Supplementary Information

Shape-Shifting in Contorted Dibenzotetrathienocoronenes

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I. Synthesis

General. All reactions were run in oven-dried glassware (130 ^{o}C), and monitored by TLC using silica gel 60 F_{254} pre-coated plates (EM Science). Anhydrous and oxygen-free solvents were obtained from a Schlenk manifold system with purification columns packed with activated alumina and supported copper catalyst (Glass Contour, Irvine, CA). Column chromatography was performed on a CombiFlash® Rf system using RediSepTM normal phase silica columns (ISCO, Inc., Lincoln, NE). ^{1}H NMR (300MHz, 400MHz), and ^{13}C NMR (75MHz, 100MHz) spectra were recorded on Bruker DRX-300 and Bruker DRX-400 spectrometers at room temperature unless otherwise noted. HRMS were recorded on JEOL JMS-HX110A/110A Tandem mass spectrometer. The photochemistry was carried out according to a reported procedure (reference 22 in manuscript). IR spectra were recorded in powder form on Thermo Scientific NICOLET iS10 with SMART iTR module and were shown in Figure S1 for selected molecules. Compound **4a** and **4g** were purchased from Aldrich. Crystal structure of C60 in the co-crystal was modeled as rigid bodies by using FRAG command.

General Procedure for Synthesis of Compounds 4b-4f. The synthesis of **4e** is used as example, with the other compounds prepared in identical fashion. A 25-mL two-necked round-bottomed flask was purged with nitrogen, charged with bis(1,5-cyclooctadiene)di-μ-methoxy-diiridium(I) ([Ir(OMe)(COD)]$_2$) (26 mg, 0.04 mmol, Alfa Aesar) and 4,4'-di-*tert*-butyl-2,2'-bipyridine (dtbpy) (21 mg, 0.08 mmol, Aldrich), and purged with nitrogen again. Anhydrous hexane (15 mL) and pinacolborane (0.5g, 1.98

mmol, Frontier Scientific) were then added by syringe, and the flask was immersed in an oil bath at room temperature. The mixture was stirred for 5 min to give a dark red solution and charged with 2-dodecylthiophene (666 mg, 3.96 mmol). The solution was then stirred at 50 °C for 8 - 12 hours. Subsequently, the mixture was removed from the oil bath and allowed to cool to room temperature. After chromatography on a silica gel column (40 % CH_2Cl_2: Hexane), product **4e** was isolated as a colorless oil in 86 % yield. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.89 (t, J = 6.8 Hz, 3H), 1.26 (br, 18H), 1.34 (s, 12H), 1.68 (quint, J = 7.6 Hz, 2H), 2.85 (t, J= 7.6 Hz, 2H), 6.90 (d, J = 3.6 Hz, 1H), 7.47 (d, J = 3.6 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 12.27, 22.83, 24.88, 29.22, 29.50, 29.68, 29.78, 30.29, 31.83, 32.06, 83.97, 125.94, 137.48, 153.90; HRMS (FAB+) cald. for $C_{22}H_{39}$ $B_1O_2S_1$: 378.2768, found: 378.2774.

2-(5-butyl-2-thienyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4b). 63**%.** ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.95 (t, J = 7.2 Hz, 3H), 1.34 (br, 12H), 1.41(m, 2H), 1.69 (quint, J = 7.6 Hz, 2H), 2.87 (t, J= 7.6 Hz, 2H), 6.87 (d, J = 3.6 Hz, 1H), 7.50 (d, J = 3.6 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 13.77, 22.08, 24.69, 29.76, 33.76, 83.69, 125.78, 137.33, 153.48; HRMS (FAB+) cald. for $C_{14}H_{23}B_1O_2S_1$: 268.1671, found: 268.1576.

2-(5-hexyl-2-thienyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4c). 88%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.95 (t, J = 7.2 Hz, 3H), 1.34 (br, 12H), 1.41(m, 2H), 1.69 (quint, J = 7.6 Hz, 2H), 2.87 (t, J= 7.6 Hz, 2H), 6.87 (d, J = 3.6 Hz, 1H), 7.50 (d, J = 3.6 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.02, 22.51, 24.67, 28.69, 30.07, 31.53, 31.62, 83.62, 125.71, 137.30, 153.45; HRMS (FAB+) cald. for $C_{16}H_{27}$ $B_1O_2S_1$: 294.1828, found: 294.1816.

2-(5-octyl-2-thienyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4d). 86%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.89 (t, J = 7.2 Hz, 3H), 1.26 (br, 10H), 1.32(s, 12H), 1.68 (quint, J = 7.6 Hz, 2H), 2.85 (t, J= 7.6 Hz, 2H), 6.85 (d, J = 3.6 Hz, 1H), 7.47 (d, J = 3.6 Hz, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm):

14.24, 22.81, 24.90, 29.23, 29.35, 29.47, 30.32, 31.84, 32.01, 84.01, 125.96, 137.50, 153.94; HRMS (FAB+) cald. for $C_{18}H_{31}B_1O_2S_1$: 322.2138, found: 322.2129.

4,4,5,5-tetramethyl-2-(5-(perfluorohexyl)thiophen-2-yl)-1,3,2-dioxaborolane (4f). 56%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 1.38 (s, 12H), 7.51 (d, J = 3.6 Hz, 1H), 7.63 (m, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 24.88, 84.91, 131.23, 136.79; LRMS (FAB+) cald. for $C_{16}H_{14}B_1F_{13}O_2S_1$: 528.06, found: 528.09.

General Ramirez Olefination Procedure.

6,13-bis(dibromomethylene)-6,13-dihydropentacene (**3**). CBr_4 (4.30 g, 12.9 mmol), PPh_3 (6.8 g, 25.8 mmol), and anhydrous toluene (150 ml) were added to a 250 ml two-necked round-bottomed flask and stirred at room temperature for 5 minutes. 6,13-pentacenequinone was then added to the flask and the solution was stirred at 80 ^{o}C for 12 hours. The solution was cooled to room temperature, with the precipitate removed by filtration and rinsed with toluene. The filtrate was tried under reduced pressure, and the crude product was subjected to column chromatography (20 % CH_2Cl_2: Hexane). Compound **3** was isolated as a white solid in 86% yield. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 7.51 (m, 4H), 7.85 (m, 4H), 8.26 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 90.62, 127.30, 128.25, 131.94, 133.46, 139.79; HRMS (FAB+) cald. for $C_{24}H_{12}Br_4$: 619.7634, found: 615.7637.

General procedure for the Suzuki-Miyaura Coupling (**5a-5g**). The synthesis of **5c** is used as example, with the other compounds prepared in identical fashion. 6 ml THF and 1.5 ml H_2O were added to a 25 ml two-necked round-bottomed flask, and the solution was bubbled with argon for 10 minutes. Na_2CO_3 (1.07 g, 1.01 mol), $Pd(PPh_3)_2Cl_2$ (70 mg, 0.10 mmol), **3** (784 mg, 126 mmol), and **4c** (1.86 g, 630 mmol) were then added to the solution, and the mixture was stirred at 70 ^{o}C for 4 hours. The solution was then cooled to room temperature and washed sequentially with H_2O and brine. Compound **5c** was isolated *via* column chromatography (10% CH_2Cl_2: Hexane) as a yellow solid in 98 % yield. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.88 (t, J = 7.2 Hz, 12H), 1.27 (br, 44H), 1.61 (quint, J = 7.2 Hz, 8H), 2.73 (t, J= 7.2 Hz, 8H),

6.59 (d, *J* = 3.6 Hz, 4H), 6.90 (d, *J* = 3.6 Hz, 4H), 7.32 (m, 4H), 7.56 (m, 4H), 7.87 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.25, 22.67, 28.78, 30.22, 31.64, 31.72, 123.65, 125.82, 126.19, 126.60, 128.06, 128.45, 131.99, 136.15, 137.36, 140.99, 146.47; LRMS (FAB+) cald. for $C_{64}H_{72}S_4$: 968.45, found: 968.66.

6,13-bis(dithiophen-2-ylmethylene)-6,13-dihydropentacene (5a). 98%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 6.95 (t, *J* = 4.4 Hz, 4H), 7.16 (d, *J* = 3.6 Hz, 4H), 7.33 (m, 4H), 7.55 (m, 4H), 7.84 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 125.49, 126.13, 126.21, 126.72, 126.81, 128.10, 128.85, 132.00, 135.65, 138.59, 143.39; HRMS (FAB+) cald. for $C_{16}H_{27}$ $B_1O_2S_1$: 632.0761, found: 632.0743.

6,13-bis(bis(5-butylthiophen-2-yl)methylene)-6,13-dihydropentacene (5b). 87%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.84 (t, *J*= 7.2 Hz, 12H), 1.28 (quint, 8H), 1.56 (quint, 8H), 2.71 (t, J=7.2Hz, 8H), 6.57 (d, *J* = 3.6 Hz, 4H), 6.88 (d, *J* = 3.2 Hz, 4H), 7.30 (m, 4H), 7.54 (m, 4H), 7.84 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 13.92, 22.12, 29.87, 33.78, 123.67, 125.82, 126.17, 126.58, 128.06, 128.45, 131.97, 136.12, 137.35, 140.91, 146.39; HRMS (FAB+) cald. for $C_{56}H_{56}S_4$: 856.3265, found: 856.3237.

6,13-bis(bis(5-octylthiophen-2-yl)methylene)-6,13-dihydropentacene (5d). 93%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.95 (t, *J*= 7.2 Hz, 12H), 1.30 (br, 40H), 1.65 (quint, 8H), 2.77 (t, J=7.2Hz, 8H), 6.63 (d, *J* = 3.6 Hz, 4H), 6.94 (d, *J* = 3.6 Hz, 4H), 7.35 (m, 4H), 7.60 (m, 4H), 7.91 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.29, 22.83, 29.13, 29.36, 29.50, 30.22, 31.70, 32.07, 123.64, 125.81, 126.17, 126.59, 128.05, 128.44, 131.96, 136.13, 137.31, 140.94, 146.44; LRMS (FAB+) cald. for $C_{72}H_{88}S_4$: 1080.58, found: 1080.61.

6,13-bis(bis(5-dodecylthiophen-2-yl)methylene)-6,13-dihydropentacene (5e). 73%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.90 (t, *J*= 7.2 Hz, 12H), 1.28 (br, 72H), 1.60 (quint, 8H), 2.72 (t, J=7.2Hz, 8H), 6.58 (d, *J* = 3.6 Hz, 4H), 6.88 (d, *J* = 3.6 Hz, 4H), 7.31 (m, 4H), 7.56 (m, 4H), 7.85 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.29, 22.87, 29.17, 29.55, 29.73, 29.86, 30.23, 31.72, 32.10, 123.64, 125.82,

126.18, 126.59, 128.06, 128.44, 131.97, 136.15, 137.29, 140.93, 146.47; HRMS (FAB+) cald. for $C_{88}H_{120}S_4$: 1306.8384, found: 1306.8359.

6,13-bis(bis(5-(perfluorohexyl)thiophen-2-yl)methylene)-6,13-dihydropentacene (5f). 56%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 7.19 (d, J = 3.6 Hz, 4H), 7.31 (d, J = 3.6 Hz, 4H), 7.37 (m, 4H), 7.51 (m, 4H), 7.77 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 115.60, 122.60, 127.25, 127.96, 129.26, 130.12, 132.19, 133.63, 147.13, 155.09, 161.08; LRMS (FAB+) cald. for $C_{64}H_{20}F_{52}S_4$: 1903.96, found: 1903.30.

6,13-bis(bis(5'-hexyl-[2,2'-bithiophen]-5-yl)methylene)-6,13-dihydropentacene (5g). 53%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.90 (t, J= 7.2 Hz, 12H), 1.33 (br, 72H), 1.66 (quint, 8H), 2.76 (t, J=7.2Hz, 8H), 6.61 (d, J = 3.6 Hz, 4H), 6.85 (d, J = 3.6 Hz, 4H), 6.94 (d, J = 3.6 Hz, 4H), 7.03 (d, J = 3.6 Hz, 4H), 7.32 (m, 4H), 7.60 (m, 4H), 7.96 (s, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.22, 22.72, 28.90, 30.32, 31.71, 122.59, 123.57, 124.81, 125.01, 126.28, 126.81, 128.23, 129.88, 132.13, 134.84, 135.60, 138.46, 138.68, 141.41, 145.52 ; LRMS (FAB+) cald. for $C_{80}H_{80}S_8$: 1296.40, found: 1296.64.

General Procedure for Synthesis of Dibenzotetrathienocoronenes (**1a-1h**). The synthesis of **1c** is used as example, with the other compounds prepared in identical fashion. A mixture of **5c** (365 mg, 0.37 mmol), iodine (477 mg, 1.89 mmol), and propylene oxide (10 ml) in anhydrous benzene (350 ml) were irradiated with UV light (Hanovia 450 W high-pressure quartz Hg vapor lamp). The whole reaction system was submerged in a water bath and simultaneously cooled by circulating water. The mixture was bubbled with nitrogen during the reaction. After 4 hours, the solvent was removed under reduced pressure, and the product **1c** was isolated by column chromatography (20 %, CH_2Cl_2: Hexane) as a yellow solid in 91 % yield. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.99 (t, J= 7.2 Hz, 12H), 1.46 (m, 16H), 1.59 (quint, 8H), 1.97 (quint, J=7.2Hz, 8H), 3.10 (t, J= 3.6Hz, 8H), 7.58 (m, 4H), 8.17 (m, 4H), 8.91 (m, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.36, 22.91, 29.36, 31.17, 31.86, 31.91, 118.90, 120.93, 121.32, 122.38, 123.64, 125.58, 127.54, 128.71, 133.79, 134.00, 146.62 ; HRMS (FAB+) cald. for $C_{64}H_{64}S_4$: 960.3891, found: 960.3874.

Dibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene (1a). 92%. ^{1}H-NMR (400 MHz, $C_2D_2Cl_4$), δ (ppm): 7.94 (m, 4H), 8.72 (d, J= 6.0 Hz, 4H), 9.32 (d, J= 6.0 Hz, 4H), 9.36 (m, 4H); ^{13}C-NMR could not be obtained due to the poor solubility of the compound; the crystal structure is available online.

2,9,12,19-tetrabutyldibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene (1b). 89%. ^{1}H-NMR (300 MHz, $CDCl_3$), δ (ppm): 1.10 (t, *J*= 7.2 Hz, 12H), 1.61 (m, 8H), 1.98 (quint, 8H), 3.17 (t, *J*= 7.5 Hz, 8H), 7.66 (m, 4H), 8.28 (s, 4H), 9.02 (m, 4H); ^{13}C-NMR (75 MHz, $CDCl_3$) δ (ppm): 13.92, 22.12, 29.87, 33.78, 123.66, 125.82, 126.58, 128.06, 128.45, 131.96, 136.12, 137.96, 140.91, 146.39; HRMS (FAB+) cald. for $C_{56}H_{48}S_4$: 848.2639, found: 848.2650.

2,9,12,19-tetraoctyldibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene (1d). 86%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.93 (t, *J*= 6.8 Hz, 12H), 1.36 (br, 24H), 1.49 (m, 8H), 1.57 (m, 8H), 1.97 (quint, *J*= 7.2Hz, 8H), 3.11 (t, *J*= 7.6 Hz, 8H), 7.58 (m, 4H), 8.19 (s, 4H), 8.92 (m, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm):14.31, 22.89, 29.57, 29.68, 29.70, 31.21, 31.91, 32.13, 118.95, 120.97, 121.40, 122.43, 123.66, 125.63, 127.60, 128.76, 134.07, 146.70; LRMS (FAB+) cald. for $C_{72}H_{80}S_4$: 1072.51, found: 1072.49.

2,9,12,19-tetradodecyldibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene (1e). 92%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.88 (t, *J*= 6.8 Hz, 12H), 1.27 (br, 56H), 1.49 (quint, 8H), 1.60 (quint, 8H), 2.03 (quint, *J*= 7.2Hz, 8H), 3.22 (t, *J*= 7.6 Hz, 8H), 7.70 (m, 4H), 8.36 (s, 4H), 9.10 (m, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm): 14.18, 22.83, 29.53, 29.68, 29.70, 31.37, 31.96, 32.10, 121.40, 121.93, 122.85, 123.92, 125.92, 127.92, 128.64, 129.12, 134.24, 134.52, 147.09; HRMS (FAB+) cald. for $C_{88}H_{112}S_4$: 1296.7647, found: 1296.7728.

2,9,12,19-tetrahexyldibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene 1,1,10,10,11,11,20,20-octaoxide (1h). Compound **1c** (2.3 mg) was dissolved in 10 ml dichloromethane and mCPBA (40 mg) was added at 0 ^{o}C. Upon addition of mCPBA, the solution changed from yellow to

orange. The solution was stirred for another 30 minutes and quenched with saturated Na_2CO_3. The crude product was extracted with dichloromethane and dried under vacuum, with **1h** produced as an orange solid in quantitative yield. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 0.93 (t, J= 6.8 Hz, 12H), 1.40 (m, 12H), 1.56 (m, 12H), 1.98 (quint, J= 7.2 Hz, 8H), 2.91 (t, J= 7.6 Hz, 8H), 7.98 (s, 4H), 8.09 (m, 4H), 8.87 (m, 4H); **1h** is too insoluble for obtaining ^{13}C-NMR.; LRMS (FAB+) cald. for $C_{64}H_{64}O_8S_4$: 1088.35, found: 1088.73.

2,9,12,19-tetrakis(perfluorohexyl)dibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene (1f). 86%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 8.13 (m, 4H), 9.31 (m, 4H), 9.35 (m, 4H); **1f** has poor solubility for obtaining ^{13}C-NMR.; LRMS (FAB+) cald. for $C_{64}H_{12}F_{52}S_4$: 1896.95, found: 1892.26.

2,9,12,19-tetrakis(5-hexylthiophen-2-yl)dibenzo[5,6:11,12]coroneno[2,1-b:3,4-b':8,7-b'':9,10-b''']tetrathiophene (1g). 89%. ^{1}H-NMR (400 MHz, $CDCl_3$), δ (ppm): 1.00 (t, J= 6.8 Hz, 12H), 1.42 (m, 24H), 1.70 (m, 8H), 2.74 (t, J= 7.6 Hz, 8H), 6.52 (d, J= 3.2 Hz, 4H), 6.63 (d, J= 3.2 Hz, 4H), 6.82 (m, 4H), 7.44 (s, 4H), 7.84 (m, 4H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm):14.37, 22.92, 29.31, 30.48, 31.70, 31.91, 118.49, 119.20, 120.15, 120.94, 121.14, 124.37, 124.54, 124.85, 126.44, 127.59, 132.65, 133.14, 134.96, 136.33, 145.62; LRMS (FAB+) cald. for $C_{80}H_{72}S_8$: 1288.34, found: 1288.47.

