. ^{13}C NMR of compound 4 recorded in CDCl_3 .



Observed Mass: 928.2172 [M⁺]



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
928.2172	1	C ₅₉ H ₃₆ N ₄ O ₄ S ₂	928.2172	0.0	22.9	1	100.00	44.0	odd	ok

Figure S13. HRMS spectrum of compound **5**.

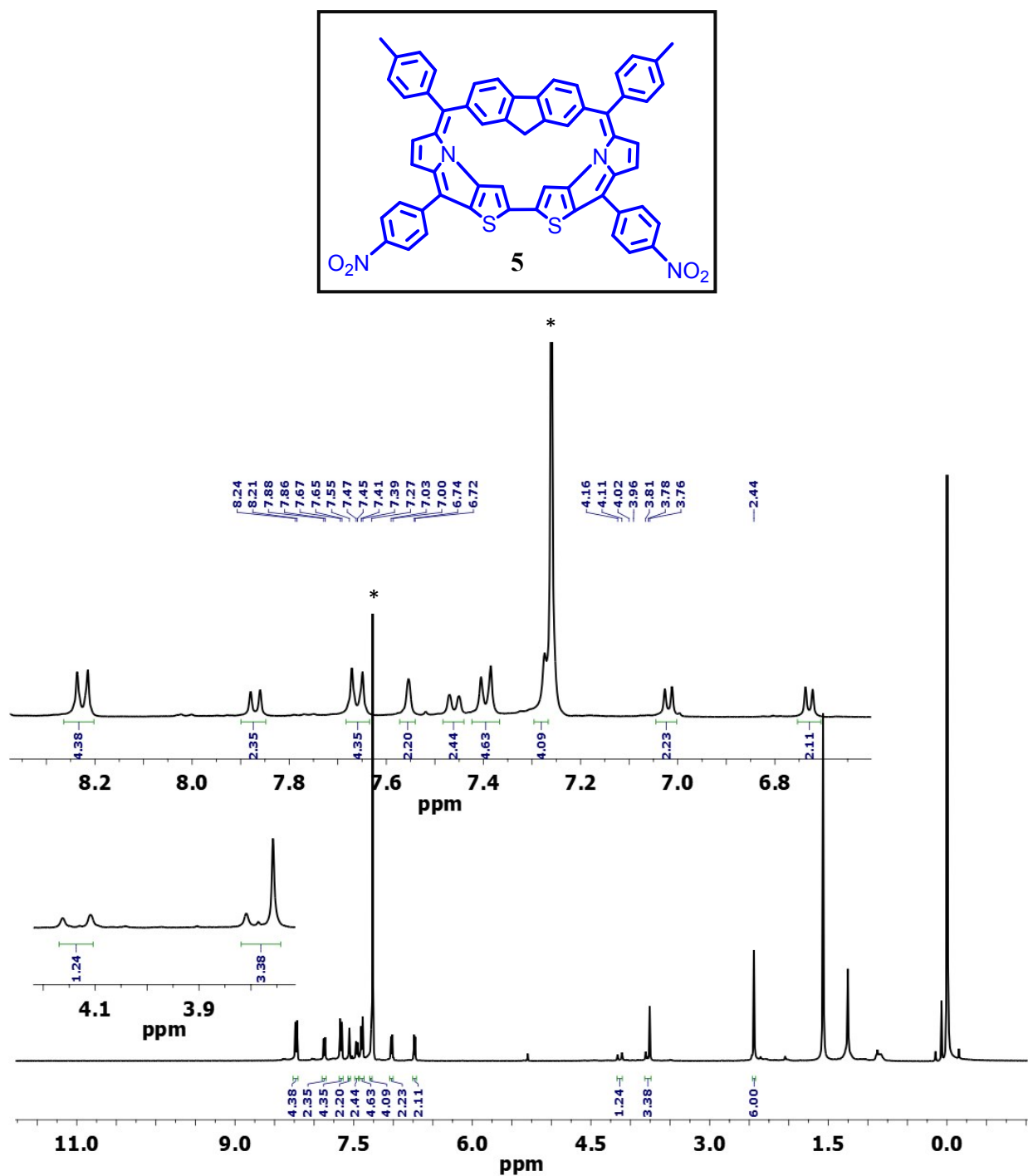


Figure S14. ^1H NMR of compound **5** recorded in CDCl_3 .

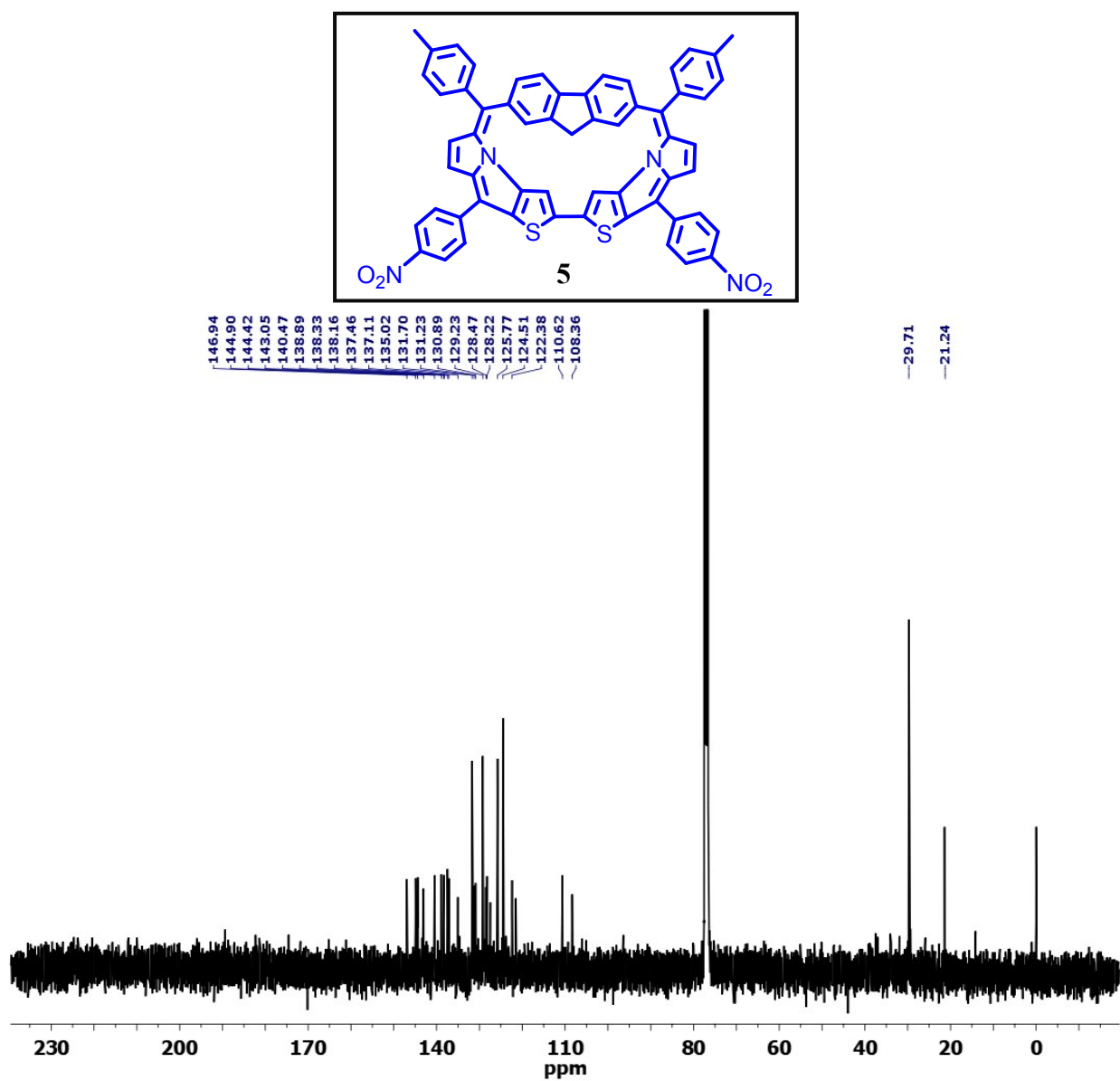
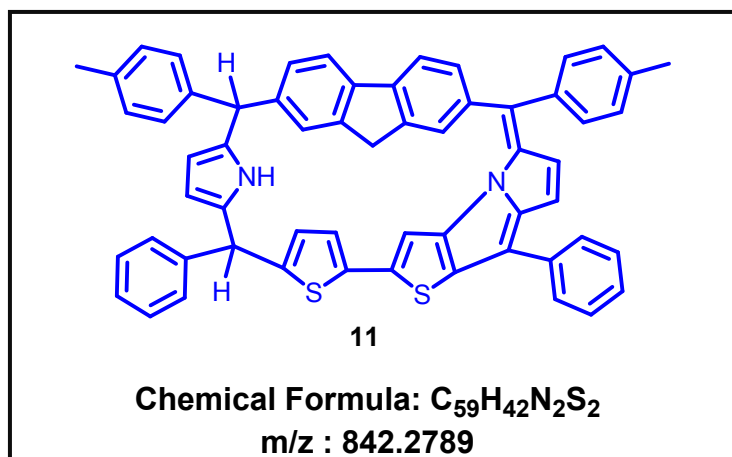


Figure S15. ^{13}C NMR of compound **5** recorded in CDCl_3 .



Observed Mass: 842.2790 [M⁺]

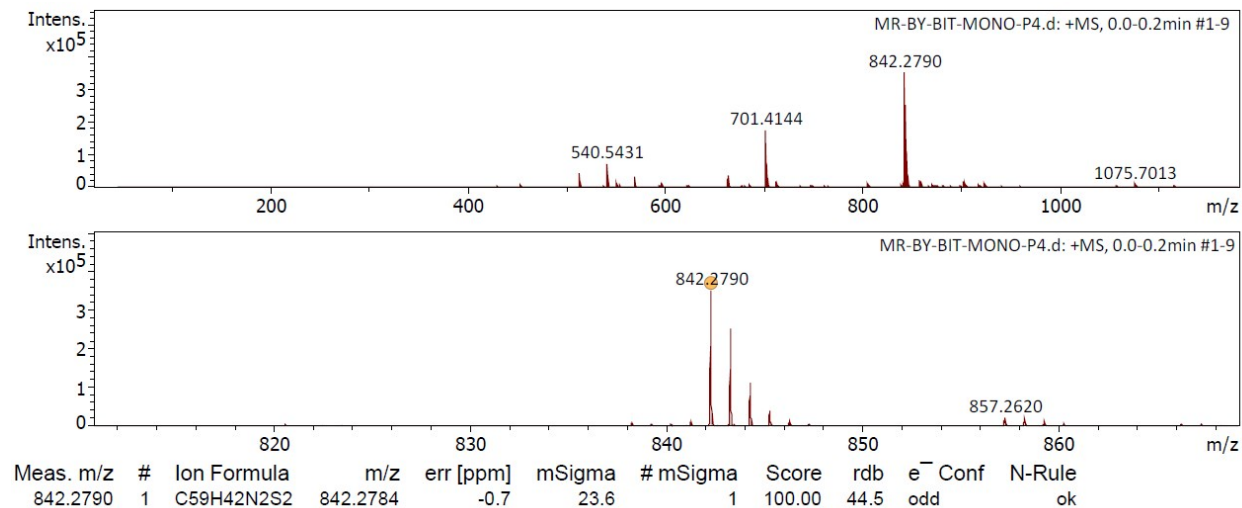


Figure S16. HRMS spectrum of compound **11**.

