Supporting Information for:

1,1,*n*,*n*-Tetramethyl[*n*](2,11)teropyrenophanes (*n*=7–9): A Series of Armchair SWCNT Segments

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I. General Experimental Conditions, Procedures and Characterization Data

All reactions were performed under an atmosphere of nitrogen unless otherwise indicated. Experiments involving moisture sensitive compounds were carried out using anhydrous solvents and oven-dried (120 °C) glassware. Solvents for these reactions were dried and distilled according to standard procedures. All other solvents and chemicals were used as received. Solvents were removed under reduced pressure using a rotary evaporator. Chromatographic separations were achieved using Silicycle silica gel 60, particle size 40-63 μm. Column dimensions are recorded as height × diameter. Thin-layer chromatography (tlc) was performed using commercially precoated plastic-backed POLYGRAM® SIL G/UV254 silica gel plates, layer thickness 200 μm. Compounds on tlc plates were visualized using a UV lamp (254 and 365 nm). Melting points were obtained using a Fisher-Johns apparatus. Infrared (IR) spectra were recorded using neat samples on a Bruker TENSOR 27 instrument. ^{1}H (500.133 MHz) and ^{13}C (125.77 MHz) nuclear magnetic resonance (NMR) spectra were obtained from $CDCl_3$ solutions using a Bruker Avance 500 MHz spectrometer. Chemical shifts (δ) are relative to internal standards: TMS (δ_H = 0.00 ppm) and $CDCl_3$ (δ_H = 7.27 ppm; δ_C = 77.23 ppm), respectively. ^{1}H NMR data are presented as follows: chemical shift (δ, ppm), multiplicity (s = singlet, br s = broad singlet, d = doublet, br d = broad doublet, t = triplet, q = quartet, m = multiplet), coupling constants (J, Hz). Low-resolution and high-resolution mass spectrometric (MS) data were obtained using an Agilent 1100 Series LC/MSD instrument and a Waters Micromass® GCT PremierTM instrument. MS data are presented as follows: ionization mode, *m/z* (relative intensity), assignment (when appropriate), calculated mass and found mass for the given formula.

2,8-Dichloro-2,8-dimethylnonane (7)

A solution of dimethyl pimelate (**4**) (10.7 g, 56.7 mmol) in anhydrous THF (100 mL) was added dropwise over a period of 30 min to a stirred 0 °C solution of methylmagnesium bromide (3.0 M, 85 mL, 0.26 mol). After the addition was complete, the reaction mixture was heated at reflux for 12 h. The reaction mixture was cooled to room temperature and quenched by the addition of a saturated solution of ammonium chloride (100 mL). The layers were separated and the aqueous layer was extracted with ether (2 × 50 mL). The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield a white solid, which was recrystallized from heptane to give 2,8-dimethyl-2,8-nonanediol (8.76 g, 82%) as a white powder: m.p. 71–72 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.72 (br s, 2H), 1.48–1.45 (m, 4H), 1.39–1.31 (m, 6H), 1.21 (s, 12H); ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 71.12, 44.01, 30.79, 29.30, 24.41; LCMS (APCI negative) *m/z* 187 $[M–H]^+$; HRMS (CI) calculated for $C_{11}H_{25}O_2$

([M+H]$^+$) 189.1855, found 189.1849. A mixture of 2,8-dimethyl-2,8-nonanediol (3.42 g, 18.2 mmol) and concentrated aqueous HCl solution (50 mL) was stirred at room temperature for 2 h. The reaction mixture was poured into a large excess of ice water (200 mL) and extracted with dichloromethane (3 × 40 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (2 × 50 mL), washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to give 2,8-dichloro-2,8-dimethylnonane (**7**) (3.80 g, 93%) as a light yellow oil, which was used subsequently without purification. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.78–1.75 (m, 4H), 1.59 (s, 12H), 1.53–1.49 (m, 4H), 1.36–1.33 (m, 2H); ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 71.30, 46.20, 32.61, 29.96, 25.21; LCMS (APCI-positive) *m/z* (rel. int.) 225 [M+H]$^+$; no HRMS data could be obtained for this compound.

2,10-Dichloro-2,10-dimethylundecane (9)

A solution of dimethyl azelate (**6**) (10.8 g, 49.9 mmol) in anhydrous THF (100 mL) was added dropwise over a period of 30 min to a stirred 0 °C solution of methylmagnesium bromide (3.0 M, 75 mL, 0.23 mol). After the addition was complete, the reaction mixture was heated at reflux for 12 h. The reaction mixture was cooled to room temperature and quenched by the addition of a saturated solution of ammonium chloride (100 mL). The layers were separated and the aqueous layer was extracted with ether (3 × 50 mL). The combined organic layers were dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield a white solid, which was recrystallized from heptane to give 2,10-dimethyl-2,10-undecanediol (9.05 g, 84%) as a white powder: m.p. 64–66 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.52 (br s, 2H), 1.48–1.45 (m, 4H), 1.38–1.32 (m, 10H), 1.21 (s, 12H); ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 71.21, 44.17, 30.32, 29.80, 29.41, 24.52; IR (cm^{-1}, neat): 3366, 2964, 2930, 2860, 1472, 1362; LCMS (APCI negative) *m/z* 216 (25) 215 [M–H]$^+$; HRMS (CI) calculated for $C_{13}H_{29}O_2$ ([M+H]$^+$) 217.2168, found 217.2160. A mixture of 2,10-dimethyl-2,10-undecanediol (1.75 g, 8.10 mmol) and concentrated aqueous HCl solution (40 mL) was stirred at room temperature for 2 h. The reaction mixture was poured into a large excess of ice water (100 mL) and extracted with dichloromethane (3 × 30 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (2 × 50 mL), washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to give 2,10-dichloro-2,10-dimethylundecane (**9**) (1.88 g, 92%) as a light yellow oil, which was used subsequently without purification. ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.79–1.75 (m, 4H), 1.58 (s, 12H), 1.48–1.44 (m, 4H), 1.31–1.25 (m, 6H); ^{13}C NMR (125.77 MHz, $CDCl_3$): δ 71.42, 46.32, 32.45, 29.90,

29.74, 25.01; LCMS (APCI-positive) *m/z* (rel. int.) 253 $[M+H]^+$; no HRMS data could be obtained for this compound.

2,8-Bis(2-pyrenyl)-2,8-dimethylnonane (10)

Aluminum chloride (1.64 g, 12.3 mmol) was added to a stirred 0 °C solution of pyrene (6.21 g, 30.7 mmol) and 2,8-dichloro-2,8-dimethylnonane (**7**) (1.38 g, 6.14 mmol) in dichloromethane (100 mL). The resulting slurry was allowed to warm to room temperature and stirred for 4 h. The reaction was poured into ice water (200 mL) and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 100 mL) and the combined organic extracts were washed with a saturated solution of sodium bicarbonate (50 mL), washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The yellow residue was subjected to column chromatography (25 × 6.5 cm; 1:9 dichloromethane/hexanes) to yield 2,8-bis(2-pyrenyl)-2,8-dimethylnonane (**10**) as a white solid (1.40 g, 41%): R_f = 0.26 (1:9 dichloromethane/hexanes); m.p. 207–209 °C (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.19 (d, J=7.5 Hz, 4H), 8.16 (s, 4H), 8.08–8.00 (m, 10H), 1.79–1.76 (m, 4H), 1.51 (s, 12H), 1.19–1.15 (m, 2H) 1.07–1.02 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.09, 131.41, 131.32, 128.04, 127.56, 125.82, 125.08, 124.99, 123.25, 123.18, 45.54, 38.54, 31.35, 29.89, 25.21; LCMS (APCI-positive) *m/z* (rel. int.) 559 (12), 558 (47), 557 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{43}H_{40}$ ($[M]^+$) 556.3130, found 556.3128.

2,10-Bis(2-pyrenyl)-2,10-dimethylundecnane (12)

Aluminum chloride (1.78 g, 13.4 mmol) was added to a stirred 0 °C solution of pyrene (6.73 g, 33.3 mmol) and 2,10-dichloro-2,10-dimethylundecane (**9**) (1.68 g, 6.67 mmol) in dichloromethane (100 mL). The resulting slurry was allowed to warm to room temperature and stirred for 4 h. The reaction was poured into ice water (300 mL) and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 100 mL) and the combined organic extracts were washed with a saturated solution of sodium bicarbonate (50 mL), washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The oily orange residue was subjected to column chromatography (25 × 6.5 cm; 1:9 dichloromethane/hexanes) to yield 2,10-bis(2-pyrenyl)-2,10-dimethylundecane (**12**) as an orange oil

(1.67 g, 43%): R_f = 0.28 (1:9 dichloromethane/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09–8.05 (m, 8H), 7.98–7.95 (m, 8H), 7.91–7.87 (m 2H) 1.74–1.71 (m, 4H), 1.47 (s, 12H), 1.08–1.02 (m, 6H) 1.01–0.93 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 147.88, 131.14, 131.08, 127.80, 127.34, 125.64, 124.88, 124.81, 123.05, 122.97, 45.31, 38.40, 30.45, 29.72, 29.51, 24.91; LCMS (APCI-positive) *m/z* (rel. int.) 587 (13), 586 (49), 585 ($[M+H]^+$, 100), 385 (7), 384 (18), 383 ($M–C_{16}H_{10}$, 42); HRMS (EI) calculated for $C_{45}H_{44}$ ($[M]^+$) 584.3443, found 584.3441.

2,8-Bis(6-formylpyren-2-yl)-2,8-dimethylnonane (13)

Titanium(IV) chloride (0.453 g, 2.39 mmol) was added to a stirred 0 °C solution of 2,8-bis(2-pyrenyl)-2,8-dimethylnonane (**10**) (0.531 g, 0.953 mmol) and dichloromethyl methyl ether (0.274 g, 2.39 mmol) in dichloromethane (25 mL). The cooling bath was removed and the resulting mixture was stirred at room temperature for 2 h. The reaction mixture was poured into ice water (100 mL) and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 30 mL) and the combined organic extracts were washed with a saturated solution of sodium bicarbonate (40 mL), washed with brine (40 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The solid brown residue was subjected to column chromatography (30 × 3 cm; dichloromethane) to yield 2,8-bis(6-formylpyren-2-yl)-2,8-dimethylnonane (**13**) as a bright yellow solid (0.488 g, 84%): R_f = 0.26 (dichloromethane); m.p. 165–168 °C (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.62 (s, 2H), 9.27 (d, *J*=9.2 Hz, 2H), 8.16 (d, *J*=7.9 Hz, 2H), 8.13–8.10 (m, 4H), 8.08 (d, *J*=9.2 Hz, 2H), 8.01 (d, *J*=8.9 Hz, 2H), 7.97 (d, *J*=8.9 Hz, 2H), 7.85 (d, *J*=7.8 Hz, 2H) 1.77–1.74 (m, 4H), 1.49 (s, 12H), 1.14–1.11 (m, 2H) 0.99–0.97 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 193.34, 148.82, 135.77, 132.28, 131.49, 131.45, 131.30, 131.19, 131.11, 130.66, 127.60, 127.32, 125.29, 124.85, 124.62, 123.14, 122.62, 45.41, 38.72, 30.37, 29.80, 25.10; LCMS (APCI-positive) *m/z* (rel. int.) 615 (11), 614 (49), 613 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{45}H_{40}O_2$ ($[M]^+$) 612.3028, found 612.3020.

2,10-Bis(6-formylpyren-2-yl)-2,10-dimethylundecane (15)

Titanium(IV) chloride (0.67 g, 3.5 mmol) was added to a stirred 0 °C solution of 2,10-bis(2-pyrenyl)-2,10-dimethylundecnane (**12**) (0.82 g, 1.4 mmol) and dichloromethyl methyl ether (0.40 g, 3.5 mmol) in dichloromethane (30 mL). The cooling bath was removed and the resulting mixture was stirred at room temperature for 2 h. The reaction mixture was poured into ice water (100 mL) and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 30 mL) and the combined organic

extracts were washed with washed with a saturated solution of sodium bicarbonate (40 mL), washed with brine (40 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The solid brown residue was subjected to column chromatography (20 × 3.5 cm; dichloromethane) to yield 2,10-bis(6-formylpyren-2-yl)-2,10-dimethylundecane (**15**) as a light brown oil (0.77 g, 88%): R_f = 0.26 (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.73 (s, 2H), 9.32 (d, J=9.2 Hz, 2H), 8.38 (d, J=7.9 Hz, 2H), 8.22 (d, J=9.2 Hz, 2H), 8.20–8.14 (m, 6H) 8.10 (d, J=8.9 Hz, 2H), 8.00 (d, J=8.9 Hz, 2H), 1.75–1.72 (m, 4H), 1.49 (s, 12H), 1.08–1.04 (m, 6H) 0.98–0.93 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 193.52, 148.94, 135.75, 132.22, 131.54, 131.51, 131.33, 131.25, 131.15, 130.63, 127.67, 127.36, 125.33, 124.96, 124.70, 123.26, 122.63, 45.36, 38.69, 30.41, 29.84, 29.61 25.12; LCMS (APCI-positive) *m/z* (rel. int.) 643 (14), 642 (54), 641 ($[M+H]^+$, 100), 613 (16); HRMS (EI) calculated for $C_{47}H_{44}O_2$ ($[M]^+$) 640.3341, found 640.3335.

2,8-Bis(6-(bromomethyl)pyren-2-yl)-2,8-dimethylnonane (16)

Sodium borohydride (0.082 g, 2.2 mmol) was added to a stirred 0 °C solution of 2,8-bis(6-formylpyren-2-yl)-2,8-dimethylnonane (**13**) (0.385 g, 0.627 mmol) in THF (20 mL). The resulting slurry was allowed to slowly warm to room temperature over a 16 h period. THF was evaporated under reduced pressure and the solid residue was taken up into dichloromethane (30 mL). This solution was cooled to 0 °C and an aqueous 1 M HCl solution was added until the solution was at acidic pH. The layers were separated and the aqueous layer was extracted with dichloromethane (2 × 20 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (30 mL), washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield 2,8-bis(6-(hydroxymethyl)pyren-2-yl)-2,8-dimethylnonane as a light yellow oil (0.359 g, 93%). Purification of this compound was not necessary and the crude material was used in subsequent experiments: R_f = 0.18 (1:9 EtOAc/dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, J=9.2 Hz, 2H), 8.07 (s, 4H), 8.04 (d, J=7.7 Hz, 2H), 8.00 (d, J=9.2 Hz, 2H) 7.97–7.95 (m, 4H), 7.93 (d, J=7.7 Hz, 2H) 5.27 (s, 4H) 1.99 (br s, 2H), 1.76–1.73 (m, 4H), 1.46 (s, 12H), 1.00–0.97 (m, 2H), 0.91–0.87 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.22, 133.98, 131.50, 131.42, 130.96, 128.99, 128.53, 128.10, 127.56, 126.07, 125.30, 124.87, 123.57, 123.48, 123.35, 123.18, 64.25, 45.44, 38.61, 30.47, 29.51, 25.31; LCMS (APCI-positive) *m/z* (rel. int.) 597 (12), 596 (51), 595 (100, $[M–OH]^+$); HRMS (EI) calculated for $C_{45}H_{44}O_2$ ($[M]^+$) 616.3341, found 616.3334. Phosphorus tribromide (0.090 g, 0.33 mmol) was added to a stirred 0 °C solution of 2,8-bis(6-(hydroxymethyl)pyren-2-yl)-2,8-dimethylnonane (0.273 g, 0.443 mmol) in dichloromethane (15 mL). After 4 h, water (15 mL) was added. The layers were separated and the

aqueous layer was extracted with dichloromethane (2 × 20 mL). The combined organic extracts were washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield 2,8-bis(6-(bromomethyl)pyren-2-yl)-2,8-dimethylnonane (**16**) as a light yellow solid (0.292 g, 89%). Purification of **16** was not necessary and the crude material was used in subsequent experiments: R_f = 0.24 (15% dichloromethane/hexanes); m.p. 103–106 °C (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.34 (d, J=9.9 Hz, 2H), 8.16–8.11 (m, 6H), 8.03 (d, J=7.8 Hz, 2H), 8.00–7.94 (m, 6H), 5.26 (s, 4H), 1.78–1.74 (m, 4H), 1.49 (s, 12H), 1.12–1.08 (m, 2H), 1.00–0.96 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.55, 133.22, 131.40, 130.96, 130.77, 129.32, 128.88, 128.69, 127.76, 127.52, 125.49, 125.03, 123.91, 123.88, 123.24, 123.07, 45.45, 38.63, 32.73, 30.46, 29.87, 25.15; LCMS (APCI-positive) *m/z* (rel. int.) 667 (12), 666 (53), 665 (98, $[M(^{81}Br)–Br]^+$), 664 (52) 663 (100, $[M(^{79}Br)–Br]^+$); No HRMS data could be obtained for this compound.

2,9-Bis(6-(bromomethyl)pyren-2-yl)-2,9-dimethyldecane (17)

Sodium borohydride (0.356 g, 9.57 mmol) was added to a stirred 0 °C solution of 2,9-bis(6-formylpyren-2-yl)-2,9-dimethyldecane (**14**) (1.50 g, 2.39 mmol) in THF (30 mL). The resulting slurry was allowed to slowly warm to room temperature over a 12 h period. The solvent was evaporated under reduced pressure and the solid residue was taken up in dichloromethane (30 mL). This solution was cooled to 0 °C and an aqueous 1 M HCl solution was added until the solution was at acidic pH. The layers were separated and the aqueous layer was extracted with dichloromethane (2 × 30 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (50 mL), washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield 2,9-bis(6-(hydroxymethyl)pyren-2-yl)-2,9-dimethyldecane as a clear straw-colored oil (1.43 g, 95%). This compound was used in further experiments without purification: R_f = 0.35 (1:9 EtOAc/dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.23 (d, J=9.2 Hz, 2H), 8.07 (s, 4H), 8.05 (d, J=7.7 Hz, 2H), 8.00 (d, J=9.2 Hz, 2H) 7.96–7.94 (m, 4H), 7.93 (d, J=7.7 Hz, 2H), 5.27 (s, 4H) 1.99 (br s, 2H), 1.76–1.73 (m, 4H), 1.46 (s, 12H), 1.08–1.05 (m, 4H), 0.98–0.94 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.22, 133.98, 131.50, 131.42, 130.96, 128.99, 128.53, 128.10, 127.56, 126.07, 125.30, 124.87, 123.57, 123.48, 123.35, 123.18, 64.25, 45.44, 38.61, 30.47, 29.51, 25.31; LCMS (APCI-positive) *m/z* (rel. int.) 615 (15), 614 (50), 613 (100, ($[M–OH]^+$); HRMS (EI) calculated for $C_{46}H_{46}O_2$ ($[M]^+$) 630.3498, found 630.3496. Phosphorus tribromide (0.398 g, 1.48 mmol) was added to a stirred solution of 2,9-bis(6-(hydroxymethyl)pyren-2-yl)-2,9-dimethyldecane (1.24 g, 1.97 mmol) in dichloromethane (25 mL) at 0 °C. The resulting mixture was allowed to warm to room temperature and stirred for 1 h. Water (25 mL)

was added and the layers were separated. The aqueous layer was extracted with dichloromethane (2 × 30 mL). The combined organic extracts were washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield 2,9-bis(6-(bromomethyl)pyren-2-yl)-2,9-dimethyldecane (**17**) as a light yellow solid (1.38 g, 92%). This material was used in further experiments without purification: R_f = 0.22 (15% dichloromethane/hexanes); m.p. 193–194 °C ($CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.29 (d, J=9.2 Hz, 2H), 8.14–8.12 (m, 6H), 8.03 (d, J=7.8 Hz, 2H), 7.99 (d, J=8.9 Hz, 2H) 7.94 (d, J=8.9 Hz, 2H), 7.92 (d, J=7.8 Hz, 2H), 5.21 (s, 4H), 1.75–1.73 (m, 4H), 1.46 (s, 12H), 1.10–1.08 (m, 4H), 0.99–0.94 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.55, 133.21, 131.41, 130.97, 130.76, 129.31, 128.88, 128.69, 127.76, 127.52, 125.47, 125.03, 123.91, 123.88, 123.24, 123.07, 45.45, 38.64, 32.74, 30.49, 29.88, 25.17; LCMS (APCI-positive) *m/z* (rel. int.) 679 (12), 678 (41), 677 (100, $[M(^{81}Br)–Br]^+$), 676 (42), 675 (92, $[M(^{79}Br)–Br]^+$); HRMS (EI) calculated for $C_{46}H_{44}Br_2$ ($[M]^+$) 754.1810, found 754.1804.

2,10-Bis(6-(bromomethyl)pyren-2-yl)-2,10-dimethylundecane (18)

Sodium borohydride (0.124 g, 3.28 mmol) was added to a stirred 0 °C solution of 2,10-bis(6-formylpyren-2-yl)-2,10-dimethylundecane (**15**) (0.610 g, 0.952 mmol) in THF (30 mL). The resulting slurry was allowed to slowly warm to room temperature over a 12 h period. THF was evaporated under reduced pressure and the solid residue was taken up into dichloromethane (30 mL). This solution was cooled to 0 °C and an aqueous 1 M HCl solution was added until the solution was at acidic pH. The layers were separated and the aqueous layer extracted with dichloromethane (2 × 30 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (30 mL), washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield 2,10-bis(6-(hydroxymethyl)pyren-2-yl)-2,10-dimethylundecane as a clear straw-colored oil (0.581 g, 94%). Purification of this compound was not necessary and the crude material was used in subsequent experiments: R_f = 0.13 (1:9 EtOAc/dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32 (d, J=9.2 Hz, 2H), 8.21–8.17 (m, 6H), 8.08 (d, J=7.8 Hz, 2H), 8.04 (d, J=8.9 Hz, 2H) 8.01–7.98 (m, 4H), 5.24 (s, 4H) 1.93 (br s, 2H), 1.79–1.75 (m, 4H), 1.52 (s, 12H), 1.13–1.07 (m, 6H), 1.02–0.97 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.06, 133.77, 131.31, 131.22, 130.75, 128.80, 128.34, 127.91, 127.35, 125.87, 125.10, 124.67, 123.39, 123.28, 123.15, 122.98, 64.05, 45.26, 38.61, 30.35, 29.68, 29.42, 25.41; LCMS (APCI-positive) *m/z* (rel. int.) 629 (12), 628 (51), 627 (100, $[M–OH]^+$); HRMS (EI) calculated for $C_{47}H_{48}O_2$ ($[M]^+$) 644.3654, found 644.3643. Phosphorus tribromide (0.160 g, 0.591 mmol) was added to a stirred 0 °C solution of 2,10-bis(6-(hydroxymethyl)pyren-2-yl)-2,10-dimethylundecane (0.510 g, 0.791

mmol) in dichloromethane (20 mL). The reaction was allowed to warm to room temperature and after 1 h, water (20 mL) was added. The layers were separated and the aqueous layer was extracted with dichloromethane (2 × 30 mL). The combined organic extracts were washed with water (50 mL), washed with brine (50 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure to yield 2,10-bis(6-(bromomethyl)pyren-2-yl)-2,10-dimethylundecane (**18**) as a light yellow solid (0.542 g, 89%). Purification of **18** was not necessary and the crude material was used in subsequent experiments: R_f = 0.22 (15% dichloromethane/hexanes); m.p. 182–183 °C (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.36 (d, J=9.3 Hz, 2H), 8.22–8.16 (m, 6H), 8.10–8.04 (m, 4H), 8.02–7.98 (m, 4H), 5.31 (s, 4H), 1.77–1.74 (m, 4H), 1.51 (s, 12H), 1.14–1.11 (m, 6H), 1.03–0.99 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 148.37, 132.00, 131.19, 130.75, 130.54, 129.79, 128.67, 128.48, 127.53, 127.30, 125.26, 124.80, 123.70, 123.67, 123.02, 122.84, 45.91, 38.88, 32.45, 30.40, 29.88, 25.01 (only 22 of 23 signals observed); LCMS (APCI-positive) *m/z* (rel. int.) 693 (12), 692 (44), 691 (100, $[M(^{81}Br)–Br]^+$), 690 (46), 689 (92, $[M(^{79}Br)–Br]^+$); HRMS (EI) calculated for $C_{47}H_{46}Br_2$ ($[M]^+$) 768.1966, found 768.1961.

1,1,7,7-Tetramethyl[7.2](7,1)pyrenophane (19)

A solution of *n*-butyllithium (0.50 M, 0.31 mL, 0.16 mmol) in hexanes was added to a stirred –15 °C solution of 2,8-bis(6-(bromomethyl)pyren-2-yl)-2,8-dimethylnonane (**16**) (0.179 g, 0.241 mmol) in THF (20 mL). After 10 min, water (20 mL) was added to the reaction mixture. THF was evaporated under reduced pressure and the resulting aqueous solution was extracted with dichloromethane (3 × 30 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (30 mL), washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The residue was preadsorbed on silica gel and purified by column chromatography (30 × 2 cm; 15% dichloromethane/hexanes) to yield 1,1,7,7-tetramethyl[7.2](7,1)pyrenophane (**19**) as a clear, colorless oil (0.080 g, 57%): R_f= 0.38 (15% dichloromethane/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.31–8.26 (m, 2H), 8.16–8.03 (m, 6H), 8.00–7.95 (m, 2H), 7.90–7.88 (m, 2H), 7.34 (s, 2H) 6.59–6.48 (m, 2H), 3.88 (s, 4H) 1.60–1.28 (m, 16H), 1.05–1.00 (m, 2H), 0.65–0.55 (m, 2H), 0.39–0.28 (m, 2H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 146.13, 130.93, 130.06, 130.00, 129.83, 127.67, 127.13, 127.09, 125.27, 125.10, 124.70, 123.02, 122.52, 122.28, 122.21, 46.01, 38.38, 36.82, 30.39, 29.51 25.71 (only 21 of 23 signals observed); LCMS (APCI-positive) *m/z* (rel. int.) 585 (14), 584 (51), 583 (100, $[M+H]^+$); HRMS (EI) calculated for $C_{45}H_{42}$ ($[M]^+$) 582.3287, found 582.3280.

1,1,8,8-Tetramethyl[8.2](7,1)pyrenophane (20)

A solution of *n*-butyllithium (1.0 M, 0.40 mL, 0.40 mmol) in hexanes was added to a stirred –15 °C solution of 2,9-bis(6-(bromomethyl)pyren-2-yl)-2,9-dimethyldecane (**17**) (0.401 g, 0.529 mmol) in THF (45 mL). After 10 min, water (15 mL) was added to the reaction mixture. THF was evaporated under reduced pressure and the resulting aqueous solution was extracted with dichloromethane (3 × 30 mL). The combined organic extracts were washed with an aqueous 1 M HCl solution (30 mL), washed with a saturated solution of sodium bicarbonate (30 mL), washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The resulting residue was preadsorbed on silica gel and purified by column chromatography (25 × 3 cm; 15% dichloromethane/hexanes) to yield 1,1,8,8-tetramethyl[8.2](7,1)pyrenophane (**20**) as a clear, colorless oil (0.186 g, 59%): R_f = 0.32 (15% dichloromethane/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.22 (br d, 2H), 8.15 (br d, 2H), 8.02 (d, J=9.4 Hz, 2H), 7.89–7.84 (m, 4H), 7.35 (s, 2H) 6.68–6.50 (m, 4H), 3.89 (s, 4H) 1.66–1.58 (m, 4H), 1.43–1.28 (m, 12H), 1.12–1.06 (m, 4H), 0.57–0.43 (m, 2H), 0.30–0.18 (m, 2H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 146.10, 131.05, 129.98, 129.91, 129.80, 127.62, 127.16, 127.00, 125.54, 125.04, 125.02, 124.67, 122.85, 122.53, 122.36, 122.05, 46.44, 38.11, 36.47, 31.45, 30.48, 24.22; LCMS (APCI-positive) *m/z* (rel. int.) 599 (12), 598 (53), 597 (100 $[M+H]^+$); HRMS (EI) calculated for $C_{46}H_{44}$ ($[M]^+$) 596.3443, found 596.3436.

1,1,9,9-Tetramethyl[9.2](7,1)pyrenophane (21)

A solution of *n*-butyllithium (0.50 M, 0.61 mL, 0.31 mmol) in hexanes was added to a stirred –15 °C solution of 2,10-bis(6-(bromomethyl)pyren-2-yl)-2,10-dimethylundecane (**18**) (0.420 g, 0.548 mmol) in THF (30 mL). After 10 min, water (25 mL) was added to the reaction mixture. THF was evaporated under reduced pressure and the resulting aqueous solution was extracted with dichloromethane (3 × 25 mL). The combined organic extracts were washed with an aqueous solution of 1 M HCl (30 mL), washed with a saturated solution of sodium bicarbonate (30 mL), washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The resulting residue was preadsorbed on silica gel and purified by column chromatography (25 × 2.5 cm; 15% dichloromethane/hexanes) to yield 1,1,9,9-tetramethyl[9.2](7,1)pyrenophane (**21**) as a clear, colorless oil (0.177 g, 53%): R_f = 0.31 (15% dichloromethane/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J=9.0 Hz, 2H), 8.08 (d, J=9.1 Hz, 2H), 8.00 (d, J=9.2 Hz, 2H), 7.97–7.92 (m, 4H), 7.69 (br s, 2H), 7.24 (br d, 2H) 7.12 (d, J=9.0 Hz, 2H), 4.02 (s, 4H) 1.71–1.67 (m, 4H), 1.50 (s, 12H), 1.01–0.96 (m, 6H), 0.78–0.73 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) 146.62, 136.18, 130.95, 130.34, 129.67, 129.62, 127.73, 127.26, 126.89, 126.34, 124.81, 124.78,

123.24, 122.91, 122.53, 122.43, 45.58, 38.31, 35.65, 30.64, 29.67, 29.35, 25.05; LCMS (APCI-positive) *m/z* (rel. int.) 613 (13), 612 (54), 611 ($[M+H]^+$ 100), 598 (11), 597 (22); HRMS (EI) calculated for $C_{47}H_{46}$ ($[M]^+$) 610.3600, found 610.3600.

