Electronic Supplementary Material (ESI) for Chemical Science


# Accessing Extended and Partially Fused Hexabenzocoronenes using a Benzannulation / Cyclodehydrogenation Approach

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**Supplementary Information**

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**A. Materials.** All reagents were purchased from commercial sources and used without further purification. $CH_2Cl_2$, PhMe, and MeOH were purchased from commercial sources and purified using a custom-built alumina-column based solvent purification system. Other solvents were purchased from commercial sources and used without further purification

**Instrumentation.** Infrared spectra were recorded on a Thermo Nicolet iS10 with a diamond ATR attachment and are uncorrected. Ultraviolet/visible/near infrared absorbance spectra were recorded on a Cary 5000 spectrophotometer with a Hg lamp.

Photoemission and excitation spectra were recorded on a Horiba Jobin Yvon Fluorolog-3 fluorescence spectrophotometer equipped with a 450 W Xe lamp, double excitation and double emission monochromators, a digital photon-counting photomultiplier and a secondary InGaAs detector for the NIR range. Correction for variations in lamp intensity over time and wavelength was achieved with a solid-state silicon photodiode as the reference. The spectra were further corrected for variations in photomultiplier response over wavelength and for the path difference between the sample and the reference by multiplication with emission correction curves generated on the instrument.

MALDI-TOF mass spectrometry was performed on a Waters MALDI micro MX MALDI-TOF mass spectrometer using positive ionization and a reflectron detector. MALDI samples were prepared by depositing the analyte dissolved in a saturated dithranol or tetracyanoquinodimethane solution onto a stainless steel sample plate. The plate was dried in air before loading it into the instrument. Calibration of the mass range was performed by addition of poly(ethylene-oxide) standards.

Gas chromatography/electron impact mass spectrometry was performed on an Agilent 6890N Network GC System with a JEOL JMS-GCmate II Mass Spectrometer (magnetic sector).

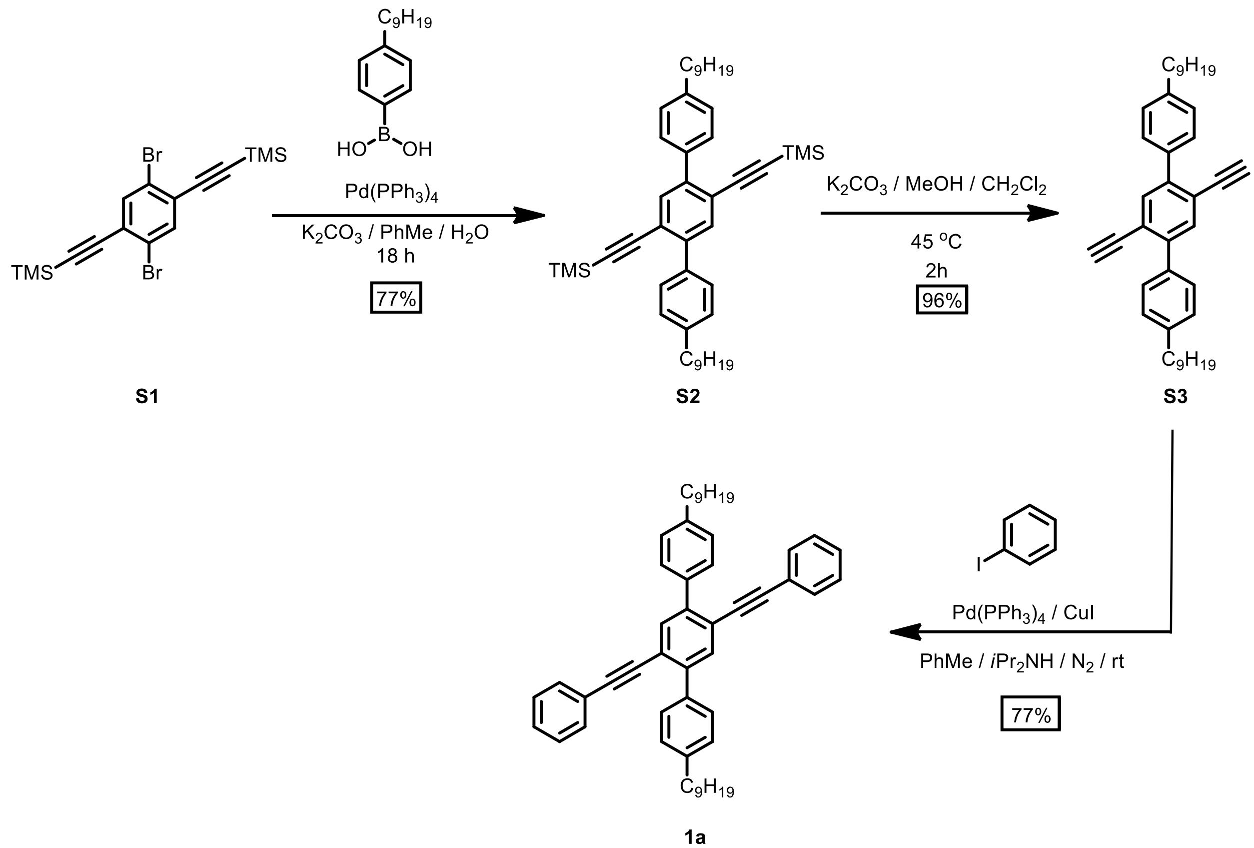
NMR spectra were recorded on a Varian 400 MHz, a Varian 500 MHz or a Bruker ARX 300 MHz spectrometer using a standard $^1H/X$ Z-PFG probe at ambient temperature with a 20 Hz sample spin rate.

Electrochemistry experiments were performed on a Princeton Applied Research VersaSTAT 3 potentiostat using a standard three electrode configuration with a Pt-button electrode as the working electrode, a coiled Pt wire as counter and a Pt wire as the quasi-reference electrode. Potentials were reported relative to $Fc/Fc^+$ redox couple.

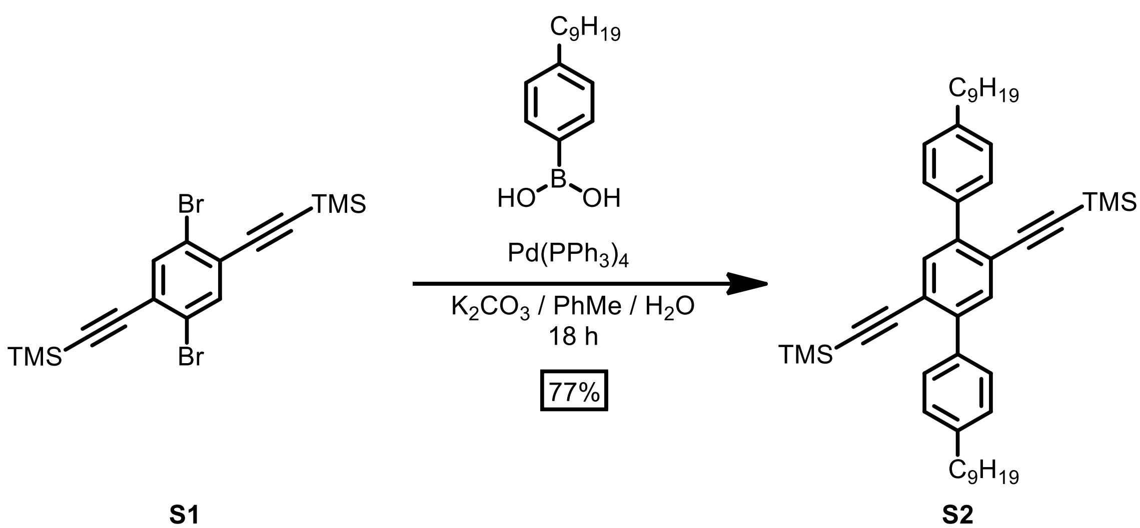
1,4-dibromo-2,5-diiodobenzene[1] and **S1**[2] were prepared from reported protocols.

## B. Synthetic Procedures

**Scheme S1.** Overall synthesis of **1a**.

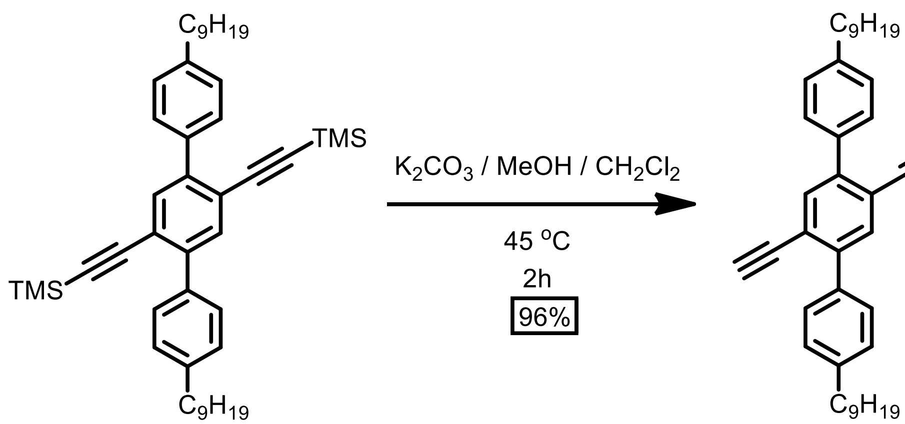



**Scheme S2.** Synthesis of **S2**.




**Synthesis of S2: S1** (0.650 g, 1.518 mmol), 4-*n*-nonylbenzeneboronic acid (0.829 g, 3.339 mmol), $K_2CO_3$ (0.629 g, 4.553 mmol), $Pd(PPh_3)_4$ (0.175 g, 0.152 mmol) were dissolved in a mixture of PhMe (15 mL) and water (3 mL), subjected to three freeze-pump-thaw cycles and backfilled with a $N_2$ atmosphere. The mixture was heated to 100 °C for 18 h. The solution was cooled to rt, filtered through celite, and washed with additional $CH_2Cl_2$ (250 mL). The solvent was evaporated and the resulting oil was purified by chromatography ($SiO_2$, hexanes to 1% *v/v* EtOAc/hexanes) to give **S2** (0.786 g, 77% yield) as a yellow oil that solidified slowly. **S2:** $^1$H NMR (400 MHz, $CDCl_3$) δ 7.59 (s, 2H), 7.55 (d, $J$ = 7.8 Hz, 4H ), 7.24 (d, $J$ = 7.8 Hz, 4H), 2.68 (t, $J$ = 7.8 Hz, 4H), 1.68 (m, 4H), 1.39-1.25 (m, 24H), 0.95-0.91 (m, 6H), 0.18 (s, 18H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 142.81, 142.73, 136.75, 134.49, 129.49, 128.27, 121.95, 104.98, 99.54, 36.12, 32.31, 31.94, 30.12, 30.00, 29.77, 29.67, 23.09, 14.53, 0.42. IR (solid, ATR) 2956, 2923, 2853, 2155, 1521, 1479, 1376, 1248, 1187, 1017, 906, 863, 839, 758, 722, 699 cm$^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{46}H_{66}Si_2]^+$ 674.4703, found 674.4706.

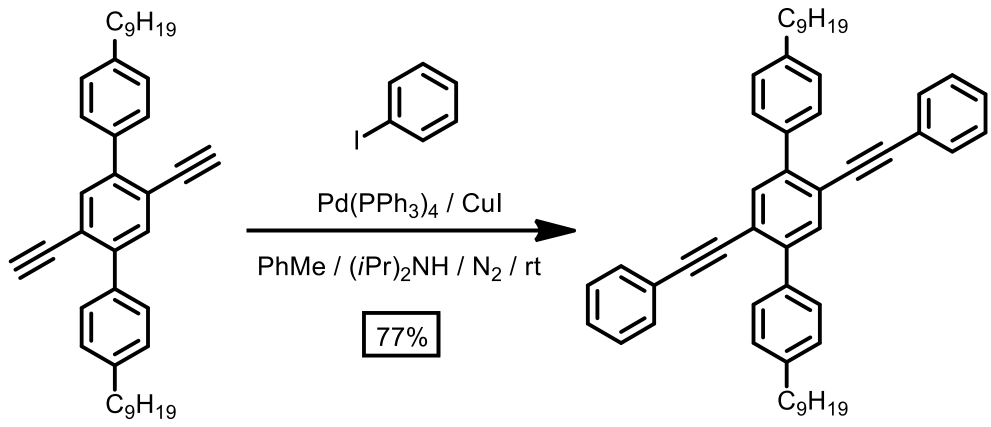
**Scheme S3.** Synthesis of **S3**.




**S2** **S3**

**Synthesis of S3:** $K_2CO_3$ (2.87 g, 20.7 mmol) was suspended in MeOH (41 mL) and a solution of **S2** (1.400 g, 2.073 mmol) dissolved in $CH_2Cl_2$ (10 mL) was added. The mixture was stirred at 45 °C for 2 h, after which it was cooled to rt and poured into aqueous HCl (2M, 10 mL). The solution was washed with $Et_2O$ (3x50 mL), and the combined organic layers were washed with brine (20 mL), dried ($MgSO_4$) and filtered. The solvent was evaporated to give **S3** (1.060 g, 96% yield) as a white solid that was used without further purification. **S3:** $^1$H NMR (300 MHz, $CDCl_3$) δ 7.63 (s, 2H), 7.55 (d, $J$ = 8.0 Hz, 4H), 7.25 (d, $J$ = 8.0 Hz, 4H), 3.14 (s, 2H), 2.66 (t, $J$ = 7.6 Hz, 4H), 1.67 (m, 4H), 1.40-1.25 (m, 24H), 0.91-0.87 (m, 6H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 142.89, 142.71, 136.33, 135.11, 129.11, 128.30, 121.07, 82.91, 81.74, 35.92, 32.06, 31.54, 29.72, 29.69, 29.59, 29.50, 22.84, 14.28. IR (solid, ATR) 3287, 2953, 2918, 2851, 1522, 1480, 1468, 1414, 1376, 1265, 1139, 1018, 902, 841, 823, 721, 666 cm$^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{40}H_{50}]^+$ 530.3913, found 530.3896.

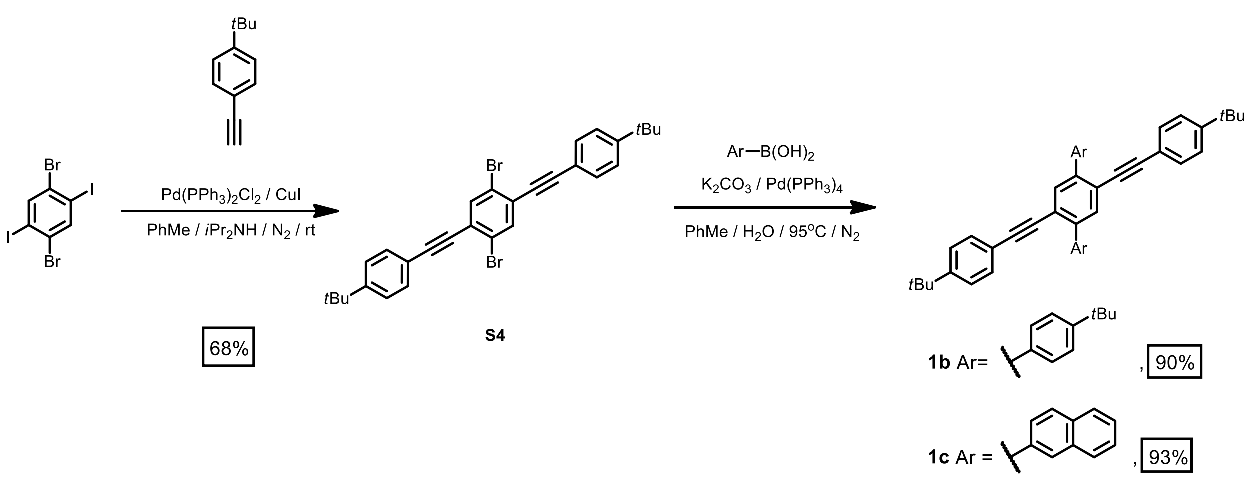
**Scheme S4.** Synthesis of **1a**.



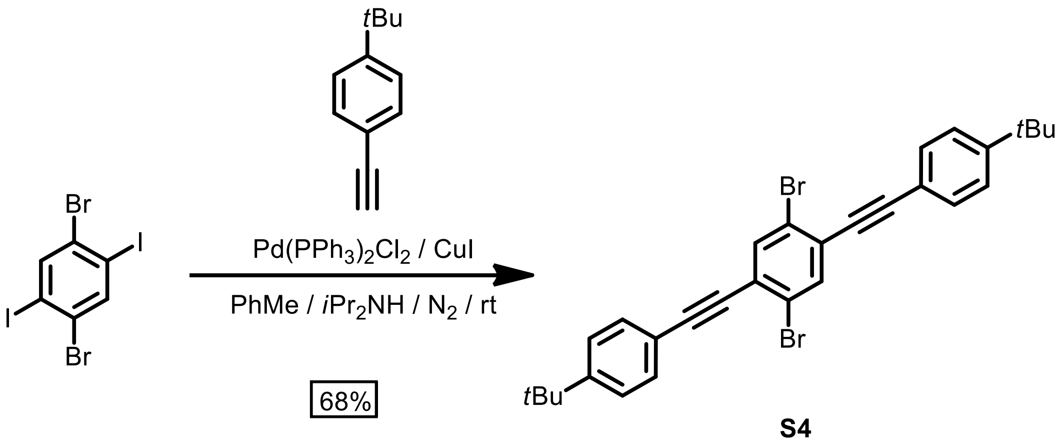

**S3** **1a**

**Synthesis of 1a: S3** (0.300 g, 0.565 mmol), iodobenzene (0.346 mg, 1.695 mmol) and freshly distilled $i$Pr$_2$NH (9 mL) were dissolved in anhydrous PhMe (28 mL), subjected to three freeze-pump-thaw cycles, and backfilled with $N_2$. $Pd(PPh_3)_4$ (33 mg, 0.028 mmol) and CuI (11 mg, 0.057 mg) were added, and another freeze-pump-thaw cycle was performed. After stirring for 2 h at rt, the reaction mixture was filtered through celite and washed with $CH_2Cl_2$ (150 mL). The solvent was evaporated and the crude product was purified by chromatography ($SiO_2$, 3% *v*/*v* EtOAc/hexanes) to give **1a** (0.296 g, 77% yield) as a yellow solid. **1a:** $^1$H NMR (400 MHz, $CDCl_3$) δ 7.72 (s, 2H), 7.67 (d, $J$ = 8.1 Hz, 4H), 7.39-7.33 (m, 4H), 7.33-7.27 (m, 6H), 2.70 (t, $J$ = 7.5 Hz, 4H), 1.69 (m, 4H), 1.44-1.23 (m, 24H), 0.93-0.86 (m, 6H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 142.69, 142.33, 136.89, 133.89, 131.56, 129.32, 128.41, 128.38, 128.19, 123.50, 121.73, 93.78, 89.63, 35.92, 32.07, 31.70, 29.77, 29.75, 29.53, 29.52, 22.85, 14.29. IR (solid, ATR) 3061, 2954, 2922, 2851, 1597, 1572, 1496, 1466, 1441, 1377, 1261, 1189, 1122, 1068, 1027, 1018, 903, 853, 834, 810, 752, 723, 687 cm$^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{52}H_{58}]^+$ 682.4539, found 682.4551.

**Scheme S5.** Overall syntheses of the dialkynes **1b** and **1c.**

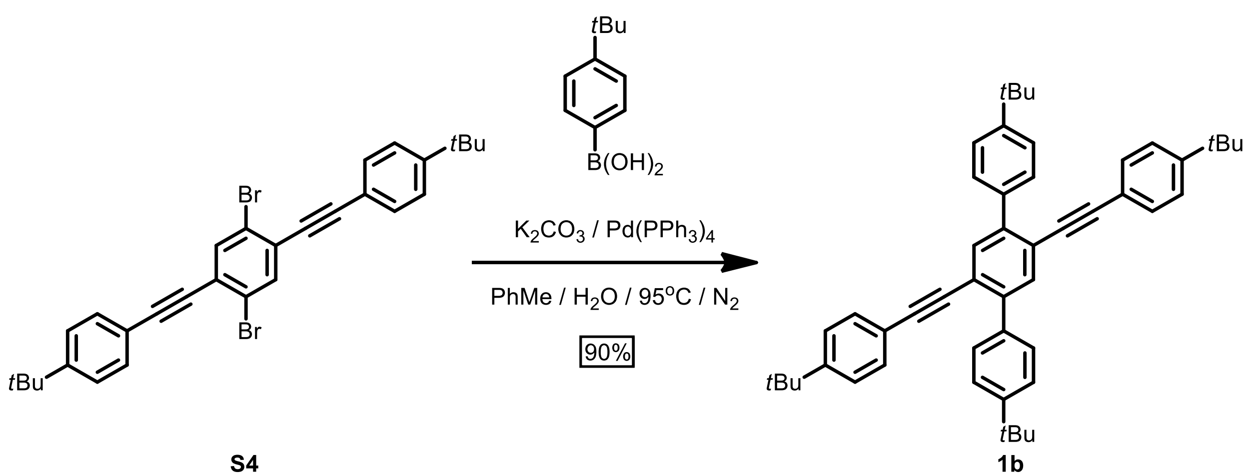


**Scheme S6.** Synthesis of **S4**



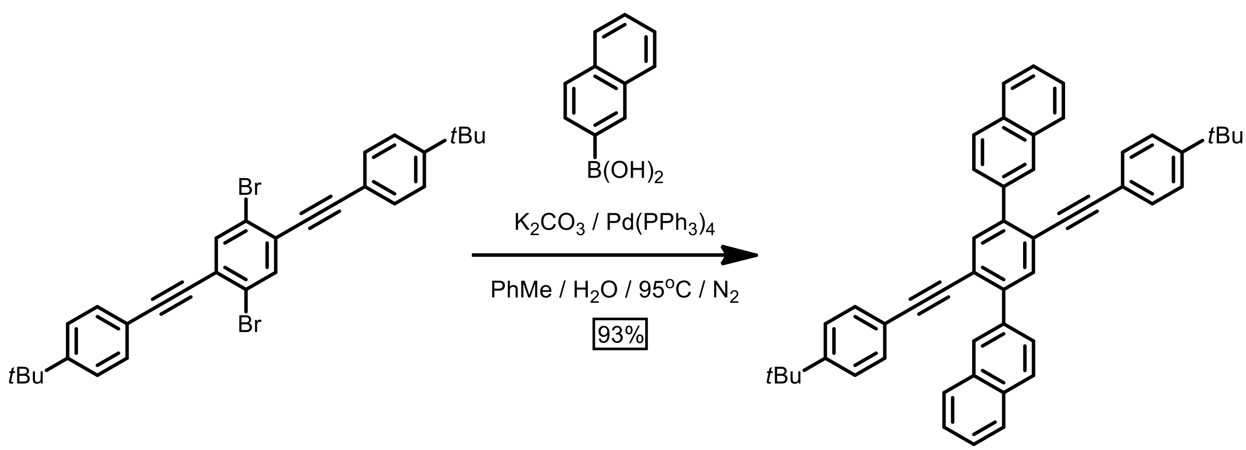

**Synthesis of S4:** Anhydrous PhMe (31 mL) and freshly distilled *i*$Pr_2NH$ (10 mL) were added to a 100 mL flask and sparged with $N_2$ for 20 min. 1,4-dibromo-2,5-diiodobenzene (3.000 g, 6.15 mmol), 1-(*tert*-butyl)-4-ethynylbenzene (2.433 g, 15.38 mmol), $Pd(PPh_3)_2Cl_2$ (216 mg, 0.308 mmol) and CuI (117 mg, 0.615 mmol) were added to the solution, in sequence. The mixture was stirred at rt for 14 h. The crude reaction mixture was filtered through a pad of $SiO_2$ gel and washed with additional $CH_2Cl_2$ (200 mL). Evaporation of the solvent provided the crude product as a solid, which was purified by chromatography ($SiO_2$, hexanes) to provide **S4** (2.310 g, 68% yield) as a white powder. $^1$H and $^{13}$C NMR spectroscopy were consistent with the report of Hseuh *et al.*[3] **S4:** $^1$H NMR (300 MHz, $CDCl_3$) δ 7.77 (s, 2H), 7.58 – 7.47 (m, 4H), 7.46 – 7.35 (m, 4H), 1.34 (s, 18H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 152.68, 136.05, 131.70, 126.58, 125.63, 123.81, 119.46, 97.03, 86.49, 77.58, 77.16, 76.74, 35.06, 31.30.

**Scheme S7.** Synthesis of **1b**




**Synthesis of 1b: S4** (0.400 g, 0.729 mmol), 4-*tert*-benzeneboronic acid (0.286 g, 1.605 mmol), and $K_2CO_3$ (0.465 g, 3.36 mmol) were added to a 50 mL flask equipped with a condenser. The flask was evacuated under high vacuum and backfilled with $N_2$ three times. Degassed solvents, PhMe (7.3 mL) and DI $H_2O$ (2.4 mL) were added under positive $N_2$ pressure at 77 K. The mixture was subjected to three freeze-pump-thaw cycles and the catalyst, $Pd(PPh_3)_4$ (0.042 g, 0.036 mmol) was quickly added under $N_2$ while still frozen. The flask was subjected to two more freeze-pump-thaw cycles to ensure air-free atmosphere. It was heated to 95°C, stirred for 12 hours and cooled down to rt. The mixture was transferred to a 250 mL beaker and the product crashed out upon addition of MeOH (70 mL). It was filtered through a coarse fritted funnel, and the ppt was washed with $H_2O$ (100 mL) and additional MeOH (125 mL) to give the product **1b** (0.428 g, 90% yield) as an off-white powder. $^1$H NMR (300 MHz, $CDCl_3$) δ 7.71 (s, 2H), 7.69 (d, *J* = 8.4 Hz, 4H), 7.51 (d, *J* = 8.4 Hz, 4H), 7.33 (d, *J* = 8.7 Hz, 4H), 7.28 (d, *J* = 8.7 Hz, 4H), 1.42 (s, 18H), 1.31 (s, 18H). $^{13}$C NMR (75 MHz, $CDCl_3$) δ 151.67, 150.70, 142.09, 136.79, 133.81, 131.30, 129.13, 125.42, 125.02, 121.79, 120.54, 93.96, 89.11, 34.94, 34.81, 31.58, 31.31. IR (solid, ATR) 3035, 2959, 2903, 2866, 1505, 1480, 1462, 1393, 1362, 1268, 1202, 1112,1104, 1013, 905, 838 cm$^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{50}H_{54}]^+$ 654.4226, found 654.4234.

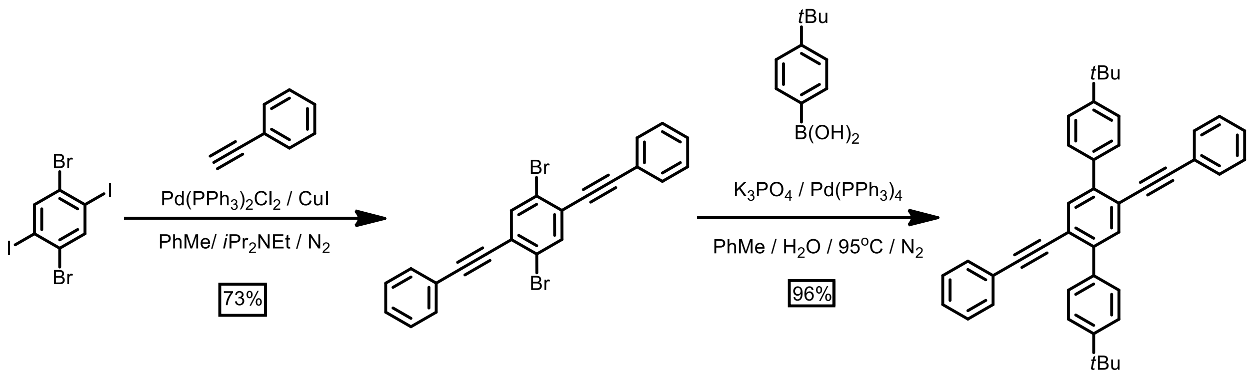
**Scheme S8.** Synthesis of **1c**




**S4** **1c**

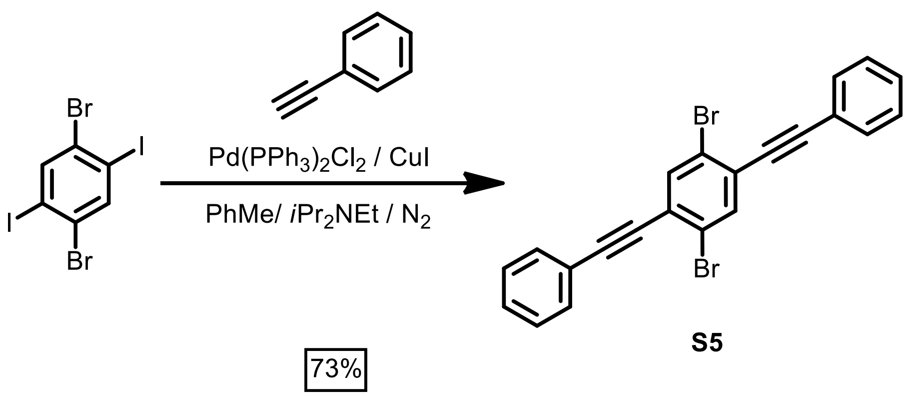
**Synthesis of 1c: 1c** was synthesized using a similar procedure as that used to prepare **1b**. **S4** (0.300 g, 0.547 mmol), 2-naphthaleneboronic acid (0.207 g, 1.204 mmol), $K_2CO_3$ (0.348 g, 2.52 mmol), $Pd(PPh_3)_4$ (0.032 g, 0.027 mmol), PhMe (5.5 mL) and $H_2O$ (1.8 mL) were used. MeOH (50 mL) was added and the resulting precipitate was recovered by filtration through a coarse fritted funnel. The crude solid was washed with $H_2O$ (50 mL) and additional MeOH (100 mL) to provide the product **1c** (0.325 g, 93% yield) as an off-white powder. $^1$H NMR (500 MHz, $CDCl_3$) δ 8.23 (s, 2H), 8.00 – 7.88 (m, 8H), 7.86 (s, 2H), 7.53 (dd, *J* = 6.3, 3.2 Hz, 4H), 7.32 – 7.18 (m, 8H), 1.28 (s, 18H). $^{13}$C NMR (125 MHz, $CDCl_3$) δ 151.94, 142.55, 137.41, 134.35, 133.60, 133.18, 131.41, 128.57, 128.51, 127.90, 127.76, 127.58, 126.32, 125.46, 122.38, 120.45, 94.63, 88.92, 34.98, 31.33. IR (solid, ATR) 3031, 2962, 2865, 2209, 1598, 1516, 1506, 1489, 1464, 1395, 1363, 1348, 1194, 1130, 1117, 1105, 1017, 982, 967, 955, 946, 911, 898, 868, 861, 847, 830, 823, 775, 771, 754, 736, 713, 695 $cm^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{50}H_{42}]^+$ 642.3287, found 642.3278.

**Scheme S9.** Overall synthesis of **1d**




S5 1d

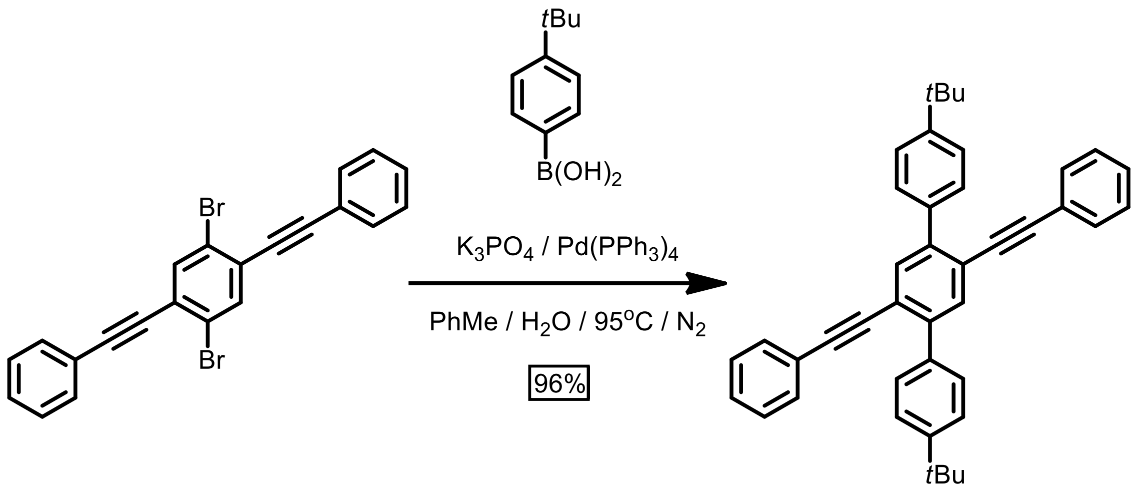
**Scheme S10.** Synthesis of **S5**




S5

**Synthesis of S5:** Anhydrous PhMe (41 mL) and freshly distilled *i*$Pr_2NH$ (10 mL) were added to a 100 mL flask and bubbled with $N_2$ for 20 min. 1,4-dibromo-2,5-diiodobenzene (1.000 g, 2.05 mmol), ethynylbenzene (0.461 g, 4.51 mmol), $Pd(PPh_3)_2Cl_2$ (72 mg, 0.103 mmol) and CuI (39 mg, 0.205 mmol) were added to the solution, in sequence. The mixture was stirred at rt for 20 min. The crude reaction mixture was poured into a 1 M HCl solution (50 mL) and extracted with $CH_2Cl_2$ (3x50 mL). Combined organic layers were dried ($MgSO_4$), filtered and the solvent was evaporated. The crude product was purified by flash column chromatography ($SiO_2$, 1% v/v EtOH/hexanes) to give **S5** (0.650 g, 73% yield) as a white powder. $^1H$ and $^{13}C$ NMR spectroscopy were consistent with the report of Liang *et al.*[4] **S5:** $^1H$ NMR (400 MHz, $CDCl_3$) δ 7.79 (s, 2H), 7.61 – 7.54 (m, 4H), 7.42 – 7.34 (m, 6H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ 136.15, 131.94, 129.27, 128.61, 126.54, 123.86, 122.44, 96.80, 86.96.

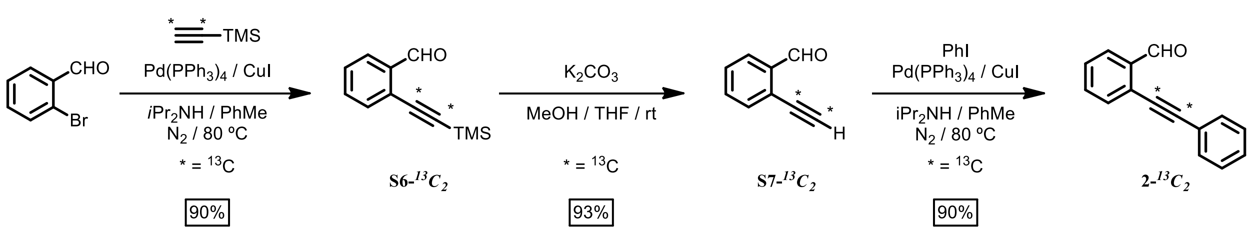
**Scheme S11.** Synthesis of **1d**



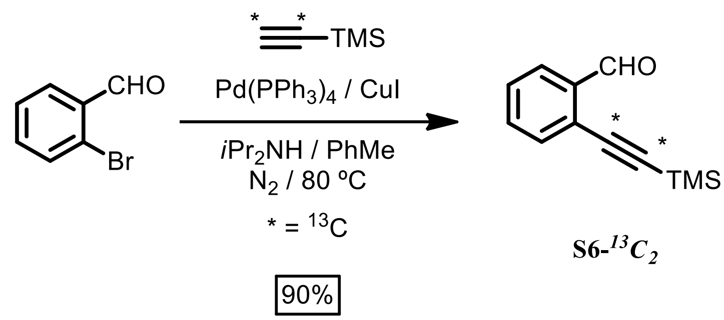

**S5** **1d**

Synthesis of **1d**: **1d** was synthesized using a similar procedure as that used to prepare **1b**. **S5** (0.200 g, 0.459 mmol), 4-*tert*-benzeneboronic acid (0.204 g, 1.146 mmol), $K_3PO_4$ (0.292 g, 1.376 mmol), $Pd(PPh_3)_4$ (0.053 g, 0.046 mmol), PhMe (4.6 mL) and $H_2O$ (1.5 mL) were used. After 13h the reaction mixture was cooled to rt and MeOH was added until precipitation was complete. The precipitate was collected using a coarse fritted funnel and washed with $H_2O$ (50 mL) and MeOH (50mL), dried and **1d** (0.240g, 96% yield) was isolated as an off-white powder. **1d**: $^1$H NMR (400 MHz, CDCl3) δ 7.72 (s, 2H), 7.69 (d, J = 8.5 Hz, 4H), 7.52 (d, J = 8.5 Hz, 4H), 7.37-7.32 (m, 4H), 7.32-7.27 (m, 6H), 1.41 (s, 18H). $^{13}$C NMR (100 MHz, CDCl3) δ 150.81, 142.30, 136.71, 133.80, 131.56, 129.14, 128.40, 128.38, 125.06, 123.51, 121.79, 93.86, 89.69, 34.82, 31.56. IR (solid, ATR) 3033, 2961, 2867, 1595, 1572, 1498, 1477, 1443, 1385, 1362, 1266, 1200, 1175, 1160, 1110, 1068, 1014, 965, 912, 908, 898, 852, 837, 829, 752, 688 cm-1. HRMS (EI, *m/z*): calcd for $[C_{42}H_{38}]^+$ 542.2974, found 542.2969.

**Scheme S12.** Synthesis of **2-*$^{13}C_2$***



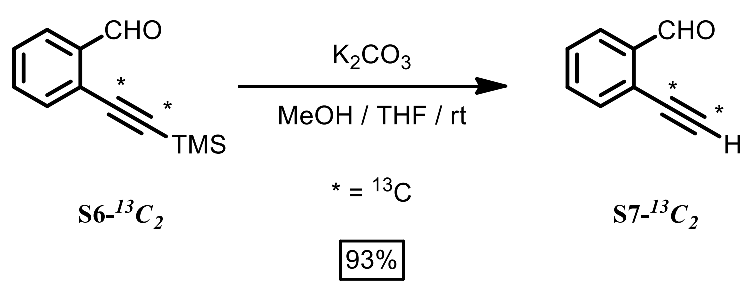
**Scheme S13.** Synthesis of **S6-$^{13}C_2$**



**S6-$^{13}C_2$**

**Synthesis of S6-$^{13}C_2$.** 2-bromobenzaldehyde (0.526 g 2.84 mmol), CuI (5 mg, 0.028 mmol), and $Pd(PPh_3)_4$ (15 mg, 0.013 mmol) were loaded in a 25 mL Schlenk flask equipped with a magnetic stirrer. The flask was evacuated under dynamic vacuum to 150 mtorr and backfilled with $N_2$ three times. Anhydrous PhMe (3 mL) and anhydrous $i$Pr$_2$NH (1 mL) were added via cannula under $N_2$. The mixture was bubbled with $N_2$ for 20 min and trimethylsilylacetylene-$^{13}C_2$ (99% atom $^{13}$C, 0.435 mL, 300 mg, 2.994 mmol) was added dropwise with stirring. The mixture was heated to 80 ºC and stirred for 12 h, after which it was quenched with saturated $NH_4Cl$ (*aq*), and extracted with $CH_2Cl_2$ (3 x 10 mL). The combined organic extracts were rinsed with saturated $NH_4Cl$ (*aq*), water, and brine. The solution was dried over anhydrous $MgSO_4$, filtered over celite, and concentrated to dryness. The obtained dark residue was purified by column chromatography ($SiO_2$, 5% *v*/*v* THF/hexanes) to provide **S6-$^{13}C_2$** (0.554 g, 90% yield) as a yellow oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 10.56 (d, $J_{CH}$ = 0.76 Hz, 1H), 7.91 (d, $J$ = 7.95 Hz, 1H), 7.57 (m, $J$ = 7.85, 1.71, 0.70 Hz, 1H), 7.54 (m, $J$ = 7.75, 0.68 Hz, 1H), 7.43 (m, $J$ = 7.75, 0.68 Hz, 1H), 0.28 (d, $J_{CH}$ = 2.48 Hz, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 102.74 (d, $J_{CC}$ = 136.2 Hz), 100.02 (d, $J_{CC}$ = 136.3 Hz). EI-MS: calcd for $[C_{10}{}^{13}C_2H_{14}OSi]^+$ 204.09, found 203.15.

**Scheme S14.** Synthesis of **S7-$^{13}C_2$**

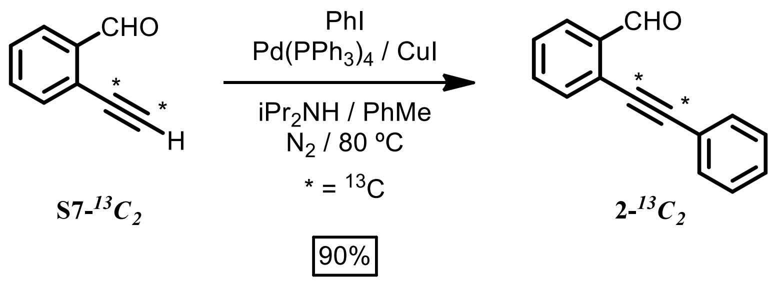


**S6-$^{13}C_2$** **S7-$^{13}C_2$**

**Synthesis of S7-$^{13}C_2$. S6-$^{13}C_2$** (0.554 g, 2.71 mmol), and $K_2CO_3$ (3.74 g, 27.11 mmol) were suspended in THF (6 mL) and MeOH (2 mL). The suspension was stirred at rt for 30 min. The mixture was added to 1 M HCl (3 mL), extracted with $CH_2Cl_2$ (3 x 2 mL), after which the combined organic extracts were dried over anhydrous $MgSO_4$, filtered over celite, and concentrated to dryness to afford **S7-$^{13}C_2$** (0.335 g, 93% yield) as a yellow solid. $^1$H NMR (400

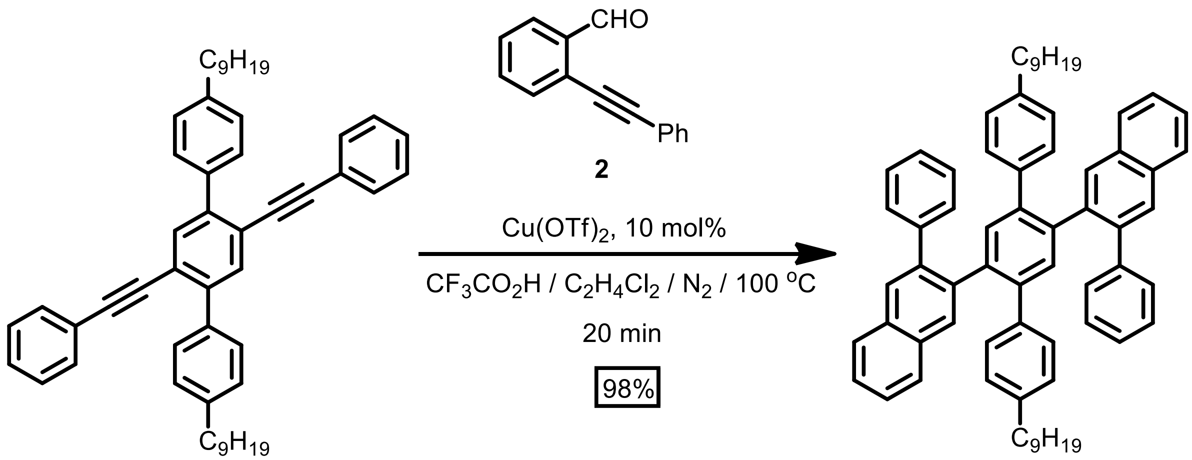
MHz, $CDCl_3$) δ 10.54 (d, $J_{CH}$ = 0.65 Hz, 1H), 7.94 (m, $J$ = 7.60, 1.29 Hz, 1H), 7.60 (m, $J$ = 7.06, 7.33, 7.06, 7.56 Hz, 2H), 7.49 (m, $J$ = 7.33, 1.02 Hz, 1H), 3.46 (dd, $J$ = 192.22, 55.95 Hz, 9H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 82.73 (m, $J$ = 535.66, 8.54, 2.33 Hz), 81.01 (m, $J$ = 534.92, 0.29 Hz). HRMS (EI, *m/z*): calcd for $[C_7H_6O^{13}C_2]^+$ 132.0486, found 132.0488

**Scheme S15.** Synthesis of **2-*$^{13}C_2$***



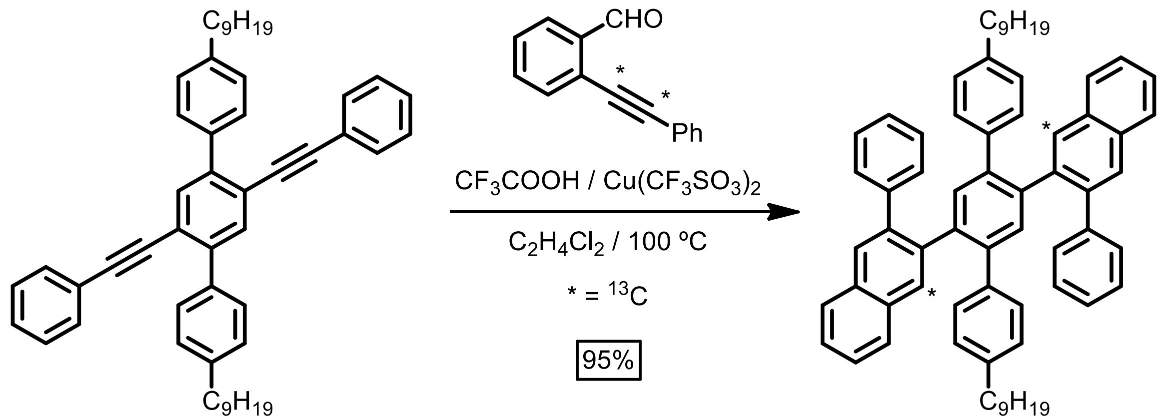

**Synthesis of 2-*$^{13}C_2$*. S7-*$^{13}C_2$*** (0.335 g, 2.53 mmol), CuI (5 mg, 0.027 mmol), and $Pd(PPh_3)_4$ (16 mg, 0.014 mmol) were loaded in a 25 mL Schlenk flask equipped with a magnetic stirrer. The flask was evacuated under dynamic vacuum to 150 mtorr and backfilled with $N_2$ three times. A mixture containing anhydrous PhMe (5 mL), anhydrous *i*$Pr_2NH$ (2 mL), and PhI (0.608 g) were added via cannula under $N_2$. The mixture was stirred at rt for 10 h, after which it was quenched with saturated $NH_4Cl$ (*aq*) and extracted with PhMe (3 x 10 mL). The combined organic extracts were rinsed with saturated $NH_4Cl$ (*aq*), water, and brine. The solution was dried over anhydrous $MgSO_4$, filtered over celite and concentrated to dryness. The obtained dark residue was purified by column chromatography ($SiO_2$, 5% *v*/*v* THF/hexanes) to provide **2-*$^{13}C_2$*** (0.506 g, 90% yield) as a green oil. $^1$H NMR (400 MHz, $CDCl_3$) δ 10.66 (s, 1H), 7.97 (d, $J$ = 7.27 Hz, 1H), 7.65 (m, $J$ = 5.45, Hz, 1H), 7.61-7.56 (m, 3H), 7.46 (m, $J$ = 7.48, 1H), 7.39 (m, $J$ = 2.51, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 96.52 (d, $J_{CC}$ = 184.82 Hz), 84.97 (d, $J_{CC}$ = 182.02 Hz). HRMS (EI, *m/z*): calcd for $[C_{13}H_{10}O^{13}C_2]^+$ 208.0799, found 208.0800.

**Scheme S16.** Synthesis of **3a**.




**Synthesis of 3a:** Dialkyne **1a** (0.273 g, 0.400 mmol) and benzaldehyde **2** (0.330 g, 1.600 mmol) were dissolved in 1,2-dichloroethane (16 mL) under $N_2$. $Cu(OTf)_2$ (58 mg, 0.160 mmol) and $CF_3CO_2H$ (0.135 mL, 1.760 mmol) were added in quick succession. The solution was heated to reflux for 20 min, after which it was cooled to rt and poured into a saturated aqueous $NaHCO_3$ solution (50 mL). The aqueous layer was washed with extracted with $CH_2Cl_2$ (3x50 mL), and the combined organic layers were dried ($MgSO_4$) and filtered. The solvent was evaporated to provide the product as a crude solid, which was purified by chromatography ($SiO_2$, 2% v/v EtOAc/hexanes) to give **2a** (0.348 g, 98% yield) as an off-white solid. **2a:** $^1$H NMR (500 MHz, $CDCl_3$) δ 8.05 (s, 2H), 7.67 (d, $J$ = 8.1 Hz, 4H), 7.88-7.84 (m, 4H), 7.66 (s, 2H), 7.53-7.48 (m, 6H), 7.22-7.17 (m, 2H), 7.16-7.11 (m, 2H), 6.77 (d, $J$ = 7.7 Hz, 8H), 6.55 (d, $J$ = 8.1 Hz, 4H), 2.52 (td, $J$ = 8.0 Hz, 2.2 Hz, 4H), 1.60 (m, 4H), 1.39-1.25 (m, 24H), 0.94-0.89 (m, 6H). $^{13}$C NMR (125 MHz, $CDCl_3$) δ 141.1, 140.9, 140.0, 139.6, 139.2, 139.1, 137.8, 133.9, 133.1, 132.9, 130.6, 129.4, 129.0, 128.9, 127.9, 127.9, 127.8, 127.5, 126.2, 35.7, 32.1, 31.8, 29.8, 29.7, 29.5, 29.4, 22.9, 14.3. IR (solid, ATR) 3053, 2953, 2923, 2852, 1941, 1671, 1596, 1489, 1456, 1371, 1260, 1074, 1014, 914, 889, 796, 772, 759, 746, 695 cm$^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{68}H_{70}]^+$ 886.5478, found 886.5509.

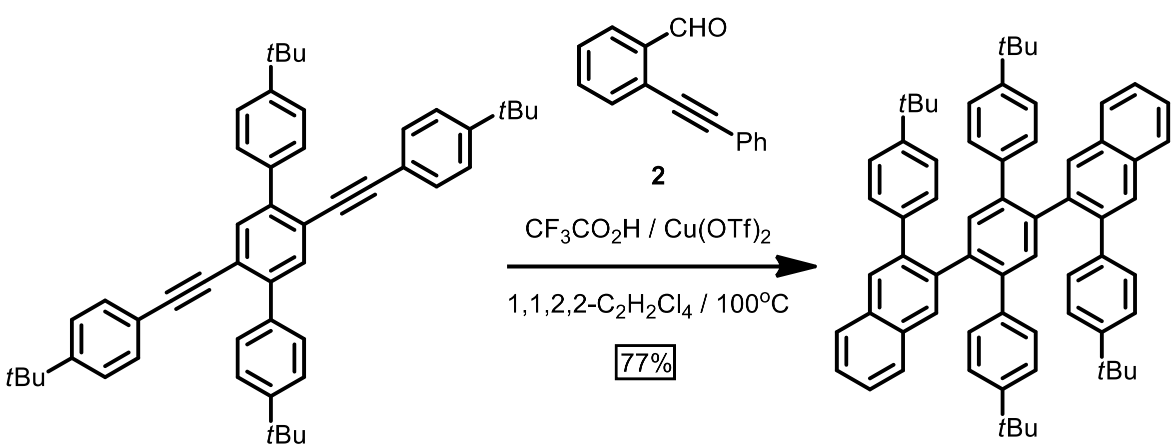
**Scheme S17.** Synthesis of **3a-*$^{13}C_2$***.




**1a** **3a-*$^{13}C_2$***

**Synthesis of 3a-*$^{13}C_2$*: 3a-*$^{13}C_2$*** was synthesized using a similar procedure as that used to prepare **3a. 1a** (0.050 g, 0.073 mmol), **2-*$^{13}C_2$*** (0.090 g, 439 mmol), $Cu(OTf)_2$ (0.009 g, 0.026 mmol), $CF_3COOH$ (0.028 mL, 0.042 g, 0.439 mmol), 1,2-dichloroethane (1.3 mL) were used. **3a-*$^{13}C_2$*** was isolated as a yellow solid (0.062 g, 95% yield). $^1$H NMR (500 MHz, $CDCl_3$) δ 8.07 (d, $J_{CH}$ = 159.17 Hz, 2H), 7.87 (m, 4H), 7.67 (s, 2H), 7.52 (m, $J$ = 3.64 Hz, 6H), 7.20-7.13 (m, 4H), 6.78-6.77 (m, 8H), 6.57-6.55 (d, $J$ = 8.35 Hz, 4H) 2.52 (t, $J$ = 7.6 Hz, 4H), 1.61 (t, $J$ = 7.2 Hz, 4H), 1.33 (m, br, 24H), 0.93 (t, $J$ = 6.7 Hz, 6H). $^{13}$C NMR (125 MHz, $CDCl_3$) δ 130.58 (s). MS: (*m*/*z* MALDI-TOF, TCNQ) calcd for $[C_{66}H_{70}{}^{13}C_2]^+$ 888.5477, found 888.5207.