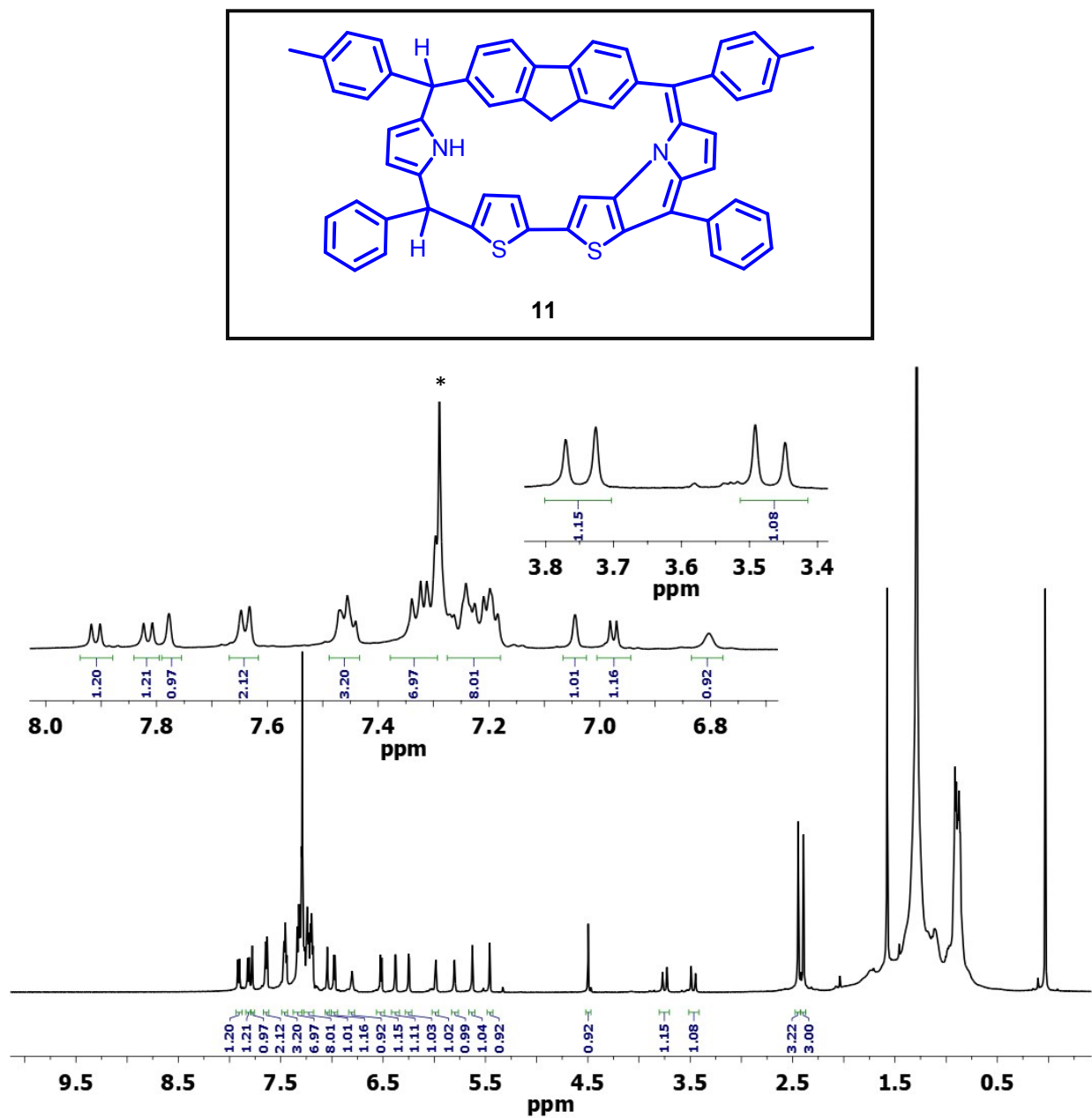


Figure S17. ^1H NMR of compound **11** recorded in CDCl_3 .

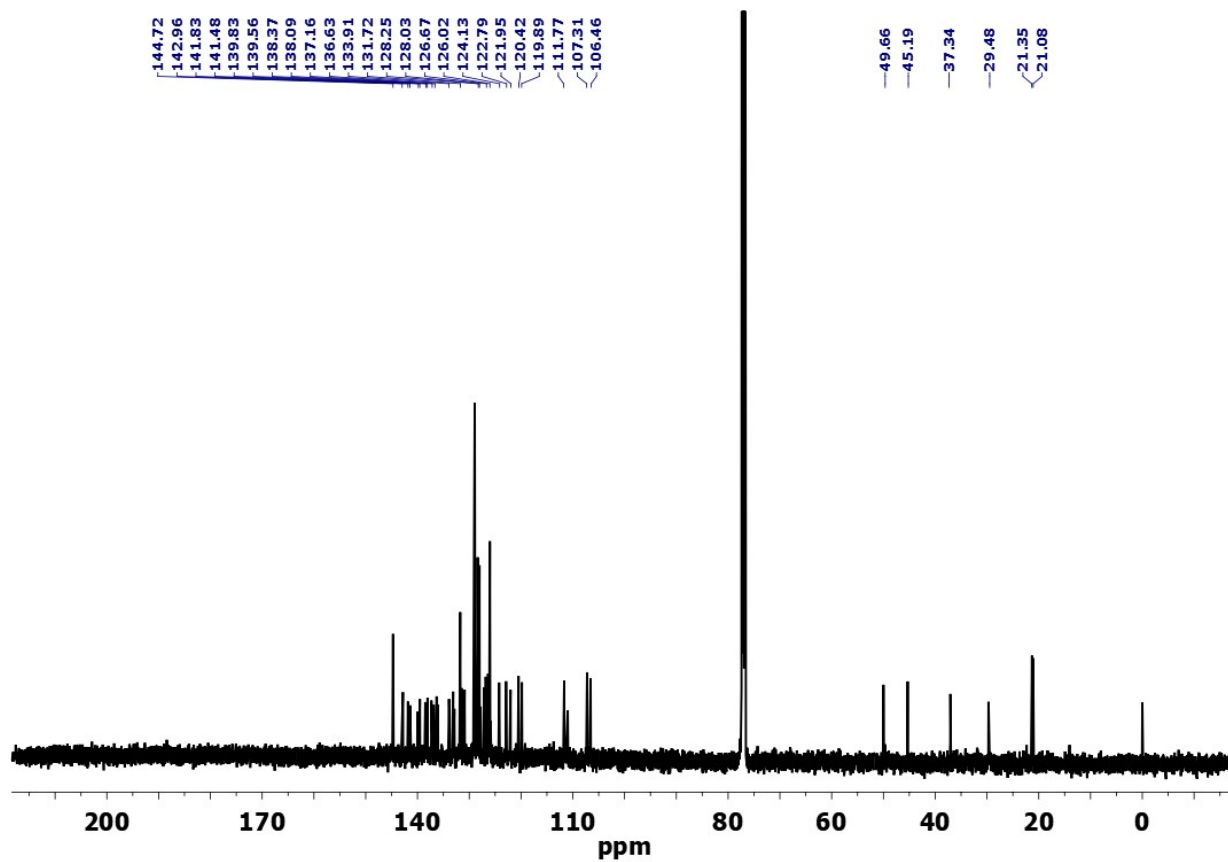
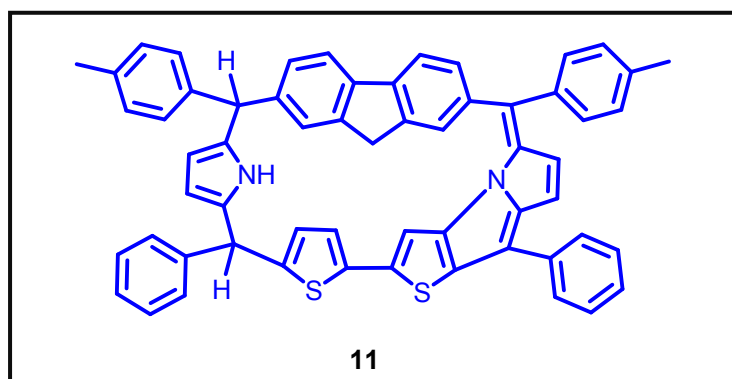
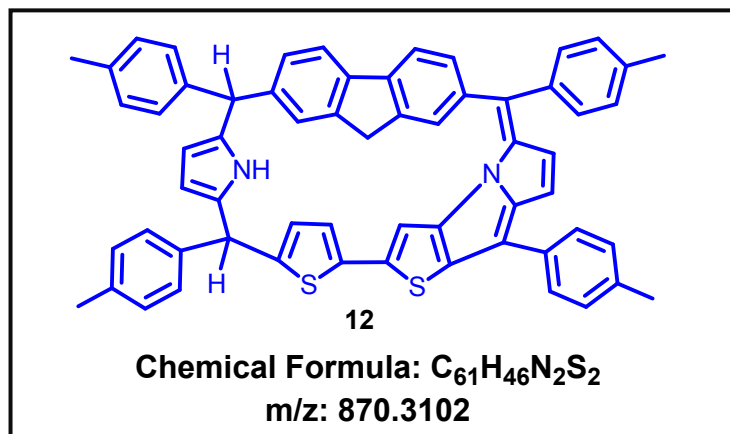


Figure S18. ^{13}C NMR of compound 11 recorded in CDCl_3 .



Observed Mass: 870.3097 [M⁺]

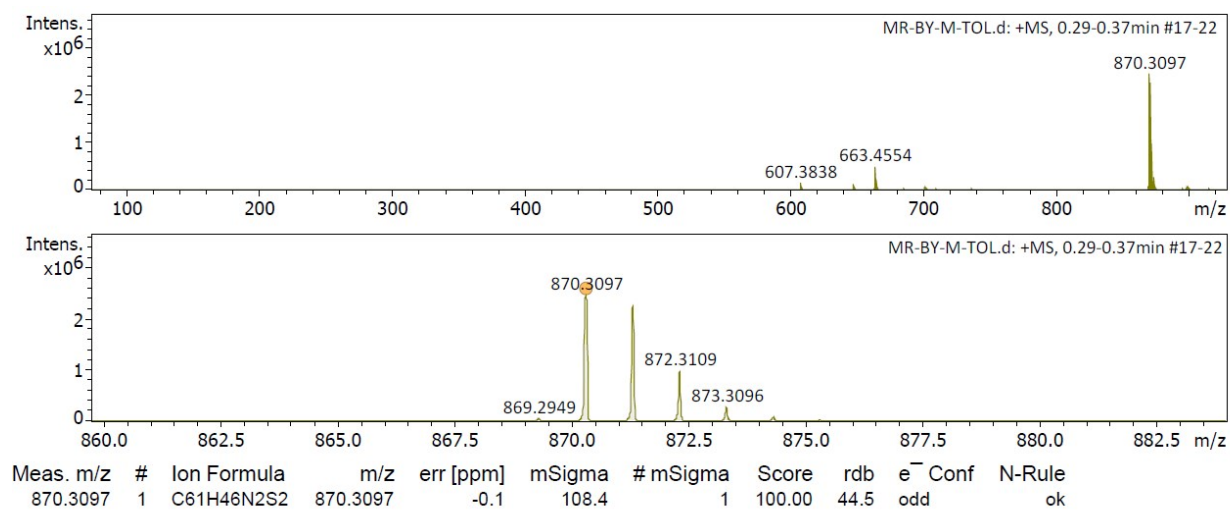


Figure S19. HRMS spectrum of compound **12**.