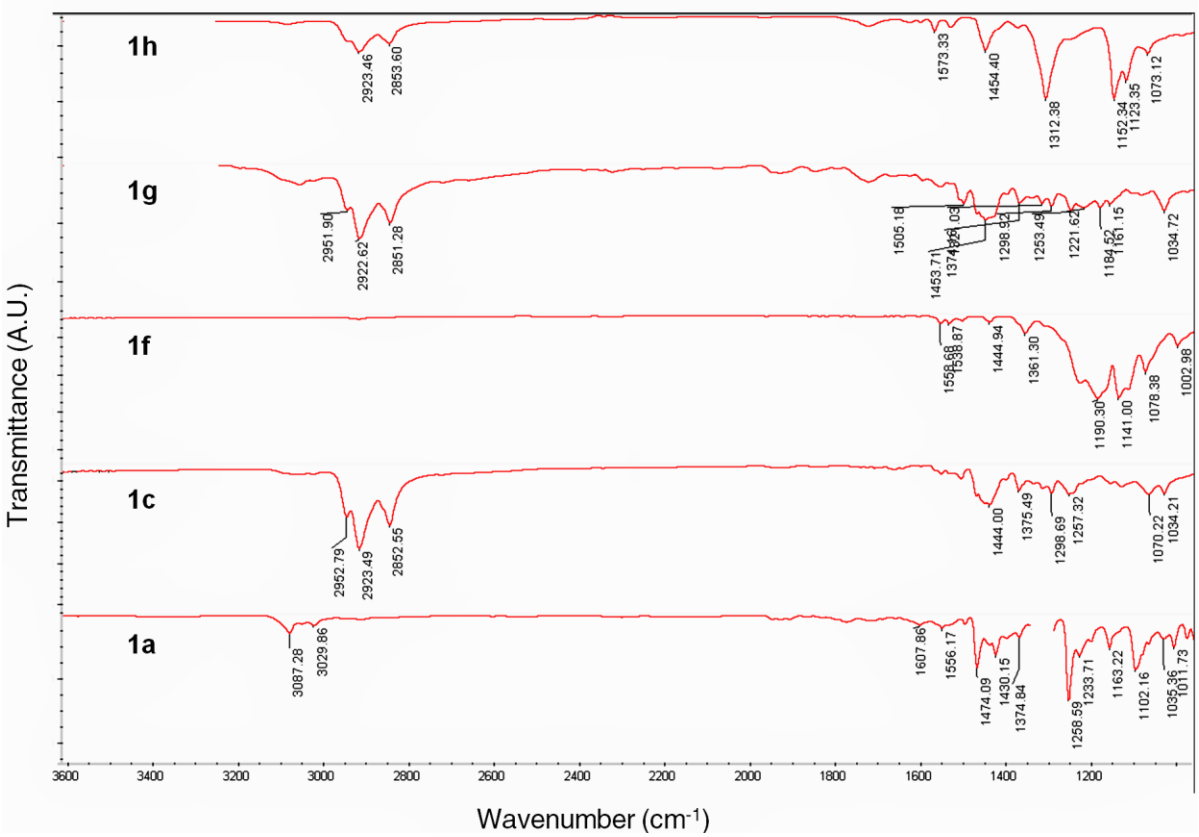


Figure S1. IR spectra for selected molecules to further reinforce the reliability of compounds 1f and 1h due to their poor solubility.

II. General procedure for cyclic voltammetry Measurements

A CH Instruments electrochemical workstation was used for cyclic voltammetry measurements. The experiments were performed in a single-compartment cell using a platinum wire auxiliary (BAS), a Ag/AgCl reference (BAS), and a glassy carbon working electrode (BAS). Prior to electrochemical measurements, the working electrodes were polished on PSA microcloth (Buehler) with 1.0 μm alumina micropolish and 0.05 μm alumina micropolish and then thoroughly sonicated in water, isopropanol, and dichloromethane to remove residual alumina particles. The supporting electrolyte for electrochemical measurements was 0.1 M tetrabutylammonium tetrafluoroborate (Fluka) in anhydrous

dichloromethane (Fluka). For experimental consistency, electrochemical potentials were standardized against the ferrocene/ferrocenium couple. The HOMO and LUMO energy values were calculated by using a value of -4.8 eV for ferrocene with respect to vacuum. This value is obtained from a value of -4.6 eV below vacuum level for the standard hydrogen electrode (SHE) and a redox potential of 0.2 V versus (SHE) for ferrocene.

III. Summary of DFT calculation of electronic structures, and determination of molecular ground-state geometries.

In order to simplify the calculations, the longer alky and perfluoroalkyl groups have been modeled by methyl groups and perfluoromethyl groups in **4c**, **4f** and **4i**. In a similar vein, hexyl-thiophene is modeled with thiophene in **4g**. In all cases, **UD**, **BF** and **TSD** stand for up-down-up-down-up-down, butterfly and up-down-down-twist-up-down conformations, respectively.

In each case the geometries were optimized using the B3LYP functional and the 6-31G** double-zeta basis set. At each optimized geometry the single-point wavefunction was recalculated using the larger 6-311G** triple-zeta basis set in order to determine the conformational energy differences more accurately.

The different conformations were determined by choosing an initial geometry that was as close as possible to the chemically intuitive conformations; the optimum, local-minimum geometries were then determined by typical gradient-based methods. Jaguar (Schrodinger LLC, New York) was used throughout.

Tetramethyl DBTTC (model for 4c-UD)

6-31G**:

final total energy (Hartree): -3284.07299

HOMO energy (Hartree): -0.17970 (-4.89 eV)

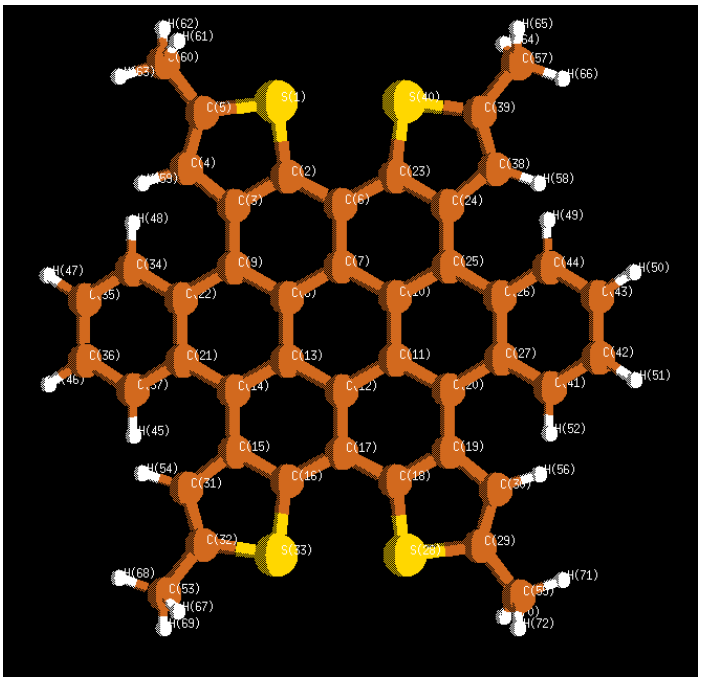
LUMO energy (Hartree): -0.05949 (-1.62 eV)

6-311G**:

final total energy (Hartree): -3284.49385

HOMO energy (Hartree): -0.18791 (-5.11 eV)

LUMO energy (Hartree): -0.06854 (-1.865 eV)



final geometry:

angstroms

atom	x	y	z
S1	0.0147818787	-0.0278373064	0.0018244006
C2	0.0061029596	-0.0087148414	1.7625091459
C3	1.3087656643	0.0174675913	2.2737599901
C4	2.2906986217	-0.0505341721	1.2192713814
C5	1.7671298329	-0.0757417261	-0.0362410779
C6	-1.1375818625	-0.1005818229	2.5984827644
C7	-0.9218570460	-0.3468108988	3.9896703895
C8	0.4059890067	-0.2537306558	4.5334458216
C9	1.5048223288	0.0551726220	3.6959540095
C10	-2.0341896249	-0.6853212627	4.8363835078
C11	-1.8179396102	-0.9342413408	6.2466683898
C12	-0.4893785853	-0.8422241487	6.7904351708
C13	0.6217372605	-0.4981044821	5.9448489637
C14	1.9300045965	-0.4143980459	6.4777321454
C15	2.1649594534	-0.9351138387	7.7945388812
C16	1.0730672087	-1.2218819615	8.6223392154
C17	-0.2710100848	-1.0952512208	8.1799043611
C18	-1.4144986767	-1.1983370345	9.0151715576
C19	-2.7179872363	-1.2217770714	8.5047795874
C20	-2.9166304618	-1.2473317551	7.0824360437
C21	2.9620975065	0.2432061029	5.6986624357
C22	2.7537218897	0.4703574619	4.3071315609

C23	-2.4795955291	0.0330035642	2.1551309241
C24	-3.5722010846	-0.2406875477	2.9851144684
C25	-3.3415992785	-0.7616207733	4.3027077560
C26	-4.3763235369	-1.4170500891	5.0786084573
C27	-4.1676775046	-1.6542851320	6.4685612869
S28	-1.4213126772	-1.1971876992	10.7761119272
C29	-3.1735434951	-1.1533554172	10.8164880583
C30	-3.6983938295	-1.1655999567	9.5613440783
C31	3.4132842179	-1.2914295152	8.4226061853
C32	3.2872595381	-1.7829566901	9.6848478083
S33	1.6063171703	-1.8432527848	10.1815259704
C34	3.7200618592	1.2269061033	3.5976672542
C35	4.8559504886	1.7181888302	4.2093937816
C36	5.0554604261	1.5034490298	5.5806500920
C37	4.1162526244	0.7978035500	6.3057556663
C38	-4.8183078327	0.1213627284	2.3557556199
C39	-4.6896442750	0.6039656277	1.0903785181
S40	-3.0086277906	0.6491750751	0.5926019746
C41	-5.1373325131	-2.4118096131	7.1722815852
C42	-6.2758267723	-2.8931711693	6.5572450806
C43	-6.4752211313	-2.6677761427	5.1874969295
C44	-5.5330021497	-1.9615733165	4.4669434200
H45	4.2326915046	0.7299496950	7.3776300190
H46	5.9174759211	1.9316719901	6.0837961188
H47	5.5627074590	2.3131357499	3.6382688286

H48	3.5302288042	1.4966124875	2.5690325118
H49	-5.6487745262	-1.8854236965	3.3947426628
H50	-7.3392710121	-3.0887255231	4.6816331536
H51	-6.9849766701	-3.4891077194	7.1243991675
H52	-4.9485459501	-2.6907923927	8.1985076926
C53	4.3696209400	-2.2603457035	10.6040839814
H54	4.3733839596	-1.2389684828	7.9286772753
C55	-3.9022055857	-1.0930867102	12.1240024441
H56	-4.7626041266	-1.0786721126	9.3934365502
C57	-5.7694000869	1.0821508232	0.1685999620
H58	-5.7784562972	0.0789189931	2.8507647131
H59	3.3545878871	-0.1371020847	1.3898000224
C60	2.4971438850	-0.1534118804	-1.3420927126
H61	2.1999244377	-1.0328854843	-1.9243353531
H62	2.3086301309	0.7295079466	-1.9637776513
H63	3.5739859412	-0.2139734659	-1.1625072410
H64	-5.6198581421	2.1264807933	-0.1278653472
H65	-5.8128177616	0.4844085318	-0.7491414305
H66	-6.7408632950	1.0069719312	0.6647898668
H67	4.2274179061	-3.3081272934	10.8919239099
H68	5.3409890093	-2.1740324399	10.1095200117
H69	4.4076080860	-1.6697101208	11.5266784338
H70	-3.6045884412	-0.2214157205	12.7176455764
H71	-4.9792573632	-1.0305052262	11.9464827129
H72	-3.7126974042	-1.9842247188	12.7335584312

Tetramethyl DBTTC (model for 4c-BF)

6-31G**:

Final total energy (Hartree): -3284.07419

HOMO energy (Hartree): -0.17842 (-4.85625 eV)

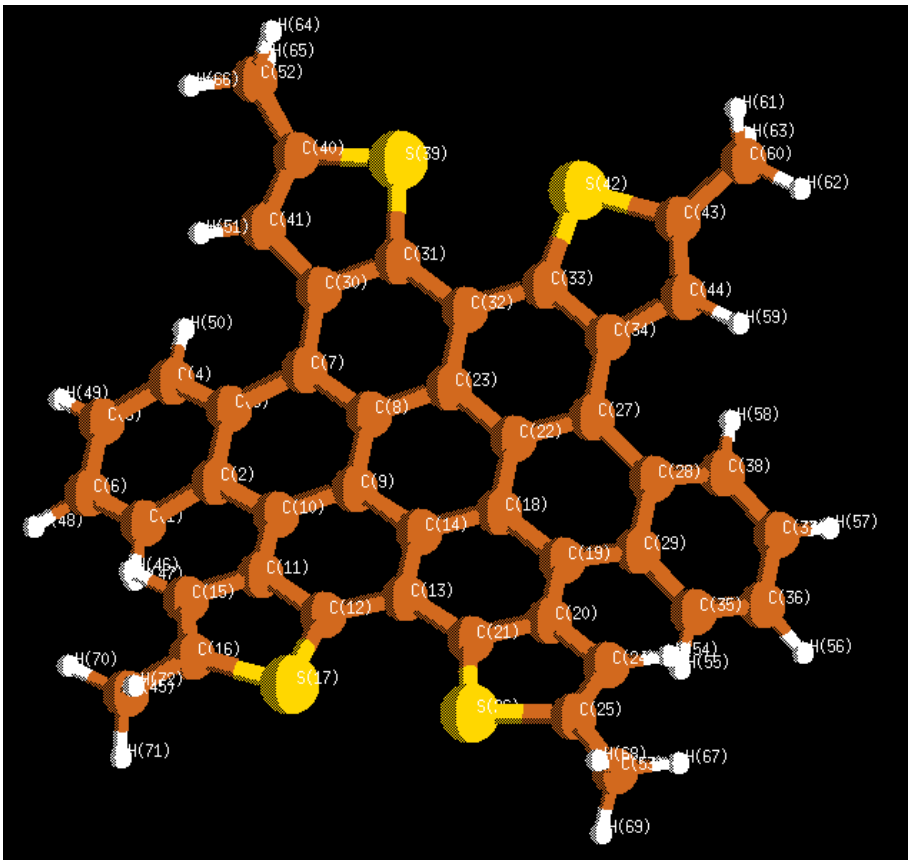
LUMO energy (Hartree): -0.05903 (-1.60668 eV)

6-311g**:

Final total energy (Hartree): -3284.49494

HOMO energy (Hartree): -0.18668 (-5.08107 eV)

LUMO energy (Hartree): -0.06811 (-1.85382 eV)



final geometry:

angstroms

atom	x	y	z
C1	0.0071289903	-0.0906763913	0.0069146366
C2	-0.0007965446	-0.0341180764	1.4218856644
C3	1.2493800618	0.0026277112	2.1053185049
C4	2.4379828806	-0.0155942085	1.3352231455
C5	2.4126261667	-0.0285836684	-0.0457751049
C6	1.1827999264	-0.0678852879	-0.7178950894
C7	1.2708055727	-0.0895804612	3.5541567307
C8	0.1263897311	-0.5956956818	4.2106158368
C9	-1.1458564369	-0.6207526674	3.5190155528
C10	-1.2287596612	-0.1491404095	2.1895341423
C11	-2.5242179855	0.1409695347	1.6484153349
C12	-3.6734037465	-0.2549638266	2.3502073341
C13	-3.6116761123	-0.9207643681	3.6056218171
C14	-2.3226343419	-1.0733111065	4.2062637106
C15	-2.8598235524	0.8871651164	0.4611181208
C16	-4.1942879397	1.0204307537	0.2368766646
S17	-5.1318426950	0.2300297745	1.4892431213
C18	-2.1871688885	-1.7385977334	5.4717732928
C19	-3.3010322862	-2.3642069655	6.0751746986
C20	-4.6071359913	-2.0763676751	5.5590082199
C21	-4.7345532520	-1.3846129401	4.3448333945
C22	-0.9121674955	-1.7249964368	6.1582673988

C23	0.2053905235	-1.0365314418	5.5750974871
C24	-5.8928721629	-2.3379312113	6.1574658646
C25	-6.9538023986	-1.9107584339	5.4216326271
S26	-6.4305440533	-1.1486427937	3.9327478937
C27	-0.7905130587	-2.3449435101	7.4214603103
C28	-1.8003004403	-3.3112507713	7.8136484715
C29	-3.0584382749	-3.3177512280	7.1434331220
C30	2.4173424505	0.2477326948	4.3457225848
C31	2.4706131243	-0.1476866743	5.6904943751
C32	1.4087224557	-0.8494067200	6.3248825693
C33	1.4202919161	-1.3151980032	7.6679193795
C34	0.3532598900	-2.0339031746	8.2272618119
C35	-3.9752996159	-4.3539731517	7.4451160448
C36	-3.6954748798	-5.3242808442	8.3877269612
C37	-2.4560897309	-5.3200086391	9.0434918752
C38	-1.5261198487	-4.3436007650	8.7434646628
S39	3.9694658966	0.3916165010	6.4423973637
C40	4.4768234371	1.2048578043	4.9748201684
C41	3.5657106714	1.0394216025	3.9787738468
S42	2.6922766737	-1.0537348119	8.8580385949
C43	1.7552815879	-1.8429879527	10.1117151290
C44	0.5667986520	-2.2950185199	9.6294209163
C45	-4.8770450659	1.7442930800	-0.8830709533
H46	-2.1301578426	1.3657307166	-0.1763852113
H47	-0.9255006821	-0.2268820898	-0.5217928639

H48	1.1511369255	-0.1308901941	-1.8017457358
H49	3.3443498155	-0.0601845516	-0.6031332062
H50	3.3919541455	-0.0942075056	1.8368819153
H51	3.6820525291	1.5253449382	3.0198653444
C52	5.7590325750	1.9792029449	4.9392652128
C53	-8.4116699323	-2.0075105611	5.7520944621
H54	-6.0240802958	-2.7757743167	7.1372958301
H55	-4.8882728288	-4.4353029115	6.8725556390
H56	-4.4148145356	-6.1153729727	8.5785757845
H57	-2.2045207732	-6.1082829658	9.7470717578
H58	-0.5382112331	-4.4157159015	9.1770450085
H59	-0.1684978453	-2.7519761483	10.2770069390
C60	2.2795138314	-1.9283220959	11.5125879721
H61	2.4733172458	-0.9359399806	11.9354581317
H62	1.5492010054	-2.4317277341	12.1520638388
H63	3.2169885789	-2.4940066929	11.5613703104
H64	5.7762092908	2.7726891636	5.6950249839
H65	6.6272627204	1.3352817910	5.1208108135
H66	5.8847426365	2.4444049835	3.9576434078
H67	-8.5398946760	-2.4625911335	6.7379498709
H68	-8.8918316208	-1.0225727750	5.7680231532
H69	-8.9521855260	-2.6231596825	5.0237998021
H70	-4.1309024160	2.2075632982	-1.5344737470
H71	-5.4838723205	1.0666582502	-1.4947008634
H72	-5.5407523291	2.5339234408	-0.5130058475

Tetramethyl DBTTC (model for 4c-TSD)

6-31G**:

final total energy (Hartree): -3284.06740

HOMO energy (Hartree): -0.17942 (-4.88347 eV)

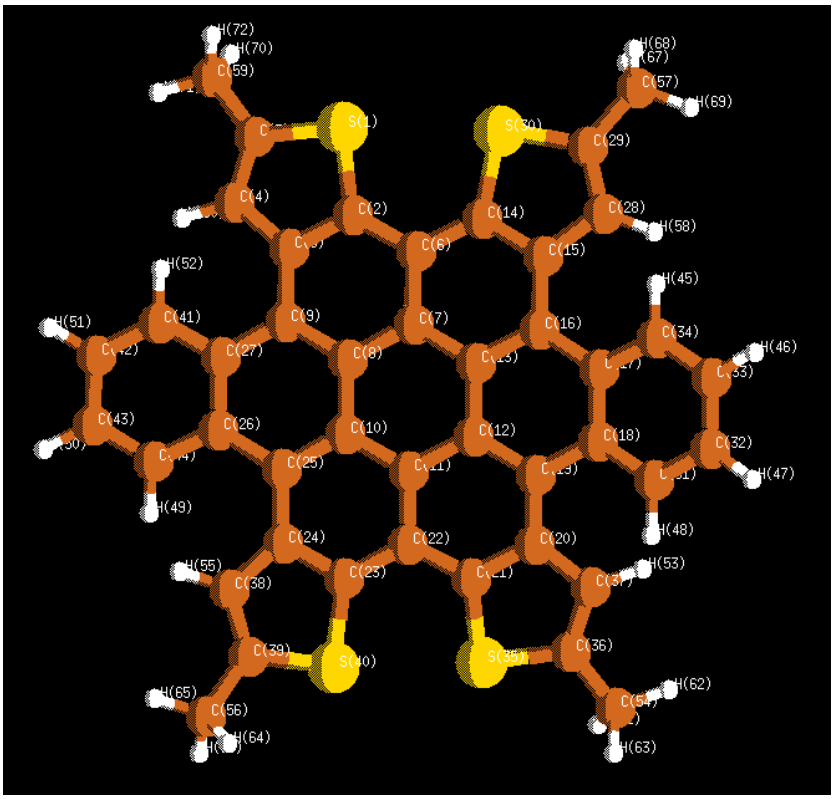
LUMO energy (Hartree): -0.05972 (-1.62546 eV)