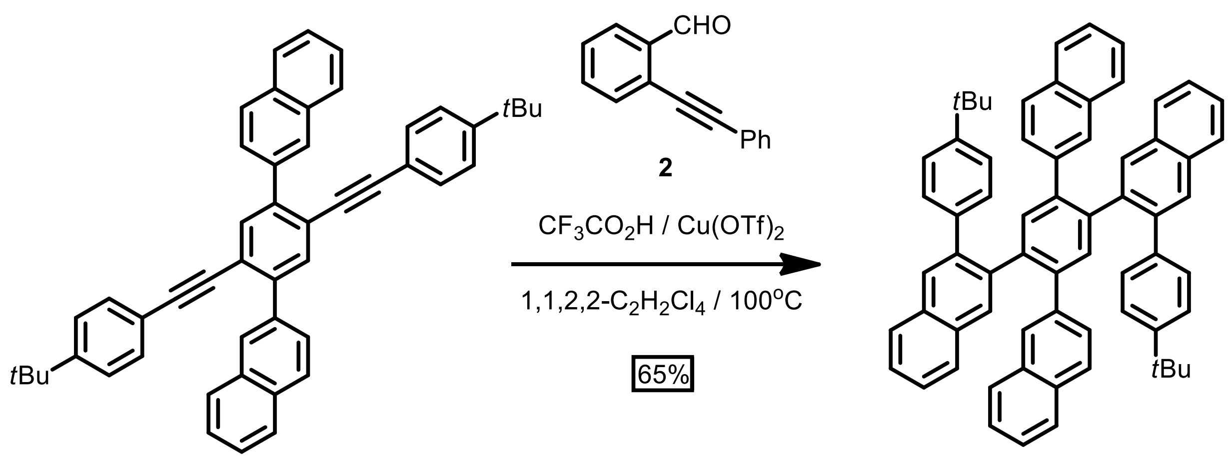
**Scheme S18.** Synthesis of **3b**.




**1b** **3b**

**Synthesis of 3b: 3b** was synthesized using a similar procedure that was used to prepare **3a**. **1b** (0.329 g, 0.502 mmol), benzaldehyde **2** (0.518 g, 2.51 mmol), $Cu(OTf)_2$ (18 mg, 0.050 mmol) and $CF_3CO_2H$ (0.19 mL, 2.51 mmol) 1,1,2,2-tetrachloroethane (5 mL) were used. **3b** (0.330 g, 77% yield) was isolated as an off-white powder. **3b:** $^1$H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 2H), 7.91-7.88 (m, 4H), 7.70 (s, 2H), 7.59 (s, 2H), 7.55-7.52 (m, 4H), 7.18 (d, $J$ = 8.3 Hz, 4H), 6.96 (d, $J$ = 8.4 Hz, 4H), 6.66 (d, $J$ = 8.3 Hz, 4H), 6.56 (d, $J$ = 8.4 Hz, 4H), 1.39 (s, 18H), 1.34 (s, 18H). $^{13}$C NMR (100MHz, $CDCl_3$) δ 148.9, 148.9, 140.0, 139.5, 139.4, 139.3, 138.0, 137.4, 133.8, 133.1, 133.0, 130.4, 128.8, 128.5, 128.5, 127.9, 127.7, 126.2, 126.1, 124.7, 124.2, 34.5, 34.5, 31.5, 31.5. IR (solid, ATR) 3052, 2960, 2865, 1516, 1489, 1473, 1458, 1393, 1362, 1269, 1214, 1199, 1132, 1111, 1022, 1011, 947, 919, 888, 852, 831, 748, 687, 668 cm$^{-1}$. HRMS (MALDI-TOF, *m/z*): calcd for $[C_{66}H_{66}]^+$ 858.5159, found 858.517

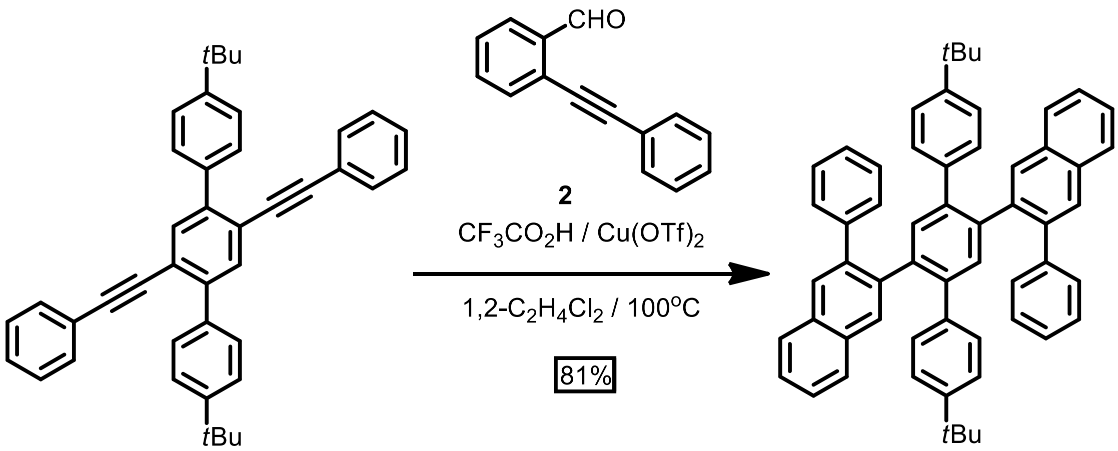
**Scheme S19.** Synthesis of **3c**.




**1c** **3c**

**Synthesis of 3c: 3c** was synthesized using a similar procedure that was used to prepare **3a**. **1c** (0.305 g, 0.474 mmol), benzaldehyde **2** (0.490 g, 2.37 mmol), $Cu(OTf)_2$ (17 mg, 0.047 mmol), $CF_3CO_2H$ (0.18 mL, 2.37 mmol) 1,1,2,2-tetrachloroethane (5.0 mL) were used. After purification by flash column chromatography ($SiO_2$, 3% *v*/*v* EtOAc/hexanes), **3c** was isolated as a white powder (0.260g, 65% yield). **3c:** $^1$H NMR (400 MHz, $CDCl_3$) δ 8.18 (s, 2H), 7.93 – 7.86 (m, 2H), 7.86 – 7.77 (m, 2H), 7.76 – 7.69 (m, 4H), 7.60 (s, 2H), 7.56 – 7.46 (m, 4H), 7.46 – 7.35 (m, 8H), 7.09 – 7.04 (m, 4H), 7.03 (d, $J$ = 1.8 Hz, 2H), 6.82 (dd, $J$ = 8.5, 1.8 Hz, 2H), 6.59 – 6.49 (m, 4H), 1.36 (s, 18H). $^{13}$C NMR (101 MHz, $CDCl_3$) δ 149.16, 140.52, 139.90, 139.44, 138.99, 138.21, 137.96, 134.16, 133.41, 133.21, 132.87, 132.00, 130.40, 128.96, 128.82, 128.40, 128.00, 127.92, 127.75, 127.47, 127.42, 126.76, 126.30, 126.24, 125.69, 125.54, 124.18, 53.09, 34.54, 31.75, 31.59, 22.82, 14.29, 0.16. IR (solid, ATR) 3054, 2959, 2865, 1788, 1596, 1507, 1489, 1452, 1394, 1361, 1260, 1215, 1177, 1088, 1215, 891, 856, 819, 742 cm$^{-1}$. HRMS (MALDI-TOF, *m/z*): calcd for $[C_{66}H_{54}]^+$ 846.4220, found 846.419.

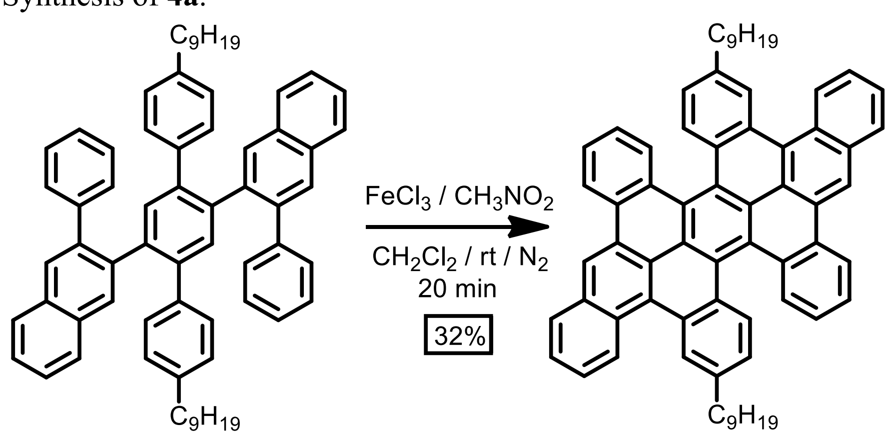
**Scheme S20.** Synthesis of **3d**.




**1d** **3d**

**Synthesis of 3d: 3d** was synthesized using a similar procedure that was used to prepare **3a**. **1d** (0.180 g, 0.332 mmol), benzaldehyde **2** (0.205 g, 1.00 mmol), $Cu(OTf)_2$ (12 mg, 0.033 mmol), $CF_3CO_2H$ (0.08 mL, 1.00 mmol) 1,2-dichloroethane (8.3 mL) were used. After purification by flash column chromatography ($SiO_2$, 2% *v*/*v* EtOAc/hexanes), **3d** was isolated as a white powder (0.201g, 81% yield). **3d:** $^1H$ NMR (400 MHz, $CDCl_3$) δ 8.07 (s, 2H), 7.87 (dd, $J$ = 6.1, 3.3 Hz, 4H), 7.65 (s, 2H), 7.54 (s, 2H), 7.51 (dd, $J$ = 6.1, 3.3 Hz, 4H), 7.18 (t, $J$ = 7.3 Hz, 2H), 7.11 (t, $J$ = 7.5 Hz, 4H), 6.97 (d, $J$ = 8.2 Hz, 4H), 6.71 (d, $J$ = 7.3 Hz, 4H), 6.57 (d, $J$ = 8.2 Hz, 4H), 1.30 (s, 18H). $^{13}C$ NMR (100 MHz, $CDCl_3$) δ 149.03, 141.01, 139.89, 139.55, 139.23, 139.08, 137.40, 133.81, 133.03, 132.93, 130.58, 129.21, 128.86, 128.69, 127.90, 127.75, 127.42, 126.19, 126.11, 124.70, 34.48, 31.48. IR (solid, ATR) 3056, 3029, 2900, 2864, 1490, 1477, 1459, 1437, 1372, 1363, 1270, 1027, 1113, 1011, 950, 915, 888, 835, 797, 772, 756, 745, 720, 696, 668 $cm^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{58}H_{50}]^+$ 746.3913, found 746.3921.

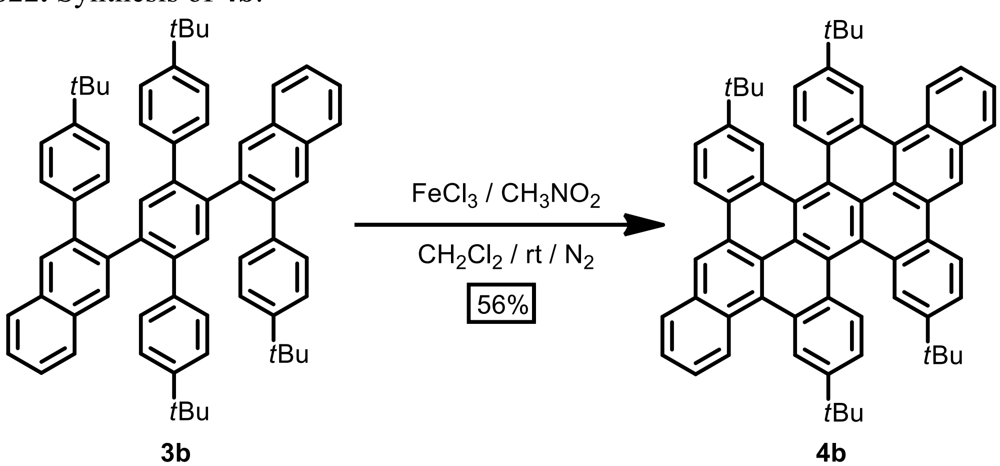
**Scheme S21.** Synthesis of **4a**.




**3a** **4a**

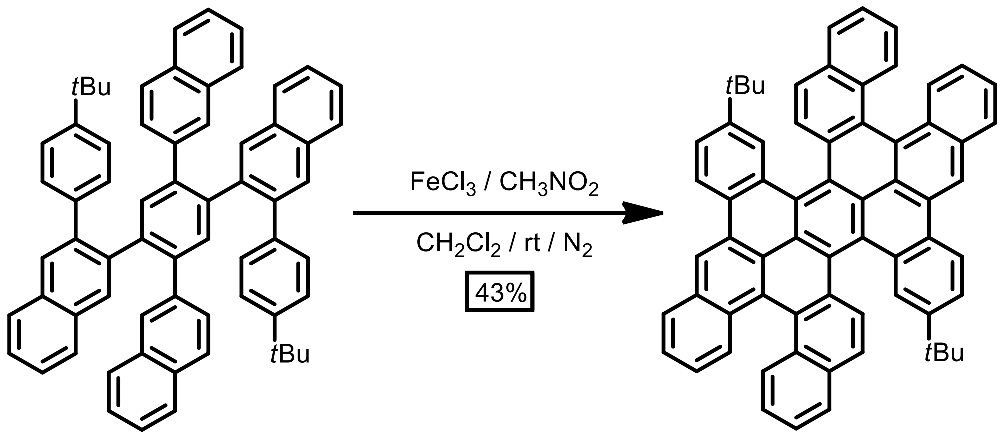
**Synthesis of 4a: 3a** (0.100 g, 0.113 mmol) was dissolved in $CH_2Cl_2$ (55.0 mL) under $N_2$ at rt. $FeCl_3$ (0.548 g, 3.381 mmol) dissolved in $CH_3NO_2$ (5.0 mL) was added dropwise over 6 min, while the solution was bubbled with $N_2$. Vigorous $N_2$ flow through the solution was maintained for 20 min, after which the reaction mixture was poured into a separatory funnel that contained $H_2O$ (100 mL). The organic phase was separated and the aqueous phase was washed with $CH_2Cl_2$ (3 x 50 mL). The combined organic phases were dried ($MgSO_4$), filtered, and the solvent was removed. Purification by chromatography ($SiO_2$, 1:8 *v*/*v* $CH_2Cl_2$/hexanes) provided **4a** (0.032 g, 32% yield) as an orange solid. **4a:** $^1$H NMR (500 MHz, $CDCl_3$) δ 9.36 (s, 2H), 9.35 (d, *J* = 8.4 Hz, 2H), 8.96 (dd, *J* = 8.5, 1.2 Hz, 2H), 8.90 (dd, *J* = 8.2, 1.2 Hz, 2H), 8.68 (d, *J* = 1.8 Hz, 2H), 8.51 (d, *J* = 8.5 Hz, 2H), 8.40 (dd, *J* = 7.8, 1.6 Hz, 2H), 7.88 – 7.73 (m, 4H), 7.62 (ddd, *J* = 8.2, 6.8, 1.3 Hz, 2H), 7.38 (ddd, *J* = 8.1, 6.8, 1.2 Hz, 2H), 7.13 (dd, *J* = 8.5, 1.8 Hz, 2H), 2.78 (td, *J* = 7.3, 5.1 Hz, 4H), 1.69 (p, *J* = 7.6 Hz, 4H), 1.47 – 1.12 (m, 24H), 0.89 – 0.81 (m, 6H). $^{13}$C NMR (125 MHz, $CDCl_3$) δ 141.23, 133.01, 131.55, 131.27, 130.95, 130.74, 130.34, 129.10, 129.10, 128.87, 128.39, 128.28, 128.02, 127.67, 126.92, 126.56, 126.04, 125.91, 125.82, 124.68, 124.39, 124.13, 121.94, 121.36, 36.37, 32.03, 31.54, 29.72, 29.69, 29.54, 29.47, 22.80, 14.25. IR (solid, ATR) 3050, 2920, 2850, 1606, 1464, 1354, 1154, 904, 878, 834, 810, 785, 759, 744, 715cm$^{-1}$. HRMS (MALDI-TOF, *m/z*): calcd for $[C_{68}H_{62}]^+$ 878.4846, found 878.487.

**Scheme S22.** Synthesis of **4b**.




**Synthesis of 4b: 4b** was synthesized using a similar procedure that was used to prepare **4a**. **3b** (0.076 g, 0.089 mmol), $FeCl_3$ (0.433 g, 2.671 mmol), $CH_2Cl_2$ (45 mL) and $CH_3NO_2$ (4.5 mL) were used. The reaction mixture was stirred for 20 min before workup. Purification of the crude product by chromatography ($SiO_2$, 1:8 *v*/*v* $CH_2Cl_2$/hexanes) provided **4b** (0.043 g, 56% yield) as an orange solid. **4b:** $^1$H NMR (400 MHz, $CDCl_3$) δ 9.42 (d, *J* = 8.5 Hz, 2H), 9.35 (s, 2H), 9.00 (dd, *J* = 15.6, 1.9 Hz, 4H), 8.85 (d, *J* = 8.8 Hz, 2H), 8.51 (d, *J* = 8.7 Hz, 2H), 8.40 (d, *J* = 7.4 Hz, 2H), 7.85 (ddd, *J* = 8.4, 6.7, 1.3 Hz, 2H), 7.78 (ddd, *J* = 8.4, 6.7, 1.3 Hz, 2H), 7.69 (dd, *J* = 8.6, 2.0 Hz, 2H), 7.37 (dd, *J* = 8.7, 2.0 Hz, 2H), 1.46 (s, 18H), 1.25 (s, 18H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 149.19, 148.80, 133.09, 131.13, 130.94, 130.04, 129.07, 128.72, 128.62, 128.59, 128.57, 128.27, 128.13, 128.04, 125.94, 125.89, 125.53, 125.45, 125.31, 124.92, 124.60, 123.78, 123.68, 121.64, 121.49, 35.26, 34.83, 31.44, 31.09. IR (solid, ATR) 3050, 2962, 2902, 2867, 1608, 1489, 1476, 1465, 1457, 1393, 1369, 1264, 902, 881, 824, 748 $cm^{-1}$. HRMS (MALDI-TOF, *m/z*): calcd for $[C_{66}H_{58}]^+$ 850.4533, found 850.447.

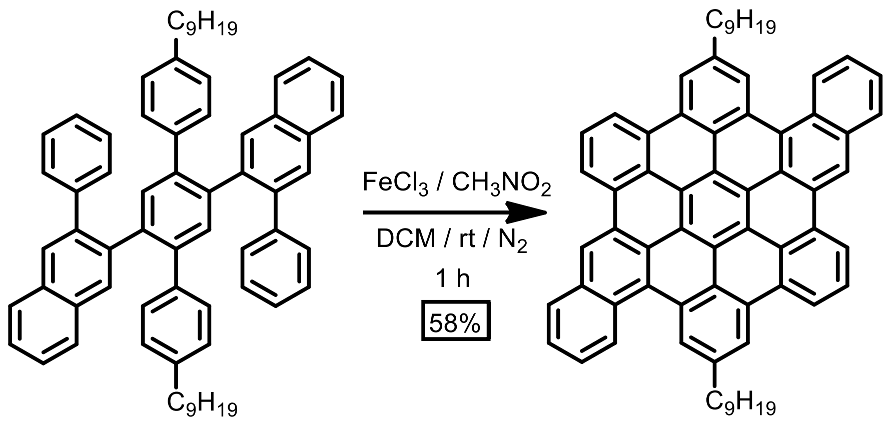
**Scheme S23.** Synthesis of **4c**.




**3c** **4c**

**Synthesis of 4c: 4c** was synthesized using a similar procedure that was used to prepare **4a**. **3c** (0.180 g, 0.212 mmol), $FeCl_3$ (0.620 g, 3.825 mmol), $CH_2Cl_2$ (21 mL) and $CH_3NO_2$ (4.0 mL) were used. The reaction mixture was stirred for 45 min before workup. Purification of the crude product by chromatography ($SiO_2$, 5% *v*/*v* EtOAc/hexanes) provided **4c** (0.076 g, 43% yield) as a red solid. **4c:** $^1H$ NMR (500 MHz, $CDCl_3$) δ 9.42 (s, 2H), 9.18 (d, *J* = 2.0 Hz, 2H), 8.96 (d, *J* = 8.6 Hz, 2H), 8.69 (dd, *J* = 8.7, 3.5 Hz, 4H), 8.38 (d, *J* = 8.1 Hz, 2H), 8.15 (d, *J* = 8.6 Hz, 2H), 7.85 – 7.79 (m, 2H), 7.77 (dd, *J* = 8.5, 2.1 Hz, 2H), 7.72 (d, *J* = 8.7 Hz, 4H), 7.52 (ddd, *J* = 8.3, 6.7, 1.4 Hz, 2H), 7.47 – 7.38 (m, 2H), 7.22 (ddd, *J* = 8.5, 6.7, 1.4 Hz, 2H), 1.28 (s, 18H). $^{13}C$ NMR (126 MHz, $CDCl_3$) δ 149.29, 132.89, 132.16, 131.90, 130.91, 129.83, 129.65, 129.61, 129.58, 129.53, 128.65, 128.44, 128.41, 128.26, 128.23, 128.18, 128.04, 128.01, 127.69, 127.59, 127.54, 127.52, 127.21, 126.23, 126.21, 126.17, 126.16, 126.12, 125.82, 125.48, 125.07, 124.64, 124.29, 123.86, 123.68, 123.66, 122.81, 122.25, 77.41, 77.36, 77.16, 76.90, 35.07, 35.06, 31.35, 31.23, 31.22, 31.18, 31.16, 31.13, 30.80, 29.87, 0.17. IR (solid, ATR) 3064, 2959, 2925, 2859, 1735, 1507, 1455, 1361, 1261, 822, 753 $cm^{-1}$. HRMS (MALDI-TOF, *m/z*): calcd for $[C_{66}H_{46}]^+$ 838.3594, found 838.351.

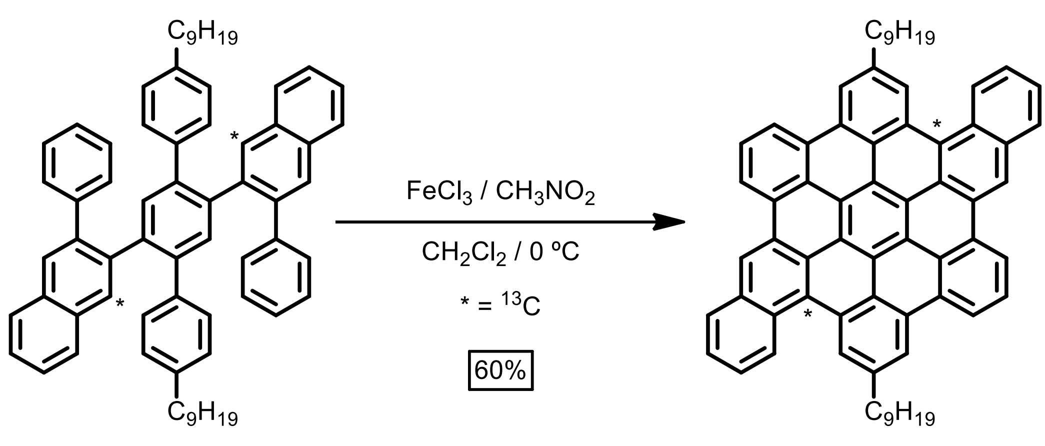
**Scheme S24.** Synthesis of **5a**.




**3a** **5a**

**Synthesis of 5a: 3a** (0.100 g, 0.113 mmol) was dissolved in $CH_2Cl_2$ (11.3 mL) under $N_2$. $FeCl_3$ (0.329 g, 2.029 mmol) dissolved in $CH_3NO_2$ (2 mL) was added dropwise over 5 min. The solution was stirred at rt, during which time product formation was monitored by MALDI-TOF mass spectrometry. After the reaction was complete (1 h), the reaction mixture was poured into MeOH (50 mL), forming a precipitate. The precipitate was recovered by filtration and washed with additional MeOH (100 mL) to give **5a** (0.057 g, 58% yield) as a yellow-brown powder. **5a:** $^1$H NMR (400 MHz, 1,2-$CD_4Cl_2$) δ 9.22-8.68 (m, 10H), 8.16-8.07 (m, 2H), 7.92-7.80 (m, 2H), 7.63-7.47 (m, 6H), 3.05 (m, 4H), 1.89 (m, 4H), 1.45-0.46 (m, 30H). $^{13}$C NMR (75 MHz, 2:1 $CS_2$:$CD_2Cl_2$) δ 130.3-118.3 (br) 32.9, 30.6, 30.4, 27.1, 23.8, 15.0. IR (solid, ATR) 3049, 2951, 2920, 2850, 1933, 1671, 1599, 1489, 1456, 1376, 1321, 1260, 1027, 908, 878, 847, 823, 746, 722, 699, 669, 653 $cm^{-1}$. HRMS (EI, *m/z*): calcd for $[C_{68}H_{58}]^+$ 874.4539, found 874.4519.

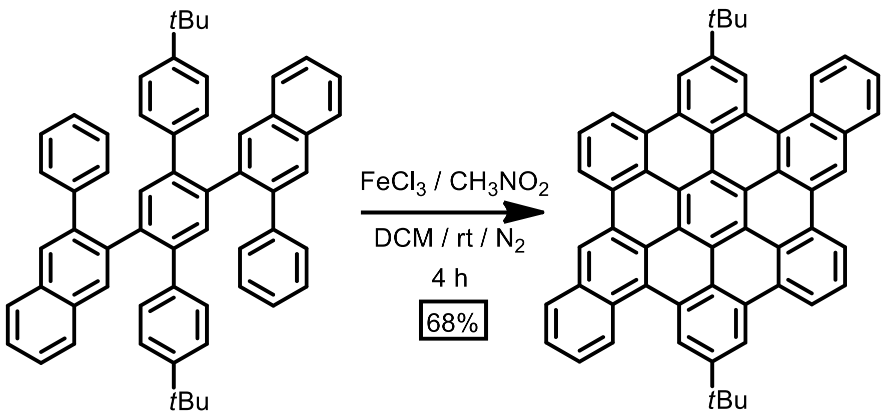
**Scheme S25.** Synthesis of **5a-*$^{13}C_2$***.




**3a-*$^{13}C_2$*** **5a-*$^{13}C_2$***

**Synthesis of 5a-*$^{13}C_2$*: 5a-*$^{13}C_2$*** was synthesized using a similar procedure as that used to prepare **5a**. **5a-*$^{13}C_2$*** (0.025g 0.028 mmol), $FeCl_3$ (0.137 g, 0.843 mmol), $CH_3NO_2$ (1 mL), 1,2-dichloroethane (14 mL). **5a-*$^{13}C_2$*** was isolated as an orange solid (0.015 g, 60% yield). $^{1}$H NMR (500 MHz, $C_2D_2Cl_4$, 135 ºC) δ (ppm) 9.21 (d, $J$ = 7.4 Hz, 1H), 9.16 (s, 1H), 9.01 (s, 1H), 8.95 (d, $J$ = 7.2 Hz, 1H), 8.87 (d, $J$ = 7.7 Hz, 1H), 8.33 (d, $J$ = 7.4 Hz, 1H), 7.98 (t, $J$ = 7.7 Hz, 1H), 7.79 (m, 2H), 3.19 (t, $J$ = 7.8 Hz, 2H), 2.10 (t, $J$ = 7.5 Hz, 2H), 1.76 – 1.70 (m, 2H), 1.66 – 1.59 (m, 2H), 1.57 – 1.33 (m, 8H), 0.99 (t, $J$ = 6.9 Hz, 3H). $^{13}$C NMR (125 MHz, $C_2D_2Cl_4$, 135 ºC) δ (ppm) 126.47 (s). HRMS (MALDI-TOF, *m/z*): calcd for $[C_{66}H_{58}{}^{13}C_2]^+$ 876.4539, found 876.461.

**Scheme S26.** Synthesis of **5d**




**3d** **5d**

**Synthesis of 5d:** The compound **5d** was synthesized using a similar procedure used to prepare **5a**. **3d** (0.048 g, 0.064 mmol), $FeCl_3$ (0.188 g, 1.157 mmol), $CH_2Cl_2$ (6.0 mL) and $CH_3NO_2$ (1.0 mL) were used. The reaction mixture was stirred for 4 h before precipitation using MeOH. Upon filtration **5d** (0.032 g, 68% yield) was isolated as an orange solid. NMR characterization attempts were not successful due to low solubility of the compound. **5d:** IR (solid, ATR) 3054, 2952, 2865, 1598, 1583, 1475, 1464, 1391, 1361, 1279, 1252, 1199, 908, 876, 823, 748, 723, 696 cm$^{-1}$. HRMS (MALDI-TOF, *m/z*): calcd for $[C_{66}H_{54}]^+$ 734.2968, found 734.302.