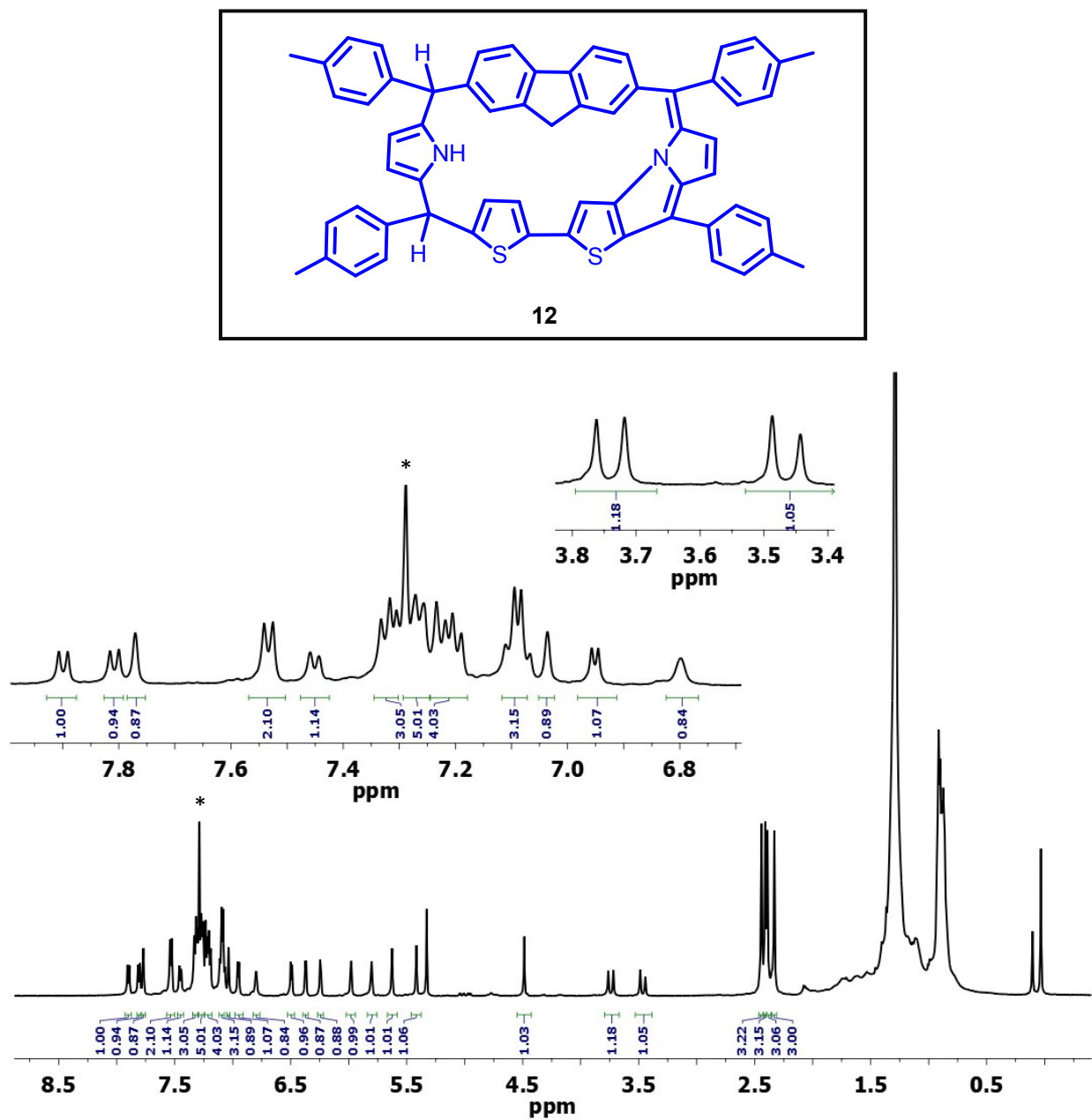


Figure S20. ^1H NMR of compound **12** recorded in CDCl_3 .

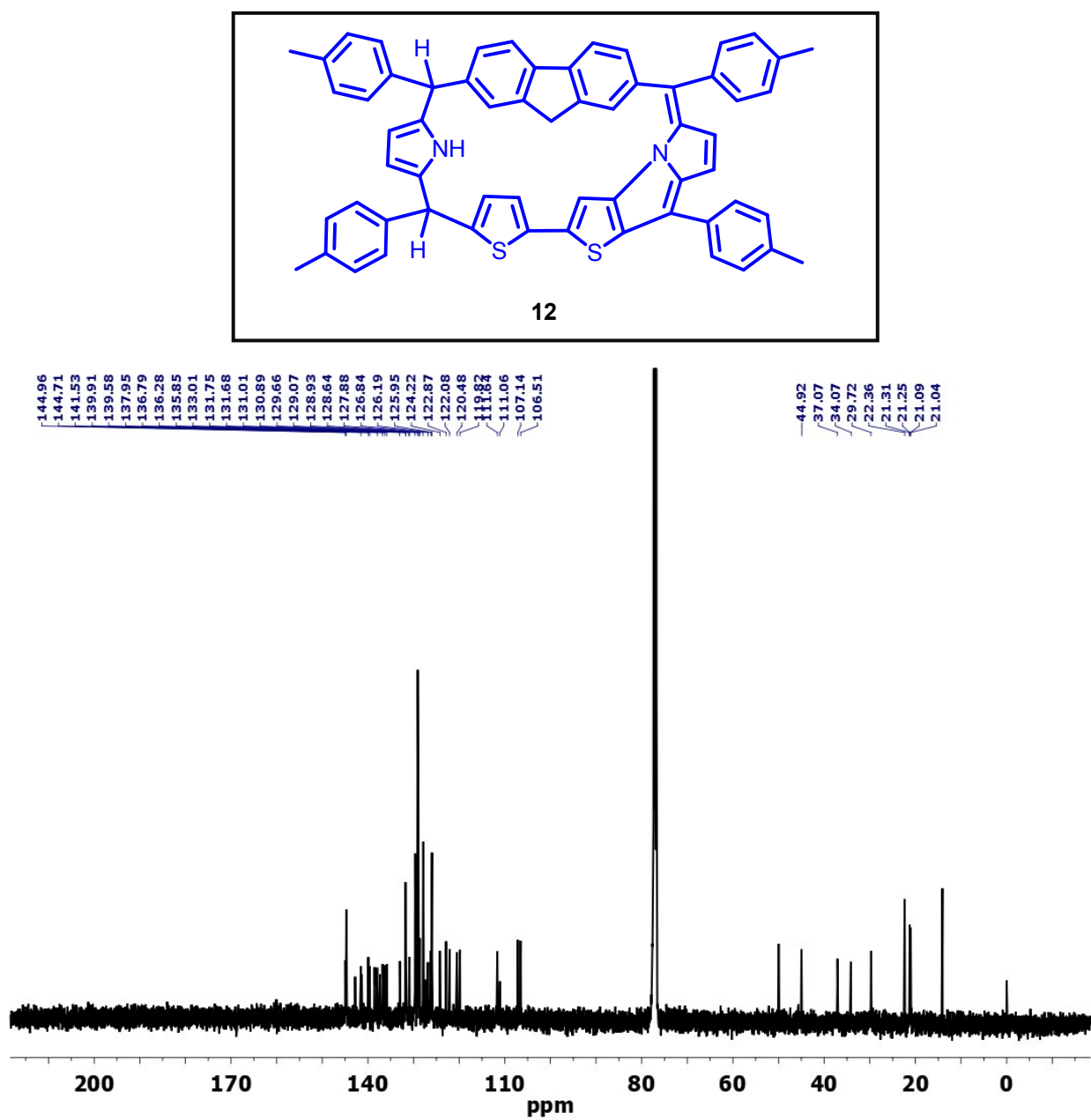
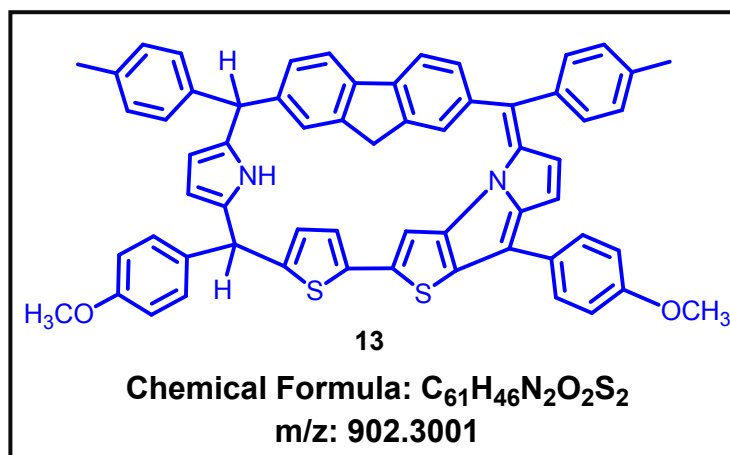
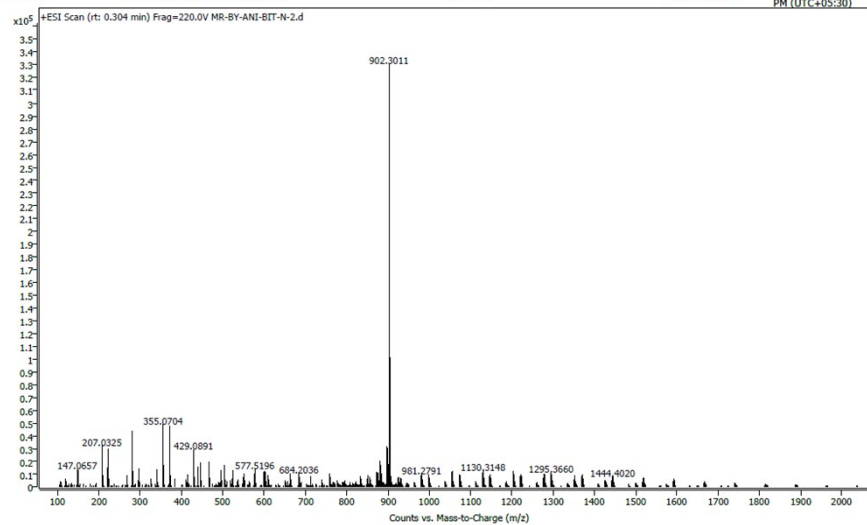


Figure S21. ^{13}C NMR of compound 12 recorded in CDCl_3 .