6-311G**:

final total energy (Hartree): -3284.48792

HOMO energy (Hartree): -0.18753 (-5.103 eV)

LUMO energy (Hartree): -0.06866 (-1.868 eV)



final geometry:

angstroms

atom	x	y	z
S1	-0.0061846611	0.0210408307	0.0022204883
C2	-0.0016044739	0.0192569623	1.7638499879
C3	1.3075277791	0.0020999110	2.2641003488
C4	2.2750618878	0.0925111903	1.1955181007
C5	1.7402329355	0.1033080641	-0.0541851356
C6	-1.1436643781	0.1244934241	2.6033162886
C7	-0.9180662519	0.2982950350	4.0060280144
C8	0.4234245332	0.2713964210	4.5369596531
C9	1.5244401329	0.0021415364	3.6871270390
C10	0.6444767356	0.5139639903	5.9510395249
C11	-0.4723081841	0.8723419322	6.7850951363
C12	-1.8123038287	0.7985951246	6.2772216712
C13	-2.0412609316	0.4564405000	4.8912071153
C14	-2.4863752192	0.1734464138	2.1352748893
C15	-3.5839480043	0.3140222962	2.9961973644
C16	-3.3678077146	0.3448815176	4.4116599661
C17	-4.4512516133	0.2281421216	5.3727048557
C18	-4.2301210465	0.6270269451	6.7216095205
C19	-2.9139032005	1.0896473483	7.1157269088
C20	-2.6650684343	1.7714188657	8.3512449407
C21	-1.3568305779	1.8337517652	8.8434950905
C22	-0.2551545248	1.2808322768	8.1362676215

C23	1.0326675059	1.0604399248	8.6865577457
C24	2.1036583535	0.5757203049	7.9252058522
C25	1.9529425843	0.4520064134	6.4955895388
C26	3.0767604121	0.1952949084	5.6173486661
C27	2.8405457058	-0.1854862658	4.2654577524
C28	-4.8151982109	0.4887764900	2.2653700730
C29	-4.6819944878	0.4219205282	0.9143542037
S30	-3.0138081981	0.1538398701	0.4528410176
C31	-5.2637458123	0.4193422410	7.6683553621
C32	-6.4779889428	-0.1313964358	7.3085671007
C33	-6.6913676448	-0.5387249250	5.9835734399
C34	-5.6900402844	-0.3766758863	5.0459988236
S35	-1.2959442841	2.7272076944	10.3593139789
C36	-3.0174210398	3.0604797318	10.2893914878
C37	-3.5865404607	2.4968343764	9.1895747079
C38	3.2047200624	0.1888033755	8.7769043137
C39	3.0104957679	0.4312202547	10.1013282767
S40	1.4395531563	1.1454317919	10.3965285724
C41	3.9214537281	-0.7541920080	3.5406947960
C42	5.2125367138	-0.7394963485	4.0262949390
C43	5.4797253795	-0.1126627148	5.2547885571
C44	4.4288532337	0.3247418624	6.0341989838
H45	-5.8336135677	-0.7899032361	4.0579078747
H46	-7.6211475049	-1.0243126571	5.7019438527
H47	-7.2426455363	-0.2946696896	8.0623693529

H48	-5.0755565763	0.6309121149	8.7122331563
H49	4.6457447410	0.8117737701	6.9726586974
H50	6.5008334562	0.0072396692	5.6038735662
H51	6.0147968750	-1.1907132564	3.4501518208
H52	3.7218058024	-1.2449088233	2.5988791329
H53	-4.6310439719	2.6435042291	8.9503691856
C54	-3.6769735642	3.8893324278	11.3486989792
H55	4.0901170581	-0.3229096835	8.4318645946
C56	3.9349163304	0.1319689084	11.2414256922
C57	-5.7455382056	0.5682436542	-0.1303448463
H58	-5.7649981732	0.7152966129	2.7276284135
C59	2.4547770426	0.2039715096	-1.3669213969
H60	3.3368117317	0.2130693699	1.3464456742
H61	-3.2185853697	4.8806678532	11.4358641518
H62	-4.7346905641	4.0257419098	11.1072245890
H63	-3.6151938926	3.4124707800	12.3336664226
H64	3.4761125816	-0.5484472714	11.9677626798
H65	4.8481595473	-0.3381727797	10.8669773600
H66	4.2209899680	1.0416256339	11.7817173647
H67	-5.5254784067	1.3873714931	-0.8239950399
H68	-5.8558320696	-0.3445757548	-0.7268119941
H69	-6.7076293939	0.7766102717	0.3456128034
H70	2.1395187837	1.0870575148	-1.9344414088
H71	3.5327129682	0.2764014768	-1.1984470008

H72	2.2701860607	-0.6731160722	-1.9979306376

Tetratrifluoromethyl DBTTC (model for 1f-UD)

6-31G**:

final total energy (Hartree): -4474.90858

HOMO energy (Hartree): -0.20979 (-5.71009 eV)

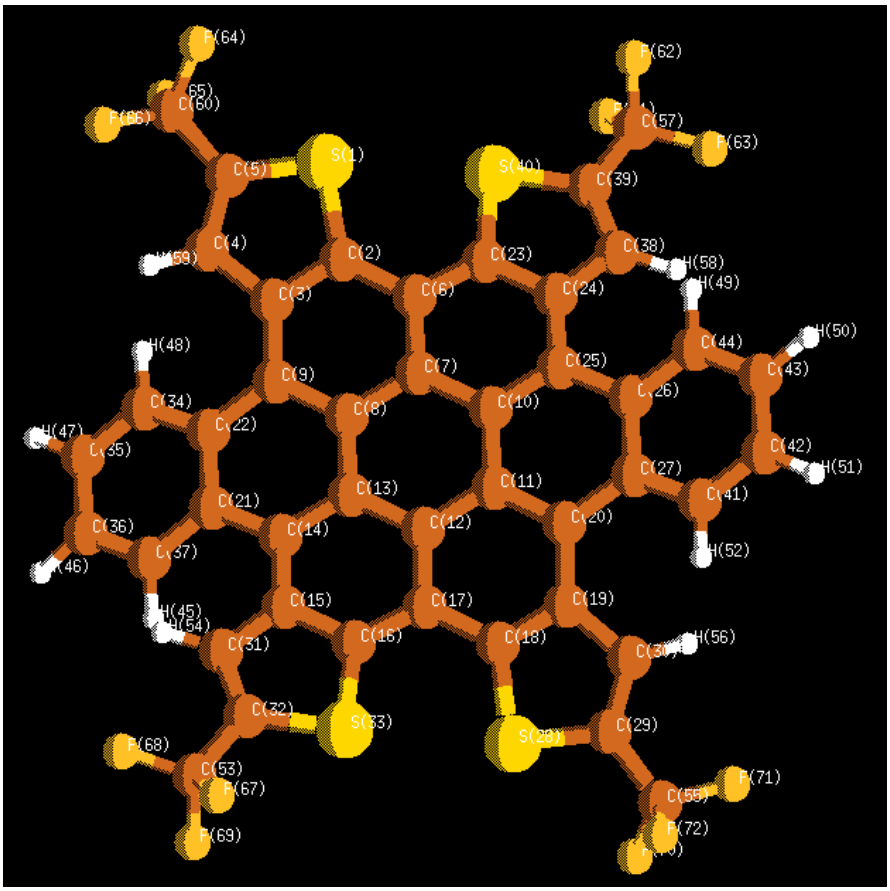
LUMO energy (Hartree): -0.09137 (-2.486918 eV)

6-311G**:

final total energy (Hartree): -4475.71645950335

HOMO energy (Hartree): -0.21987 (-5.98444 eV)

LUMO energy (Hartree): -0.10232 (-2.78496 eV)



final geometry:

angstroms

atom	x	y	z
S1	-0.0189921555	-0.0205134970	-0.0127640037
C2	0.0007283898	-0.1206521572	1.7410242868
C3	1.3070788500	-0.1134448918	2.2473239430
C4	2.2796731666	-0.0934487487	1.1855021494
C5	1.7209776243	-0.0184409297	-0.0516469357
C6	-1.1388383626	-0.2320801923	2.5812711420
C7	-0.9293525833	-0.4896707553	3.9678078929
C8	0.4048046169	-0.4353928377	4.5043690780
C9	1.5065904697	-0.1249009358	3.6703370324
C10	-2.0549707620	-0.7745732849	4.8217685698
C11	-1.8385914658	-1.0315199449	6.2336378462
C12	-0.4979829660	-1.0084630986	6.7631376831
C13	0.6199384642	-0.6986823030	5.9110709827
C14	1.9318191974	-0.6449969375	6.4378244656
C15	2.1608951282	-1.1656150425	7.7555118172
C16	1.0669869736	-1.4294574264	8.5895905848
C17	-0.2748643855	-1.2724616337	8.1480109373
C18	-1.4099945592	-1.3276032684	8.9984111019
C19	-2.7226554695	-1.2768184228	8.5086558241
C20	-2.9433928043	-1.2813020287	7.0844569234
C21	2.9703950455	0.0134990367	5.6701845260

C22	2.7593275908	0.2718116114	4.2852656479
C23	-2.4741327009	-0.0635987422	2.1337351996
C24	-3.5821861852	-0.2739719754	2.9654847971
C25	-3.3714864918	-0.7819457656	4.2975023022
C26	-4.4356403095	-1.3619974508	5.0950697979
C27	-4.2255159180	-1.6044665103	6.4856521393
S28	-1.3606152695	-1.3424880951	10.7527609306
C29	-3.0954803012	-1.2059656075	10.8195099671
C30	-3.6738407247	-1.1735414213	9.5882813073
C31	3.4048969620	-1.5056493916	8.3927529334
C32	3.2504789089	-1.9475030468	9.6684716934
S33	1.5806145936	-2.0130220129	10.1668386471
C34	3.7236561003	1.0458407478	3.5924890891
C35	4.8644070549	1.5155147094	4.2108163329
C36	5.0687540787	1.2659570554	5.5750714057
C37	4.1277824630	0.5504904229	6.2870975024
C38	-4.8031712843	0.1346946301	2.3126388976
C39	-4.6086932173	0.5720491418	1.0384743347
S40	-2.9388912044	0.5356230628	0.5528517600
C41	-5.2380441174	-2.2837822825	7.2089457308
C42	-6.4186899957	-2.6826119327	6.6150945542
C43	-6.6205356134	-2.4531921838	5.2465906699
C44	-5.6386536513	-1.8259946319	4.5065598869
H45	4.2457559596	0.4708338551	7.3576729214
H46	5.9324770646	1.6802291418	6.0860153571

H47	5.5684306419	2.1247787157	3.6523463605
H48	3.5295013839	1.3564343925	2.5772794061
H49	-5.7672628374	-1.7568589283	3.4362164628
H50	-7.5203671121	-2.8121560746	4.7563059330
H51	-7.1615000893	-3.2195123232	7.1972397719
H52	-5.0571295066	-2.5732004129	8.2335097515
C53	4.3432870452	-2.3156737035	10.6194571217
H54	4.3723295778	-1.4683973827	7.9162037578
C55	-3.7679986560	-1.1159780106	12.1521552456
H56	-4.7358469586	-1.0261048545	9.4630207837
C57	-5.6212681418	1.0810431262	0.0640249562
H58	-5.7756550733	0.1577384137	2.7809676693
H59	3.3471899659	-0.1688695920	1.3228231651
C60	2.4349897414	0.1505791124	-1.3531830402
F61	-5.3030683891	2.3181834535	-0.3798264765
F62	-5.6988958076	0.2896512736	-1.0303192113
F63	-6.8471706374	1.1409678878	0.6179189080
F64	1.8833722561	-0.6009265360	-2.3305870898
F65	2.3878096292	1.4348649597	-1.7773909226
F66	3.7341729875	-0.1906104099	-1.2418145817
F67	4.1348544249	-3.5225668658	11.1881327991
F68	5.5349569868	-2.3523904927	9.9885951540
F69	4.4442413843	-1.4216450507	11.6294168745
F70	-3.3031690406	-0.0736290683	12.8768673054
F71	-5.0997477849	-0.9636157975	12.0160041708

F72	-3.5523157278	-2.2270733126	12.8934654589

Tetratrifluoromethyl DBTTC (model for 1f-BF)

6-31g**:

final total energy (Hartree): -4474.91147

HOMO energy (Hartree): -0.20842 (-5.6728 eV)

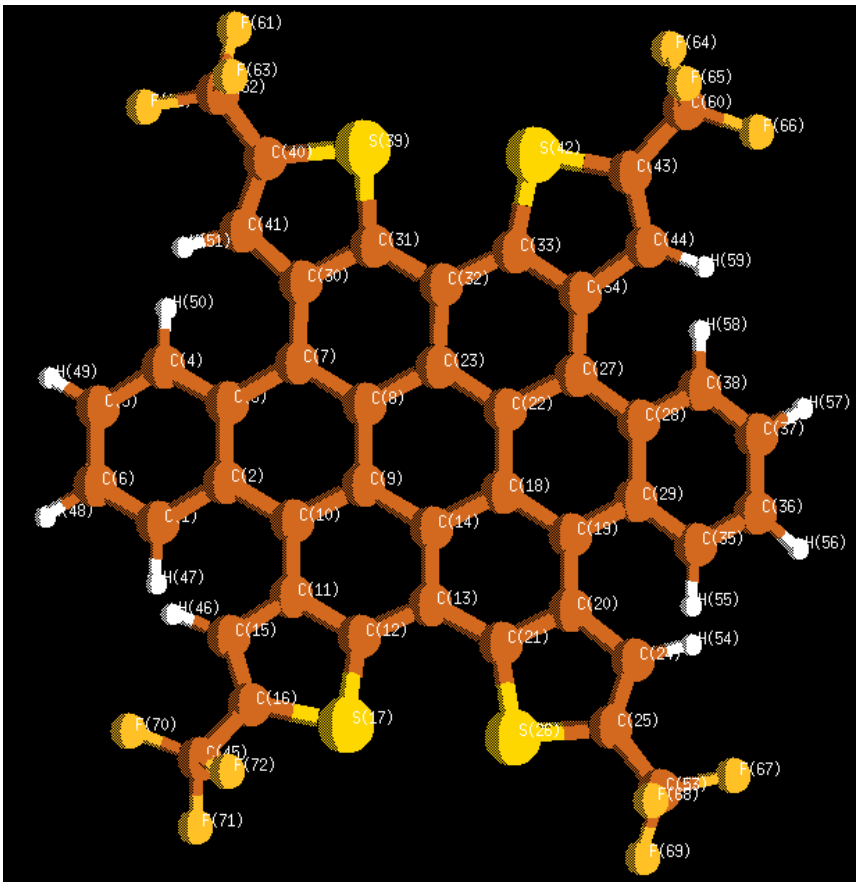
LUMO energy (Hartree): -0.08981(-2.44446 eV)

6-311G**:

final total energy (Hartree): -4475.71929

HOMO energy (Hartree): -0.21844 (-5.94552 eV)

LUMO energy (Hartree): -0.10081(-2.74386 eV)



final geometry:

angstroms

atom	x	y	z
C1	0.0243897422	-0.1215134830	-0.0329325707
C2	0.0267665083	-0.1169965140	1.3826870842
C3	1.2799655805	-0.1118152774	2.0597726326
C4	2.4662787844	-0.1183597592	1.2875675353
C5	2.4322880459	-0.0886650118	-0.0929061697
C6	1.1985050844	-0.0881558640	-0.7597935695
C7	1.3022798168	-0.2181089223	3.5062280573
C8	0.1615051616	-0.7269098049	4.1645537028
C9	-1.1089926558	-0.7508839434	3.4729956423
C10	-1.1933343692	-0.2488250708	2.1546980501
C11	-2.4892917673	0.0762852362	1.6336176229
C12	-3.6364221423	-0.3425042706	2.3243799543
C13	-3.5679570092	-1.0560074752	3.5530161873
C14	-2.2847656011	-1.2116460559	4.1573418179
C15	-2.8248112383	0.9080858497	0.5078580234
C16	-4.1639815194	1.0731390491	0.3461196173
S17	-5.1035392701	0.2218190789	1.5400128701
C18	-2.1581143631	-1.8615070859	5.4338988502
C19	-3.2782162398	-2.4734385844	6.0451886131
C20	-4.5824983032	-2.2056823751	5.5019356743
C21	-4.6946346294	-1.5308531188	4.2749619405
C22	-0.8872799217	-1.8252066008	6.1315710267

C23	0.2348468465	-1.1484036252	5.5369102443
C24	-5.8807987674	-2.4511256144	6.0785539980
C25	-6.9063439604	-2.0289729036	5.2917405799
S26	-6.3692095403	-1.3029867172	3.8052689431
C27	-0.7781355530	-2.4011572438	7.4173774250
C28	-1.7966872295	-3.3437668249	7.8416026920
C29	-3.0476999831	-3.3796504275	7.1564254669
C30	2.4362025854	0.1506132411	4.3018116600
C31	2.4832891127	-0.2135368965	5.6572002072
C32	1.4280867226	-0.9281359497	6.2910237409
C33	1.4308439946	-1.3517688003	7.6486441636
C34	0.3610048436	-2.0586435126	8.2219163522
C35	-3.9741980664	-4.3939548009	7.5018785851
C36	-3.7097947180	-5.3141050837	8.4974337821
C37	-2.4797704754	-5.2794415659	9.1690409740
C38	-1.5412863812	-4.3246199767	8.8308496222
S39	3.9404465030	0.3897897169	6.4335074382
C40	4.4227156887	1.1876200230	4.9611498665
C41	3.5548859168	0.9783845352	3.9367616551
S42	2.6965138221	-1.0283605640	8.8237540280
C43	1.7486594256	-1.7708733490	10.0825179759
C44	0.5619040155	-2.2581628481	9.6338118737
C45	-4.8578330618	1.9217319016	-0.6690670801
H46	-2.1054249864	1.4204002156	-0.1129674974
H47	-0.9125207274	-0.2248182987	-0.5628373563

H48	1.1627231699	-0.1099939780	-1.8446589977
H49	3.3598551271	-0.1120858454	-0.6566412018
H50	3.4223853462	-0.2190411004	1.7826187644
H51	3.6784523773	1.4546535318	2.9754359549
C52	5.6116121048	2.0933711847	4.9535698259
C53	-8.3686458167	-2.0562755242	5.5955217147
H54	-6.0508494110	-2.8663547572	7.0601043137
H55	-4.8786630078	-4.5079732484	6.9217663485
H56	-4.4340369730	-6.0917194316	8.7197865460
H57	-2.2411934162	-6.0296510404	9.9166733378
H58	-0.5599506694	-4.3844736207	9.2793254382
H59	-0.1647648026	-2.6910230255	10.3045201192
C60	2.2350387133	-1.7494088887	11.4959864828
F61	6.6669825456	1.5364544900	5.5873172096
F62	5.9864386013	2.3848237589	3.6915592273
F63	5.3542376418	3.2633761422	5.5799960242
F64	3.5033762868	-2.2065878234	11.5932631621
F65	2.2325430946	-0.4998457139	12.0107484370
F66	1.4553295220	-2.5164227114	12.2846080071
F67	-8.6131510718	-2.7027358514	6.7514000010
F68	-8.8776162038	-0.8085356086	5.7049975183
F69	-9.0681374765	-2.6727803152	4.6161069890
F70	-3.9673704479	2.5637722635	-1.4508468846
F71	-5.6629554040	1.1906033056	-1.4716010084
F72	-5.6414302982	2.8544879882	-0.0827916203