12,22-Diformyl-1,1,7,7-tetramethyl[7.2](7,1)pyrenophane (22)

A solution of titanium(IV) chloride (1.0 M, 0.28 mL, 0.28 mmol) in dichloromethane was added to a stirred 0 °C solution of 1,1,7,7-tetramethyl[7.2](7,1)pyrenophane (**19**) (0.064 g, 0.11 mmol) and dichloromethyl methyl ether (0.032 g, 0.28 mmol) in dichloromethane (12 mL). The cooling bath was removed and after 2 h the reaction was poured into ice water (30 mL). The layers were separated and the aqueous layer was extracted with dichloromethane (2 × 10 mL). The combined organic extracts were washed with brine (20 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The solid brown residue was subjected to column chromatography (25 × 2 cm; dichloromethane) to yield 12,22-diformyl-1,1,7,7-tetramethyl[7.2](7,1)pyrenophane (**22**) as a bright yellow solid (0.052 g, 74%): R_f = 0.42 (dichloromethane); m.p. 292 °C (dec.) (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.93 (s, 2H), 9.35 (d, *J*=9.2 Hz, 2H), 8.53 (s, 2H), 8.15 (d, *J*=9.2 Hz, 2H), 7.96 (s, 2H) 7.37 (s, 2H), 6.60 (br s, 2H), 6.47 (br s, 2H), 3.92 (br s, 4H), 1.42–1.40 (m, 12H), 1.29–1.21 (m, 4H), 0.82–0.77 (m, 2H), 0.55–0.48 (m, 2H), 0.28–0.19 (m, 2H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 193.27, 147.20, 135.99, 134.82, 134.43, 132.74, 130.59, 130.08, 129.85, 129.64, 128.75, 127.44, 124.72, 124.42, 124.37, 122.46, 122.33, 121.80, 45.57, 38.46, 38.30, 30.18, 25.59; LCMS (APCI-positive) *m/z* (rel. int.) 641 (10), 640 (49), 639 (100, $[M+H]^+$); HRMS (EI) calculated for $C_{47}H_{42}O_2$ ($[M]^+$) 638.3185, found 638.3181.

13,23-Diformyl-1,1,8,8-tetramethyl[8.2](7,1)pyrenophane (23)

A solution of titanium(IV) chloride (1.0 M, 0.50 mL, 0.50 mmol) in dichloromethane was added to a stirred 0 °C solution of 1,1,8,8-tetramethyl[8.2](7,1)pyrenophane (**20**) (0.120 g, 0.201 mmol) and dichloromethyl methyl ether (0.058 g, 0.50 mmol) in dichloromethane (10 mL). The cooling bath was removed and after 3 h the reaction was poured into ice water (50 mL). The layers were separated and the aqueous layer was extracted with dichloromethane (2 × 15 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (20 mL), washed with brine (20 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The solid brown residue was subjected to column chromatography (30 × 2.5 cm; dichloromethane) to yield 13,23-diformyl-1,1,8,8-tetramethyl[8.2](7,1)pyrenophane (**23**) as a bright yellow solid (0.102 g, 77%): R_f = 0.28

(dichloromethane); m.p. 296–297 °C (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$, T = –25 °C) δ 10.95 (s, 2H), 9.36 (d, J=9.2 Hz, 2H), 8.62 (s, 2H), 8.16 (d, J=9.2 Hz, 2H), 8.00 (s, 2H) 7.44 (s, 2H), 6.78 (d, J=9.1 Hz, 2H), 6.59 (d, J=9.1 Hz, 2H), 3.95 (s, 4H), 1.77 (s, 2H), 1.70–1.65 (m, 2H), 1.49–1.45 (m, 2H), 1.37 (s, 6H), 1.31 (s, 6H) 1.01–0.96 (m, 2H) 0.58–0.51 (m, 2H) 0.15–0.10 (m, 2H); ^{13}C NMR (125.77 MHz, $CDCl_3$ T = –25 °C) δ 193.60, 147.41, 135.98, 134.70, 132.87, 130.74, 130.46, 130.18, 129.70, 129.26, 127.59, 124.86, 124.70, 124.42, 122.48, 122.38, 121.98, 46.09, 38.40, 36.43, 32.16, 30.13, 28.09, 24.02; LCMS (APCI-positive) *m/z* (rel. int.) 655 (12), 654 (53), 653 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{48}H_{44}O_2$ ($[M]^+$) 652.3341, found 652.3328.

14,24-Diformyl-1,1,9,9-tetramethyl[9.2](7,1)pyrenophane (24)

A solution of titanium(IV) chloride (1.0 M, 0.35 mL, 0.35 mmol) in dichloromethane was added to a stirred 0 °C solution of 1,1,9,9-tetramethyl[9.2](1,7)pyrenophane (**21**) (0.085 g, 0.14 mmol) and dichloromethyl methyl ether (0.040 g, 0.35 mmol) in dichloromethane (15 mL). The cooling bath was removed and after 2 h the reaction was poured into ice water (50 mL). The layers were separated and the aqueous layer was extracted with dichloromethane (2 × 30 mL). The combined organic extracts were washed with a saturated solution of sodium bicarbonate (30 mL), washed with brine (30 mL), dried over $MgSO_4$, filtered and concentrated under reduced pressure. The yellow residue was subjected to column chromatography (25 × 2.5 cm; dichloromethane) to yield 14,24-diformyl-1,1,9,9-tetramethyl[9.2](7,1)pyrenophane (**24**) as a bright yellow oil (0.075 g, 81%): R_f= 0.24 (dichloromethane); ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.83 (s, 2H), 9.24 (d, J=9.2 Hz, 2H), 8.43 (s, 2H), 8.11 (d, J=9.2 Hz, 2H), 8.00 (s, 2H) 7.69 (s, 2H), 7.14 (br s, 4H), 3.99 (s, 4H), 1.58–1.55 (m, 4H), 1.40 (s, 12H), 0.87–0.84 (m, 6H), 0.66–0.63 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 193.16, 147.69, 135.33, 134.16, 132.76, 130.42, 130.24, 129.95, 129.79, 129.72, 127.17, 124.84, 124.73, 124.51, 122.61, 122.45, 122.20, 45.43, 38.38, 35.29, 29.91, 29.83, 29.57, 24.90; LCMS (APCI-positive) *m/z* (rel. int.) 669 (14), 668 (55), 667 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{49}H_{46}O_2$ ($[M]^+$) 666.3498, found 666.3494.

1,1,7,7-Tetramethyl[7.2.2](7,1,3)pyrenophane-18-monoene (25)

Titanium(IV) chloride (0.174 g, 0.917 mmol) was added to a 0 °C slurry of zinc dust (0.120 g, 1.83 mmol) and THF (10 mL). After the addition was complete, the reaction was heated to reflux for 1 h, at which point a dark black color persisted, indicative of the low-valent titanium species. Pyridine (0.1 mL) was added to the mixture and stirring at reflux was continued for 10 min. A solution of 12,22-diformyl-1,1,7,7-tetramethyl[7.2](7,1)pyrenophane (**22**) (0.076 g, 0.12 mmol) in THF (10 mL) was then added.

The resulting mixture was heated at 70 °C for 4 h, after which it was poured, without significant cooling, into chloroform (20 mL). The resulting solution was concentrated under reduced pressure and adsorbed on silica gel in preparation for column chromatography. Aqueous work-up for this reaction is not recommended as layer separation can be quite difficult and the yields are lower. The preadsorbed sample was subjected to column chromatography (25 × 2.5 cm; 15% dichloromethane/hexanes) to yield 1,1,7,7-tetramethyl[7.2.2](7,1,3)pyrenophane-18-monoene (**25**) (0.026 g, 36%): R_f = 0.60 (1:9 EtOAc/hexanes); mp >300 °C (dec.) ($CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (s, 2H), 7.80 (d, J=9.2 Hz, 2H), 7.63 (d, J=9.0 Hz, 2H), 7.62 (s, 2H), 7.53 (br s, 2H), 7.52 (br s, 2H), 7.48 (d, J=9.2 Hz, 2H), 7.42 (d, J=9.0 Hz, 2H) 4.29–4.25 (m, 2H), 3.74–3.70 (m, 2H) 1.42–1.37 (m, 4H) 1.34 (s, 6H), 1.33 (s, 6H) 0.76–0.70 (m, 2H), 0.28–0.24 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 145.64, 137.69, 136.14, 130.14, 130.04, 130.01, 128.28, 128.04, 126.29, 125.76, 123.99, 123.64, 122.42, 122.27, 122.21, 122.02, 46.13, 38.45, 31.02, 30.47, 28.77, 28.69, 26.54 (only 23 of 24 signals observed); LCMS (APCI-positive) *m/z* (rel. int.) 609 (16), 608 (56), 607 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{47}H_{42}$ ($[M]^+$) 606.3287, found 606.3277.

1,1,8,8-Tetramethyl[8.2.2](7,1,3)pyrenophane-19-monoene (26)

Titanium(IV) chloride (0.047 g, 0.25 mmol) was added to a 0 °C slurry of zinc dust (0.032 g, 0.50 mmol) and THF (5 mL). After the addition was complete, the reaction was heated to reflux for 1 h, at which point a dark black color persisted, indicative of the low-valent titanium species. Pyridine (0.05 mL) was added to the mixture and stirring at reflux was continued for 10 min. A solution of 13,23-diformyl-1,1,8,8-tetramethyl[8.2](7,1)pyrenophane (**23**) (0.020 g, 0.031 mmol) in THF (5 mL) was then added. The mixture was heated at 70 °C for 4 h, after which it was poured, without significant cooling, into chloroform (15 mL). The resulting solution was concentrated under reduced pressure and adsorbed on silica gel in preparation for column chromatography. Aqueous work-up for this reaction is not recommended as layer separation can be quite difficult and the yields are lower. The preadsorbed sample was subjected to column chromatography (25 × 2 cm; 1:5 dichloromethane/heaxanes) to afford 1,1,8,8-tetramethyl[8.2.2](7,1,3)pyrenophane-19-monoene (**26**) as a pale-green oil (0.010 g, 52%): R_f = 0.61 (1:9 EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 2H), 7.82 (d, J=9.2 Hz, 2H) 7.66–7.64 (m, 4H), 7.56 (d, J=1.4 Hz, 2H), 7.54 (d, J=1.4 Hz, 2H), 7.48 (d, J=9.1 Hz, 2H), 7.44 (d, J=9.2 Hz, 2H), 4.31–4.26 (m, 2H), 3.76–3.71 (m, 2H), 1.54–1.50 (m, 4H), 1.33 (s, 6H) 1.32 (s, 6H), 1.05–1.02 (m, 4H), 0.34–0.30 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 145.37, 138.21, 135.82, 130.01, 128.58, 128.56, 126.12, 125.33, 124.02, 123.99, 123.01, 122.98, 122.96, 122.36, 122.16, 46.72, 38.33, 30.78, 29.65, 24.74;

LCMS (APCI-positive) *m/z* (rel. int.) 623 (11), 622 (54), 621 ($[M+H]^+$, 100), HRMS (EI) calculated for $C_{48}H_{44}$ ($[M]^+$) 620.3443, found 620.3438.

1,1,9,9-Tetramethyl[9.2.2](7,1,3)pyrenophane-20-monoene (27)

Titanium(IV) chloride (0.103 g, 0.544 mmol) was added to a 0 °C slurry of zinc dust (0.142 g, 1.09 mmol) in THF (15 mL). After the addition was complete, the reaction was heated to reflux for 1 h, at which point a dark black color persisted, indicative of the low-valent titanium species. Pyridine (0.15 mL) was added to the mixture and stirring at reflux was continued for 10 min. A solution of 14,24-diformyl-1,1,9,9-tetramethyl[9.2](7,1)pyrenophane (**24**) (0.069 g, 0.10 mmol) in THF (10 mL) was then added. The mixture was heated at 70 °C for 4 h, after which it was poured, without significant cooling, into chloroform (40 mL). The resulting solution was concentrated under reduced pressure and adsorbed on silica gel in preparation for column chromatography. Aqueous work-up for this reaction is not recommended as layer separation can be quite difficult and the yields are lower. The preadsorbed sample was subjected to column chromatography (30 × 2 cm; 1:5 dichloromethane/hexanes) to give 1,1,9,9-tetramethyl[9.2.2](7,1,3)pyrenophane-20-monoene (**27**) as a light green oil (0.033 g, 51%): R_f = 0.64 (1:9 EtOAc/hexanes); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (s, 2H), 7.84 (d, J=9.2 Hz, 2H), 7.81 (s, 2H), 7.68 (d, J=9.0 Hz, 2H), 7.62 (br s, 2H), 7.61 (br s, 2H), 7.55 (d, J=9.2 Hz, 2H), 7.50 (d, J=9.0 Hz, 2H), 4.31–4.24 (m, 2H), 3.80–3.73 (m, 2H), 1.53–1.50 (m, 4H) 1.32 (s, 6H), 1.31 (s, 6H), 0.88–0.83 (m, 6H), 0.63–0.58 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 146.05, 137.38, 135.73, 130.18, 130.16, 129.38, 129.32, 128.24, 127.81, 126.47, 126.00, 123.74, 123.59, 122.65, 122.30, 122.16, 122.13, 45.92, 38.14, 30.64, 30.15, 29.36, 29.25, 28.67, 24.95; LCMS (APCI-positive) *m/z* (rel. int.) 637 (15), 636 (54), 635 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{49}H_{46}$ ($[M]^+$) 634.3600, found 634.3602.

1,1,7,7-Tetramethyl[7](2,11)teropyrenophane (28)

A solution of 1,1,7,7-tetramethyl[7.2.2](7,1,3)pyrenophane-18-monoene (**25**) (65.0 mg, 0.107 mmol) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (487 mg, 2.15 mmol), which was added in equal portions over 1 h intervals, in *m*-xylene (5 mL) was heated at 130 °C for 14 h. The hot solvent was evaporated under a stream of nitrogen gas. The residue was taken up into EtOAc and adsorbed on silica gel in preparation for column chromatography. The preadsorbed sample was subjected to column chromatography (39 × 1.5 cm; 5% EtOAc/hexanes) to yield 1,1,7,7-tetramethyl[7](2,11)teropyrenophane (**28**) (22 mg, 36%, (50% borsm)), which exhibits yellow fluorescence at 365 nm, and **25** (20 mg, 31% recovery). R_f = 0.27 (1:9 EtOAc/hexanes); m.p. >300 °C (dec.); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (s,

4H), 8.26 (d, *J*=9.5 Hz, 4H), 7.62 (d, *J*=9.5 Hz, 4H) 7.29 (s, 4H), 1.35 (s, 12H), 0.78–0.74 (m, 4H), 0.08-0.01 (m, 2H), –1.12 to –1.18 (m, 4H); ^{13}C NMR δ 144.50, 128.75, 127.89, 126.97, 126.03, 125.44, 124.89, 124.18, 123.54, 123.18, 77.65, 47.74, 38.23, 31.18, 28.42, 24.27; LCMS (APCI-positive) *m/z* (rel. int.) 605 (14), 604 (43), 603 (82, $[M+H]^+$); HRMS (EI) calculated for $C_{47}H_{38}$ ($[M]^+$) 602.2974, found 602.2974.

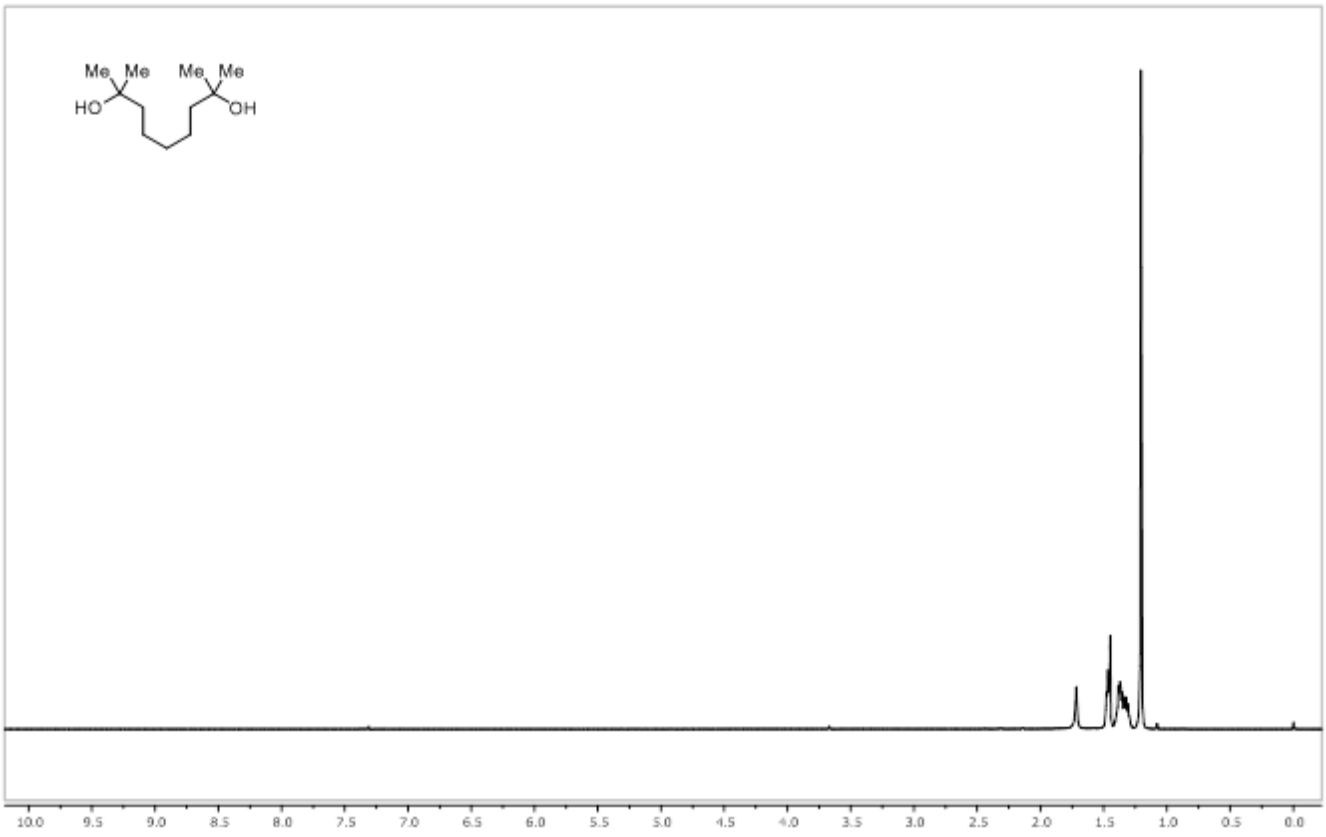
1,1,8,8-Tetramethyl[8](2,11)teropyrenophane (1)

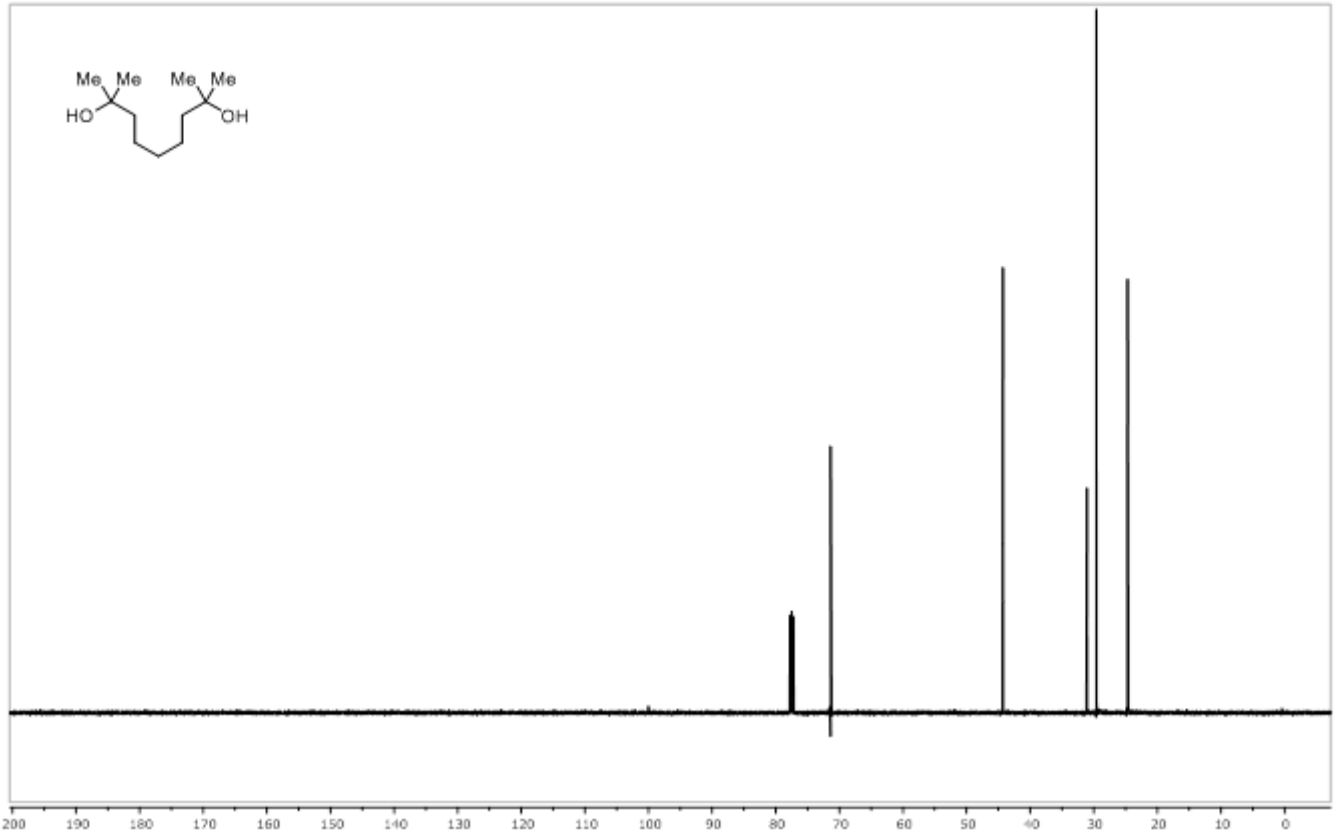
A solution of 1,1,8,8-tetramethyl[8.2.2](7,1,3)pyrenophane-19-monoene (**26**) (0.022 g, 0.036 mmol) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (0.032 g, 0.14 mmol) in *m*-xylene (5 mL) was heated at 145 °C for 48 h. The hot solvent was evaporated under a stream of nitrogen gas. The residue was taken up into dichloromethane and adsorbed on silica gel in preparation for column chromatography. The preadsorbed sample was subjected to column chromatography (30 × 2.0 cm; 5% EtOAc/hexanes) to yield 1,1,8,8-tetramethyl[8](2,11)teropyrenophane (**1**) as an orange solid (0.020 g, 90%), which exhibits yellow fluorescence at 365 nm: R_f = 0.33 (1:9 EtOAc/hexanes); m.p. >300 °C (dec.) (EtOH); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.62 (s, 4H), 8.39 (d, *J*=9.5 Hz, 4H), 7.71 (d, *J*=9.5 Hz, 4H), 7.42 (s, 4H), 1.32 (s, 12H), 0.74–0.70 (m, 4H), –0.24 to –0.27 (m, 4H), –0.65 to –0.70 (m, 4H); ^{13}C NMR (125.77 MHz, $CDCl_3$) δ 145.34, 128.57, 127.75, 127.45, 127.36, 125.92, 125.15, 124.56, 123.68, 123.30, 77.68, 47.77, 38.53, 30.12, 29.78, 27.16, 23.96; LCMS (APCI-positive) *m/z* (rel. int.) 619 (13), 618 (52), 617 ($[M+H]^+$, 100); HRMS (CI) calculated for $C_{48}H_{41}$ ($[M+H]^+$) 617.3208, found 617.3211.

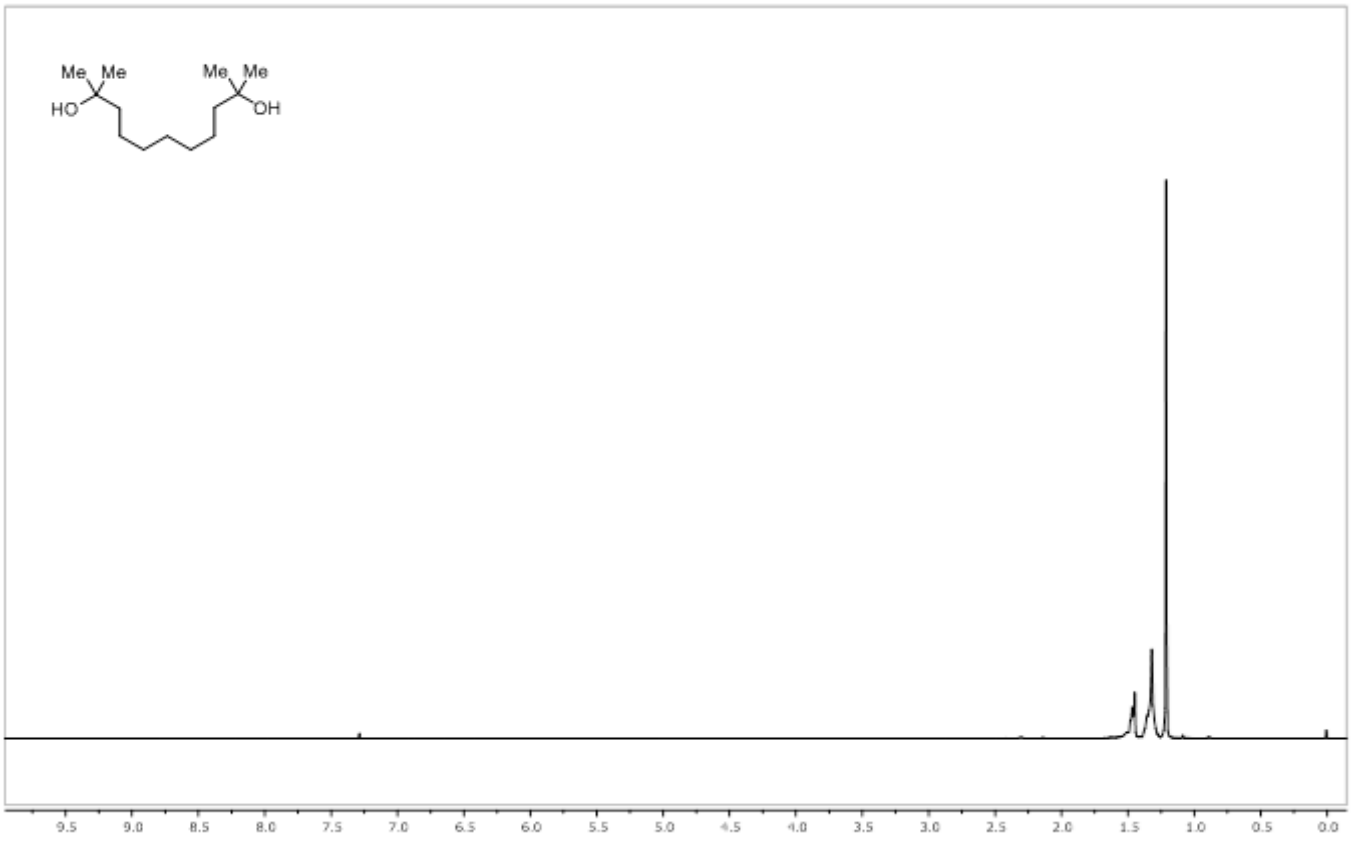
1,1,9,9-Tetramethyl[9](2,11)teropyrenophane (29)

A solution of 1,1,9,9-tetramethyl[9.2.2](7,1,3)pyrenophane-20-monoene (**27**) (0.025 g, 0.039 mmol) and 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (0.039 g, 0.17 mmol) in *m*-xylene (6 mL) was heated at 145 °C for 36 h. The hot solvent was evaporated under a stream of nitrogen gas. The residue was taken up into dichloromethane and adsorbed on silica gel in preparation for column chromatography. The preadsorbed sample was subjected to column chromatography (30 × 2.0 cm; 5% EtOAc/hexanes) to yield 1,1,9,9-tetramethyl[9](2,11)teropyrenophane (**29**) as an orange solid (0.023 g, 95%), which exhibits yellow fluorescence at 365 nm. R_f = 0.40 (1:9 EtOAc/hexanes); m.p. >300 °C (dec.) ($CHCl_3$); ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (s, 4H), 8.52 (d, *J*=9.5 Hz, 4H), 7.80 (d, *J*=9.5 Hz, 4H) 7.50 (s, 4H), 1.37 (s, 12H), 0.81–0.78 (m, 4H), –0.51 to –0.55 (m, 4H), –0.99 to –1.03 (m, 6H); (APCI-positive) *m/z* (rel. int.) 633 (16), 632 (54) 631 ($[M+H]^+$, 100); HRMS (EI) calculated for $C_{49}H_{42}$ ($[M]^+$) 630.3287, found 630.3282.