Observed Mass: 902.3011 [M⁺]

Name	Rack Pos.	Instrument	Operator
Inj. Vol. (ul)	Plate Pos.	IRM Status	Acc. Time (Local)
Data File	Method (Acq)	Comment	06-01-2021 5:46:13 PM (UTC+05:30)



Name	Rack Pos.	Instrument	Operator
Inj. Vol. (ul)	Plate Pos.	IRM Status	Acc. Time (Local)
Data File	Method (Acq)	Comment	06-01-2021 5:46:13 PM (UTC+05:30)

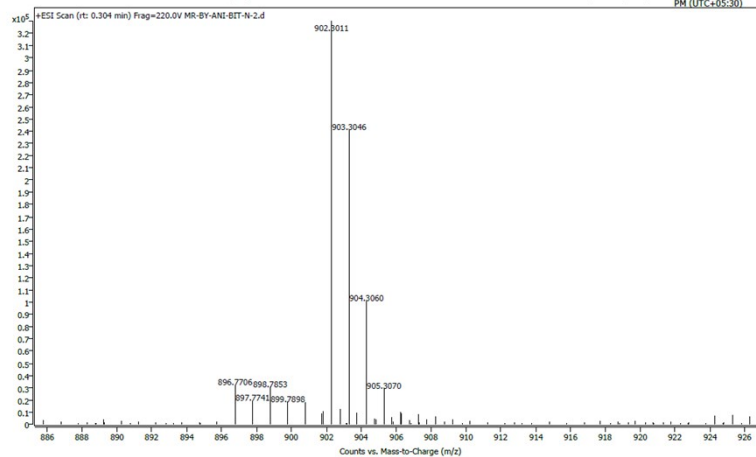


Figure S22. HRMS spectrum of compound 13.

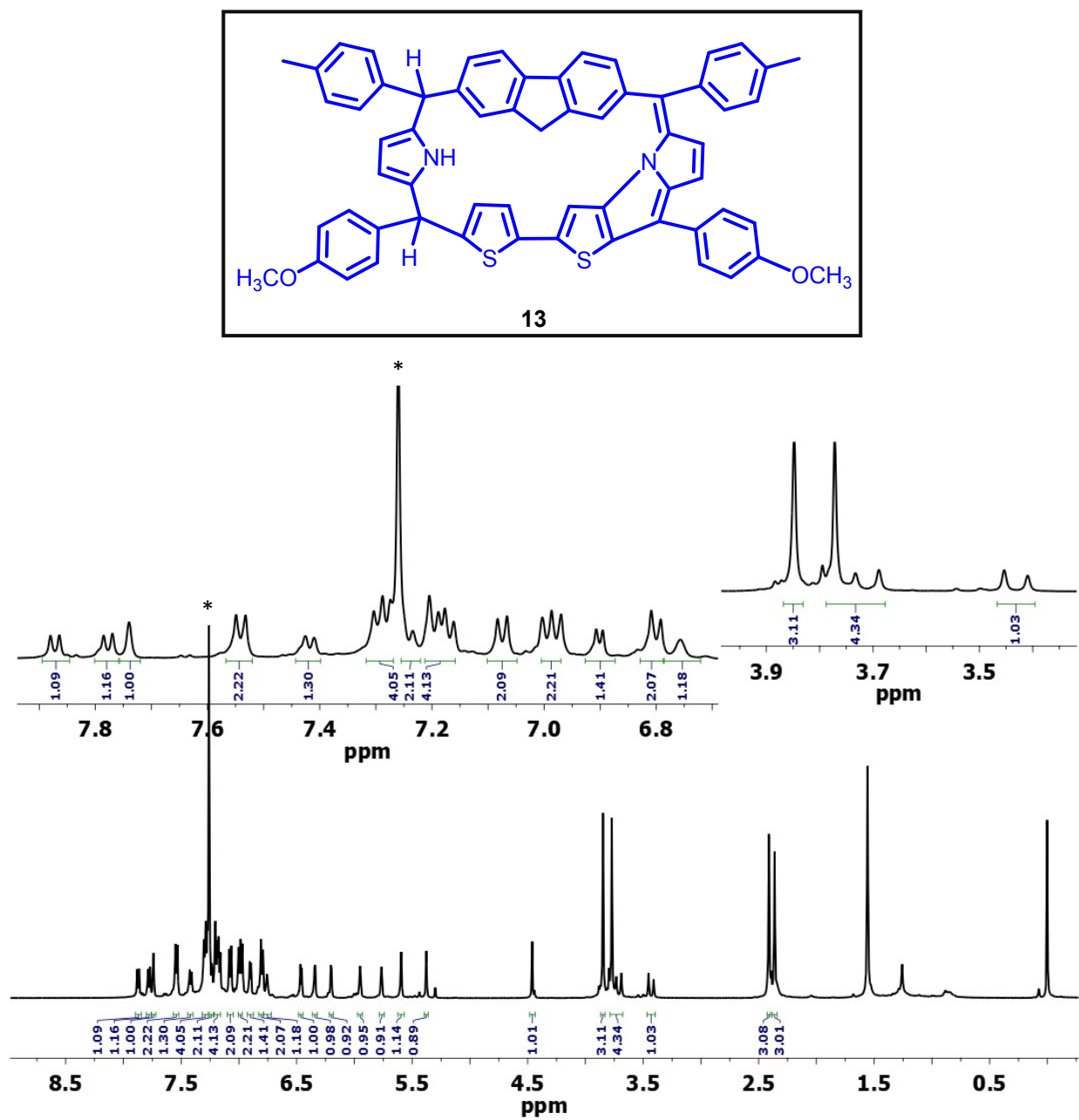


Figure S23. ^1H NMR of compound **13** recorded in CDCl_3 .

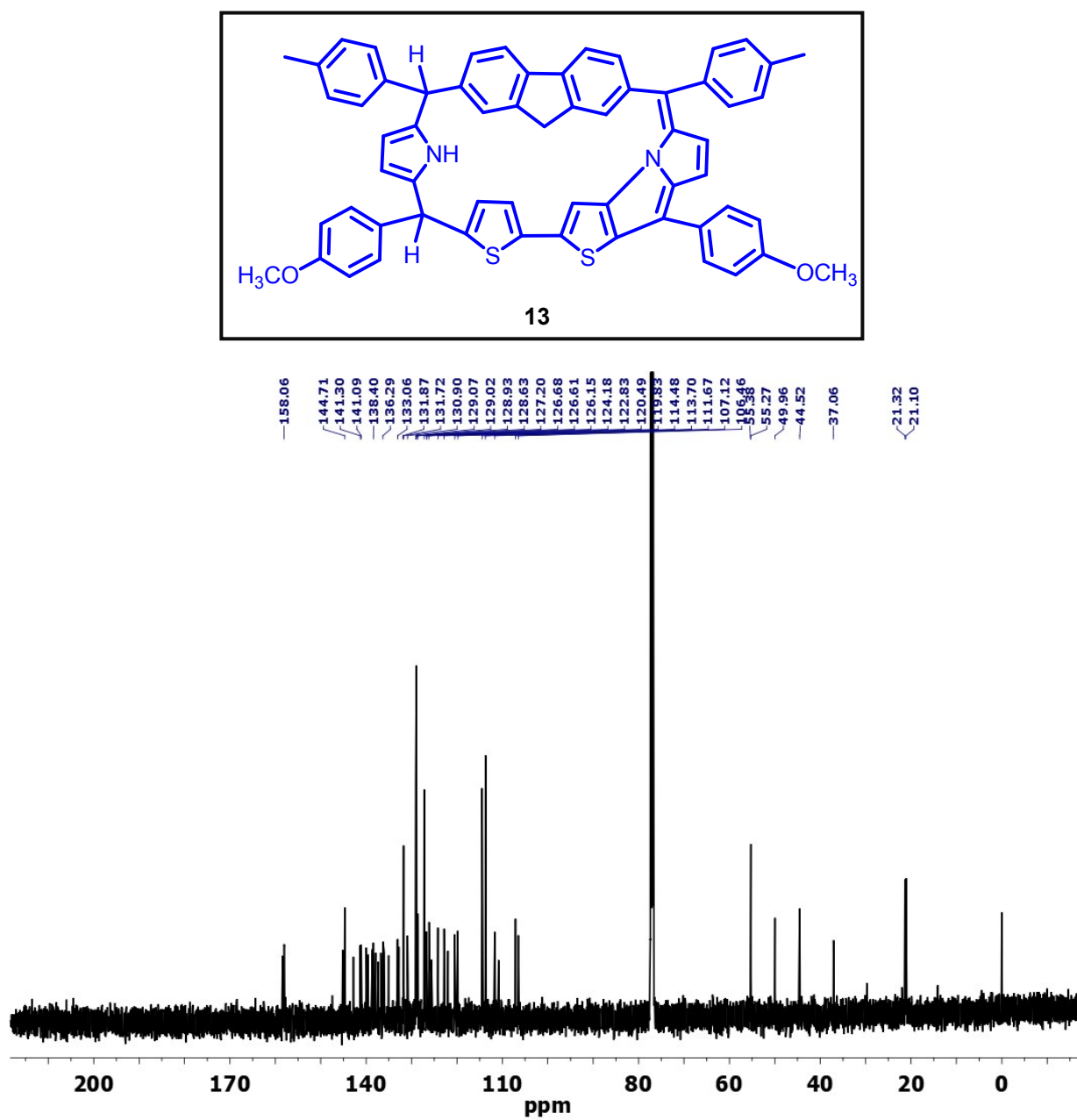


Figure S24. ^{13}C NMR of compound **13** recorded in CDCl_3 .

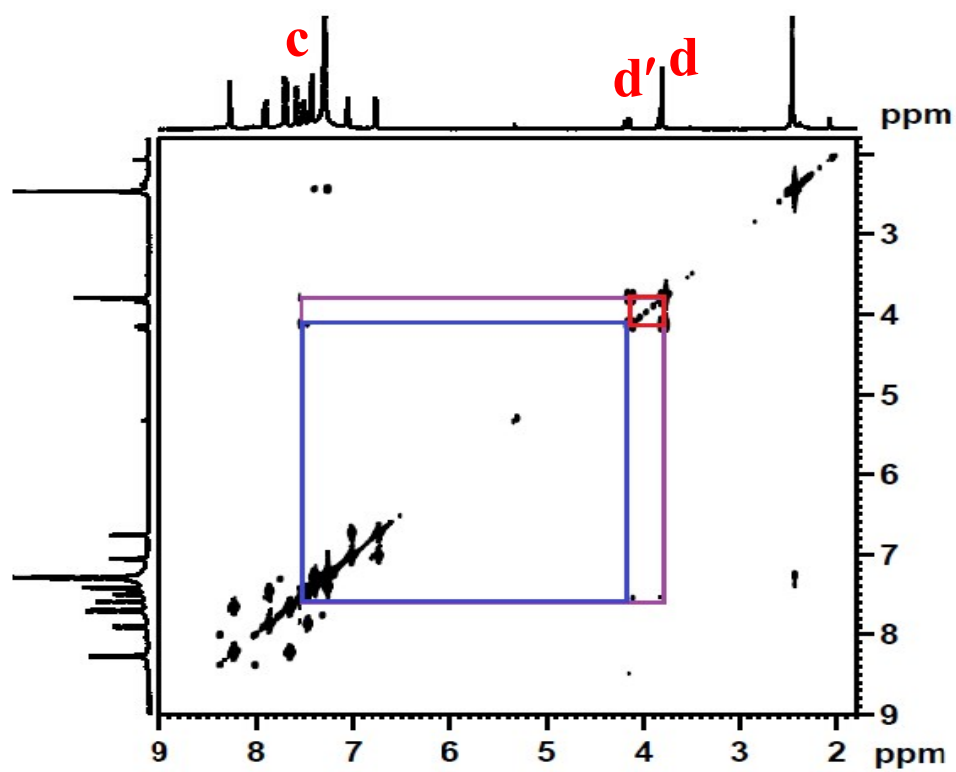
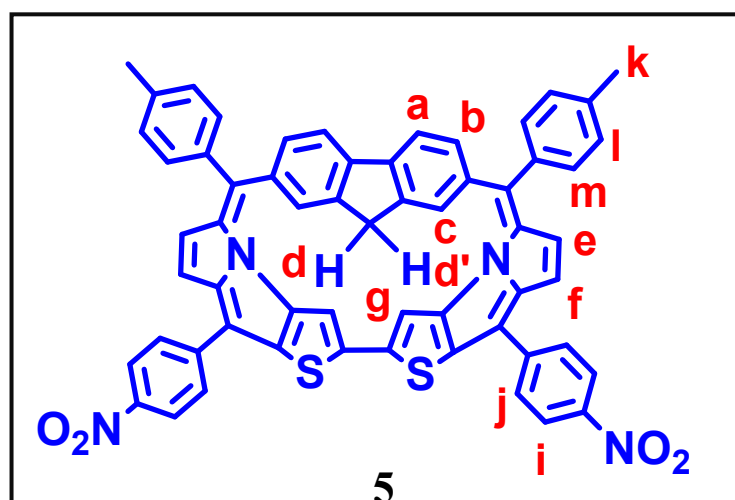


Figure S25. ¹H-¹H NOESY spectrum of compound **5** recorded in CDCl₃.