Tetrathienyl DBTTC (model for 1g-UD)

6-31G**:

final total energy (Hartree): -5334.05427

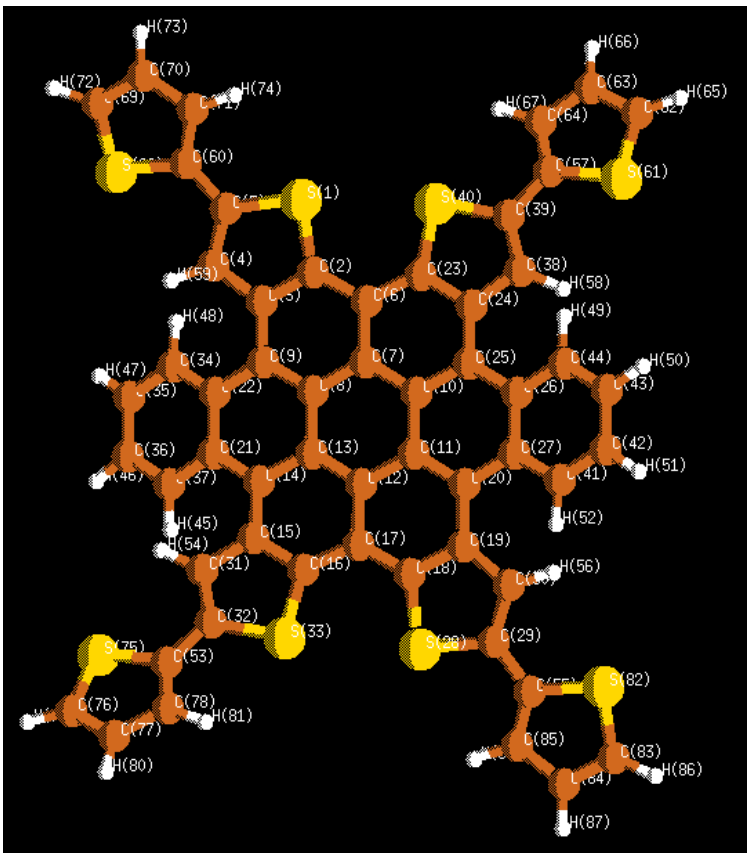
HOMO energy (Hartree): -0.18377 (-5.00187 eV)

LUMO energy (Hartree): -0.07442 (-2.02557 eV)

6-311G**:

final total energy (Hartree): -5334.66873 HOMO energy (Hartree): -0.19209 (-5.22832 eV)

LUMO energy (Hartree): -0.08369 (-2.27788 eV)



final geometry:

angstroms

atom	x	y	z
S1	0.0719469480	-0.1196574294	0.0186826999
C2	-0.0095338615	-0.0405709343	1.7777739437
C3	1.2749909020	0.0417137828	2.3307327559
C4	2.2993609443	-0.0462864411	1.3377534144
C5	1.8356909449	-0.1370318665	0.0554921428
C6	-1.1724261391	-0.1226835599	2.5934685584
C7	-0.9789326494	-0.3358049945	3.9971355032
C8	0.3336526848	-0.2174423438	4.5617607232
C9	1.4363458701	0.1202697291	3.7485513484
C10	-2.0950129835	-0.6578085352	4.8472510343
C11	-1.8834148527	-0.9314739314	6.2564395311
C12	-0.5535972913	-0.8726933670	6.8040149668
C13	0.5427066790	-0.4788750273	5.9659928460
C14	1.8464315298	-0.3804740001	6.4938408742
C15	2.0995309322	-0.9669367248	7.7707724491
C16	1.0327442210	-1.3339978085	8.6017118407
C17	-0.3206655016	-1.1967533878	8.1811148194
C18	-1.4643457271	-1.3292772815	9.0133456488
C19	-2.7725593145	-1.2763918852	8.5080999169
C20	-2.9866567836	-1.2391873841	7.0865753333
C21	2.8673792981	0.3288605365	5.7516978646
C22	2.6638787269	0.5755533443	4.3666021494

C23	-2.5111310786	0.0098409945	2.1402746688
C24	-3.6108476041	-0.1924610790	2.9864508908
C25	-3.4047667033	-0.6969944493	4.3165159728
C26	-4.4707467774	-1.2969941592	5.0945793953
C27	-4.2613150456	-1.5712331192	6.4780879256
S28	-1.4628787982	-1.4366909036	10.7691114132
C29	-3.2177539850	-1.2975327408	10.8228115724
C30	-3.7431240894	-1.2138756998	9.5620412889
C31	3.3660793459	-1.3320180593	8.3180356628
C32	3.3023854857	-1.9072899289	9.5548171556
S33	1.6304288580	-2.0341447722	10.1081182038
C34	3.6065808206	1.3766900310	3.6770984834
C35	4.7244715087	1.8848874026	4.3079306326
C36	4.9225605350	1.6454418826	5.6758822484
C37	3.9995801332	0.9002268991	6.3821074473
C38	-4.8372859227	0.2095652526	2.3636731191
C39	-4.7047859919	0.6262704054	1.0674866677
S40	-3.0219464124	0.5631935243	0.5509062243
C41	-5.2676388797	-2.2818913600	7.1807719318
C42	-6.4486049780	-2.6662713969	6.5791332844
C43	-6.6542778800	-2.3966345481	5.2187541947
C44	-5.6736421084	-1.7498075533	4.4950889255
H45	4.1126969484	0.8099792669	7.4534350210
H46	5.7716646883	2.0831549110	6.1921650653
H47	5.4193485127	2.5089813562	3.7540788570

H48	3.4158422980	1.6566905589	2.6505588987
H49	-5.8027625628	-1.6558572358	3.4273592555
H50	-7.5552853067	-2.7409993040	4.7196997675
H51	-7.1886240930	-3.2215013608	7.1479509714
H52	-5.0825817561	-2.5996920969	8.1957925066
C53	4.4338259255	-2.3744320977	10.3290189517
H54	4.2966926145	-1.2484646987	7.7764205838
C55	-3.9264348697	-1.2742358220	12.0863849388
H56	-4.7956126949	-1.0329967313	9.3998638492
C57	-5.7530425343	1.0753321431	0.1741056276
H58	-5.7839553323	0.2661776968	2.8806321728
H59	3.3514728393	-0.1233292658	1.5702714763
C60	2.6349174556	-0.2538296871	-1.1470043063
S61	-7.4275530183	0.6445387511	0.4904108938
C62	-7.9698363914	1.5171608097	-0.9058744912
C63	-6.9271340270	2.0882660423	-1.5810420961
C64	-5.6664634642	1.8376242727	-0.9695588319
H65	-9.0240915920	1.5522705318	-1.1421559739
H66	-7.0527586345	2.6764210155	-2.4825318843
H67	-4.7260487710	2.2229900862	-1.3468300487
S68	4.3350346910	0.1966614648	-1.1138476614
C69	4.5410694844	-0.2625894612	-2.7726850873
C70	3.3731214052	-0.7146923220	-3.3209838958
C71	2.2884566501	-0.7088992184	-2.3990247847
H72	5.5104751212	-0.1665428490	-3.2409564559

H73	3.2876180880	-1.0499144398	-4.3480461801
H74	1.2896450446	-1.0517544623	-2.6426020075
S75	6.0385862839	-1.7534209782	9.9600256597
C76	6.7640530260	-2.7748057276	11.1571766730
C77	5.8295304591	-3.5269127877	11.8131795860
C78	4.5036393221	-3.2995683479	11.3450401038
H79	7.8344314705	-2.7534204870	11.3061798792
H80	6.0769549541	-4.2294427139	12.6004122041
H81	3.6316353646	-3.8201089553	11.7247906509
S82	-5.6480908192	-1.6228482225	12.1507905036
C83	-5.6851927261	-1.3833708918	13.8675806511
C84	-4.4490042619	-1.0707809534	14.3609356769
C85	-3.4486908176	-1.0087015055	13.3507794338
H86	-6.6168985076	-1.4903873682	14.4050553221
H87	-4.2568578144	-0.8830573610	15.4108346943
H88	-2.4120697379	-0.7573494786	13.5445220330

Tetrathienyl DBTTC (model for 1g-BF)

6-31G**:

final total energy (Hartree): -5334.05561

HOMO energy (Hartree): -0.18257 (-4.96921 eV)

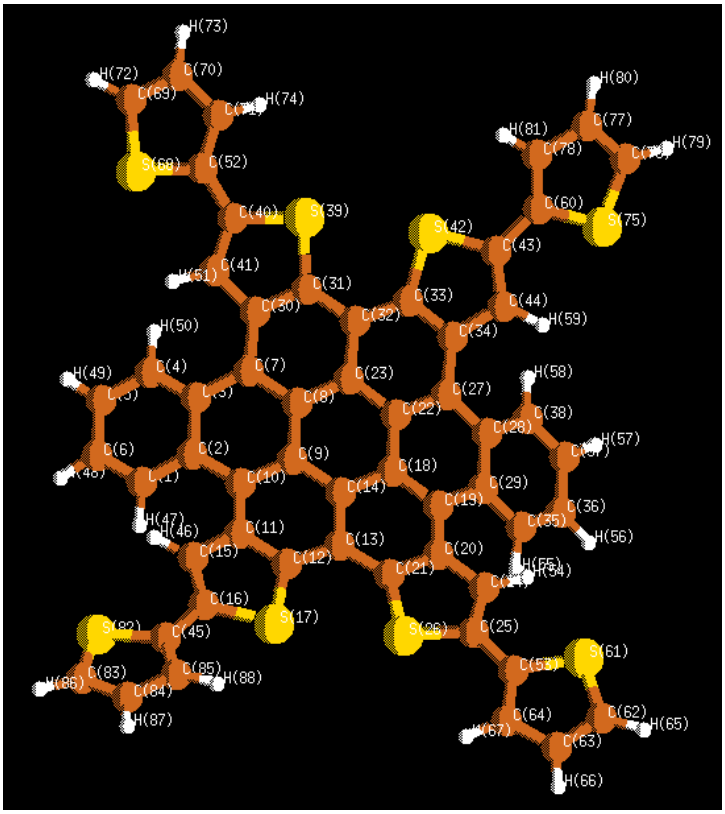
LUMO energy (Hartree): -0.07315 (-1.991 eV)

6-311G**:

final total energy (Hartree): -5334.66995

HOMO energy (Hartree): -0.19098 (-5.19811 eV)

LUMO energy (Hartree): -0.08235 (-2.24141 eV)



final geometry:

angstroms

atom	x	y	z
C1	0.0412276663	-0.1990529200	-0.0321122413
C2	0.0137450136	-0.1120713312	1.3812935994
C3	1.2556170056	-0.0583902182	2.0786240303
C4	2.4553883238	-0.0930459738	1.3276480247
C5	2.4484172886	-0.1383018437	-0.0523044046
C6	1.2278792583	-0.1924447479	-0.7394915530
C7	1.2557080673	-0.1182170934	3.5269465716
C8	0.1109716370	-0.6196336855	4.1811665380
C9	-1.1534783954	-0.6604189721	3.4771882875
C10	-1.2197000550	-0.2146532093	2.1410902519
C11	-2.5109135583	0.0715558458	1.5910000991
C12	-3.6762479889	-0.2853118355	2.2935568816
C13	-3.6313727741	-0.9341547660	3.5596556459
C14	-2.3376212590	-1.0994821770	4.1571597895
C15	-2.8092182816	0.8019774406	0.3958971231
C16	-4.1434248185	0.9664361548	0.1483125604
S17	-5.1170427475	0.2069400066	1.4064297762
C18	-2.1902872306	-1.7702571398	5.4166894538
C19	-3.2930524135	-2.4080603277	6.0142331773
C20	-4.5950310695	-2.0931801606	5.5179204647
C21	-4.7521297841	-1.3806967346	4.3183485651

C22	-0.9244597824	-1.7495347252	6.1149194470
C23	0.1858536493	-1.0413501051	5.5496070833
C24	-5.8404999827	-2.3429467321	6.1662652026
C25	-6.9376975520	-1.8862403105	5.4938102885
S26	-6.4646967506	-1.1003157085	3.9853538740
C27	-0.8101600081	-2.3768298662	7.3745541284
C28	-1.8103868297	-3.3549280799	7.7586084110
C29	-3.0608968220	-3.3676418063	7.0771209248
C30	2.3806920895	0.2597119997	4.3295072888
C31	2.4242294664	-0.1004943014	5.6862265286
C32	1.3759001956	-0.8269674888	6.3146178832
C33	1.3819125113	-1.3048386407	7.6541590223
C34	0.3199118344	-2.0516178750	8.1923382681
C35	-3.9834992211	-4.4000439578	7.3765511631
C36	-3.7144518200	-5.3597709423	8.3323518955
C37	-2.4811729576	-5.3507697328	8.9990888133
C38	-1.5445369289	-4.3813014667	8.6976881195
S39	3.8810706200	0.5157323106	6.4544968352
C40	4.3959523228	1.2978944326	4.9643073321
C41	3.5021412485	1.0676567793	3.9558411401
S42	2.6417981372	-1.0489552740	8.8546426721
C43	1.6934205539	-1.8615752877	10.0946125490
C44	0.5104013644	-2.3220198421	9.5868431419
C45	-4.7417241333	1.6769522584	-0.9650508638
H46	-2.0589835490	1.2747432880	-0.2207758976

H47	-0.8833079187	-0.3457390643	-0.5724988134
H48	1.2109821887	-0.2778691496	-1.8218253477
H49	3.3873122612	-0.1813948035	-0.5959679985
H50	3.4021384483	-0.1589390577	1.8447486176
H51	3.6179532680	1.5154010865	2.9799322518
C52	5.6077799197	2.0880186564	4.9216456519
C53	-8.3102734118	-1.9913850941	5.9458061842
H54	-5.9211222083	-2.7972884887	7.1420826075
H55	-4.8889099627	-4.4891192523	6.7933318680
H56	-4.4375842081	-6.1463014399	8.5257109227
H57	-2.2386231301	-6.1310097334	9.7142087215
H58	-0.5612345310	-4.4529675417	9.1414444458
H59	-0.2404333191	-2.7714253232	10.2205807015
C60	2.1822862396	-1.9754712425	11.4528916804
S61	-8.6390206793	-2.5607209595	7.5810831285
C62	-10.3502732962	-2.4446642444	7.3318155687
C63	-10.6495086049	-1.9912646107	6.0783149129
C64	-9.4918526739	-1.7325283849	5.2895877964
H65	-11.0280500649	-2.7128262268	8.1296976588
H66	-11.6629930006	-1.8459829182	5.7232689867
H67	-9.5298208189	-1.3790970516	4.2656609030
S68	5.9694037951	3.0991861521	3.5302509938
C69	7.4605596611	3.6299944591	4.2395233013
C70	7.6628209804	3.0704051913	5.4699095999
C71	6.6110498606	2.1941967960	5.8589845052

H72	8.0919487371	4.3250733655	3.7042377502
H73	8.5349517259	3.2730223505	6.0805931340
H74	6.5997970284	1.6489769827	6.7960375687
S75	1.5263507613	-3.1950980482	12.5344022988
C76	2.5461448512	-2.6658985670	13.8326586535
C77	3.3518275553	-1.6292644393	13.4517442508
C78	3.1470307222	-1.2364234568	12.0996319300
H79	2.4879595532	-3.1539886109	14.7952879049
H80	4.0638894797	-1.1530572511	14.1155557489
H81	3.6767873453	-0.4198071186	11.6235448026
S82	-3.8291254178	1.9123389719	-2.4499367880
C83	-5.1197143478	2.8260446475	-3.1594406480
C84	-6.1909086142	2.9256621826	-2.3159552894
C85	-5.9788098717	2.2720253822	-1.0692019543
H86	-5.0085224959	3.2296129534	-4.1559650713
H87	-7.1006980762	3.4568528531	-2.5698729382
H88	-6.7017705911	2.2641390167	-0.2614768532

DBTTC tetramethyl tetrasulfone (model for 1h-UD)

6-31G**

final total energy (Hartree): -3885.46340

HOMO energy (Hartree): -0.22077 (6.01 eV)

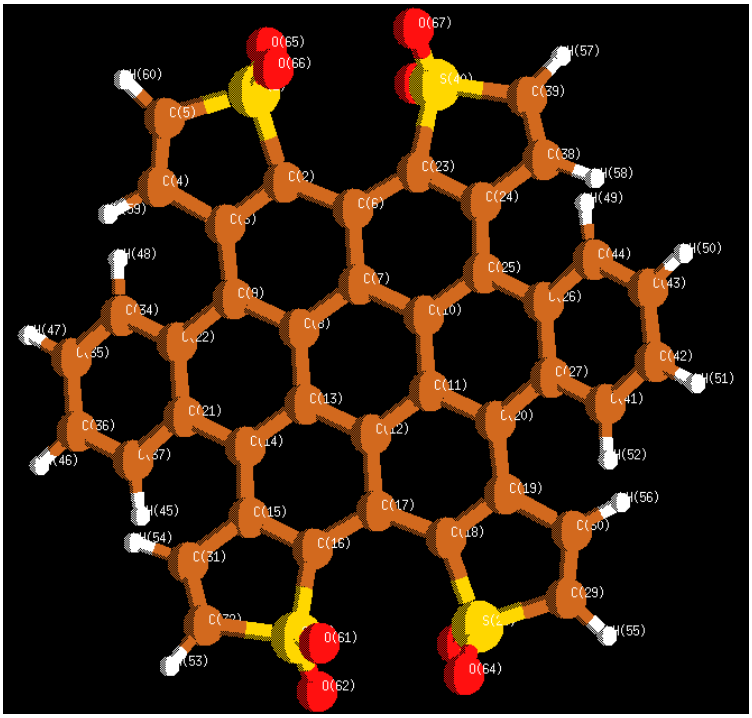
LUMO energy: -0.11825 (3.22 eV)

basis: 6-311G**

final total energy (Hartree): -3886.04293

HOMO energy (Hartree): -0.23115 (6.29 eV)

LUMO energy (Hartree): -0.12940 (3.52 eV)



final geometry:

angstroms

atom	x	y	z
C1	0.0000000000	0.0000000000	0.0000000000
C2	0.0000000000	0.0000000000	1.4148707688
C3	1.2474389605	0.0000000000	2.0994734490
C4	2.4377180093	-0.0003714832	1.3343238337
C5	2.4081864511	-0.0471357946	-0.0465769600
C6	1.1781634881	-0.0466870546	-0.7203056503
C7	1.2619807870	0.1492439635	3.5430882969
C8	0.1071681398	0.6367180457	4.1992817746
C9	-1.1603748013	0.6366110785	3.5025342701
C10	-1.2244591344	0.1471275274	2.1771968527
C11	-2.5147291028	-0.1626419684	1.6540112454
C12	-3.6533307412	0.3385441872	2.2607003872
C13	-3.6097981057	1.0797895958	3.4692332931
C14	-2.3446218939	1.0872755428	4.1633558928
C15	-2.2695822400	1.5433562967	5.5155910683
C16	-3.4250736698	2.0329941538	6.1694519446
C17	-4.5628465982	2.3264332786	5.3604182271
C18	-4.6594565429	1.8132589119	4.0784702542
C19	-5.6502352951	3.2632687914	5.7136601704
C20	-6.5723003935	3.4672412970	4.7676386268
S21	-6.1868306933	2.4665404471	3.3212382421