^{1}H and ^{13}C NMR Spectra



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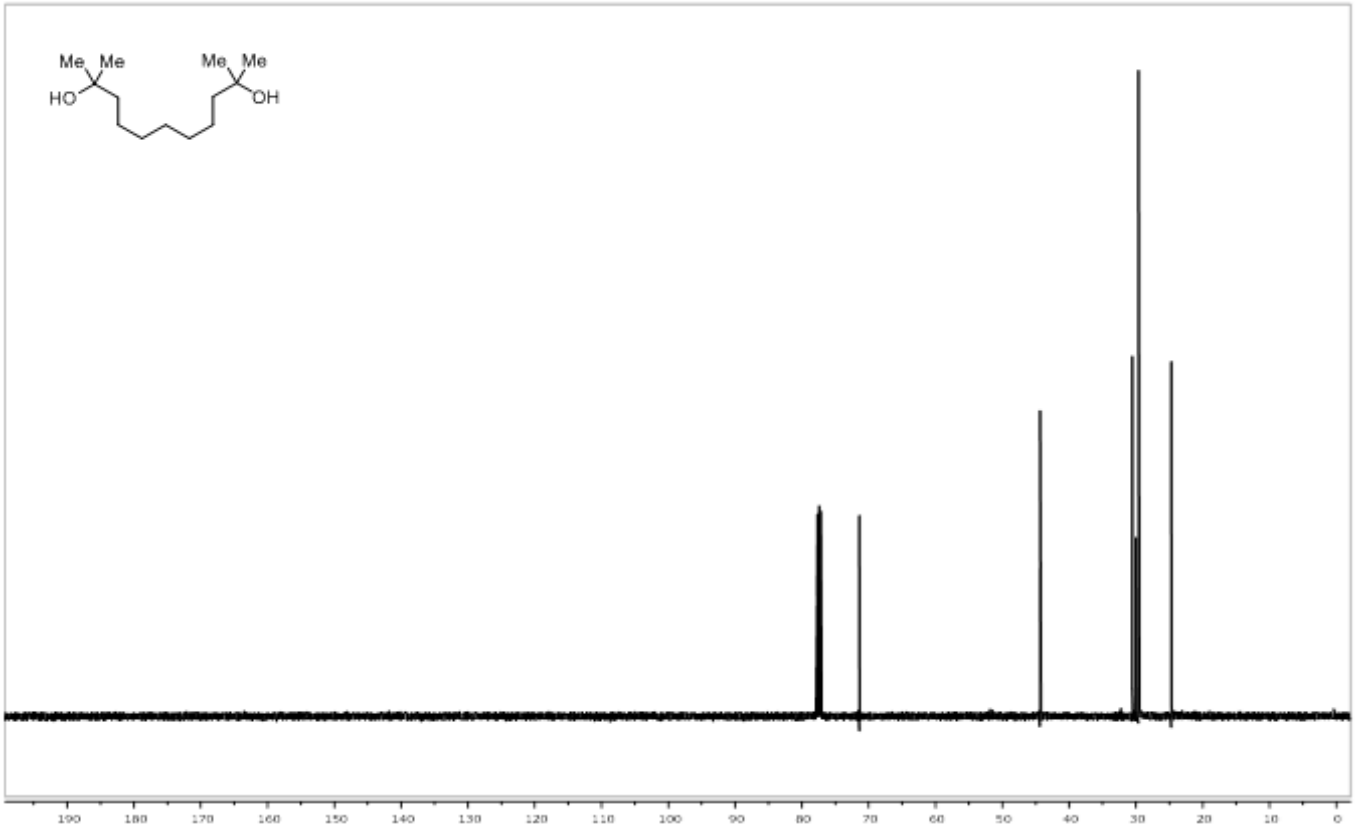
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10
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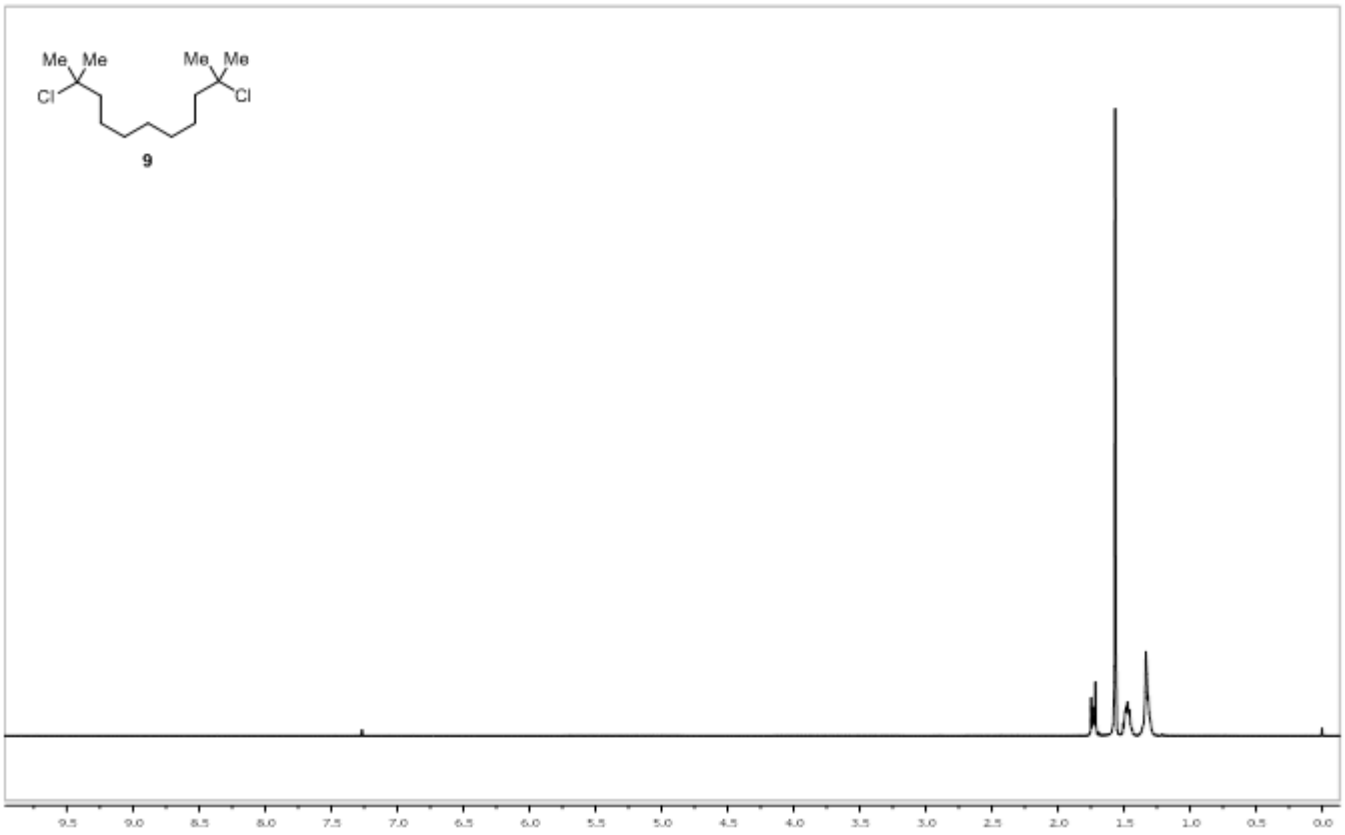

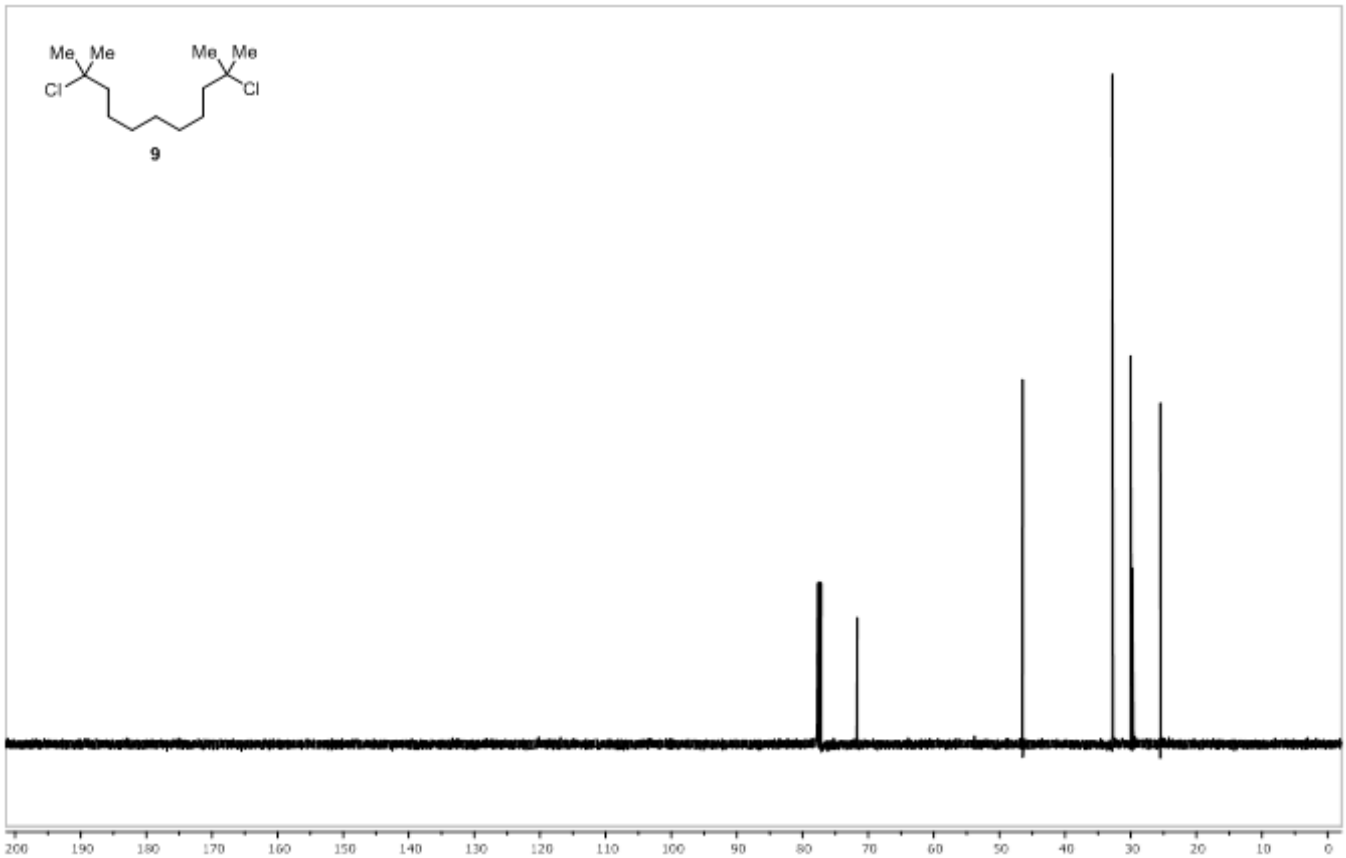

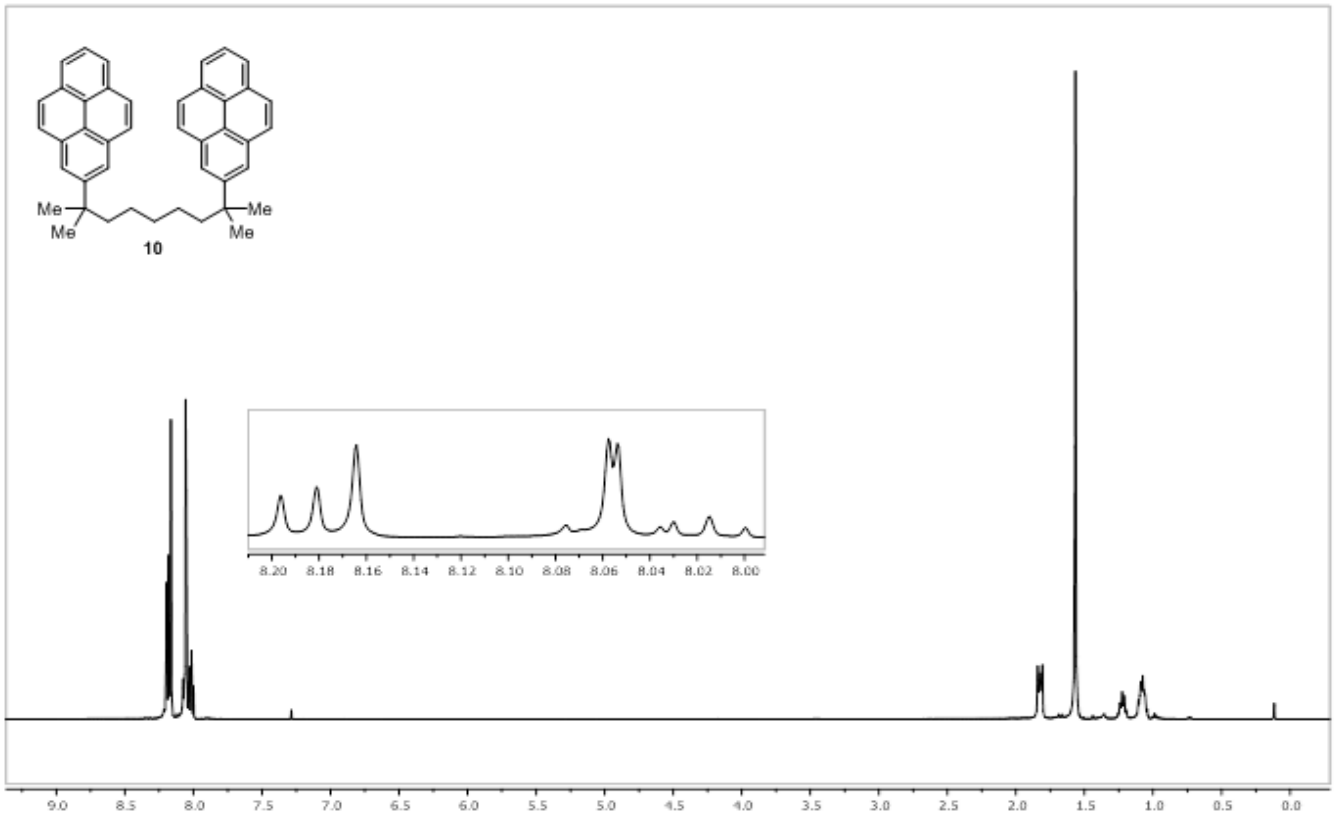
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Me
Me
Me
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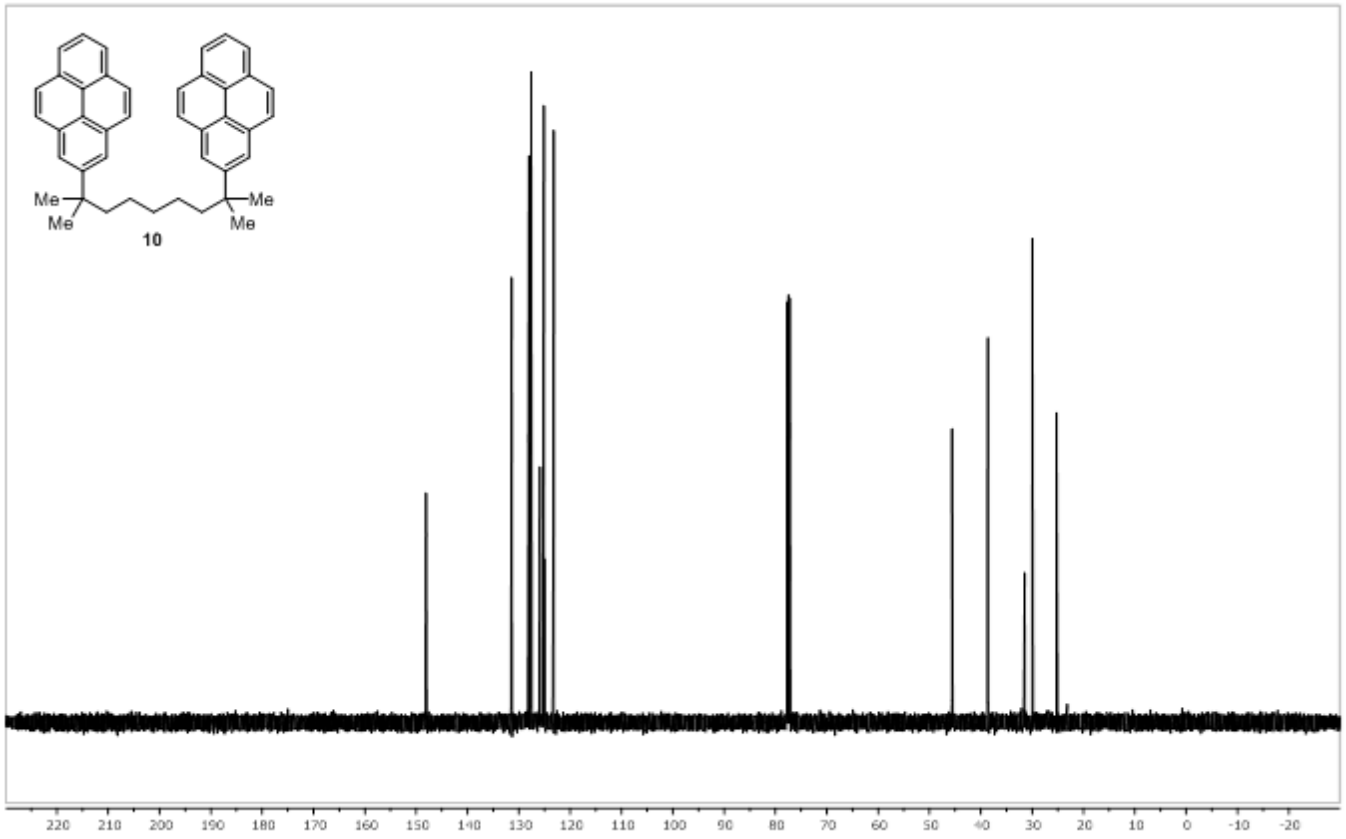
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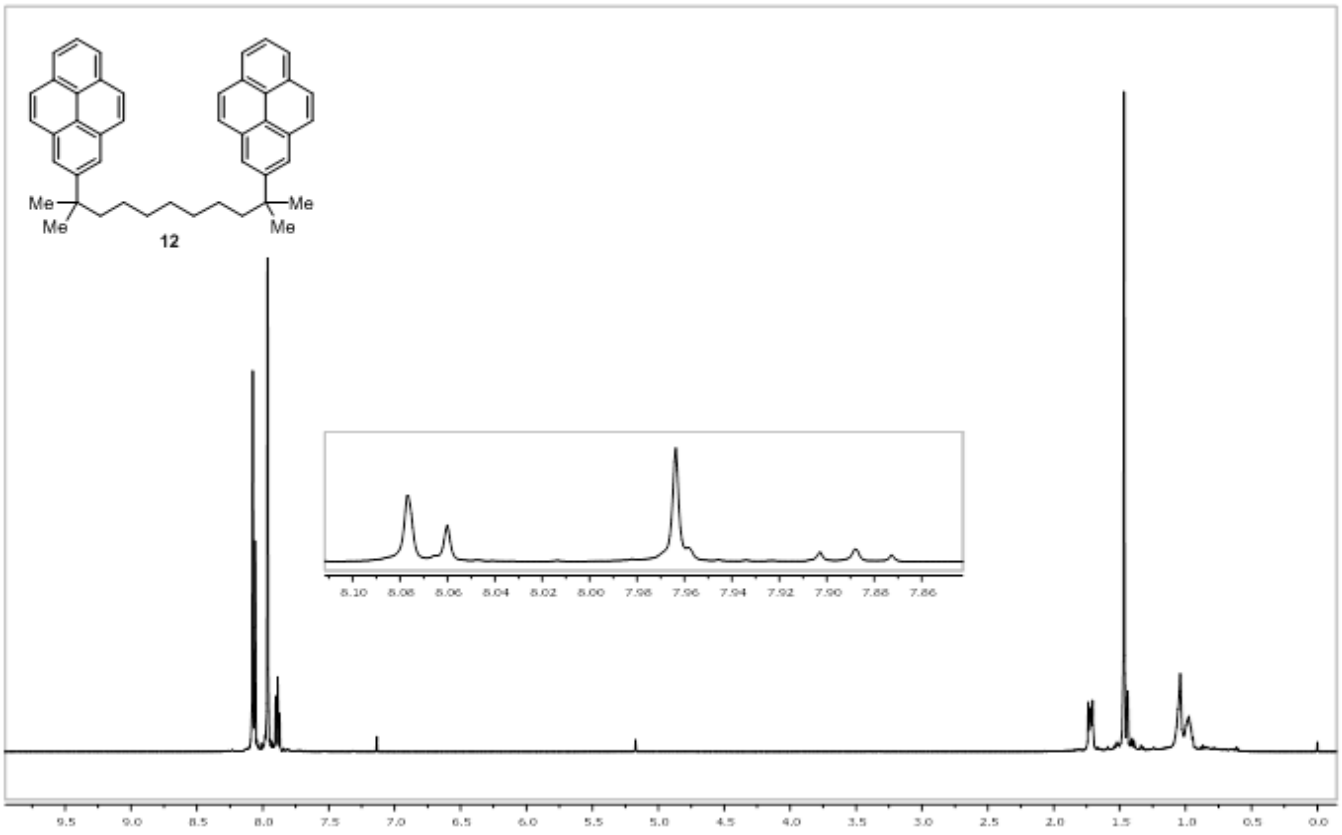