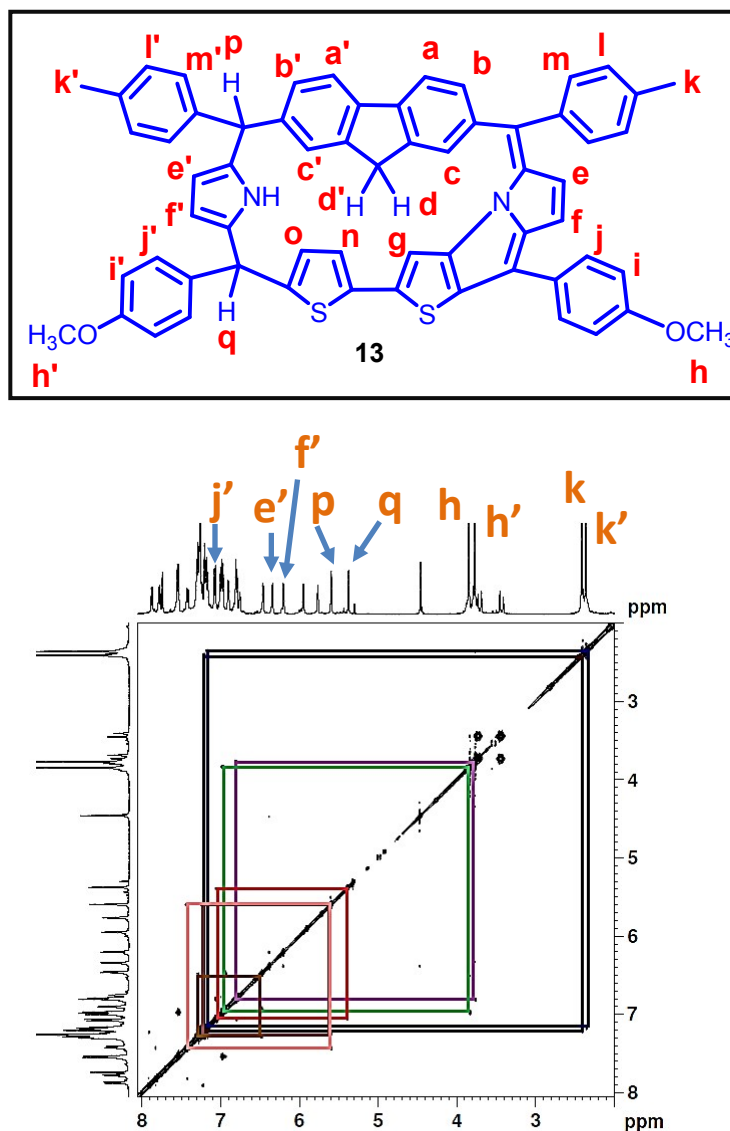


Figure S26. ^1H - ^1H NOESY spectrum of compound **13** recorded in CDCl_3 .

In ^1H NMR spectra of intermediate **13**, two singlets appeared for $-\text{OCH}_3$ protons (*type h & h'*) at 3.84 and 3.77 ppm corresponding to three protons each. The *h'* type protons showed NOE correlation with a resonance appeared at 6.80 ppm (*type i'*) which in turn showed cross peak correlation with a resonance at 7.08 ppm (*type j*). The *type j'* proton showed NOE correlation with a resonance at 6.19 ppm (*type f*) which in turn showed correlation with 6.34 ppm assigned as *type e'*. In addition to that two singlets were observed at 5.37 and 5.59 ppm assigned as *meso* sp^3 protons (*q* and *p* type) protons based on ^{13}C and HSQC NMR studies. The *q* type proton

showed a NOE correlation with one of the $-\text{OCH}_3$ aryl proton at 7.08 ppm assigned as j' type proton which in turn showed correlation with a resonance at 6.19 ppm as f' type proton. This indicated that the q type proton is located near the bithiophene moiety of the fused macrocycle. Similarly the p type proton showed one NOE correlation with one of the $-\text{CH}_3$ aryl proton at 7.28 ppm assigned as m' type proton which in turn showed correlation with a resonance at 7.18 ppm assigned as type l' proton and another correlation with one of the aryl protons (type b') of fluorene moiety which indicated that p type proton is located near the fluorene moiety of the fused macrocycle. All these NMR characteristics concluded that both the meso sp^3 protons (type p and q) are on the same side of the fused macrocycle. In addition to that, the singlet resonance observed in the region of 4.46 ppm was due to one proton of bithiophene moiety and assigned as type g protons. The two protons of $-\text{CH}_2$ group of fluorene moiety appeared as two doublets at 3.72 ppm (type d) and 3.411 ppm (type d'). All other mono fused calixsapphyrin intermediates having different meso-aryl substituents such as macrocycles **11**, **12** and **13** showed similar NMR features and the resonances of each of these mono fused calixsapphyrin intermediates were identified and assigned by adopting similar strategy as described for macrocycle **13**. Thus, 1D and 2D NMR spectroscopy was very useful in deducing the molecular structures of these mono fused calixsapphyrin intermediates **11-13**.

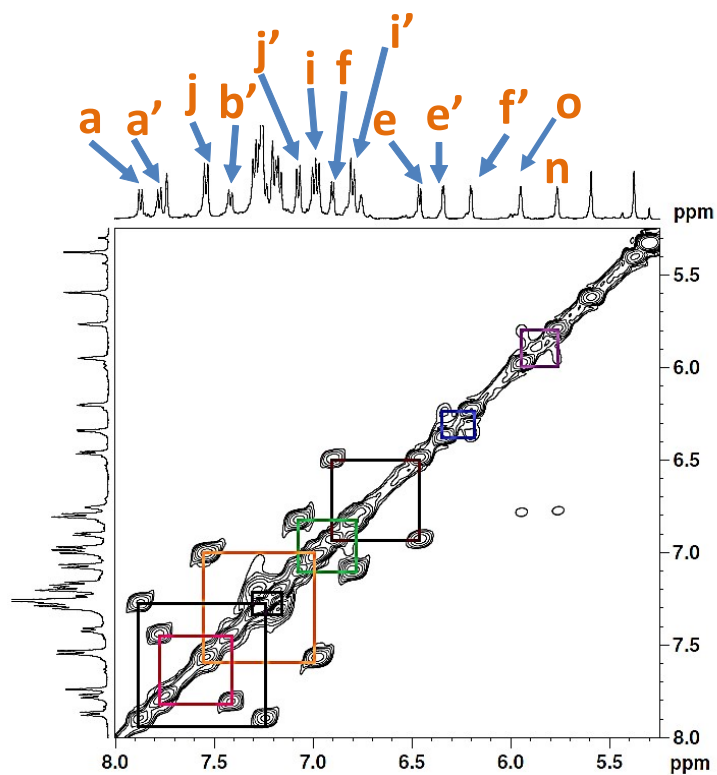
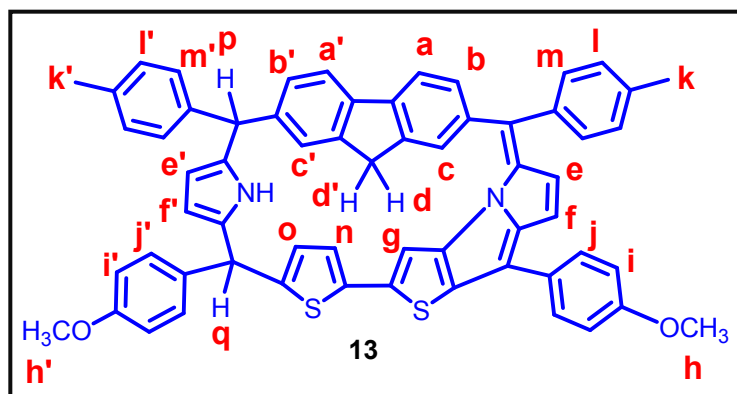


Figure S27. ¹H-¹H COSY spectrum of compound **13** recorded in CDCl₃.

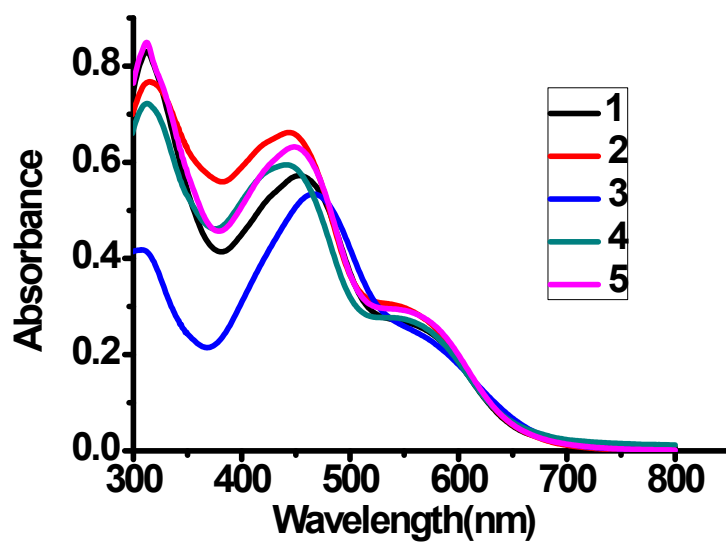


Figure S28. Comparison of absorption spectra of compounds **1-5** recorded in CHCl_3 .