## C. NMR Spectra

**Figure S1.** $^{1}$H NMR of **S2** (300 MHz, $CDCl_3$, 300 K).

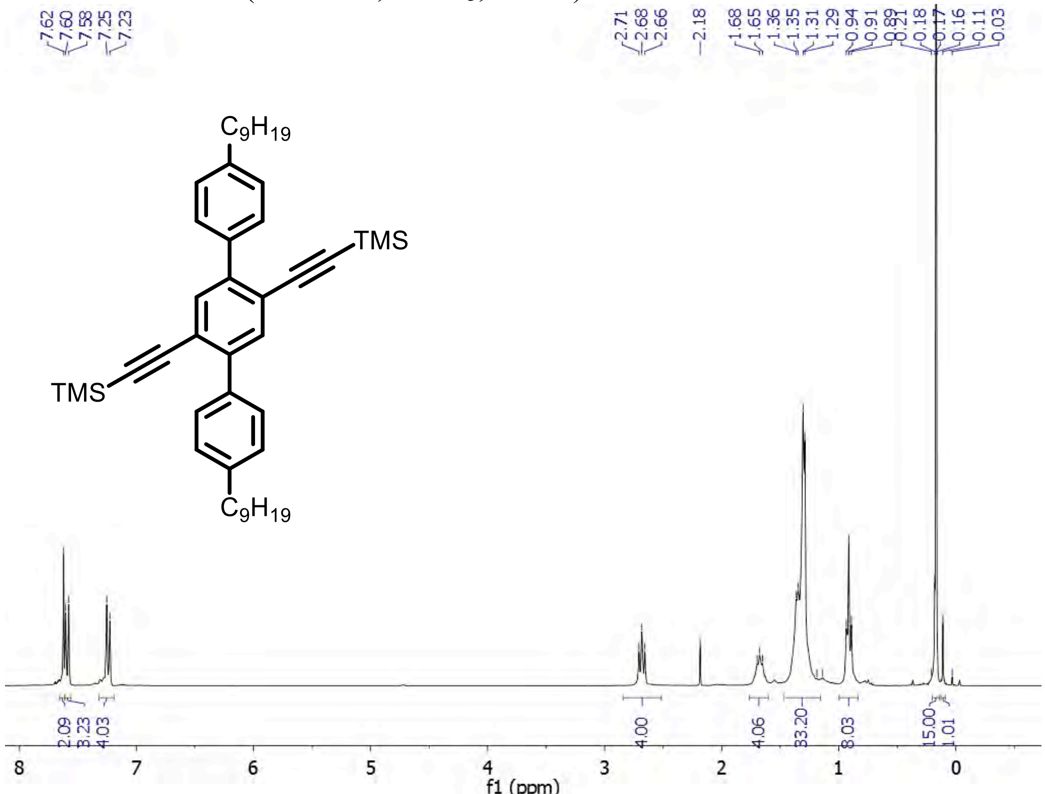


**Figure S2.** $^{13}$C NMR of **S2** (75 MHz, $CDCl_3$, 300 K).

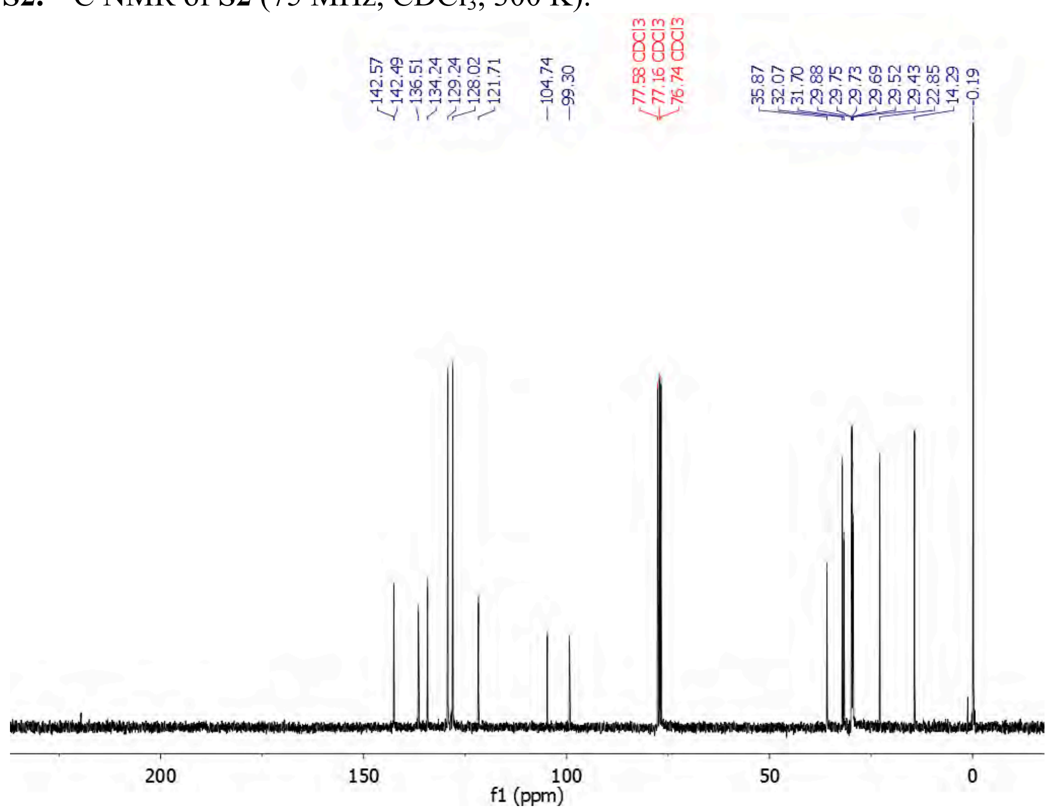


**Figure S3.** $^{1}$H NMR of **S3** (300 MHz, $CDCl_3$, 300 K).

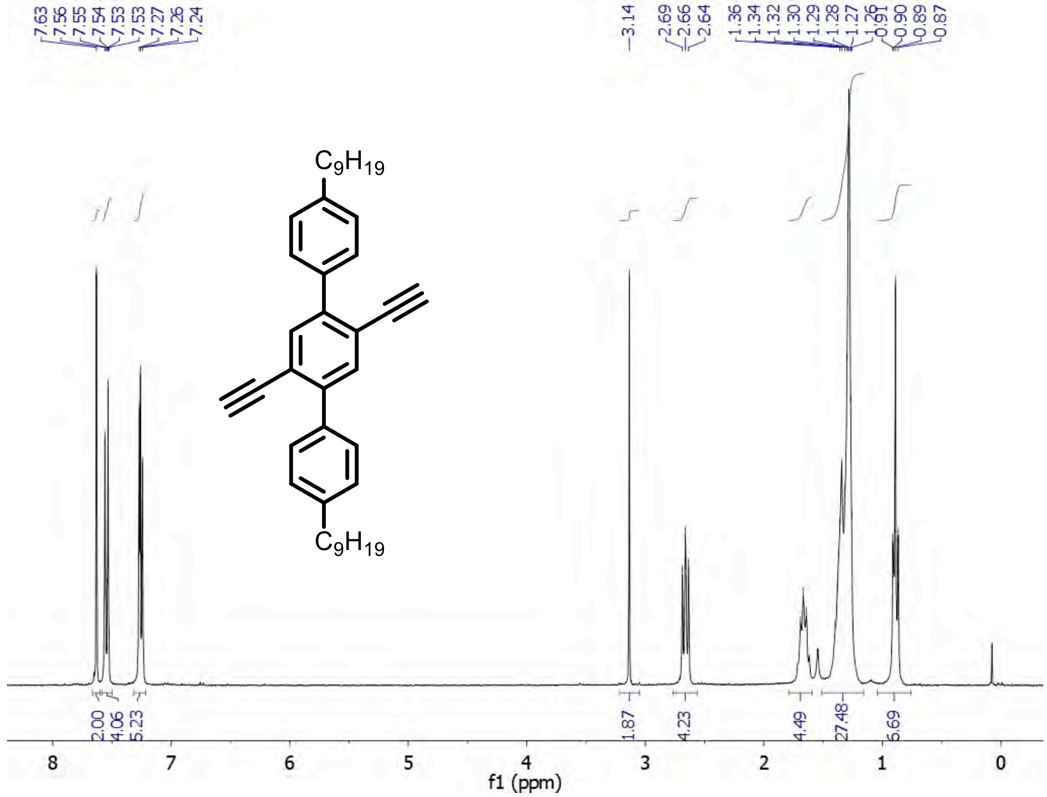


**Figure S4.** $^{13}$C NMR of **S3** (75 MHz, $CDCl_3$, 300 K).

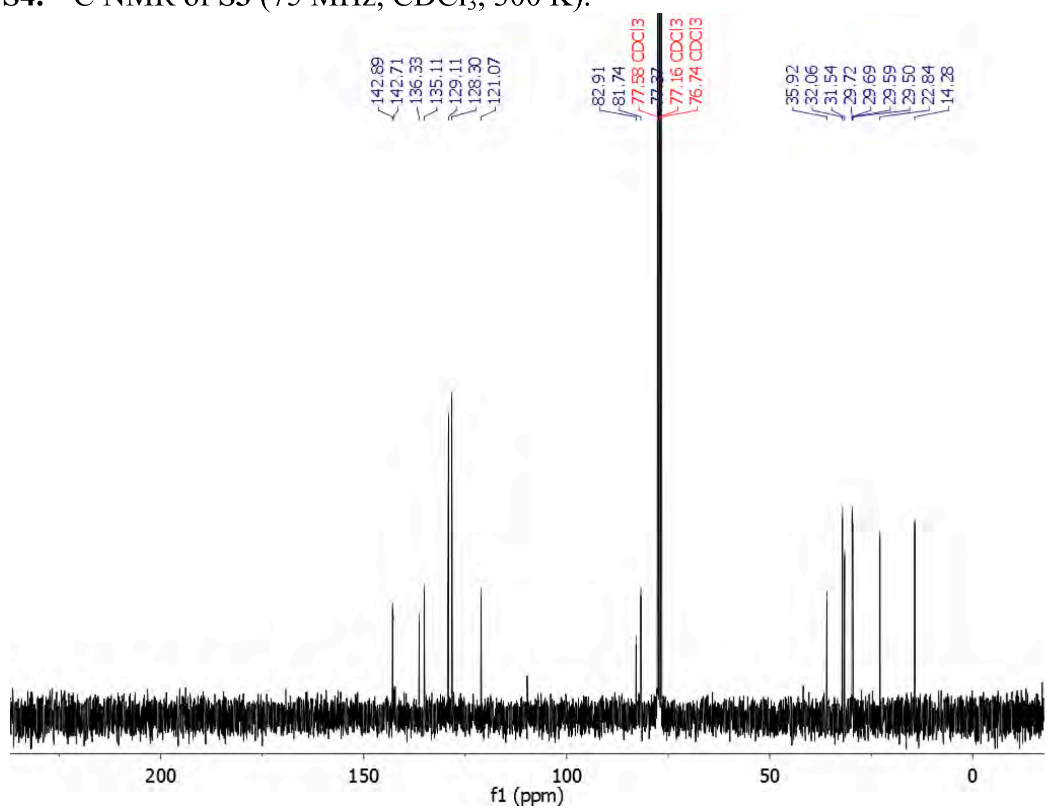


**Figure S5.** $^{1}$H NMR of **1a** (400 MHz, $CDCl_3$, 298 K).

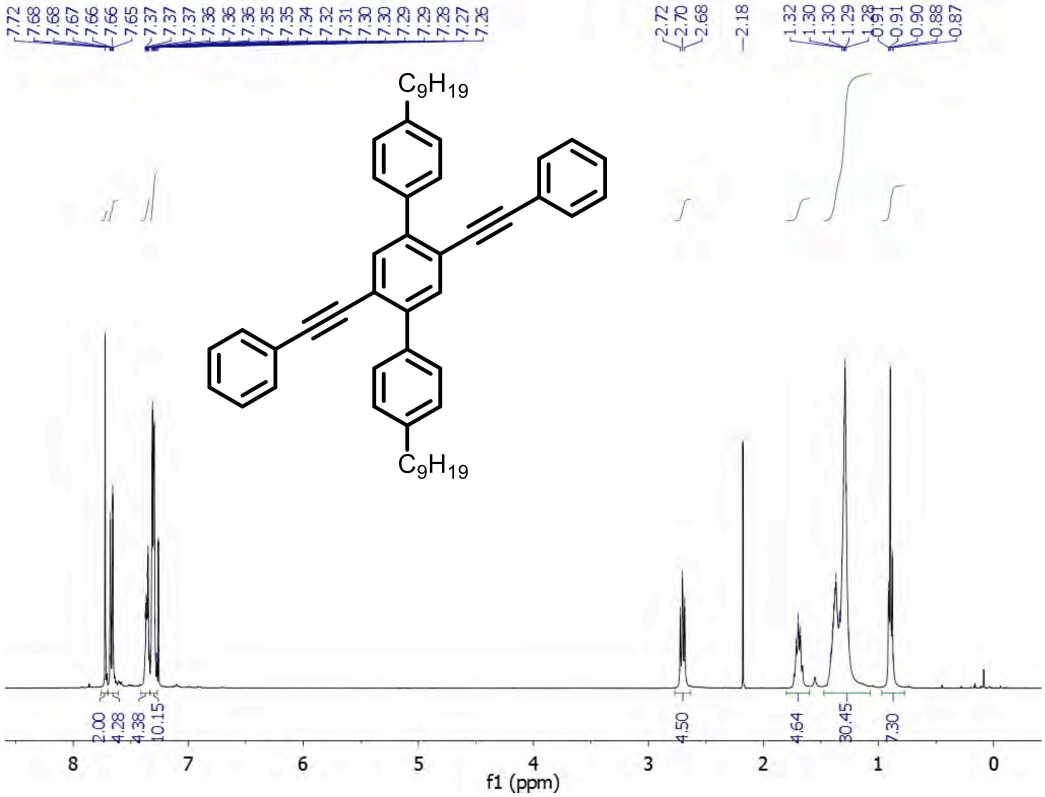



**Figure S6.** $^{13}$C NMR of **1a** (100 MHz, $CDCl_3$, 298 K).

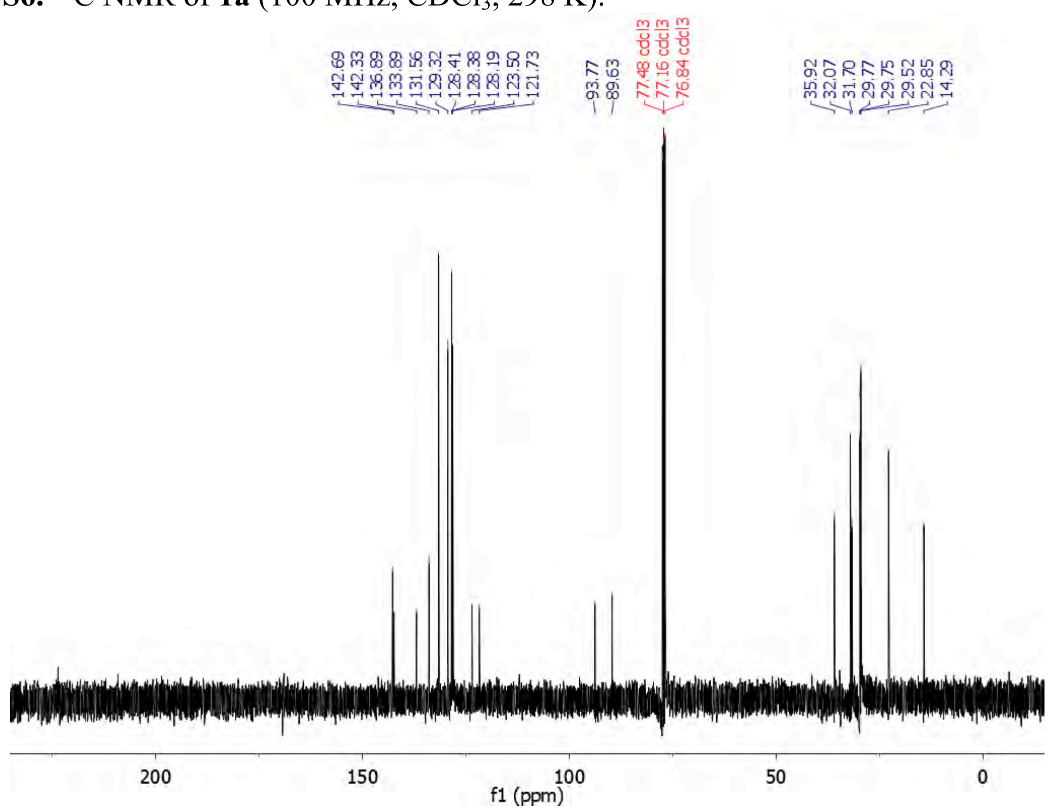


**Figure S5.** $^{1}H$ NMR of **S4** (300 MHz, $CDCl_3$, 298 K).

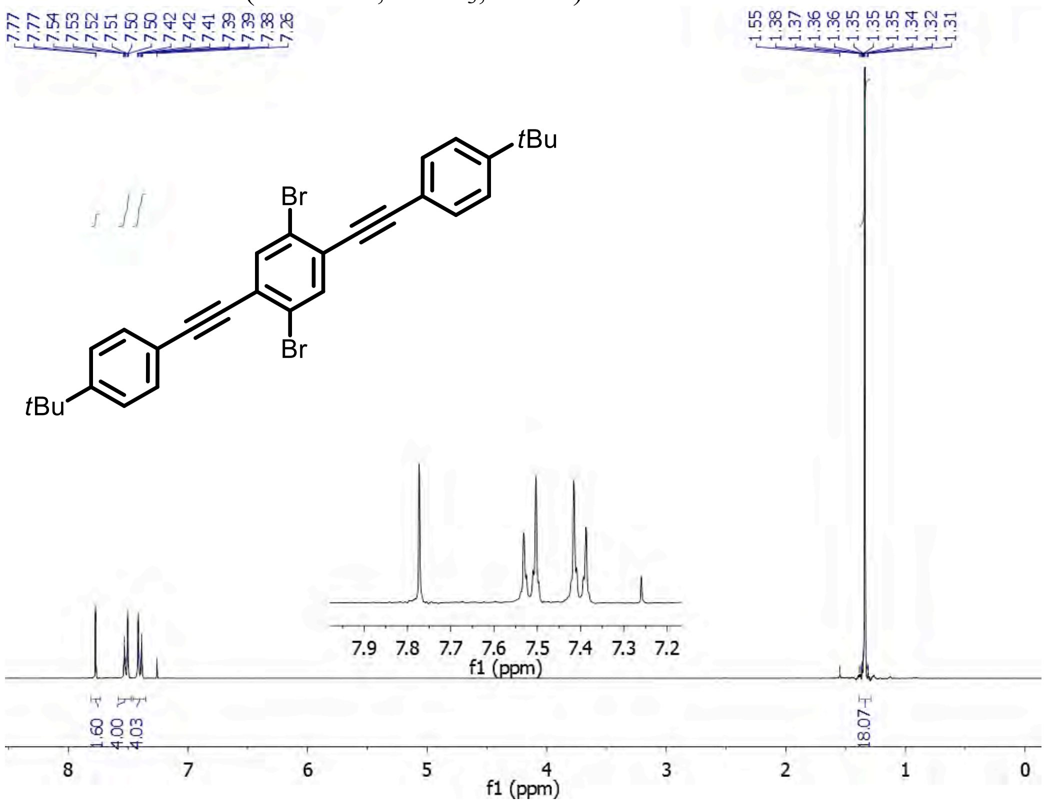


**Figure S6.** $^{13}C$ NMR of **S4** (75 MHz, $CDCl_3$, 298 K).

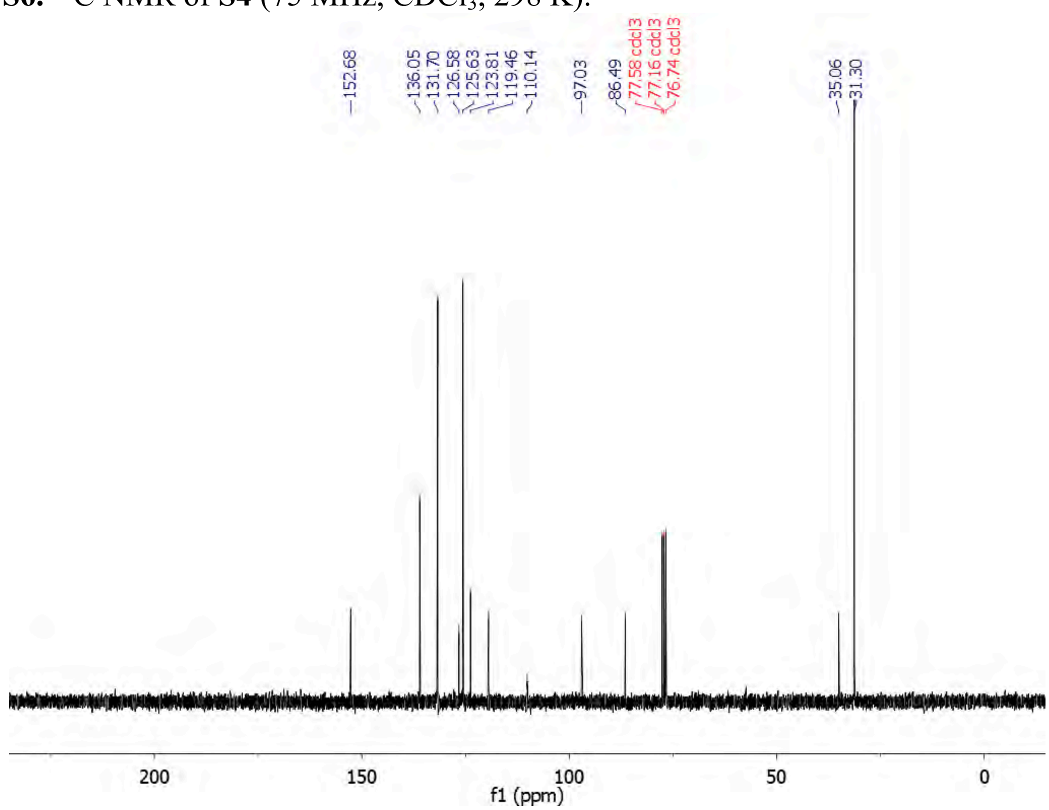


**Figure S7.** $^{1}H$ NMR of **1b** (300 MHz, $CDCl_3$, 300 K).

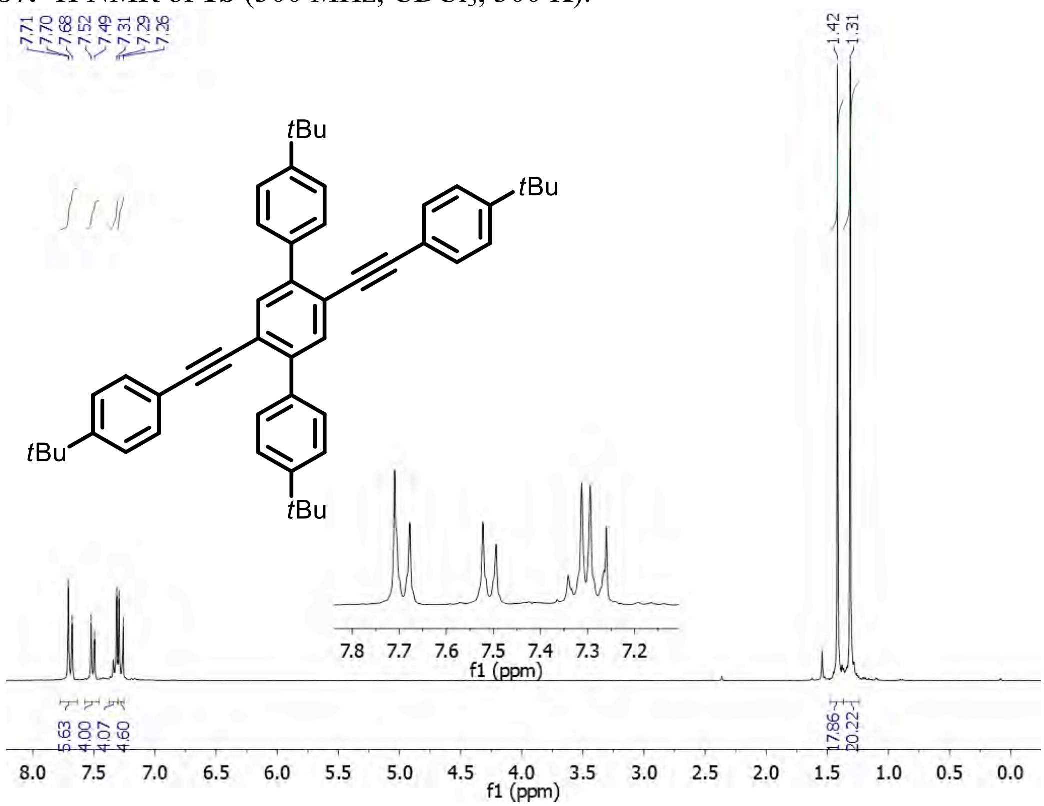



**Figure S8.** $^{13}C$ NMR of **1b** (75 MHz, $CDCl_3$, 300 K).

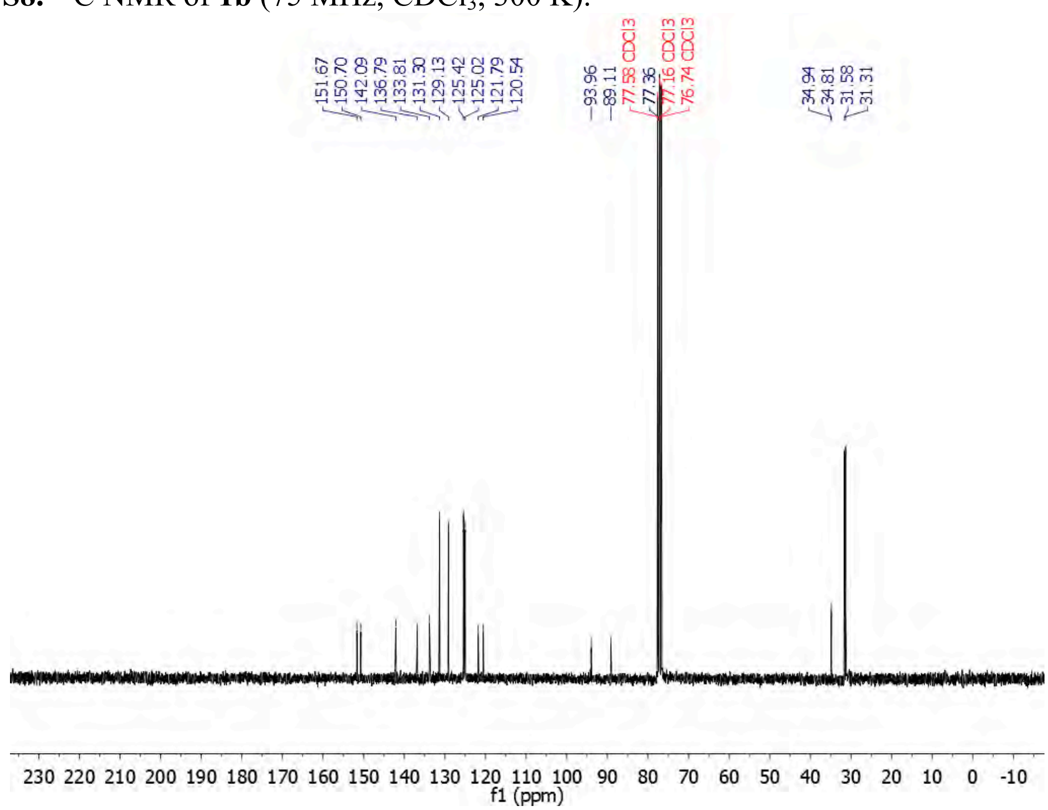


**Figure S9.** $^{1}$H NMR of **1c** (500 MHz, $CDCl_3$, 328 K).

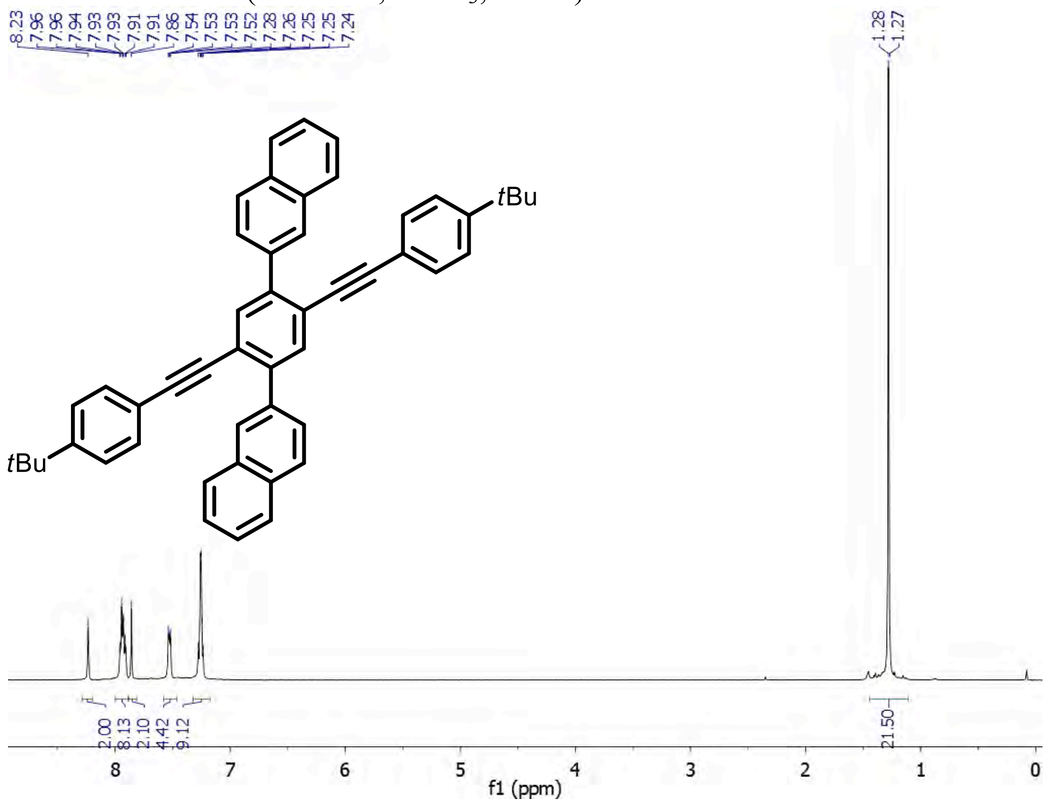



**Figure S10.** $^{13}$C NMR of **1c** (125 MHz, $CDCl_3$, 328 K).

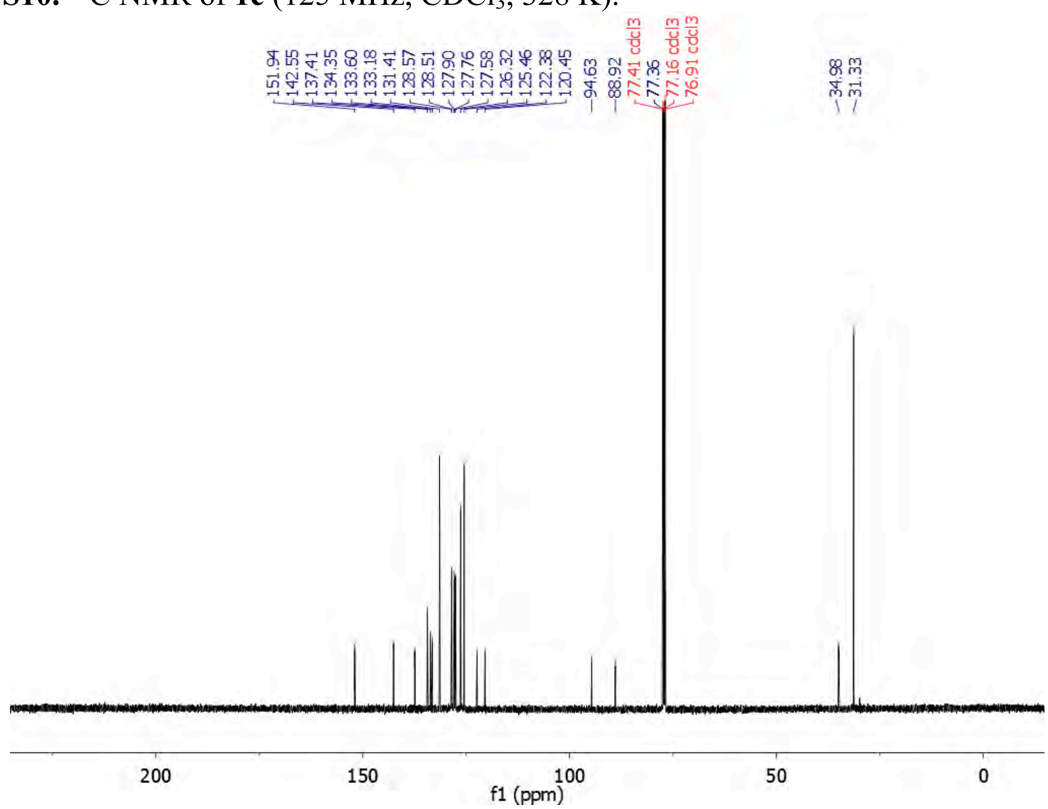


**Figure S11.** $^1$H NMR of **S5** (400 MHz, $CDCl_3$, 297 K).

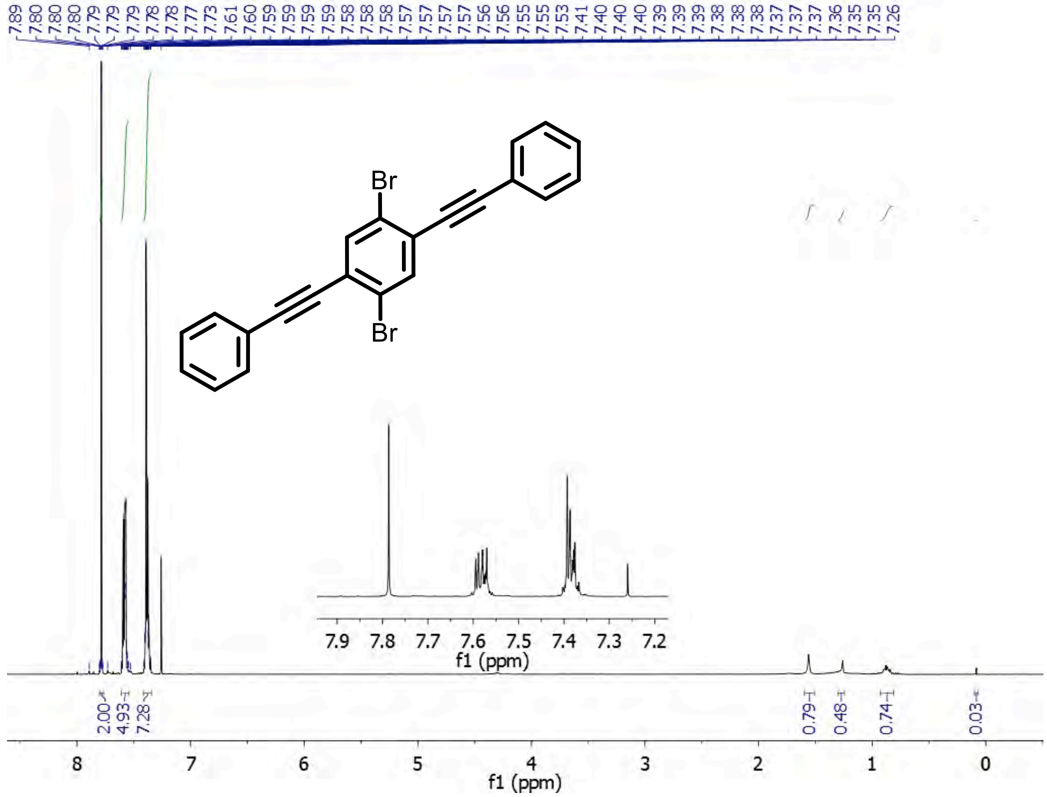



**Figure S12.** $^{13}$C NMR of **S5** (100 MHz, $CDCl_3$, 297 K).

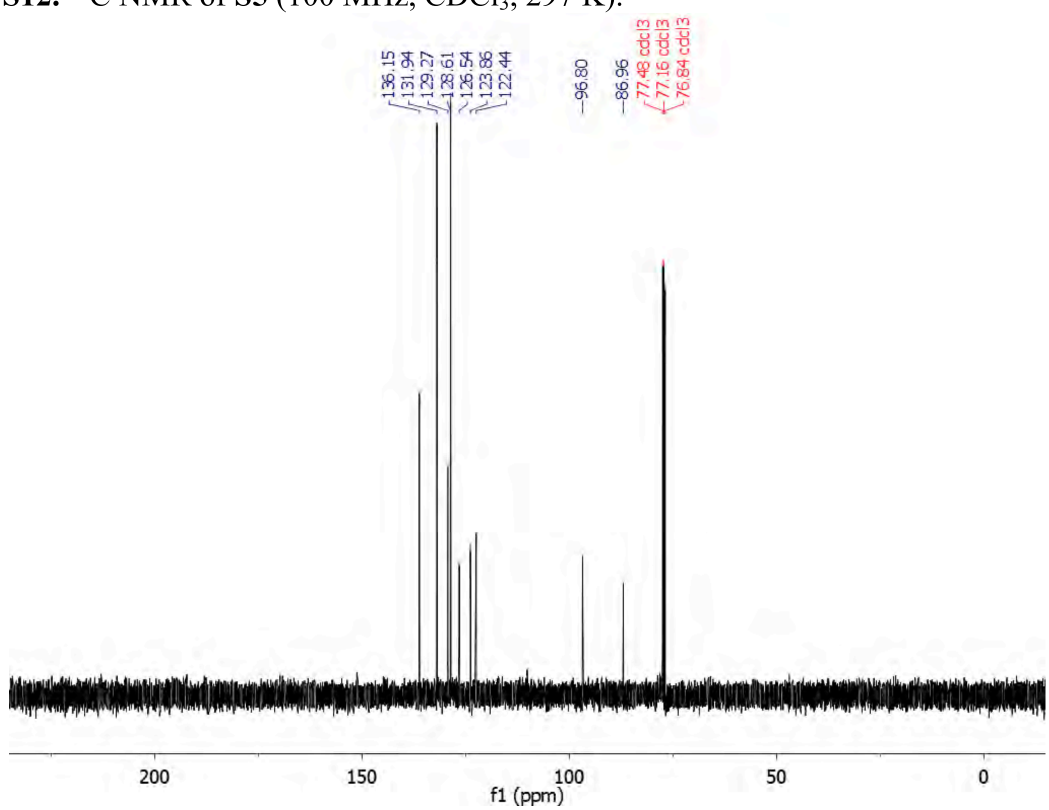


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**Figure S13.** $^{1}$H NMR of **1d** (400 MHz, $CDCl_3$, 295 K).

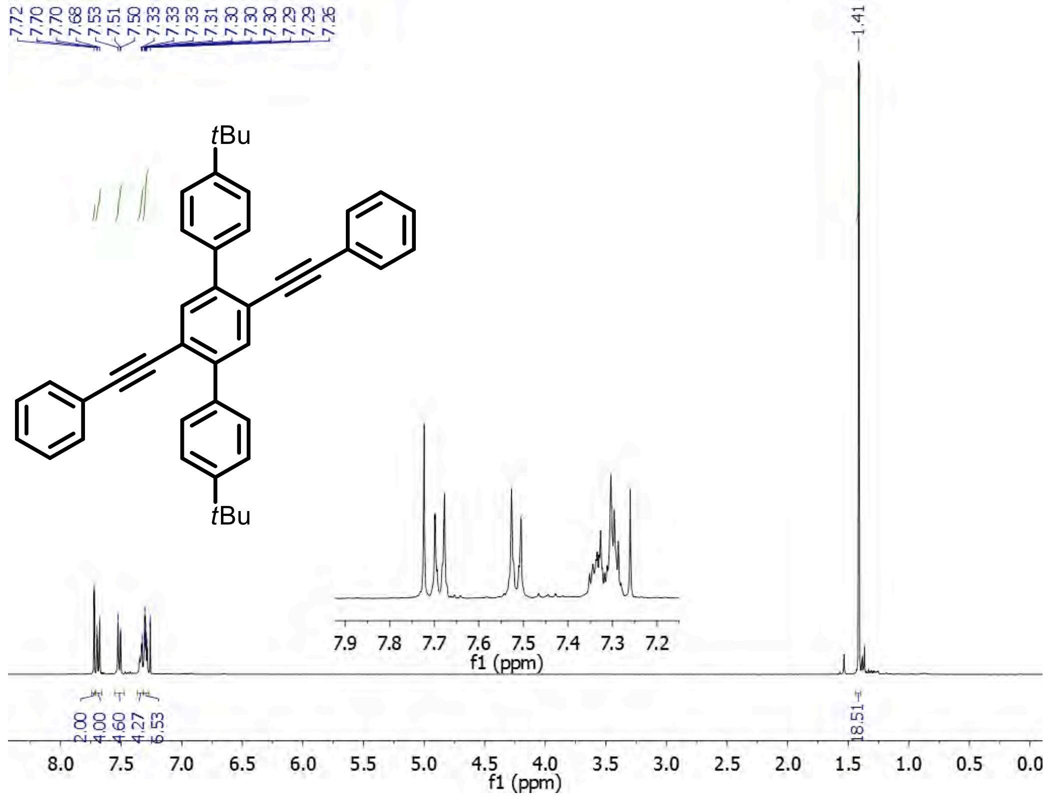


**Figure S14.** $^{13}$C NMR of **1d** (100 MHz, $CDCl_3$, 295 K).

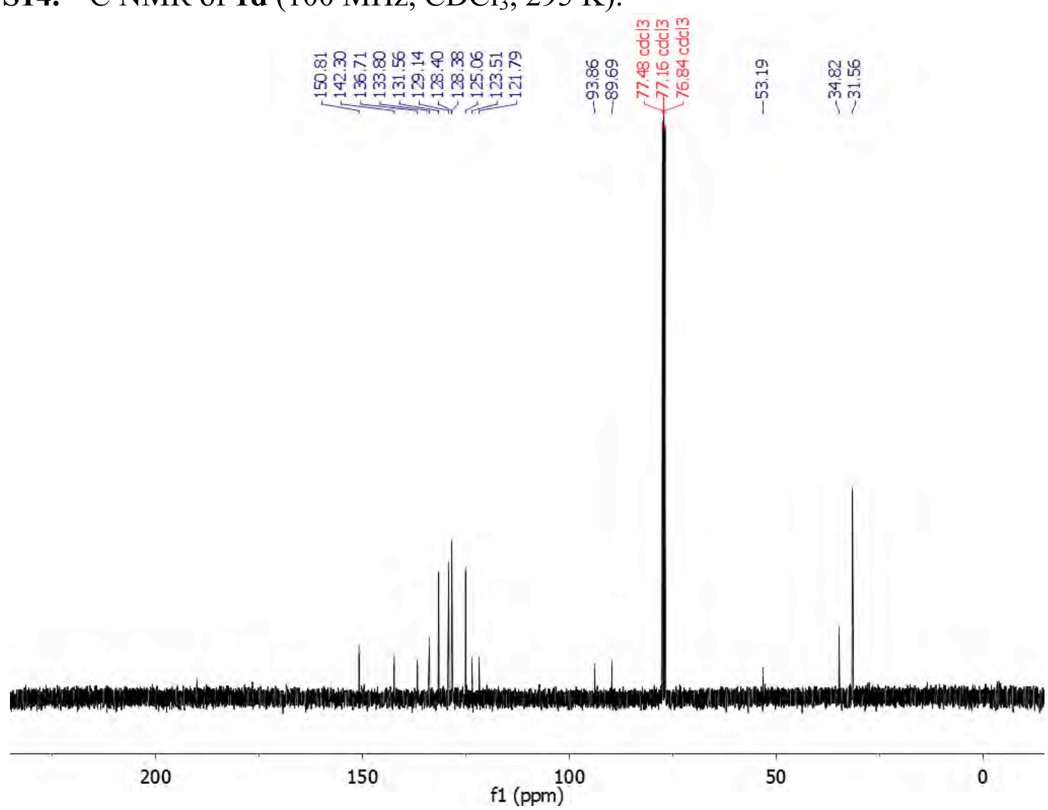

**Figure S15.** $^{1}$H NMR spectrum of **S6-$^{13}$*C$_2$*** (400 MHz, $CDCl_3$, 298 K).

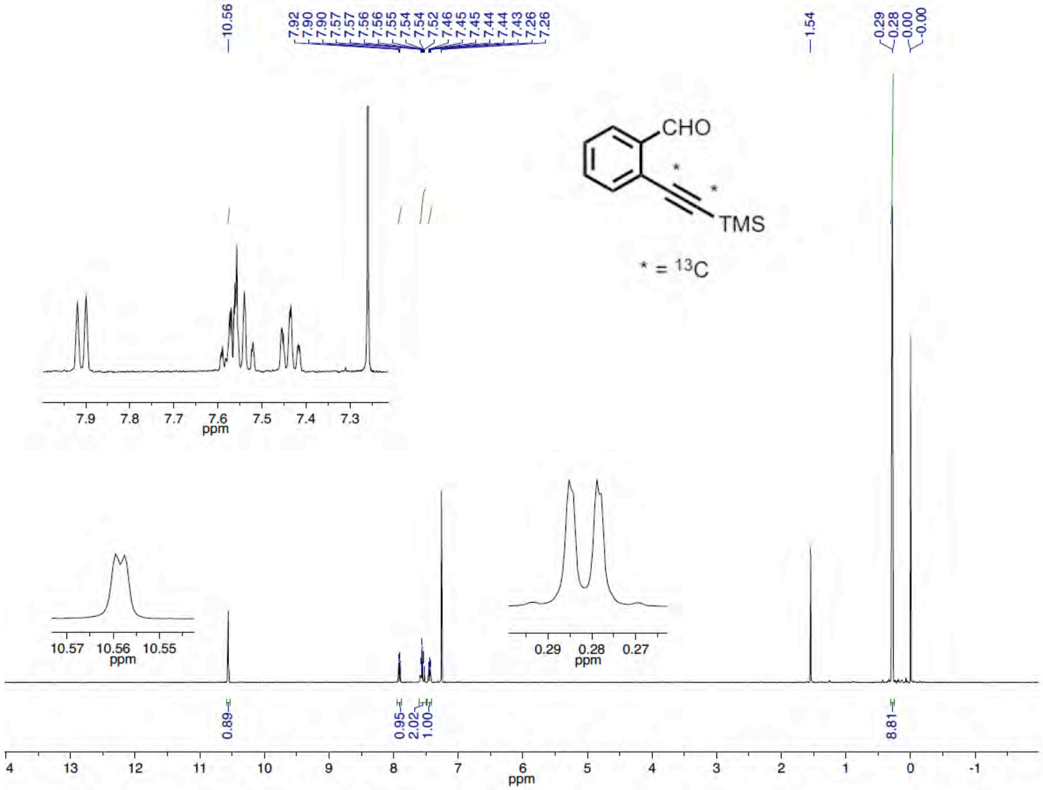


**Figure S16.** $^{13}$C NMR spectrum of **S6-$^{13}$*C$_2$*** (100 MHz, $CDCl_3$, 298 K).

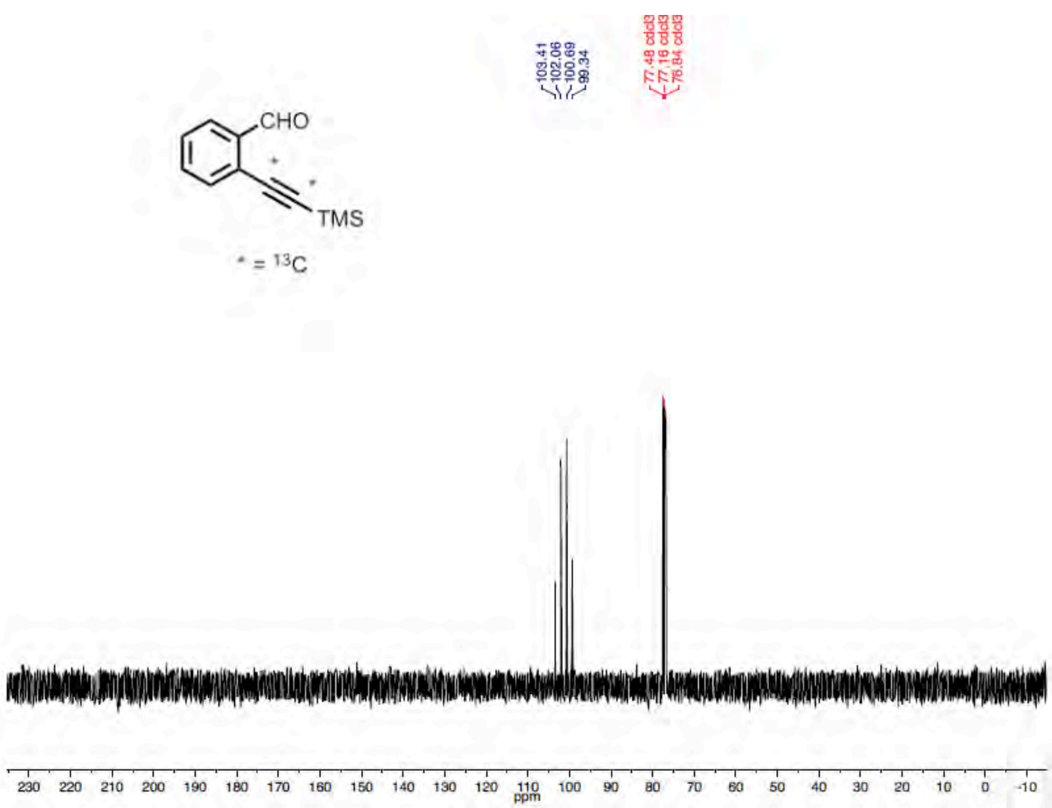

**Figure S17.** $^{1}$H NMR spectrum of **S7-$^{13}C_2$** (400 MHz, $CDCl_3$, 298 K).

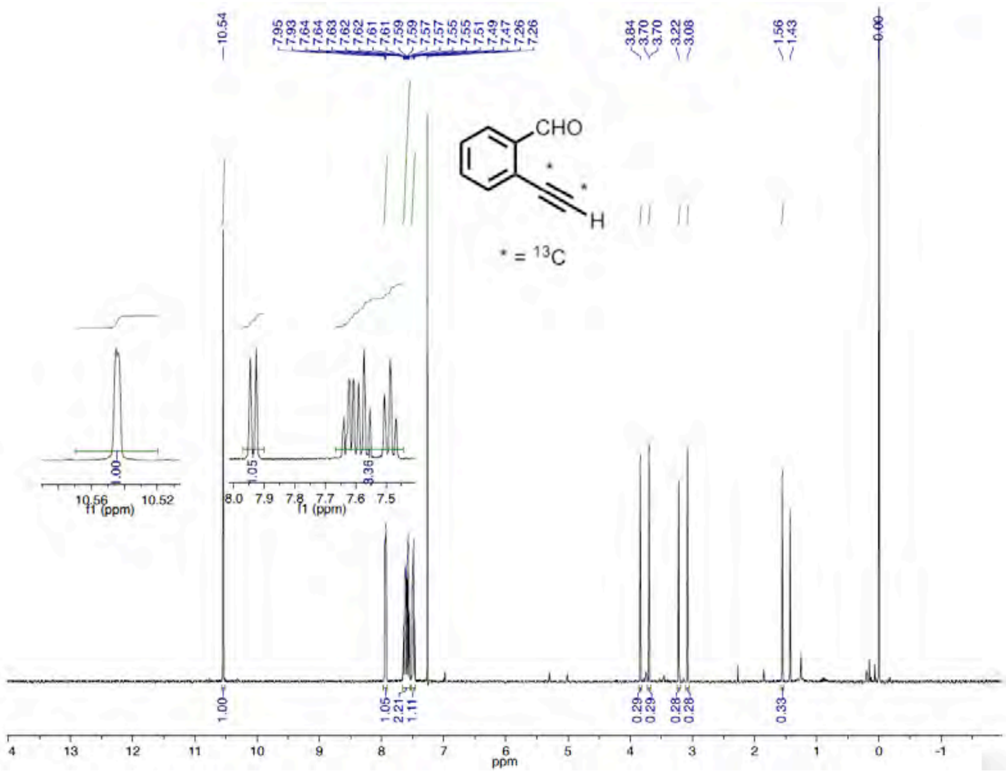

**Figure S18.** $^{13}$C NMR spectrum of **S7-$^{13}C_2$** (100 MHz, $CDCl_3$, 298 K).

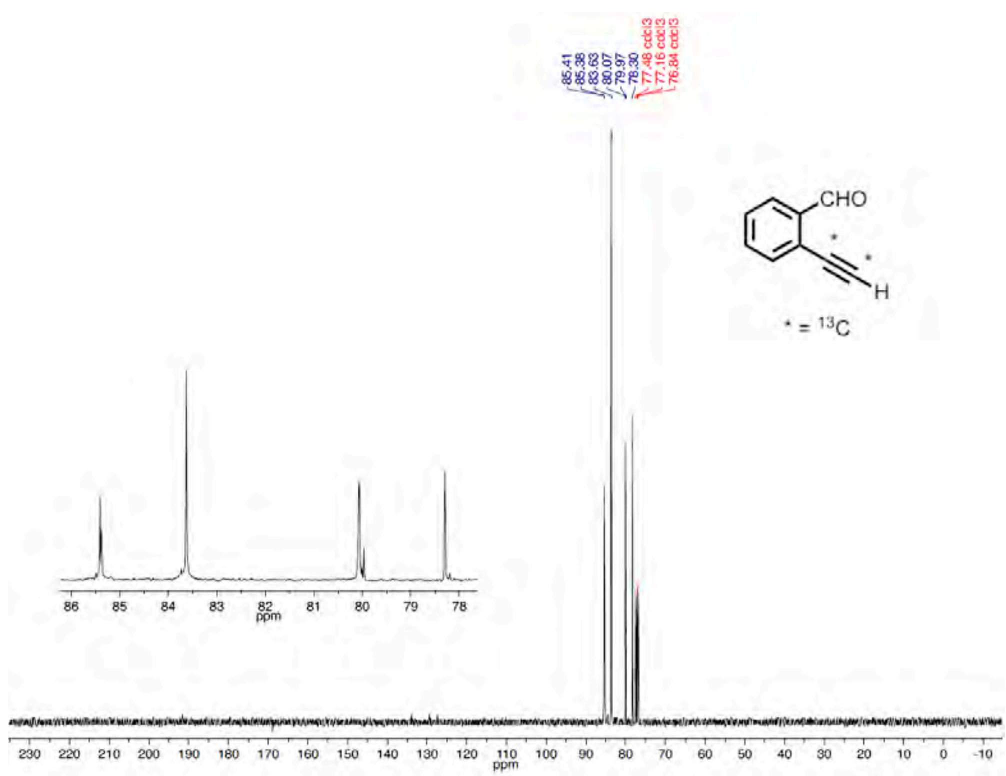

**Figure S19.** $^{1}$H NMR spectrum of **2-$^{13}C_2$** (400 MHz, $CDCl_3$, 298 K).

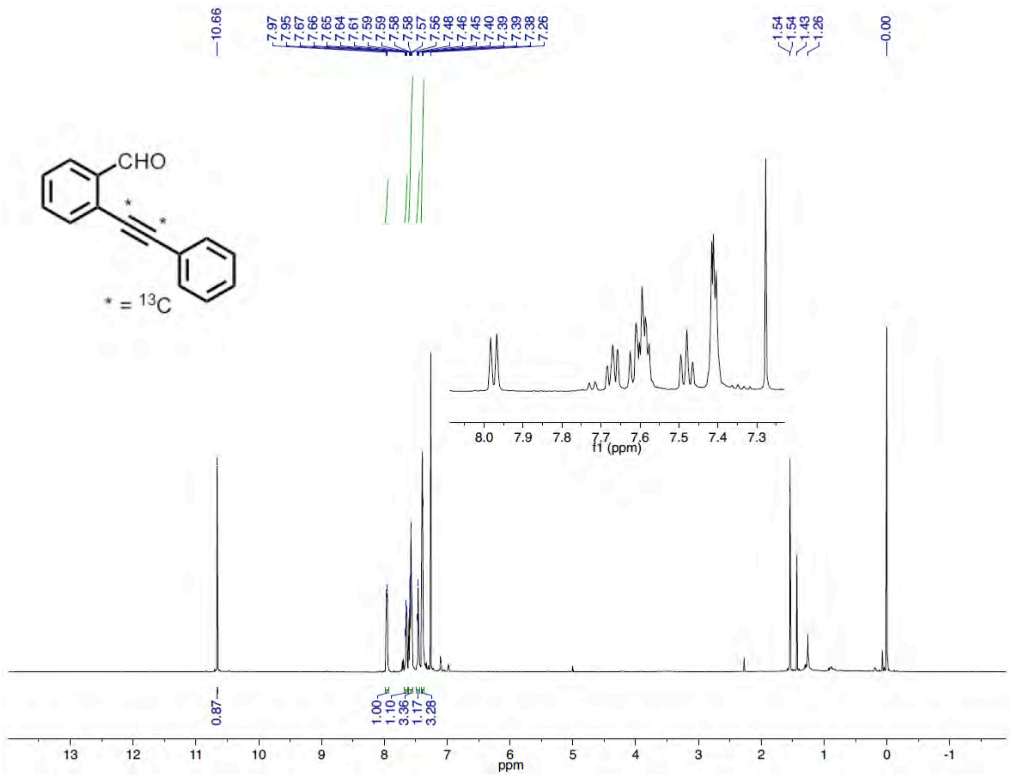

**Figure S20.** $^{13}$C NMR spectrum of **2-$^{13}C_2$** (100 MHz, $CDCl_3$, 298 K).

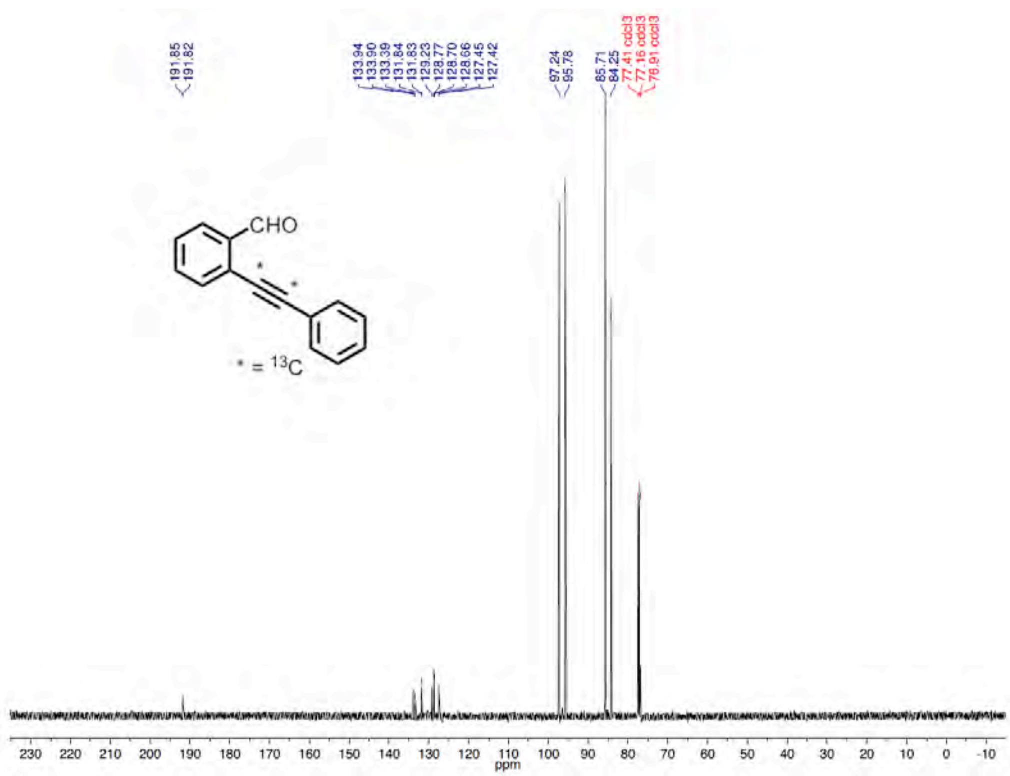

**Figure S21.** $^{1}$H NMR of **3a** (500 MHz, $CDCl_3$, 298 K).

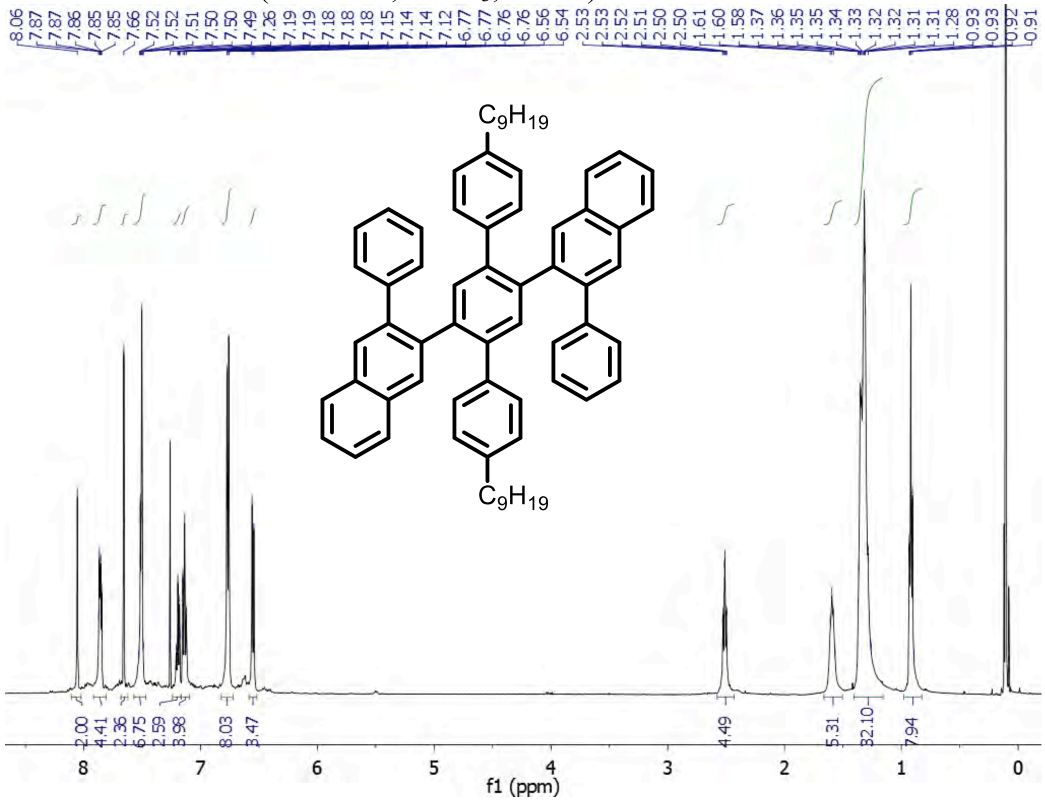


**Figure S22.** $^{13}$C NMR of **3a** (125 MHz, $CDCl_3$, 298 K).

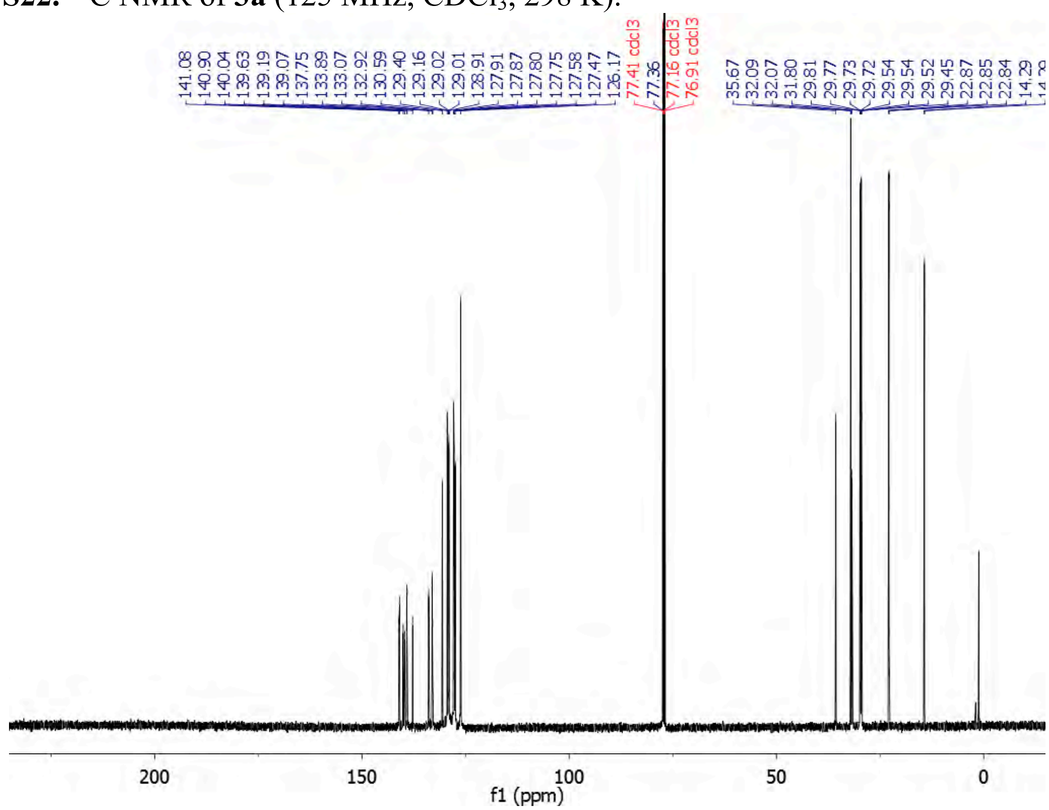

**Figure S23.** [1]H NMR spectrum of **3a-*13C2*** (500 MHz, $CDCl_3$, 298 K).

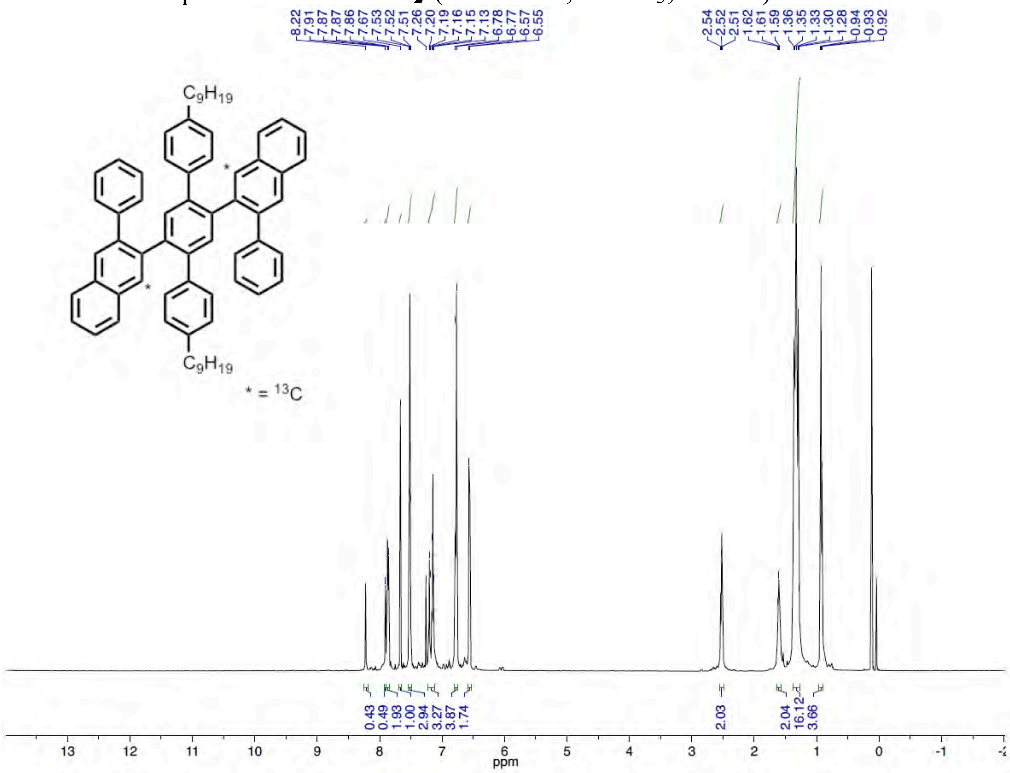

**Figure S24.** Partial [1]H NMR spectra (500 MHz, $CDCl_3$, 298K) of **3a** and **3a-*13C2*** that indicate [13]C-[1]H coupling at the labeled position.

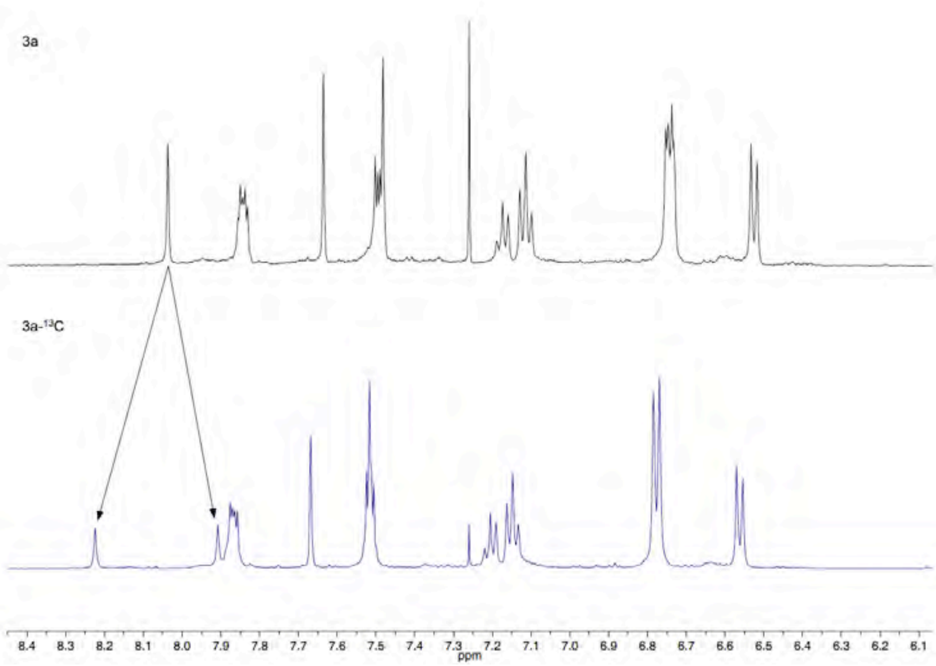

**Figure S25.** $^{13}$C NMR spectrum of **3a-*$^{13}C_2$*** (125 MHz, $CDCl_3$, 298 K).

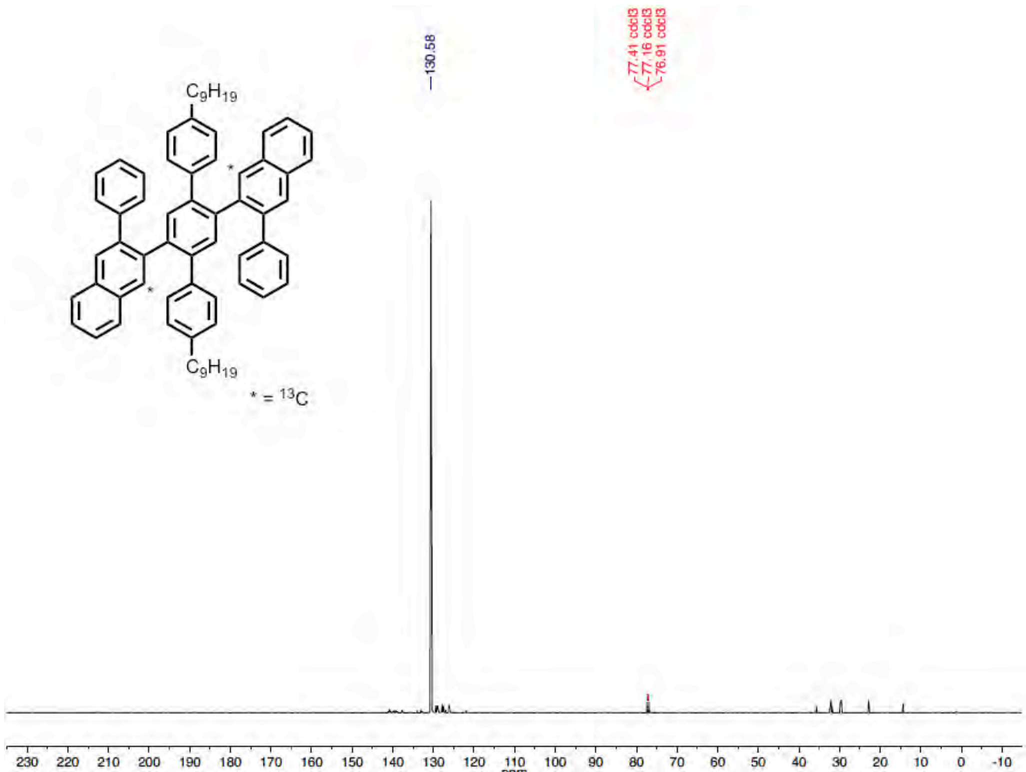

**Figure S26.** $^{1}$H NMR of **3b** (400 MHz, $CDCl_3$, 297 K).

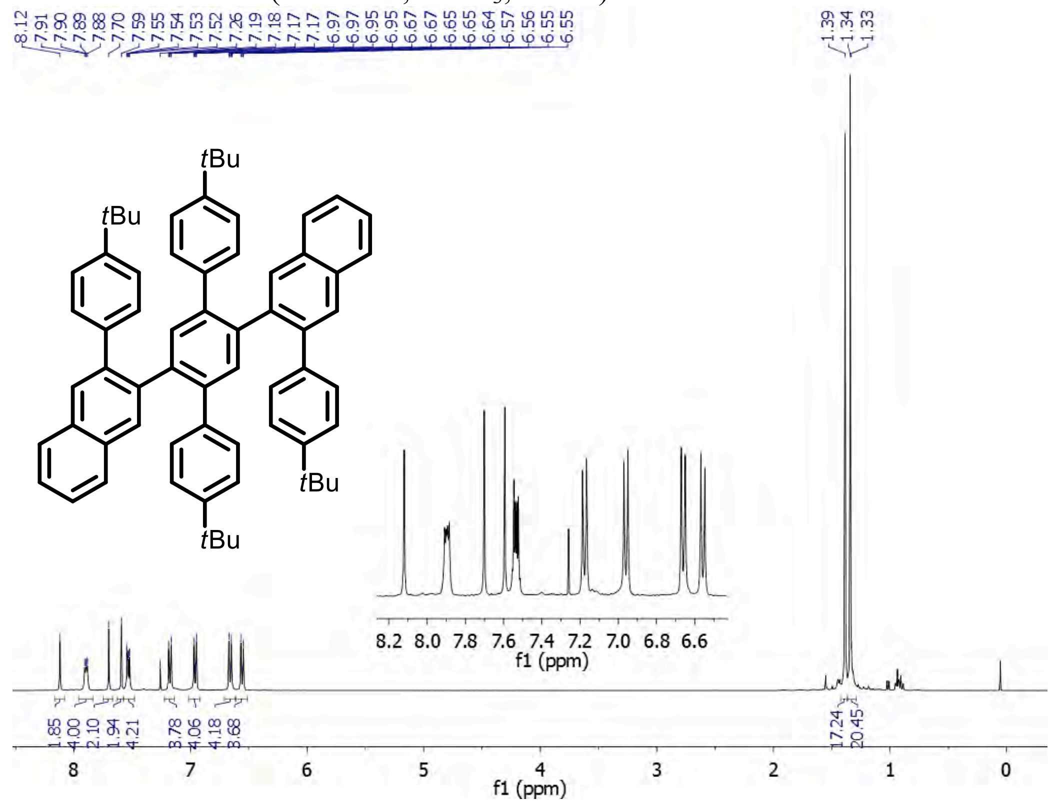


**Figure S27.** $^{13}$C NMR of **3b** (100 MHz, $CDCl_3$, 297 K).

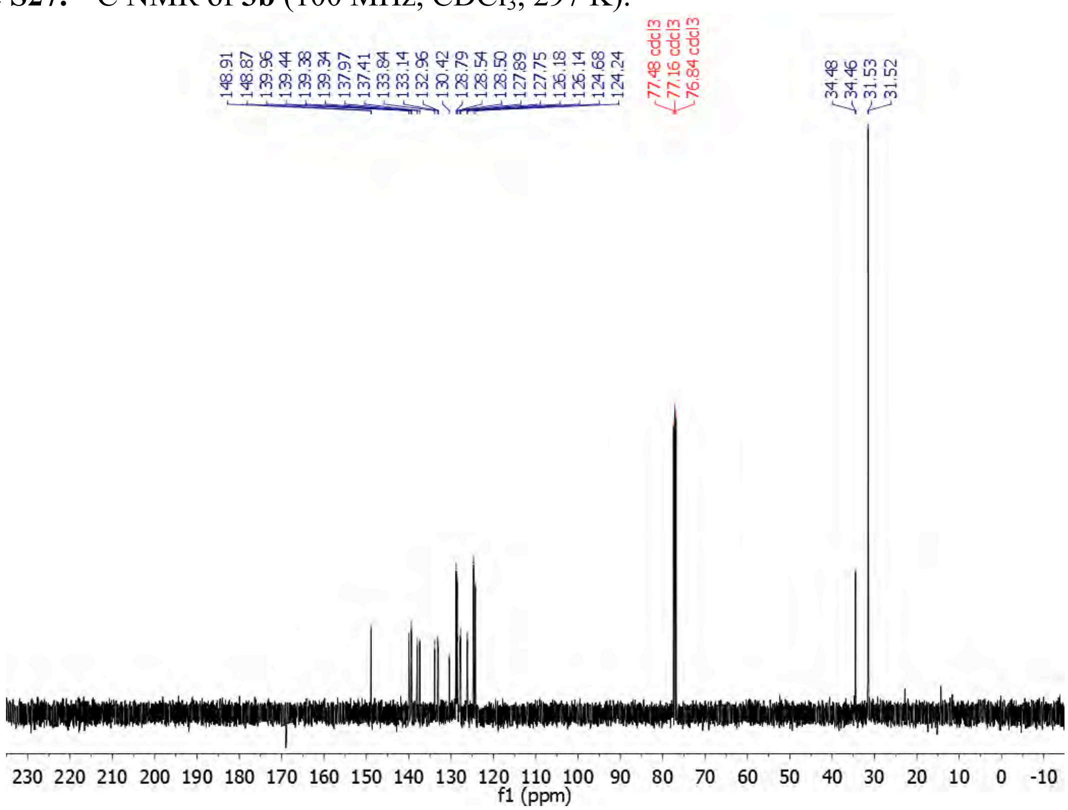

**Figure S28.** $^{1}$H NMR of **3c** (400 MHz, $CDCl_3$, 295 K).

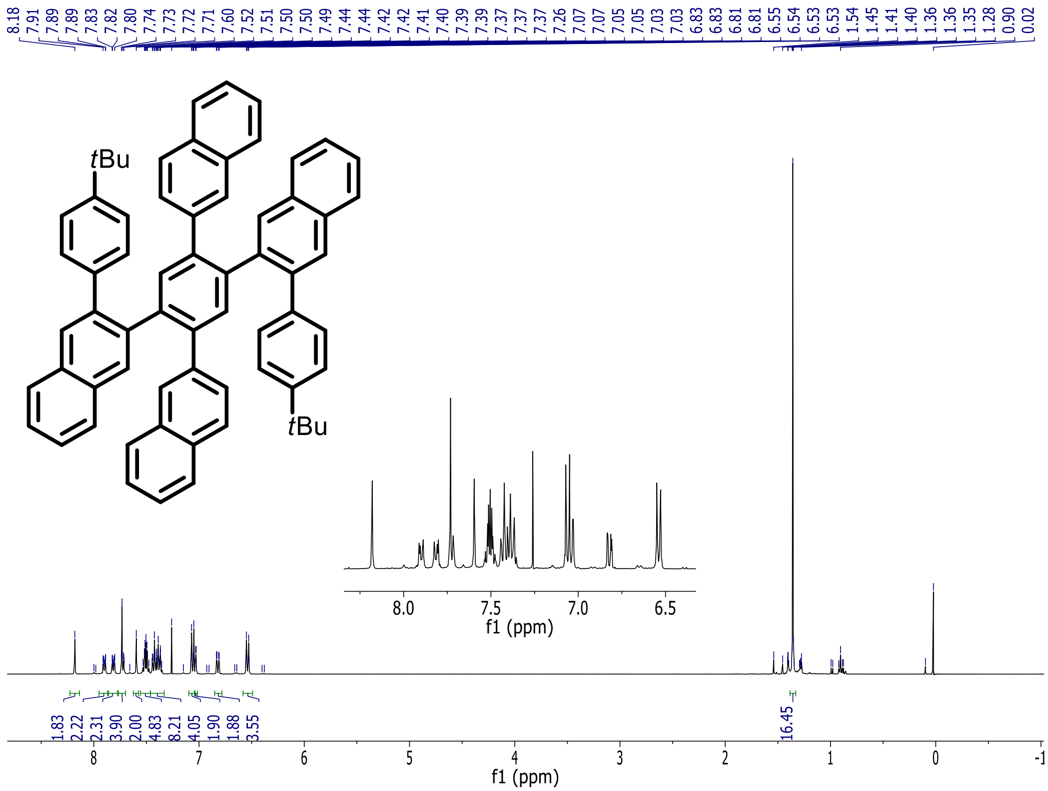


**Figure S29.** $^{13}$C NMR of **3c** (100MHz, $CDCl_3$, 295 K).

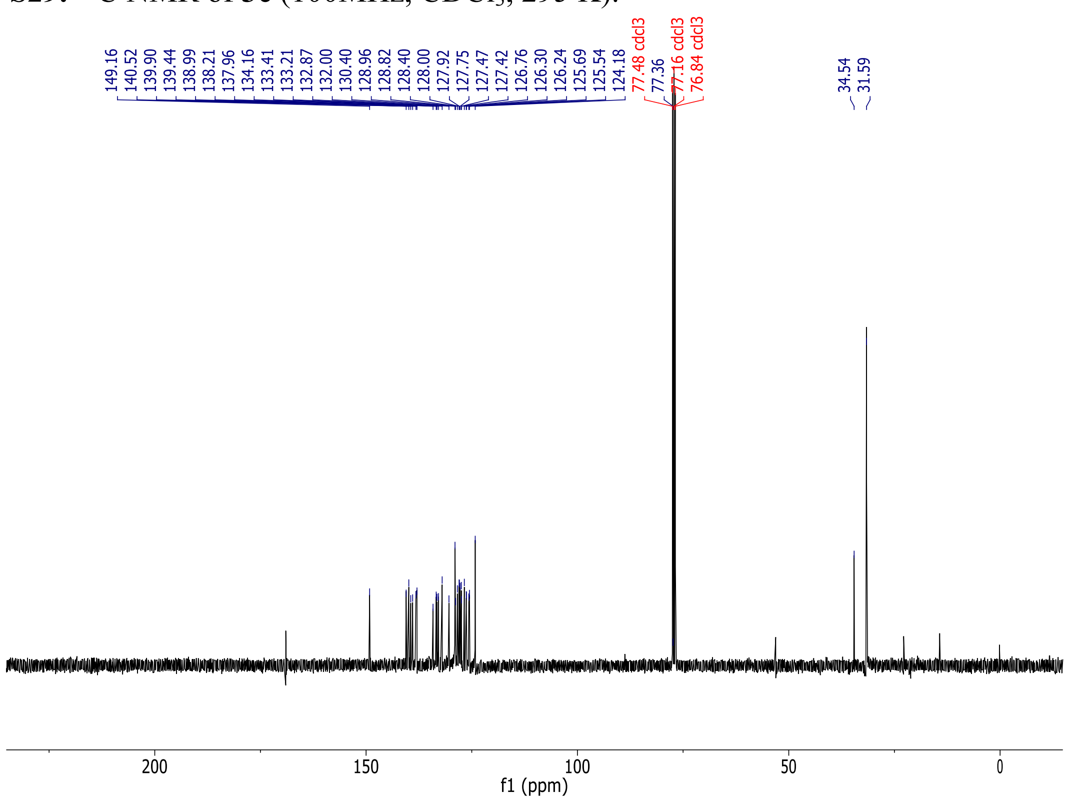

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**Figure S30.** $^{1}$H NMR of **3d** (400 MHz, $CDCl_3$, 295 K).