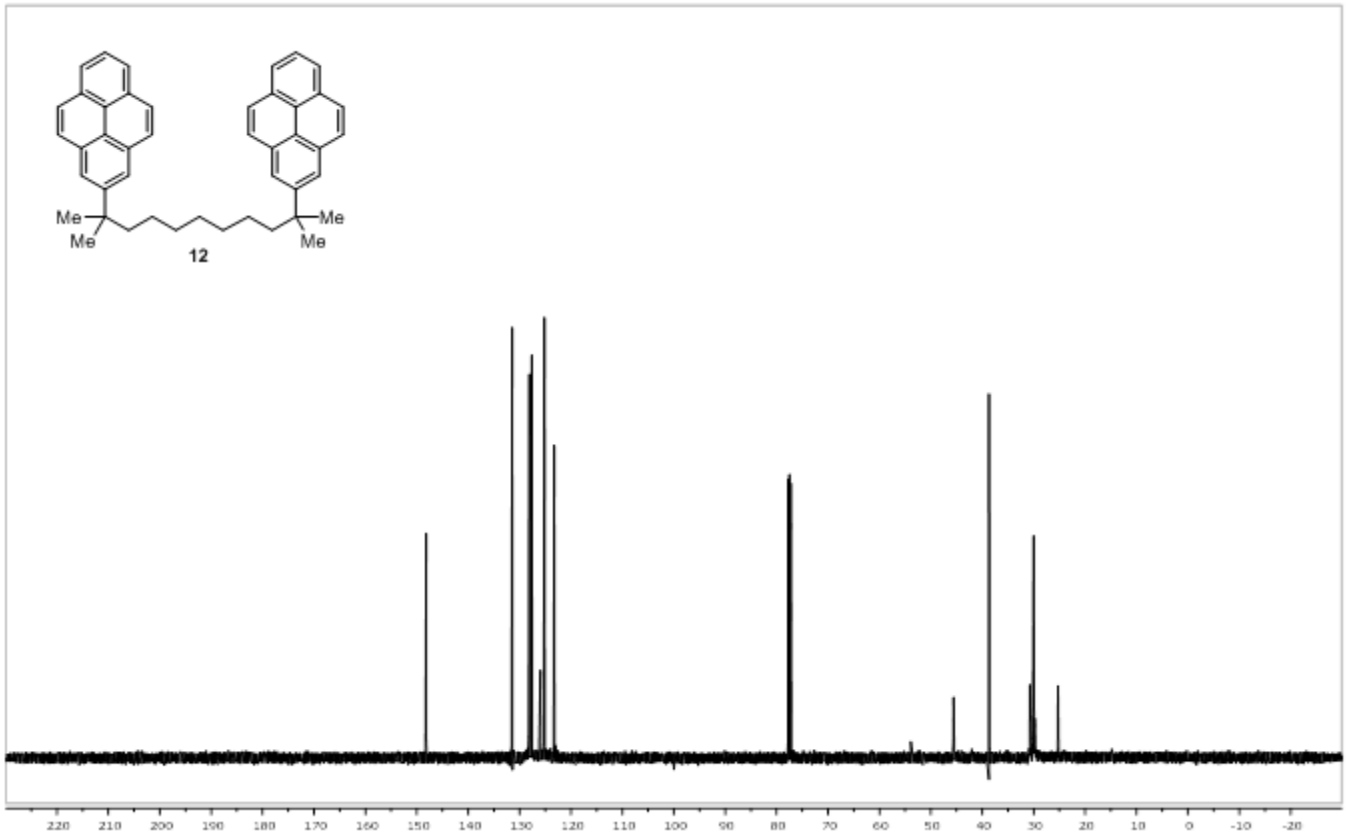

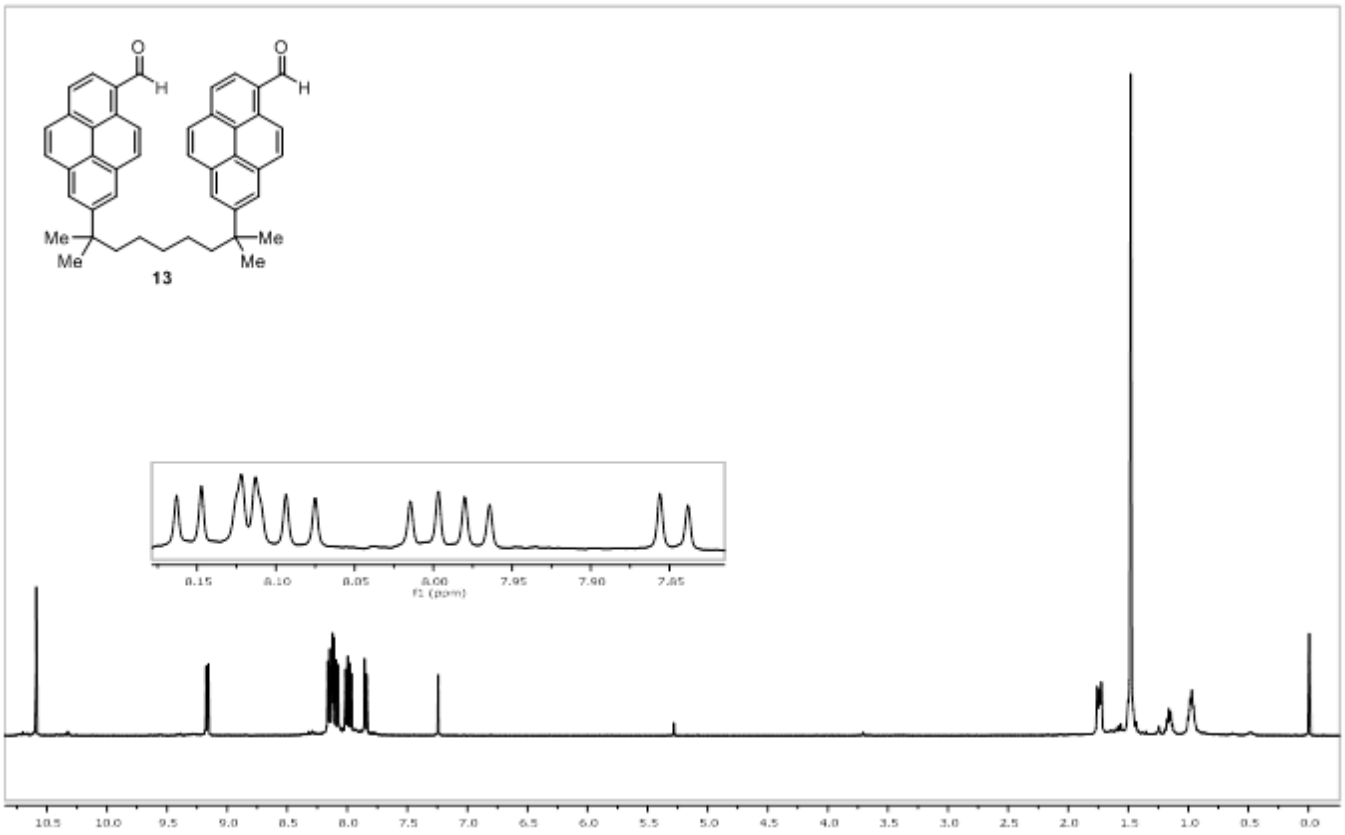

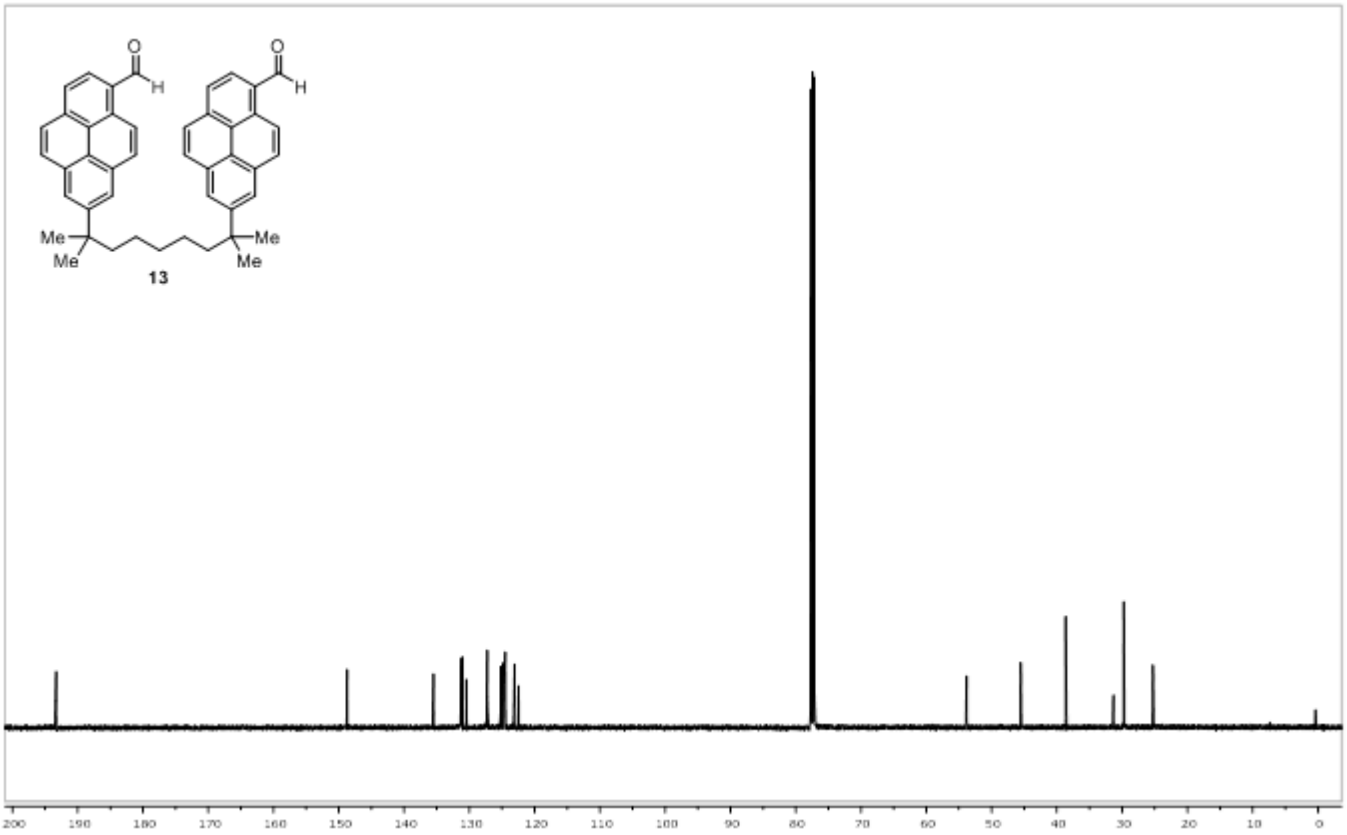

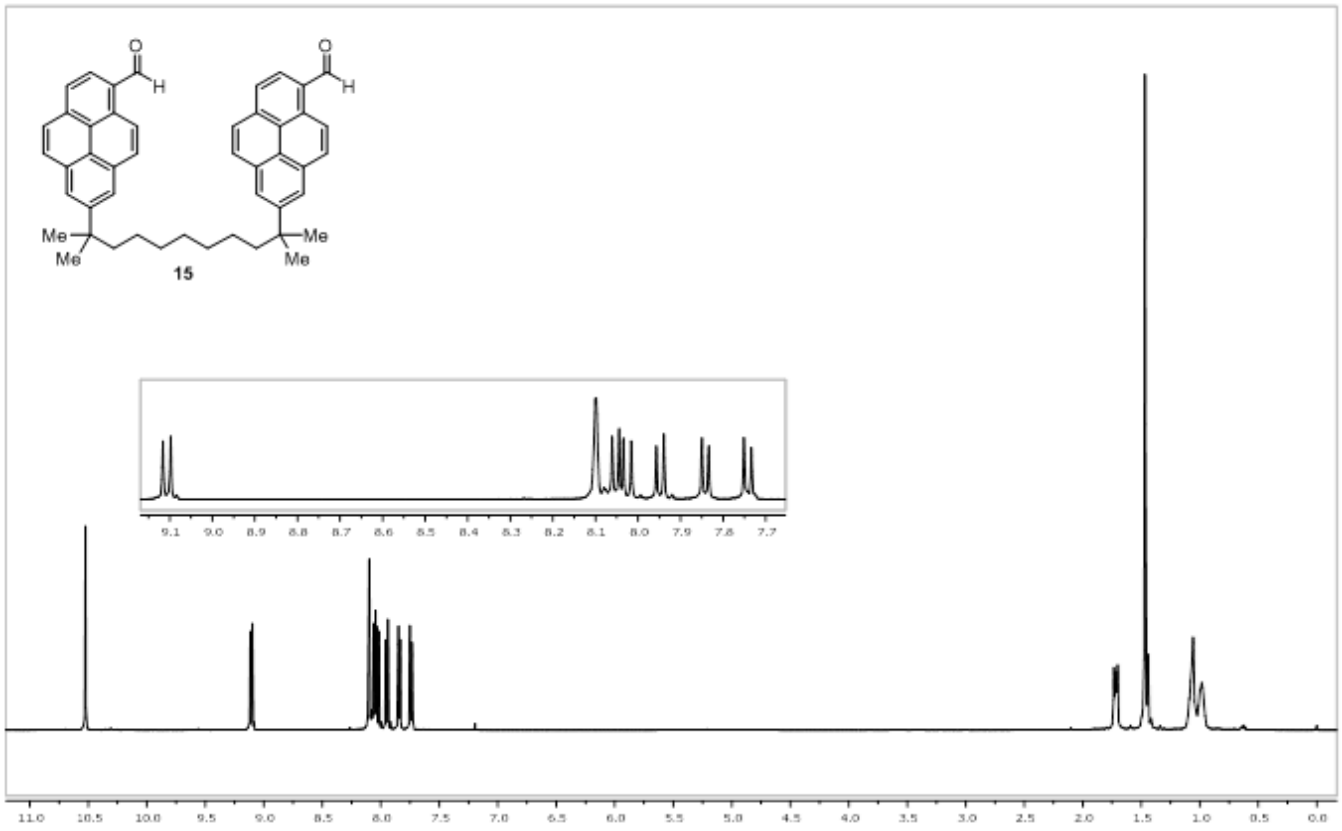
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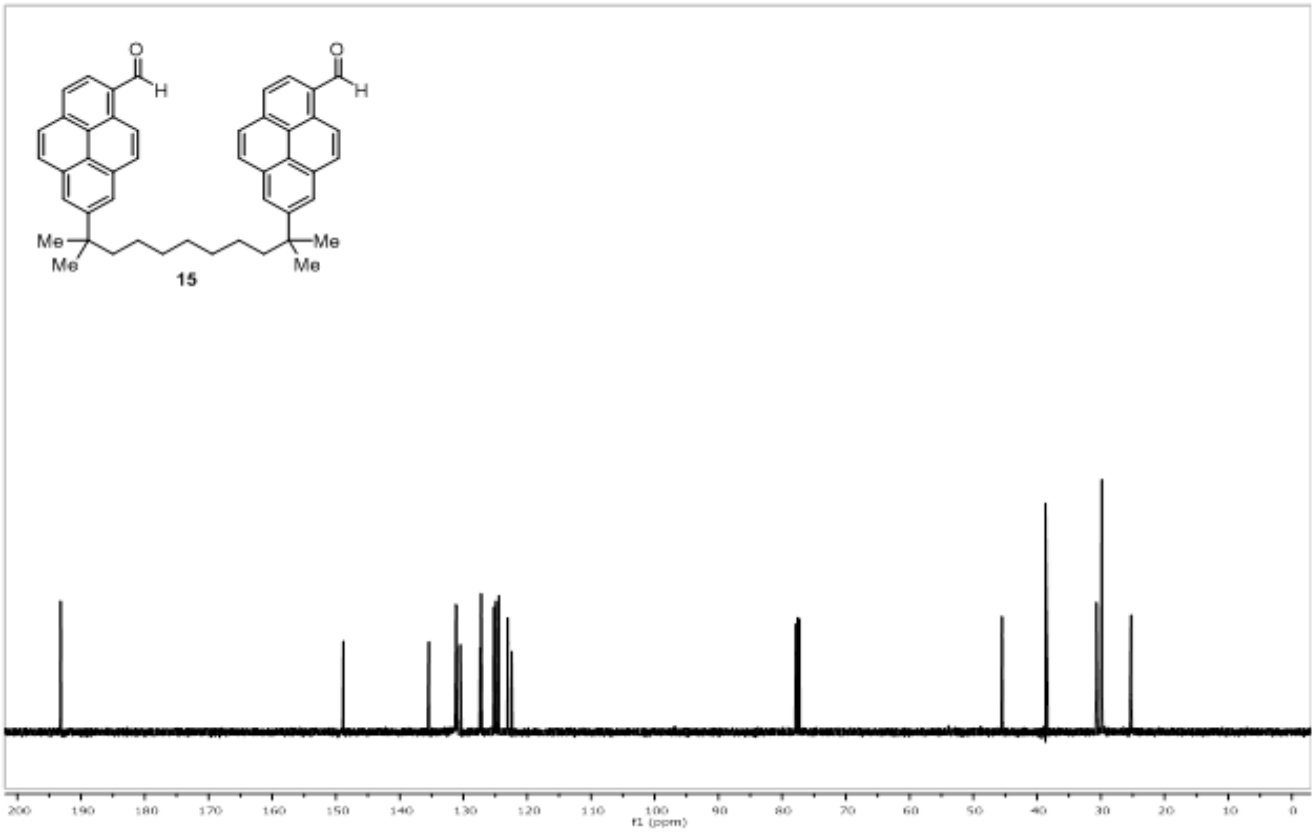
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Me
Me
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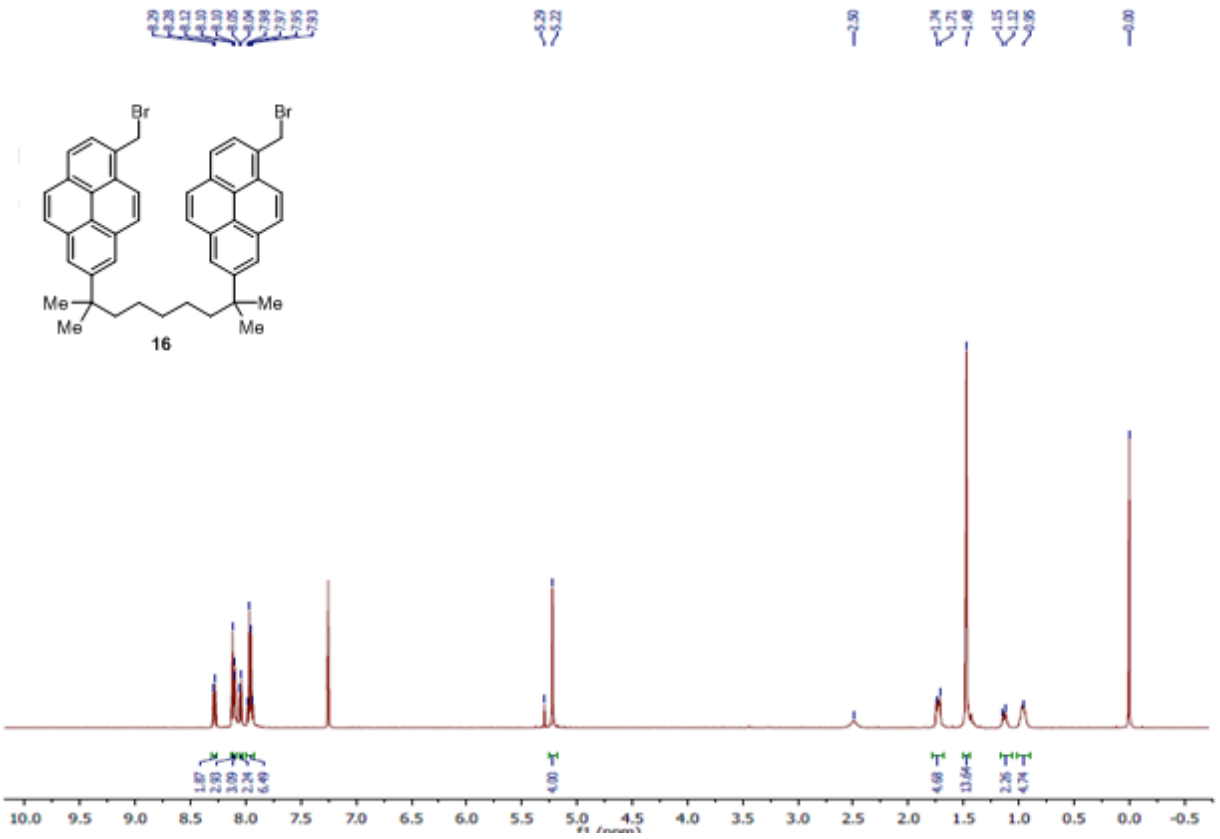
f1 (ppm)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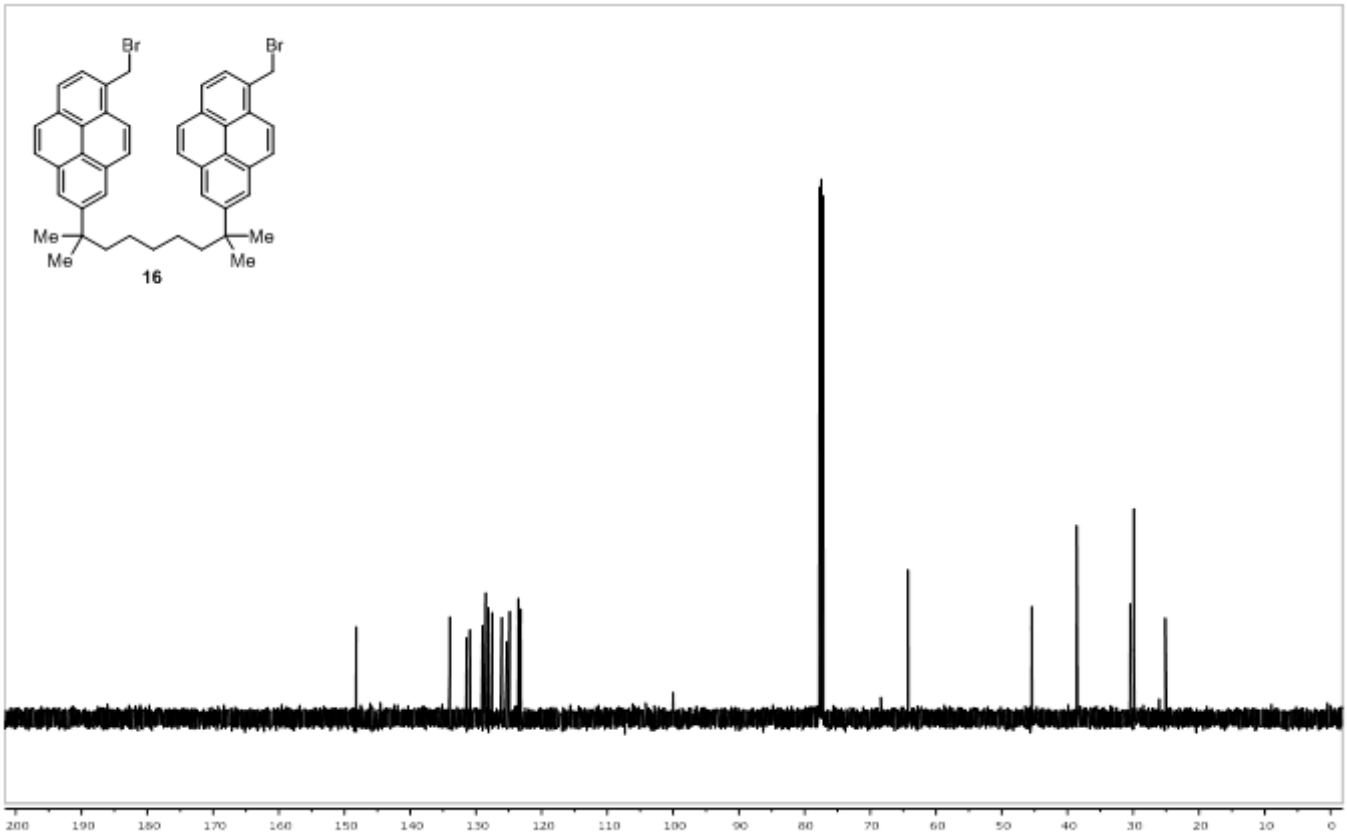
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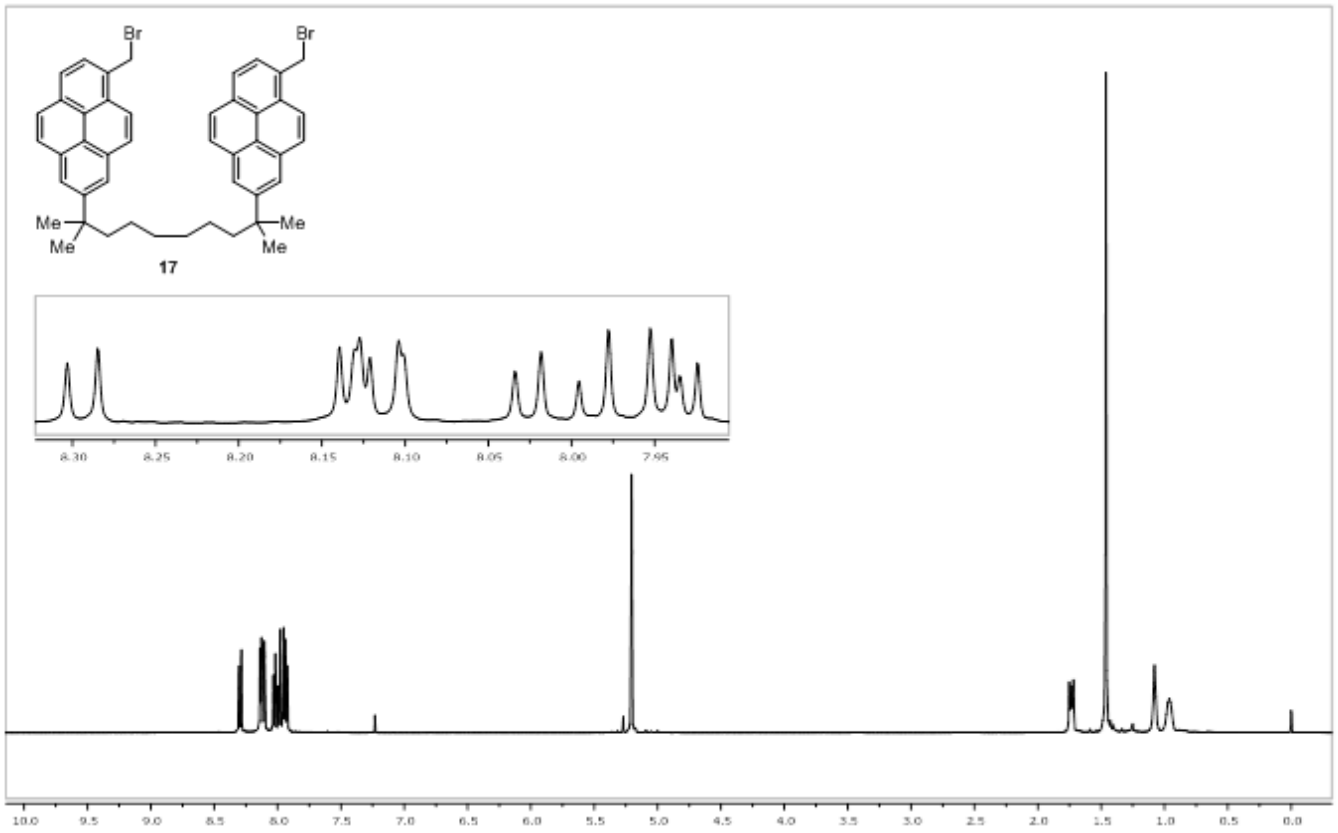