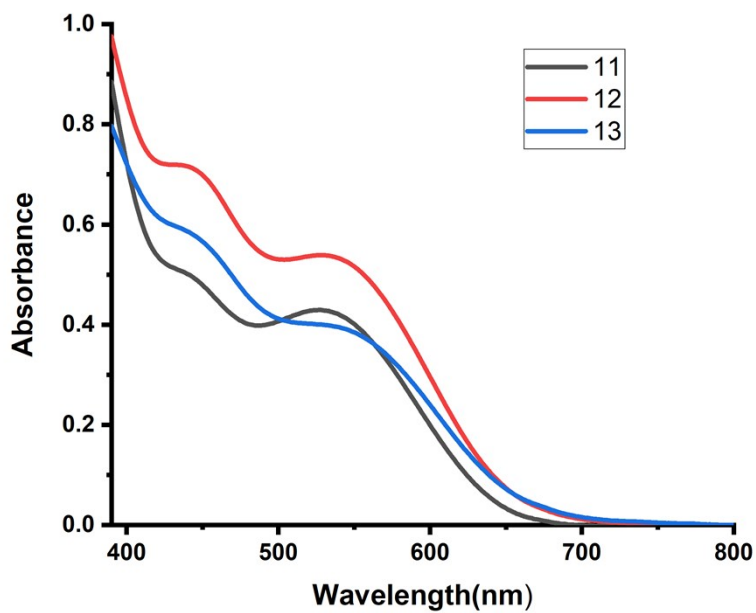


Figure S29. Comparison of absorption spectra of compounds **11-13** recorded in CHCl_3 .

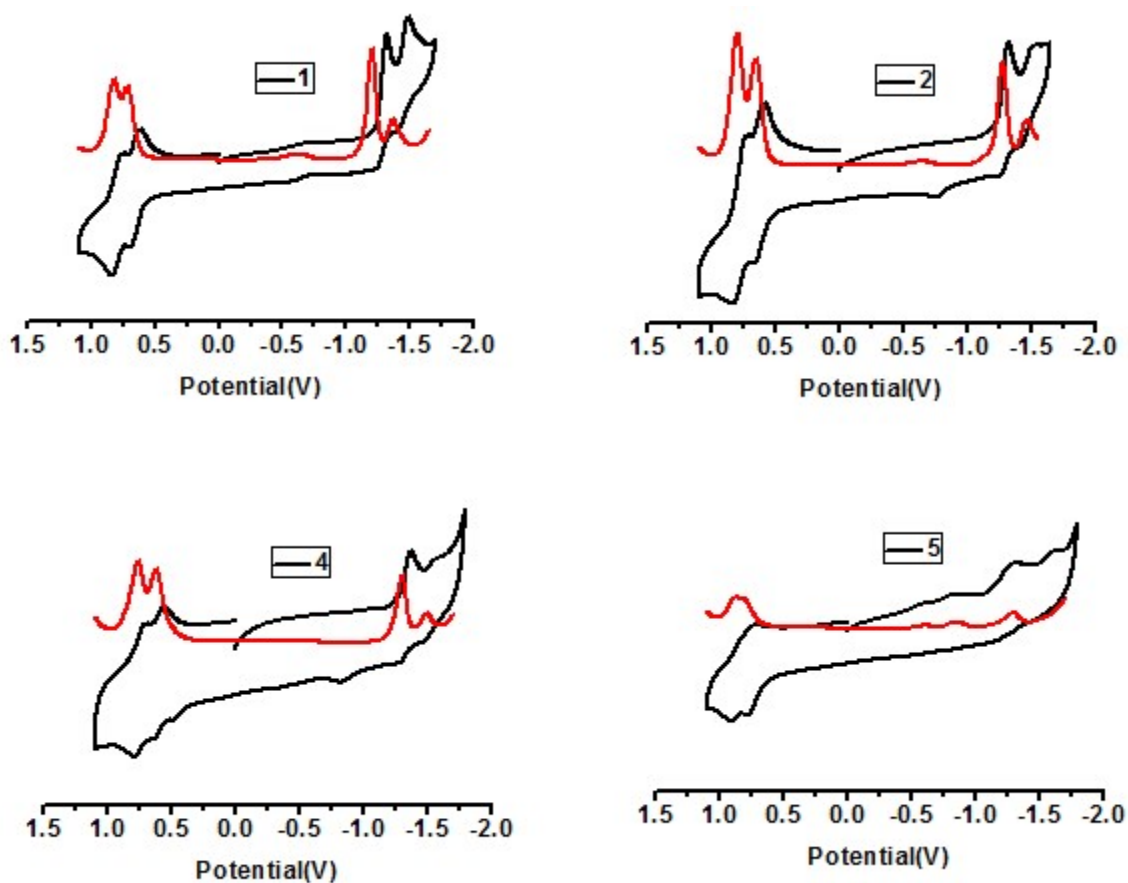


Figure S30. Cyclic voltammograms (black lines) along with differential pulse voltammograms (red lines) of the compounds **1**, **2**, **4** and **5** recorded in CH_2Cl_2 containing 0.1 M TBAP as the supporting electrolyte and a saturated calomel electrode (SCE) as the reference electrode at scan rates of 50 mVs^{-1} .

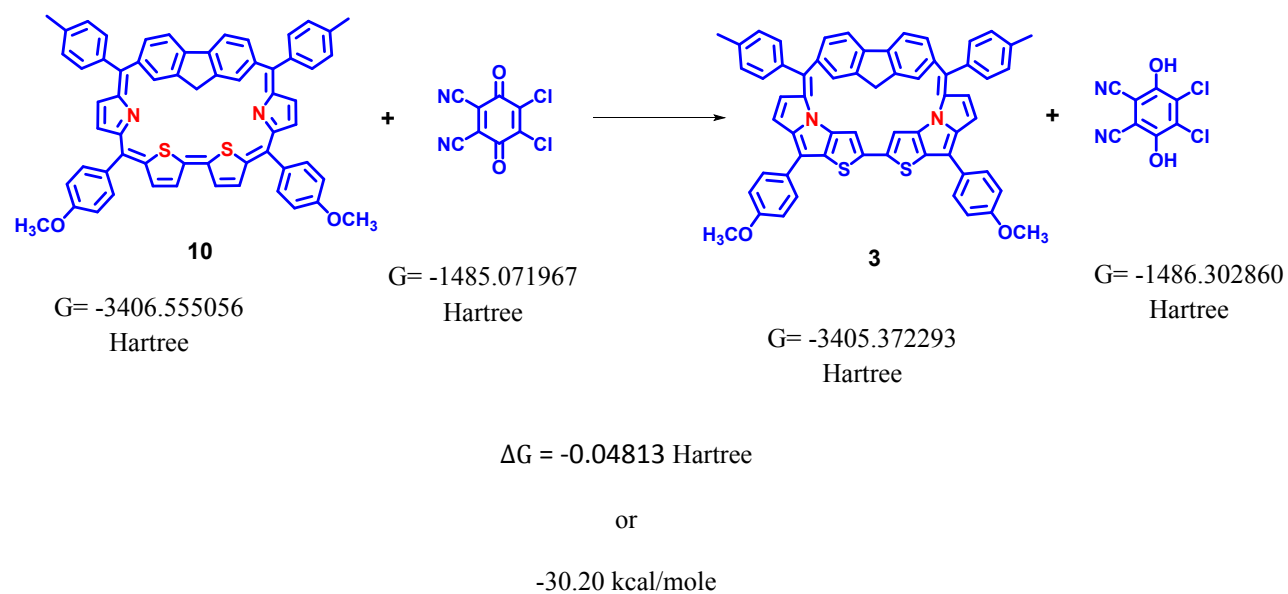


Figure S31: Calculation for the stability of compound **3** over compound **10**.

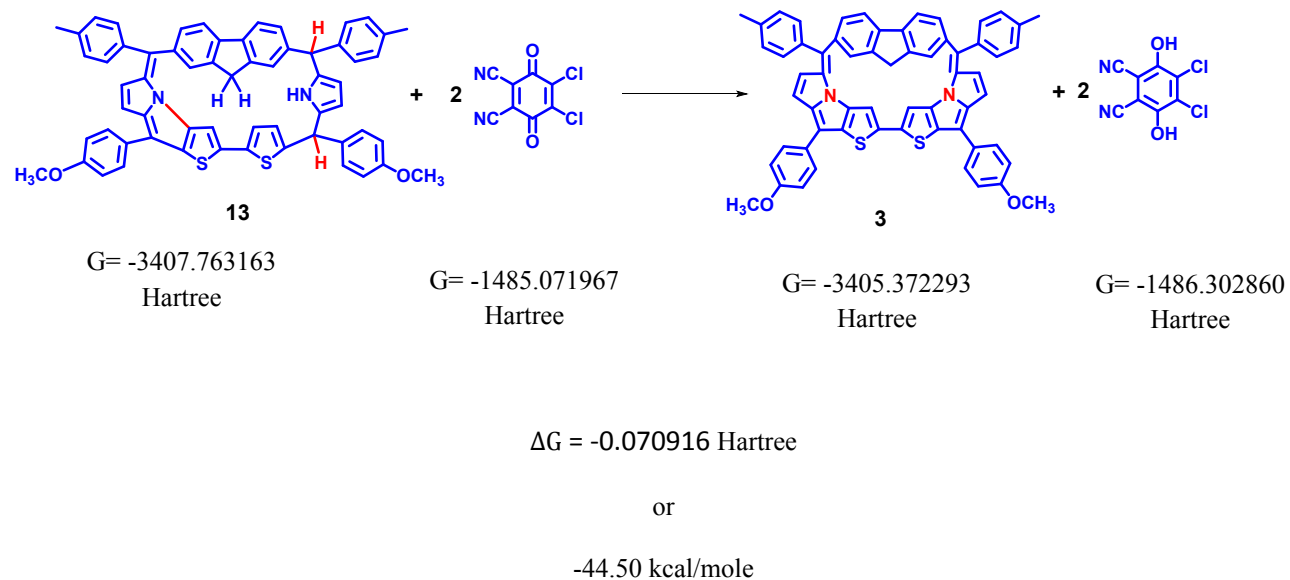


Figure S32: Calculation for the stability of compound **3** over compound **13**.

Figure S33: Cartesian coordinates of the S0 optimized structures of the compounds **10**.

Sum of imaginary frequencies= 0; # Total Energy (hartree) = -3406.402378.