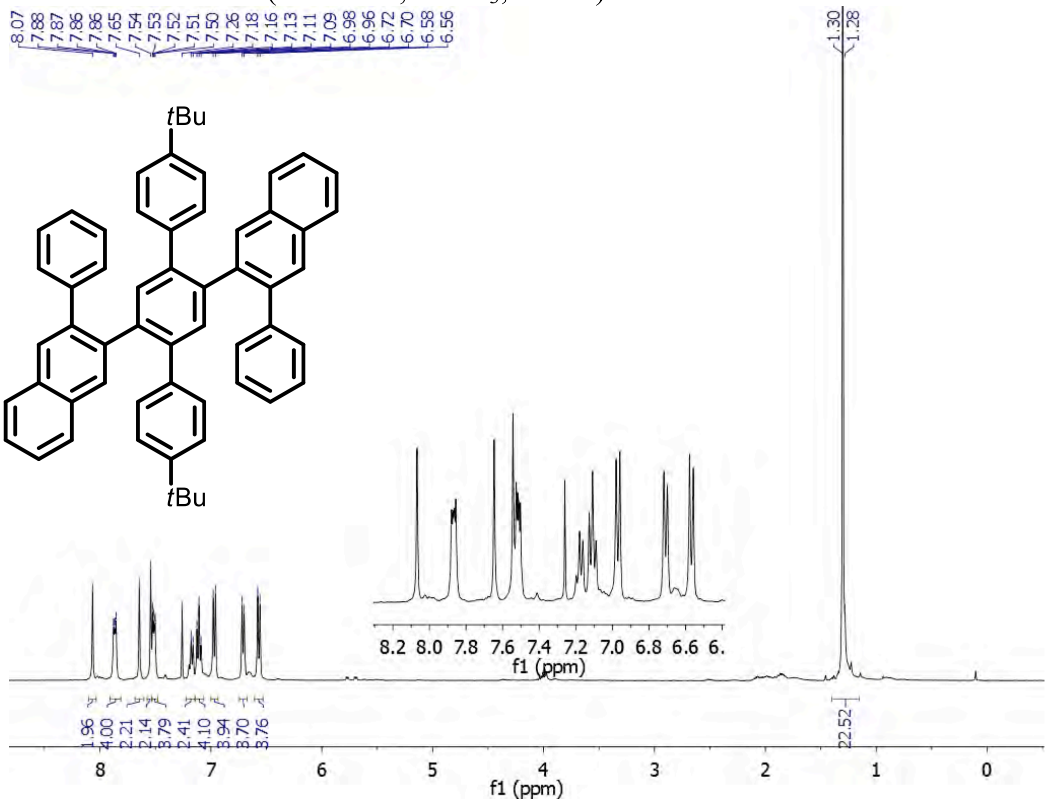

**Figure S31.** $^{13}$C NMR of **3d** (100MHz, $CDCl_3$, 295 K).

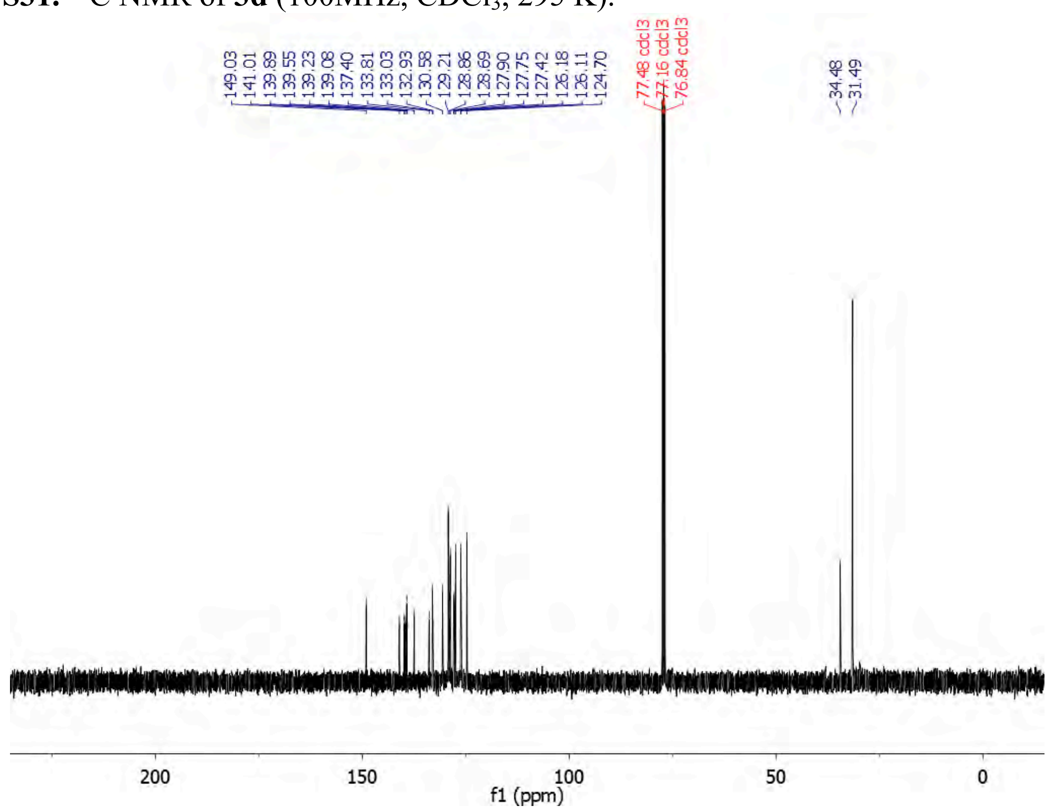

**Figure S32.** $^{1}$H NMR of **4a** (500 MHz, $CDCl_3$, 295 K).

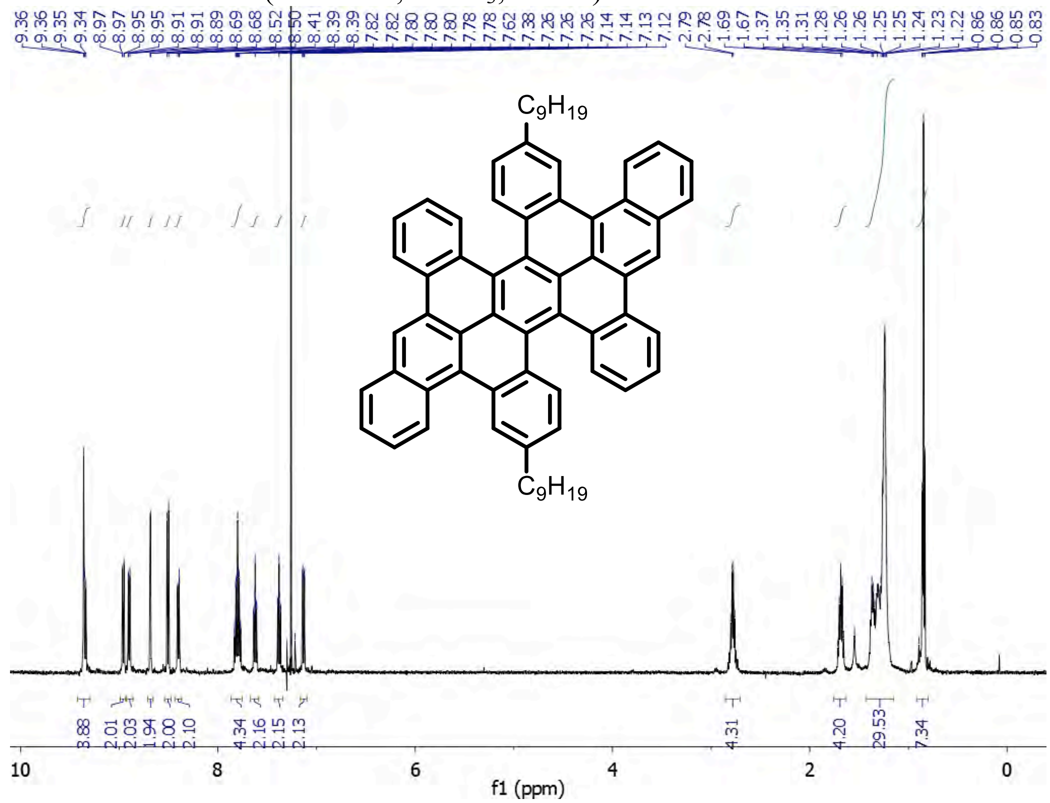

**Figure S33.** $^{13}$C NMR of **4a** (125 MHz, $CDCl_3$, 295 K).

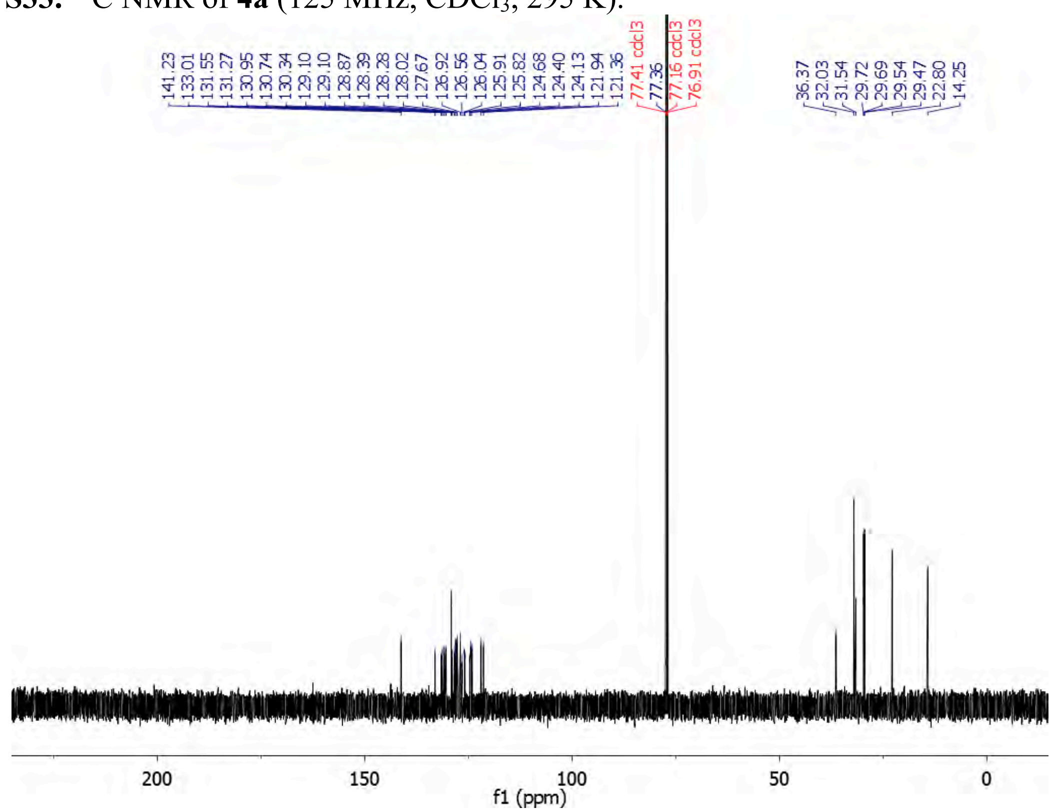

**Figure S34.** $^{1}$H NMR of **4b** (500 MHz, $CDCl_3$, 295 K).

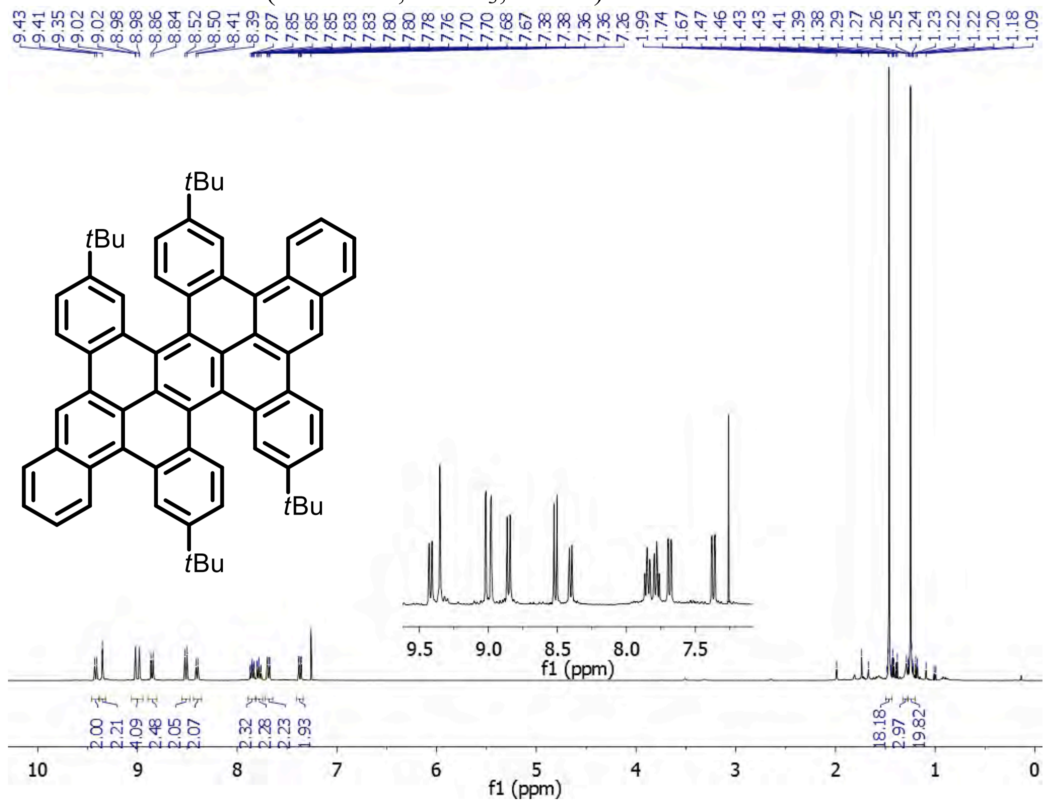


**Figure S35.** $^{13}$C NMR of **4b** (125 MHz, $CDCl_3$, 295 K).

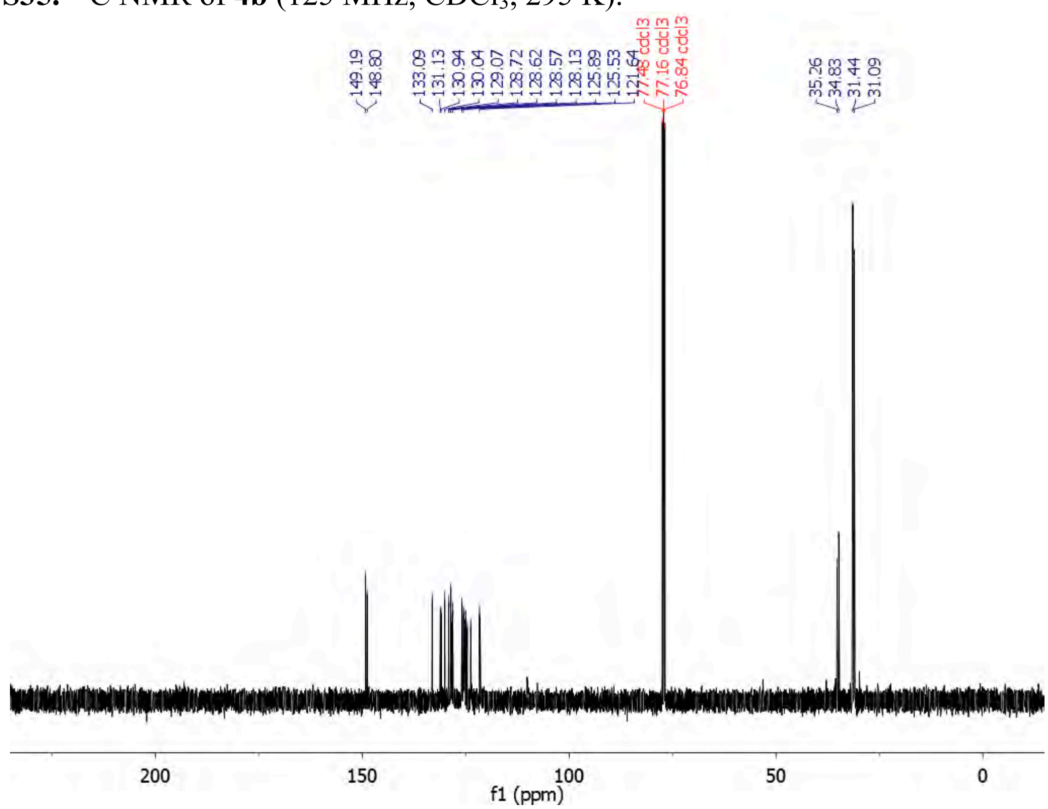

**Figure S36.** $^{1}$H NMR of **4c** (500 MHz, $CDCl_3$, 298 K).

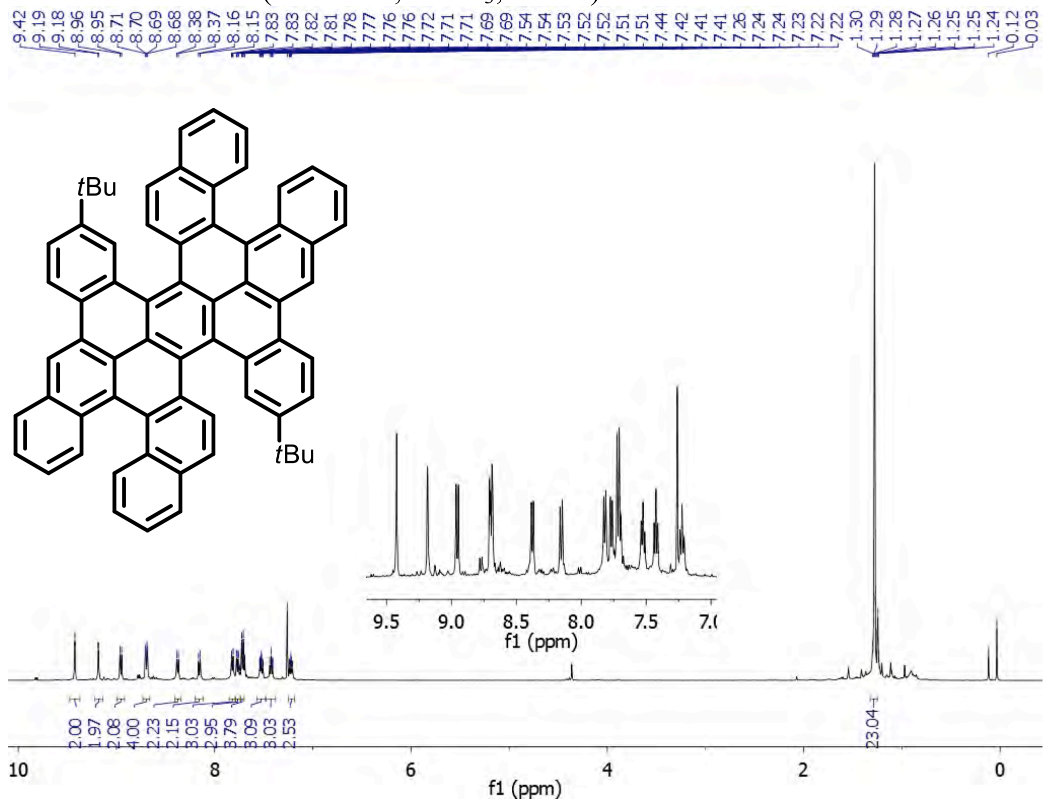


**Figure S37.** $^{13}$C NMR of **4c** (125 MHz, $CDCl_3$, 298 K).

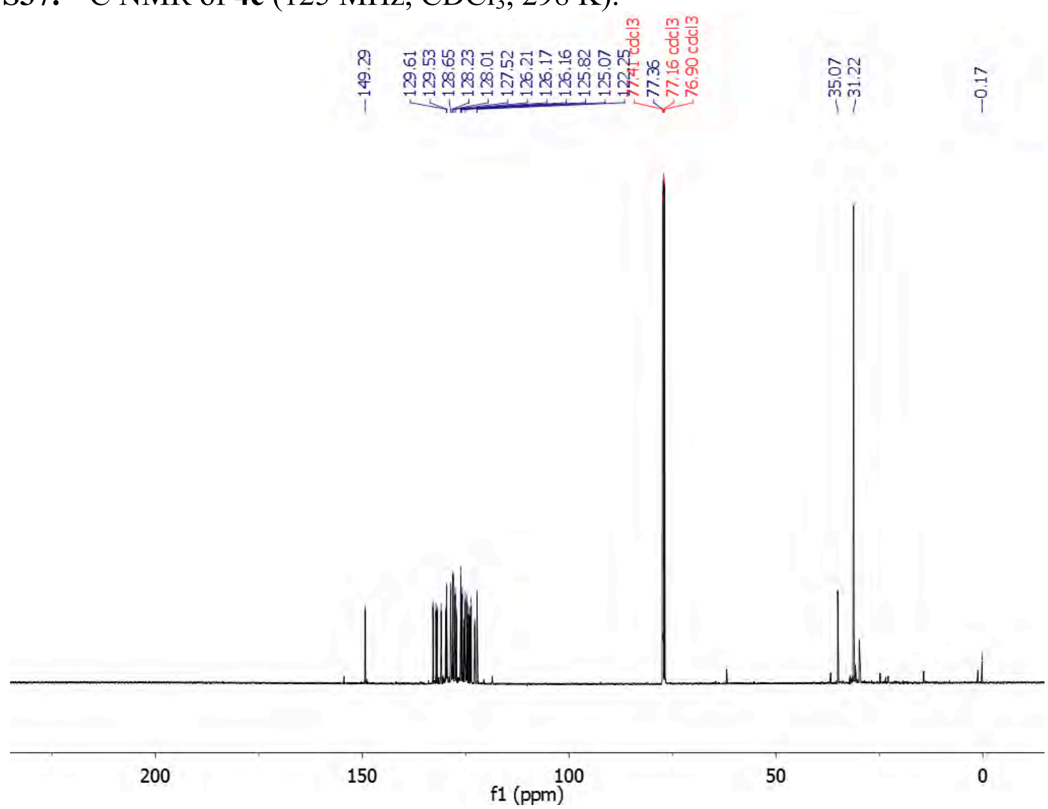

**Figure S38.** $^{1}$H NMR of **5a** (300 MHz, *o*-$C_6D_4Cl_2$, 353 K).

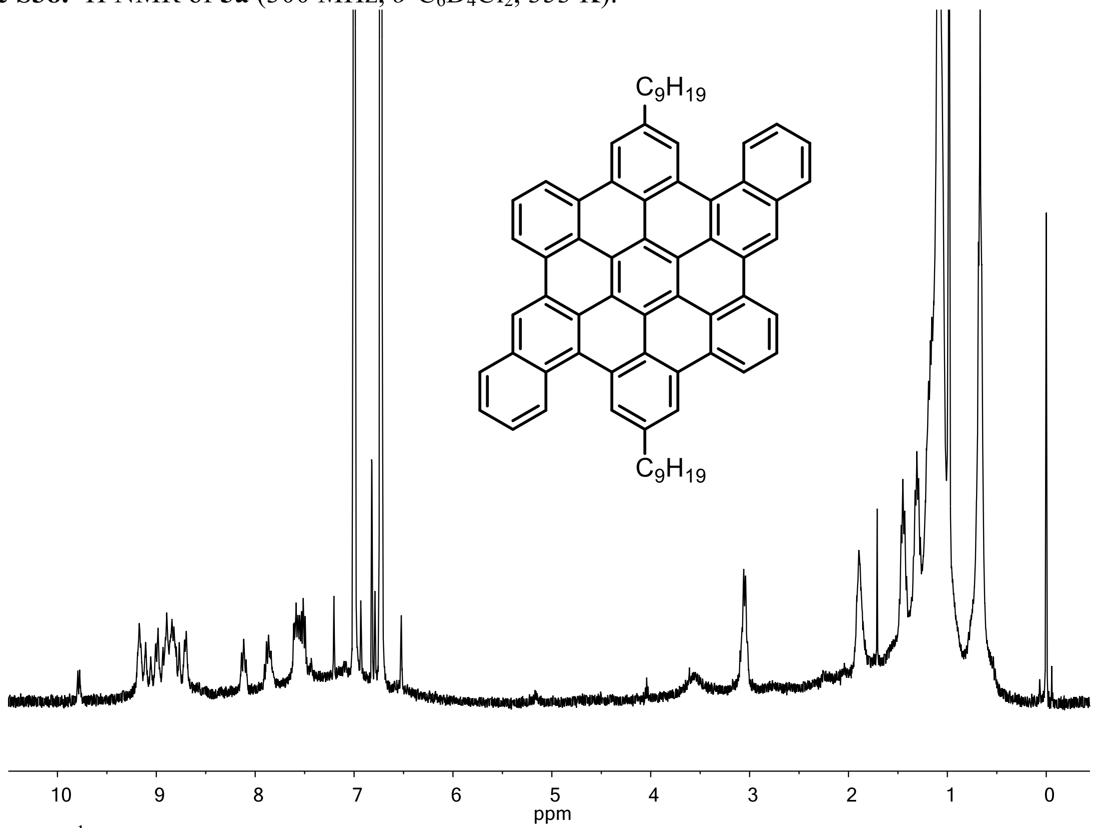


**Figure S39.** $^{1}$H NMR of **5a** (300 MHz, *o*-$C_6D_4Cl_2$, 353 K), aromatic region.

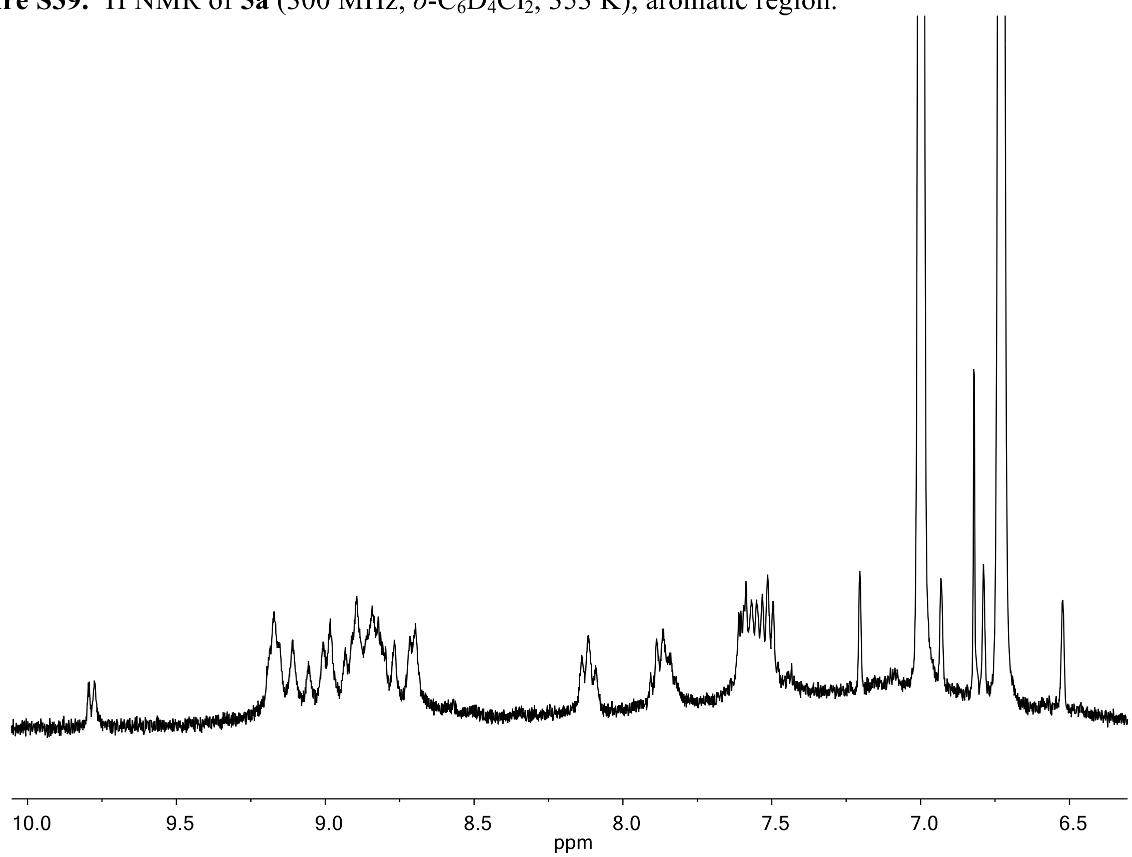

**Figure S40.** $^{13}C$ NMR of **5a** (75 MHz, 2:1 $CS_2$:$CD_2Cl_2$, 298 K).

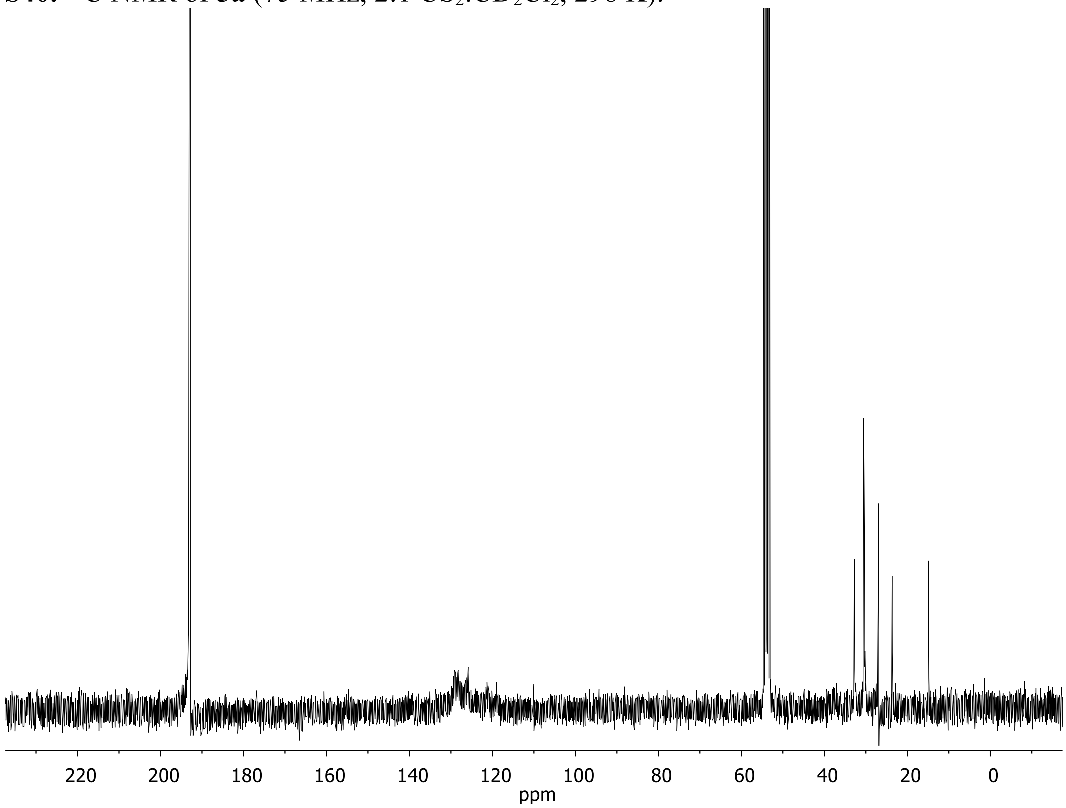

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**Figure S41.** $^{1}$H NMR spectrum of **5a-$^{13}$*C*$_2$** (500 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

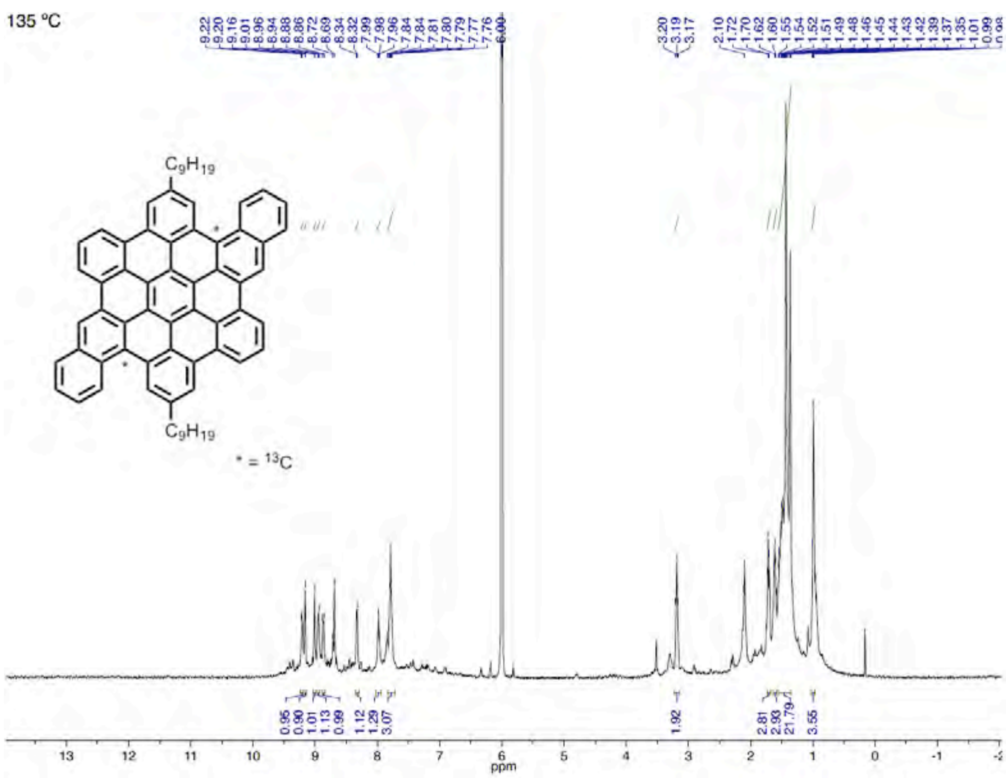



**Figure S42.** $^{1}$H NMR spectrum of **5a-$^{13}$*C*$_2$** (500 MHz, 1,2-$C_2H_2Cl_4$, 408 K). 1H signal assignment of aromatic region.

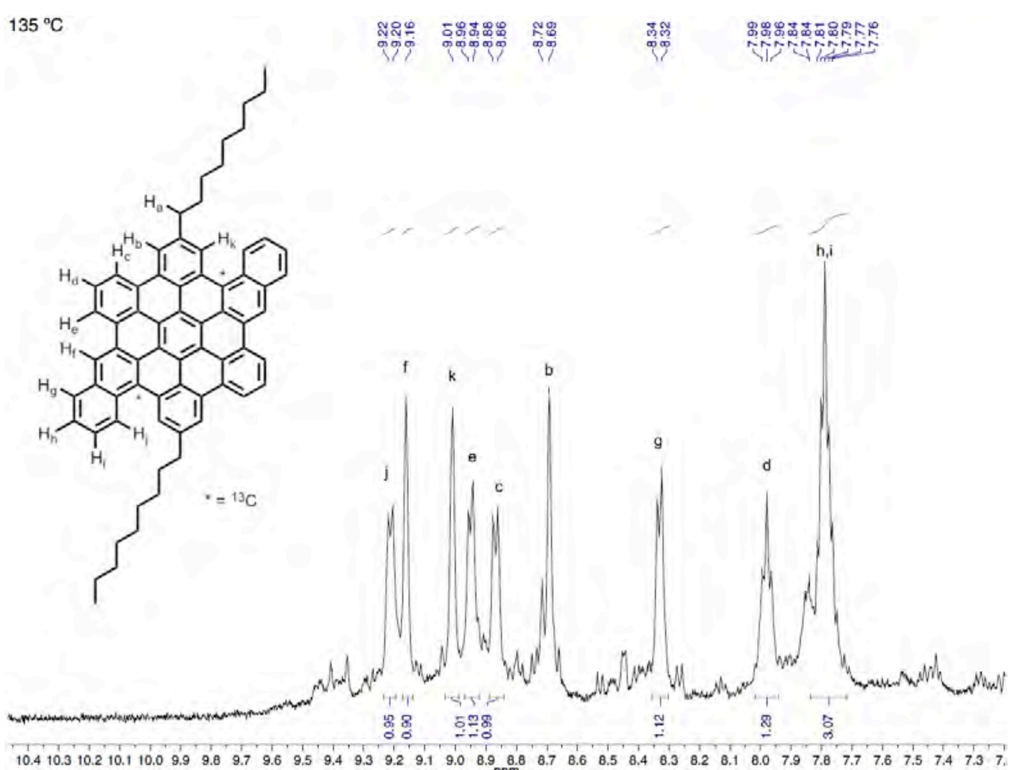
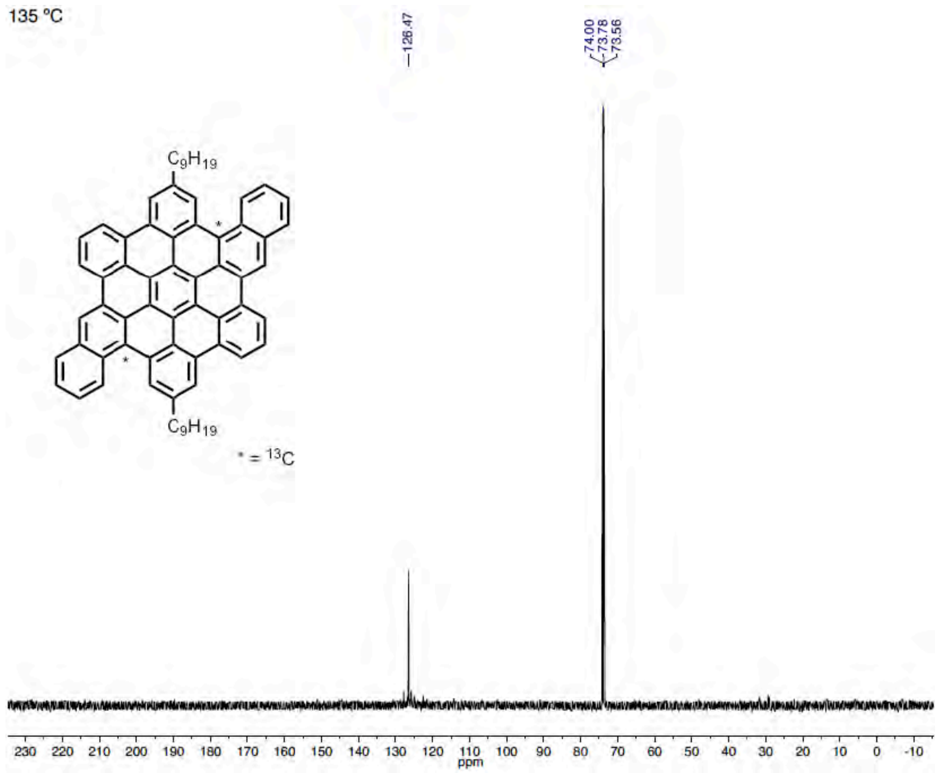
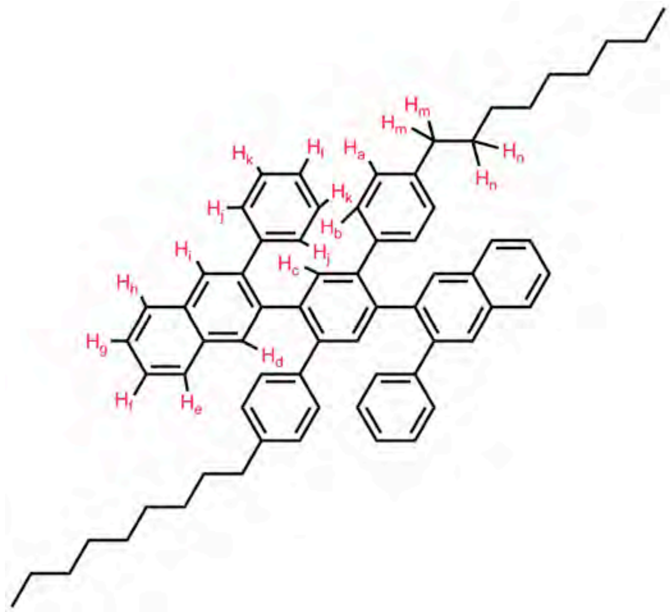


**Figure S43.** $^{13}$C NMR spectrum of **5a-*$^{13}$C$_2$***. (125 MHz, 1,2-$C_2H_2Cl_4$, 408 K)



## D. 2D NMR Spectra and Structural Assignments of Selected Compounds

**Peak assignments for the compound 3a:**




The peak corresponding to the proton $H_d$ was assigned using the COESY and ROESY spectra (full assignments below). This is the proton signal that splits into two signals in the $^{13}$C-labeled benzannulated compound **$^{13}C_2$-3a** (Figure S24) due to the proton-carbon coupling.