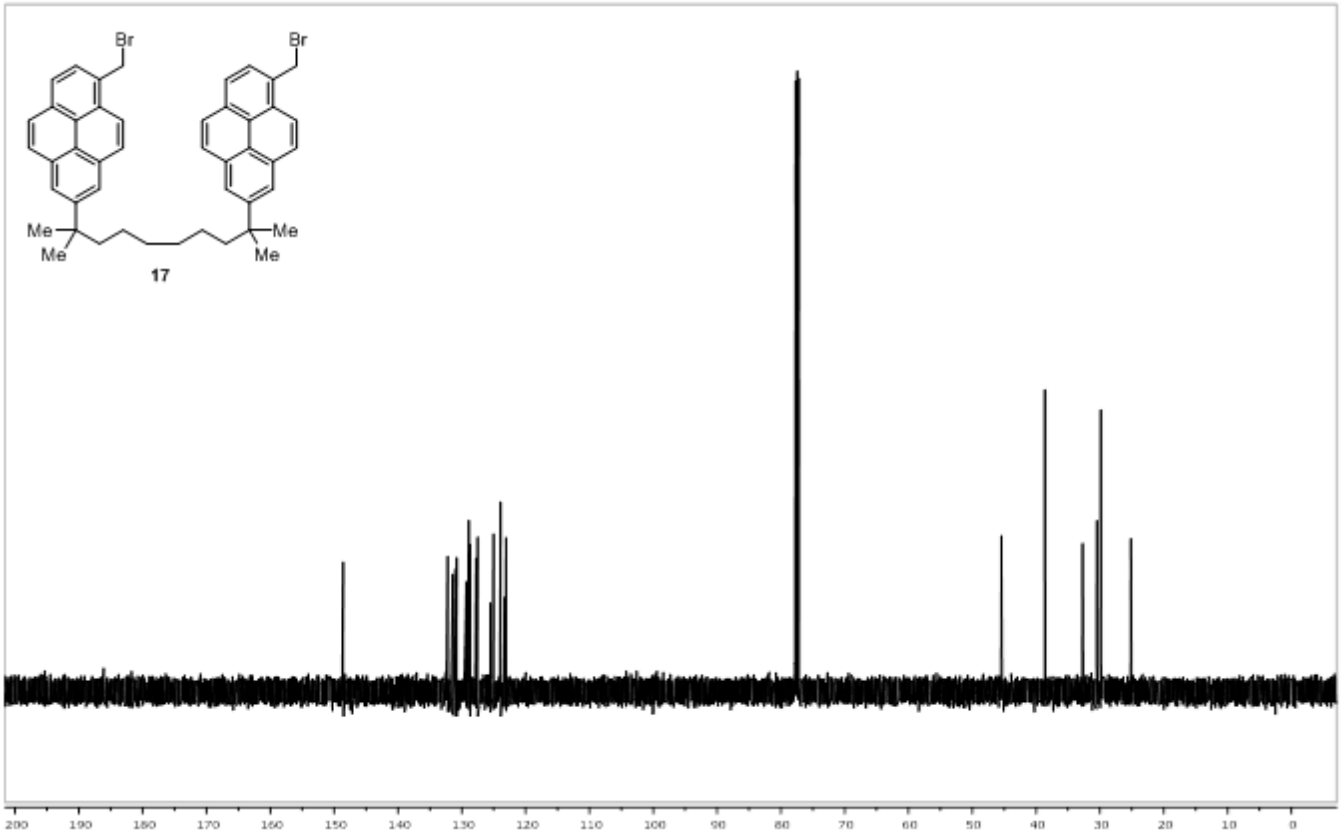

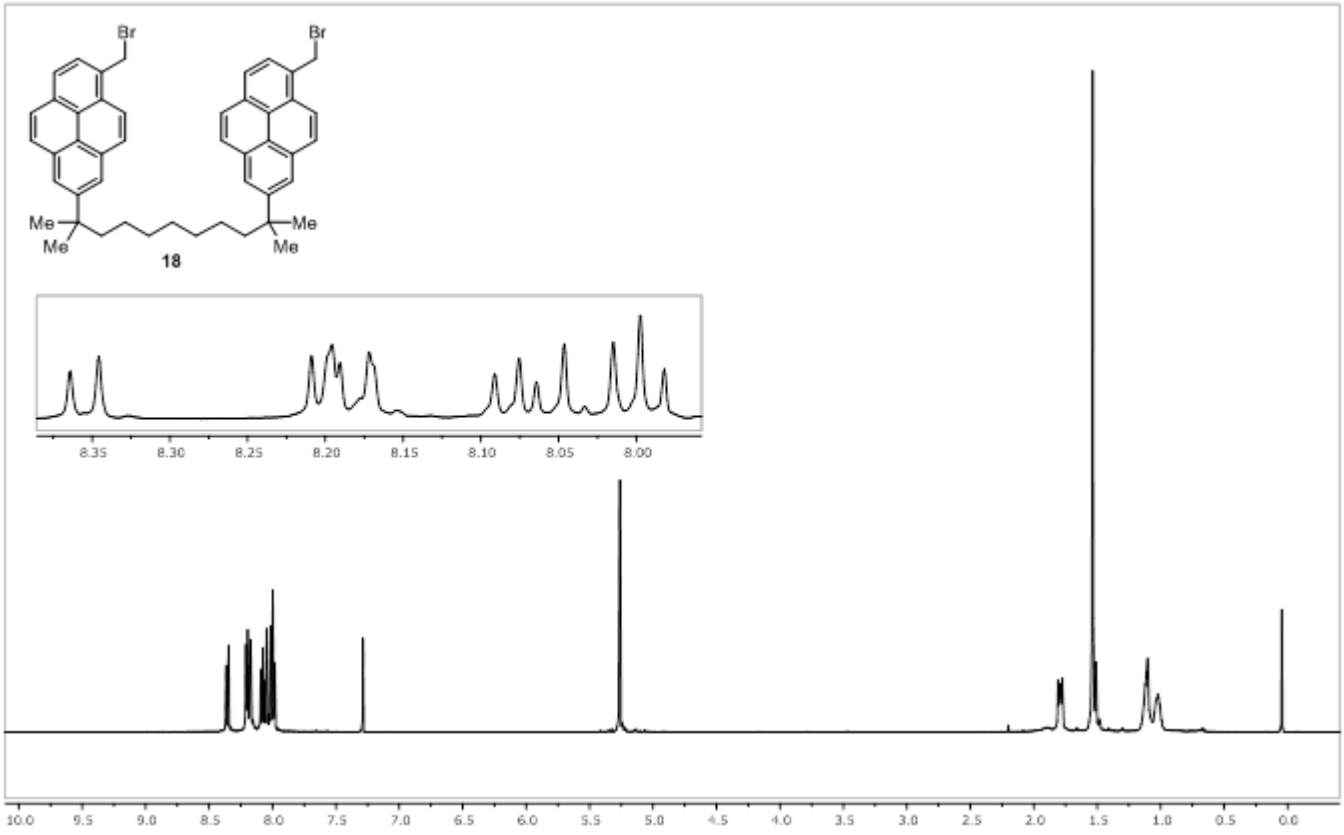

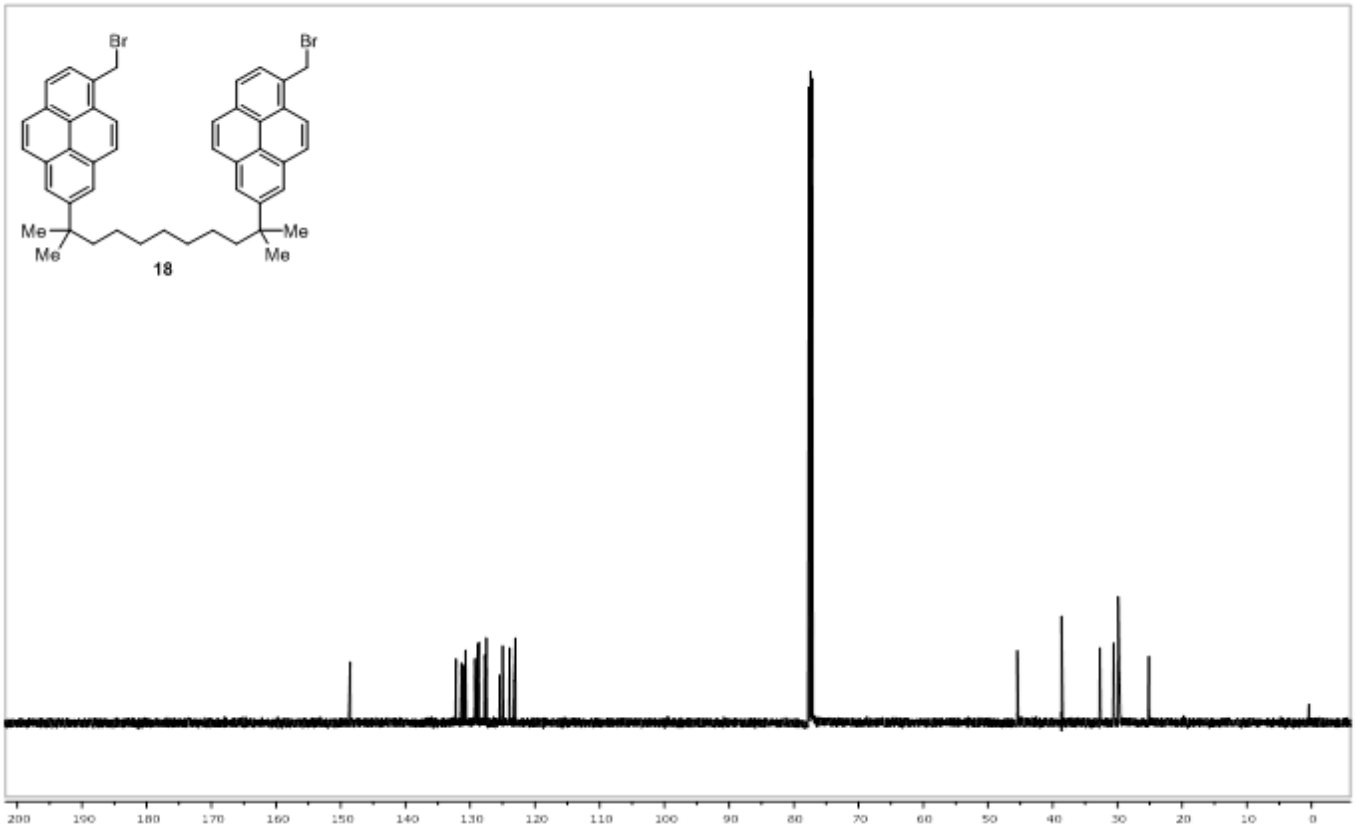

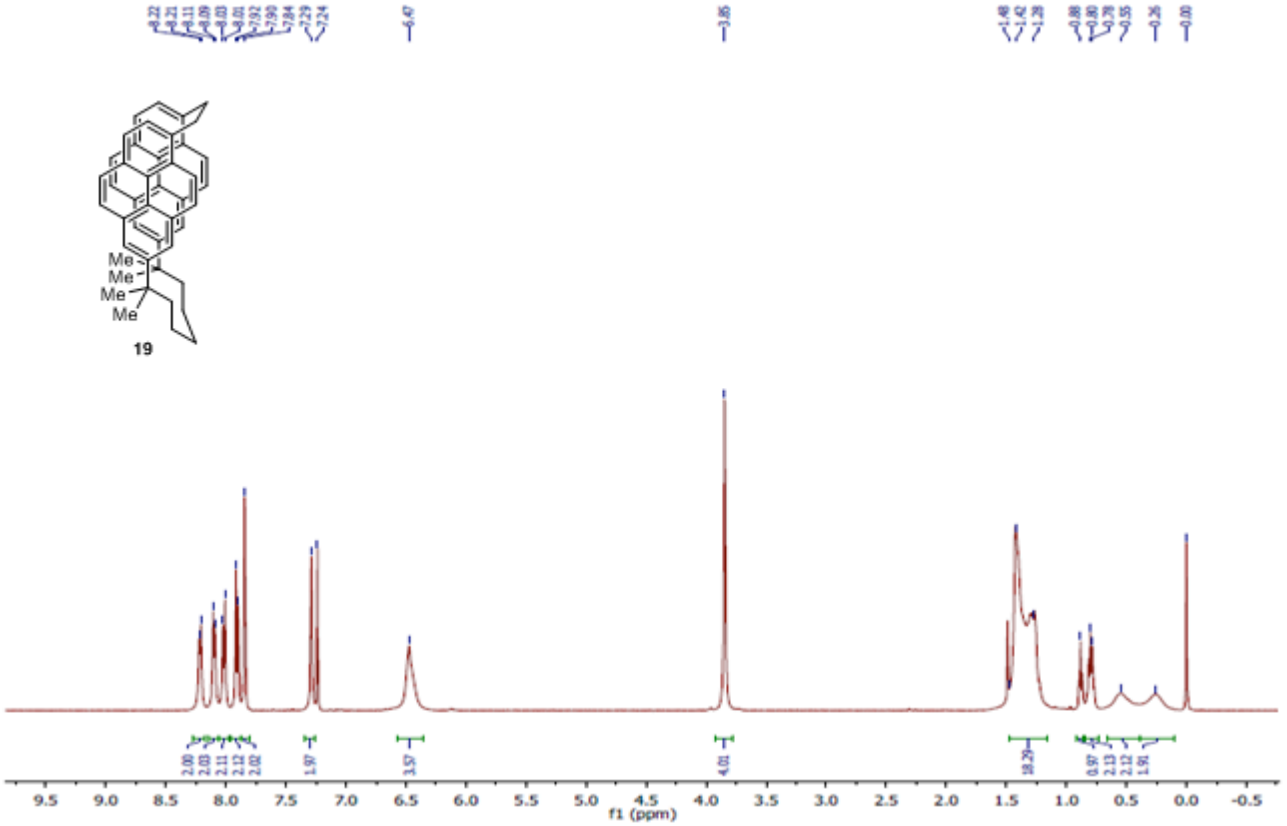
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Me
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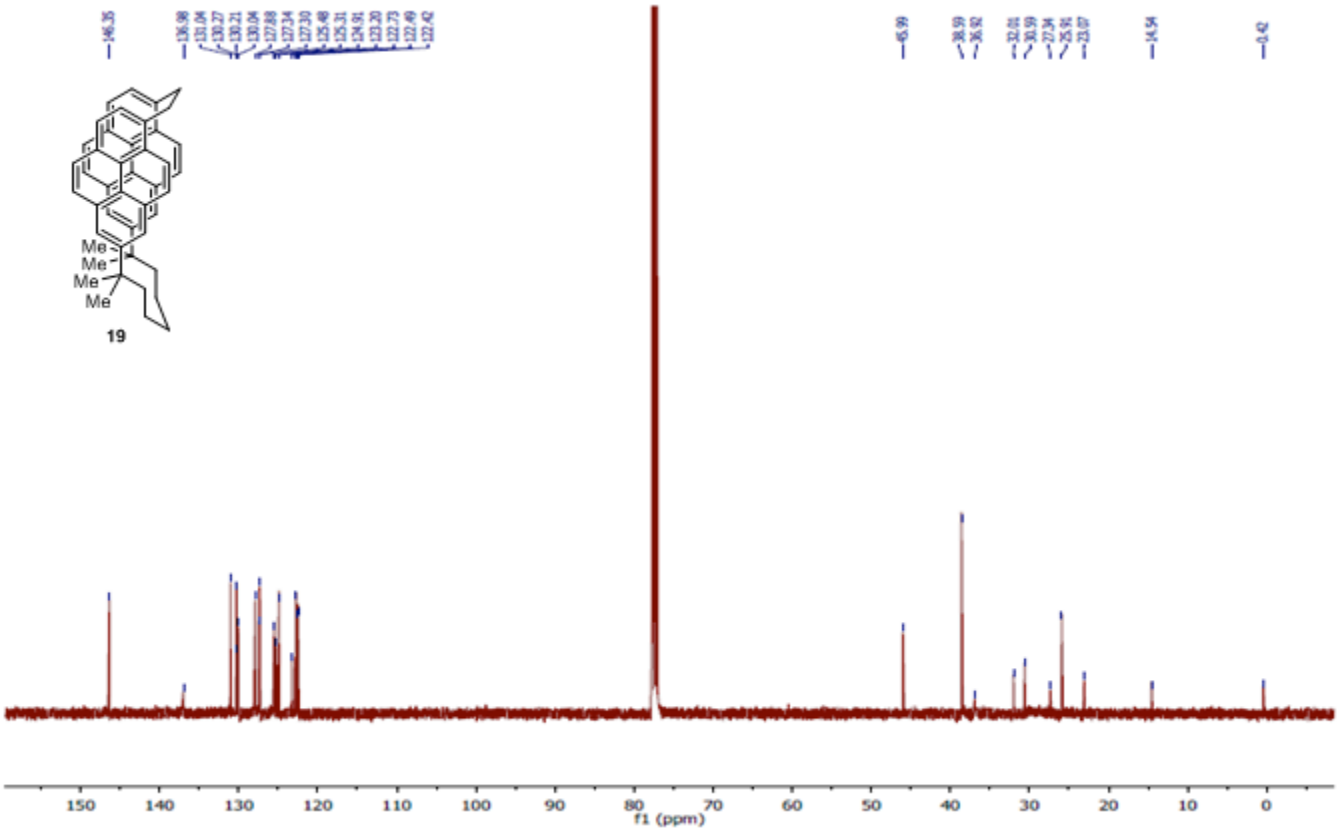
f1 (ppm)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Me
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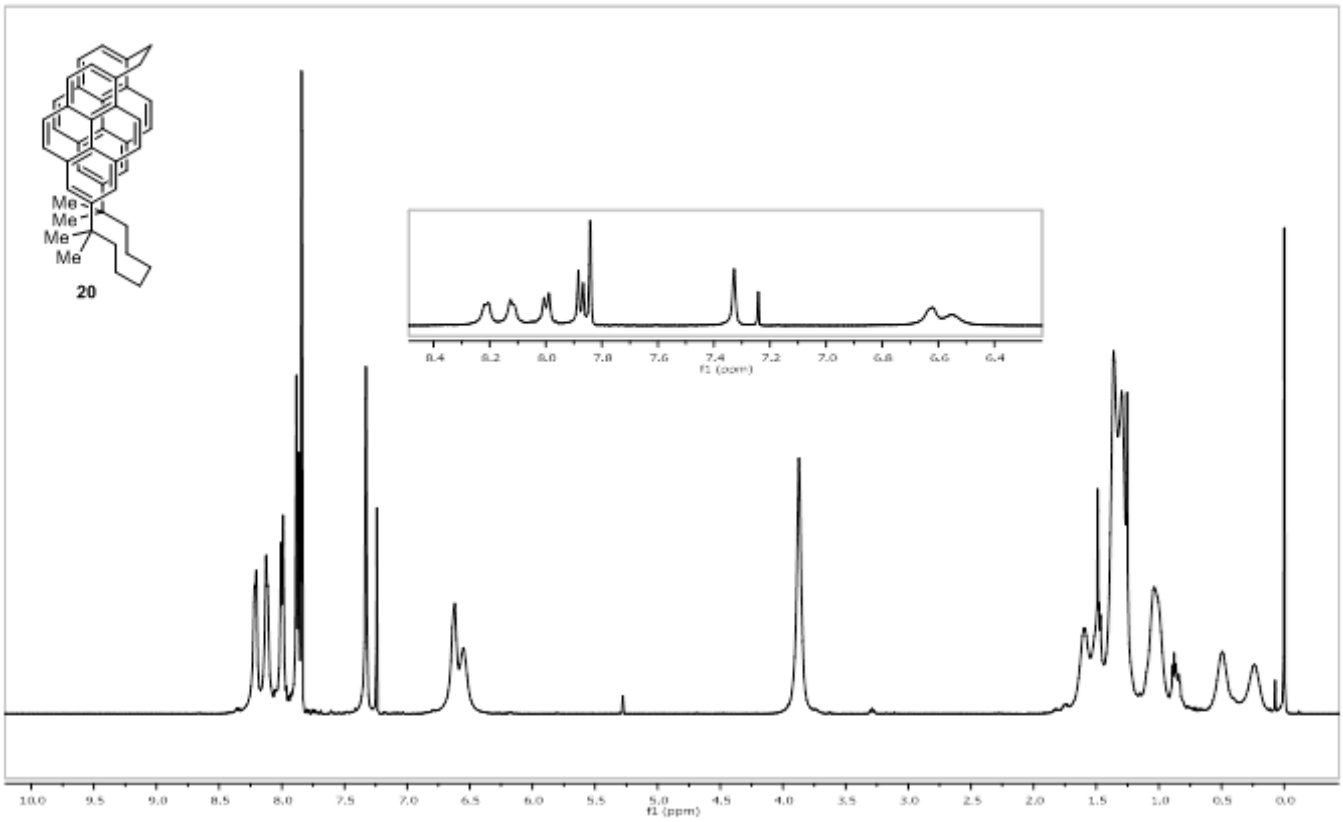
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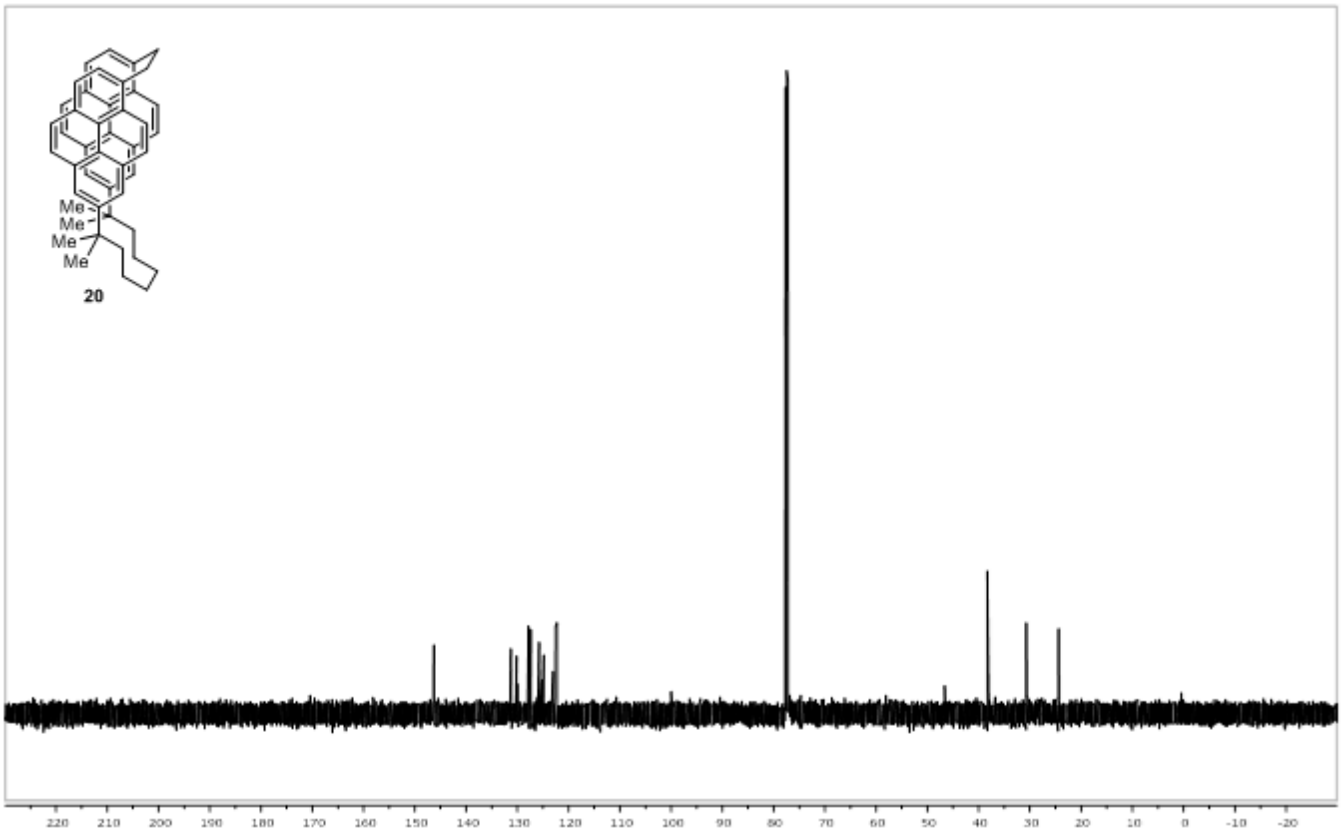
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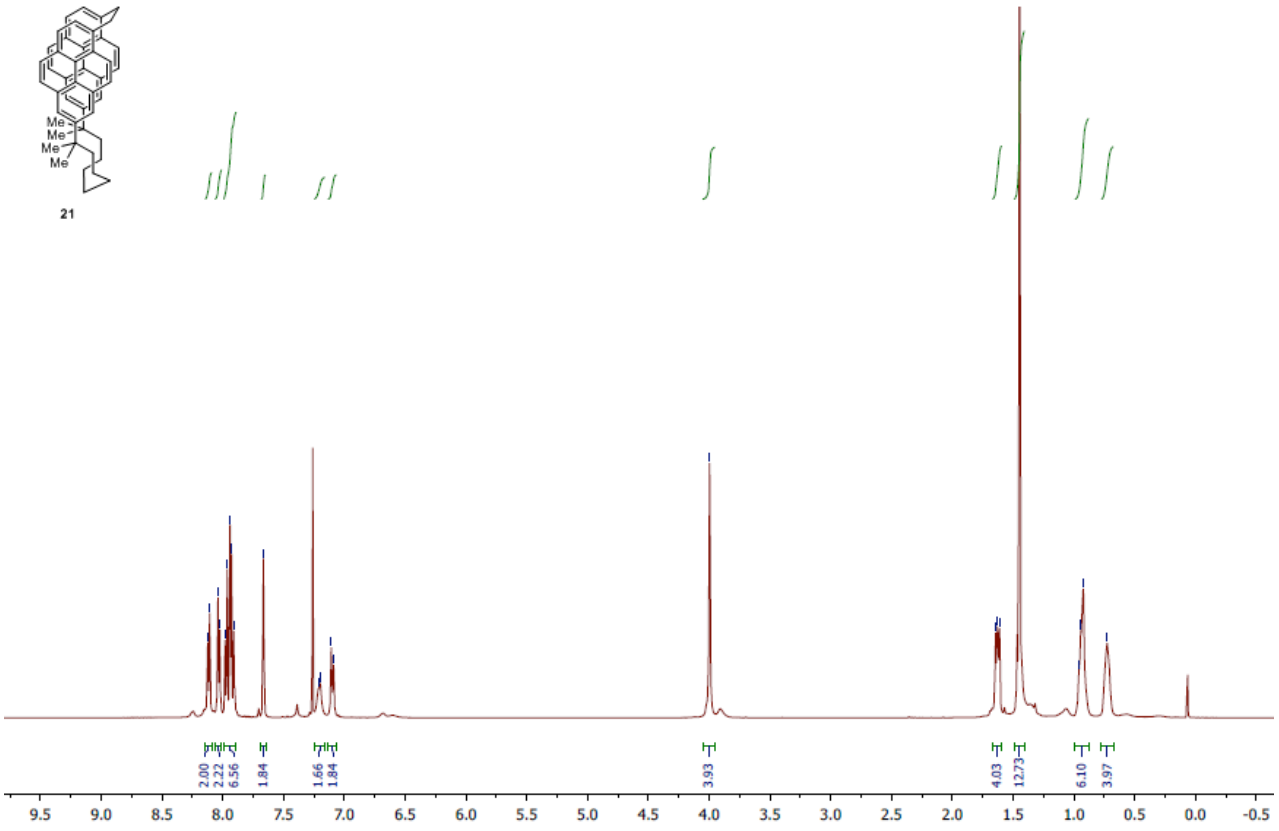