C22	0.1814375782	1.0858345675	5.5538262800
C23	-1.0021741810	1.5402644494	6.2139548327
C24	-0.9379284901	2.0230651903	7.5422434224
C25	-2.1655657453	2.1761592437	8.3011056826
C26	-3.4116999799	2.1853422292	7.6128336999
C27	2.3967759407	-0.1547257867	4.3515267329
C28	2.4915508083	0.3437386897	5.6393247357
C29	1.4444660932	1.0782947433	6.2520295047
C30	1.4894653720	1.8050757790	7.4689469882
C31	0.3533244990	2.3126140161	8.0750728806
S32	2.9441884731	2.4568040034	8.3594487301
C33	1.9252099319	3.4465531360	9.4654647280
C34	0.6334972120	3.2422825357	9.1895375272
C35	3.4775827538	-1.0966524653	3.9922314555
C36	4.3914464756	-1.3216470395	4.9412348779
S37	4.0074528515	-0.3349100514	6.3974214537
C38	-4.6044756805	2.1927913099	8.3745171636
C39	-4.5800741404	2.2376391286	9.7553930946
C40	-3.3524163188	2.2259116000	10.4330501847
C41	-2.1722069121	2.1714117170	9.7164484663
C42	-2.7886554779	-1.1139217526	0.5561296654
C43	-4.0797766003	-1.3428481156	0.2958921465
S44	-5.1050938620	-0.3478520509	1.3923320422
O45	-7.2205183270	1.4377859389	3.1700887158
O46	-5.8455833285	3.3627610130	2.2085400847

O47	3.6492540891	-1.2412791399	7.4964775697
O48	5.0516130147	0.6801518407	6.5677580199
O49	3.6990252574	3.3611255894	7.4817640219
O50	3.6279944080	1.4252292906	9.1454330761
O51	-5.8092311849	0.6600979961	0.5936668969
O52	-5.8409953441	-1.2475590706	2.2905946475
H53	-1.2405820317	2.0522514402	10.2540735439
H54	-3.3266800731	2.2075786232	11.5182033016
H55	-5.5121866904	2.2289778018	10.3118680581
H56	-5.5580533955	2.0893431945	7.8744208625
H57	-0.9356466253	0.1085665282	-0.5332429160
H58	1.1487858799	-0.0317708869	-1.8053868650
H59	3.3380612124	-0.0326112672	-0.6066086908
H60	3.3922523447	0.1087358099	1.8316546721
C61	2.6052485875	4.3227941206	10.4581577695
H62	-0.1607151606	3.7740376319	9.6962270063
C63	5.5783477553	-2.2186783883	4.9891501801
H64	3.4786731017	-1.6223208723	3.0467153722
C65	-4.7575238229	-2.2482328327	-0.6720844237
H66	-1.9893755089	-1.6436553239	0.0539372952
H67	-5.6514472100	3.8006785506	6.6525947477
C68	-7.7697562092	4.3502333020	4.7170713546
H69	3.2275097919	3.7235959745	11.1326129591
H70	3.2667251537	5.0334703543	9.9501662473
H71	1.8732963425	4.8781892504	11.0499026197

H72	5.6818758779	-2.7744252032	4.0538665263
H73	6.4906143105	-1.6359364197	5.1604166278
H74	5.4855151444	-2.9292625468	5.8181372047
H75	-5.3899367225	-1.6708876474	-1.3561436793
H76	-4.0244509476	-2.8107650181	-1.2555447720
H77	-5.4091508714	-2.9526316576	-0.1429258829
H78	-7.8729536405	4.9167750881	5.6459233119
H79	-7.6919952743	5.0510592783	3.8782983044
H80	-8.6764551730	3.7546689710	4.5606345686

DBTTC tetramethyl tetrasulfone (model for 1h-BF)

6-31G**

final total energy (Hartree): -3885.45577

HOMO energy (Hartree): -0.21959 (5.97 eV)

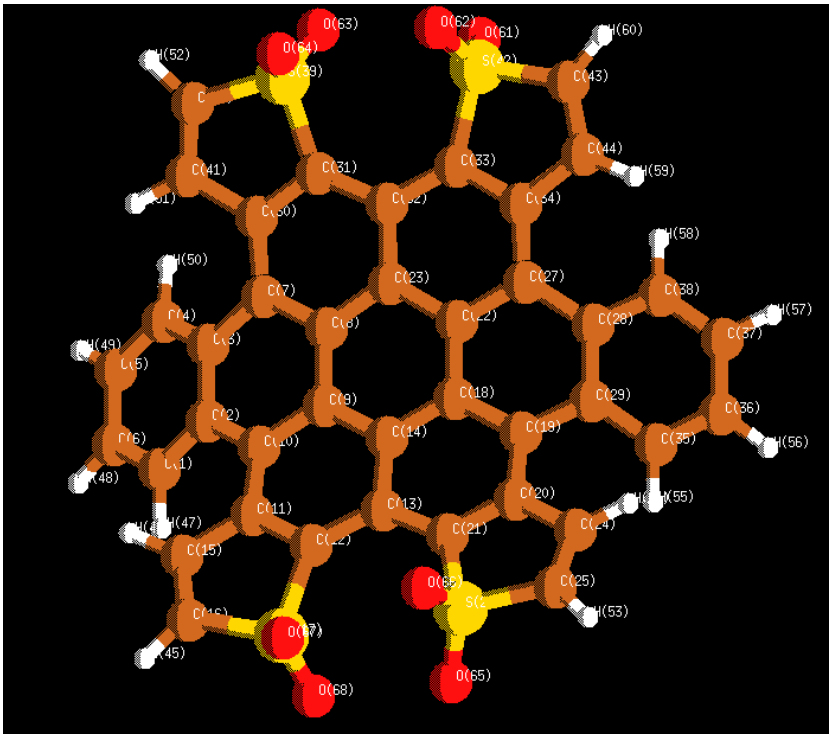
LUMO energy (Hartree): -0.11907 (3.24 eV)

6-311G**

final total energy (Hartree): -3886.03433

HOMO energy (Hartree): -0.22989 (6.26 eV)

LUMO energy (Hartree): -0.13023 (3.54 eV)



final geometry:

angstroms

atom	x	y	z
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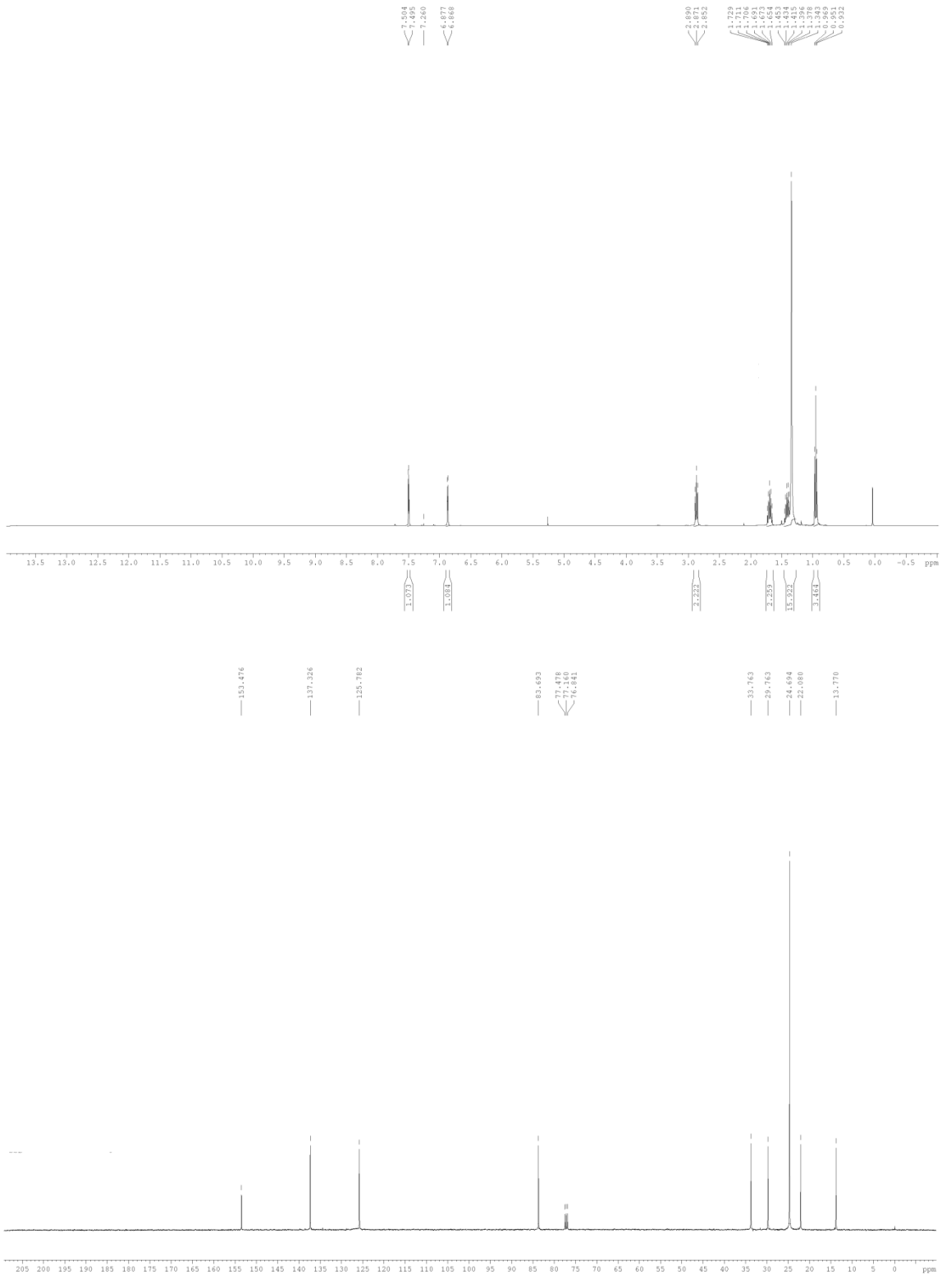
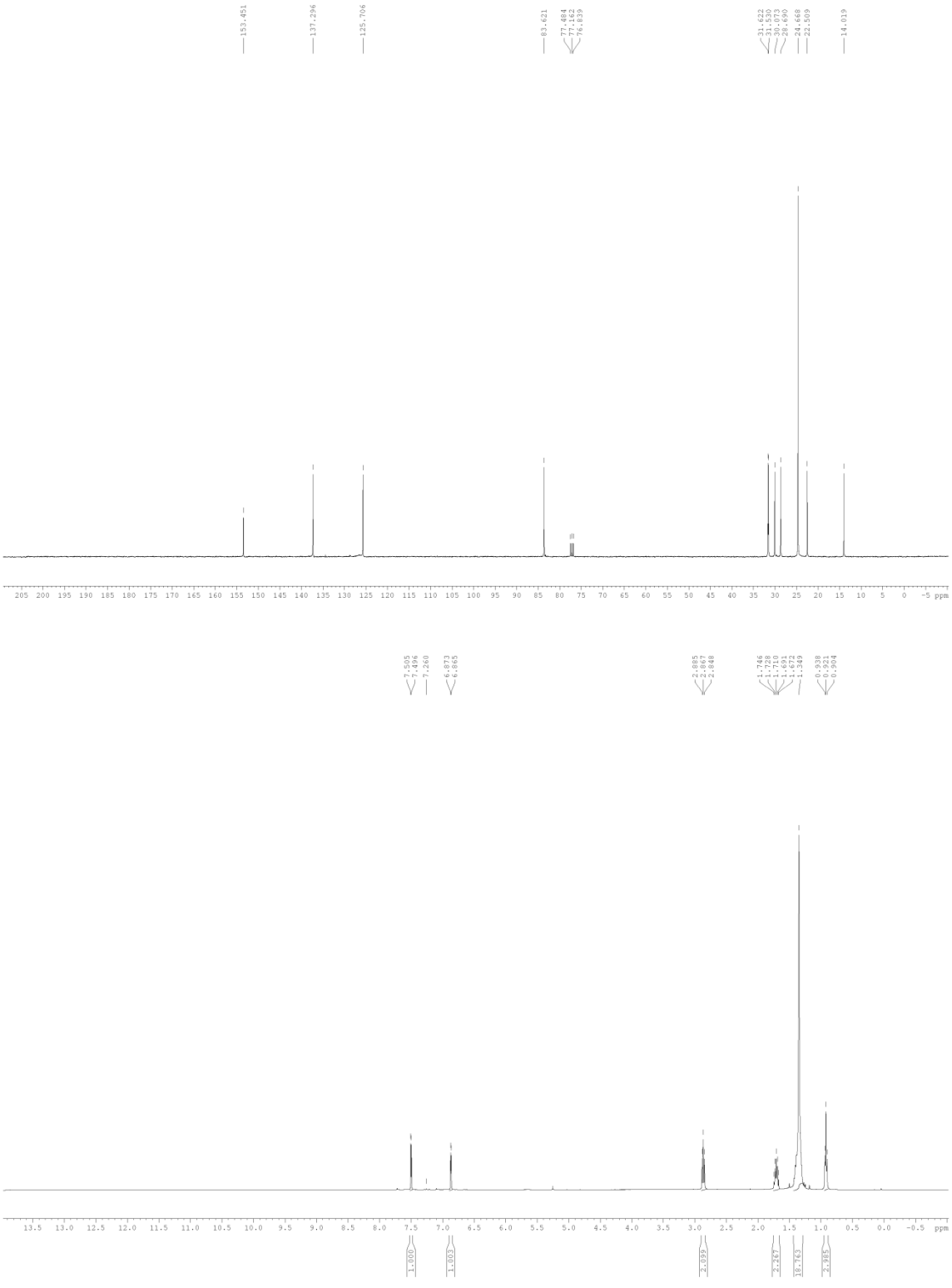
C2	0.0000000000	0.0000000000	1.4145487658
C3	1.2499215831	0.0000000000	2.0965947715
C4	2.4370112921	-0.0049746084	1.3281064595
C5	2.4067274359	0.0419957907	-0.0534697932
C6	1.1770024696	0.0458603074	-0.7240000984
C7	1.2642104365	-0.1631193549	3.5435833899
C8	0.1325863731	-0.7397206442	4.1641588274
C9	-1.1358634052	-0.7573222006	3.4657207913
C10	-1.2242279019	-0.1785322272	2.1812806106
C11	-2.5214562600	0.1208256005	1.6829356942
C12	-3.6628420518	-0.3628842387	2.3113809329
C13	-3.6146259644	-1.1130915433	3.5168780000
C14	-2.3003352090	-1.2925815311	4.0950486071
C15	-2.7973769271	1.0054609004	0.5319191493
C16	-4.0772956387	1.1031041648	0.1652295832
S17	-5.0862247499	0.0736774834	1.2381227934
C18	-2.1204429794	-2.0737170407	5.2761598475
C19	-3.1917620459	-2.8263513255	5.8049252117
C20	-4.5021314905	-2.4955300826	5.3568680278
C21	-4.6953449309	-1.6555017301	4.2686496530
C22	-0.8599348231	-2.0420777572	5.9813402455

C23	0.2191394548	-1.2430777608	5.4959869138
C24	-5.7470190652	-2.8806745014	6.0539984220
C25	-6.8777444236	-2.3902275994	5.5415086358
S26	-6.4941425564	-1.3305196364	4.1436178637
C27	-0.7283265616	-2.7530282106	7.1928276094
C28	-1.6583358756	-3.8325884455	7.4708146513
C29	-2.8975984923	-3.8727950665	6.7706294230
C30	2.3791573126	0.1518463636	4.3689353800
C31	2.4394053341	-0.2810575694	5.6889330916
C32	1.3917088047	-1.0112296882	6.3084865338
C33	1.3153773136	-1.4892289480	7.6488268758
C34	0.3091028622	-2.3413219419	8.0790316756
C35	-3.7367128065	-4.9983045121	6.9469716131
C36	-3.3960416908	-6.0265988124	7.8068964676
C37	-2.1743542117	-5.9857304825	8.4941348392
C38	-1.3161875902	-4.9173460844	8.3107204150
S39	4.1004968726	0.1563064745	6.3278658349
C40	4.5148447646	1.0999434950	4.8547036622
C41	3.5242413734	0.9940963648	3.9652282138
S42	2.2770751796	-0.9884133118	9.1229420247
C43	1.2862930632	-2.0046068575	10.2263099486
C44	0.3273661509	-2.6198148176	9.5299199667
C45	-4.7563895959	1.9081096256	-0.8861892369
H46	-2.0111897130	1.5864432231	0.0685388289
H47	-0.9339971113	-0.1137322890	-0.5340349217

H48	1.1442688360	0.0296394919	-1.8089615561
H49	3.3362699584	0.0219467588	-0.6138656109
H50	3.3921815901	-0.1235406374	1.8207209314
H51	3.5199861681	1.5412962575	3.0323091177
C52	5.7858157745	1.8745290673	4.8427235460
C53	-8.2990827653	-2.5086500812	5.9666740491
H54	-5.7297753508	-3.4691274138	6.9605132614
H55	-4.6278291485	-5.0995386254	6.3420948307
H56	-4.0517902355	-6.8857298963	7.9069344524
H57	-1.8777820060	-6.8125190441	9.1319958616
H58	-0.3351250357	-4.9478056462	8.7670106542
H59	-0.4360698853	-3.2257167315	9.9985847959
C60	1.6009742060	-1.9780820816	11.6810535697
O61	3.6516661936	-1.4974723329	9.0929141868
O62	1.9915831276	0.4146891607	9.4492511675
O63	4.9338878932	-1.0505165092	6.3979391580
O64	4.0434042026	1.1015181459	7.4474186023
O65	-7.0659236342	-1.8948932370	2.9169248988
O66	-6.7970570757	0.0437463972	4.5622799076
O67	-6.0503767518	0.9470370237	1.9140684799
O68	-5.5290119336	-1.1110709163	0.4928105185
H69	-8.3858476424	-3.1365683596	6.8568600022
H70	-8.7142262381	-1.5185171017	6.1851478211
H71	-8.9025618524	-2.9446664291	5.1625007597
H72	-4.0336489011	2.5236658552	-1.4267722060

H73	-5.2680036505	1.2530077196	-1.6006069256
H74	-5.5162517907	2.5566999725	-0.4369706111
H75	1.5398108172	-0.9534880120	12.0645966287
H76	0.9038020150	-2.6080812101	12.2391780056
H77	2.6225422726	-2.3327421860	11.8576418825
H78	5.8209043904	2.5575460471	5.6985242370
H79	6.6470329187	1.2018643097	4.9266053459
H80	5.8774856175	2.4523913974	3.9196041702