**Figure S44.** Full COSY spectrum of **3a** (500 MHz, 500 MHz, $CDCl_3$, 295 K).

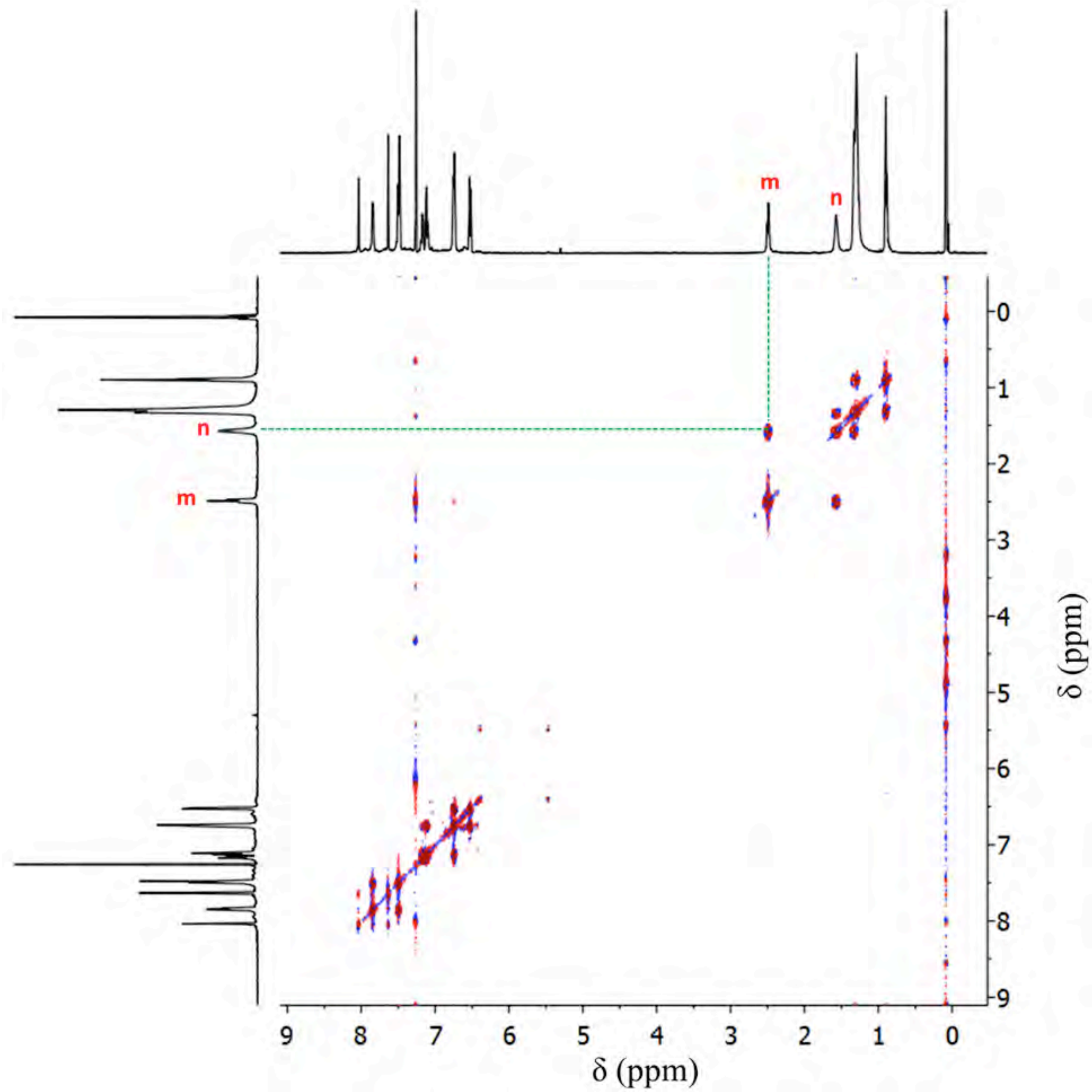


**Figure S45.** Partial COSY spectrum of **3a** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 295 K).

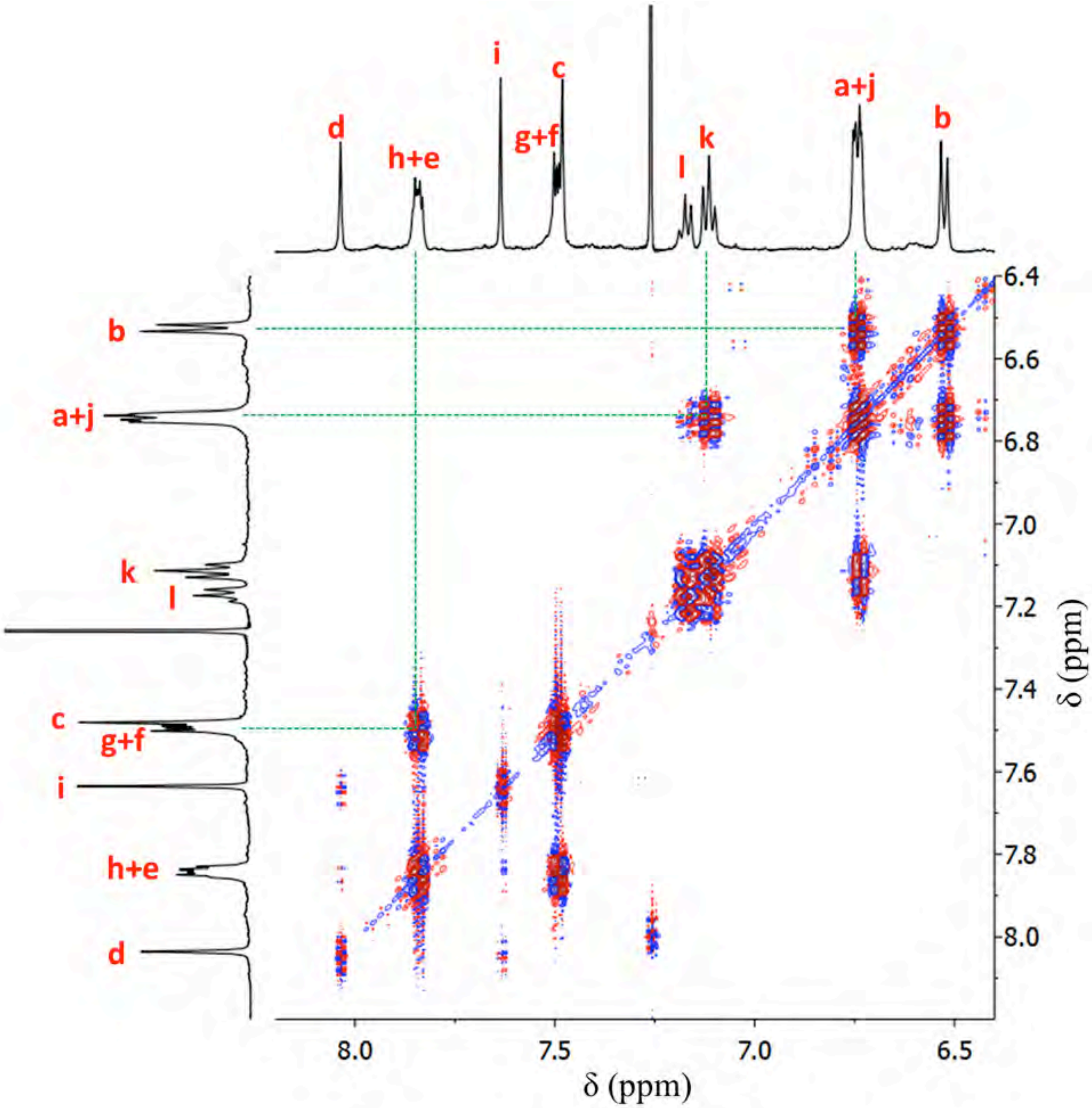


**Figure S46.** Full ROESY spectrum of **3a** (500 MHz, 500 MHz, $CDCl_3$, 295 K).

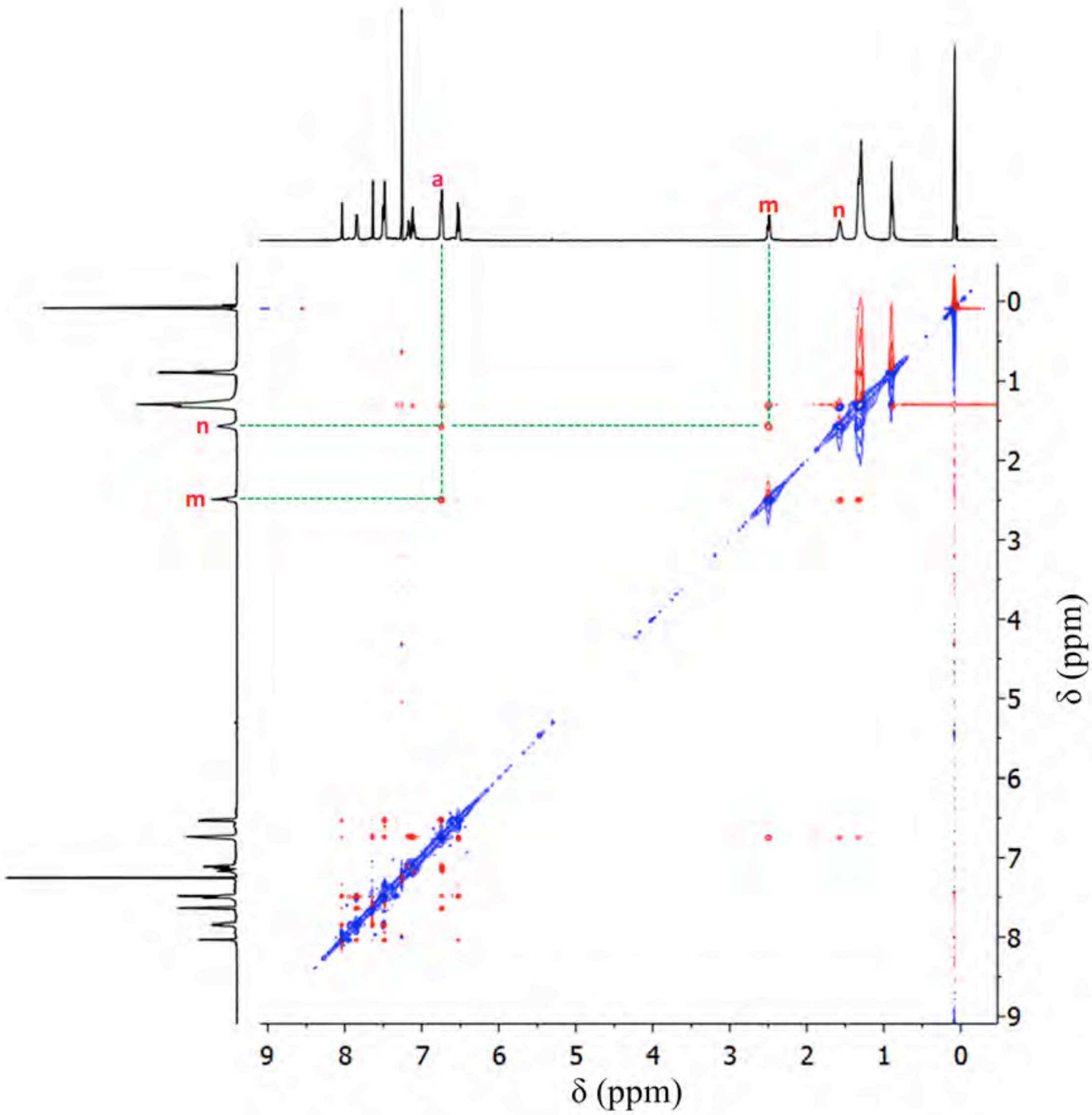


**Figure S47.** Partial ROESY spectrum of **3a** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 295 K).

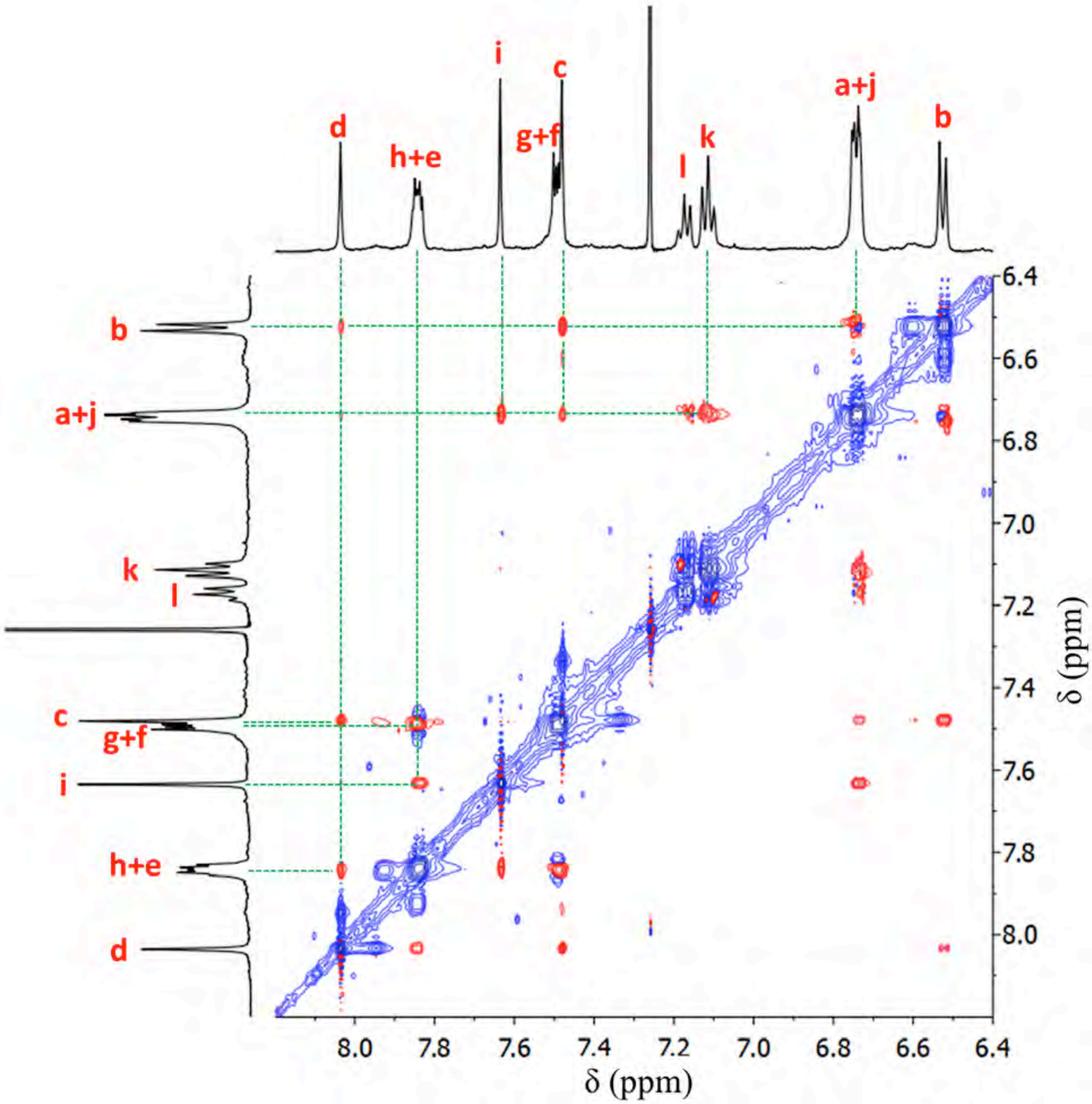


**Figure S48.** Full HSQC spectrum of **3a** (500 MHz, 125 MHz, $CDCl_3$, 295 K).

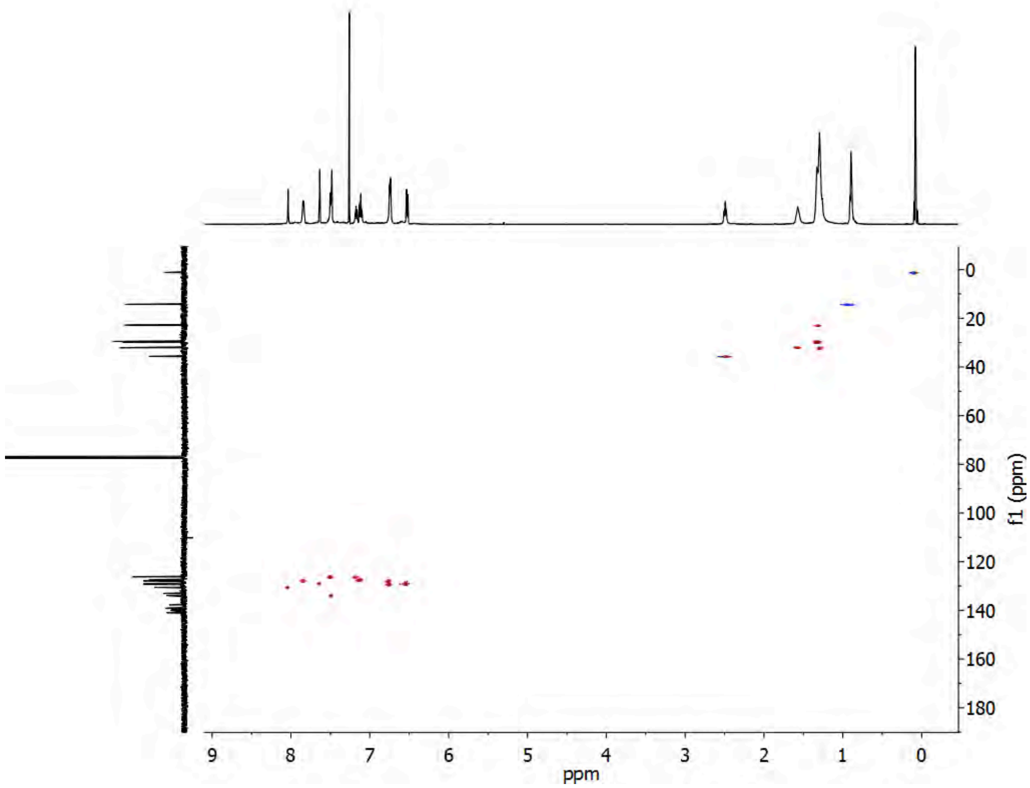



**Figure S49.** Partial HSQC spectrum of **3a** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 295 K).

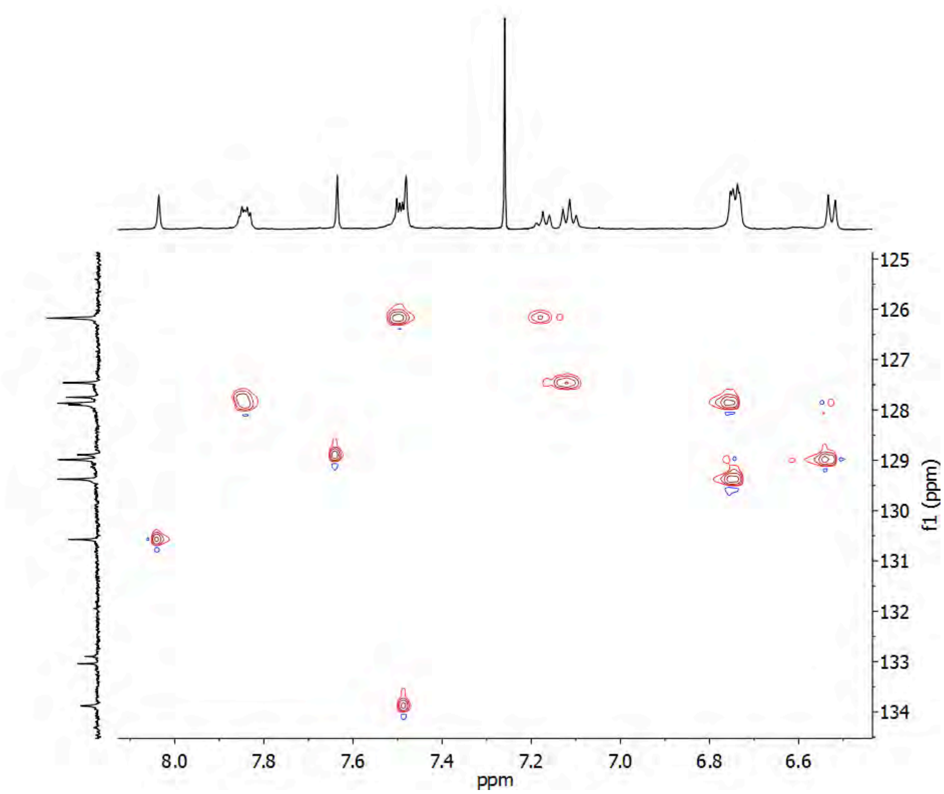


**Figure S50.** Full HMBC spectrum of **3a** (500 MHz, 125 MHz, $CDCl_3$, 295 K).

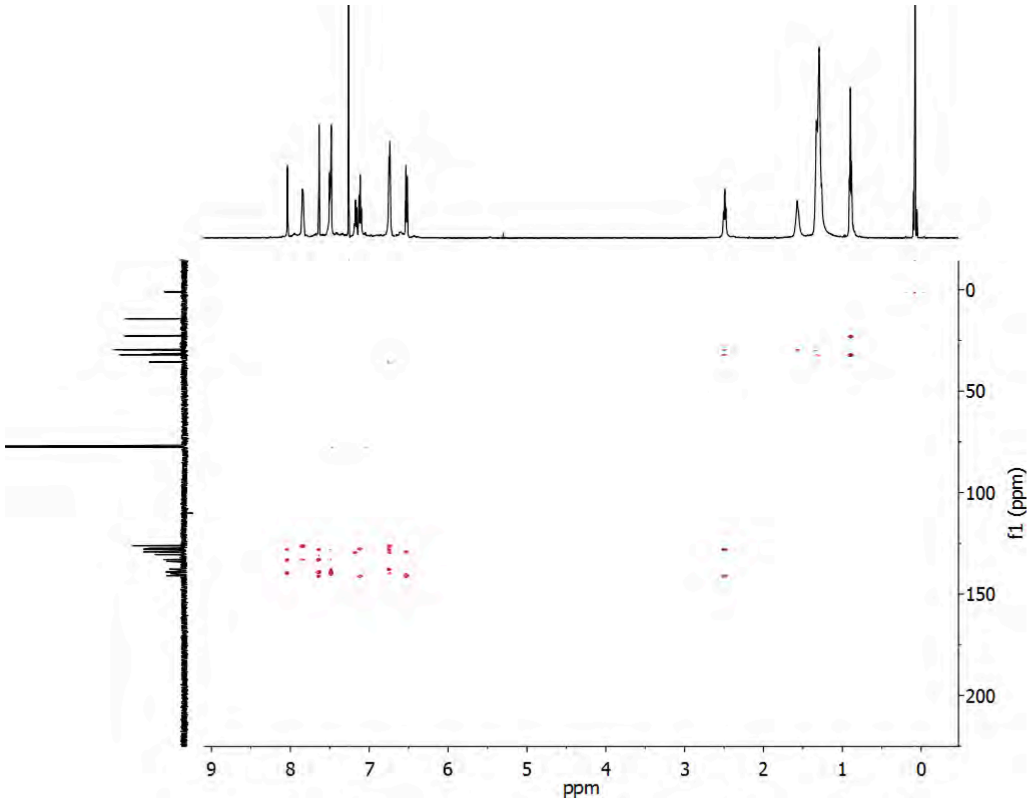
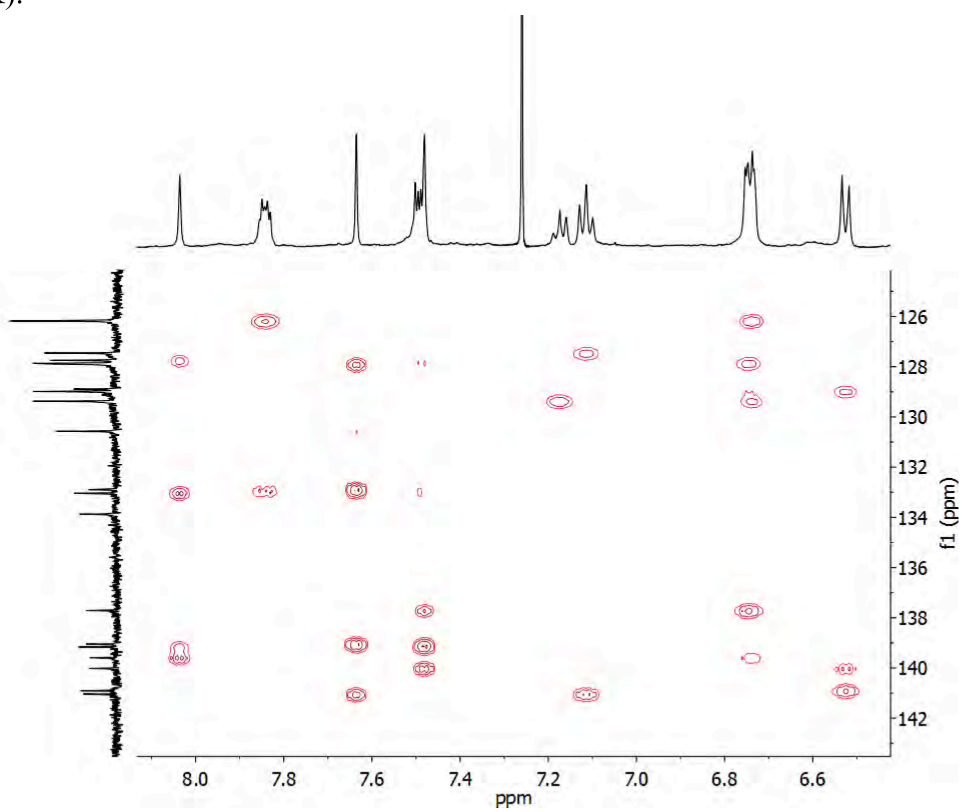
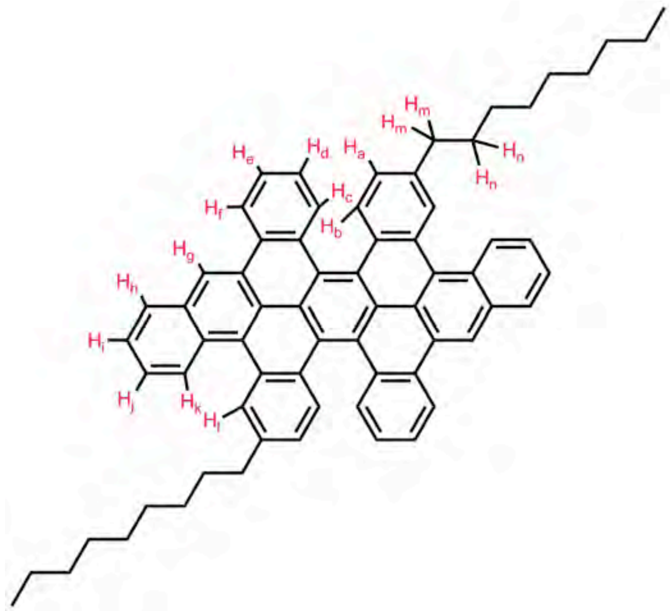



**Figure S51.** Partial HMBC spectrum of **3a** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 295 K).



**Peak assignments for the compound 4a:**




COSY spectrum indicates a 1,2,4-trisubstituted aromatic spin system, which contains $H_a$, $H_b$ and $H_l$. $H_a$ is coupled to both $H_b$ and $H_l$, whereas $H_b$ and $H_k$ are only coupled to $H_a$. Therefore, $H_a$ is in position 2 on the aromatic ring. Coupling constant between $H_a$ and $H_b$ is consistent with *o*-substitution pattern. Coupling constant between $H_l$ and $H_a$ is consistent with *m*- substitution pattern. As a result, $H_b$ and $H_l$ are at positions 1 and 4, respectively. As expected, this is the ring the nonyl chain is attached to, assigned using ROESY crosspeaks between $H_a$ and $H_m$ and $H_l$ and $H_m$.

ROESY crosspeak between $H_b$ and $H_c$ indicates that a C-C bond didn't form between these two carbons. Note that after extended reaction time, this bond does form, forming the compound **5a**.

Rest of the protons on the periphery of the molecule can be assigned by using the ROESY and COSY crosspeaks as shown below.

**Figure S52.** Full COSY spectrum of **4a** (500 MHz, 500 MHz, $CDCl_3$, 295 K).

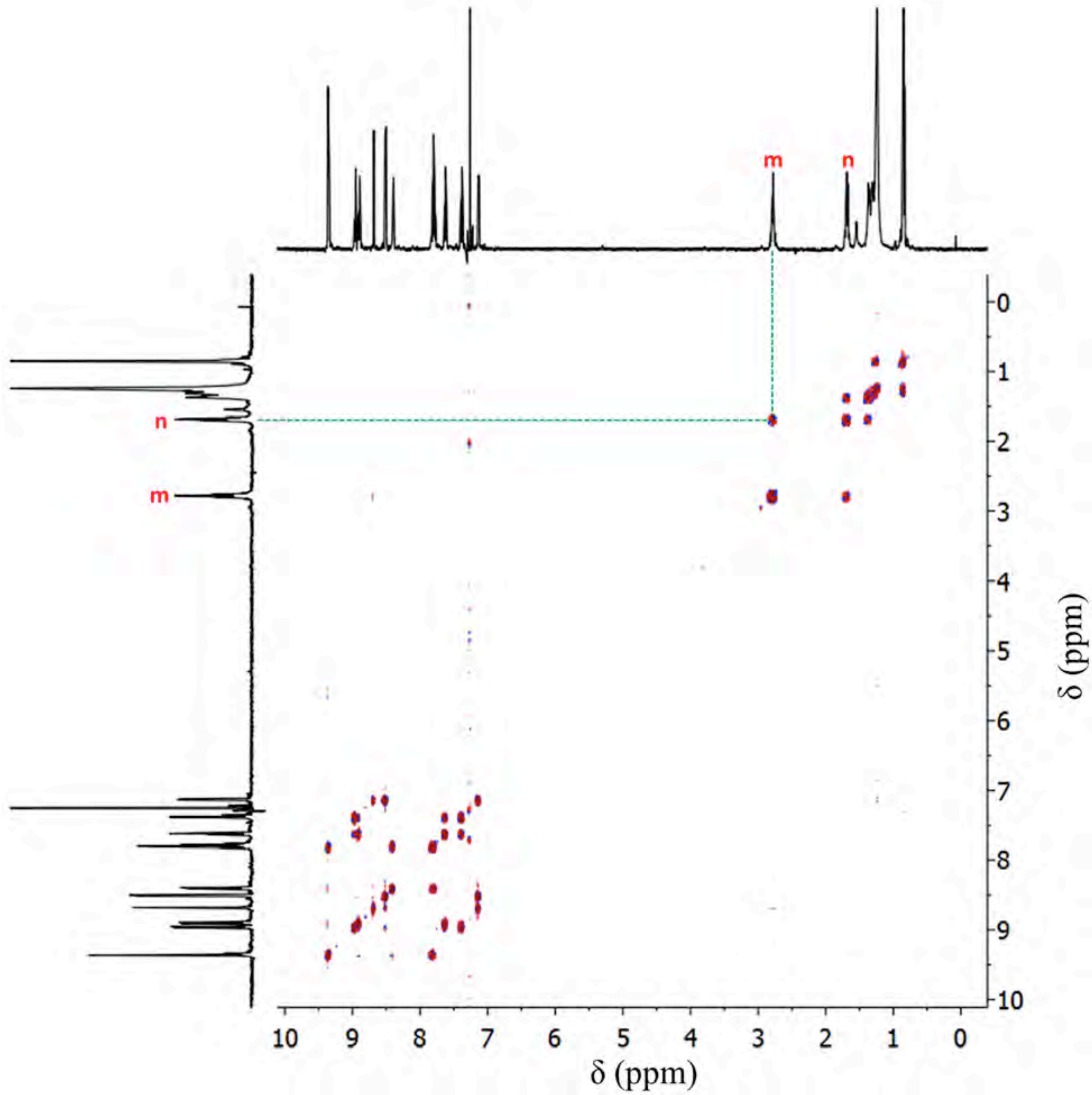


**Figure S53.** Partial COSY spectrum of **4a** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 295 K).

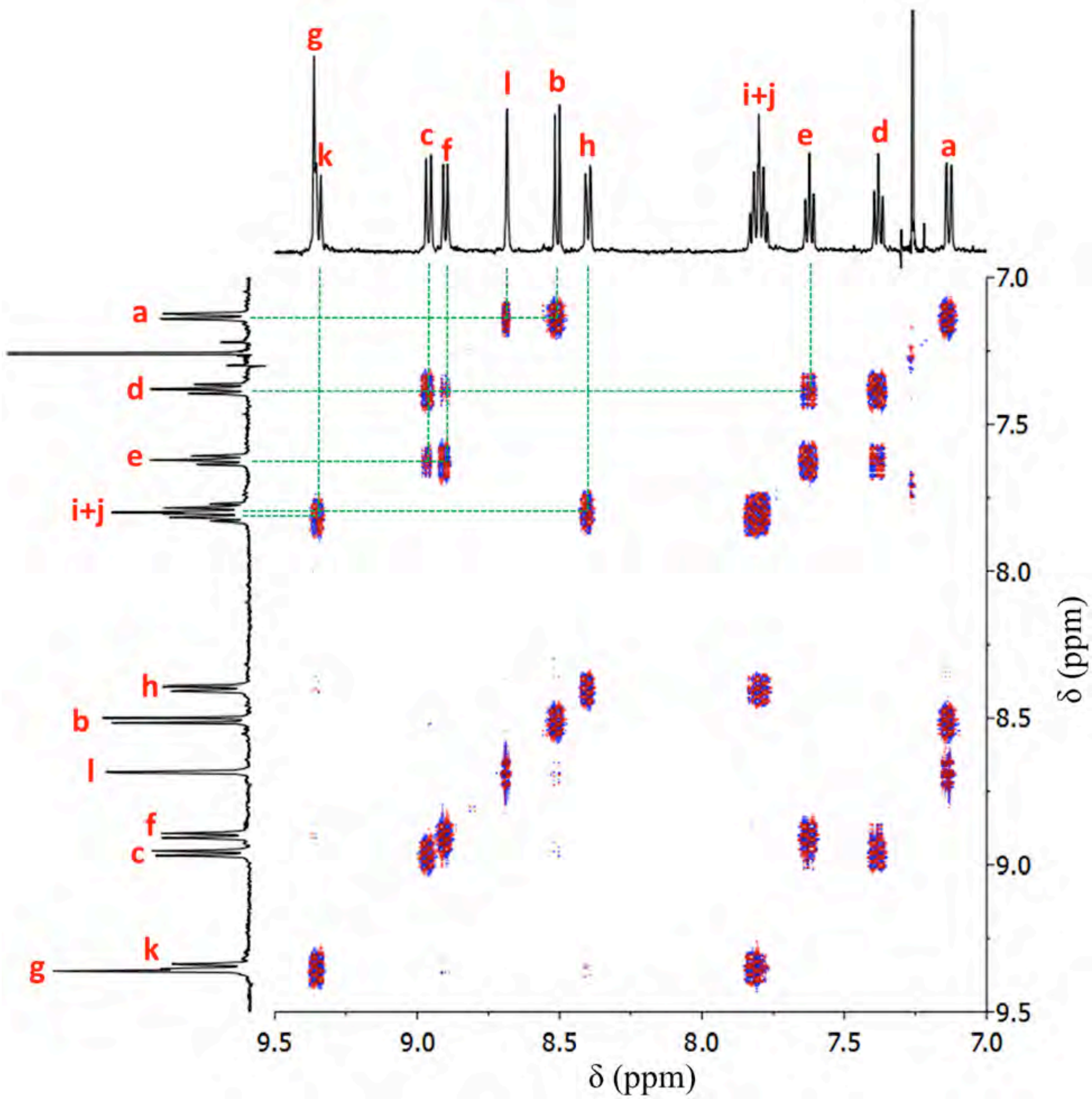


**Figure S54.** Full ROESY spectrum of **4a** (500 MHz, 500 MHz, $CDCl_3$, 295 K).

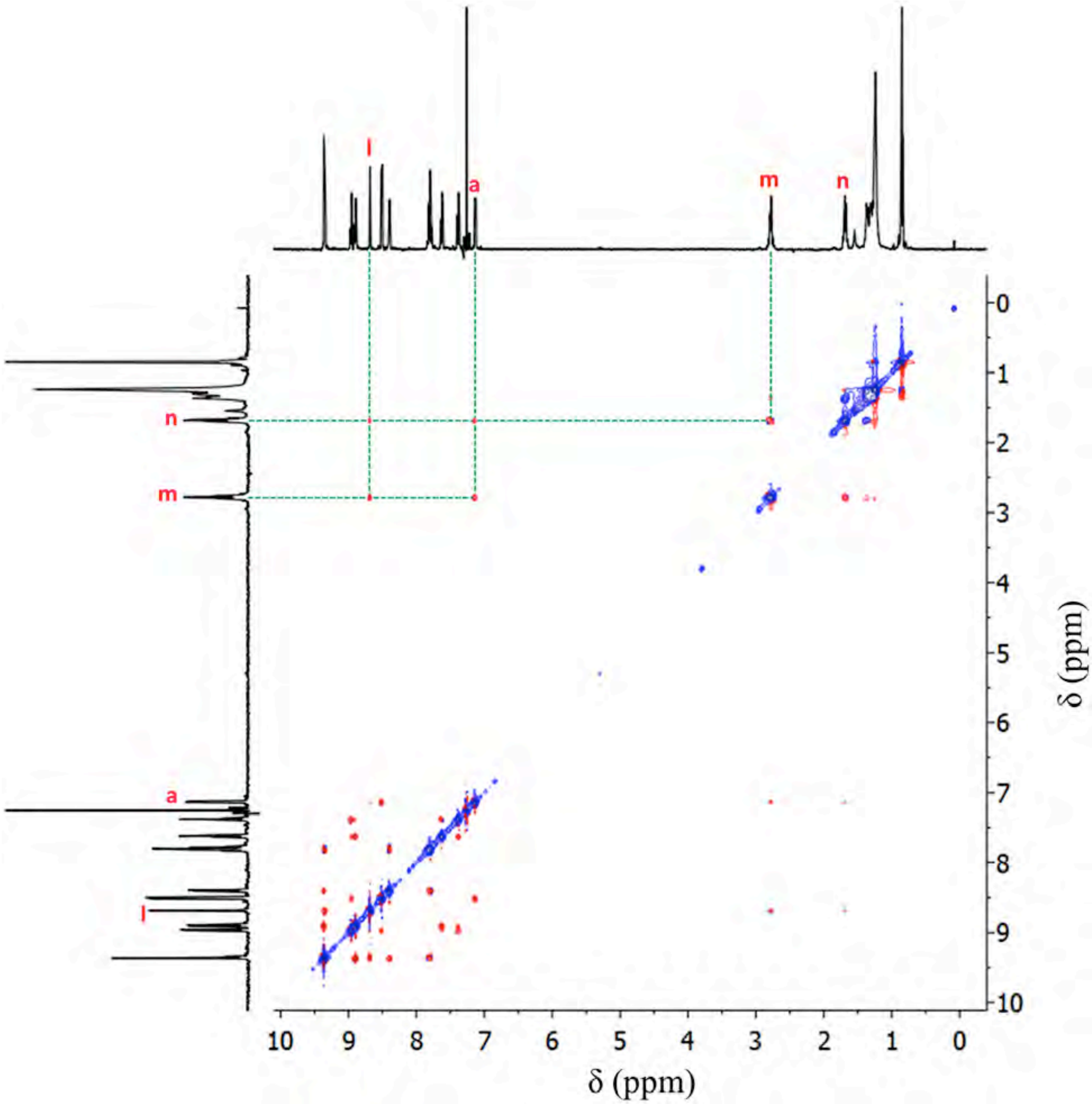


**Figure S55.** Partial ROESY spectrum of **4a** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 295 K).

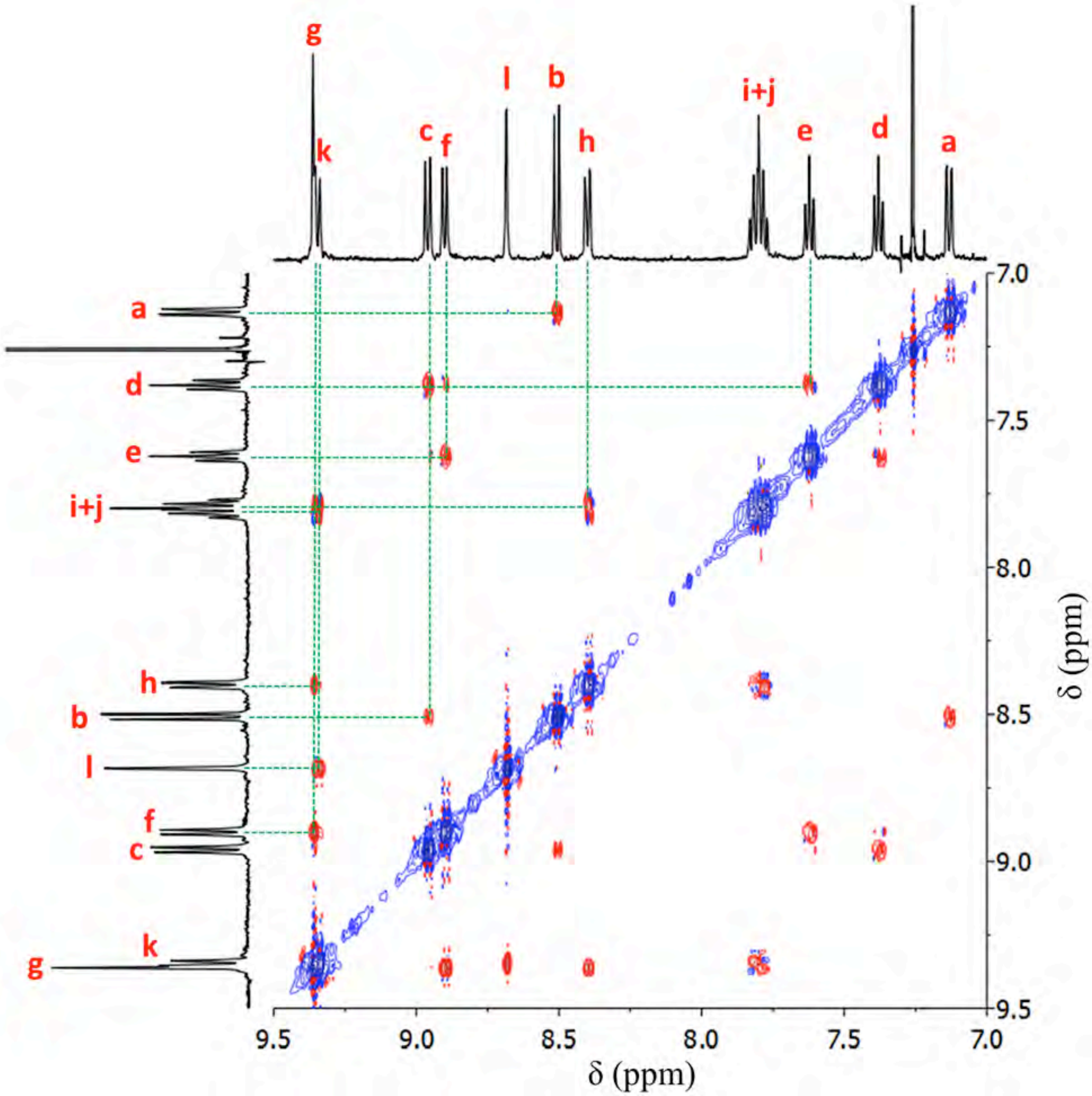


**Figure S56.** Full HSQC spectrum of **4a** (500 MHz, 125 MHz, $CDCl_3$, 295 K).

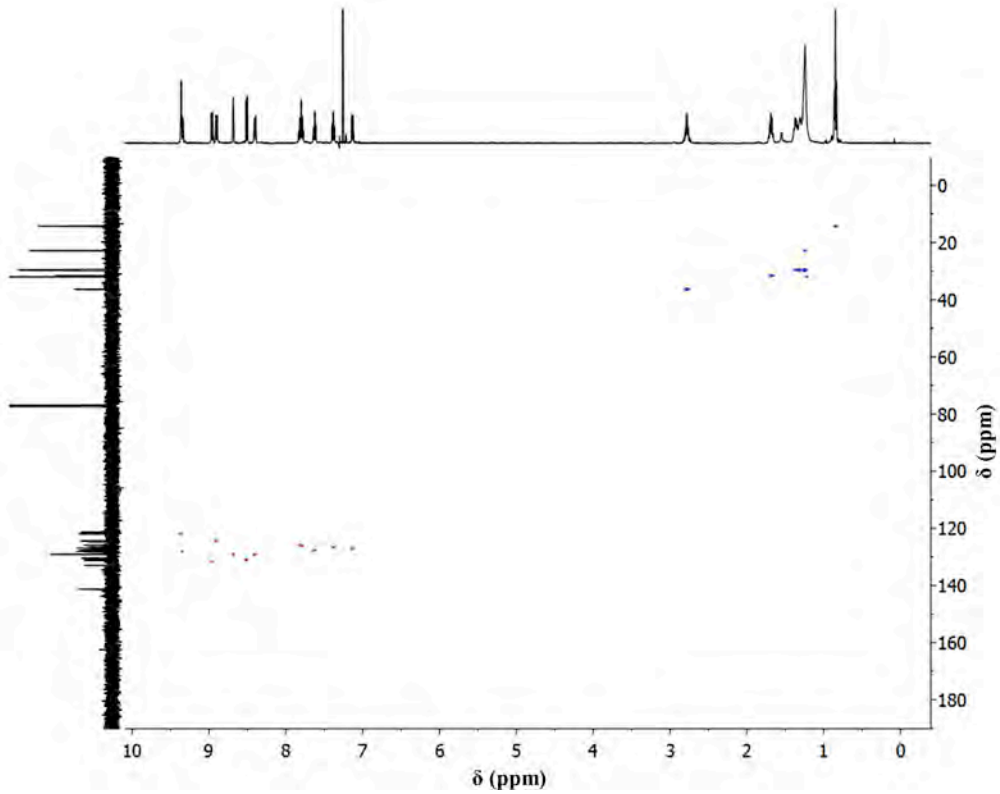



**Figure S57.** Partial HSQC spectrum of **4a** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 295 K).

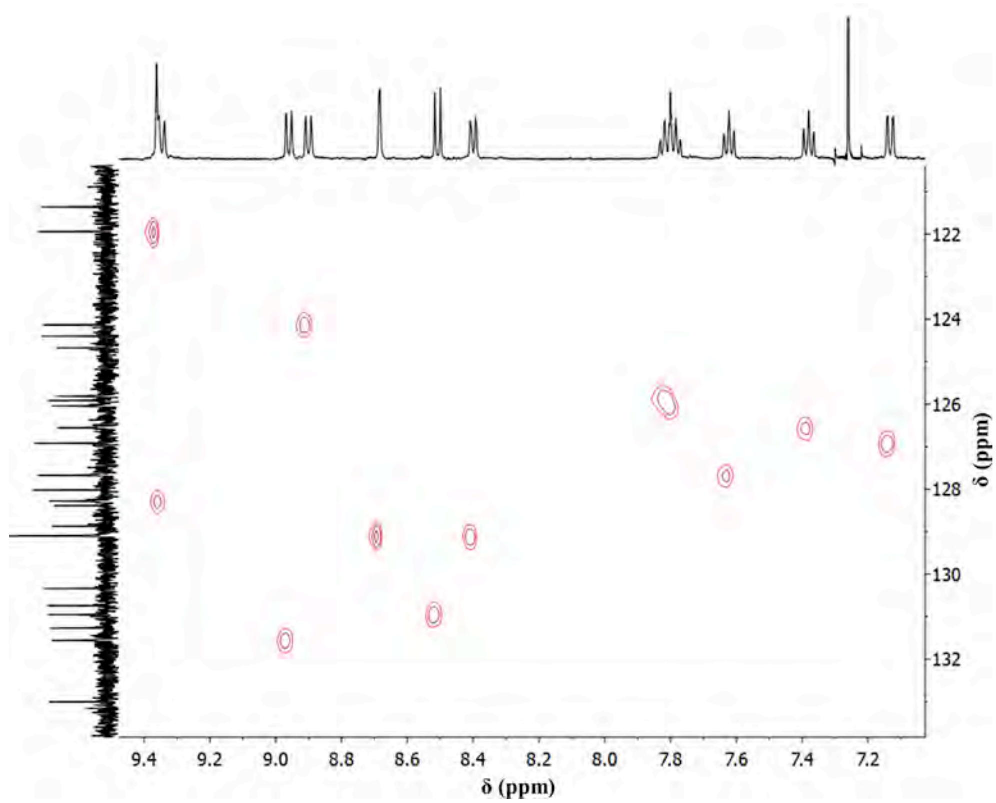


**Figure S58.** Full HMBC spectrum of **4a** (500 MHz, 125 MHz, $CDCl_3$, 295 K).

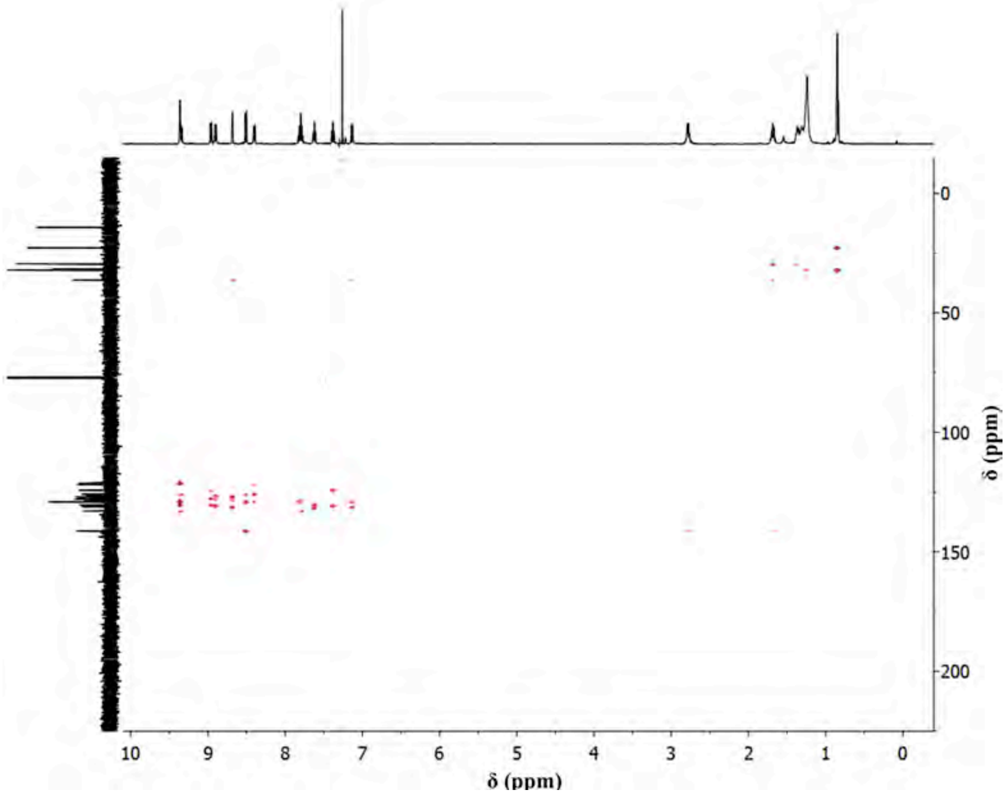
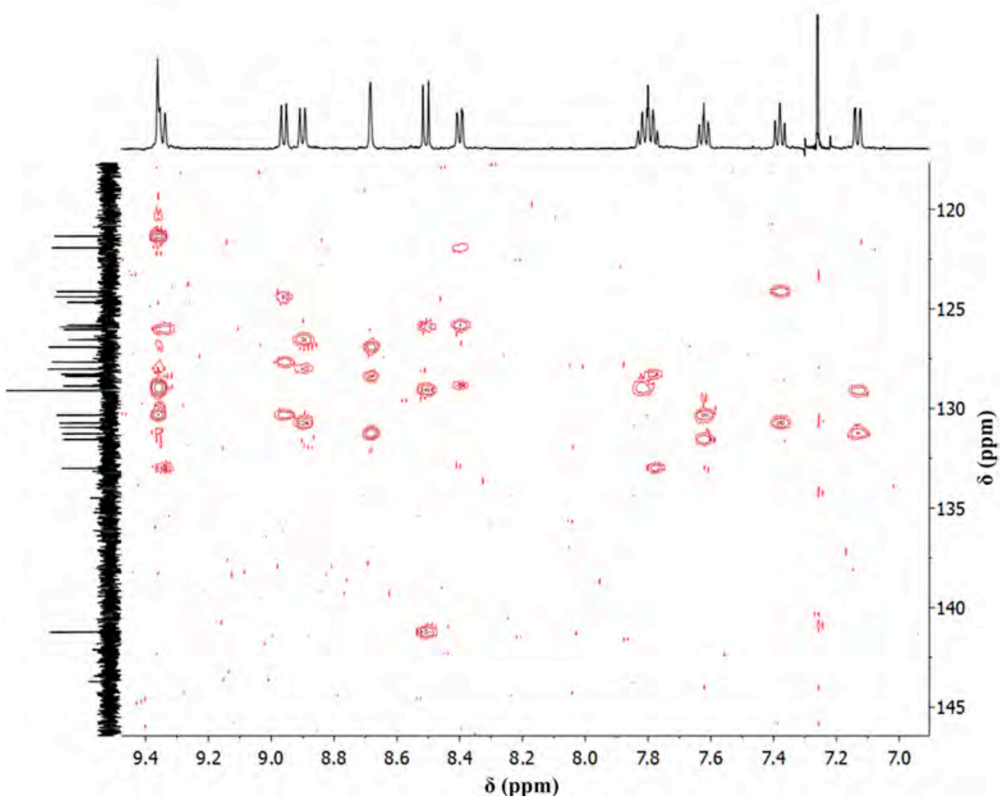
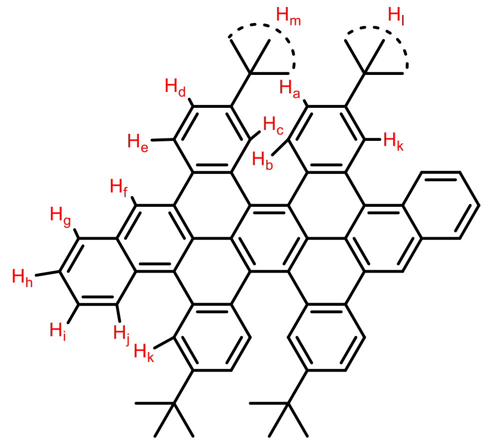



**Figure S59.** Partial HMBC spectrum of **4a** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 295 K).



**Peak assignments for the compound 4b:**




COSY spectrum indicates two 1,2,4-trisubstituted aromatic spin systems. First one contains $H_a$, $H_b$ and $H_k$. $H_a$ is coupled to both $H_b$ and $H_k$, whereas $H_b$ and $H_k$ are only coupled to $H_a$. Therefore, $H_a$ is in position 2 on the aromatic ring. Coupling constant between $H_a$ and $H_b$ is consistent with *o*- substitution pattern. Coupling constant between $H_k$ and $H_a$ is consistent with *m*- substitution pattern. As a result, $H_b$ and $H_k$ are at positions 1 and 4, respectively. The second such spin system involves protons $H_c$, $H_d$ and $H_e$. By a similar analysis, $H_c$, $H_d$ and $H_e$ are at positions 4,2, and 1, respectively. Location of these two spin systems can be assigned based on ROESY crosspeaks between $H_e$ and $H_f$, and $H_i$ and $H_k$.

ROESY crosspeak between $H_b$ and $H_c$ is a clear indication of an incomplete cyclodehydrogenation; because in the case of complete fusion, these two proton signals wouldn't be observed.

The two *t*-butyl groups can be assigned based on the ROESY spectrum. $H_m$ has crosspeaks with $H_c$ and $H_d$, and $H_l$ has crosspeaks with $H_a$ and $H_k$.

Rest of the protons on the periphery of the molecule can be assigned by using the ROESY and COSY crosspeaks as shown below.