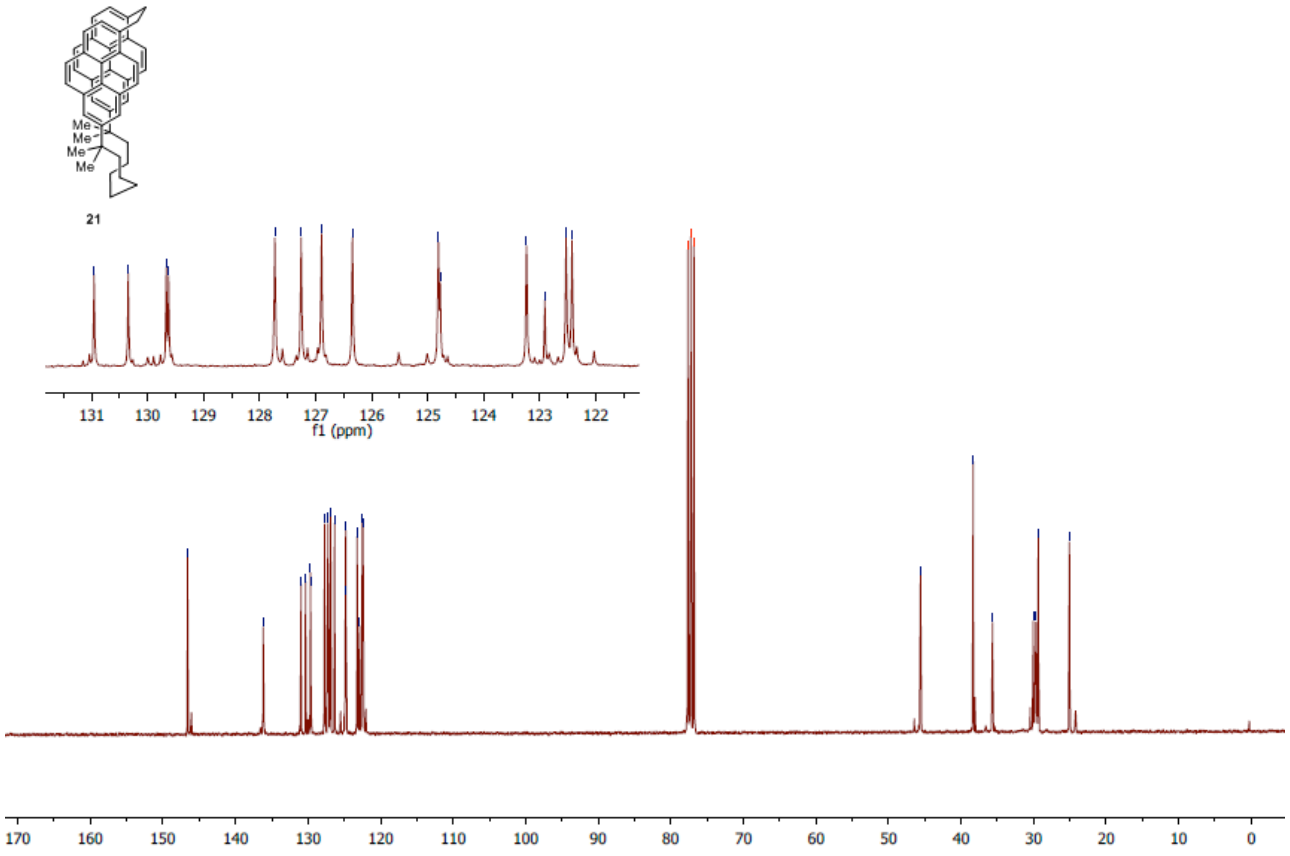

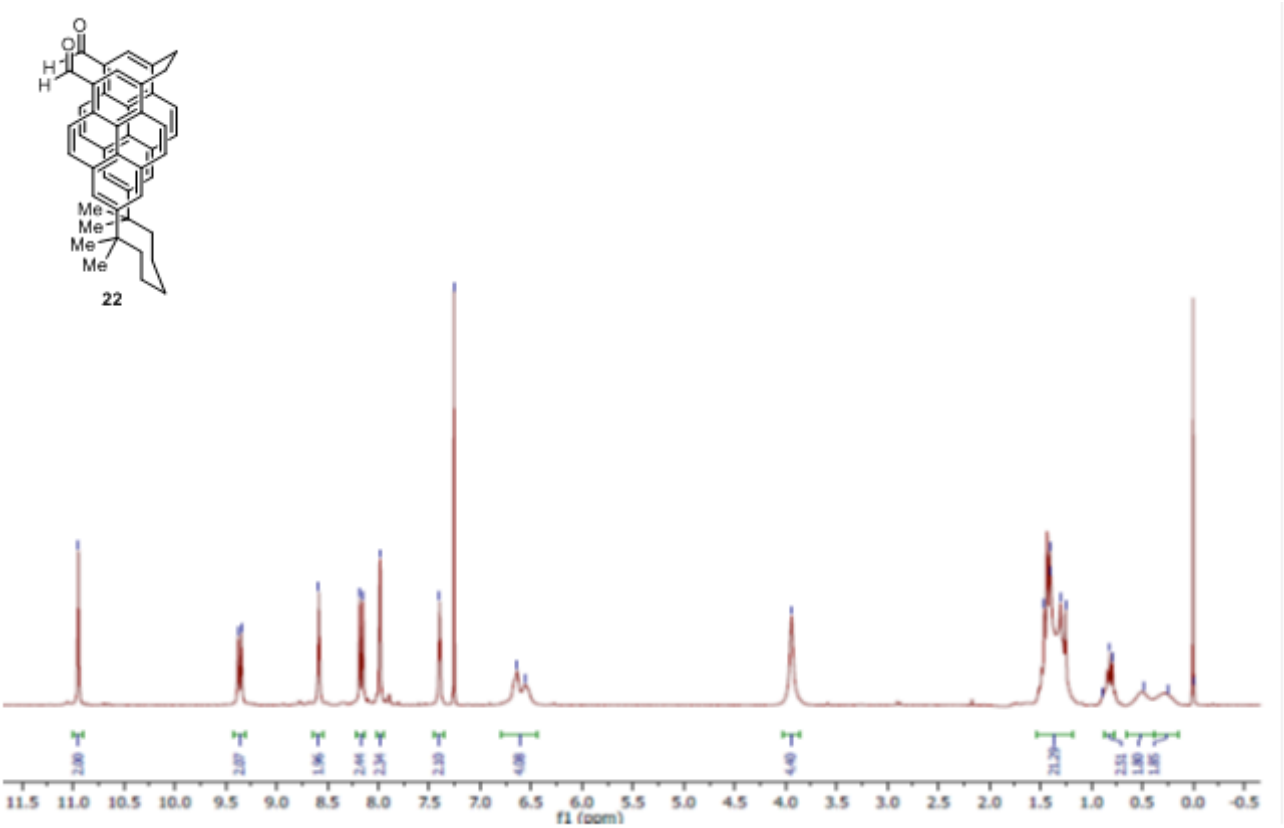
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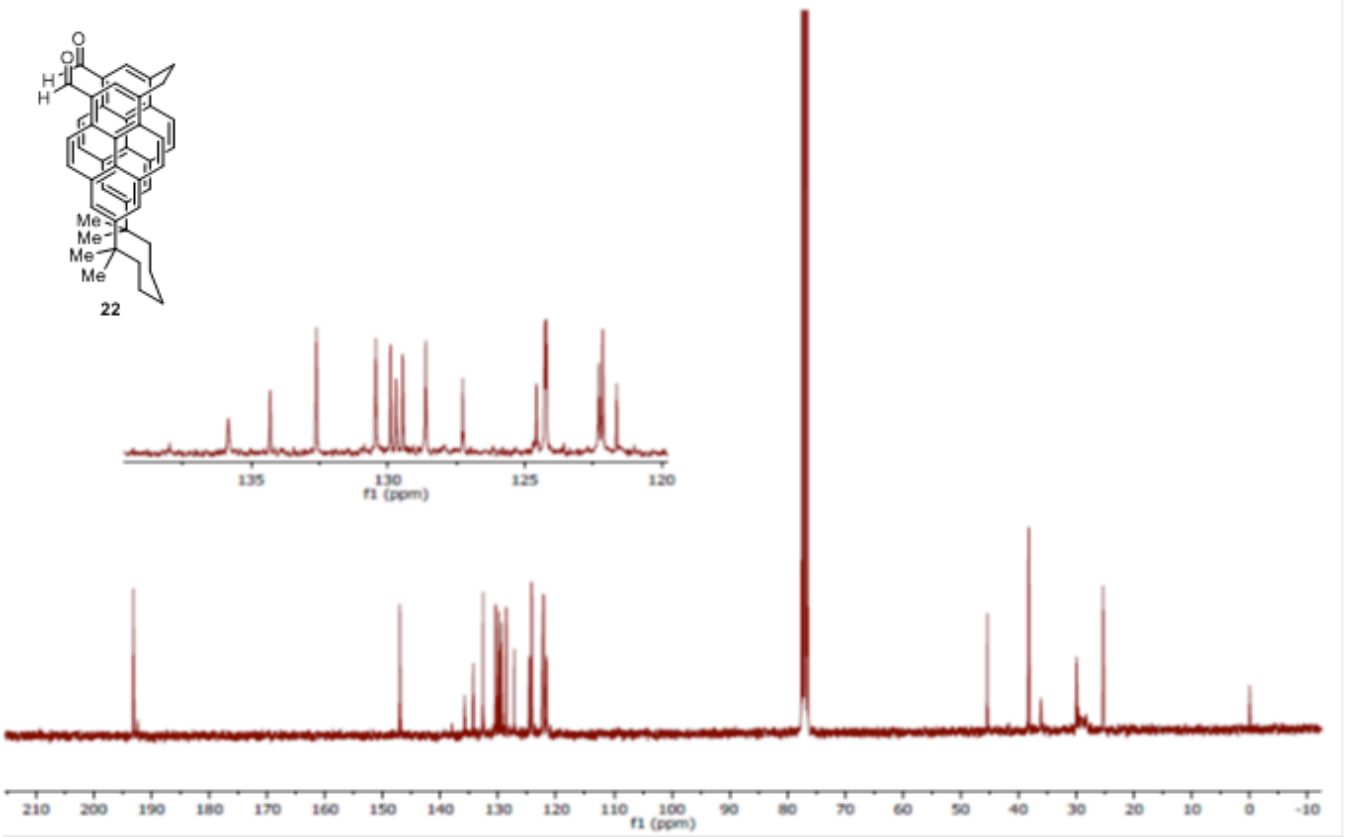
Me
Me
22
f1 (ppm)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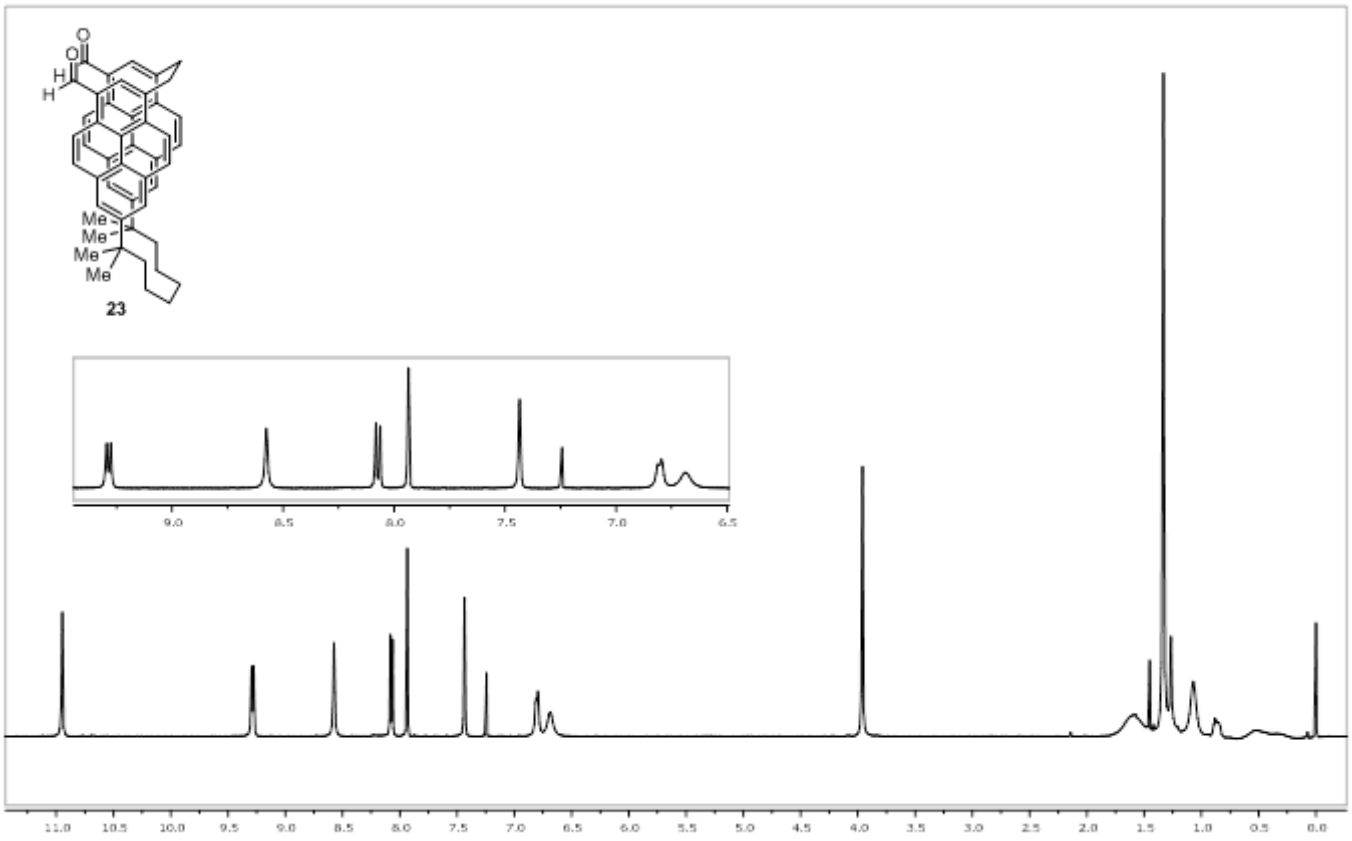
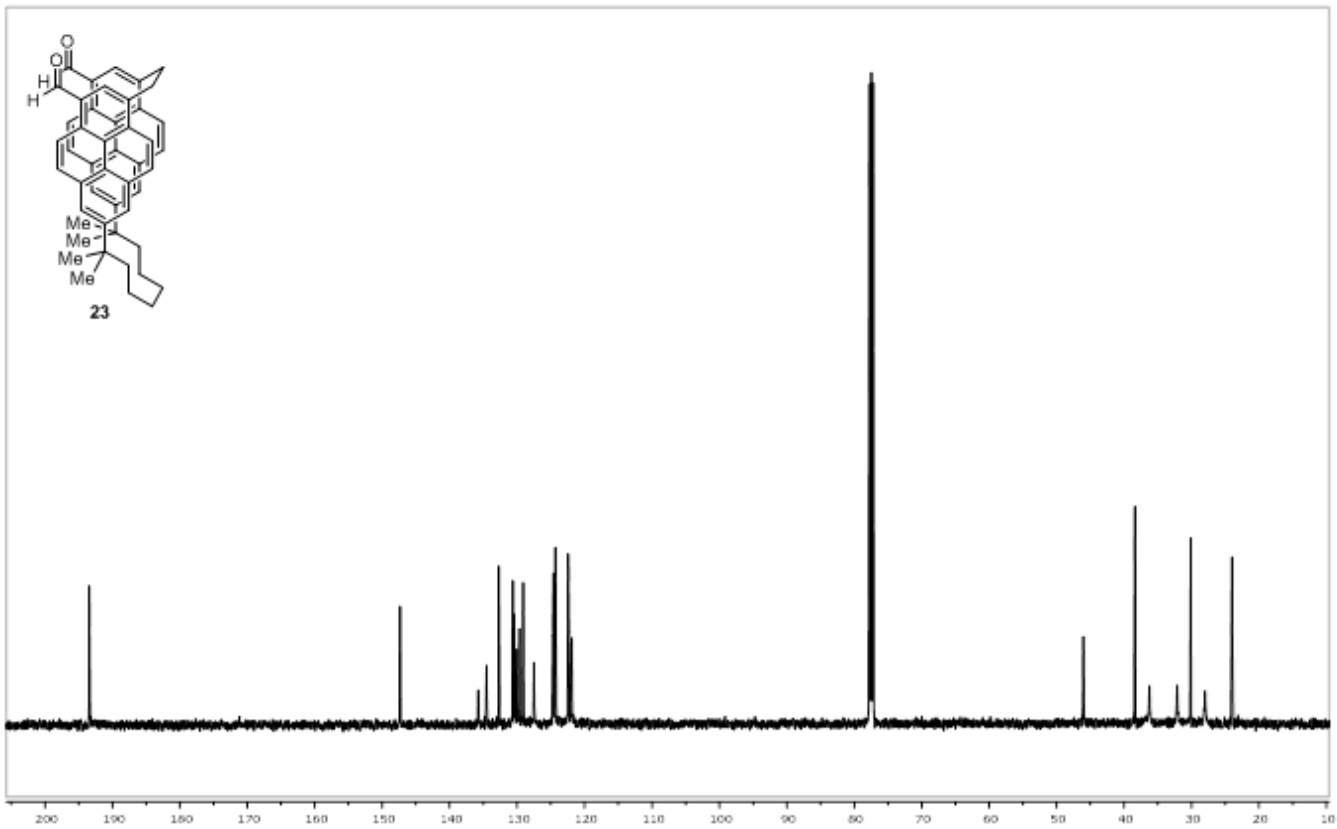
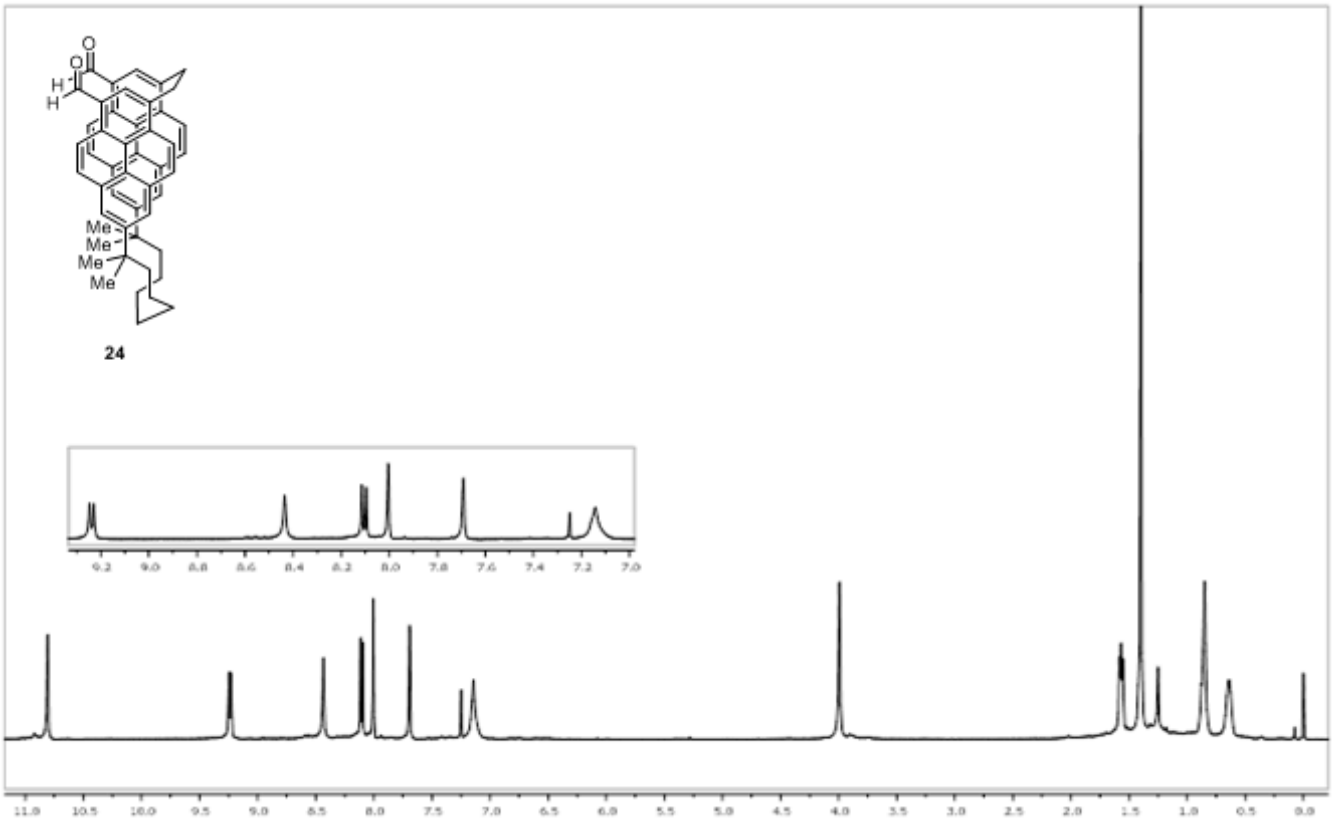
f1 (ppm)
f1 (ppm)







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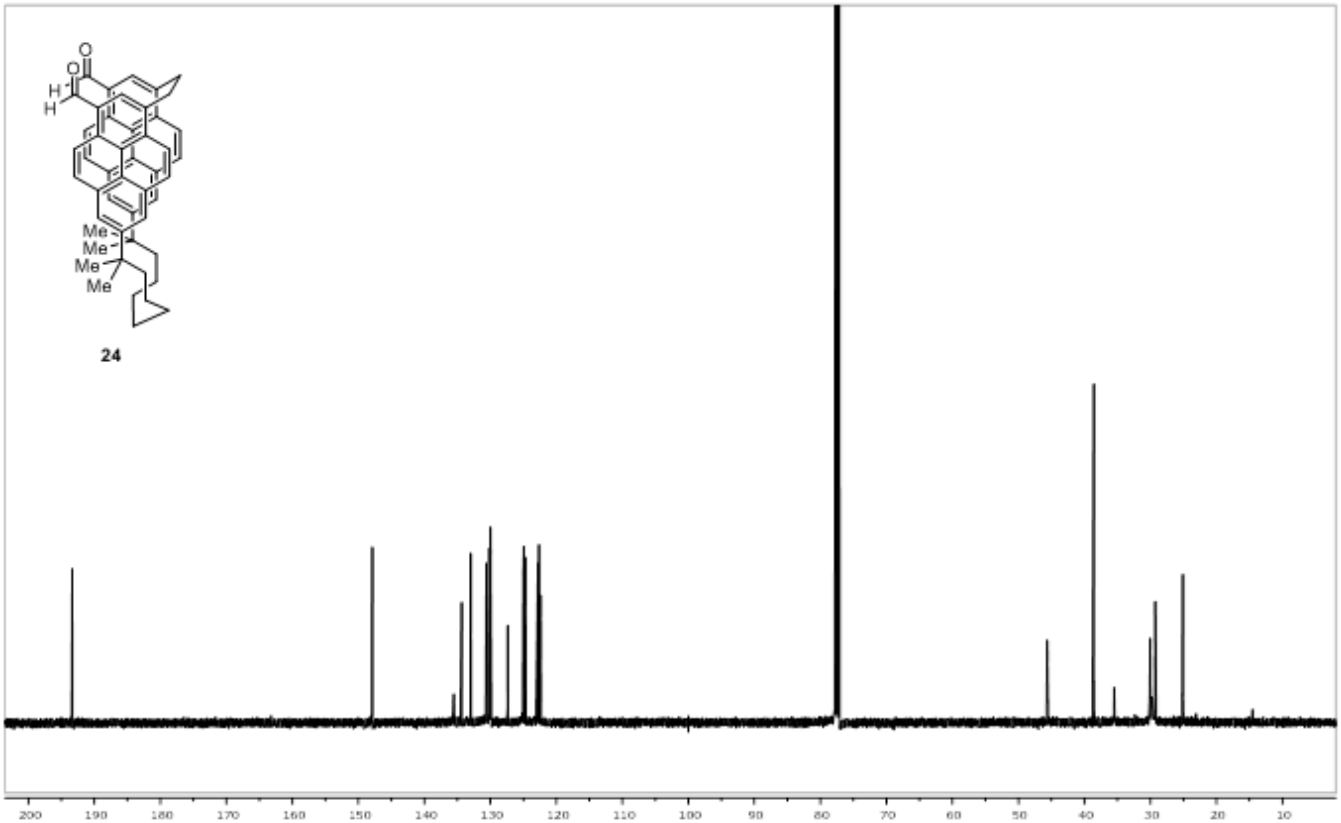