Atoms	X	Y	Z	Atoms	X	Y	Z
C	1.15758400	-2.62049300	0.84615200	C	-8.94473700	-6.80701600	-0.34067100
C	0.71269300	-3.70911700	0.05814900	C	8.91683000	-6.80240200	-0.31266300
C	-0.74152100	-3.71003900	0.05293700	H	-0.02523000	-2.00211600	2.56033600
C	-1.19336700	-2.62098900	0.83645800	H	-0.01982000	-0.83342600	1.24674900
C	-0.02063800	-1.90741600	1.46553200	H	-1.34119900	-5.36131500	-1.22055600
C	-1.66824600	-4.51685600	-0.62065400	H	-3.73644800	-4.78819000	-1.10164400
C	-3.01619100	-4.19469300	-0.54926700	H	-2.86864100	-1.43862600	1.46421200
C	-3.47043700	-3.05794800	0.16697400	H	2.82690800	-1.43951200	1.49119200
C	-2.52985800	-2.29366600	0.89493500	H	3.71707300	-4.78187900	-1.07660600
C	2.49339100	-2.29318700	0.91692200	H	1.32366100	-5.35718200	-1.21412100
C	3.44066300	-3.05532700	0.19505200	H	-7.48043900	-1.40814800	0.52735200
C	2.99237800	-4.19020900	-0.52813400	H	-7.31419800	1.26232300	0.44958900
C	1.64534700	-4.51361100	-0.61008300	H	-3.53087700	4.69872900	-0.60571500
C	4.84250000	-2.65112600	0.15336300	H	-1.01335900	5.02730600	-0.71233200
C	-4.87168000	-2.65299900	0.10931700	H	6.51400000	2.76595500	-1.79384300
C	-5.90607900	-3.70519200	-0.01948200	H	8.19146700	4.55869700	-1.74394900
C	-5.24422400	-1.31029900	0.14519200	H	6.60852900	5.93529500	2.00906100
C	5.87763300	-3.70238200	0.02220100	H	4.91131500	4.11907300	1.94795900
C	5.21709300	-1.30938900	0.20895500	H	5.01339800	-4.98593600	1.52464600
C	-6.60319100	-0.80585000	0.34085500	H	6.73153900	-6.73925900	1.33131100
C	-6.51705100	0.54626400	0.31248000	H	8.69554400	-4.47786000	-1.74413000
C	-5.10381000	0.86036000	0.07719200	H	6.97714700	-2.72176100	-1.55005900
N	-4.36214500	-0.24798400	0.00208300	H	-5.05298400	-4.97216000	1.50321300
N	4.33980600	-0.24331400	0.06788400	H	-6.77073300	-6.72685600	1.31747600
C	5.08148400	0.86265200	0.17536300	H	-8.71094400	-4.49976900	-1.79789200
C	-3.25549400	2.55578200	-0.21164300	H	-6.99323700	-2.74250700	-1.61151300
C	-2.82033600	3.89587900	-0.46631900	H	-6.46108000	2.71064500	-1.99467000
C	-1.47087300	4.06529400	-0.52561400	H	-8.16499400	4.52099600	-2.02517600
C	-0.70509500	2.87513700	-0.32581900	H	-6.70832800	5.93582400	1.76434100
S	-1.81754500	1.49885800	-0.10477000	H	-5.02380600	4.14720600	1.78293600
C	0.69097100	2.87628600	-0.30641200	H	-9.72153800	-6.66043900	0.42043400
C	3.23785400	2.55953500	-0.12741900	H	-8.52576600	-7.80602300	-0.18486900
S	1.79977300	1.49921500	-0.07179200	H	-9.43832800	-6.79394700	-1.31653800
C	4.57186700	2.19831300	0.03643300	H	8.49499600	-7.80306300	-0.17631200
C	-4.59197100	2.19395500	-0.07523500	H	9.68588000	-6.66852800	0.45857500
C	5.58275300	3.30619500	0.06715800	H	9.42042600	-6.77539400	-1.28311700
C	-5.60925300	3.29641300	-0.10200500	C	-8.66022400	7.25143400	0.77917200
C	6.52671900	3.45600200	-0.95545700	H	-7.74968300	7.85282400	0.89728200
C	7.48257900	4.47501800	-0.92875400	H	-8.90192200	6.77632600	1.73856200
C	7.50701500	5.37243400	0.14494900	H	-9.48406100	7.90292900	0.48441000
C	6.57084100	5.23585700	1.18039100	C	9.36687100	6.58644300	-0.73633400
C	5.62672100	4.21881400	1.13716200	H	8.90517000	6.79326800	-1.71032200
C	5.82233000	-4.86848300	0.81059900	H	10.02342500	5.71201500	-0.83019300
C	6.79449000	-5.85642800	0.69975500	H	9.96064900	7.44918800	-0.43112300
C	7.85384600	-5.73552100	-0.21178300	O	8.39181800	6.40332700	0.27815800
C	7.89910100	-4.58748100	-1.01225700	O	-8.52583700	6.29501800	-0.26031900
C	6.93425100	-3.58895100	-0.89965900	C	1.45946400	4.06994300	-0.47079800
C	-5.85678100	-4.86249800	0.78215200	H	1.00527200	5.03410700	-0.65427600
C	-6.82865000	-5.85119500	0.67554800	C	2.80715300	3.90214000	-0.37548300
C	-7.88141400	-5.74003500	-0.24479300	H	3.51923800	4.70844600	-0.48367200
C	-7.92001700	-4.60135400	-1.05892800	C	6.48976200	0.54177900	0.43006700
C	-6.95555300	-3.60201100	-0.95070800	C	6.57356600	-0.81088900	0.43465200
C	-6.51496900	3.41716600	-1.17195500	H	7.28507200	1.25377800	0.59565800
C	-7.47039400	4.42398700	-1.19726000	H	7.44639300	-1.41815800	0.62592800
C	-7.55234600	5.34539100	-0.14254000				
C	-6.66335800	5.24231600	0.93311900				
C	-5.70576400	4.22431200	0.94126000				

Figure S34: Cartesian coordinates of the S0 optimized structures of the compounds **3**. # Sum of imaginary frequencies= 0; # Total Energy (hartree) = -3405.225927.

Atoms	X	Y	Z	Atoms	X	Y	Z
C	0.86733900	-3.50687000	-0.89037900	C	-7.02256400	4.13728200	-2.79788600
C	-0.56992800	-3.59407300	-0.63904600	C	-6.39500500	5.37266900	-2.59976300
C	-0.79197200	-3.51066300	0.75390500	C	-5.16423000	5.41855000	-1.92866000
C	0.53735900	-3.46553800	1.48426600	C	-4.57850900	4.25297600	-1.45948300
C	-1.63899500	-3.51253600	-1.53305200	C	-7.36000900	-6.05422400	4.52969700
C	-2.90575800	-3.23194200	-1.03166400	C	9.04842000	-5.18744600	-3.46507200
C	-3.12968900	-3.07857800	0.35019600	H	0.72500000	-4.38645600	2.05448300
C	-2.06959300	-3.30021300	1.25151500	H	0.59038200	-2.63656300	2.19896600
C	2.83919300	-2.87369100	0.37247000	H	-1.47900500	-3.58273300	-2.60495200
C	3.52505200	-2.65643700	-0.83813700	H	-3.73700400	-3.08426300	-1.71358500
C	2.90088200	-2.99056500	-2.05642200	H	-2.24287100	-3.18565200	2.31795000
C	1.57177800	-3.39920300	-2.09348300	H	3.33196200	-2.64313600	1.31262900
C	4.87840000	-2.05786900	-0.83603700	H	3.45270800	-2.85673300	-2.98148600
C	-4.45651600	-2.61305800	0.81800900	H	1.07956200	-3.57026000	-3.04648700
C	-5.20365500	-3.46994700	1.76039200	H	-7.18253800	-1.67786900	0.68472800
C	-4.98448300	-1.43252600	0.34880200	H	-7.45430200	0.66352300	-0.53884500
C	5.95730500	-2.83309100	-1.49237000	H	7.14567800	1.43657300	1.19512200
C	5.14334800	-0.84429200	-0.24953100	H	7.36608400	-0.92418500	-0.00252600
C	-6.38906400	-1.04187100	0.32233200	H	-1.33726500	-1.05704300	0.32730200
C	-6.52860300	0.14496100	-0.33314100	H	1.47641000	-0.82949000	-0.89734500
C	-5.22506000	0.60587100	-0.71207900	H	2.63011100	3.79974200	2.79640100
N	-4.30045800	-0.36871600	-0.31168400	H	3.24803200	5.96613200	3.81986700
N	4.23811900	0.16957800	0.18155300	H	7.06755100	5.79833400	1.85540200
C	4.96298900	1.22282900	0.76019400	H	6.43430100	3.68466700	0.79876300
C	6.34820300	0.85696400	0.75204500	H	5.26717800	-4.73549000	-0.74438400
C	6.46433800	-0.34606400	0.12804900	H	7.03147200	-6.05799600	-1.83321300
C	-3.19167400	1.49057100	-0.92408000	H	8.66415100	-2.47628700	-3.54517400
C	-3.02099300	0.19577700	-0.41157900	H	6.89356400	-1.15174800	-2.46578900
C	-1.67308800	-0.13839200	-0.12585000	H	-4.48466900	-5.31887500	0.91064900
C	-0.80541000	0.90099900	-0.41081900	H	-5.69419800	-6.77382100	2.48051900
S	-1.66199600	2.30132300	-1.09399000	H	-7.27935200	-3.31637500	4.46942100
C	0.61943000	1.00238300	-0.13427700	H	-6.05303100	-1.85748500	2.91531800
C	1.63962300	0.09283000	-0.36103600	H	-6.89739400	2.01764300	-2.52417700
C	2.88882000	0.55832900	0.13335300	H	-7.96523100	4.06787700	-3.32777700
C	2.82459700	1.83031900	0.72261700	H	-4.68997000	6.38324000	-1.78139800
S	1.21002800	2.46501200	0.68605900	H	-3.63848000	4.31694000	-0.92050100
C	4.12185200	2.27894800	1.11255300	H	-6.78351600	-6.94805800	4.78820100
C	-4.57488500	1.76907900	-1.14000100	H	-8.30090700	-6.39636500	4.08019700
C	4.49167900	3.55801000	1.72235600	H	-7.61326600	-5.53397700	5.45789200
C	-5.19340000	2.99673800	-1.64154600	H	9.37258700	-6.03124100	-2.84784300
C	3.59727000	4.23970000	2.57353000	H	9.92895000	-4.58411000	-3.70386200
C	3.93756400	5.44849700	3.16121600	H	8.67234400	-5.60369100	-4.40823700
C	5.19366100	6.02370700	2.92045800	C	-8.13127800	6.58670900	-3.70353000
C	6.09683400	5.36960000	2.07449800	H	-8.94219900	6.19226600	-3.07758700
C	5.73857900	4.15735500	1.48447100	H	-8.08770600	6.01018500	-4.63663200
C	6.01083500	-4.23425500	-1.35598300	H	-8.33635300	7.63220700	-3.93829200
C	7.00915600	-4.97982300	-1.97290100	O	-6.88836000	6.57455700	-3.02081400
C	7.98924800	-4.36828200	-2.76827200	C	6.68744400	7.84125700	3.33611500
C	7.92842700	-2.97763400	-2.92097100	H	6.84169900	8.09404900	2.27914000
C	-5.10247000	-4.87380000	1.68419500	H	7.51961500	7.21223000	3.67794400
C	-5.78800500	-5.69438500	2.57279600	H	6.66766200	8.75982100	3.92437400
C	-6.59804500	-5.15782600	3.58415400	O	5.43362300	7.21304300	3.54764900
C	-6.68259400	-3.76280100	3.67771000				
C	-5.99855600	-2.93411600	2.79247100				
C	-6.41838500	2.97161600	-2.32673700				

Figure S35: Cartesian coordinates of the S0 optimized structure of the compound *type a*.

Sum of imaginary frequencies= 0; # Total Energy (hartree) = -3407.611859.