**Figure S60.** Full COSY spectrum of **4b** (500 MHz, 500 MHz, $CDCl_3$, 298 K).

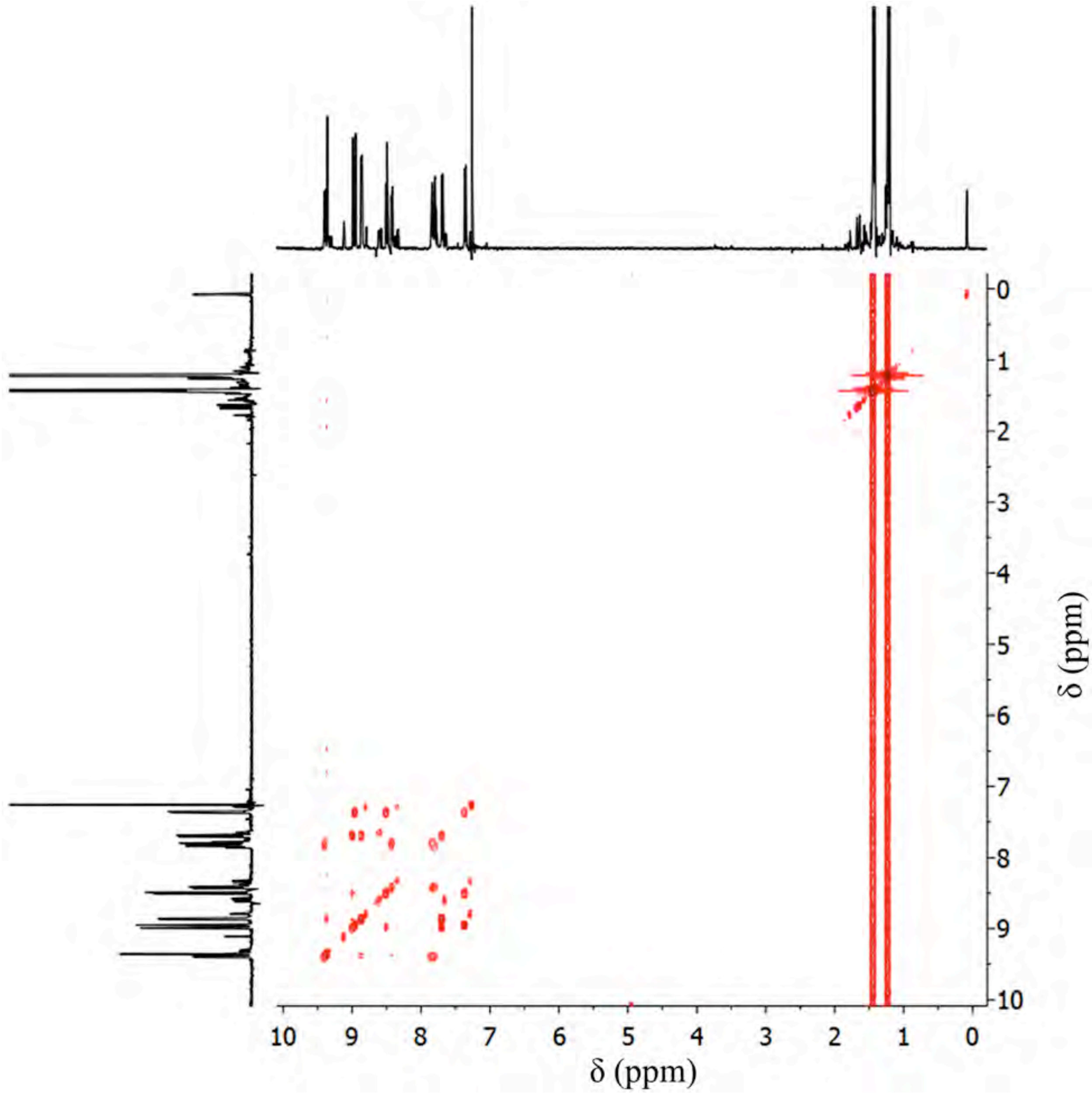


**Figure S61.** Partial COSY spectrum of **4b** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 298 K).

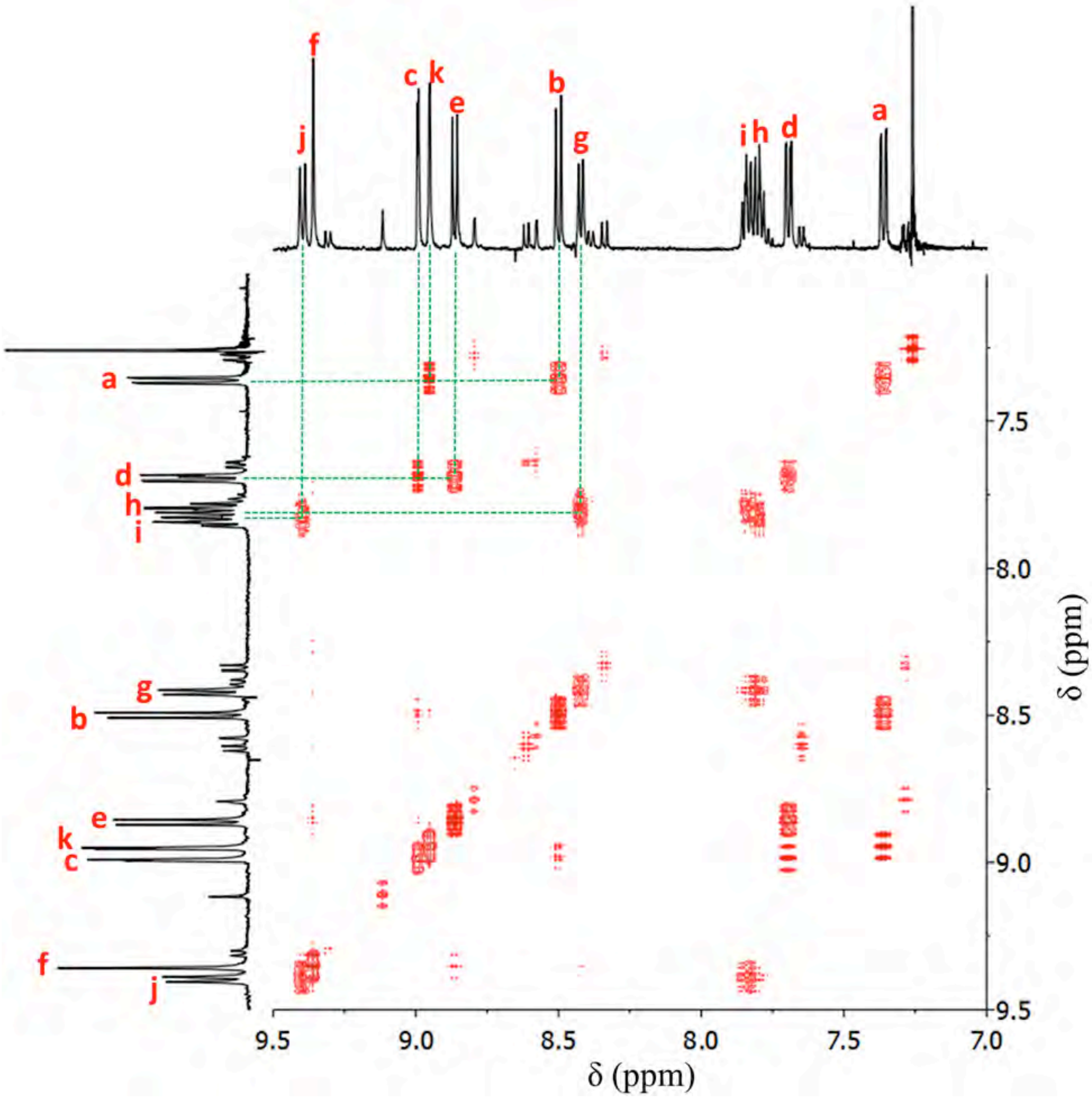


**Figure S62.** Full ROESY spectrum of **4b** (500 MHz, 500 MHz, $CDCl_3$, 298 K).

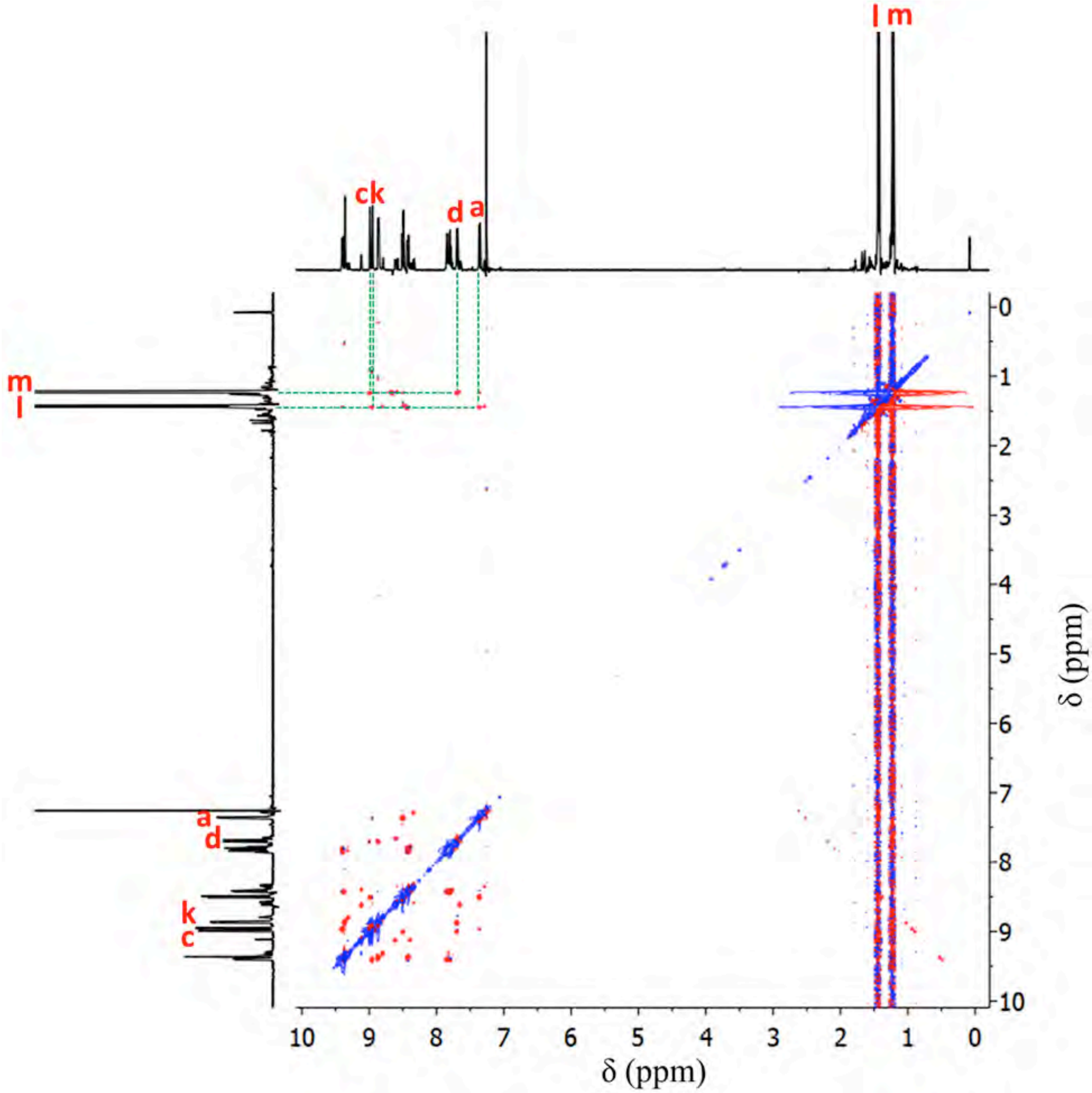


**Figure S63.** Partial ROESY spectrum of **4b** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 298 K).

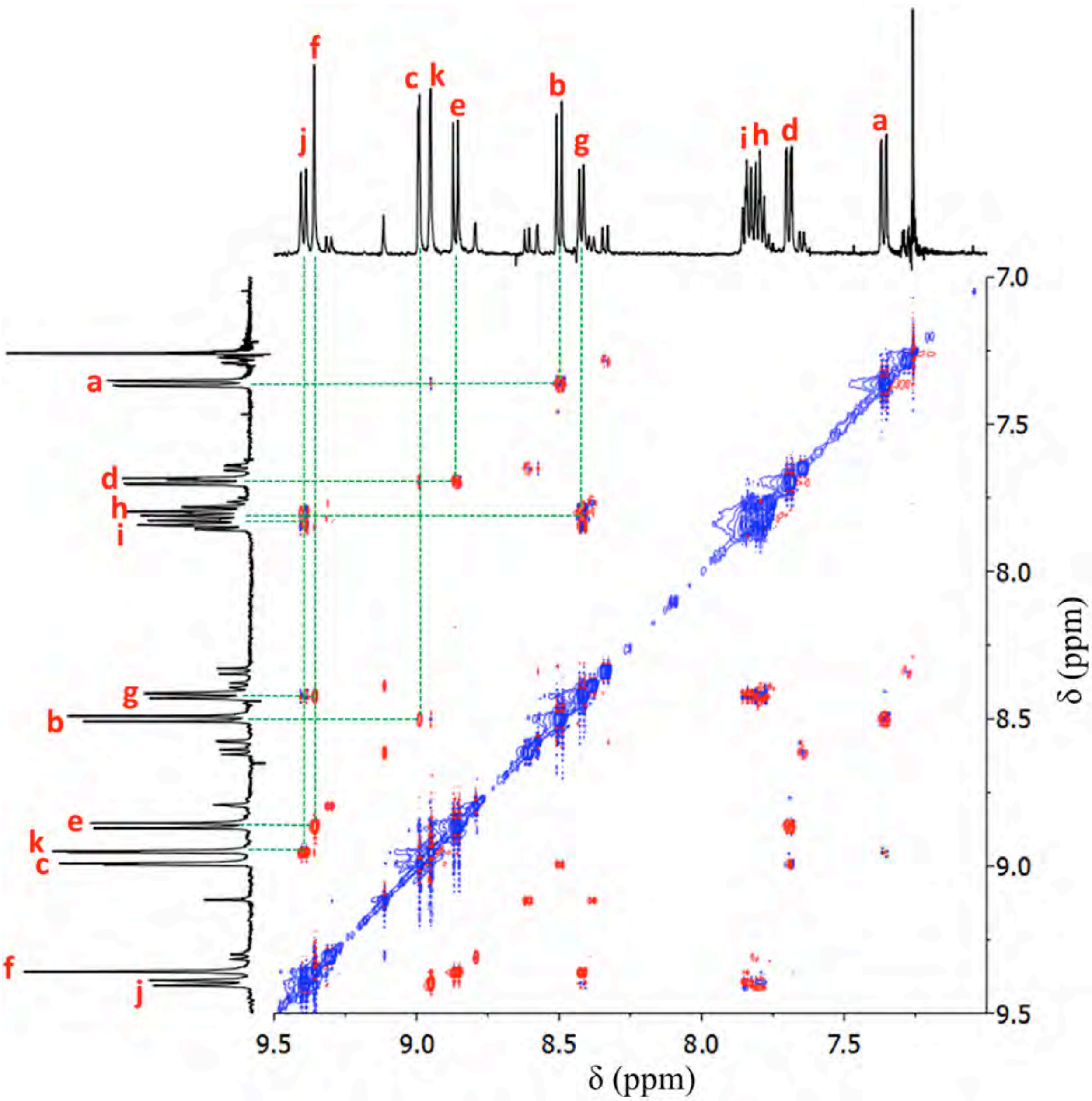


**Figure S64.** Full HSQC spectrum of **4b** (500 MHz, 125 MHz, $CDCl_3$, 298 K).

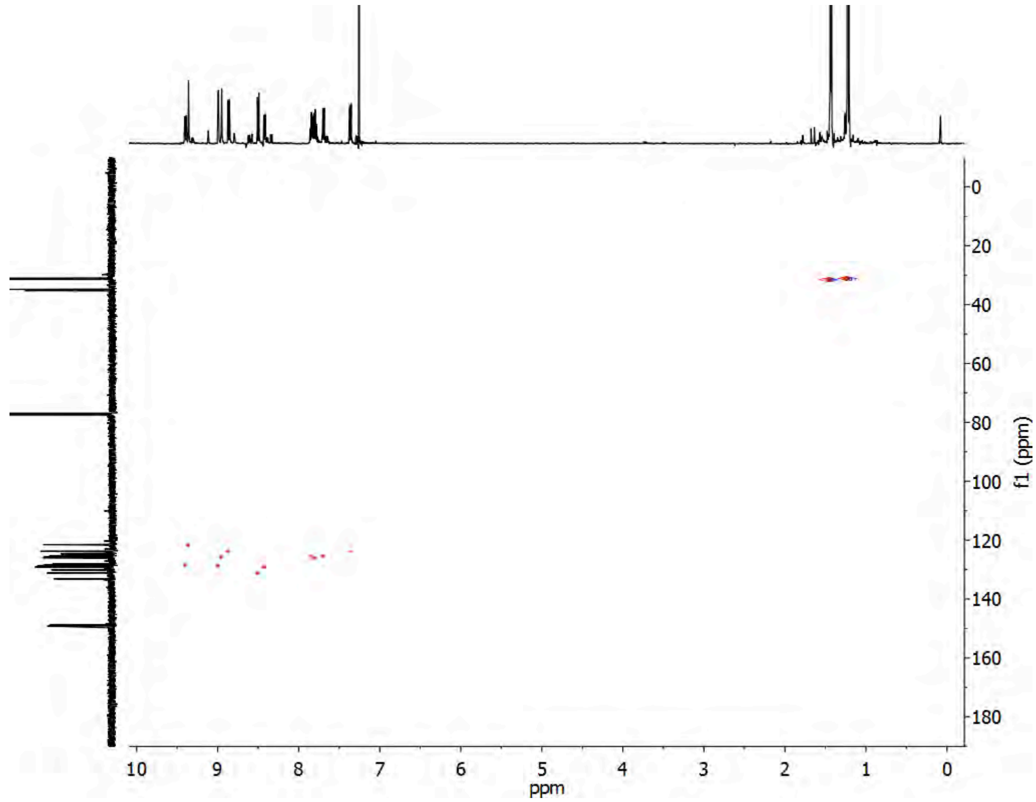



**Figure S65.** Partial HSQC spectrum of **4b** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 298 K).

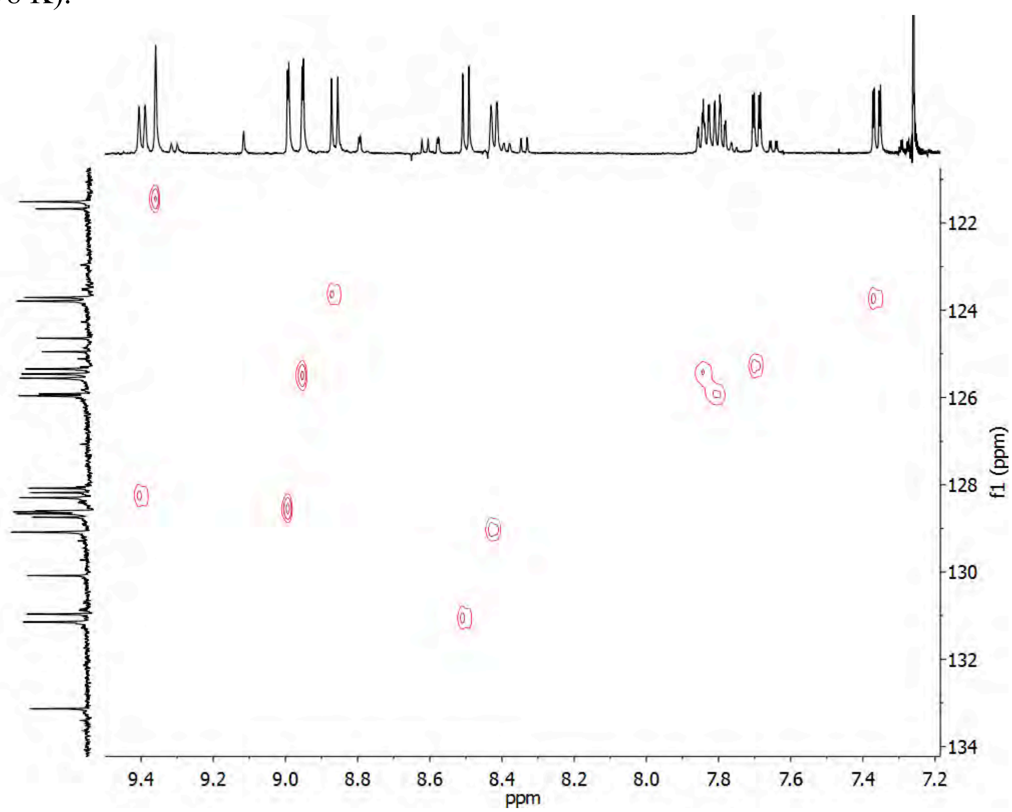


**Figure S66.** Full HMBC spectrum of **4b** (500 MHz, 125 MHz, $CDCl_3$, 298 K).

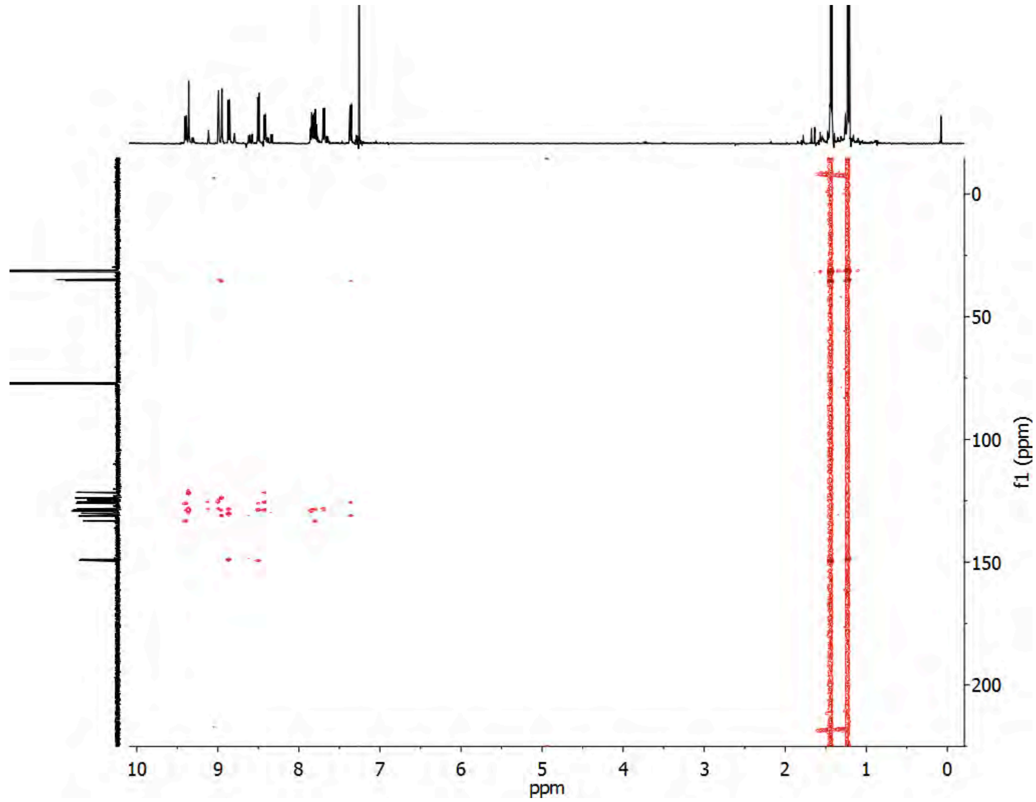
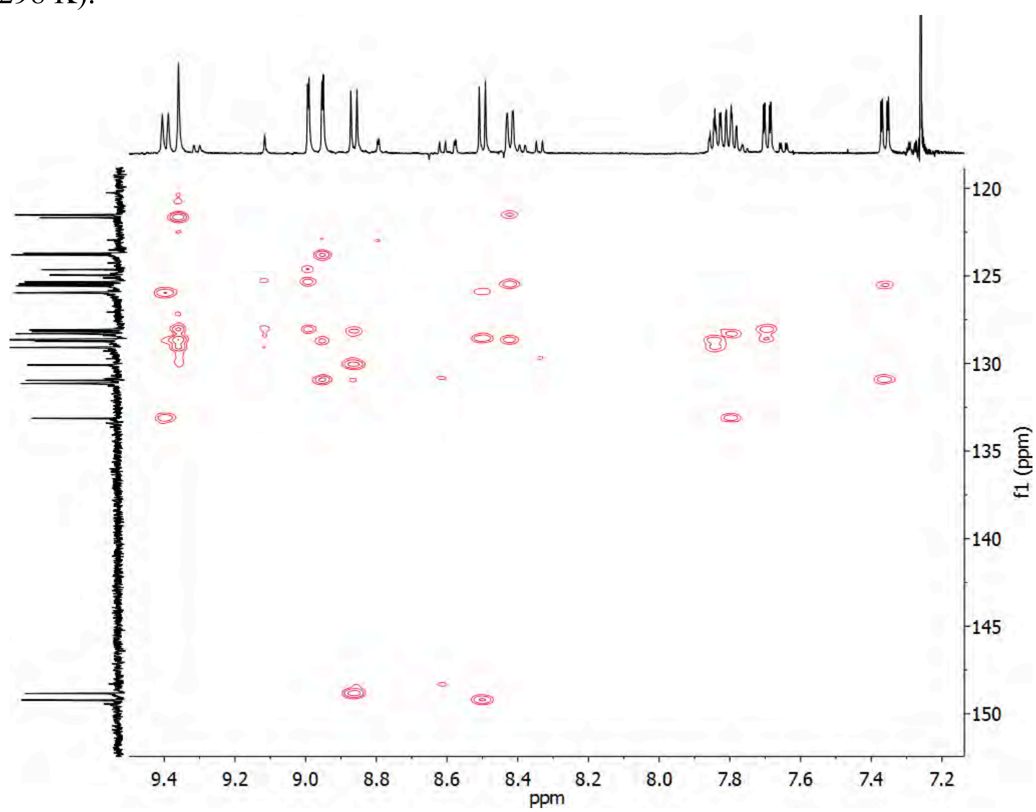



**Figure S67.** Partial HMBC spectrum of **4b** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 298 K).



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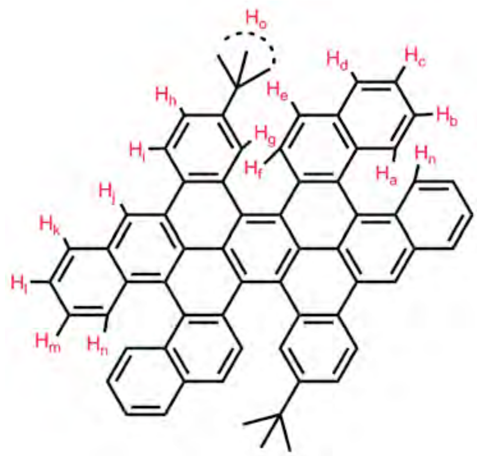
**Peak assignments for the compound 4c:**




COSY spectrum indicates a 1,2,4-trisubstituted aromatic spin system, which contains $H_g$, $H_h$ and $H_i$. $H_h$ is coupled to both $H_g$ and $H_i$, whereas $H_g$ and $H_i$ are only coupled to $H_h$. Therefore, $H_h$ is in position 2 on the aromatic ring. Based on coupling constants, $H_i$ and $H_g$ are at positions 1 and 4, respectively. Furthermore, the *t*Bu group is attached to this ring based on ROESY crosspeaks between $H_g$ and $H_o$ and $H_h$ and $H_o$.

Similar to the analyses for the compounds **4a** and **4b**, key ROESY crosspeaks allow us to determine which C-C bonds did not form in the molecule. The crosspeak between $H_f$ and $H_g$ indicates that a C-C bond didn't form at a similar position to **4a** and **4b**. This can be explained by the steric hindrance imposed by the *t*Bu group. Even after extended reaction times, this bond does not form. Another bond that does not form is the one between the carbons $H_a$ and $H_n$ are attached to, as supported by the ROESY crosspeak between two hydrogens. This is presumably due to the rigid and contorted structure of the molecule.

Rest of the protons on the periphery of the molecule can be assigned by using the ROESY and COSY crosspeaks as shown below.

**Figure S68.** Full COSY spectrum of **4c** (500 MHz, 500 MHz, $CDCl_3$, 296 K).

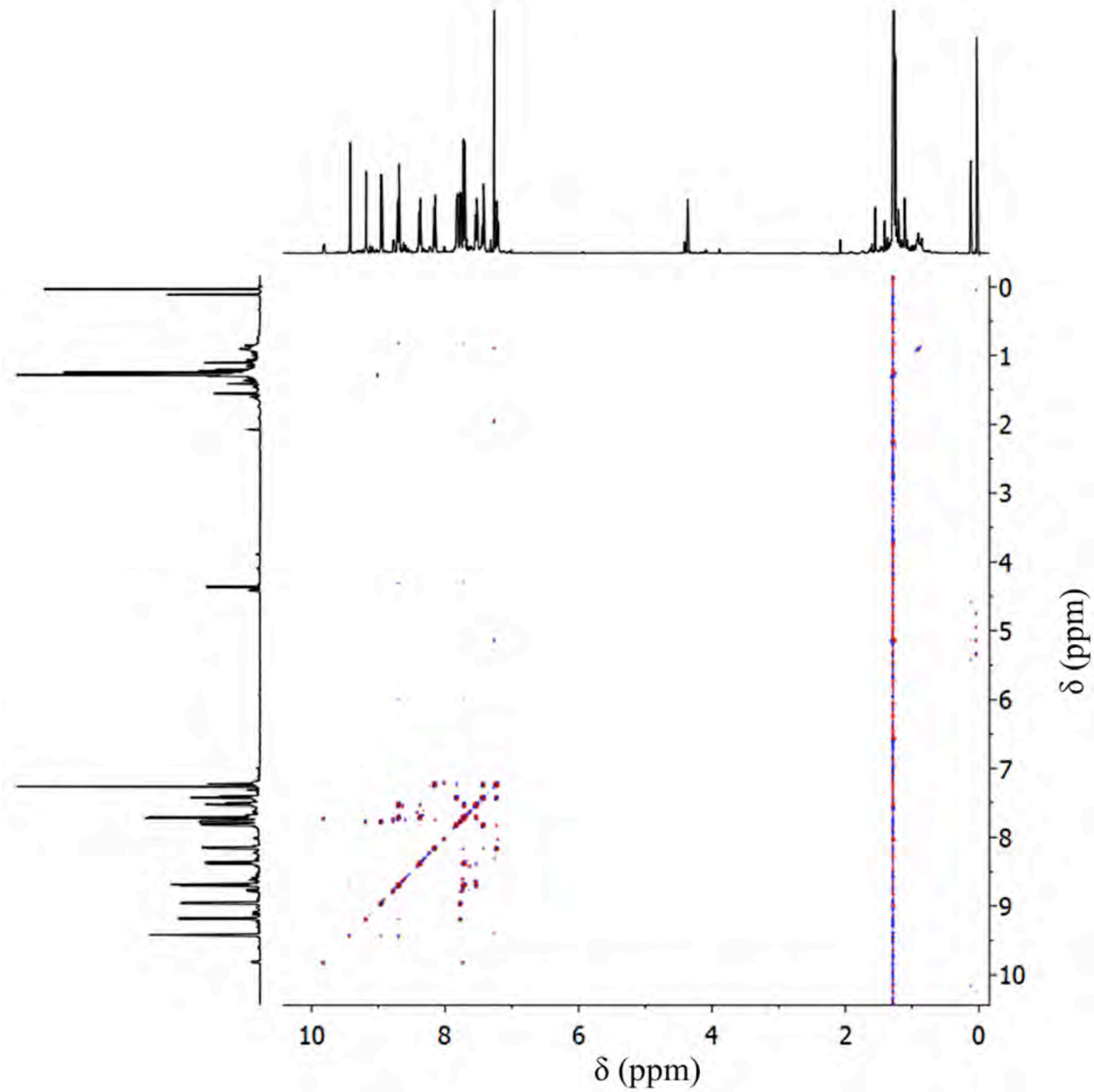


**Figure S69.** Partial COSY spectrum of **4c** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 296 K).

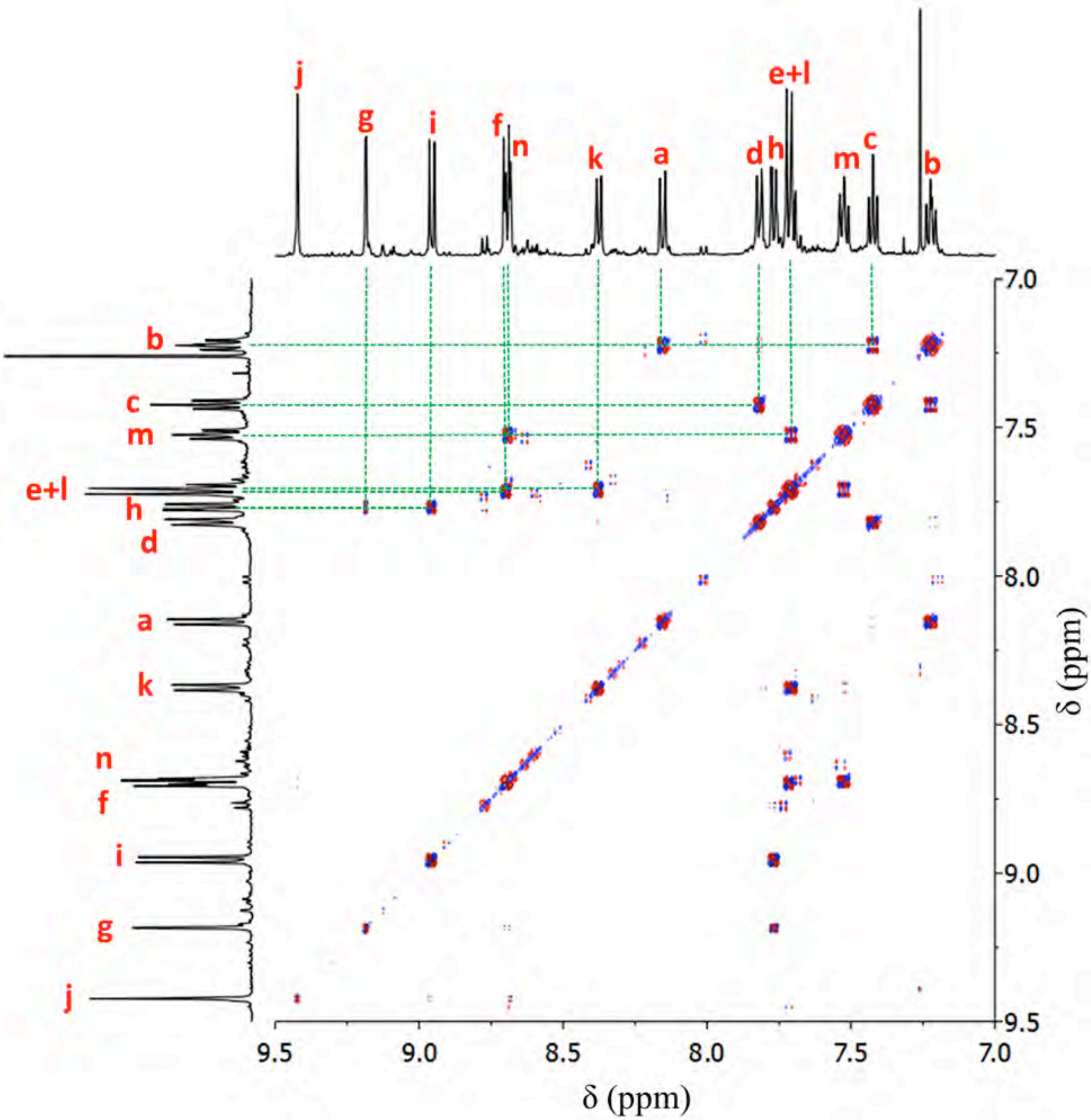


**Figure S70.** Full ROESY spectrum of **4c** (500 MHz, 500 MHz, $CDCl_3$, 296 K).

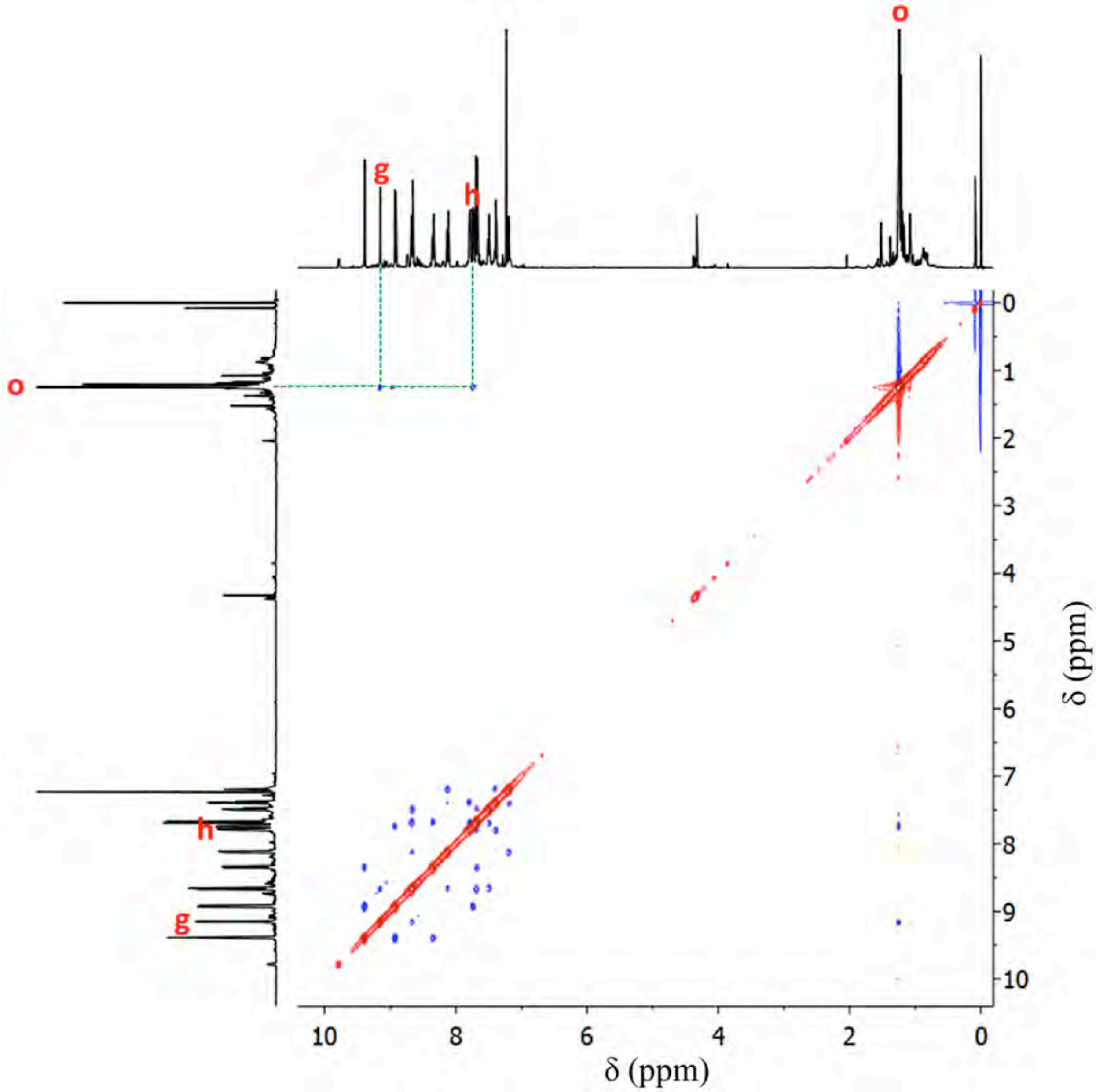


**Figure S71.** Partial ROESY spectrum of **4c** showing the aromatic region (500 MHz, 500 MHz, $CDCl_3$, 296 K).

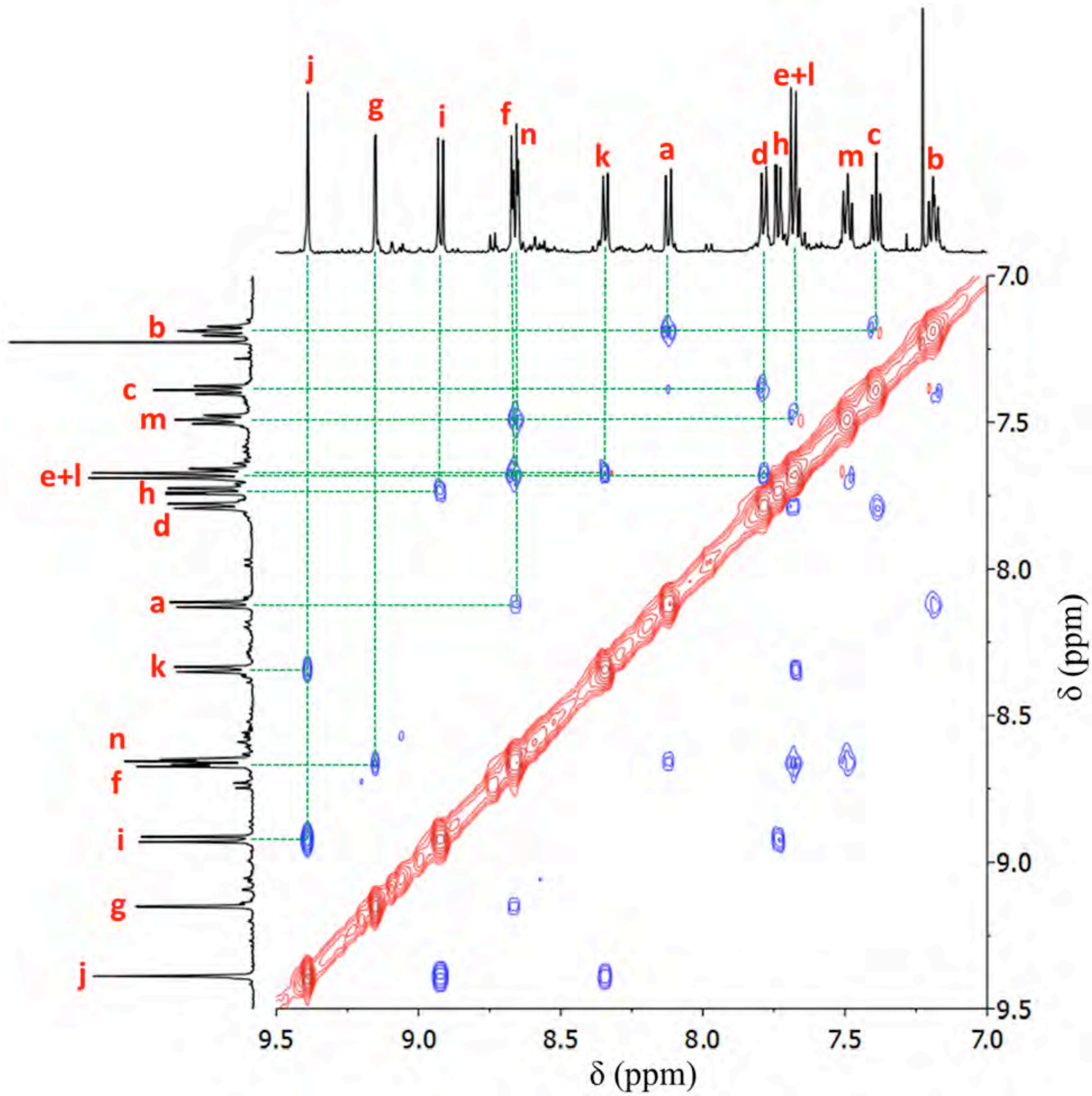


**Figure S72.** Full HSQC spectrum of **4c** (500 MHz, 125 MHz, $CDCl_3$, 296 K).

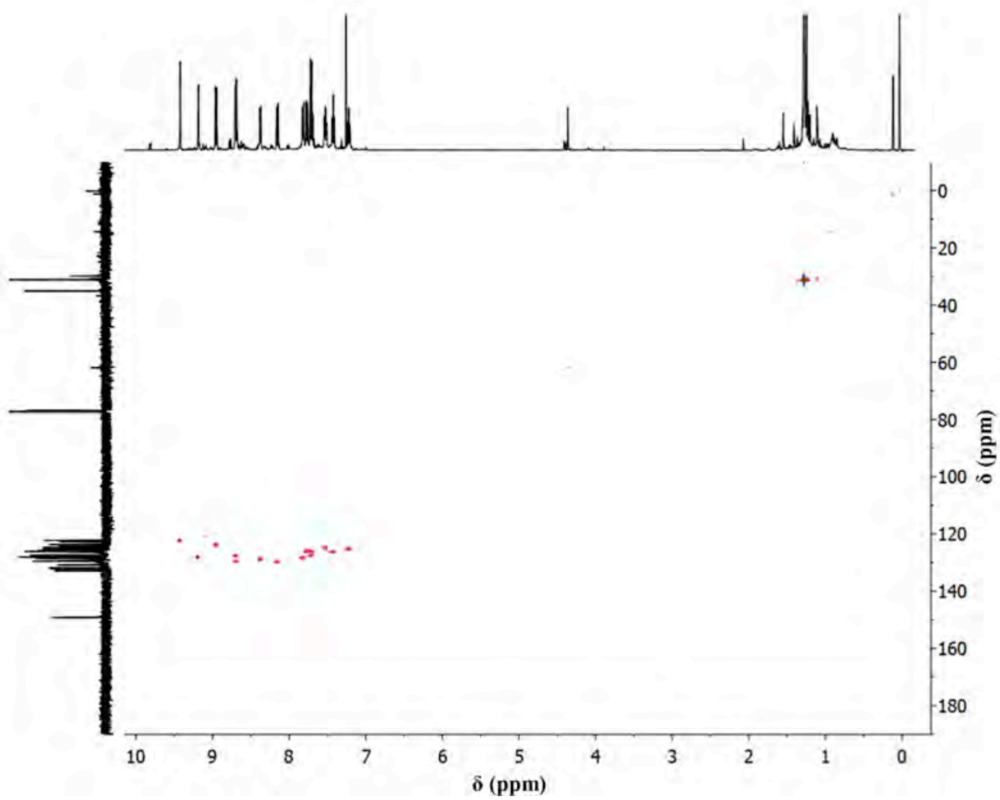



**Figure S73.** Partial HSQC spectrum of **4c** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 298 K).

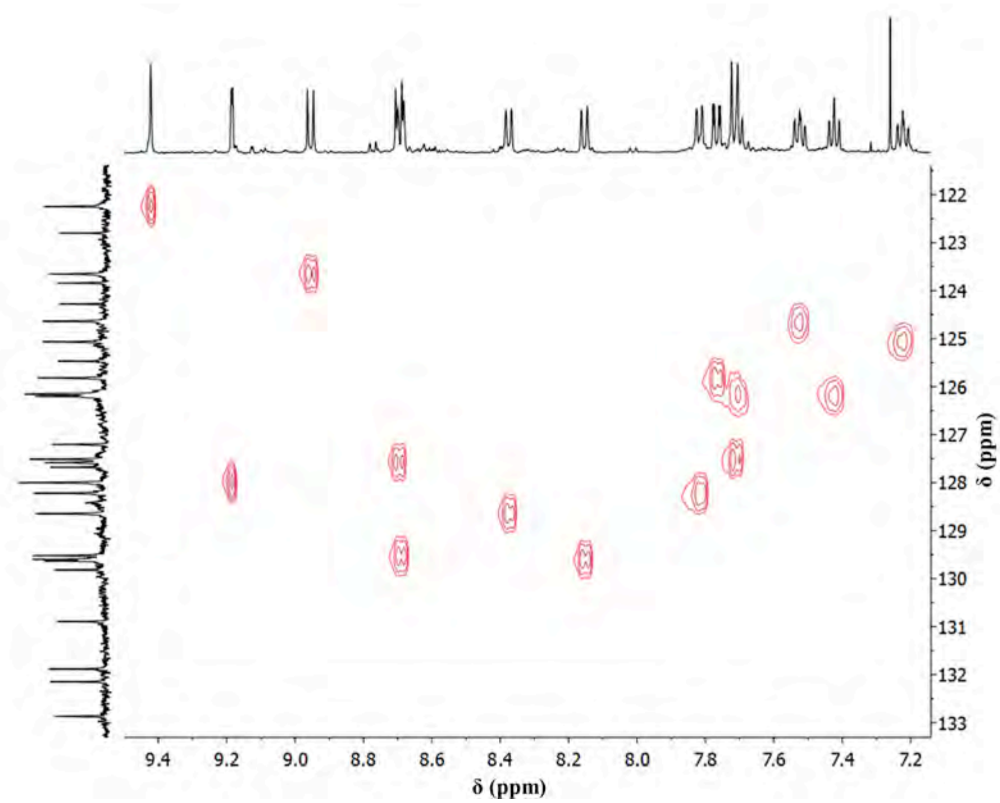


**Figure S74.** Full HMBC spectrum of **4c** (500 MHz, 125 MHz, $CDCl_3$, 296 K).

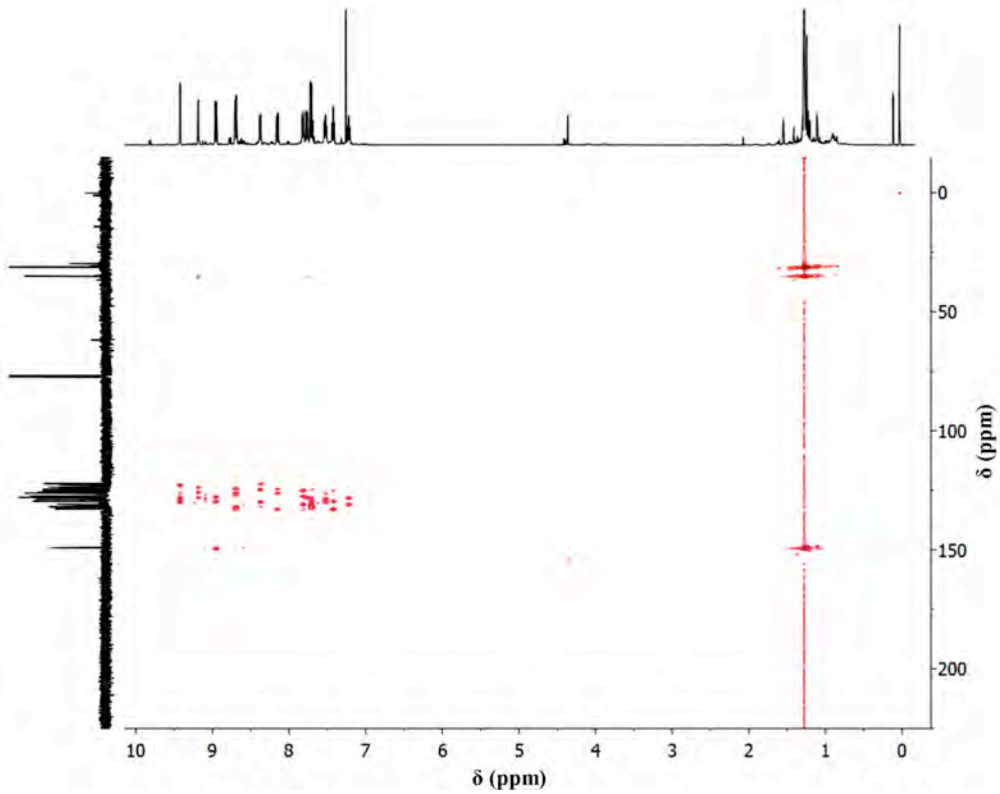
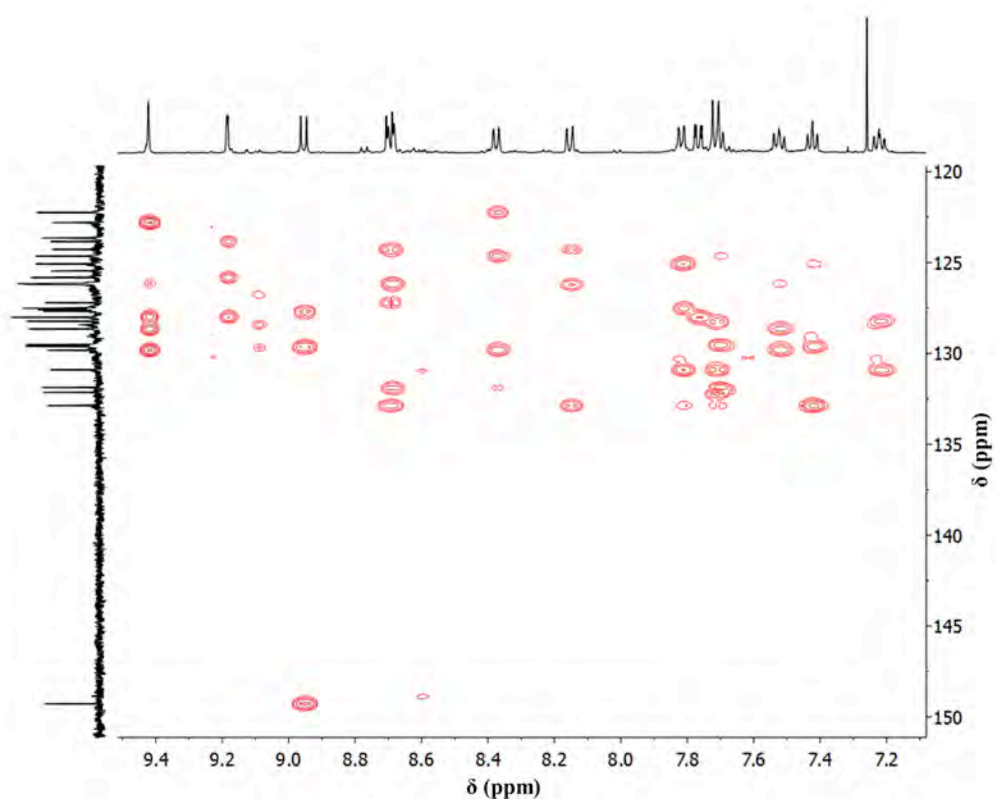