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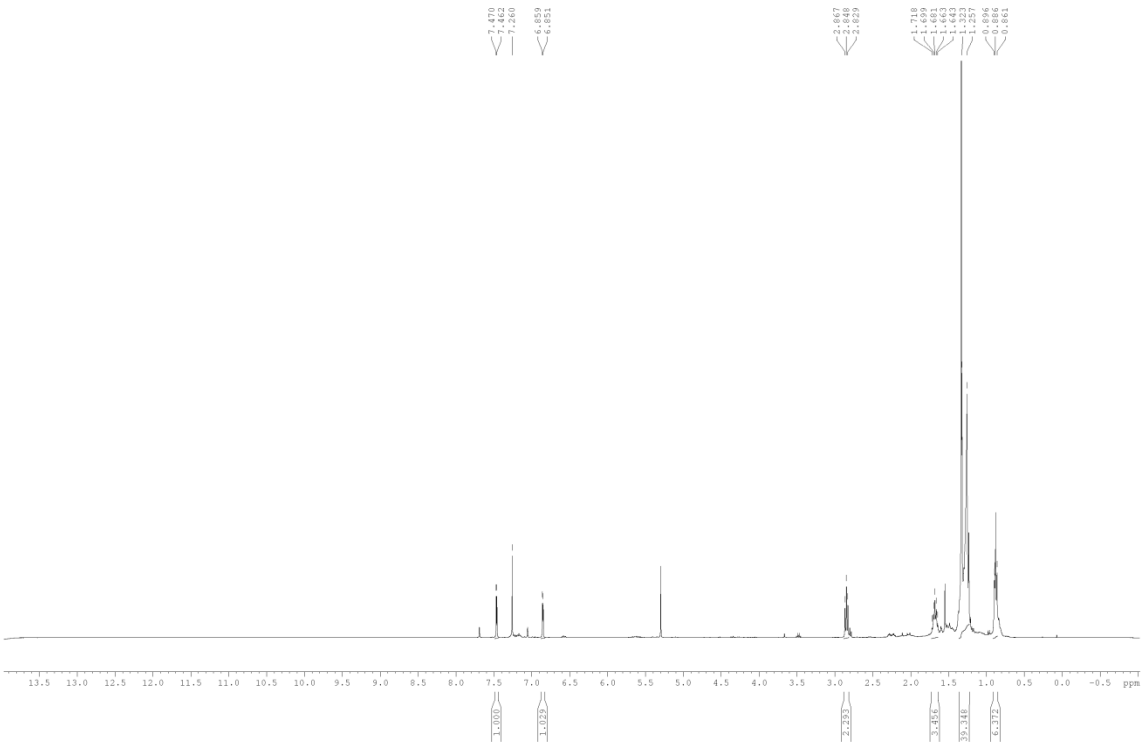
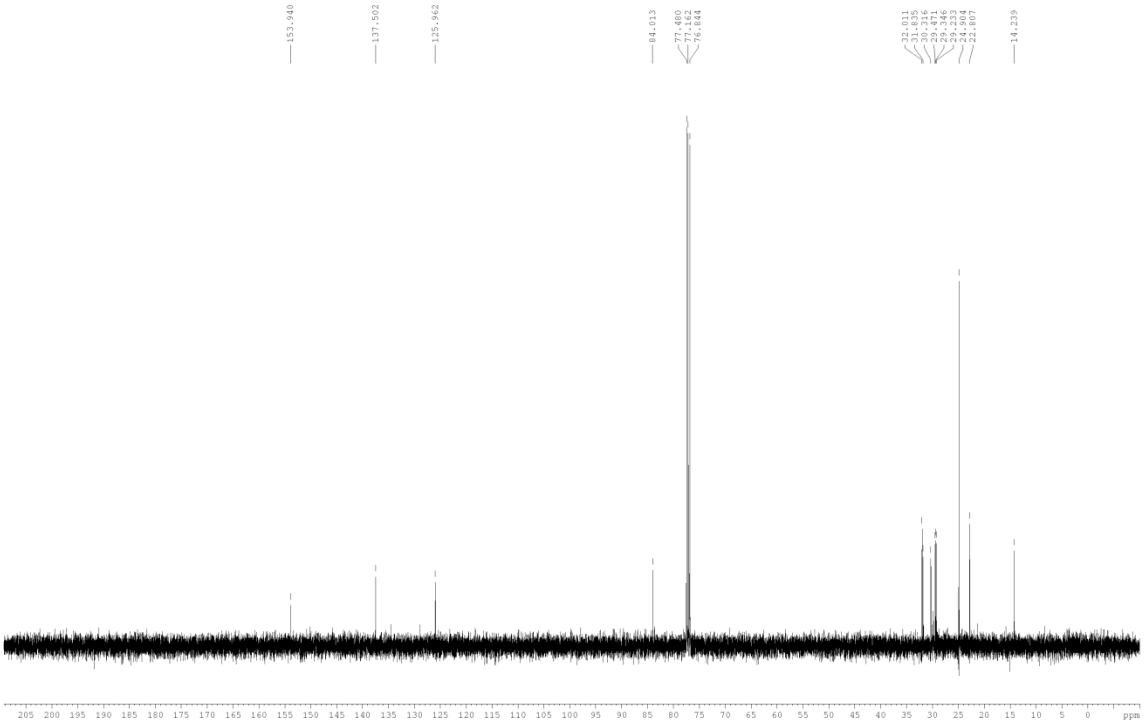
125.706
83.621
77.484
77.162
76.839
31.622
31.530
31.073
30.690
24.668
22.509
14.019
205 200 195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 ppm
7.595
7.486
7.260
6.873
6.865
2.885
2.867
2.848
1.746
1.728
1.710
1.691
1.672
1.349
0.938
0.921
0.904
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
1.000
1.003
2.099
2.247
16.763
2.985


7.470
7.462
7.260
6.859
6.851
2.667
2.648
2.629
1.718
1.699
1.681
1.663
1.643
1.625
1.257
0.896
0.886
0.861
ppm
1.000
1.029
2.293
3.456
39.348
6.372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76.844
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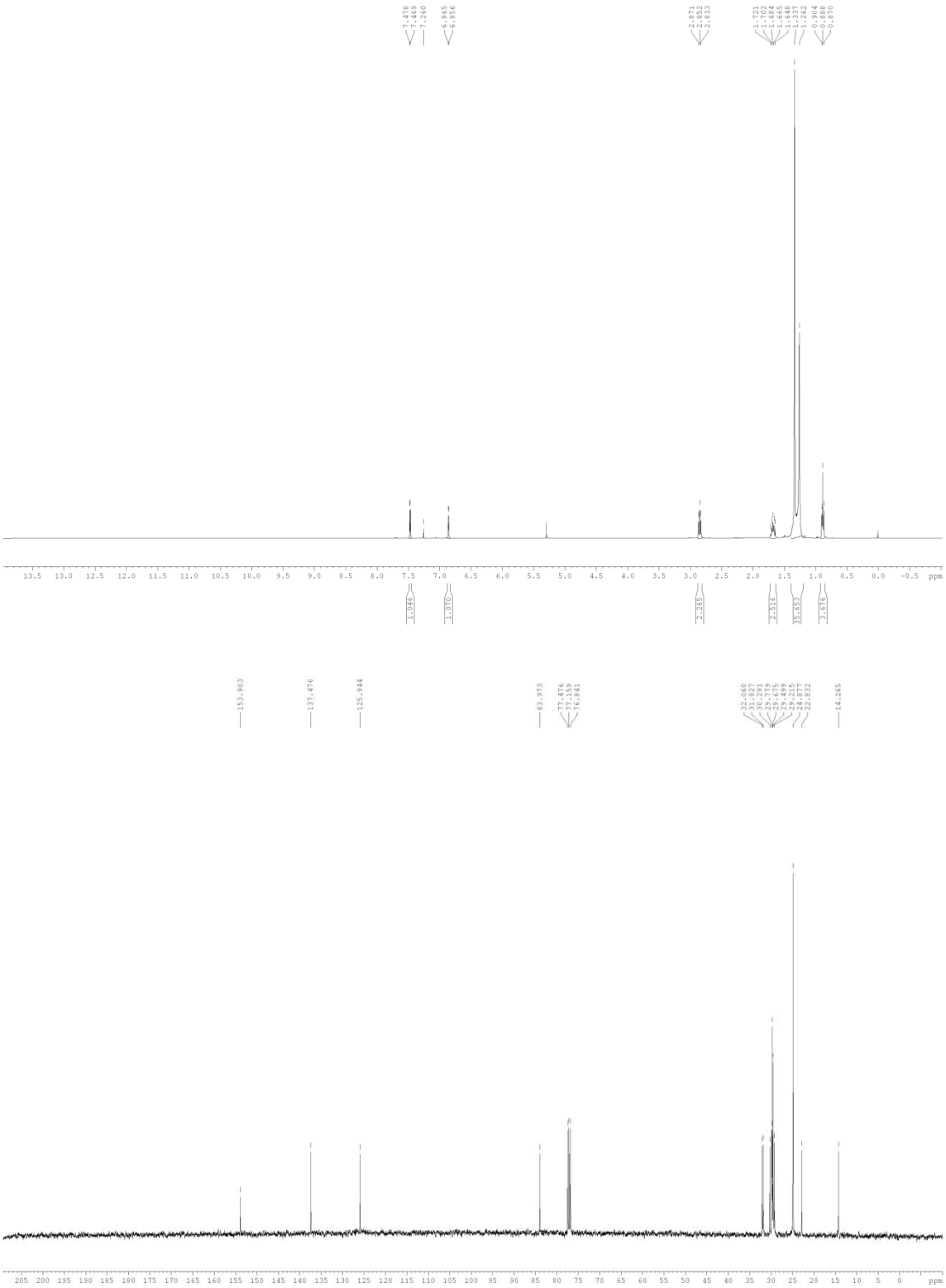
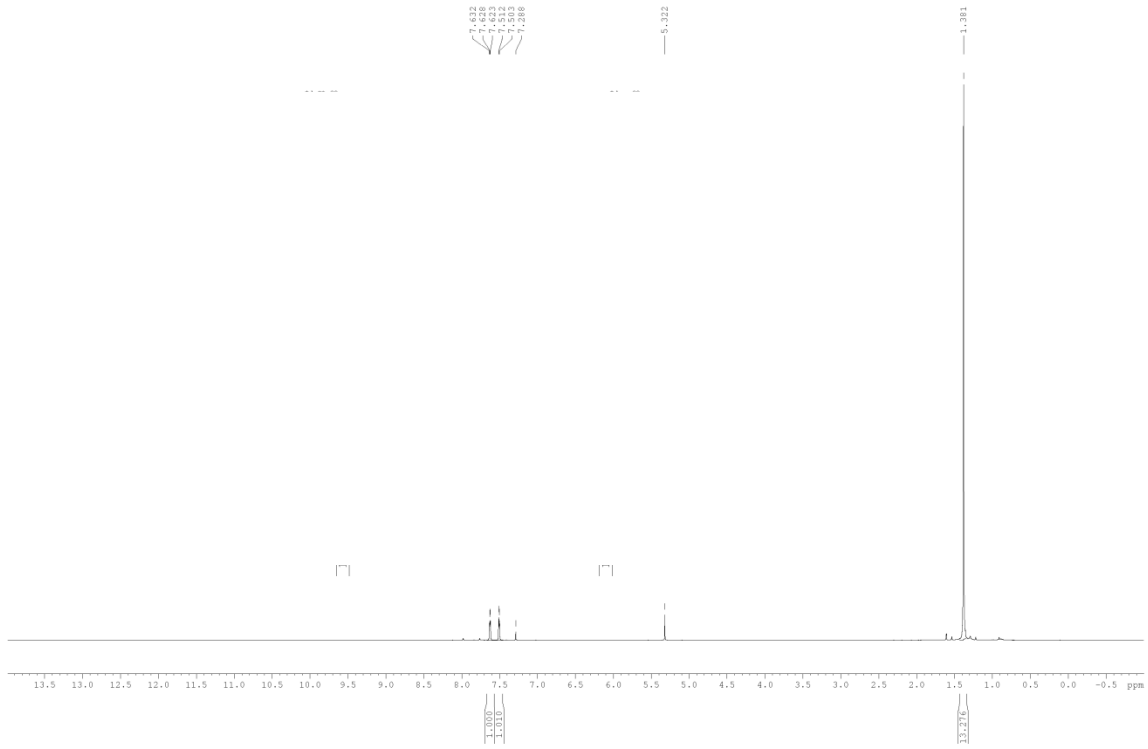
29.233
24.804
22.807
14.239
ppm