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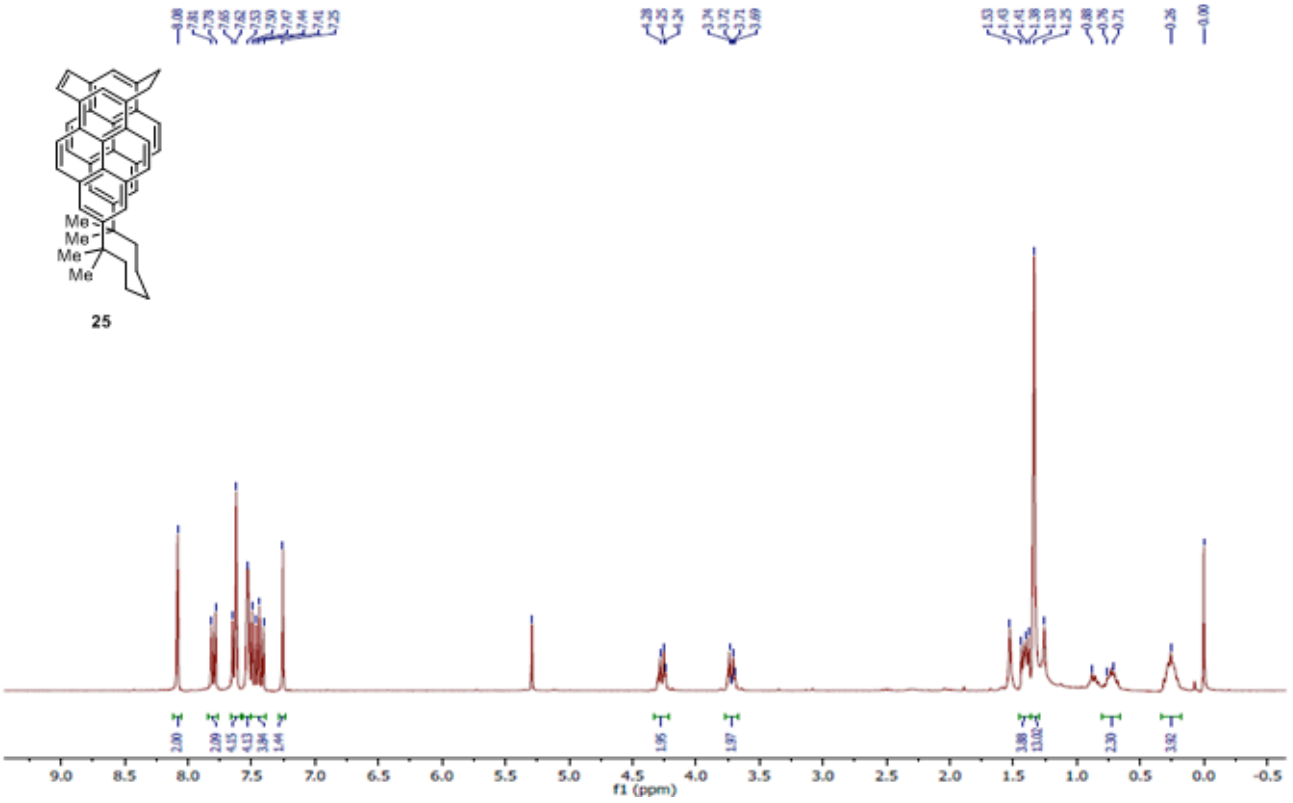
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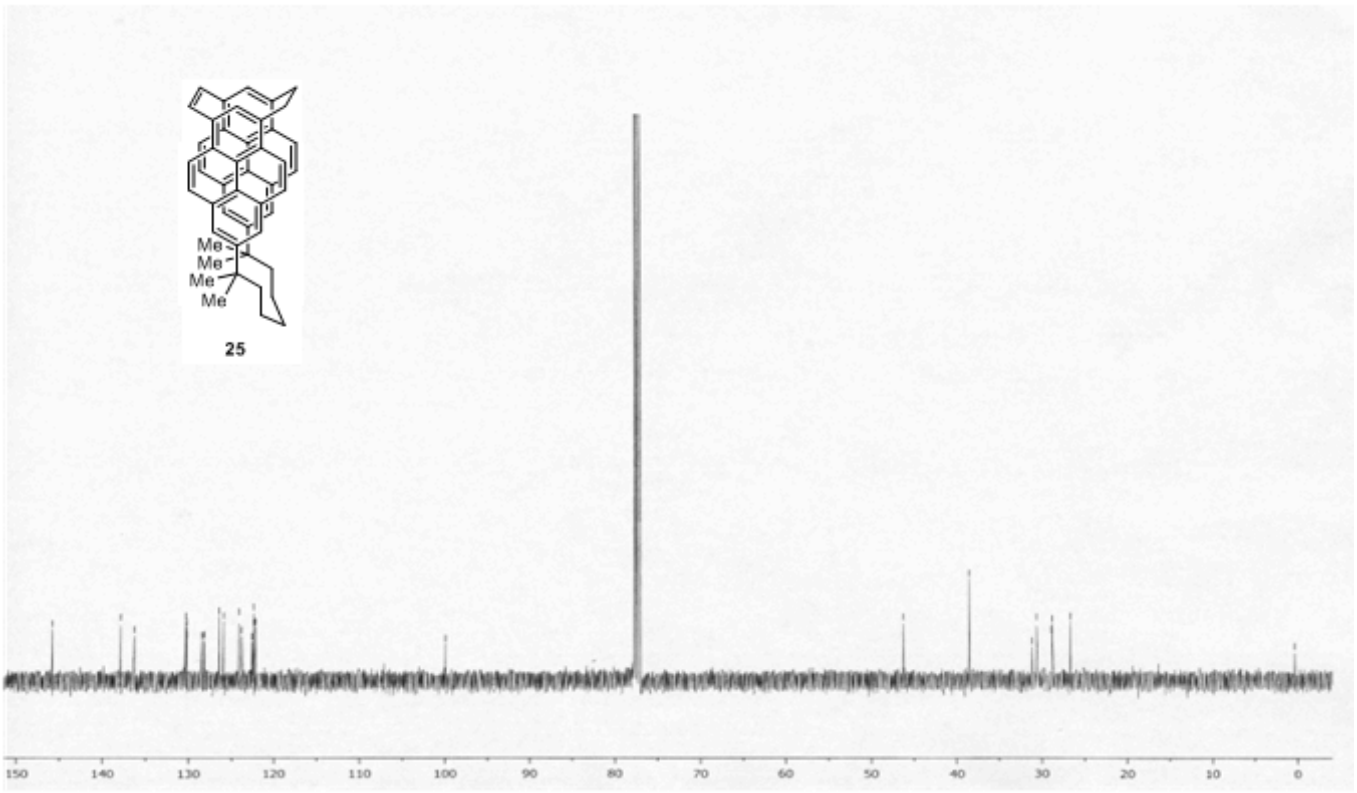
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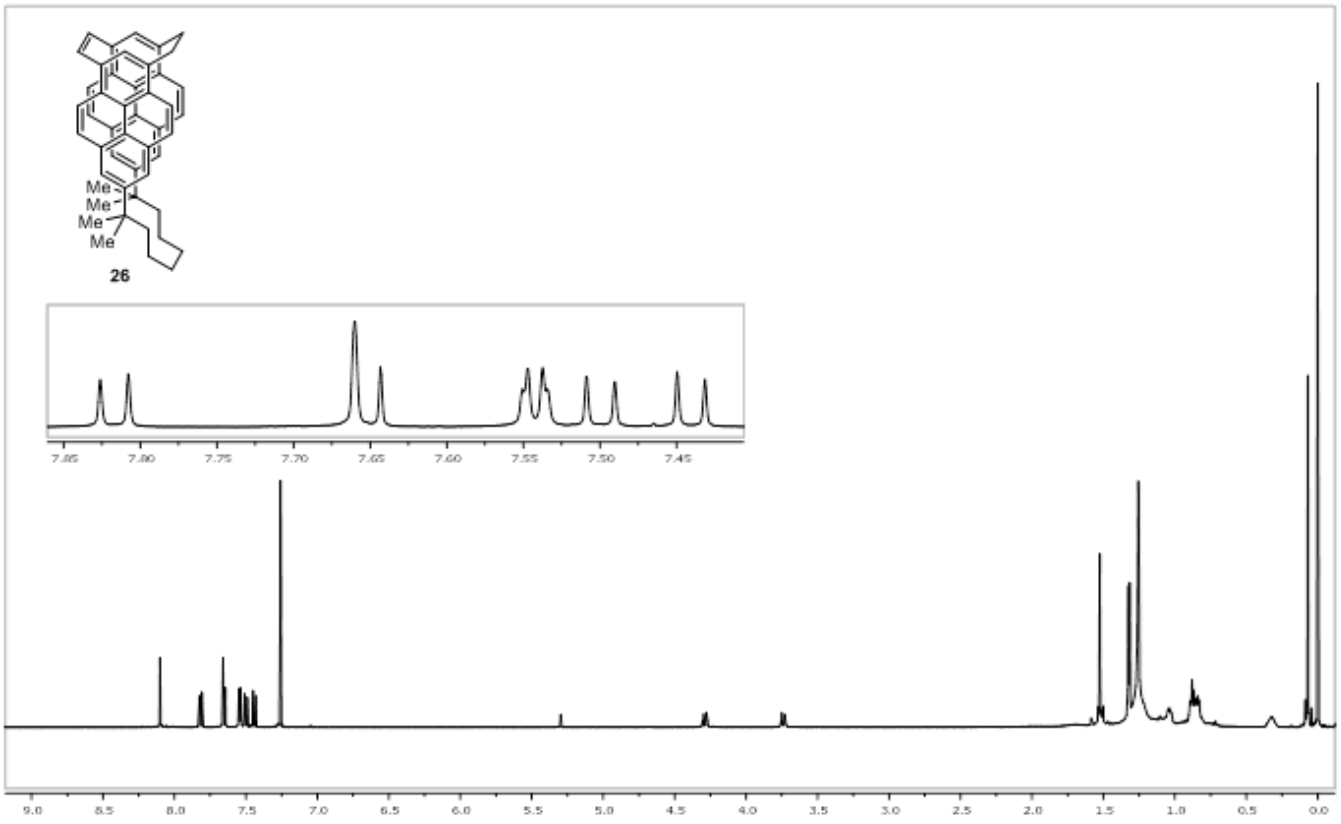
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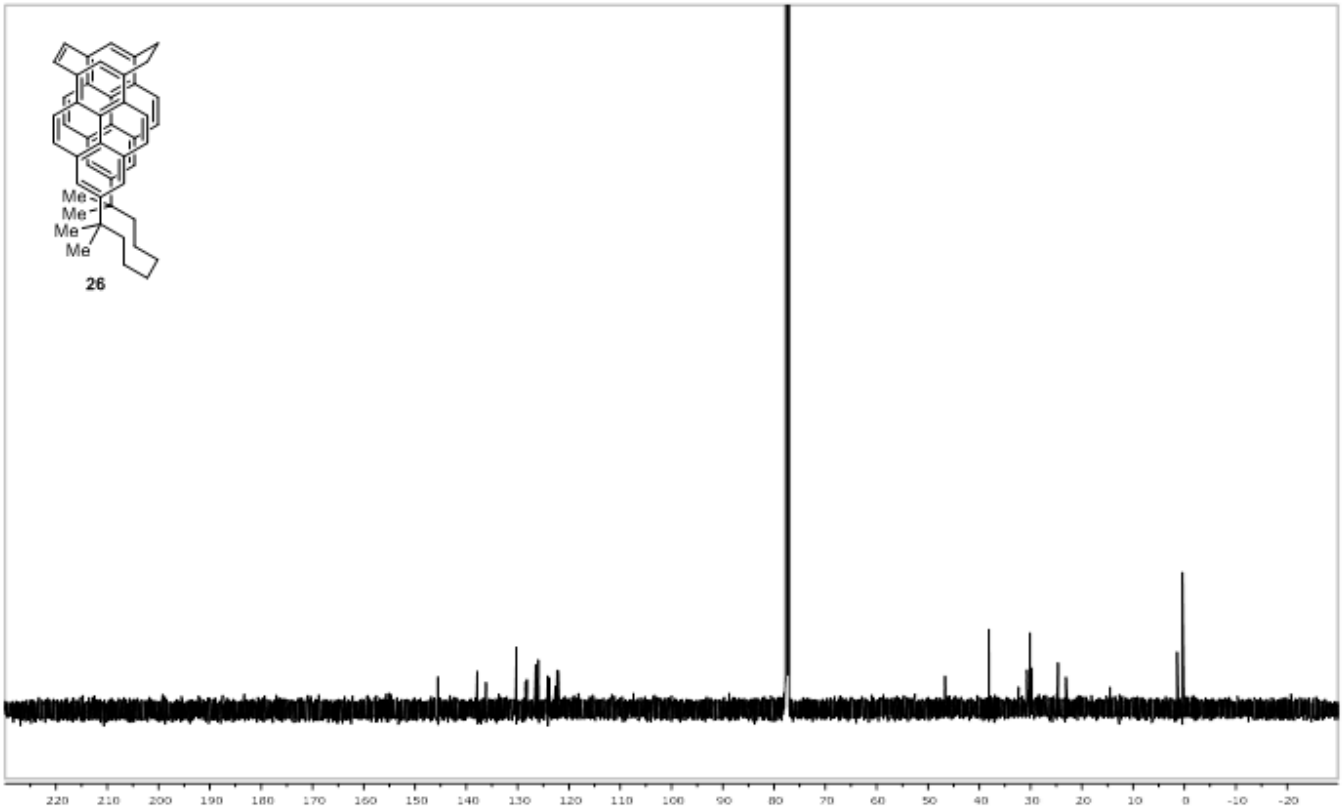
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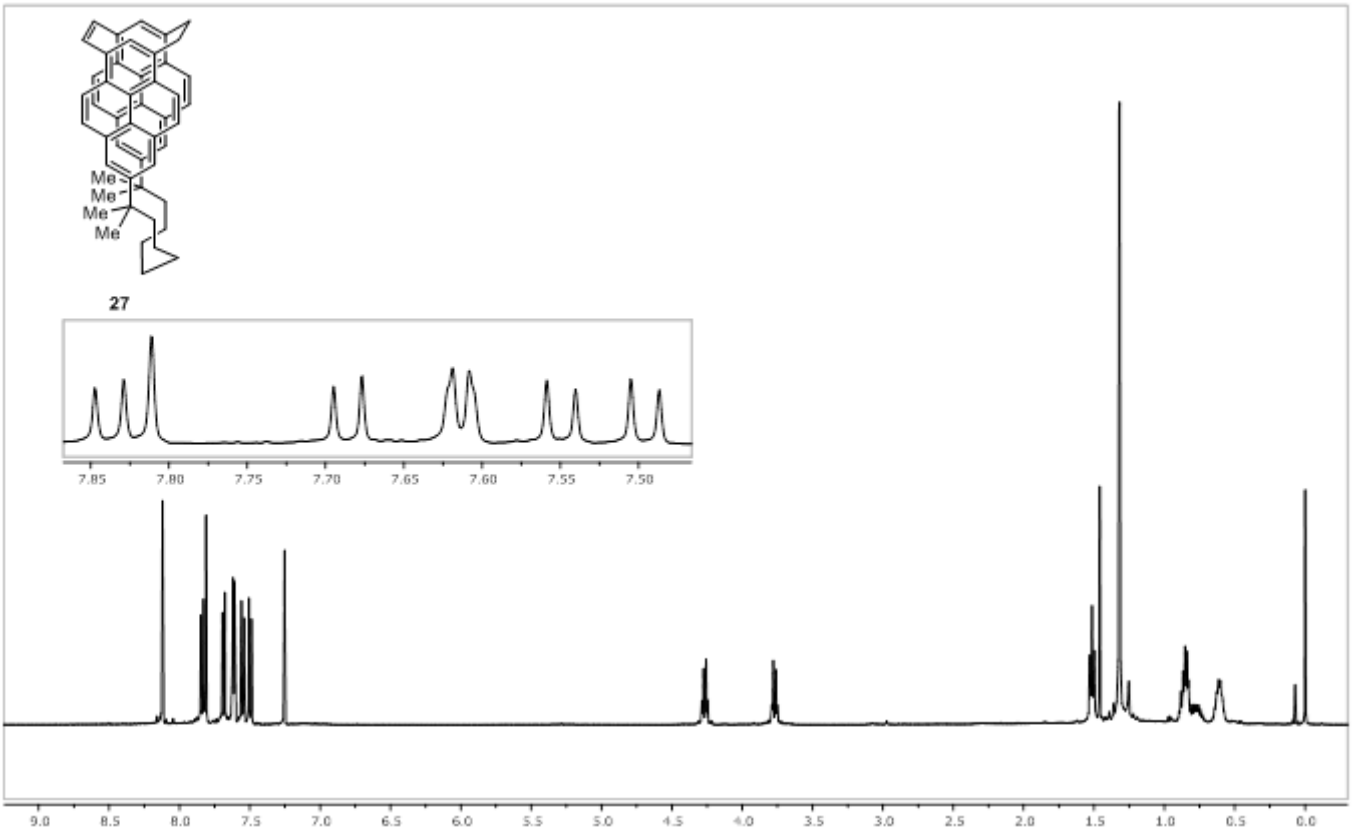
Me
Me
Me
26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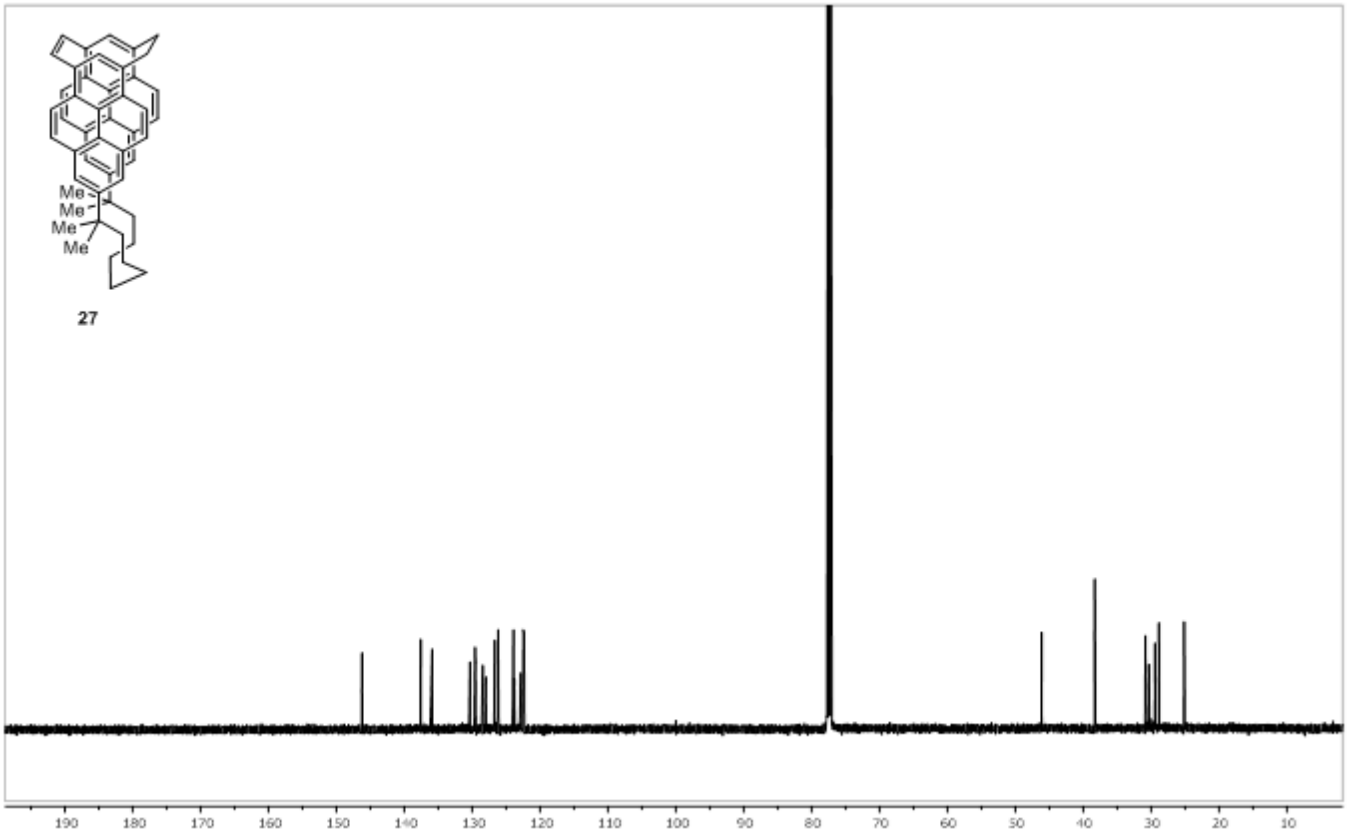
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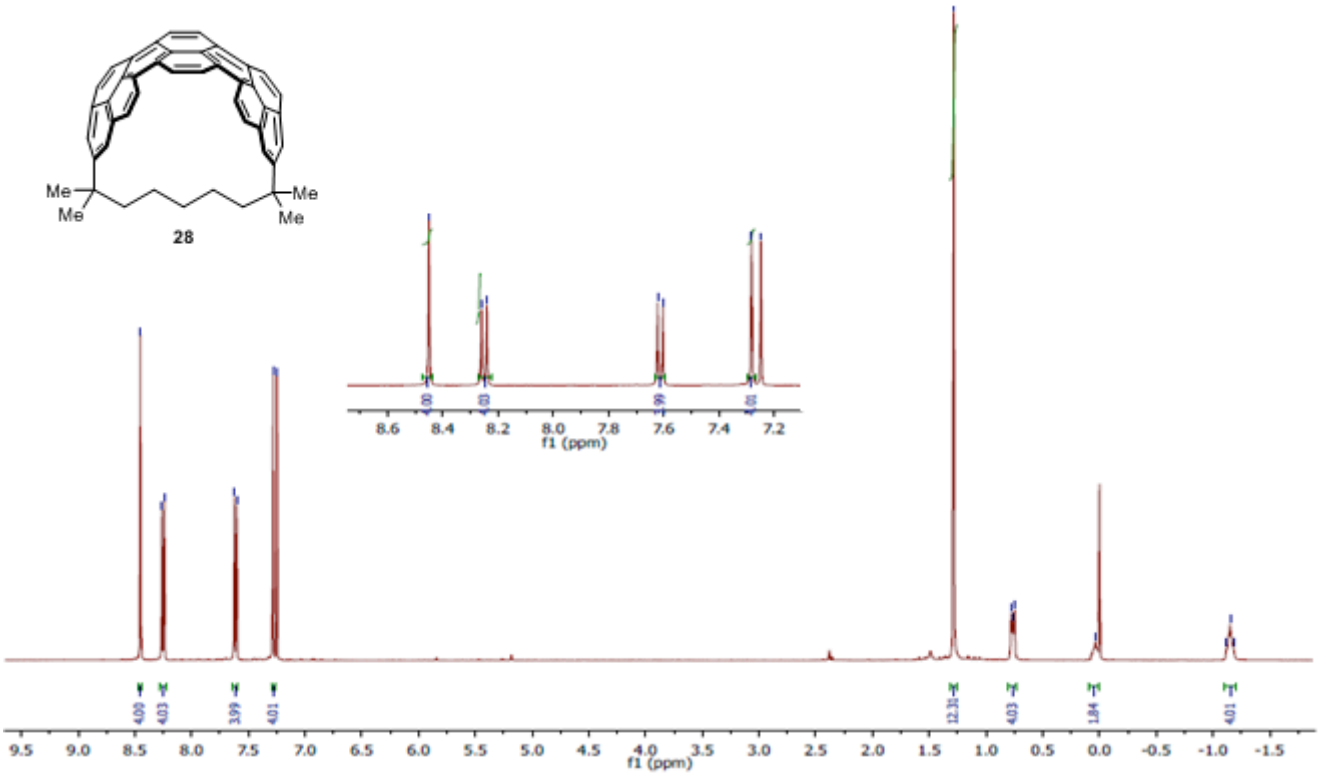
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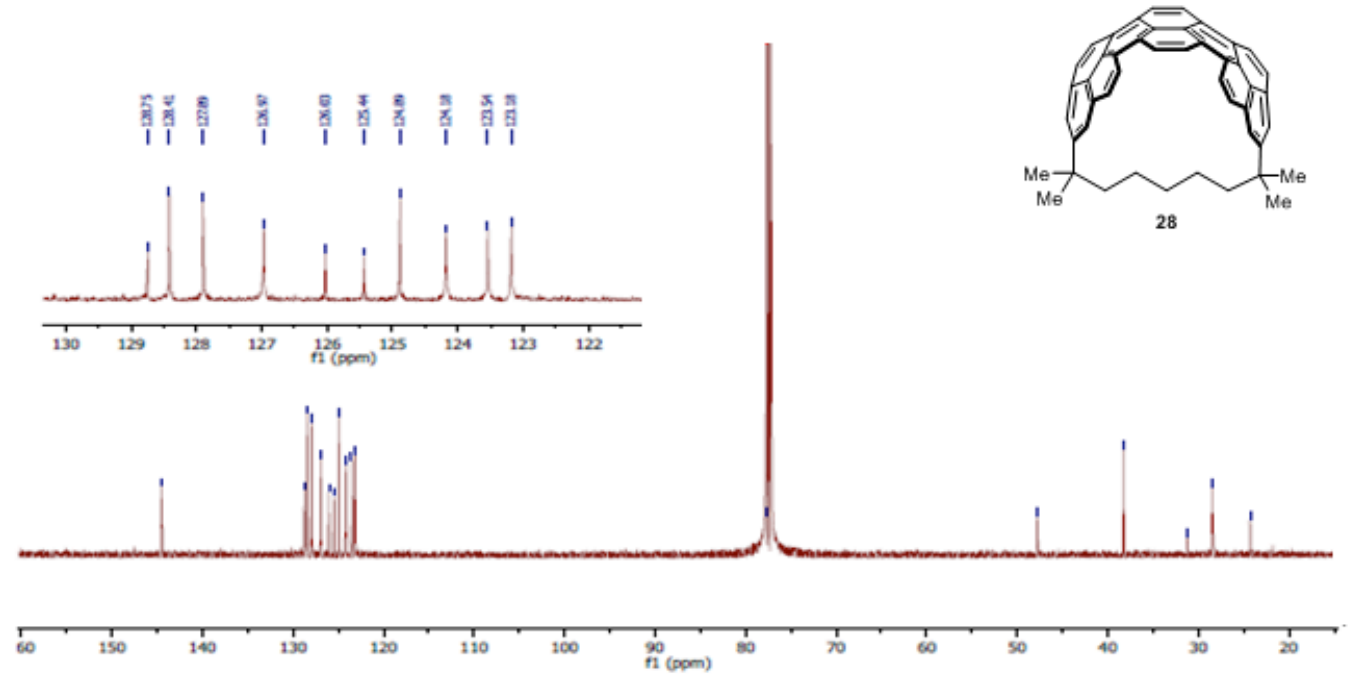
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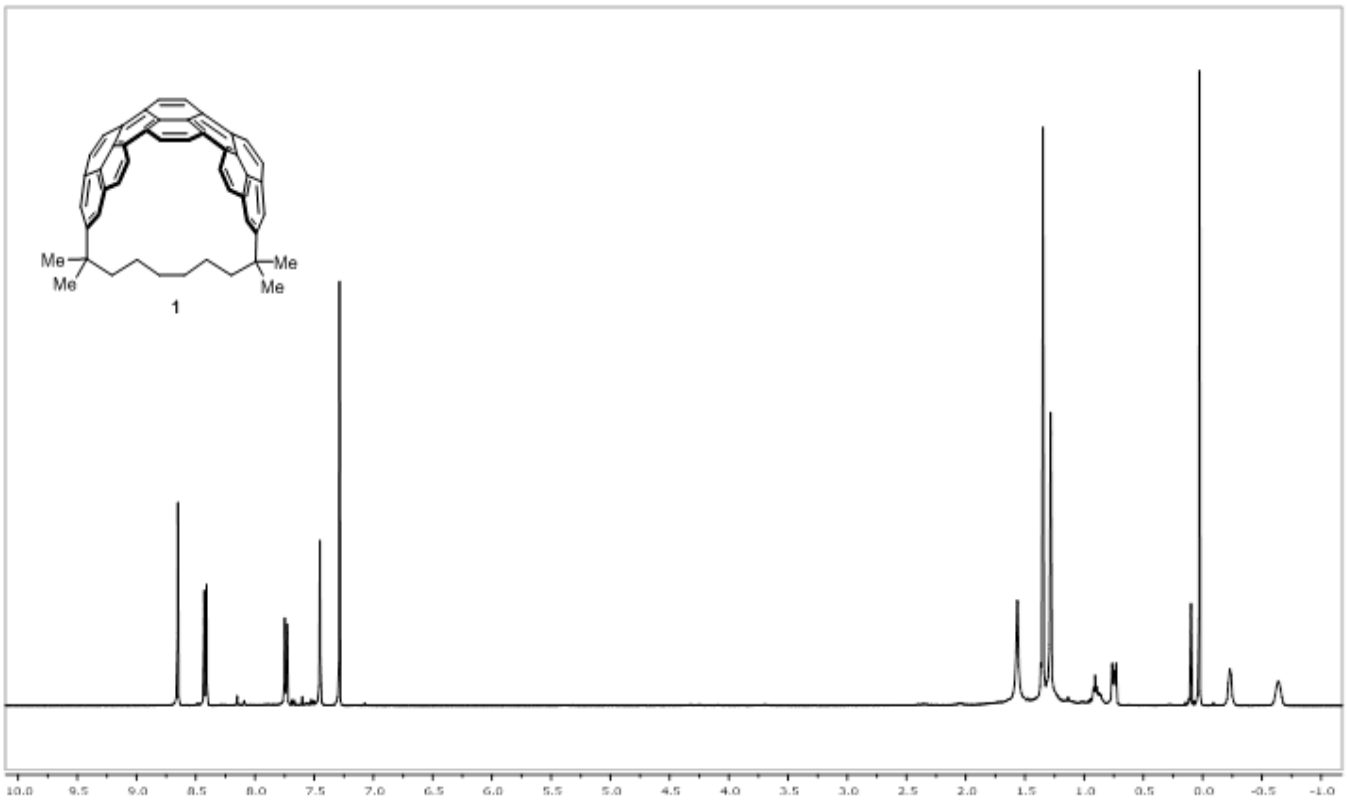
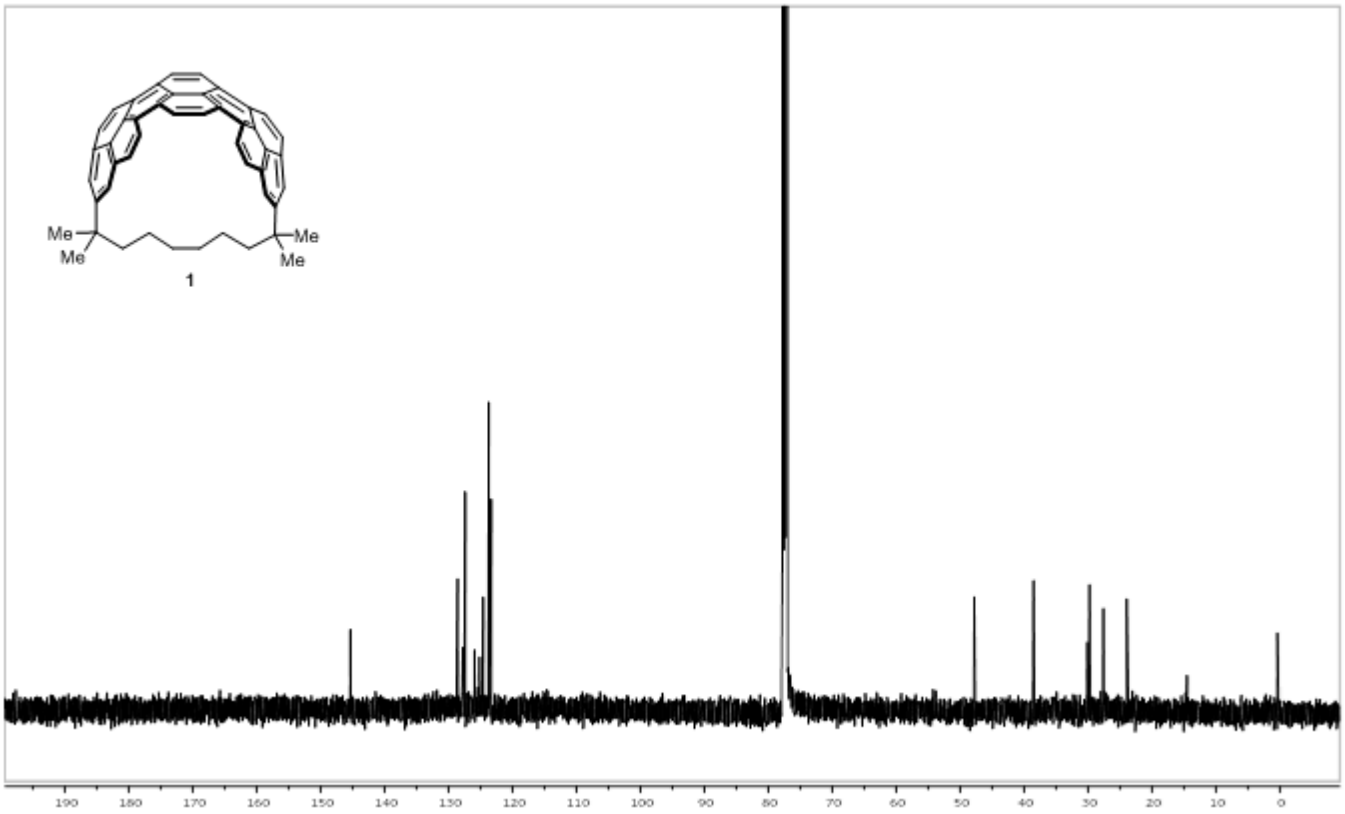
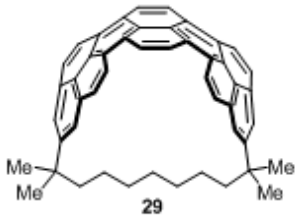
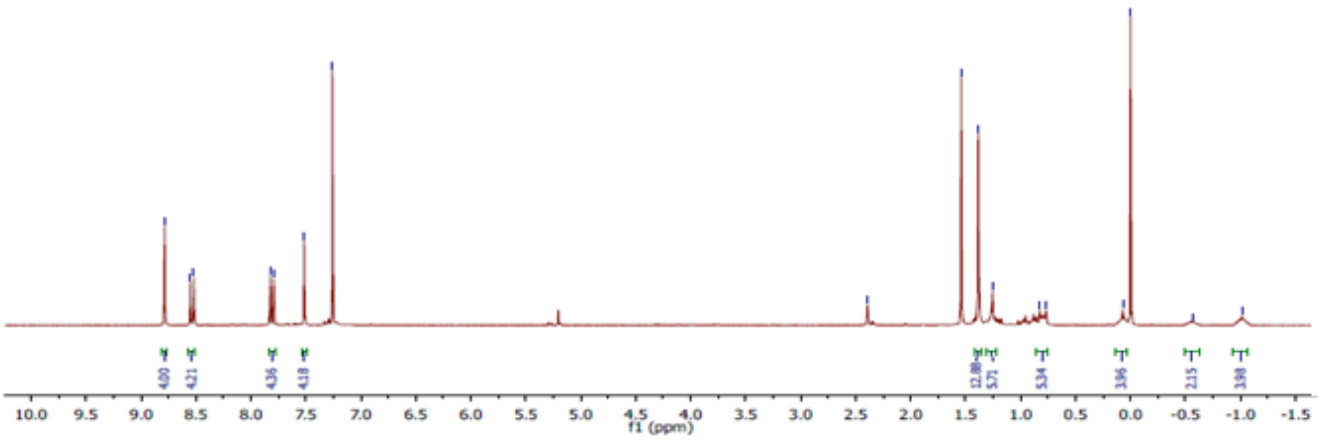
f1 (ppm)

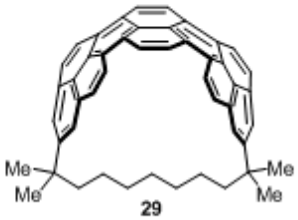






29





29

III. Additional Views of 29 in the Crystal and Structural Analysis of the Teropyrene System

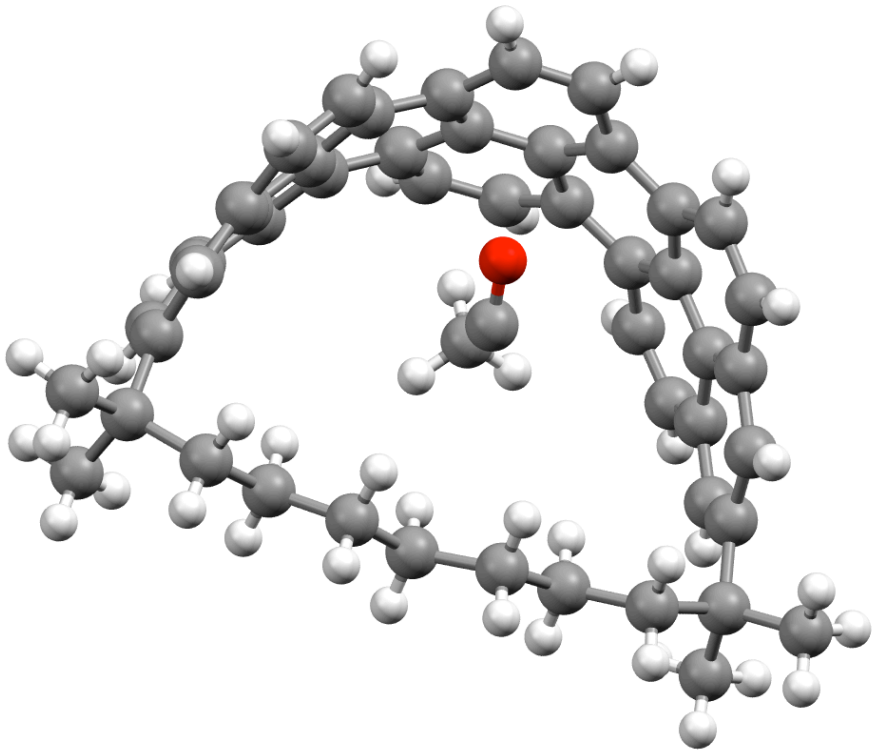


Figure SI 1: Ball-and-stick model of **29**, with minor disorder components of the ethanol molecule omitted for clarity

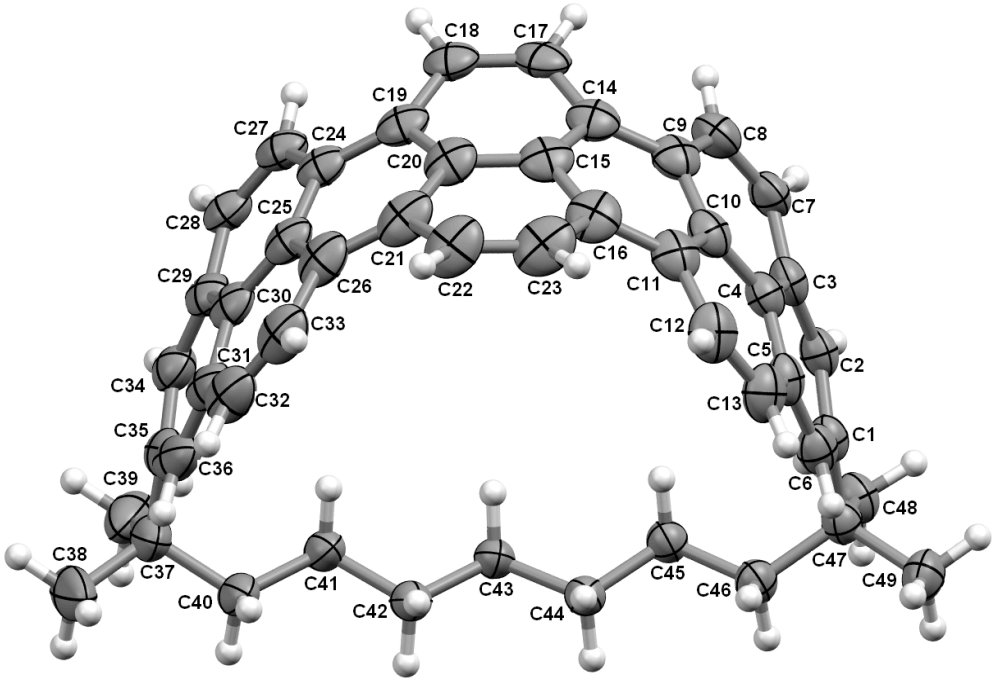
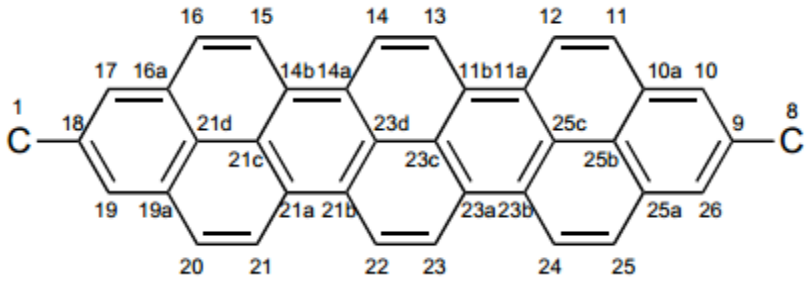


Figure SI 2: 50% probability displacement ellipsoids, with crystallographic numbering scheme. Ethanol molecule omitted for clarity.



Scheme SI 1: Technical numbering scheme as reported in: Merner, B. L.; Dawe, L. N.; Bodwell, G. J. *Angew. Chem. Int. Ed.* **2009**, *48*, 5847-5891.