**Figure S75.** Partial HMBC spectrum of **4c** showing the aromatic region (500 MHz, 125 MHz, $CDCl_3$, 296 K).



**Peak assignments for the compound 5a-$^{13}C_2$:**

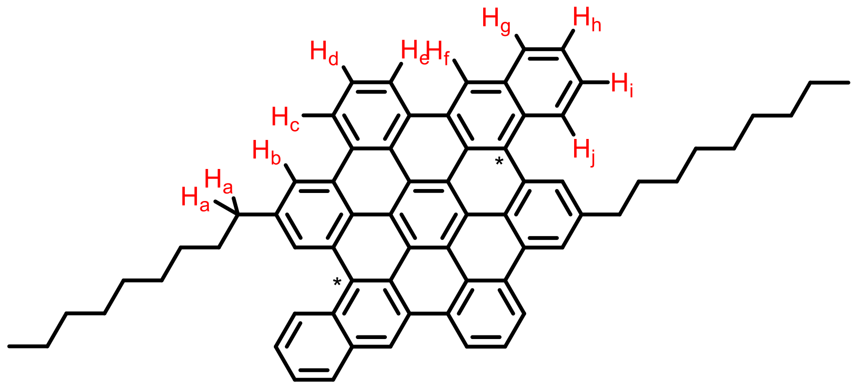


**Figure S76.** Full COSY spectrum of **5a-**$^{13}C_2$ (500 MHz, 500 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

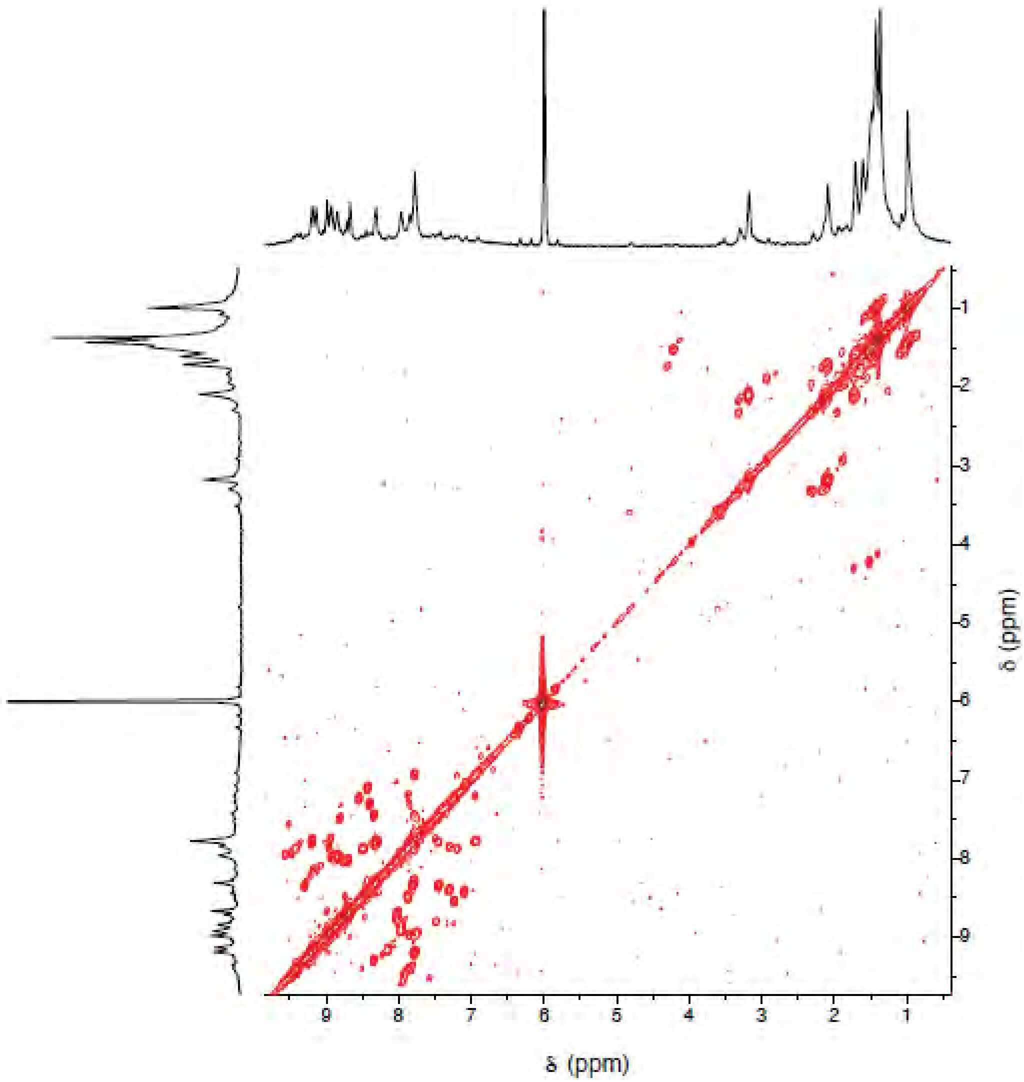


**Figure S77.** Partial COSY spectrum of **5a-**$^{13}C_2$ showing the aromatic region (500 MHz, 500 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

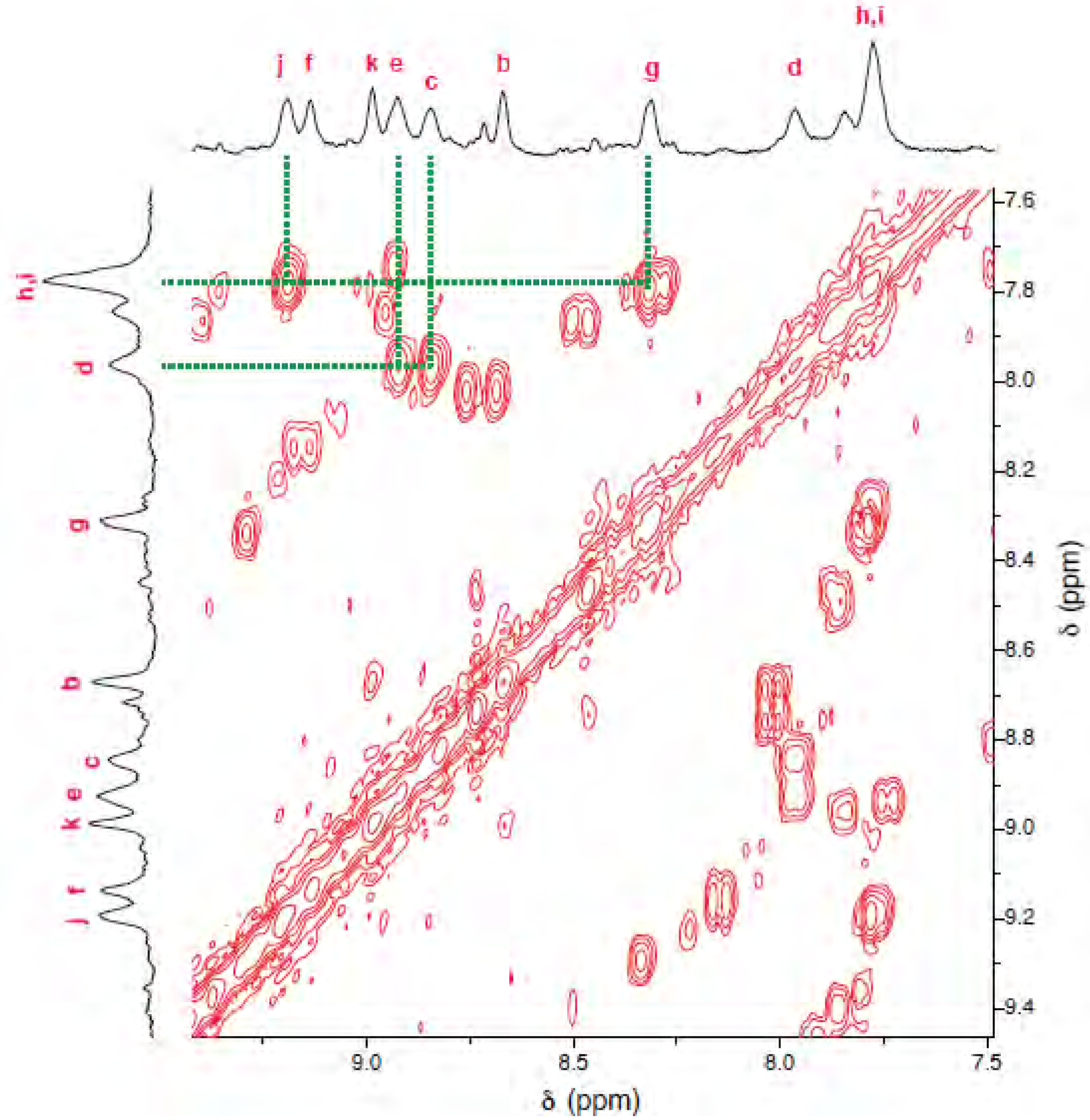


**Figure S78.** Full ROESY spectrum of **5a-$^{13}C_2$** (500 MHz, 500 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

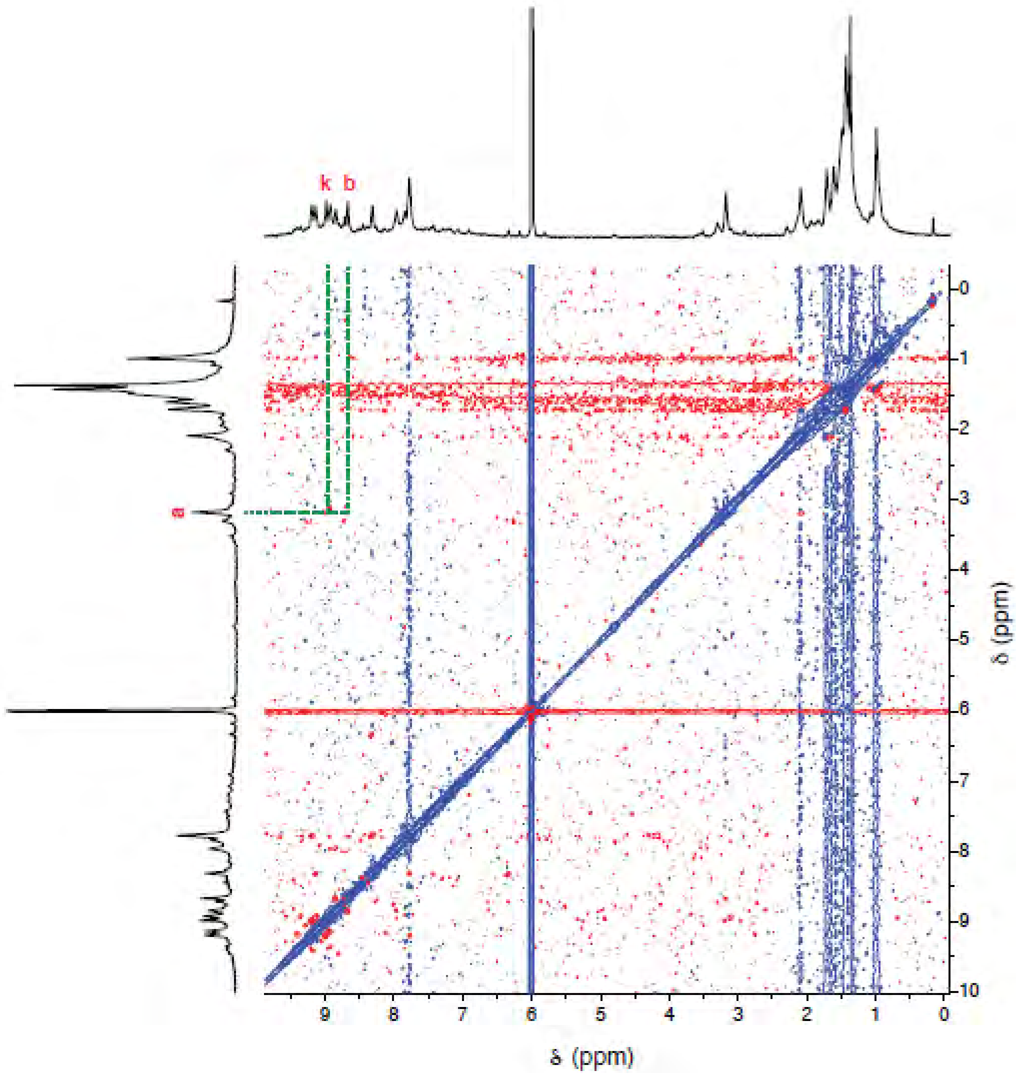


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**Figure S79.** Partial ROESY spectrum of **5a-**$^{13}$***C***$_2$ showing the aromatic region (500 MHz, 500 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

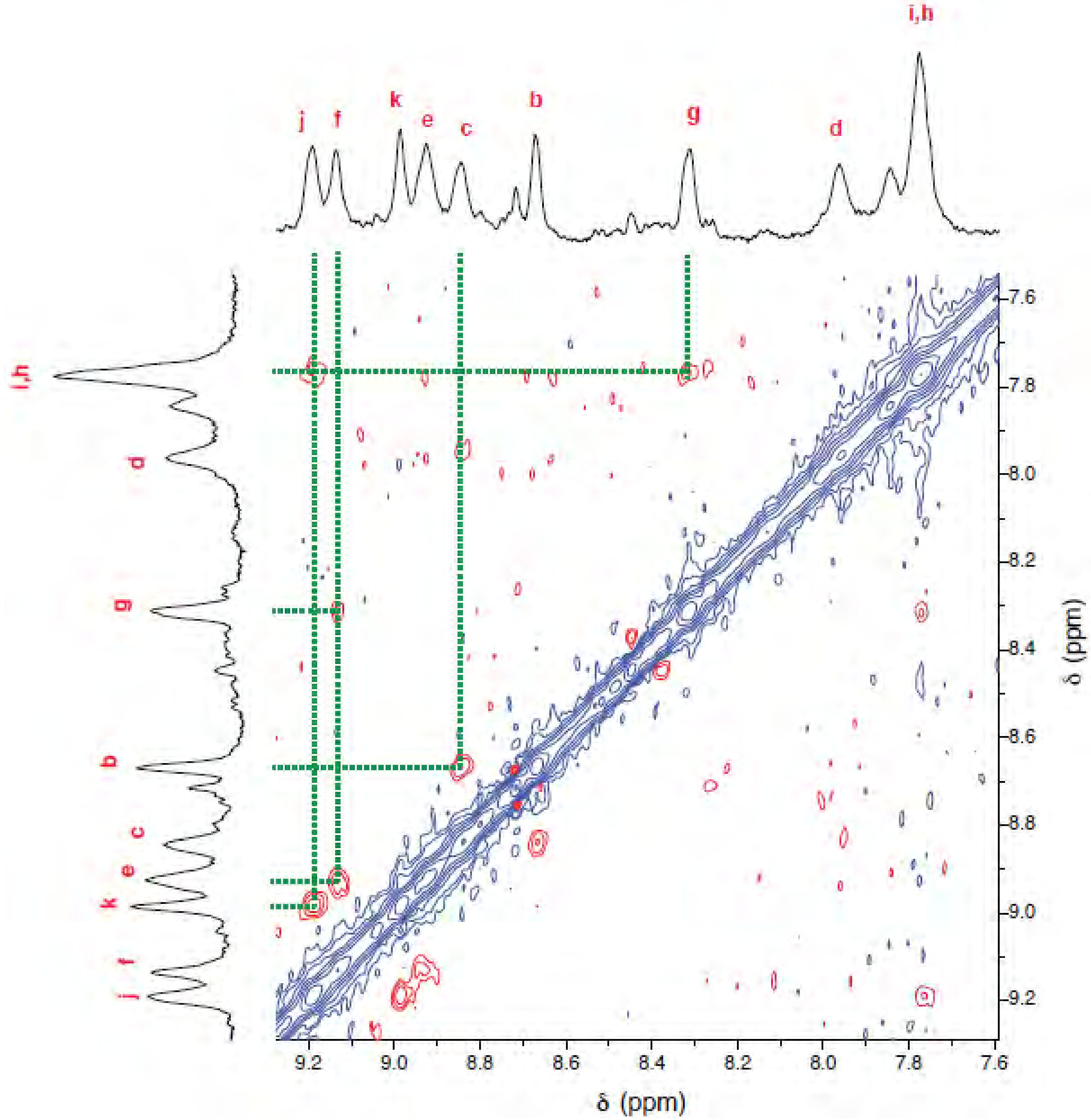


**Figure S80.** Full HSQC spectrum of **5a-**$^{13}$***C***$_2$ (500 MHz, 125 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

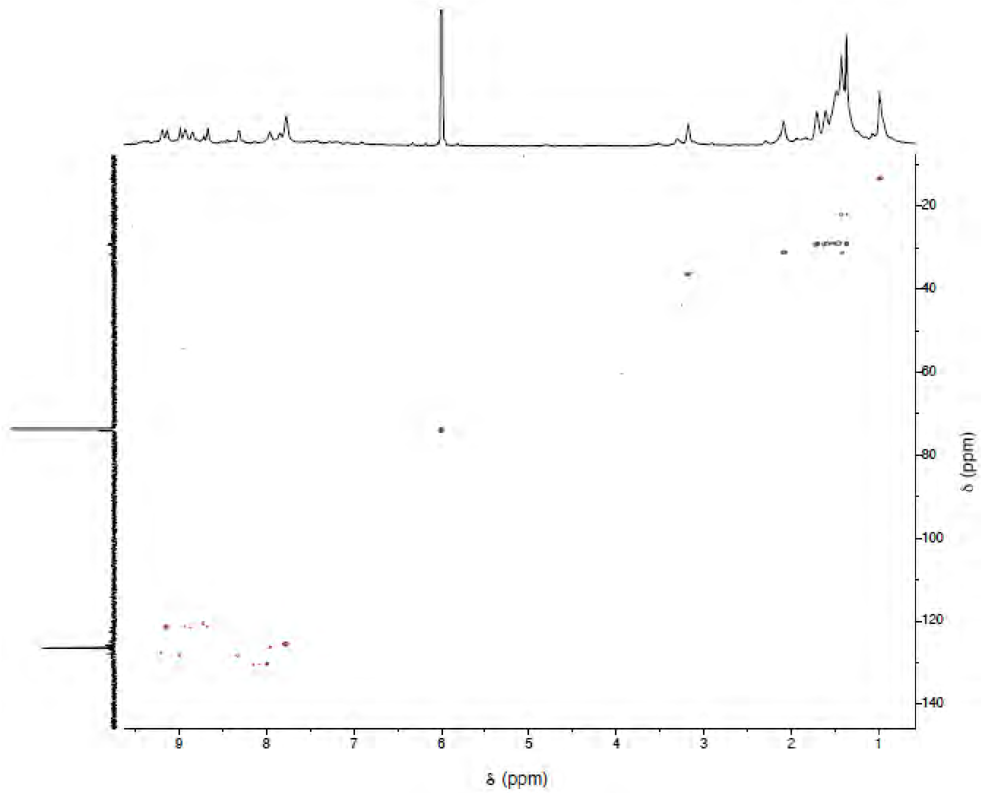



**Figure S81.** Partial HSQC spectrum of **5a-**$^{13}$***C***$_2$ showing the aromatic region (500 MHz, 125 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

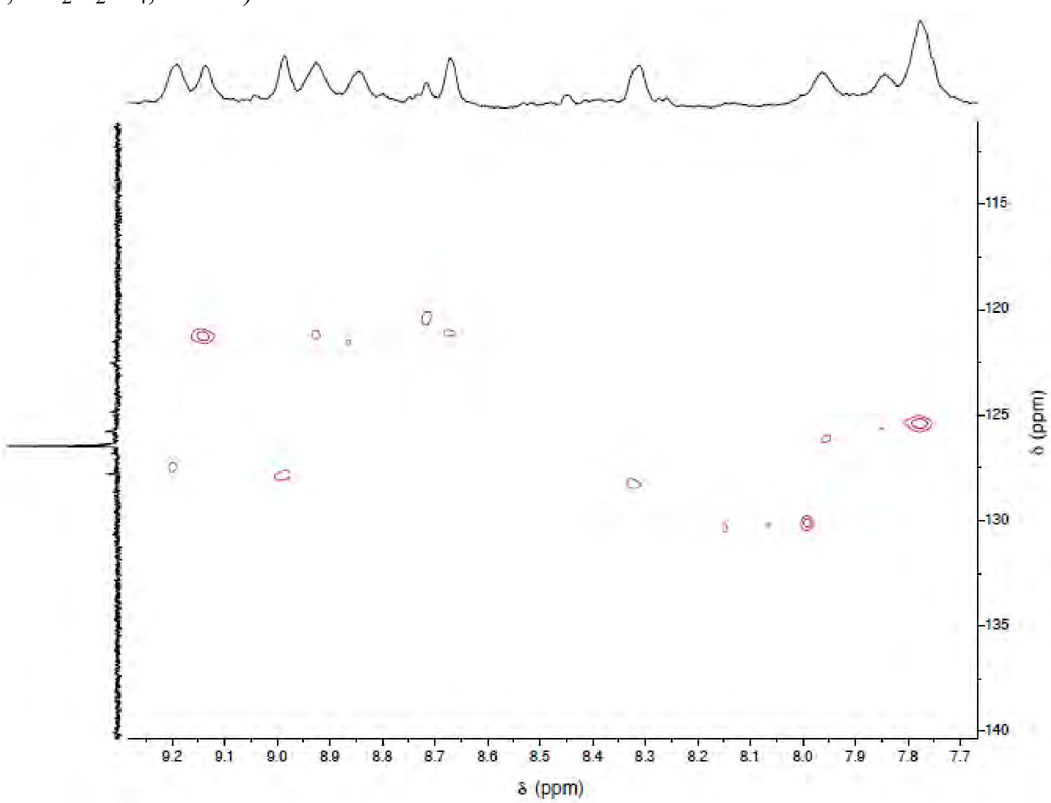


**Figure S82.** Full HMBC spectrum of **5a-*$^{13}C_2$*** (500 MHz, 125 MHz, 1,2-$C_2H_2Cl_4$, 408 K).

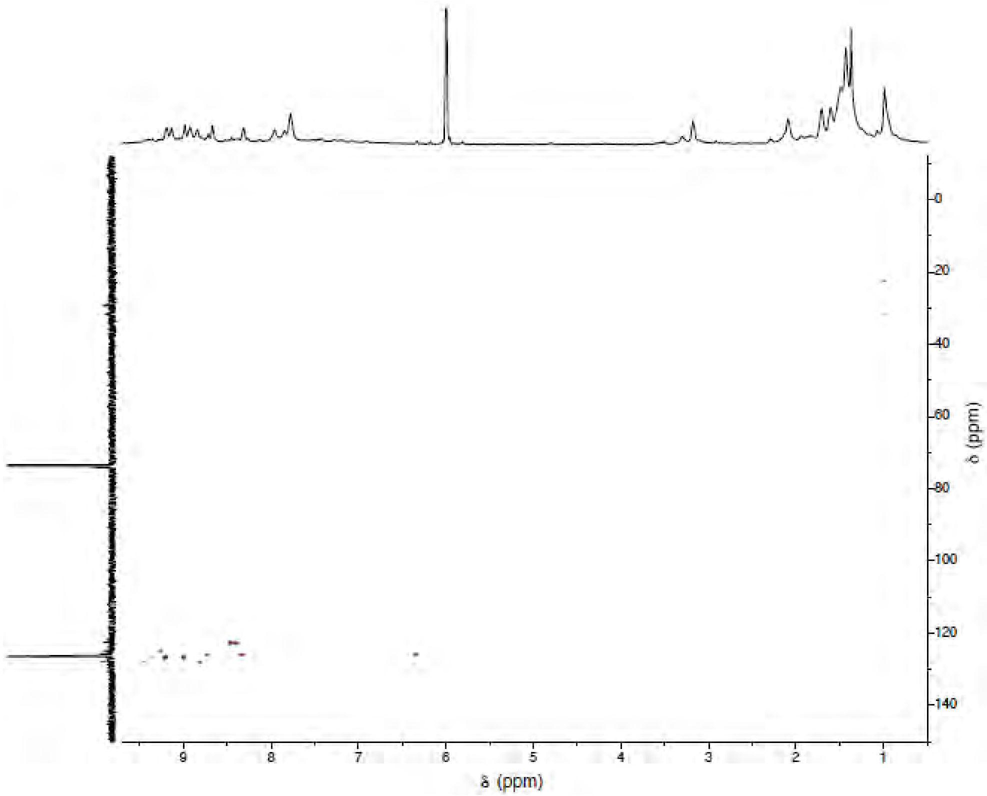
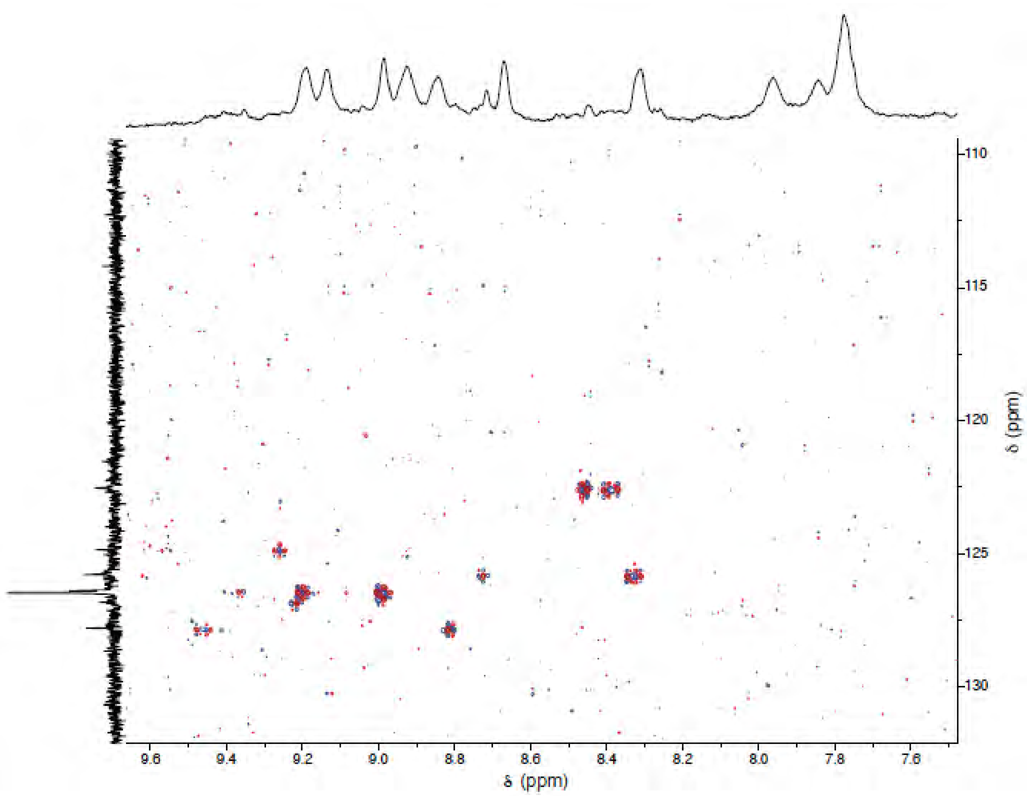


**Figure S83.** Partial HMBC spectrum of **5a-*$^{13}C_2$*** showing the aromatic region (500 MHz, 125 MHz, 1,2-$C_2H_2Cl_4$, 408 K).



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## E. UV/Vis and Fluorescence Spectroscopy

**Figure S84.** UV/Vis absorption spectra of the compounds **4a** (green) and **5a-$^{13}C_2$** (pink).

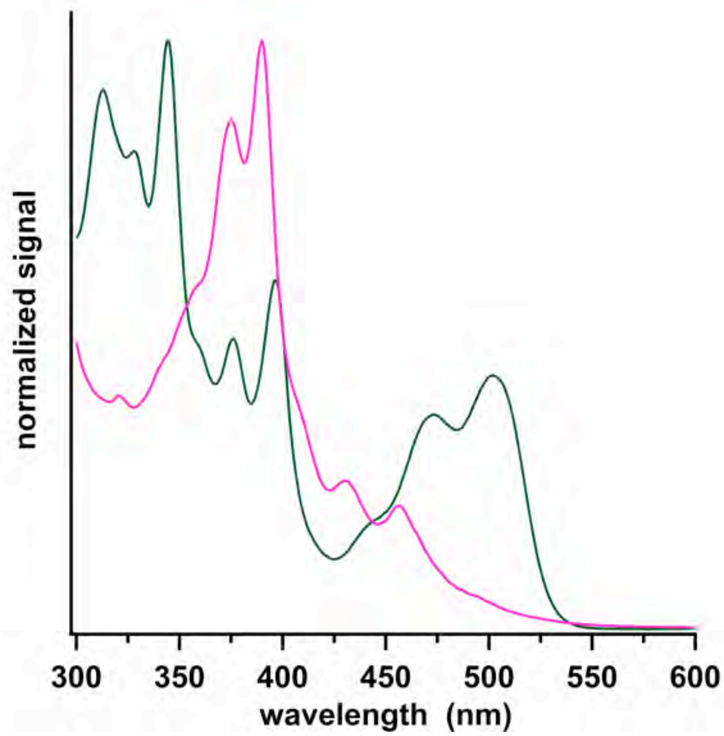
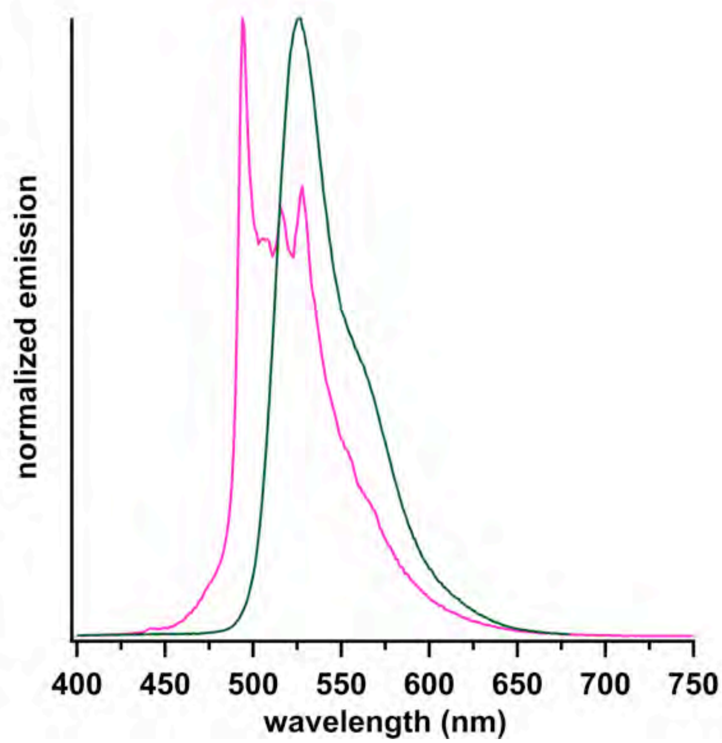


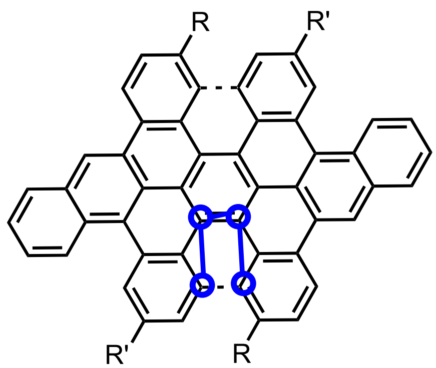

**Figure S85.** UV/Vis photoemission spectra of the compounds **4a** (green, $\lambda_{ex}$ = 344 nm) and **5a** (pink, $\lambda_{ex}$ = 389 nm).



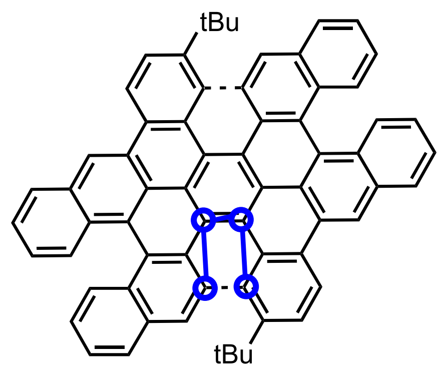
## F. DFT Calculations

DFT calculations were performed using the Gaussian 09 program, Revision A.02._ENREF_5[5] Geometries were optimized in the gas phase using the B3LYP functional and 6-31g(d) basis set on all atoms and confirmed as stationary states using frequency calculations. The torsional angles discussed the manuscript were measured from the dihedral angles illustrated in Figure S86.

**Figure S86.** Illustration of the dihedral angles measured in the optimized structures to represent torsion

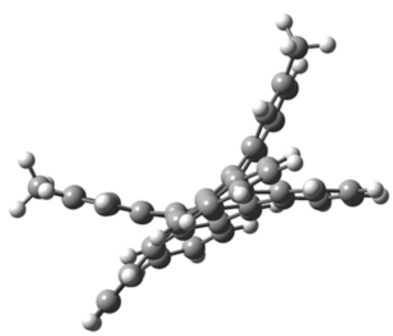



**4a, 4b, 4d**
**5a, 5b, 5d**

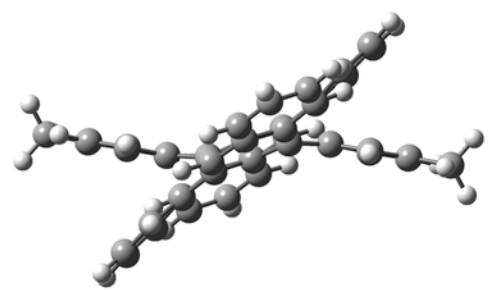



**4c, 5c**

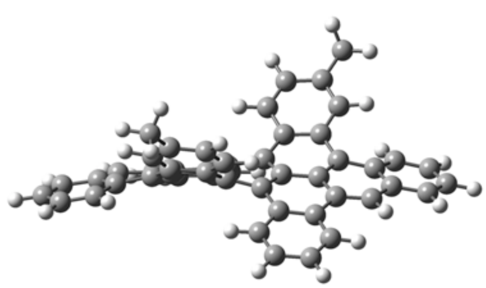
**Figure S87.** Two possible conformations of **4a**: twisted (left), and anti (right). The *n*-nonyl chains were truncated to methyl groups.



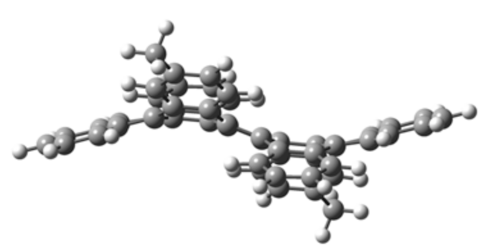
**4a-twisted angleview**



**4a-anti angleview**

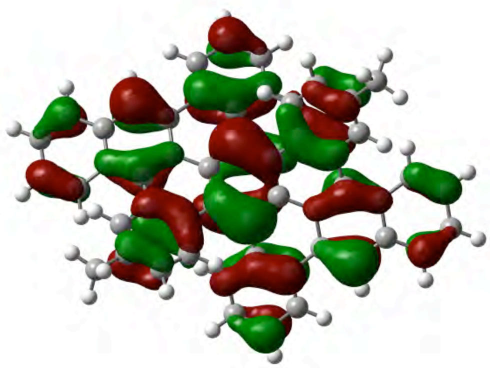
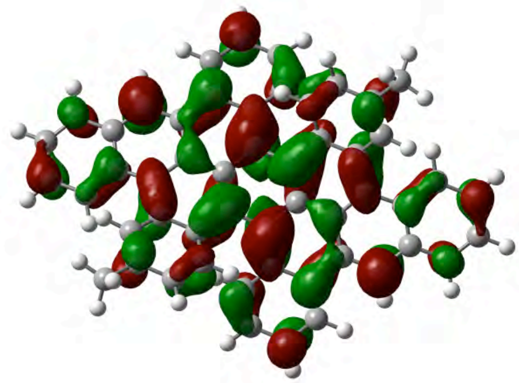
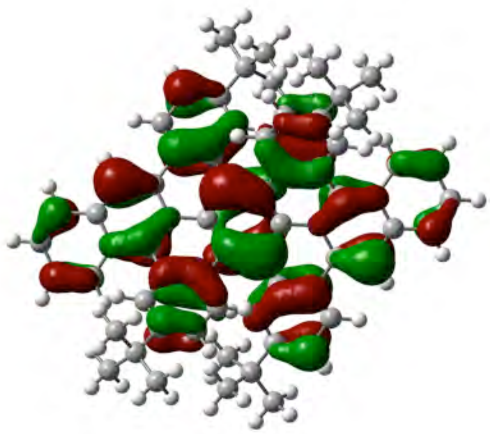
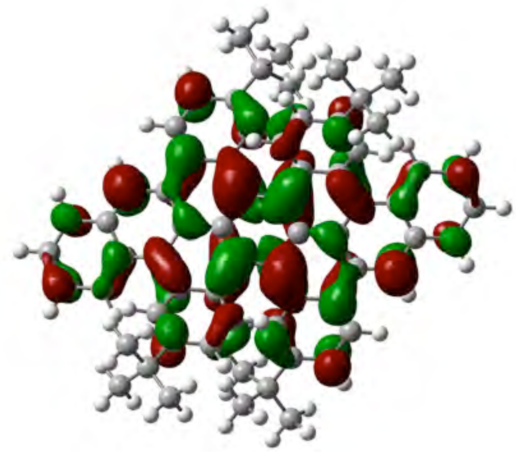
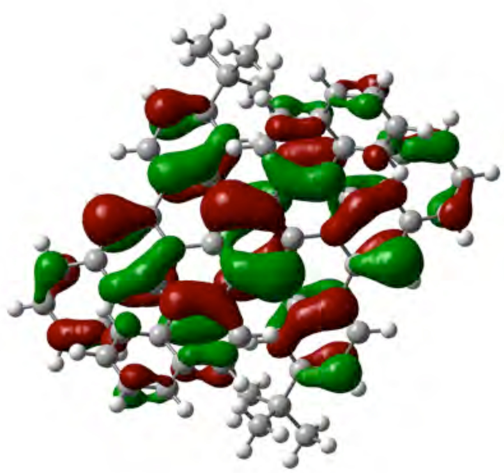
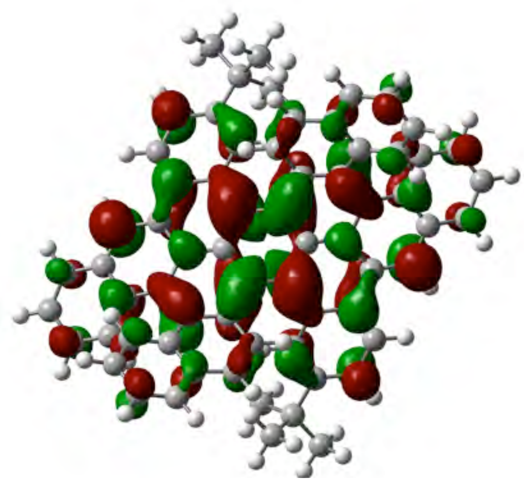


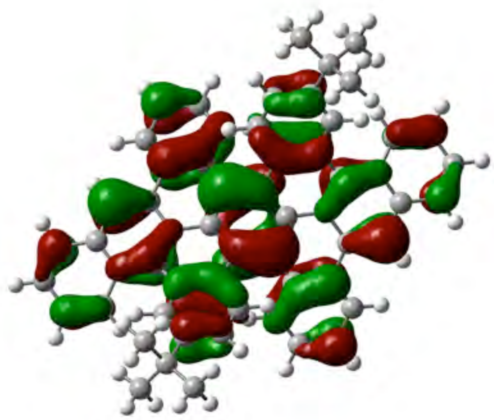
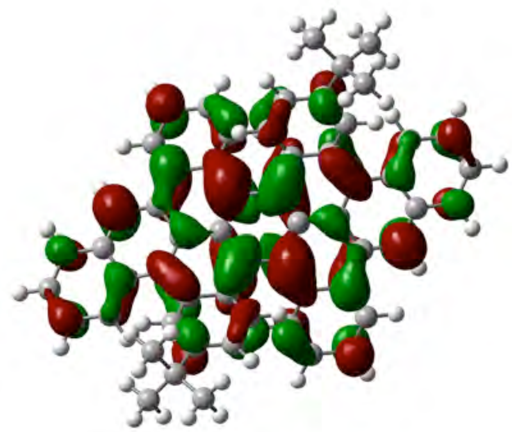
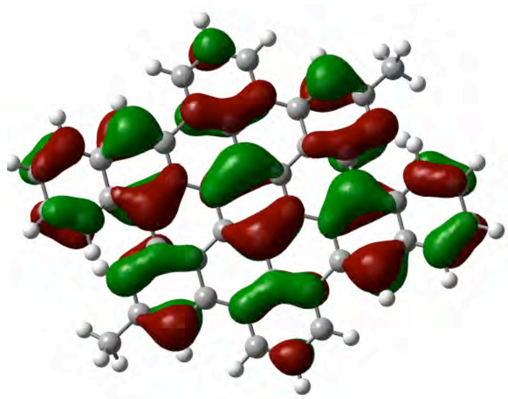
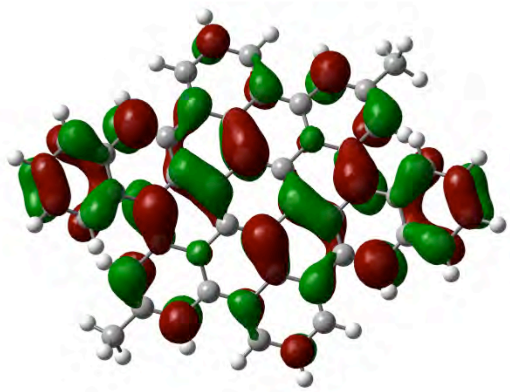
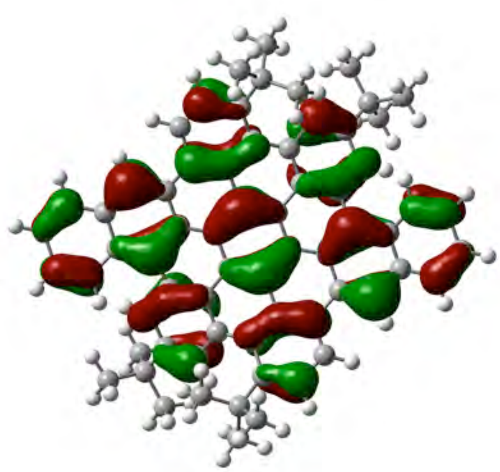
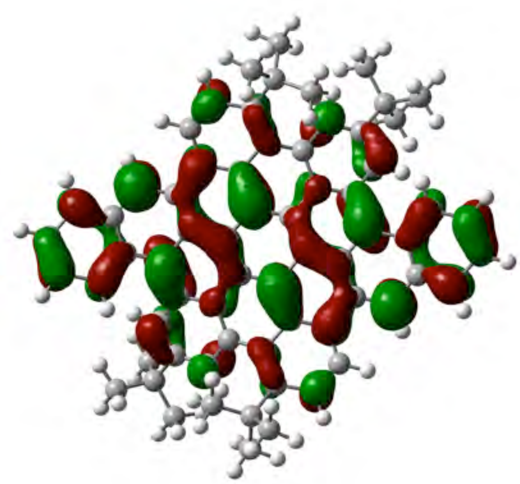
**4a-twisted sideview**



**4a-anti sideview**

**Table S1.** Calculated HOMOs and LUMOs of compounds **4a-d** and **5a-d**

| | **HOMO** | **LUMO** |
|---|---|---|
| **4a-truncated** |  |  |
| **4b** |  |  |
| **4c** |  |  |

| | **HOMO** | **LUMO** |
|---|---|---|
| **4d** |  |  |
| **5a-truncated** |  |  |
| **5b** |  |  |

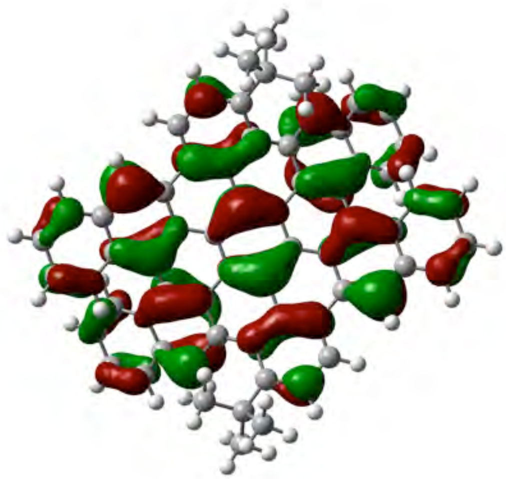
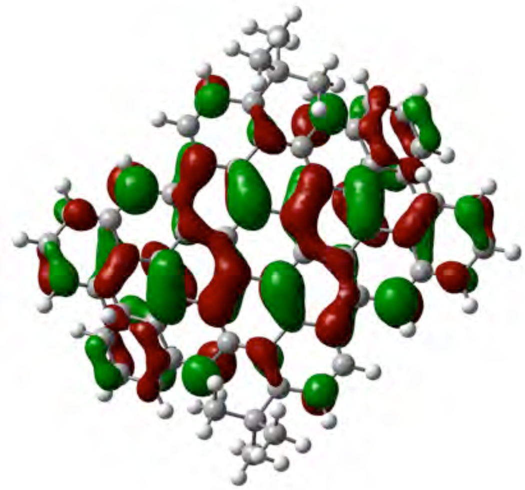
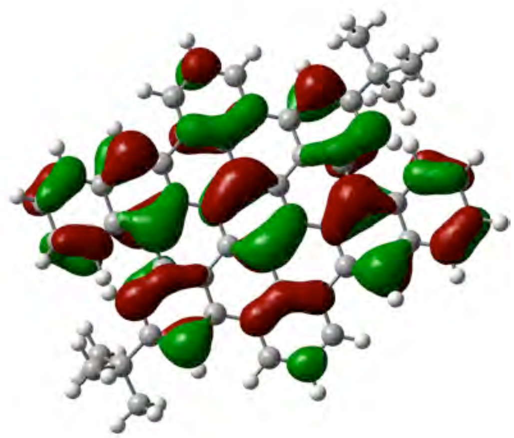
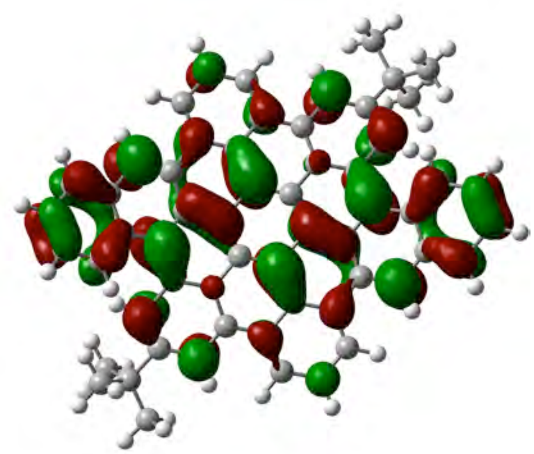
| | **HOMO** | **LUMO** |
|---|---|---|
| **5c** |  |  |
| **5d** |  |  |

**Table S2.** Cartesian coordinates of DFT computed geometries

**4a-truncated**

| | | | |
|---|---|---|---|
| C | 3.39268200 | 1.31642900 | 0.75578900 |
| C | 2.04837500 | 1.77231200 | 0.69533200 |
| C | 1.02926000 | 0.94419400 | 0.06252300 |
| C | 1.33427300 | -0.43412100 | -0.12692700 |

| | | | |
|---|---|---|---|
| C | 2.72069800 | -0.85098500 | -0.19797700 |
| C | 3.75681700 | 0.06912900 | 0.08522500 |
| C | -0.28606200 | 1.38239100 | -0.26403800 |
| C | 0.28601800 | -1.38243000 | -0.26409400 |
| C | -1.02927000 | -0.94423900 | 0.06264400 |
| C | -1.33430400 | 0.43408000 | -0.12675800 |
| C | -2.04830100 | -1.77234400 | 0.69559900 |
| C | 0.59605800 | -2.71707900 | -0.78363800 |
| C | 1.94718500 | -3.13229700 | -0.91288100 |
| C | 3.03330300 | -2.20847700 | -0.56342600 |
| C | -0.59616200 | 2.71705900 | -0.78349700 |
| C | -1.94730300 | 3.13228000 | -0.91257500 |
| C | -3.03338000 | 2.20845700 | -0.56300100 |
| C | -2.72073200 | 0.85095600 | -0.19761500 |
| C | -3.39258900 | -1.31644100 | 0.75625400 |
| C | -3.75681600 | -0.06915300 | 0.08572600 |
| C | -0.13214800 | -4.80490200 | -1.82644700 |
| C | 2.21267200 | -4.40797600 | -1.45701000 |
| C | 1.19745100 | -5.24314700 | -1.88978300 |
| C | -2.61868400 | -3.61016500 | 2.19936600 |
| C | -3.94724500 | -3.15185800 | 2.30100700 |
| C | -4.30005700 | -2.01314500 | 1.59187700 |
| H | -5.29539000 | -1.61039900 | 1.73524600 |
| C | -2.21285300 | 4.40797000 | -1.45664600 |
| C | -1.19768100 | 5.24315700 | -1.88950400 |
| H | -1.43798100 | 6.21729100 | -2.30657700 |
| C | 0.13192700 | 4.80491700 | -1.82631500 |
| H | 0.93571500 | 5.42707300 | -2.21016800 |
| C | 4.30025600 | 2.01315300 | 1.59126700 |
| C | 3.94752900 | 3.15188000 | 2.30043700 |
| C | 2.61892800 | 3.61010700 | 2.19905800 |
| H | 2.30404500 | 4.48289300 | 2.76677900 |
| C | 4.36278400 | -2.58675700 | -0.62949000 |
| C | 5.41545600 | -1.65467700 | -0.51854100 |
| C | 5.11754000 | -0.28521400 | -0.22457800 |
| C | 6.76146900 | -2.04911000 | -0.75746200 |
| C | 7.77644600 | -1.12305800 | -0.78882700 |
| H | 8.79875200 | -1.43317200 | -0.98701300 |
| C | 7.47393800 | 0.24676700 | -0.60803400 |
| H | 8.26092700 | 0.99001100 | -0.70373600 |

| | | | |
|---|---|---|---|
| C | 6.18543200 | 0.65127700 | -0.33225900 |
| H | 5.97398500 | 1.70990800 | -0.24534800 |
| C | -4.36286700 | 2.58674600 | -0.62887200 |
| C | -5.41552900 | 1.65466800 | -0.51779300 |
| C | -5.11758100 | 0.28520000 | -0.22388900 |
| C | -6.76157300 | 2.04911000 | -0.75652600 |
| C | -7.77655800 | 1.12306300 | -0.78776600 |
| H | -8.79888900 | 1.43318400 | -0.98580900 |
| C | -7.47403200 | -0.24676600 | -0.60703400 |
| H | -8.26103800 | -0.99000500 | -0.70264200 |
| C | -6.18549000 | -0.65128500 | -0.33144000 |
| H | -5.97403400 | -1.70991800 | -0.24457600 |
| H | -0.93597800 | -5.42704200 | -2.21023600 |
| H | -2.30375600 | -4.48301200 | 2.76697200 |
| H | 3.23706100 | -4.74207100 | -1.57288500 |
| H | 4.63424400 | -3.61544700 | -0.83881200 |
| H | 6.96563800 | -3.10015100 | -0.94828600 |
| H | 5.29561000 | 1.61041100 | 1.73451800 |
| H | -3.23725700 | 4.74206200 | -1.57240600 |
| H | -4.63435000 | 3.61544200 | -0.83813600 |
| H | -6.96576300 | 3.10015500 | -0.94730800 |
| C | 1.69511700 | 2.92499000 | 1.43708600 |
| H | 0.66268800 | 3.25306900 | 1.43892600 |
| C | 0.41843300 | 3.56149400 | -1.29292600 |
| H | 1.44557100 | 3.22022900 | -1.27731500 |
| C | -0.41859300 | -3.56149300 | -1.29299000 |
| H | -1.44572800 | -3.22022400 | -1.27726200 |
| C | -1.69497100 | -2.92506300 | 1.43727200 |
| H | -0.66256400 | -3.25320500 | 1.43890900 |
| C | -4.93996400 | -3.86309100 | 3.18887000 |
| H | -5.88808900 | -3.31937900 | 3.24662900 |
| H | -5.15675000 | -4.87241400 | 2.81499000 |
| H | -4.55436400 | -3.97735400 | 4.20948300 |
| C | 4.94050700 | 3.86334700 | 3.18782000 |
| H | 5.88759200 | 3.31806900 | 3.24789200 |
| H | 5.15960600 | 4.87139500 | 2.81181000 |
| H | 4.55394100 | 3.98072100 | 4.20769600 |
| H | 1.43770300 | -6.21726900 | -2.30690400 |