7.632
7.628
7.623
7.622
7.503
7.288
5.322
1.381
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
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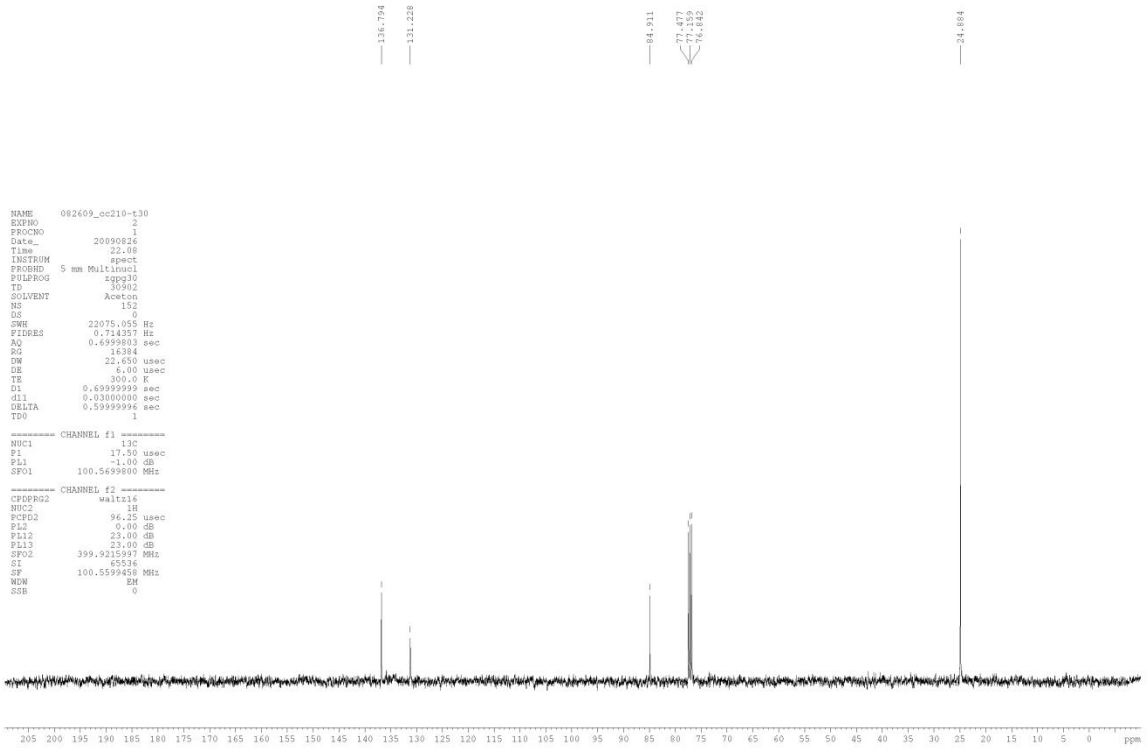
1.010
13.276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76.842
24.864
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PROCNO 1
Date_ 20090826
Time 22.08
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 30902
SOLVENT Aceton
NS 152
DS 0
SWH 22075.055 Hz
FIDRES 0.714357 Hz
AQ 0.6999803 sec
RG 16384
DW 22.650 usec
DE 6.00 usec
TE 300.0 K
D1 0.69999999 sec
d11 0.03000000 sec
DELTA 0.59999996 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 17.50 usec
PL1 -1.00 dB
SFO1 100.5699800 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 96.25 usec
PL2 0.00 dB
PL12 23.00 dB
PL13 23.00 dB
SFO2 399.9215997 MHz
SI 65536
SF 100.5599458 MHz
WDW EM
SSB 0
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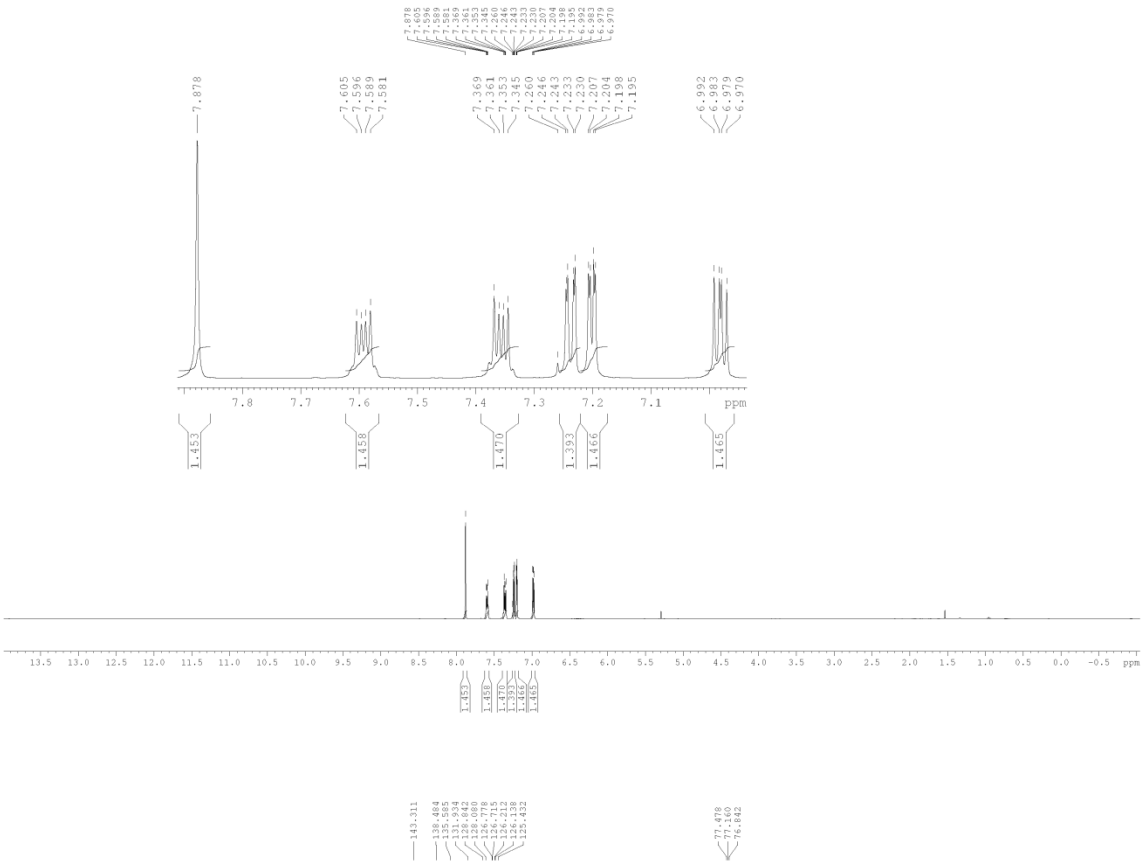
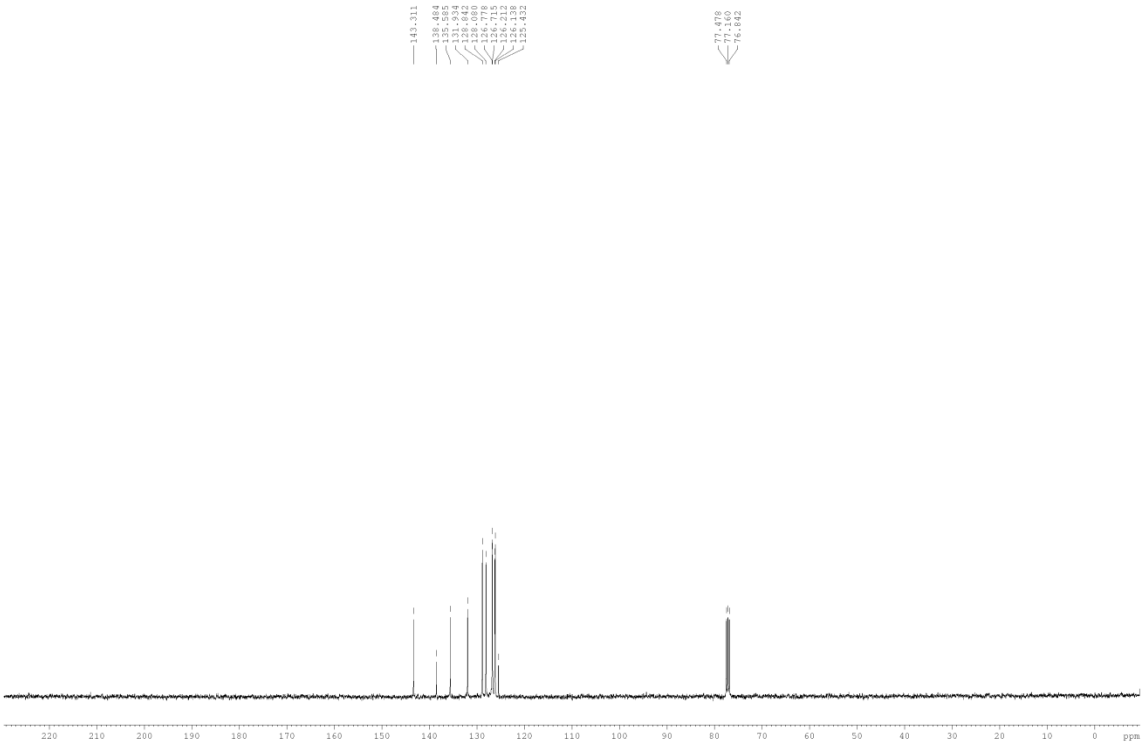
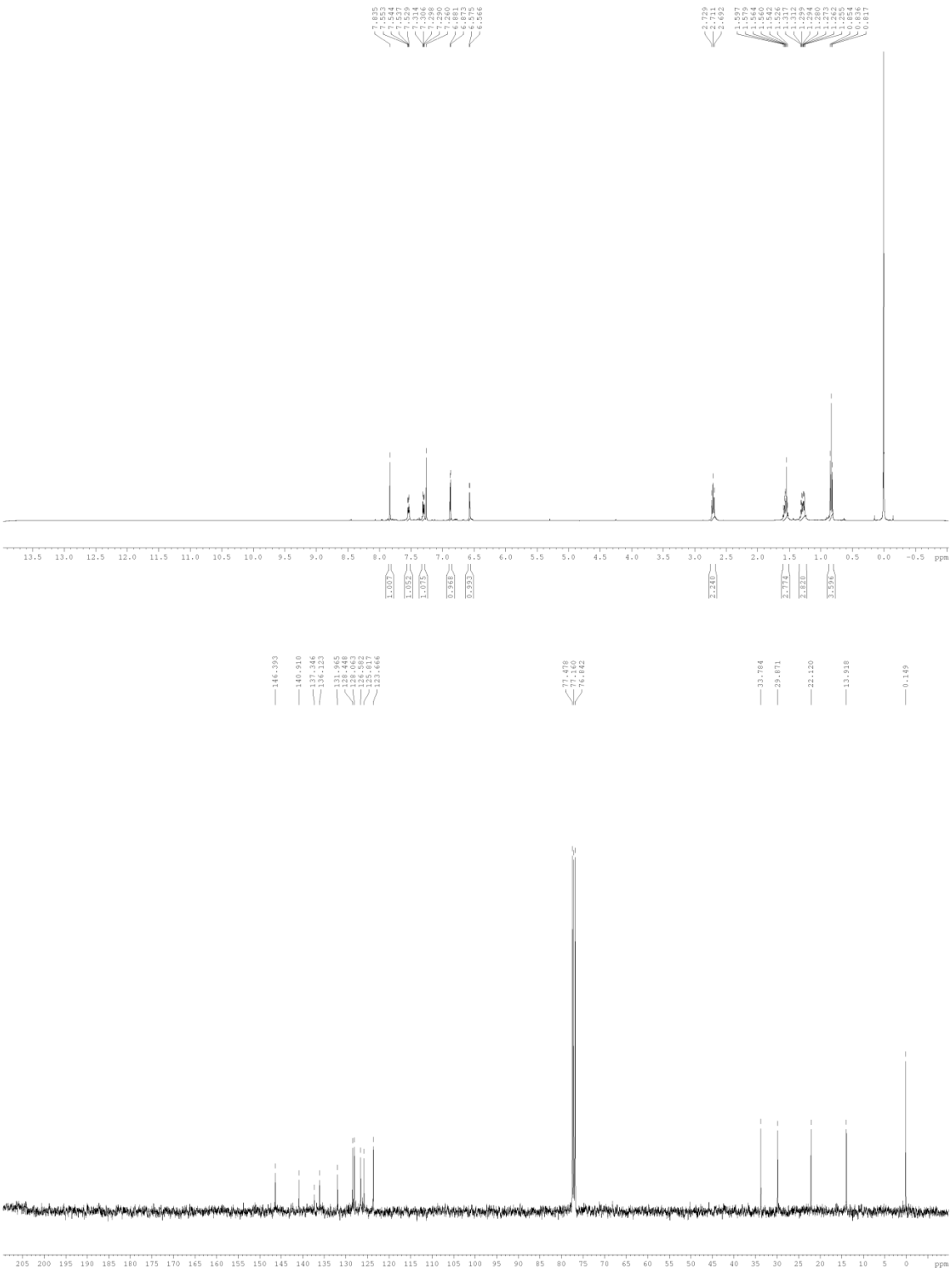
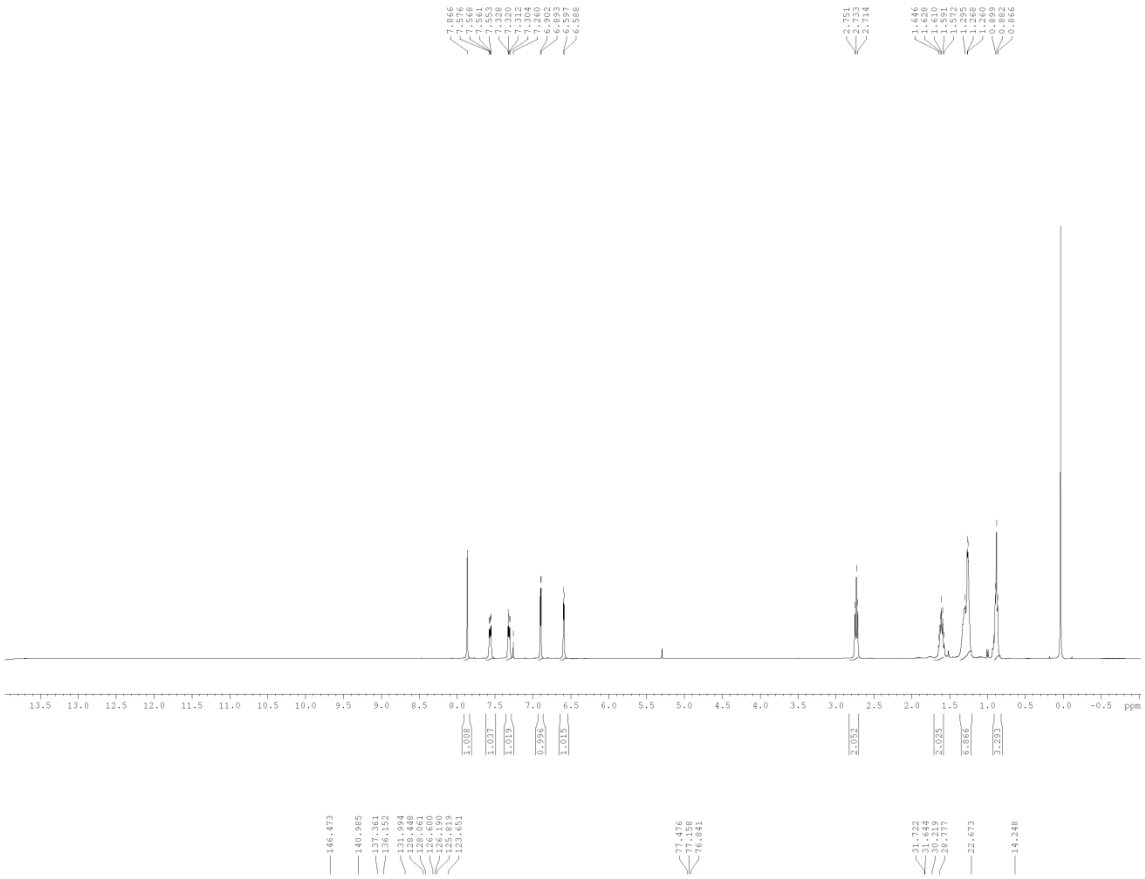
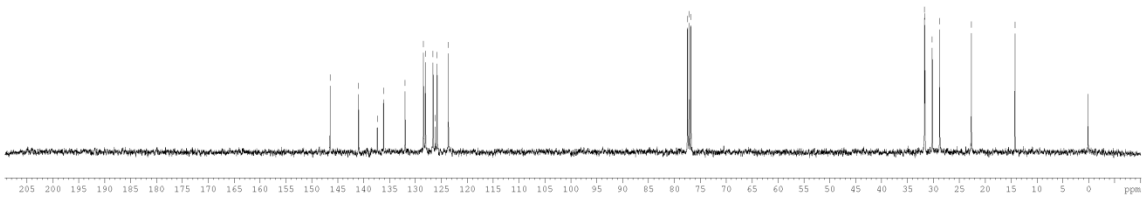
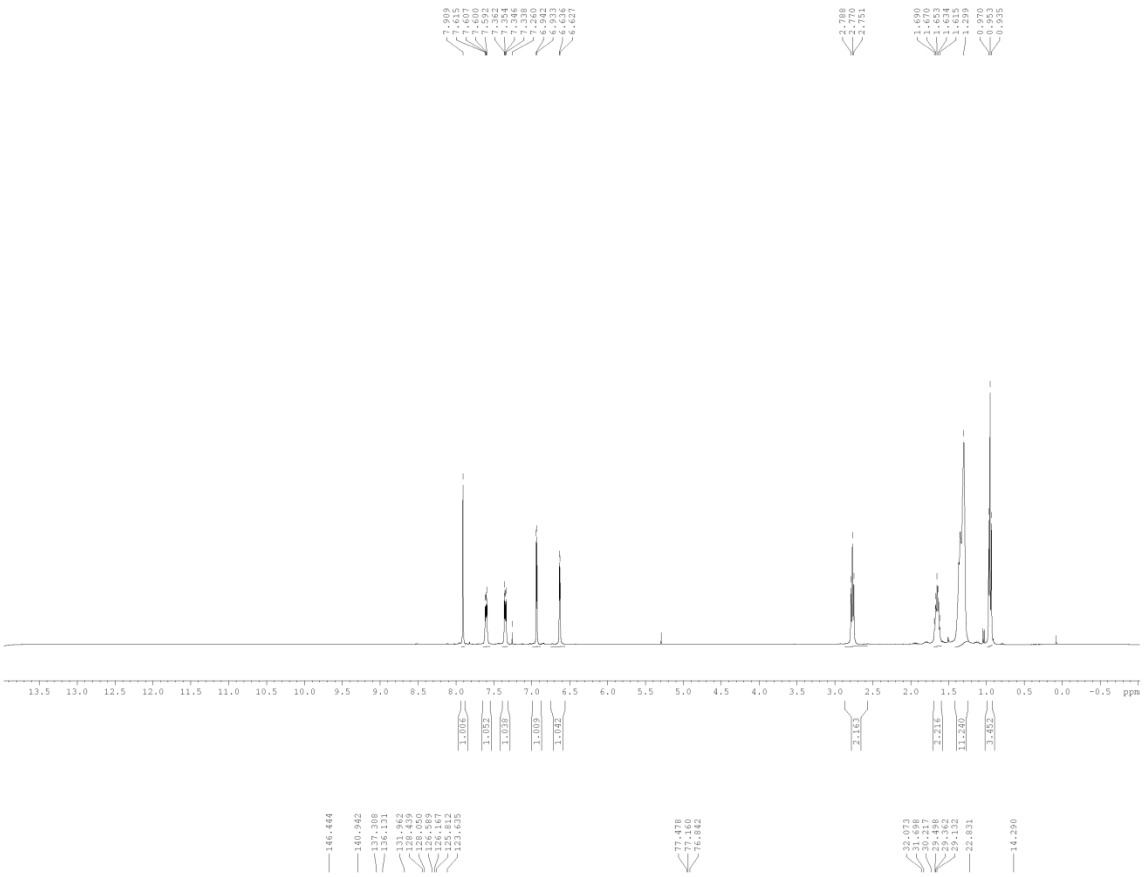