Table 1: Plane Definitions (Technical Numbering)

Plane	Atoms
1	C9-C10-C26
2	C10-C10a-C25a-C26
3	C10a-C25b-C25a
4	C11-C12-C25b-C25c-C24-C25
5	C11a-C25c-C23b
6	C11a-C11b-C23a-C23b
7	C11b-C23c-C23a
8	C12-C14-C23c-C23d-C22-C23
9	C14a-C23d-C21b
10	C14a-C14b-C21a-21b
11	C14b-C21c-C21a
12	C15-C16-C21c-C21d-C20-C21
13	C16a-C21d-C19a
14	C17-C16a-C19-C19a
15	C17-C18-C19

Table 2: Angle Calculations (Technical Numbering Scheme; ^{o})

C1 – 1(β_1)	5.9(6)
1 – 2	6.41(13)

2 – 3	7.67(13)
3 – 4	8.56(12)
4 – 5	9.63(12)
5 – 6	15.02(14)
6 – 7	16.54(14)
7 – 8	14.29(13)
8 – 9	14.11(13)
9 – 10	16.66(15)
10 – 11	13.60(15)
11 – 12	8.76(14)
12 – 13	7.93(14)
13 – 14	7.40(15)
14 – 15	7.73(15)
C1 – 1 (β_2)	5.9(5)
1 – 7 (θ_1)	63.82
5 – 11 (θ_2)	90.23
9 – 15 (θ_3)	62.06
1 – 15 (θ_{tot})	154.3
$\theta_{tot} + \beta_1 + \beta_2$	166.1

Table 3: Numbering Scheme Conversion

Technical		Crystallographic	Technical		Crystallographic
C1	=	C47	C10a	=	C3
C8	=	C37	C11a	=	C9
C9	=	C1	C11b	=	C14
C10	=	C2	C14a	=	C19
C11	=	C7	C14b	=	C24
C12	=	C8	C16a	=	C29
C13	=	C17	C19a	=	C31
C14	=	C18	C21a	=	C26
C15	=	C27	C21b	=	C21
C16	=	C28	C23a	=	C16
C17	=	C34	C23b	=	C11
C18	=	C35	C25a	=	C5
C19	=	C36	C25b	=	C4
C20	=	C32	C25c	=	C10
C21	=	C33	C23c	=	C15
C22	=	C22	C23d	=	C20
C23	=	C23	C21c	=	C25
C24	=	C12	C21d	=	C30
C25	=	C13			
C26	=	C6			

Supplemental: Full Calculations

```
-------------- Plane number  1 ---------------

Atoms Defining Plane      Distance      esd
    C1     [ 1; 0; 0; 0]      0.0000      0.0000
    C2     [ 1; 0; 0; 0]      0.0000      0.0000
    C6     [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  28.55940x + 8.17465y + 3.09176z = 12.99718
  (0.00000)  (0.00000)  (0.00000)   (0.00000)


Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
Chi-squared:      0.000

-------------- Plane number  2 ---------------

Atoms Defining Plane      Distance      esd
    C2     [ 1; 0; 0; 0]     -0.0030      0.0042
    C3     [ 1; 0; 0; 0]      0.0030      0.0042
    C5     [ 1; 0; 0; 0]     -0.0027      0.0040
    C6     [ 1; 0; 0; 0]      0.0030      0.0042

  Least-squares plane
  30.22967x + 7.08813y + 2.00030z = 11.73439
  (0.03207)  (0.02824)  (0.02544)   (0.02602)


Mean deviation from plane is   0.0029 angstrom
Weight scheem: Sigma Weights
Chi-squared:      3.464

-------------- Plane number  3 ---------------

Atoms Defining Plane      Distance      esd
    C3     [ 1; 0; 0; 0]      0.0000      0.0000
    C4     [ 1; 0; 0; 0]      0.0000      0.0000
    C5     [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  31.73673x + 5.65939y + 0.67450z = 10.22225
  (0.00000)  (0.00000)  (0.00000)   (0.00000)


Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
```

```
Chi-squared:      0.000

-------------- Plane number  4 ---------------

Atoms Defining Plane      Distance      esd
    C7     [ 1; 0; 0; 0]      0.0242      0.0042
    C8     [ 1; 0; 0; 0]      0.0108      0.0046
    C4     [ 1; 0; 0; 0]     -0.0259      0.0036
    C10    [ 1; 0; 0; 0]     -0.0341      0.0040
    C12    [ 1; 0; 0; 0]      0.0318      0.0046
    C13    [ 1; 0; 0; 0]      0.0074      0.0044

  Least-squares plane
  32.77021x + 3.90644y - 0.77925z = 8.47208
  (0.01040)  (0.02599)  (0.02140)  (0.02484)


Mean deviation from plane is   0.0224 angstrom
Weight scheem: Sigma Weights
Chi-squared:    301.893

-------------- Plane number  5 ---------------

Atoms Defining Plane      Distance      esd
    C9     [ 1; 0; 0; 0]      0.0000      0.0000
    C10    [ 1; 0; 0; 0]     -0.0000      0.0000
    C11    [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  33.15106x + 1.68404y - 2.24002z = 6.52990
  (0.00000)  (0.00000)  (0.00000)  (0.00000)


Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
Chi-squared:      0.000

-------------- Plane number  6 ---------------

Atoms Defining Plane      Distance      esd
    C9     [ 1; 0; 0; 0]      0.0084      0.0045
    C14    [ 1; 0; 0; 0]     -0.0084      0.0045
    C11    [ 1; 0; 0; 0]     -0.0092      0.0047
    C16    [ 1; 0; 0; 0]      0.0101      0.0049

  Least-squares plane
  31.77448x - 1.67152y - 4.56739z = 3.29527
  (0.02572)  (0.03453)  (0.02635)  (0.03173)
```

```
Mean deviation from plane is   0.0091 angstrom
Weight scheem: Sigma Weights
Chi-squared:     27.066

-------------- Plane number  7 ---------------

Atoms Defining Plane      Distance      esd
    C14    [ 1; 0; 0; 0]      0.0000      0.0000
    C15    [ 1; 0; 0; 0]      0.0000      0.0000
    C16    [ 1; 0; 0; 0]     -0.0000      0.0000

  Least-squares plane
  -27.75476x + 5.22979y + 6.76036z = 0.11877
   (0.00000)  (0.00000)  (0.00000)  (0.00000)


Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
Chi-squared:      0.000

-------------- Plane number  8 ---------------

Atoms Defining Plane      Distance      esd
    C17    [ 1; 0; 0; 0]     -0.0479      0.0045
    C18    [ 1; 0; 0; 0]     -0.0296      0.0047
    C15    [ 1; 0; 0; 0]      0.0729      0.0040
    C20    [ 1; 0; 0; 0]      0.0772      0.0044
    C22    [ 1; 0; 0; 0]     -0.0659      0.0054
    C23    [ 1; 0; 0; 0]     -0.0498      0.0054

  Least-squares plane
  -22.45085x + 8.02227y + 8.15167z = 2.79361
   (0.05600)  (0.02408)  (0.01443)  (0.02386)


Mean deviation from plane is   0.0572 angstrom
Weight scheem: Sigma Weights
Chi-squared:   1418.333

-------------- Plane number  9 ---------------

Atoms Defining Plane      Distance      esd
    C19    [ 1; 0; 0; 0]      0.0000      0.0000
    C20    [ 1; 0; 0; 0]      0.0000      0.0000
    C21    [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  -15.80703x + 10.22449y + 9.09896z = 5.09995
   (0.00000)   (0.00000)  (0.00000)  (0.00000)
```

```
Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
Chi-squared:      0.000

-------------- Plane number 10 ---------------

Atoms Defining Plane      Distance      esd
    C19    [ 1; 0; 0; 0]     -0.0055      0.0045
    C24    [ 1; 0; 0; 0]      0.0055      0.0045
    C21    [ 1; 0; 0; 0]      0.0079      0.0053
    C26    [ 1; 0; 0; 0]     -0.0079      0.0053

  Least-squares plane
  -6.75073x + 11.97990y + 9.54800z = 7.13790
  (0.08576)   (0.01998)  (0.01598)  (0.01618)


Mean deviation from plane is   0.0067 angstrom
Weight scheem: Sigma Weights
Chi-squared:     13.386

-------------- Plane number 11 ---------------

Atoms Defining Plane      Distance      esd
    C24    [ 1; 0; 0; 0]      0.0000      0.0000
    C25    [ 1; 0; 0; 0]      0.0000      0.0000
    C26    [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  1.09735x + 12.68032y + 9.31169z = 8.03029
 (0.00000)   (0.00000)  (0.00000)  (0.00000)


Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
Chi-squared:      0.000

-------------- Plane number 12 ---------------

Atoms Defining Plane      Distance      esd
    C27    [ 1; 0; 0; 0]     -0.0138      0.0047
    C28    [ 1; 0; 0; 0]     -0.0234      0.0047
    C25    [ 1; 0; 0; 0]      0.0365      0.0044
    C30    [ 1; 0; 0; 0]      0.0375      0.0044
    C32    [ 1; 0; 0; 0]     -0.0205      0.0058
    C33    [ 1; 0; 0; 0]     -0.0391      0.0058

  Least-squares plane
  6.17427x + 12.70036y + 8.93382z = 8.24917
```

```
 (0.07781)   (0.00967)  (0.01199)  (0.00469)


Mean deviation from plane is   0.0284 angstrom
Weight scheem: Sigma Weights
Chi-squared:    325.843

-------------- Plane number 13 ---------------

Atoms Defining Plane      Distance      esd
    C29    [ 1; 0; 0; 0]      0.0000      0.0000
    C30    [ 1; 0; 0; 0]      0.0000      0.0000
    C31    [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  10.66253x + 12.41993y + 8.45352z = 8.17402
  (0.00000)   (0.00000)  (0.00000)  (0.00000)


Mean deviation from plane is   0.0000 angstrom
Weight scheem: Sigma Weights
Chi-squared:      0.000

-------------- Plane number 14 ---------------

Atoms Defining Plane      Distance      esd
    C29    [ 1; 0; 0; 0]      0.0019      0.0045
    C34    [ 1; 0; 0; 0]     -0.0020      0.0045
    C31    [ 1; 0; 0; 0]     -0.0027      0.0053
    C36    [ 1; 0; 0; 0]      0.0033      0.0057

  Least-squares plane
  14.65462x + 11.97889y + 7.82605z = 7.82096
  (0.08127)   (0.02108)  (0.02191)  (0.01314)


Mean deviation from plane is   0.0025 angstrom
Weight scheem: Sigma Weights
Chi-squared:      1.769

-------------- Plane number 15 ---------------

Atoms Defining Plane      Distance      esd
    C34    [ 1; 0; 0; 0]      0.0000      0.0000
    C35    [ 1; 0; 0; 0]      0.0000      0.0000
    C36    [ 1; 0; 0; 0]      0.0000      0.0000

  Least-squares plane
  18.56536x + 11.30235y + 7.03444z = 7.12821
  (0.00000)   (0.00000)  (0.00000)  (0.00000)
```

Mean deviation from plane is 0.0000 angstrom

Weight scheem: Sigma Weights

Chi-squared: 0.000

Dihedral angles between least-squares planes

---

plane	plane	angle	esd
1	2	6.419	0.131
1	3	14.098	0.000
1	4	22.658	0.118
1	5	32.252	0.000
1	6	47.276	0.143
1	7	116.177	0.000
1	8	101.891	0.130
1	9	87.778	0.000
1	10	71.124	0.150
1	11	57.522	0.000
1	12	48.771	0.136
1	13	40.873	0.000
1	14	33.499	0.153
1	15	25.806	0.000
2	3	7.679	0.131
2	4	16.241	0.176
2	5	25.842	0.131
2	6	40.866	0.193
2	7	122.586	0.131
2	8	108.298	0.184
2	9	94.186	0.131
2	10	77.533	0.199
2	11	63.933	0.131
2	12	55.184	0.188
2	13	47.290	0.131
2	14	39.917	0.201
2	15	32.224	0.130
3	4	8.563	0.118
3	5	18.177	0.000
3	6	33.197	0.143
3	7	130.256	0.000
3	8	115.967	0.130
3	9	101.856	0.000
3	10	85.205	0.150
3	11	71.607	0.000
3	12	62.861	0.136
3	13	54.969	0.000
3	14	47.596	0.153
3	15	39.901	0.000

4	5	9.630	0.117
4	6	24.641	0.185
4	7	138.815	0.118
4	8	124.525	0.175
4	9	110.415	0.118
4	10	93.767	0.190
4	11	80.169	0.118
4	12	71.423	0.180
4	13	63.531	0.118
4	14	56.157	0.193
4	15	48.457	0.118
5	6	15.024	0.143
5	7	148.429	0.000
5	8	134.141	0.130
5	9	120.028	0.000
5	10	103.375	0.150
5	11	89.774	0.000
5	12	81.022	0.136
5	13	73.119	0.000
5	14	65.736	0.154
5	15	58.024	0.000
6	7	163.453	0.143
6	8	149.164	0.193
6	9	135.052	0.143
6	10	118.399	0.207
6	11	104.798	0.143
6	12	96.045	0.197
6	13	88.139	0.143
6	14	80.753	0.210
6	15	73.037	0.143
7	8	14.290	0.130
7	9	28.401	0.000
7	10	45.053	0.150
7	11	58.655	0.000
7	12	67.409	0.136
7	13	75.318	0.000
7	14	82.707	0.154
7	15	90.426	0.000
8	9	14.113	0.130
8	10	30.769	0.198
8	11	44.371	0.130
8	12	53.129	0.188
8	13	61.044	0.130
8	14	68.436	0.201
8	15	76.160	0.130
9	10	16.657	0.150
9	11	30.259	0.000
9	12	39.018	0.136
9	13	46.936	0.000
9	14	54.330	0.154

9	15	62.055	0.000
10	11	13.603	0.150
10	12	22.362	0.202
10	13	30.282	0.150
10	14	37.677	0.215
10	15	45.404	0.150
11	12	8.763	0.136
11	13	16.688	0.000
11	14	24.083	0.154
11	15	31.810	0.000
12	13	7.927	0.136
12	14	15.322	0.205
12	15	23.048	0.136
13	14	7.395	0.154
13	15	15.122	0.000
14	15	7.727	0.154

IV. DFT Calculations and Cartesian Co-ordinates for 1,1,*n*,*n*-Tetramethyl[*n*](2,11)tero-pyrenophanes (*n* = 6-9)

All calculations were performed using the Gaussian 09 package. The structures for all compounds were constructed by modifying the existing crystal structure of **N9**. All three structures were optimized using density functional theory, with the B3LYP exchange-correlation functional and the cc-pVTZ basis set.

Becke, A. D. *J. Chem. Phys.*, 1993, **98**, 5648
Kendall, R. A., Dunning, T. H. Harrison, R. J. *J. Chem. Phys.* 1992, **96**, 6796

1,1,6,6-Tetramethyl[6](2,11)teropyrenophane (E = –1775.1837652 Hartree):

C	3.604348	2.181072	-0.032186
C	3.709889	1.443523	1.152644
H	3.746586	1.953282	2.105840
C	3.648760	0.050180	1.167636
C	3.466896	-0.644614	-0.055860
C	3.590397	0.074207	-1.270397
C	3.655046	1.473498	-1.233234
H	3.653571	2.000177	-2.176682
C	3.588672	-0.710161	2.383559
H	3.884834	-0.237479	3.311532
C	3.066825	-1.960260	2.389914
H	2.939832	-2.476977	3.330321
C	2.541246	-2.545600	1.186522
C	2.918746	-1.959965	-0.053822
C	2.482482	-2.525493	-1.283726
C	2.943238	-1.913771	-2.499338
H	2.763902	-2.408578	-3.443009
C	3.464316	-0.661685	-2.494759
H	3.707570	-0.170023	-3.428283
C	1.418104	-3.402804	1.202585
C	0.717892	-3.609665	-0.014842
C	1.365364	-3.392669	-1.259003
C	0.725912	-3.748935	2.416785
H	1.280173	-3.895684	3.332905
C	-0.626930	-3.741208	2.444523
H	-1.145184	-3.882004	3.382510
C	-1.365523	-3.392606	1.259003
C	-0.718061	-3.609633	0.014841
C	-1.418264	-3.402739	-1.202585
C	-0.726088	-3.748905	-2.416784
H	-1.280355	-3.895632	-3.332904
C	0.626755	-3.741236	-2.444523
H	1.145002	-3.882058	-3.382510
C	-2.482601	-2.525379	1.283725
C	-2.918838	-1.959830	0.053822
C	-2.541365	-2.545483	-1.186522
C	-2.943328	-1.913635	2.499338

H	-2.764016	-2.408452	3.443008
C	-3.464347	-0.661526	2.494759
H	-3.707579	-0.169852	3.428283
C	-3.590392	0.074373	1.270396
C	-3.466927	-0.644455	0.055860
C	-3.648759	0.050348	-1.167636
C	-3.588708	-0.709997	-2.383559
H	-3.884850	-0.237302	-3.311531
C	-3.066919	-1.960120	-2.389914
H	-2.939951	-2.476843	-3.330321
C	-3.654971	1.473666	1.233233
H	-3.653470	2.000346	2.176681
C	-3.604240	2.181239	0.032185
C	-3.709820	1.443694	-1.152645
H	-3.746493	1.953453	-2.105841
C	-3.322174	3.692569	-0.033263
C	-4.298194	4.373375	-1.016301
H	-4.159900	4.030826	-2.041183
H	-4.142660	5.453400	-1.011874
H	-5.333904	4.179268	-0.734157
C	-3.489448	4.381453	1.329152
H	-4.512044	4.281841	1.696867
H	-3.275360	5.446964	1.231304
H	-2.818491	3.983505	2.088156
C	-1.866464	3.918184	-0.576090
H	-1.753903	3.322633	-1.485261
H	-1.796337	4.964564	-0.890735
C	-0.682181	3.628672	0.363347
H	-0.817926	2.666581	0.863786
H	-0.661432	4.383850	1.153568
C	0.682354	3.628668	-0.363376
H	0.818070	2.666597	-0.863864
H	0.661635	4.383886	-1.153559
C	1.866643	3.918090	0.576081
H	1.754044	3.322517	1.485233
H	1.796568	4.964464	0.890758
C	3.322348	3.692415	0.033265
C	4.298383	4.373172	1.016321
H	4.160058	4.030622	2.041199
H	4.142892	5.453204	1.011900
H	5.334089	4.179024	0.734191
C	3.489665	4.381306	-1.329140
H	4.512263	4.281660	-1.696842
H	3.275614	5.446824	-1.231283
H	2.818704	3.983395	-2.088160

1,1,7,7-Tetramethyl[7](2,11)teropyrenophane (28) (E = –1893.2121894 Hartree):

C	-4.092265	2.015914	0.047603
C	-4.087157	1.306394	-1.158285
H	-4.146630	1.837090	-2.099309
C	-3.884788	-0.073599	-1.204291
C	-3.672307	-0.780134	0.007873
C	-3.902262	-0.110525	1.234516
C	-4.107597	1.274916	1.228459
H	-4.185499	1.773016	2.183856
C	-3.717087	-0.792137	-2.434558
H	-4.021444	-0.321164	-3.360741
C	-3.092282	-1.994436	-2.453161
H	-2.894079	-2.472176	-3.401689
C	-2.561119	-2.571111	-1.248799
C	-3.010649	-2.042084	-0.006963
C	-2.567253	-2.602636	1.222584
C	-3.107128	-2.059547	2.436957
H	-2.910869	-2.559038	3.374639
C	-3.740423	-0.860174	2.445007
H	-4.052282	-0.415256	3.381537
C	-1.397365	-3.372783	-1.252557
C	-0.717332	-3.576144	-0.022333
C	-1.398508	-3.401062	1.210409
C	-0.676779	-3.690162	-2.455544
H	-1.210868	-3.820233	-3.385931
C	0.676779	-3.690162	-2.455544
H	1.210868	-3.820233	-3.385931
C	1.397365	-3.372783	-1.252557
C	0.717332	-3.576144	-0.022333
C	1.398508	-3.401062	1.210409
C	0.677202	-3.738874	2.406284
H	1.210100	-3.882528	3.335325
C	-0.677202	-3.738874	2.406284
H	-1.210100	-3.882528	3.335325
C	2.561119	-2.571111	-1.248799
C	3.010649	-2.042084	-0.006963
C	2.567253	-2.602636	1.222584
C	3.092282	-1.994436	-2.453161
H	2.894079	-2.472176	-3.401689
C	3.717087	-0.792137	-2.434558
H	4.021443	-0.321163	-3.360741
C	3.884788	-0.073599	-1.204291
C	3.672307	-0.780134	0.007873
C	3.902262	-0.110525	1.234516
C	3.740423	-0.860174	2.445007
H	4.052282	-0.415256	3.381537
C	3.107128	-2.059547	2.436957
H	2.910870	-2.559038	3.374638

C	4.087157	1.306395	-1.158285
H	4.146630	1.837091	-2.099309
C	4.092265	2.015914	0.047603
C	4.107597	1.274916	1.228459
H	4.185499	1.773017	2.183856
C	3.956072	3.546944	0.034370
C	4.112196	4.163200	1.433079
H	3.364502	3.802982	2.137793
H	4.005442	5.246988	1.367698
H	5.097955	3.952891	1.850784
C	5.039235	4.172131	-0.868796
H	6.037333	3.921209	-0.506863
H	4.945342	5.259542	-0.875269
H	4.962559	3.831272	-1.900675
C	2.557805	3.934951	-0.555711
H	2.516910	3.577306	-1.587953
H	2.527939	5.028020	-0.615689
C	1.296205	3.448164	0.176321
H	1.315370	2.358890	0.262000
H	1.283527	3.836492	1.198224
C	0.000000	3.879496	-0.532305
H	0.000000	3.476401	-1.550240
H	0.000000	4.969571	-0.640960
C	-1.296205	3.448164	0.176321
H	-1.315371	2.358890	0.262000
H	-1.283527	3.836492	1.198224
C	-2.557805	3.934951	-0.555711
H	-2.516911	3.577306	-1.587953
H	-2.527940	5.028020	-0.615689
C	-3.956072	3.546943	0.034370
C	-5.039235	4.172130	-0.868796
H	-4.962559	3.831271	-1.900675
H	-4.945343	5.259542	-0.875269
H	-6.037333	3.921208	-0.506863
C	-4.112197	4.163200	1.433079
H	-5.097955	3.952891	1.850784
H	-4.005442	5.246988	1.367698
H	-3.364502	3.802981	2.137793

1,1,8,8-Tetramethyl[8](2,11)teropyrenophane (1) (E = –1932.5495958 Hartree):

C	4.580085	1.823593	-0.024586
C	4.514468	1.096410	1.168674
H	4.635209	1.600908	2.117747
C	4.171680	-0.255633	1.194969
C	3.875204	-0.915452	-0.025291
C	4.158564	-0.250827	-1.243593
C	4.505962	1.106192	-1.217868
H	4.623640	1.610504	-2.166069
C	3.946044	-0.972509	2.415851
H	4.301896	-0.546580	3.345493
C	3.211768	-2.111494	2.423317
H	2.981224	-2.583782	3.367109
C	2.624003	-2.623076	1.217027
C	3.099884	-2.110641	-0.021689
C	2.604644	-2.617305	-1.254855
C	3.171769	-2.097452	-2.466329
H	2.922394	-2.560498	-3.409935
C	3.909661	-0.959216	-2.463501
H	4.248265	-0.527763	-3.397071
C	1.413116	-3.354098	1.221557
C	0.716749	-3.518905	-0.005615
C	1.394231	-3.351442	-1.242406
C	0.695355	-3.659339	2.426160
H	1.232580	-3.789166	3.354509
C	-0.659300	-3.657080	2.436298
H	-1.183172	-3.785282	3.372528
C	-1.394234	-3.351441	1.242407
C	-0.716752	-3.518904	0.005615
C	-1.413120	-3.354098	-1.221556
C	-0.695359	-3.659339	-2.426160
H	-1.232584	-3.789166	-3.354508
C	0.659296	-3.657081	-2.436297
H	1.183168	-3.785284	-3.372527
C	-2.604647	-2.617303	1.254855
C	-3.099887	-2.110639	0.021690
C	-2.624006	-2.623074	-1.217026
C	-3.171772	-2.097450	2.466329
H	-2.922398	-2.560496	3.409935
C	-3.909663	-0.959213	2.463501
H	-4.248266	-0.527760	3.397071
C	-4.158565	-0.250824	1.243594
C	-3.875206	-0.915449	0.025292
C	-4.171680	-0.255629	-1.194968
C	-3.946045	-0.972506	-2.415850
H	-4.301896	-0.546576	-3.345493
C	-3.211771	-2.111492	-2.423316
H	-2.981226	-2.583779	-3.367109

C	-4.505962	1.106196	1.217868
H	-4.623639	1.610508	2.166070
C	-4.580083	1.823597	0.024587
C	-4.514467	1.096413	-1.168674
H	-4.635207	1.600912	-2.117747
C	-4.578955	3.360182	-0.021238
C	-5.665056	3.872388	-0.989036
H	-5.495589	3.541583	-2.013147
H	-5.677603	4.963570	-0.997488
H	-6.653120	3.525115	-0.683574
C	-4.847724	3.992653	1.352397
H	-5.827059	3.702277	1.736420
H	-4.836358	5.080129	1.263439
H	-4.100131	3.719683	2.095139
C	-3.186782	3.832607	-0.562628
H	-3.034642	3.363351	-1.537863
H	-3.254278	4.908607	-0.753036
C	-1.950855	3.564414	0.313022
H	-2.000644	2.555535	0.729963
H	-1.950662	4.248305	1.166460
C	-0.622946	3.712197	-0.450253
H	-0.545952	2.898203	-1.178008
H	-0.635984	4.638250	-1.034821
C	0.622950	3.712198	0.450251
H	0.545956	2.898206	1.178009
H	0.635990	4.638252	1.034817
C	1.950859	3.564412	-0.313023
H	2.000648	2.555531	-0.729961
H	1.950667	4.248299	-1.166464
C	3.186787	3.832606	0.562625
H	3.034646	3.363354	1.537863
H	3.254284	4.908607	0.753030
C	4.578959	3.360178	0.021238
C	5.665061	3.872384	0.989035
H	5.495593	3.541582	2.013147
H	5.677611	4.963566	0.997484
H	6.653125	3.525108	0.683574
C	4.847730	3.992646	-1.352398
H	5.827065	3.702269	-1.736420
H	4.836363	5.080122	-1.263443
H	4.100138	3.719673	-2.095141

1,1,9,9-Tetramethyl[9](2,11)teropyrenophane (29) (E = –1971.8878607 Hartree)

C	-5.060312	1.611372	0.041275
C	-4.901319	0.921221	-1.164580
H	-5.062459	1.430524	-2.105240
C	-4.413480	-0.385403	-1.210103
C	-4.064093	-1.034288	0.002417
C	-4.432740	-0.428044	1.228350
C	-4.925632	0.882704	1.222092
H	-5.106228	1.353910	2.177344
C	-4.100980	-1.052026	-2.439646
H	-4.480998	-0.642404	-3.367057
C	-3.266772	-2.120135	-2.456476
H	-2.984517	-2.551378	-3.405688
C	-2.655486	-2.606281	-1.252239
C	-3.179691	-2.150553	-0.010960
C	-2.661453	-2.639491	1.219635
C	-3.282734	-2.190880	2.431723
H	-3.003155	-2.645309	3.370887
C	-4.126552	-1.128725	2.438825
H	-4.515532	-0.748834	3.375144
C	-1.408204	-3.273724	-1.255061
C	-0.716391	-3.432371	-0.023641
C	-1.409273	-3.302145	1.209514
C	-0.677422	-3.547727	-2.457332
H	-1.205866	-3.663139	-3.392410
C	0.677421	-3.547727	-2.457332
H	1.205864	-3.663139	-3.392410
C	1.408202	-3.273725	-1.255061
C	0.716389	-3.432371	-0.023641
C	1.409271	-3.302145	1.209514
C	0.677840	-3.596437	2.405595
H	1.205245	-3.725808	3.339399
C	-0.677842	-3.596437	2.405595
H	-1.205247	-3.725807	3.339399
C	2.655484	-2.606282	-1.252239
C	3.179689	-2.150554	-0.010960
C	2.661451	-2.639492	1.219635
C	3.266771	-2.120137	-2.456476
H	2.984516	-2.551380	-3.405688
C	4.100979	-1.052027	-2.439646
H	4.480998	-0.642406	-3.367057
C	4.413479	-0.385405	-1.210103
C	4.064092	-1.034289	0.002417
C	4.432740	-0.428046	1.228350
C	4.126550	-1.128727	2.438825
H	4.515531	-0.748835	3.375144
C	3.282732	-2.190881	2.431723
H	3.003153	-2.645309	3.370887

C	4.901319	0.921220	-1.164580
H	5.062460	1.430522	-2.105240
C	5.060312	1.611370	0.041275
C	4.925632	0.882702	1.222092
H	5.106229	1.353908	2.177344
C	5.200332	3.140933	0.030419
C	5.514115	3.713204	1.421541
H	4.729821	3.505015	2.147505
H	5.618863	4.797132	1.355346
H	6.451097	3.314172	1.813653
C	6.332306	3.580910	-0.918667
H	7.290718	3.171363	-0.596202
H	6.415816	4.669115	-0.927267
H	6.159271	3.259290	-1.945040
C	1.291539	3.897859	-0.426105
H	1.266826	3.515973	-1.452059
H	1.324711	4.989295	-0.510334
C	0.000001	3.478396	0.291693
H	0.000001	2.390067	0.408906
H	0.000002	3.890363	1.306283
C	-1.291537	3.897861	-0.426104
H	-1.266822	3.515978	-1.452060
H	-1.324710	4.989297	-0.510330
C	-2.569958	3.392415	0.261729
H	-2.501091	2.307410	0.367544
H	-2.609492	3.795878	1.277367
C	-3.856672	3.749838	-0.498089
H	-3.737509	3.440752	-1.540077
H	-3.974063	4.838304	-0.516802
C	-5.200330	3.140936	0.030419
C	-6.332304	3.580913	-0.918667
H	-6.159270	3.259291	-1.945040
H	-6.415811	4.669118	-0.927269
H	-7.290716	3.171368	-0.596201
C	-5.514112	3.713206	1.421541
H	-6.451094	3.314175	1.813653
H	-5.618860	4.797135	1.355346
H	-4.729818	3.505018	2.147505
C	2.569961	3.392417	0.261731
H	2.609494	3.795885	1.277367
H	2.501094	2.307412	0.367551
C	3.856674	3.749837	-0.498089
H	3.974067	4.838303	-0.516803
H	3.737511	3.440750	-1.540077