Atoms	X	Y	Z	Atoms	X	Y	Z
C	-0.21887900	-3.55860400	-0.20402500	C	-1.93470400	-0.14996600	-0.66724900
C	0.17674000	-2.87989500	0.96983800	C	-3.27046000	0.00858700	-0.22611400
C	1.62812600	-2.68914500	0.93611900	C	-3.68386600	1.34108900	-0.09712200
C	2.12731800	-3.24193600	-0.25847200	S	-2.38060700	2.43159100	-0.48412800
C	1.00521100	-3.91106600	-1.02897000	C	-5.05305600	1.40091400	0.31491000
C	2.47613900	-1.98167400	1.79336000	C	3.82018900	2.59111400	-1.75615700
C	3.79703900	-1.77149900	1.41046100	C	-5.88581700	2.58189200	0.54227200
C	4.29824900	-2.27697800	0.19653500	C	3.84517700	4.02385600	-1.23256000
C	3.45624100	-3.04538100	-0.62127000	C	-5.63557700	3.79460000	-0.13311300
C	-1.56364000	-3.73791400	-0.49719900	C	-6.42434400	4.91503400	0.07783200
C	-2.54192200	-3.19912800	0.36502300	C	-7.50096900	4.86484100	0.97531300
C	-2.12965500	-2.57756800	1.56097500	C	-7.76683500	3.67413800	1.66164500
C	-0.78292600	-2.42119600	1.87382900	C	-6.96074100	2.55666100	1.44505800
C	-3.98663900	-3.26181900	0.03617600	C	-5.57065100	-4.70990500	-1.28916700
C	5.67155500	-1.84206200	-0.31631500	C	-6.10817100	-5.95512200	-1.60362500
C	6.88591400	-2.38707600	0.44004000	C	-5.66254800	-7.12187100	-0.96952600
C	5.68273900	-0.32684700	-0.43256900	C	-4.65362000	-6.99352200	-0.00380100
C	-4.56827900	-4.57588000	-0.30908000	C	-4.11216300	-5.75340500	0.31632700
C	-4.78058100	-2.13967800	0.10565200	C	6.79216800	-3.12050500	1.62461400
C	6.54098800	0.66254700	0.00603500	C	7.93626300	-3.62503200	2.24921800
C	5.98845800	1.91982500	-0.38109400	C	9.20981700	-3.41820200	1.71401700
C	4.79778600	1.67323100	-1.03831600	C	9.30112800	-2.69242300	0.51693800
N	-4.35169400	-0.78639100	0.14988000	C	8.16407900	-2.19034100	-0.10769100
C	-5.43563400	0.05721600	0.41553900	C	3.83871000	4.31856700	0.13382300
C	-6.59927500	-0.77733500	0.52768800	C	3.80641800	5.63700900	0.59635700
C	-6.22442300	-2.07060500	0.30974500	C	3.78414800	6.69329600	-0.32054400
C	2.41519300	1.99938000	-1.80420600	C	3.79606200	6.41370800	-1.69445100
C	0.60510000	0.66390900	-2.47243800	C	3.82398400	5.09765600	-2.13518000
C	0.03111800	1.27326700	-1.38018800	C	10.44838800	-3.94567000	2.39876400
S	1.17707900	2.37417800	-0.62803700	C	-6.22004200	-8.47506600	-1.33885200
C	-1.31237300	1.06611400	-0.86169400	H	1.14982200	-4.99828300	-1.09732700

Atoms	X	Y	Z
H	0.93103300	-3.54284900	-2.05972000
H	2.10167100	-1.55011400	2.71714900
H	4.44379000	-1.15488100	2.02746200
H	3.83511600	-3.43656400	-1.56340400
H	-1.87460600	-4.23466000	-1.41212800
H	-2.88678800	-2.19240100	2.23607400
H	-0.49180900	-1.91411400	2.78901900
H	7.46318500	0.50190400	0.54483000
H	6.41812200	2.89475900	-0.20297900
H	-7.59639600	-0.42624200	0.75300000
H	-6.85149600	-2.94605300	0.38625500
H	0.05930100	-0.02552900	-3.10616700
H	-1.42714600	-1.08958600	-0.82546200
H	-4.82430100	3.85020000	-0.85232900
H	-6.23124100	5.84417900	-0.44815500
H	-8.58137800	3.60938000	2.37330000
H	-7.15485600	1.65336200	2.01498100
H	-5.91285000	-3.82783500	-1.82058700
H	-6.87851600	-6.02350500	-2.36794900
H	-4.29014100	-7.88089300	0.50894200
H	-3.33763400	-5.68530900	1.07362000
H	5.82053200	-3.31660100	2.06416400
H	7.82973100	-4.19486900	3.16918500
H	10.27623200	-2.52415400	0.06551600
H	8.26483100	-1.63439200	-1.03588400
H	3.87613600	3.50908500	0.85562600
H	3.80336300	5.82303200	1.66362700
H	3.78425600	7.24327600	-2.39360000
H	3.82809900	4.89769000	-3.20381000
H	10.19616800	-4.67346100	3.17509400
H	11.01489800	-3.13699000	2.87674600
H	11.12365100	-4.43259900	1.68706000
H	-7.23583300	-8.39510200	-1.73685300
H	-6.24589000	-9.14663500	-0.47517100

Atoms	X	Y	Z
H	-5.60647100	-8.96123600	-2.10800000
C	3.73188500	8.35648100	1.39322100
H	4.62823400	7.99854000	1.91596300
H	2.84180000	7.95447400	1.89386600
H	3.70476900	9.44634400	1.43411700
O	3.75701700	8.01648600	0.01605700
C	-9.31712000	6.02584000	2.00579400
H	-9.00270300	5.82041400	3.03722600
H	-10.08225900	5.29507600	1.71339000
H	-9.74228900	7.02924800	1.95456500
O	-8.21695400	6.01994000	1.11085900
C	1.94689700	1.07703000	-2.70948100
H	2.54397000	0.72416100	-3.54491900
N	4.64100000	0.30634700	-1.07815800
H	3.79410100	-0.14856300	-1.38723400
H	5.75460200	-2.24601100	-1.33735700
H	4.13209100	2.63997700	-2.81037700

Figure S36: Cartesian coordinates of the S0 optimized structure of the compound *type b*.

Sum of imaginary frequencies= 0; # Total Energy (hartree) = -3407.597856.

Atoms	X	Y	Z	Atoms	X	Y	Z
C	-1.39250200	-3.32515400	-0.08147400	C	-0.86536800	0.55142200	-2.36422000
C	-0.71963000	-2.79966300	1.04166500	C	-2.27613200	0.60901200	-2.25374100
C	0.71518000	-2.72801300	0.73756600	C	-2.74219700	1.62031900	-1.43629700
C	0.91885400	-3.20519500	-0.57473000	S	-1.37587500	2.52649100	-0.78316700
C	-0.38978000	-3.70790000	-1.15276600	C	-4.13008300	1.89516600	-1.04317100
C	1.78128700	-2.18467300	1.45528900	C	4.97629000	2.69278500	-0.51596700
C	3.02342900	-2.05210100	0.83097900	C	-4.66962600	3.26190300	-1.17249100
C	3.22043400	-2.46403800	-0.49491800	C	5.13596500	3.50567200	0.76267500
C	2.16133300	-3.08345000	-1.18142300	C	-4.31920600	4.07110800	-2.27608100
C	-2.78153400	-3.33628500	-0.13400100	C	-4.81989300	5.35427200	-2.42292400
C	-3.52519300	-2.79122900	0.92945300	C	-5.69525000	5.88693800	-1.46362200
C	-2.84056000	-2.32388300	2.06766500	C	-6.04505200	5.11425800	-0.35086200
C	-1.44722600	-2.33607500	2.13918200	C	-5.52577000	3.82616200	-0.21172200
C	-4.99515700	-2.52324400	0.77641900	C	-7.23678100	-3.65919000	0.52321600
C	4.52949400	-2.19435500	-1.24273100	C	-8.15238400	-4.63357300	0.90801700
C	5.48166700	-3.39311900	-1.21813700	C	-7.85521000	-5.56058600	1.91571800
C	5.23845200	-0.92795900	-0.80957900	C	-6.59349700	-5.47406200	2.51996600
C	-5.97709700	-3.54734200	1.14970400	C	-5.67440300	-4.50008300	2.14550100
C	-5.30936400	-1.27276100	0.28830200	C	5.70445400	-4.13938500	-0.05537100
C	6.54510000	-0.73529900	-0.39114800	C	6.59136000	-5.21507600	-0.05622500
C	6.77147300	0.65998100	-0.18403100	C	7.28589100	-5.58439800	-1.21523000
C	5.59518200	1.29904400	-0.48665600	C	7.05605700	-4.83912900	-2.37803400
N	-4.34740400	-0.38898400	-0.19118800	C	6.17114200	-3.76168700	-2.37865100
C	-4.87545500	0.84396300	-0.54026600	C	4.68387900	3.02178800	1.99330800
C	-6.30044400	0.72065200	-0.27483600	C	4.82578800	3.76532600	3.16483000
C	-6.55832300	-0.52779000	0.20130600	C	5.43539900	5.02620900	3.11598700
C	3.55411600	2.30900800	-0.88475900	C	5.89414100	5.52336900	1.88986400
C	2.09725300	0.53934200	-1.39313400	C	5.74255000	4.76768500	0.73253200
C	1.21976400	1.60819100	-1.41017900	C	8.26518100	-6.73440300	-1.20461600
S	2.04484300	3.13121100	-1.06958400	C	-8.83659100	-6.64022700	2.30307400
C	-0.21259700	1.51204800	-1.61955500	H	-0.36845100	-4.79378800	-1.32023400

Atoms	X	Y	Z
H	-0.62177300	-3.24881400	-2.12164000
H	1.64183600	-1.81875300	2.46863500
H	3.84188800	-1.57137200	1.35869600
H	2.31004500	-3.41475700	-2.20726900
H	-3.30283200	-3.69615500	-1.01733100
H	-3.41681300	-1.89703900	2.88334300
H	-0.94393300	-1.93300500	3.01349700
H	7.26867700	-1.52668100	-0.26260000
H	7.68814400	1.12306800	0.15206200
H	-7.02100600	1.50432000	-0.45626900
H	-7.51915100	-0.91169800	0.50936400
H	1.77617800	-0.48386300	-1.51940200
H	-0.33507400	-0.16235600	-2.98387800
H	-3.65248200	3.67049800	-3.03341600
H	-4.55363800	5.96738800	-3.27770100
H	-6.69564600	5.50827100	0.42098800
H	-5.76962100	3.25812100	0.68022100
H	-7.48345700	-2.99836800	-0.30069300
H	-9.11227400	-4.68877200	0.39946000
H	-6.32703200	-6.18208300	3.30144300
H	-4.70834900	-4.46120600	2.63854600
H	5.16951200	-3.88816800	0.85516900
H	6.74154800	-5.78180300	0.85959900
H	7.57283800	-5.10692700	-3.29649200
H	6.01426900	-3.19836700	-3.29544100
H	4.21229900	2.04435700	2.04177400
H	4.46231000	3.35680400	4.10016200
H	6.36468200	6.50072300	1.86836600
H	6.10427000	5.16632300	-0.21214300
H	7.96803000	-7.50705700	-0.48907400
H	9.27009600	-6.39794300	-0.91984400
H	8.34703500	-7.20030000	-2.19118400
H	-9.86933900	-6.32682400	2.12256400
H	-8.74369300	-6.90448000	3.36111700

Atoms	X	Y	Z
H	-8.67064900	-7.55874000	1.72530700
C	5.18283900	5.38517500	5.46530900
H	5.68878300	4.45868200	5.76594200
H	4.09772200	5.22090400	5.48016700
H	5.43453500	6.17618400	6.17326800
O	5.62809600	5.83859900	4.19704100
C	-7.01546200	7.74872800	-0.75853400
H	-6.54887700	7.84073000	0.23066700
H	-7.94864400	7.17890900	-0.66180800
H	-7.24196300	8.74480500	-1.14151300
O	-6.13502700	7.15733700	-1.70059000
C	3.41516000	0.95825300	-1.08959800
N	4.66518200	0.33619300	-0.86869400
H	-3.36227900	-0.59602300	-0.21764900
H	-2.94866600	-0.06114700	-2.77730400
H	4.24551200	-2.05830500	-2.29647600
H	5.42486800	3.27480000	-1.33449700

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