**4b**

| | | | |
|---|---|---|---|
| C | -3.56480700 | 0.72526800 | 0.73605700 |
| C | -2.67734600 | -0.38339500 | 0.67791500 |
| C | -1.37457200 | -0.23950600 | 0.03789200 |
| C | -0.88820900 | 1.08566400 | -0.15303000 |
| C | -1.83372800 | 2.18362700 | -0.22785800 |
| C | -3.20183200 | 1.96812900 | 0.05472300 |
| C | -0.50629200 | -1.31988700 | -0.28870000 |
| C | 0.50633400 | 1.31987200 | -0.28846000 |
| C | 1.37455300 | 0.23945900 | 0.03816700 |
| C | 0.88822700 | -1.08569100 | -0.15297300 |
| C | 2.67721100 | 0.38329700 | 0.67842500 |
| C | 0.96547700 | 2.61410900 | -0.80615300 |
| C | 0.04609600 | 3.68586100 | -0.94148300 |
| C | -1.36722300 | 3.49385000 | -0.59958300 |
| C | -0.96532400 | -2.61406000 | -0.80666300 |
| C | -0.04591600 | -3.68580100 | -0.94189700 |
| C | 1.36733200 | -3.49382500 | -0.59968700 |
| C | 1.83376400 | -2.18364200 | -0.22773500 |
| C | 3.56466000 | -0.72537100 | 0.73664500 |
| C | 3.20182200 | -1.96816600 | 0.05510400 |
| C | 2.73787300 | 3.97420300 | -1.85924100 |
| C | 0.51988300 | 4.89323700 | -1.48874500 |
| C | 1.82779300 | 5.04541800 | -1.91818300 |
| C | 4.14728900 | 1.60211100 | 2.20508700 |
| C | 5.02176500 | 0.50336700 | 2.30925900 |
| C | 4.69519400 | -0.63703800 | 1.57917600 |
| H | 5.30260900 | -1.52344700 | 1.70661600 |
| C | -0.51957900 | -4.89311700 | -1.48940000 |
| C | -1.82738300 | -5.04524100 | -1.91917600 |
| H | -2.12618300 | -6.00087300 | -2.33506700 |
| C | -2.73746700 | -3.97402100 | -1.86035400 |
| C | -4.69553400 | 0.63686200 | 1.57831600 |
| C | -5.02225100 | -0.50359700 | 2.30824700 |
| C | -4.14773100 | -1.60231900 | 2.20419900 |
| H | -4.33362500 | -2.50903400 | 2.76873300 |
| C | -2.28430100 | 4.52733600 | -0.67631400 |
| C | -3.67325300 | 4.30856400 | -0.56624600 |
| C | -4.15835700 | 2.99582700 | -0.26224800 |
| C | -4.59696300 | 5.36244900 | -0.81257000 |

| | | | |
|---|---|---|---|
| C | -5.95063500 | 5.12676600 | -0.84059400 |
| H | -6.64615700 | 5.93639800 | -1.04395300 |
| C | -6.43211400 | 3.81040900 | -0.64968300 |
| H | -7.49533900 | 3.60612100 | -0.74328800 |
| C | -5.56256300 | 2.77894700 | -0.36713900 |
| H | -5.95231800 | 1.77254700 | -0.27401800 |
| C | 2.28442800 | -4.52729400 | -0.67637900 |
| C | 3.67336000 | -4.30852200 | -0.56608400 |
| C | 4.15841000 | -2.99581200 | -0.26187700 |
| C | 4.59711000 | -5.36236800 | -0.81242200 |
| C | 5.95078100 | -5.12666400 | -0.84028300 |
| H | 6.64633500 | -5.93626300 | -1.04366400 |
| C | 6.43221700 | -3.81031700 | -0.64920600 |
| H | 7.49544500 | -3.60599800 | -0.74270700 |
| C | 5.56262100 | -2.77889700 | -0.36664300 |
| H | 5.95235200 | -1.77249900 | -0.27342300 |
| H | 4.33307300 | 2.50878600 | 2.76972300 |
| H | -0.15550800 | 5.73195900 | -1.61430000 |
| H | -1.95782000 | 5.53850100 | -0.89293800 |
| H | -4.20461700 | 6.35715900 | -1.01108900 |
| H | -5.30300000 | 1.52325200 | 1.70565500 |
| H | 0.15583700 | -5.73183000 | -1.61488100 |
| H | 1.95799000 | -5.53843400 | -0.89319100 |
| H | 4.20479800 | -6.35706000 | -1.01109800 |
| C | -3.00180500 | -1.53154700 | 1.43139200 |
| H | -2.31465500 | -2.36926500 | 1.43616100 |
| C | -2.27376100 | -2.78205500 | -1.30923600 |
| H | -2.94172600 | -1.93165600 | -1.27290500 |
| C | 2.27404200 | 2.78217300 | -1.30836300 |
| H | 2.94200800 | 1.93177900 | -1.27193700 |
| C | 3.00153100 | 1.53140400 | 1.43202800 |
| H | 2.31438600 | 2.36912900 | 1.43670400 |
| C | 6.26539000 | 0.50556300 | 3.21797400 |
| C | -6.26608200 | -0.50588400 | 3.21667800 |
| H | 2.12669100 | 6.00109800 | -2.33390000 |
| C | 6.10641700 | -0.57609700 | 4.31297200 |
| H | 5.99580700 | -1.57722300 | 3.88370500 |
| H | 6.98647200 | -0.58838100 | 4.96792700 |
| H | 5.22414800 | -0.37862900 | 4.93226900 |
| C | 7.52453500 | 0.19685200 | 2.37328700 |

| | | | |
|---|---|---|---|
| H | 8.41900500 | 0.19425700 | 3.00826700 |
| H | 7.45969000 | -0.78283600 | 1.88807600 |
| H | 7.66640200 | 0.95076300 | 1.59024000 |
| C | 6.47788100 | 1.86451400 | 3.91275100 |
| H | 6.60518400 | 2.67783900 | 3.18907500 |
| H | 5.64213200 | 2.12139800 | 4.57337700 |
| H | 7.38314400 | 1.82534900 | 4.52910400 |
| C | -6.47878100 | -1.86494000 | 3.91118900 |
| H | -6.60593600 | -2.67814500 | 3.18735600 |
| H | -5.64319500 | -2.12195600 | 4.57197300 |
| H | -7.38418900 | -1.82584700 | 4.52733400 |
| C | -7.52502400 | -0.19698800 | 2.37175700 |
| H | -8.41964200 | -0.19450900 | 3.00653000 |
| H | -7.46005400 | 0.78279600 | 1.88675600 |
| H | -7.66671700 | -0.95074100 | 1.58852700 |
| C | -6.10731000 | 0.57559700 | 4.31188200 |
| H | -5.22524000 | 0.37794500 | 4.93140600 |
| H | -5.99647100 | 1.57677500 | 3.88279600 |
| H | -6.98755200 | 0.58788000 | 4.96658500 |
| C | 4.18403700 | 4.07604000 | -2.37940300 |
| C | 5.16633000 | 3.87622000 | -1.20054000 |
| C | 4.43404700 | 2.98442300 | -3.44655200 |
| C | 4.47675200 | 5.44576800 | -3.02139100 |
| H | 5.03100900 | 4.65740400 | -0.44328400 |
| H | 5.02219900 | 2.90926300 | -0.70844500 |
| H | 6.20346400 | 3.92459100 | -1.55563500 |
| H | 3.75152100 | 3.10283700 | -4.29584000 |
| H | 5.46183100 | 3.05158600 | -3.82385900 |
| H | 4.29448500 | 1.97633000 | -3.04352700 |
| H | 5.51159800 | 5.47027900 | -3.38092300 |
| H | 3.82342400 | 5.64242600 | -3.87923500 |
| H | 4.35872300 | 6.26721100 | -2.30547100 |
| C | -4.18349200 | -4.07575700 | -2.38092700 |
| C | -5.16611300 | -3.87587900 | -1.20234800 |
| C | -4.43309800 | -2.98408500 | -3.44811200 |
| C | -4.47614700 | -5.44544400 | -3.02303200 |
| H | -5.03107100 | -4.65708300 | -0.44506300 |
| H | -5.02205600 | -2.90894000 | -0.71019600 |
| H | -6.20314600 | -3.92416800 | -1.55774600 |
| H | -3.75035000 | -3.10254300 | -4.29721500 |

| | | | |
|---|---|---|---|
| H | -5.46078600 | -3.05112900 | -3.82570300 |
| H | -4.29353700 | -1.97602100 | -3.04501200 |
| H | -5.51090900 | -5.46987600 | -3.38280900 |
| H | -3.82263400 | -5.64211800 | -3.88073100 |
| H | -4.35833900 | -6.26691600 | -2.30711000 |

**4c**

| | | | |
|---|---|---|---|
| C | 3.58200200 | -0.26334700 | 1.04151500 |
| C | 2.58688800 | 0.73031700 | 0.92355600 |
| C | 1.33039600 | 0.42681100 | 0.25146700 |
| C | 1.01992600 | -0.95000700 | 0.04703500 |
| C | 2.11457700 | -1.88389700 | -0.08086300 |
| C | 3.43117700 | -1.47572100 | 0.23789300 |
| C | 0.32527400 | 1.37772200 | -0.09460600 |
| C | -0.32524400 | -1.37770400 | -0.09467600 |
| C | -1.33037300 | -0.42680200 | 0.25139200 |
| C | -1.01990500 | 0.95002200 | 0.04703800 |
| C | -2.58688200 | -0.73033800 | 0.92343400 |
| C | -0.59360500 | -2.71008900 | -0.64451500 |
| C | 0.47943800 | -3.61528800 | -0.86268900 |
| C | 1.86094100 | -3.20712300 | -0.58380600 |
| C | 0.59365900 | 2.71011100 | -0.64440800 |
| C | -0.47936400 | 3.61534900 | -0.86249300 |
| C | -1.86087000 | 3.20719900 | -0.58359400 |
| C | -2.11456000 | 1.88391400 | -0.08082200 |
| C | -3.58209300 | 0.26324300 | 1.04131500 |
| C | -3.43119300 | 1.47571200 | 0.23781600 |
| C | -2.17520800 | -4.30748000 | -1.66970100 |
| C | 0.17410600 | -4.87219700 | -1.41745400 |
| C | -1.11233700 | -5.22025500 | -1.79531900 |
| C | -3.81007900 | -2.19465200 | 2.44507300 |
| C | -0.17401500 | 4.87227200 | -1.41722100 |
| C | 1.11242100 | 5.22029900 | -1.79513600 |
| H | 1.27781400 | 6.20385500 | -2.22007100 |
| C | 2.17526400 | 4.30747500 | -1.66963100 |
| C | 3.81033100 | 2.19458600 | 2.44504700 |
| H | 3.90520800 | 3.14140800 | 2.97110500 |
| C | 2.94282800 | -4.02686500 | -0.85822300 |
| C | 4.27259900 | -3.56151400 | -0.78035300 |
| C | 4.53402100 | -2.25186800 | -0.26546900 |

| | | | |
|---|---|---|---|
| C | 5.35225400 | -4.35575500 | -1.26096400 |
| C | 6.63135500 | -3.85643800 | -1.30803000 |
| H | 7.44512300 | -4.46496100 | -1.69292400 |
| C | 6.88016400 | -2.52830300 | -0.88426700 |
| H | 7.88076300 | -2.11345500 | -0.97044100 |
| C | 5.86323300 | -1.75315300 | -0.37387900 |
| H | 6.07146900 | -0.73534400 | -0.06701500 |
| C | -2.94271300 | 4.02704400 | -0.85786900 |
| C | -4.27249900 | 3.56175300 | -0.78006300 |
| C | -4.53397400 | 2.25201700 | -0.26543900 |
| C | -5.35211900 | 4.35616900 | -1.26047500 |
| C | -6.63125500 | 3.85695400 | -1.30758700 |
| H | -7.44500200 | 4.46561000 | -1.69231700 |
| C | -6.88012600 | 2.52874500 | -0.88409500 |
| H | -7.88075100 | 2.11397100 | -0.97032100 |
| C | -5.86322600 | 1.75342800 | -0.37390100 |
| H | -6.07153000 | 0.73555600 | -0.06730400 |
| H | -3.90478400 | -3.14142500 | 2.97125000 |
| H | 0.96253600 | -5.59923000 | -1.57570800 |
| H | 2.79258300 | -5.03445300 | -1.22967200 |
| H | 5.13581600 | -5.35872700 | -1.62148300 |
| H | -0.96242500 | 5.59933700 | -1.57542500 |
| H | -2.79241800 | 5.03468800 | -1.22914200 |
| H | -5.13561800 | 5.35920100 | -1.62079000 |
| C | 2.73446000 | 1.96077300 | 1.64026300 |
| H | 1.95923100 | 2.71127900 | 1.55485100 |
| C | 1.88122400 | 3.07227700 | -1.09737300 |
| H | 2.67355700 | 2.34049800 | -1.00769200 |
| C | -1.88118200 | -3.07229100 | -1.09741300 |
| H | -2.67353800 | -2.34054600 | -1.00766800 |
| C | -2.73428500 | -1.96076700 | 1.64021500 |
| H | -1.95894500 | -2.71116400 | 1.55484500 |
| H | -1.27771900 | -6.20380300 | -2.22027600 |
| C | -3.60778500 | -4.62004000 | -2.14134300 |
| C | -4.56715700 | -4.58625200 | -0.92820000 |
| C | -4.05463700 | -3.56224300 | -3.17836400 |
| C | -3.71390600 | -6.00863600 | -2.80068500 |
| H | -4.28921500 | -5.34708700 | -0.18942500 |
| H | -4.55443700 | -3.61465000 | -0.42435000 |
| H | -5.59646100 | -4.78676100 | -1.25048400 |

| | | | |
|---|---|---|---|
| H | -3.39138900 | -3.56290000 | -4.05086700 |
| H | -5.07291800 | -3.77738300 | -3.52486600 |
| H | -4.05407000 | -2.55110700 | -2.75898300 |
| H | -4.74522600 | -6.18352900 | -3.12727400 |
| H | -3.06909100 | -6.09227300 | -3.68315800 |
| H | -3.44902100 | -6.81338100 | -2.10528300 |
| C | 3.60782900 | 4.62001800 | -2.14132400 |
| C | 4.56731100 | 4.58573100 | -0.92828300 |
| C | 4.05446800 | 3.56251400 | -3.17873700 |
| C | 3.71403600 | 6.00881600 | -2.80022700 |
| H | 4.28955500 | 5.34639300 | -0.18926100 |
| H | 4.55448200 | 3.61398200 | -0.42471700 |
| H | 5.59661600 | 4.78617400 | -1.25060400 |
| H | 3.39110200 | 3.56349200 | -4.05114900 |
| H | 5.07271600 | 3.77769800 | -3.52530900 |
| H | 4.05389700 | 2.55124500 | -2.75968000 |
| H | 4.74529300 | 6.18360800 | -3.12706900 |
| H | 3.06896600 | 6.09288400 | -3.68247300 |
| H | 3.44953300 | 6.81338100 | -2.10447200 |
| C | 4.76319700 | 1.16842800 | 2.70203900 |
| C | 4.61868300 | -0.09626000 | 2.04777600 |
| C | 6.40413600 | -0.95964900 | 3.48162200 |
| H | 7.00469900 | -1.80026300 | 3.81863000 |
| C | 6.60594100 | 0.31815000 | 4.04439600 |
| H | 7.37887700 | 0.47034100 | 4.79277600 |
| C | 5.43929300 | -1.15960700 | 2.51577200 |
| H | 5.29265300 | -2.15709400 | 2.12383400 |
| C | 5.78491300 | 1.35734800 | 3.66637800 |
| H | 5.88559000 | 2.33748800 | 4.12680600 |
| C | -4.76311700 | -1.16862700 | 2.70193300 |
| C | -4.61887000 | 0.09599700 | 2.04747200 |
| C | -5.78479200 | -1.35763600 | 3.66630000 |
| H | -5.88521900 | -2.33771200 | 4.12691100 |
| C | -6.60616300 | -0.31861900 | 4.04405100 |
| H | -7.37904300 | -0.47086200 | 4.79247600 |
| C | -6.40481700 | 0.95908700 | 3.48090800 |
| H | -7.00577700 | 1.79955500 | 3.81756900 |
| C | -5.43993000 | 1.15914100 | 2.51512600 |
| H | -5.29386300 | 2.15648100 | 2.12263000 |

**4d**

| | | | |
|---|---|---|---|
| C | -3.61557100 | -0.39493200 | 0.32054500 |
| C | -2.43497700 | -1.18429300 | 0.25505200 |
| C | -1.23732200 | -0.64746200 | -0.38074600 |
| C | -1.17741900 | 0.76274900 | -0.56995300 |
| C | -2.41028700 | 1.52309000 | -0.64232000 |
| C | -3.64768700 | 0.90224600 | -0.35575300 |
| C | -0.07941400 | -1.40944500 | -0.70771900 |
| C | 0.07940700 | 1.40947000 | -0.70770600 |
| C | 1.23731500 | 0.64748300 | -0.38074100 |
| C | 1.17741200 | -0.76272600 | -0.56996600 |
| C | 2.43497000 | 1.18430100 | 0.25507300 |
| C | 0.12323900 | 2.77840400 | -1.22924900 |
| C | -1.07603900 | 3.52533200 | -1.36582600 |
| C | -2.36339300 | 2.91345600 | -1.01425300 |
| C | -0.12325000 | -2.77837900 | -1.22925700 |
| C | 1.07602600 | -3.52530600 | -1.36585400 |
| C | 2.36338500 | -2.91342700 | -1.01430100 |
| C | 2.41028000 | -1.52306600 | -0.64235000 |
| C | 3.61556700 | 0.39494200 | 0.32053900 |
| C | 3.64768100 | -0.90222400 | -0.35578300 |
| C | 1.36530400 | 4.60456800 | -2.27769700 |
| C | -1.00457300 | 4.82249300 | -1.91920500 |
| C | 0.19191900 | 5.36723700 | -2.35180500 |
| C | 3.46896500 | 2.80421300 | 1.76569800 |
| C | 4.63202600 | 2.01906900 | 1.88071600 |
| C | 4.66480300 | 0.82590200 | 1.16269500 |
| H | 5.51049200 | 0.16488700 | 1.30002100 |
| C | 1.00454800 | -4.82247200 | -1.91922000 |
| C | -0.19195300 | -5.36722100 | -2.35178800 |
| H | -0.21011900 | -6.36725500 | -2.77633700 |
| C | -1.36533800 | -4.60455500 | -2.27765500 |
| H | -2.30322800 | -4.99825200 | -2.65957500 |
| C | -4.66480200 | -0.82591000 | 1.16270000 |
| C | -4.63202400 | -2.01910300 | 1.88067700 |
| C | -3.46896900 | -2.80424600 | 1.76563600 |
| H | -3.37430100 | -3.73171000 | 2.31899200 |
| C | -3.55113400 | 3.62070400 | -1.08302000 |
| C | -4.80789200 | 2.99134600 | -0.96743300 |
| C | -4.87152300 | 1.59262400 | -0.66694300 |

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|---|---|---|---|
| C | -6.00823700 | 3.71713200 | -1.20668300 |
| C | -7.22714800 | 3.08293100 | -1.23167300 |
| H | -8.13595500 | 3.64449300 | -1.42980000 |
| C | -7.28655000 | 1.68191700 | -1.04491600 |
| H | -8.23829400 | 1.16552900 | -1.13688500 |
| C | -6.14464200 | 0.96115700 | -0.76881600 |
| H | -6.21140400 | -0.11624600 | -0.67903000 |
| C | 3.55112800 | -3.62067100 | -1.08308800 |
| C | 4.80788500 | -2.99131300 | -0.96749600 |
| C | 4.87151600 | -1.59259700 | -0.66698000 |
| C | 6.00823000 | -3.71709500 | -1.20675800 |
| C | 7.22714200 | -3.08289500 | -1.23173100 |
| H | 8.13594900 | -3.64445300 | -1.42986600 |
| C | 7.28654500 | -1.68188500 | -1.04494100 |
| H | 8.23829000 | -1.16549600 | -1.13689000 |
| C | 6.14463700 | -0.96112900 | -0.76882900 |
| H | 6.21140100 | 0.11627100 | -0.67901200 |
| H | 2.30318400 | 4.99825800 | -2.65964600 |
| H | 3.37429100 | 3.73166000 | 2.31907600 |
| H | -1.90923100 | 5.40625400 | -2.04276800 |
| H | -3.54905700 | 4.68369400 | -1.29704500 |
| H | -5.93615900 | 4.78443000 | -1.40273800 |
| H | -5.51048100 | -0.16489100 | 1.30006200 |
| H | 1.90920400 | -5.40623500 | -2.04279300 |
| H | 3.54905200 | -4.68365900 | -1.29712700 |
| H | 5.93615200 | -4.78438900 | -1.40283300 |
| C | -2.39855400 | -2.38442800 | 0.99641000 |
| H | -1.49155200 | -2.97702700 | 0.99568700 |
| C | -1.32205700 | -3.33267300 | -1.73637500 |
| H | -2.22745000 | -2.74014600 | -1.71277900 |
| C | 1.32203300 | 3.33269000 | -1.73640500 |
| H | 2.22742400 | 2.74015900 | -1.71283500 |
| C | 2.39854600 | 2.38441100 | 0.99646800 |
| H | 1.49154200 | 2.97700700 | 0.99576800 |
| C | 5.81466600 | 2.40269500 | 2.79005100 |
| C | -5.81463800 | -2.40275900 | 2.79002400 |
| H | 0.21007700 | 6.36726500 | -2.77636500 |
| C | 5.97638700 | 1.33850300 | 3.90185000 |
| H | 6.16924200 | 0.34327500 | 3.48793000 |
| H | 6.81722500 | 1.59684000 | 4.55741600 |

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|---|---|---|---|
| H | 5.07204200 | 1.27508800 | 4.51753600 |
| C | 7.11360200 | 2.46745600 | 1.95199700 |
| H | 7.96501000 | 2.73912100 | 2.58801300 |
| H | 7.34451600 | 1.50531700 | 1.48257900 |
| H | 7.03085500 | 3.21777000 | 1.15717100 |
| C | 5.61189200 | 3.77380900 | 3.46324600 |
| H | 5.49528800 | 4.57696800 | 2.72655200 |
| H | 4.73458400 | 3.78166400 | 4.11989600 |
| H | 6.48530700 | 4.01432300 | 4.07983600 |
| C | -5.61175500 | -3.77384800 | 3.46323400 |
| H | -5.49515200 | -4.57701600 | 2.72654800 |
| H | -4.73440400 | -3.78164400 | 4.11982800 |
| H | -6.48511900 | -4.01439300 | 4.07988400 |
| C | -7.11358600 | -2.46761200 | 1.95199100 |
| H | -7.96496900 | -2.73931300 | 2.58802500 |
| H | -7.34456900 | -1.50550000 | 1.48255200 |
| H | -7.03080600 | -3.21794100 | 1.15718300 |
| C | -5.97638300 | -1.33855100 | 3.90180500 |
| H | -5.07202100 | -1.27507700 | 4.51746000 |
| H | -6.16930000 | -0.34334200 | 3.48786900 |
| H | -6.81718500 | -1.59692000 | 4.55740500 |

**5a-truncated**

| | | | |
|---|---|---|---|
| C | -3.54123600 | -1.28547800 | -0.22792500 |
| C | -2.21064400 | -1.79348900 | -0.27671800 |
| C | -1.09309400 | -0.89660300 | -0.15302700 |
| C | -1.32967500 | 0.50379900 | -0.10841500 |
| C | -2.67703000 | 1.00453800 | 0.04058800 |
| C | -3.76135800 | 0.10629900 | 0.15780000 |
| C | 0.23306400 | -1.40139900 | -0.16071100 |
| C | -0.23305300 | 1.40140700 | -0.16063000 |
| C | 1.09310500 | 0.89660900 | -0.15293000 |
| C | 1.32968400 | -0.50379400 | -0.10840300 |
| C | 2.21066500 | 1.79349500 | -0.27653000 |
| C | 1.99396200 | 3.17593000 | -0.53498500 |
| C | 0.63524700 | 3.71398000 | -0.44375800 |
| C | -0.45969700 | 2.82698600 | -0.23665700 |
| C | -1.78103000 | 3.34327600 | -0.12633400 |
| C | -2.89838800 | 2.42397400 | 0.11905900 |
| C | -1.99393000 | -3.17591000 | -0.53525300 |

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|---|---|---|---|
| C | -0.63520400 | -3.71395300 | -0.44411700 |
| C | 0.45971900 | -2.82697000 | -0.23686800 |
| C | 1.78105700 | -3.34325400 | -0.12657700 |
| C | 2.89838200 | -2.42397500 | 0.11904400 |
| C | 2.67703400 | -1.00453800 | 0.04062700 |
| C | 3.54125500 | 1.28548000 | -0.22774000 |
| C | 3.76136000 | -0.10631200 | 0.15794100 |
| C | 0.38200700 | 5.09131300 | -0.53759100 |
| C | -1.98135300 | 4.72429000 | -0.25166900 |
| C | -0.91103800 | 5.58831600 | -0.45186400 |
| H | -1.08751700 | 6.65692000 | -0.53832400 |
| C | 3.08835200 | 3.97845900 | -0.88198700 |
| C | 4.37973200 | 3.46041800 | -0.98219700 |
| C | 4.58949600 | 2.12461400 | -0.64412300 |
| H | 5.58527200 | 1.71395800 | -0.75816200 |
| C | 1.98142800 | -4.72423300 | -0.25218500 |
| C | 0.91113700 | -5.58824800 | -0.45256900 |
| H | 1.08764500 | -6.65682800 | -0.53926200 |
| C | -0.38192000 | -5.09126200 | -0.53820300 |
| H | -1.19993200 | -5.78983800 | -0.66787000 |
| C | -4.58947200 | -2.12459900 | -0.64435000 |
| C | -4.37970600 | -3.46039700 | -0.98244400 |
| C | -3.08832400 | -3.97843500 | -0.88225400 |
| H | -2.93699300 | -5.02303400 | -1.13221000 |
| C | -4.16945200 | 2.88325900 | 0.40945000 |
| C | -5.23014600 | 2.00921000 | 0.72499000 |
| C | -5.02738000 | 0.59308000 | 0.64716600 |
| C | -6.48214800 | 2.52328800 | 1.16317500 |
| C | -7.48517900 | 1.68433000 | 1.58505000 |
| H | -8.43362600 | 2.08815000 | 1.92842600 |
| C | -7.25505400 | 0.28951400 | 1.61566500 |
| H | -8.01517900 | -0.37389100 | 2.01937800 |
| C | -6.06522600 | -0.23747400 | 1.16160600 |
| H | -5.89979700 | -1.30348400 | 1.25009200 |
| C | 4.16939700 | -2.88328600 | 0.40960300 |
| C | 5.23007400 | -2.00925200 | 0.72524700 |
| C | 5.02734600 | -0.59311700 | 0.64737600 |
| C | 6.48202400 | -2.52335000 | 1.16355600 |
| C | 7.48504700 | -1.68440600 | 1.58547900 |
| H | 8.43345500 | -2.08824100 | 1.92894300 |

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|---|---|---|---|
| C | 7.25496300 | -0.28958200 | 1.61601700 |
| H | 8.01508200 | 0.37381600 | 2.01975300 |
| C | 6.06518300 | 0.23742400 | 1.16185500 |
| H | 5.89978300 | 1.30344200 | 1.25029100 |
| H | 1.20004900 | 5.78988500 | -0.66709100 |
| H | 2.93701000 | 5.02305800 | -1.13194200 |
| H | -2.98150300 | 5.13863700 | -0.20500000 |
| H | -4.37091300 | 3.94681600 | 0.47330900 |
| H | -6.61819200 | 3.60208900 | 1.18293200 |
| H | -5.58524500 | -1.71394100 | -0.75839600 |
| H | 2.98160000 | -5.13854300 | -0.20562100 |
| H | 4.37081100 | -3.94685000 | 0.47351800 |
| H | 6.61803600 | -3.60215400 | 1.18335800 |
| C | 5.52881000 | 4.33515300 | -1.42761000 |
| H | 5.91643400 | 4.93869200 | -0.59584400 |
| H | 6.36091700 | 3.73610100 | -1.81150200 |
| H | 5.22133000 | 5.03128400 | -2.21575600 |
| C | -5.52878300 | -4.33513100 | -1.42786400 |
| H | -5.91636200 | -4.93872400 | -0.59611600 |
| H | -6.36091600 | -3.73607400 | -1.81169000 |
| H | -5.22131900 | -5.03121100 | -2.21606000 |

**5b**

| | | | |
|---|---|---|---|
| C | -3.49875300 | -1.23935500 | 0.30266100 |
| C | -2.82529500 | -0.01964400 | 0.01764100 |
| C | -1.40513400 | -0.01368600 | -0.18924200 |
| C | -0.69466900 | -1.24317500 | -0.17920100 |
| C | -1.42250000 | -2.49174300 | -0.14815400 |
| C | -2.83027200 | -2.49995600 | -0.01492900 |
| C | -0.72247500 | 1.22976400 | -0.21388600 |
| C | 0.72248700 | -1.22975500 | -0.21388800 |
| C | 1.40515000 | 0.01369600 | -0.18925800 |
| C | 0.69468500 | 1.24318300 | -0.17921300 |
| C | 2.82531300 | 0.01965700 | 0.01762000 |
| C | 3.53758000 | -1.20318200 | 0.10356400 |
| C | 2.90221400 | -2.44008200 | -0.36359900 |
| C | 1.46985800 | -2.46928500 | -0.29133400 |
| C | 0.76863100 | -3.70026900 | -0.34659800 |
| C | -0.69303800 | -3.72799000 | -0.24353100 |

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|---|---|---|---|
| C | -3.53756800 | 1.20319000 | 0.10358500 |
| C | -2.90221400 | 2.44009700 | -0.36358100 |
| C | -1.46985200 | 2.46929100 | -0.29134100 |
| C | -0.76860700 | 3.70026700 | -0.34665100 |
| C | 0.69306300 | 3.72799000 | -0.24356700 |
| C | 1.42252300 | 2.49174600 | -0.14817400 |
| C | 3.49877400 | 1.23935900 | 0.30265700 |
| C | 2.83029500 | 2.49995900 | -0.01493400 |
| C | 3.60355900 | -3.59816600 | -0.80706600 |
| C | 1.52568400 | -4.86781700 | -0.50111200 |
| C | 2.88192700 | -4.80266900 | -0.76838900 |
| H | 3.39110200 | -5.73338600 | -0.99401000 |
| C | 4.76850900 | -1.21352300 | 0.77612100 |
| C | 5.35895100 | -0.04537400 | 1.26889700 |
| C | 4.73303300 | 1.16982500 | 0.96926400 |
| H | 5.17378600 | 2.08902200 | 1.33283200 |
| C | -1.52564100 | 4.86781300 | -0.50123100 |
| C | -2.88188700 | 4.80266800 | -0.76848900 |
| H | -3.39103600 | 5.73337900 | -0.99417100 |
| C | -3.60355500 | 3.59818700 | -0.80707700 |
| C | -4.73301600 | -1.16983700 | 0.96925700 |
| C | -5.35895500 | 0.04535600 | 1.26887900 |
| C | -4.76852100 | 1.21350700 | 0.77610600 |
| H | -5.23142500 | 2.17221600 | 0.96333100 |
| C | -1.39807900 | -4.91816500 | -0.22480100 |
| C | -2.80672600 | -4.95782000 | -0.24489900 |
| C | -3.55024500 | -3.73387600 | -0.20125700 |
| C | -3.49288000 | -6.19915300 | -0.36162800 |
| C | -4.85782600 | -6.24404100 | -0.51132700 |
| H | -5.37012700 | -7.19693800 | -0.61207700 |
| C | -5.58805100 | -5.03482000 | -0.58441200 |
| H | -6.65669400 | -5.06102300 | -0.78004700 |
| C | -4.95390300 | -3.82052000 | -0.43471100 |
| H | -5.53111300 | -2.91217400 | -0.55067500 |
| C | 1.39810300 | 4.91816600 | -0.22483000 |
| C | 2.80675000 | 4.95782100 | -0.24490900 |
| C | 3.55026800 | 3.73387800 | -0.20125200 |
| C | 3.49290800 | 6.19915300 | -0.36163300 |
| C | 4.85785700 | 6.24403700 | -0.51131000 |
| H | 5.37016100 | 7.19693300 | -0.61205700 |

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|---|---|---|---|
| C | 5.58808200 | 5.03481500 | -0.58437300 |
| H | 6.65672900 | 5.06101500 | -0.77998600 |
| C | 4.95393000 | 3.82051600 | -0.43467700 |
| H | 5.53114000 | 2.91216800 | -0.55062200 |
| H | 5.23140200 | -2.17224000 | 0.96334700 |
| H | 1.05186500 | -5.84238400 | -0.49507000 |
| H | -0.87784100 | -5.86926300 | -0.24495800 |
| H | -2.90599200 | -7.11479700 | -0.35984500 |
| H | -5.17375400 | -2.08903900 | 1.33282700 |
| H | -1.05180800 | 5.84237200 | -0.49527200 |
| H | 0.87786700 | 5.86926600 | -0.24498700 |
| H | 2.90602200 | 7.11479700 | -0.35986500 |
| C | 6.64245900 | -0.04896100 | 2.12077000 |
| C | -6.64247400 | 0.04893500 | 2.12073500 |
| C | 6.33567800 | 0.56585500 | 3.50768700 |
| H | 7.24115400 | 0.58113500 | 4.12682700 |
| H | 5.97036200 | 1.59488700 | 3.42676900 |
| H | 5.57301600 | -0.01861200 | 4.03467200 |
| C | 7.73622500 | 0.79138700 | 1.41984600 |
| H | 7.42657700 | 1.83253900 | 1.28118200 |
| H | 8.65525600 | 0.79628400 | 2.01866500 |
| H | 7.97692600 | 0.37839100 | 0.43330300 |
| C | 7.19978500 | -1.46795300 | 2.34232500 |
| H | 6.48044500 | -2.11358300 | 2.85873800 |
| H | 7.47997200 | -1.95075300 | 1.39897500 |
| H | 8.10098100 | -1.41643400 | 2.96364400 |
| C | -7.19987600 | 1.46791400 | 2.34216600 |
| H | -6.48059300 | 2.11361600 | 2.85856900 |
| H | -7.48004000 | 1.95063100 | 1.39876600 |
| H | -8.10109900 | 1.41639400 | 2.96344400 |
| C | -7.73619300 | -0.79152200 | 1.41986500 |
| H | -7.42650400 | -1.83267500 | 1.28130300 |
| H | -8.65523400 | -0.79640000 | 2.01866600 |
| H | -7.97689000 | -0.37862500 | 0.43327900 |
| C | -6.33567300 | -0.56575500 | 3.50770500 |
| H | -5.97031300 | -1.59477800 | 3.42687200 |
| H | -5.57303900 | 0.01878600 | 4.03464900 |
| H | -7.24115300 | -0.58102500 | 4.12684000 |
| C | 5.00626000 | -3.67212000 | -1.49189800 |
| C | 5.58258200 | -2.31735000 | -1.96349800 |

| | | | |
|---|---|---|---|
| C | 6.03596300 | -4.40164700 | -0.59787300 |
| C | 4.84677400 | -4.50178400 | -2.80210200 |
| H | 4.83115700 | -1.73224800 | -2.50463900 |
| H | 5.96903900 | -1.69636700 | -1.15687900 |
| H | 6.41351600 | -2.51000900 | -2.65182600 |
| H | 5.68797200 | -5.40416100 | -0.32476400 |
| H | 6.98814100 | -4.51301900 | -1.13132800 |
| H | 6.23783000 | -3.85904700 | 0.33076100 |
| H | 5.80419200 | -4.52759600 | -3.33483900 |
| H | 4.54990500 | -5.53812500 | -2.62417600 |
| H | 4.10206700 | -4.04712500 | -3.46451000 |
| C | -5.00630900 | 3.67213700 | -1.49181300 |
| C | -5.58224000 | 2.31737200 | -1.96388500 |
| C | -6.03615100 | 4.40112900 | -0.59750700 |
| C | -4.84717000 | 4.50233100 | -2.80172800 |
| H | -4.83084900 | 1.73310400 | -2.50599100 |
| H | -5.96769600 | 1.69558200 | -1.15741900 |
| H | -6.41378500 | 2.51001700 | -2.65147900 |
| H | -5.68817500 | 5.40348300 | -0.32379200 |
| H | -6.98824300 | 4.51280900 | -1.13105100 |
| H | -6.23819200 | 3.85802900 | 0.33079200 |
| H | -5.80451300 | 4.52761100 | -3.33462100 |
| H | -4.55113900 | 5.53884700 | -2.62340900 |
| H | -4.10201100 | 4.04845400 | -3.46416000 |

**5c**

| | | | |
|---|---|---|---|
| C | -3.61119900 | -0.74297800 | 0.51205000 |
| C | -2.79637700 | 0.37022300 | 0.21273600 |
| C | -1.39478200 | 0.18496800 | -0.04314200 |
| C | -0.85626700 | -1.12879700 | -0.05654300 |
| C | -1.75644200 | -2.25152200 | -0.09482600 |
| C | -3.14984900 | -2.05169600 | 0.05189500 |
| C | -0.54624300 | 1.31768300 | -0.09154800 |
| C | 0.54623700 | -1.31768400 | -0.09155100 |
| C | 1.39477600 | -0.18497000 | -0.04313200 |
| C | 0.85626100 | 1.12879500 | -0.05652700 |
| C | 2.79637000 | -0.37022500 | 0.21275400 |
| C | 3.31210500 | -1.70633900 | 0.31968200 |
| C | 2.52590700 | -2.82962500 | -0.21220100 |
| C | 1.10432300 | -2.65229400 | -0.19573900 |

| | | | |
|---|---|---|---|
| C | 0.23084700 | -3.75804700 | -0.34148700 |
| C | -1.22269900 | -3.56753400 | -0.32013800 |
| C | -3.31211700 | 1.70633500 | 0.31965300 |
| C | -2.52590700 | 2.82962700 | -0.21219300 |
| C | -1.10432600 | 2.65229500 | -0.19571800 |
| C | -0.23084600 | 3.75805500 | -0.34141600 |
| C | 1.22269800 | 3.56753600 | -0.32010300 |
| C | 1.75643400 | 2.25152100 | -0.09480100 |
| C | 3.61119100 | 0.74297300 | 0.51207300 |
| C | 3.14984200 | 2.05169200 | 0.05191200 |
| C | 3.07273200 | -4.06543300 | -0.65487400 |
| C | 0.81549500 | -5.02221400 | -0.49657300 |
| C | 2.17882900 | -5.15203100 | -0.68854400 |
| H | 2.55978100 | -6.14400900 | -0.90557400 |
| C | 4.47565500 | -1.89796800 | 1.03574800 |
| C | -0.81549300 | 5.02223300 | -0.49641700 |
| C | -2.17882500 | 5.15205900 | -0.68840100 |
| H | -2.55978000 | 6.14405000 | -0.90537300 |
| C | -3.07272200 | 4.06545600 | -0.65483000 |
| C | -4.47568800 | 1.89796200 | 1.03569000 |
| H | -4.82494000 | 2.90489300 | 1.23267400 |
| C | -2.10460000 | -4.61505400 | -0.51714100 |
| C | -3.49848800 | -4.41241800 | -0.59756100 |
| C | -4.04289900 | -3.11123200 | -0.34888900 |
| C | -4.36401000 | -5.47749700 | -0.97629000 |
| C | -5.70513400 | -5.26187600 | -1.18105600 |
| H | -6.35375000 | -6.07899300 | -1.48486600 |
| C | -6.23245600 | -3.95680900 | -1.03101100 |
| H | -7.28057500 | -3.77011400 | -1.24850500 |
| C | -5.42632000 | -2.91664100 | -0.62592200 |
| H | -5.84863800 | -1.92370400 | -0.53790100 |
| C | 2.10460100 | 4.61504900 | -0.51714200 |
| C | 3.49848500 | 4.41240500 | -0.59758800 |
| C | 4.04289200 | 3.11122000 | -0.34889500 |
| C | 4.36401200 | 5.47746500 | -0.97635800 |
| C | 5.70512900 | 5.26182300 | -1.18114300 |
| H | 6.35374900 | 6.07892700 | -1.48498000 |
| C | 6.23244700 | 3.95675700 | -1.03107100 |
| H | 7.28056000 | 3.77005400 | -1.24858200 |
| C | 5.42630800 | 2.91660700 | -0.62594200 |

| | | | |
|---|---|---|---|
| H | 5.84861700 | 1.92366800 | -0.53788600 |
| H | 4.82490100 | -2.90489900 | 1.23274200 |
| H | 0.20356700 | -5.91639600 | -0.52894700 |
| H | -1.73899400 | -5.62144500 | -0.68892500 |
| H | -3.93199000 | -6.46364700 | -1.13001500 |
| H | -0.20356200 | 5.91641600 | -0.52869600 |
| H | 1.73899100 | 5.62143500 | -0.68894500 |
| H | 3.93200300 | 6.46361700 | -1.13010100 |
| C | 4.49020000 | -4.33680700 | -1.25461900 |
| C | 5.29072000 | -3.07746100 | -1.66139300 |
| C | 5.34251300 | -5.21954800 | -0.31309400 |
| C | 4.29382200 | -5.11913800 | -2.58875700 |
| H | 4.66463800 | -2.36758600 | -2.21261800 |
| H | 5.73671400 | -2.54661900 | -0.82148800 |
| H | 6.10980100 | -3.38155900 | -2.32306400 |
| H | 4.82831000 | -6.15581900 | -0.06907600 |
| H | 6.29461200 | -5.47614300 | -0.79379500 |
| H | 5.57425100 | -4.71512800 | 0.63047600 |
| H | 5.26921200 | -5.28610900 | -3.05928300 |
| H | 3.83178400 | -6.09957700 | -2.45192300 |
| H | 3.67280600 | -4.54895500 | -3.28835800 |
| C | -4.49016600 | 4.33684200 | -1.25462700 |
| C | -5.29065800 | 3.07750400 | -1.66147500 |
| C | -5.34253500 | 5.21955200 | -0.31312600 |
| C | -4.29373000 | 5.11921300 | -2.58873700 |
| H | -4.66454600 | 2.36766700 | -2.21271800 |
| H | -5.73666200 | 2.54661300 | -0.82160600 |
| H | -6.10972700 | 3.38161900 | -2.32315200 |
| H | -4.82833600 | 6.15580600 | -0.06903000 |
| H | -6.29459300 | 5.47618100 | -0.79388900 |
| H | -5.57435500 | 4.71510000 | 0.63040600 |
| H | -5.26909500 | 5.28616700 | -3.05932000 |
| H | -3.83172800 | 6.09966100 | -2.45184700 |
| H | -3.67265300 | 4.54906800 | -3.28831400 |
| C | -5.18746700 | 0.81850500 | 1.61020400 |
| C | -4.77277600 | -0.52758600 | 1.34420500 |
| C | -6.94280500 | 0.02347300 | 3.09906000 |
| H | -7.78035000 | 0.22045400 | 3.76258700 |
| C | -6.49098000 | -1.30184300 | 2.90157600 |
| H | -6.96638600 | -2.11942000 | 3.43668100 |

| | | | |
|---|---|---|---|
| C | 5.18743200 | -0.81851100 | 1.61026500 |
| C | 4.77275800 | 0.52758400 | 1.34424500 |
| C | 6.49098000 | 1.30182900 | 2.90160300 |
| H | 6.96639500 | 2.11941100 | 3.43669500 |
| C | 6.94279500 | -0.02348800 | 3.09909700 |
| H | 7.78034800 | -0.22046600 | 3.76261200 |
| C | 6.29322900 | -1.05958200 | 2.47084800 |
| H | 6.60213600 | -2.08873700 | 2.63877400 |
| C | 5.44068400 | 1.56778900 | 2.05038800 |
| H | 5.09757000 | 2.58837100 | 1.94037800 |
| C | -6.29326700 | 1.05957200 | 2.47078800 |
| H | -6.60219400 | 2.08872400 | 2.63869000 |
| C | -5.44068900 | -1.56779200 | 2.05035800 |
| H | -5.09756100 | -2.58837100 | 1.94034500 |

**5d**

| | | | |
|---|---|---|---|
| C | 3.76592700 | -0.04747100 | 0.01911400 |
| C | 2.67569800 | -0.96424900 | 0.05563100 |
| C | 1.32644100 | -0.48537700 | -0.07396700 |
| C | 1.08919000 | 0.91442600 | -0.11786300 |
| C | 2.19737700 | 1.83113200 | -0.26154600 |
| C | 3.51772100 | 1.33998600 | -0.36957700 |
| C | 0.24174200 | -1.40011700 | -0.06854600 |
| C | -0.24174100 | 1.40012100 | -0.06839800 |
| C | -1.32643900 | 0.48538200 | -0.07399700 |
| C | -1.08918600 | -0.91441600 | -0.11804000 |
| C | -2.67570500 | 0.96423800 | 0.05556800 |
| C | -2.92943000 | 2.33734600 | 0.30940900 |
| C | -1.82737800 | 3.29581800 | 0.20540100 |
| C | -0.49956100 | 2.82030200 | 0.00241000 |
| C | 0.57766200 | 3.74362900 | -0.11019900 |
| C | 1.93820600 | 3.24406000 | -0.34368000 |
| C | 2.92940700 | -2.33738700 | 0.30932300 |
| C | 1.82736300 | -3.29584600 | 0.20513000 |
| C | 0.49955800 | -2.82030600 | 0.00211200 |
| C | -0.57765700 | -3.74362000 | -0.11067200 |
| C | -1.93818600 | -3.24402400 | -0.34418400 |
| C | -2.19736300 | -1.83110600 | -0.26190200 |
| C | -3.76593200 | 0.04746400 | 0.01887500 |
| C | -3.51770000 | -1.33994800 | -0.36996300 |

| | | | |
|---|---|---|---|
| C | -2.04437000 | 4.68034500 | 0.28599000 |
| C | 0.30849100 | 5.11394200 | 0.00188500 |
| C | -0.98848200 | 5.57632600 | 0.19327800 |
| H | -1.17604300 | 6.64395400 | 0.26797600 |
| C | -4.22666800 | 2.73532100 | 0.66929400 |
| C | -5.27745900 | 1.82611300 | 0.79340000 |
| C | -5.02512900 | 0.49365600 | 0.44790700 |
| H | -5.81710000 | -0.23447800 | 0.56271400 |
| C | -0.30849300 | -5.11394600 | 0.00126900 |
| C | 0.98846800 | -5.57635300 | 0.19268700 |
| H | 1.17602500 | -6.64399000 | 0.26727100 |
| C | 2.04435000 | -4.68038200 | 0.28556800 |
| H | 3.04768900 | -5.07061800 | 0.40840200 |
| C | 5.02509700 | -0.49371200 | 0.44817300 |
| C | 5.27740300 | -1.82620800 | 0.79353600 |
| C | 4.22662300 | -2.73540400 | 0.66924300 |
| H | 4.40485300 | -3.77414500 | 0.90853800 |
| C | 2.98987800 | 4.09643100 | -0.62482700 |
| C | 4.28136900 | 3.62019800 | -0.93099900 |
| C | 4.55514000 | 2.21603400 | -0.85270600 |
| C | 5.29834400 | 4.51745900 | -1.36100500 |
| C | 6.52387800 | 4.05489900 | -1.77581200 |
| H | 7.28936800 | 4.74825800 | -2.11314300 |
| C | 6.76438300 | 2.66169100 | -1.80826500 |
| H | 7.70192700 | 2.28532200 | -2.20860700 |
| C | 5.81098300 | 1.77268200 | -1.36092700 |
| H | 6.00316300 | 0.71138800 | -1.45274900 |
| C | -2.98983800 | -4.09636300 | -0.62549900 |
| C | -4.28130800 | -3.62009400 | -0.93170500 |
| C | -4.55508400 | -2.21594000 | -0.85326800 |
| C | -5.29825200 | -4.51730500 | -1.36188700 |
| C | -6.52375700 | -4.05469800 | -1.77673000 |
| H | -7.28922300 | -4.74801700 | -2.11419600 |
| C | -6.76425700 | -2.66148600 | -1.80904200 |
| H | -7.70177100 | -2.28507000 | -2.20941300 |
| C | -5.81088900 | -1.77252900 | -1.36153200 |
| H | -6.00306000 | -0.71122500 | -1.45325500 |
| H | -3.04771500 | 5.07056700 | 0.40880900 |
| H | -4.40490900 | 3.77403100 | 0.90872100 |
| H | 1.11430900 | 5.83658900 | -0.04945800 |

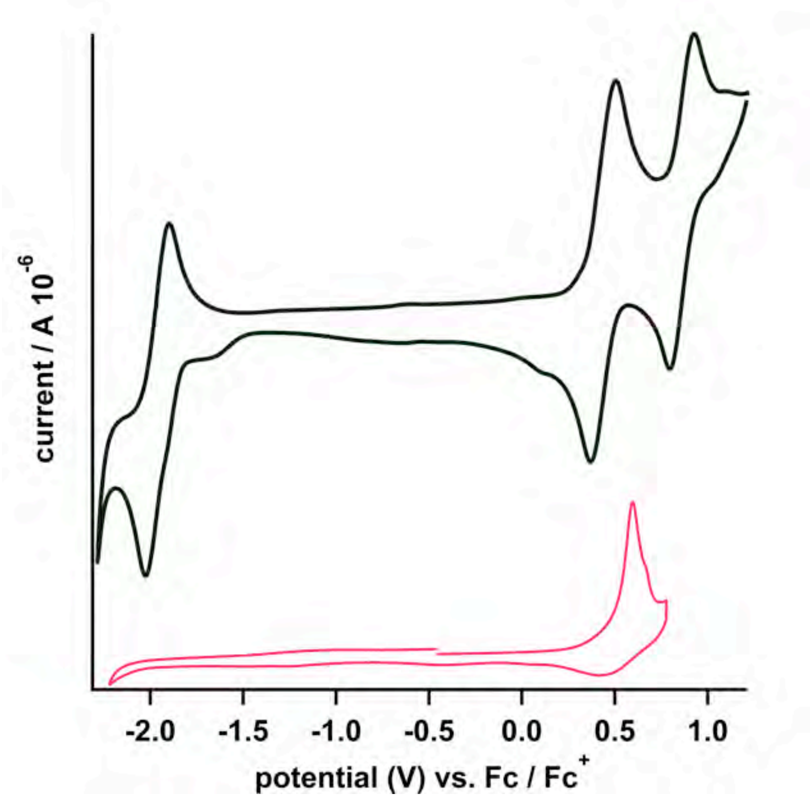
| | | | |
|---|---|---|---|
| H | 2.83112000 | 5.16719800 | -0.68851800 |
| H | 5.07271100 | 5.58113800 | -1.38097200 |
| H | 5.81706500 | 0.23440600 | 0.56310300 |
| H | -1.11430800 | -5.83658600 | -0.05020600 |
| H | -2.83107600 | -5.16712300 | -0.68930600 |
| H | -5.07261900 | -5.58098200 | -1.38196000 |
| C | -6.67459500 | 2.23075800 | 1.30154400 |
| C | 6.67451100 | -2.23089900 | 1.30172300 |
| C | -6.98517800 | 1.45813700 | 2.60603200 |
| H | -7.98059600 | 1.72739400 | 2.98013700 |
| H | -6.96879900 | 0.37418500 | 2.45227200 |
| H | -6.25268300 | 1.69628200 | 3.38554100 |
| C | -7.73922600 | 1.88180900 | 0.23451700 |
| H | -7.75958700 | 0.80981800 | 0.01176000 |
| H | -8.73860600 | 2.16520700 | 0.58676500 |
| H | -7.54599200 | 2.41642700 | -0.70274500 |
| C | -6.77735700 | 3.73816200 | 1.60225900 |
| H | -6.07437000 | 4.04810100 | 2.38380600 |
| H | -6.58980200 | 4.34692700 | 0.71015900 |
| H | -7.78725500 | 3.97434100 | 1.95568300 |
| C | 6.77733700 | -3.73836400 | 1.60212000 |
| H | 6.07432400 | -4.04851000 | 2.38356100 |
| H | 6.58986500 | -4.34694700 | 0.70987800 |
| H | 7.78722700 | -3.97456600 | 1.95555100 |
| C | 7.73922300 | -1.88165300 | 0.23487800 |
| H | 7.75952500 | -0.80961400 | 0.01234500 |
| H | 8.73858800 | -2.16504800 | 0.58716900 |
| H | 7.54612600 | -2.41609300 | -0.70251500 |
| C | 6.98492500 | -1.45854100 | 2.60640700 |
| H | 6.96849200 | -0.37455800 | 2.45287700 |
| H | 6.25237100 | -1.69690000 | 3.38579500 |
| H | 7.98032500 | -1.72781700 | 2.98054500 |

## G. Optical and Electrochemical Bandgaps

**Table S3.** Optical and electrochemical bandgaps of the compounds **4a-4c** and **5a**

| | cyclic voltammetry | | | B3LYP calculations | optical | |
|---|---|---|---|---|---|---|
| | $E_{ox,1}$ (V) | $E_{red,1}$ (V) | $\Delta(E_{ox,1} - E_{red,1})$ (V) | E (eV) | $\lambda_{max}$ (nm) (log ε) | $\lambda_{end}$ (nm) [E (eV)] |
| **4a** | 0.22 | -1.79 | 2.01 | 2.32 | 344 (4.87) | 535 (2.32) |
| **4b** | 0.22 | -1.80 | 2.02 | 2.32 | 347 (4.79) | 535 (2.32) |
| **4c** | 0.24 | -1.57 | 1.81 | 2.16 | 319 (4.65) | 575 (2.16) |
| **5a** | 0.40 | – | | 3.00 | | 490 (2.53) |

**Figure S88.** Cyclic voltammograms of **4a** (green) and **5a** (pink)

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