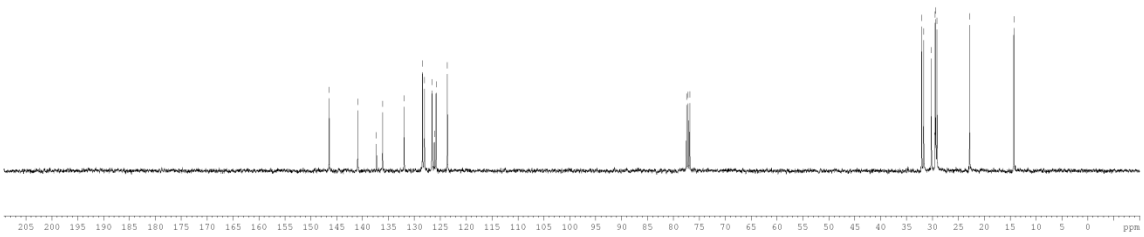


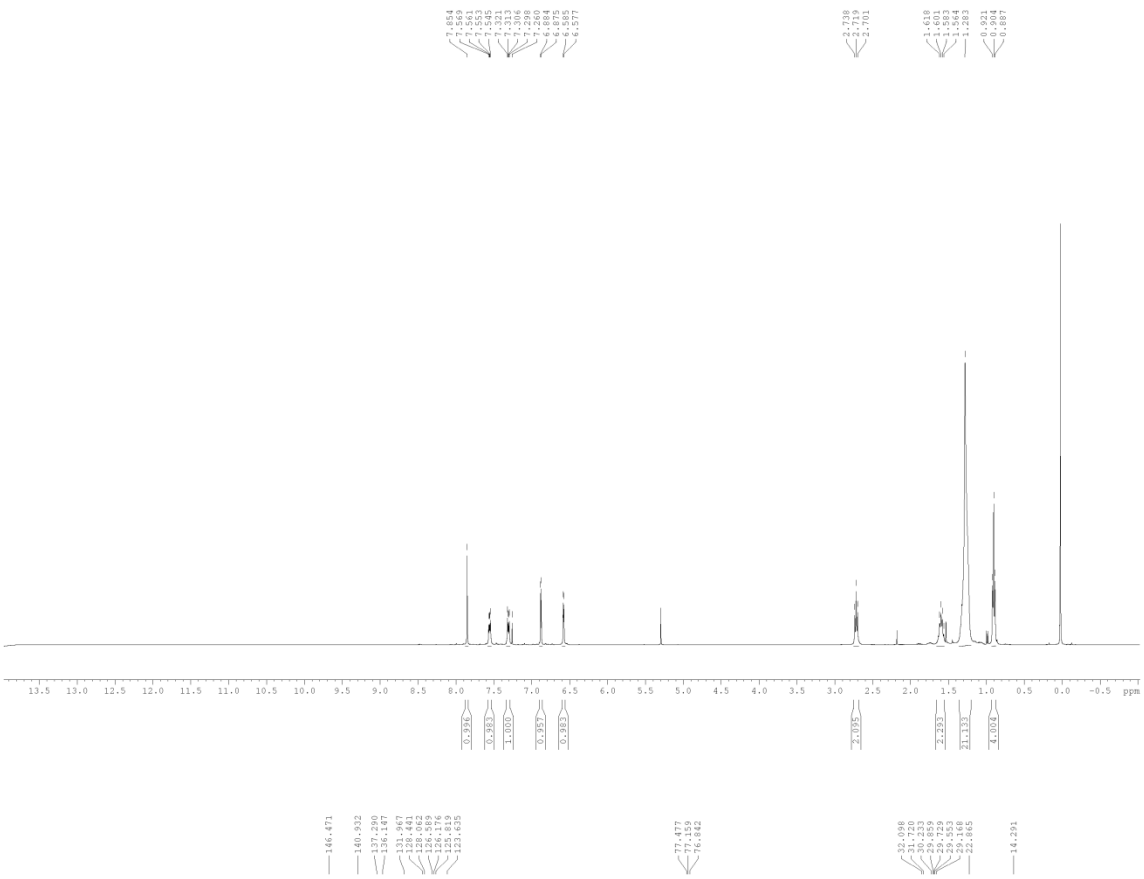


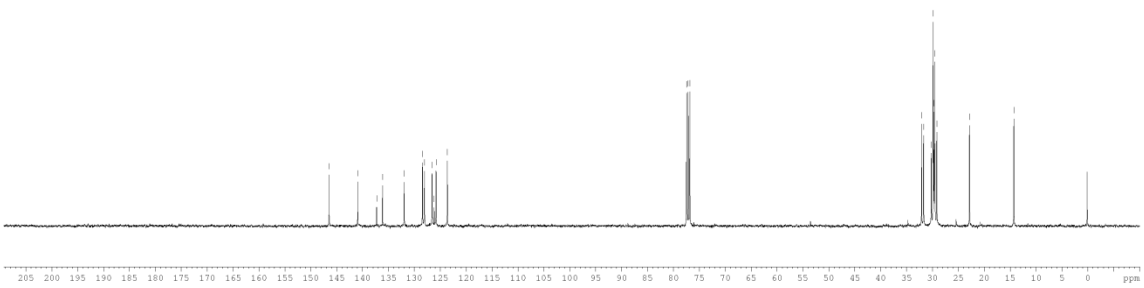


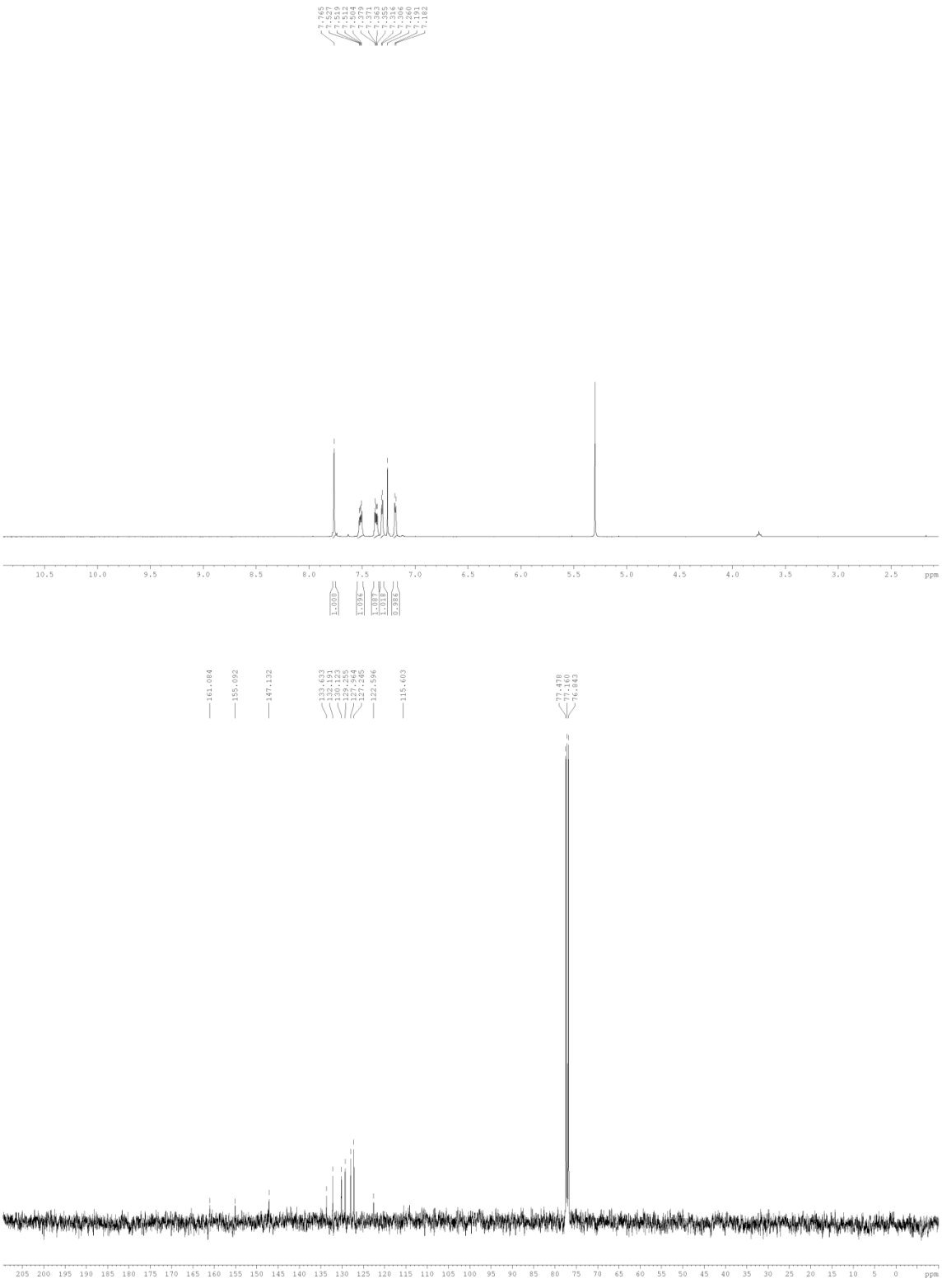


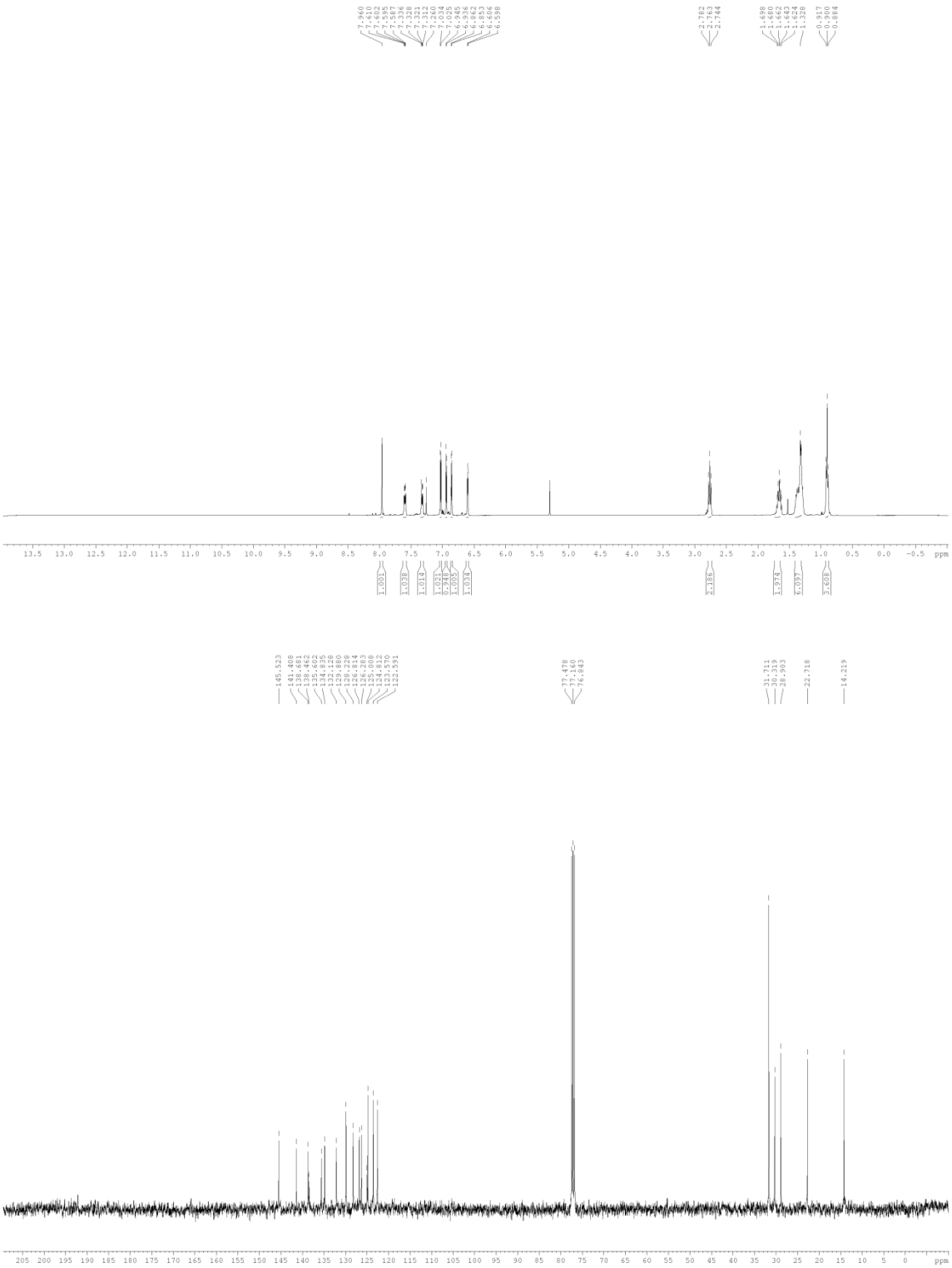


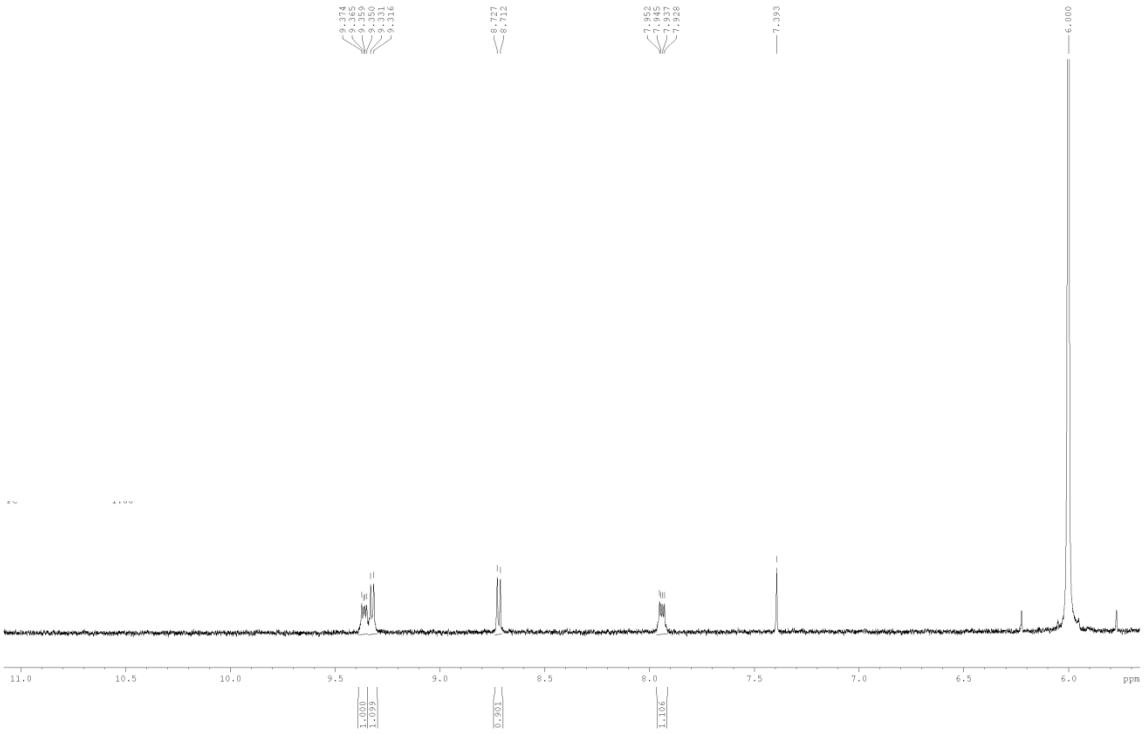


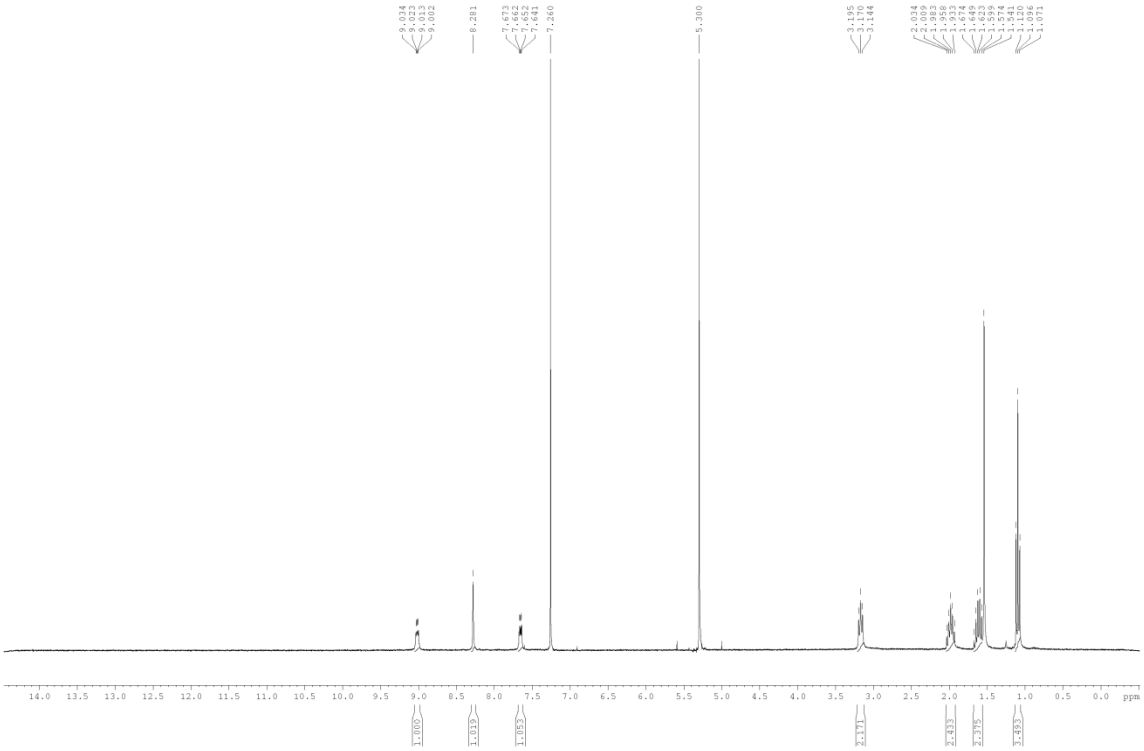


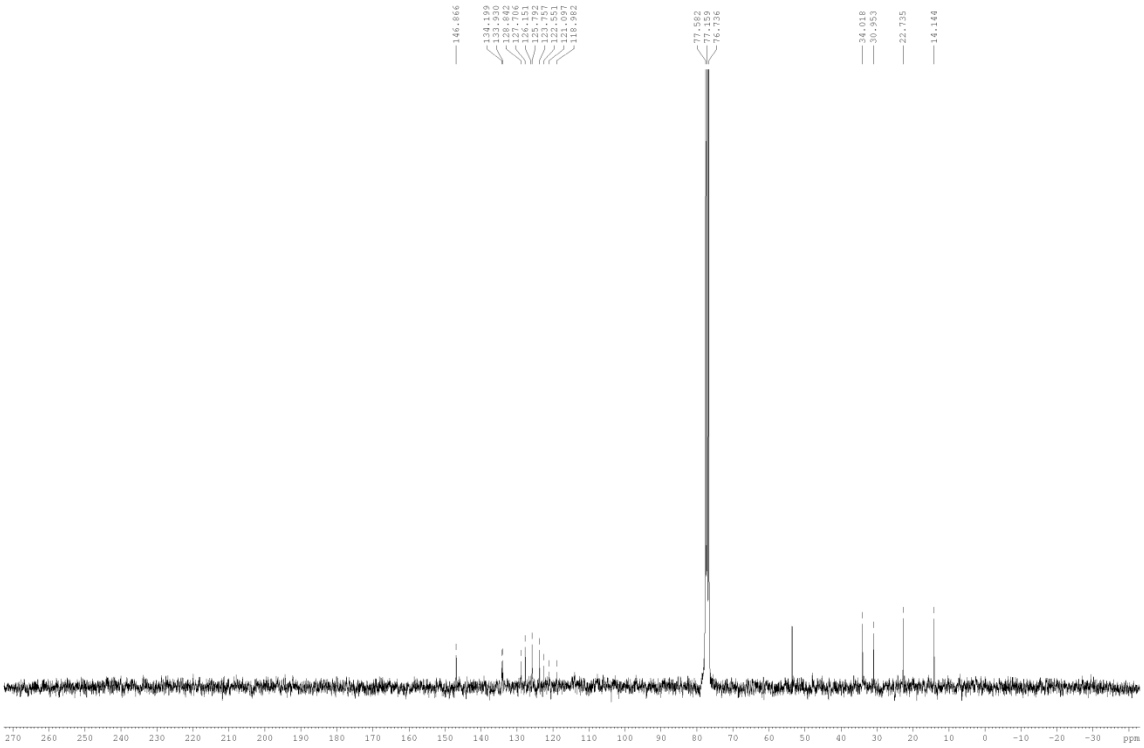


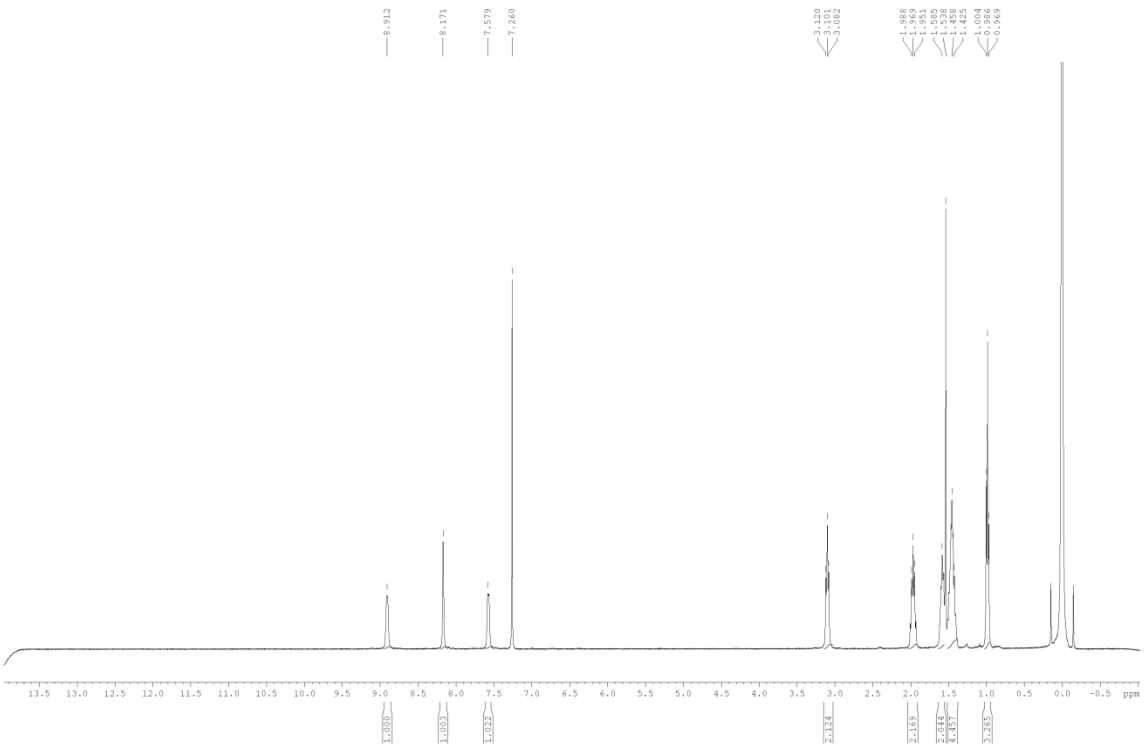


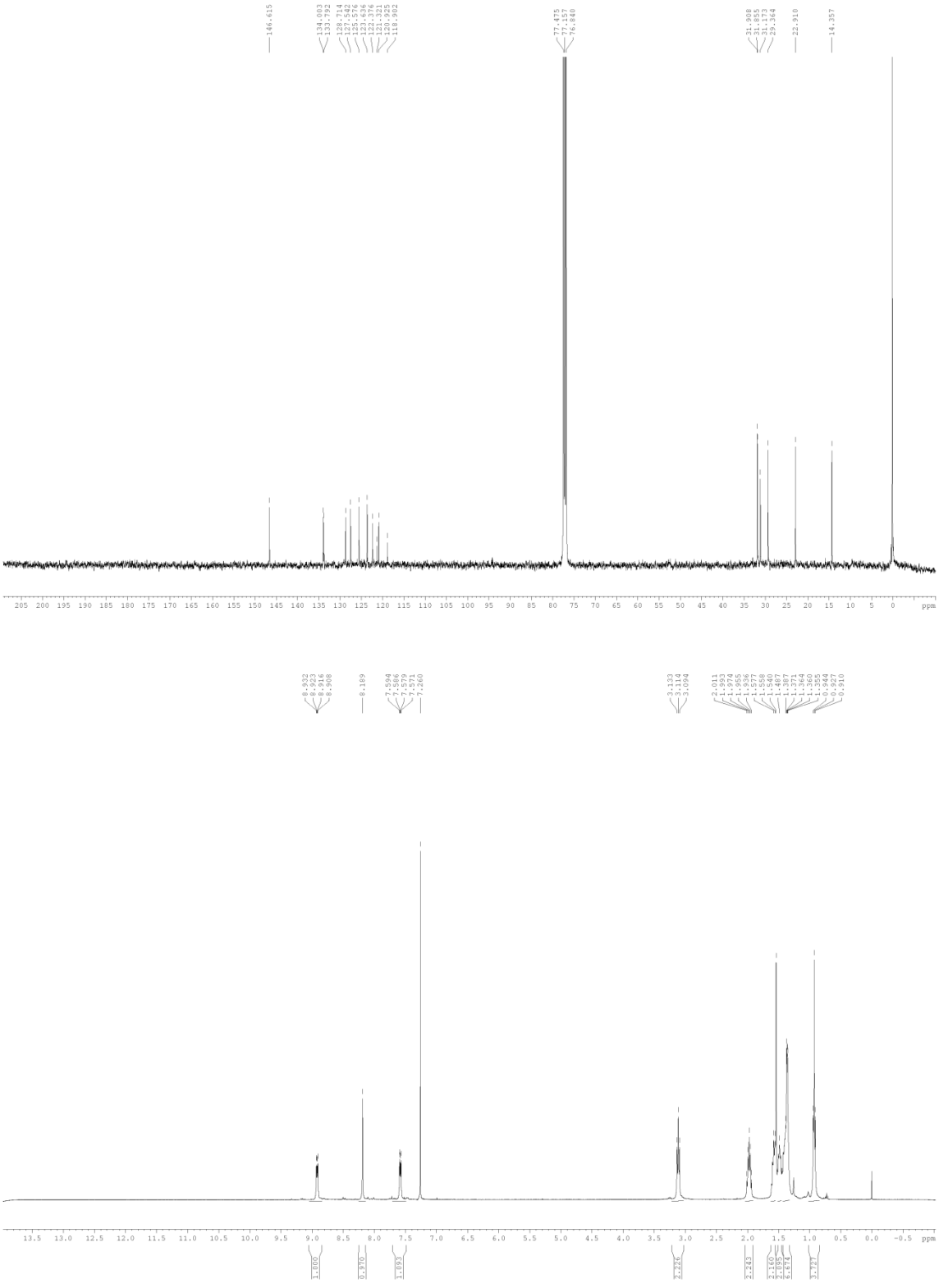


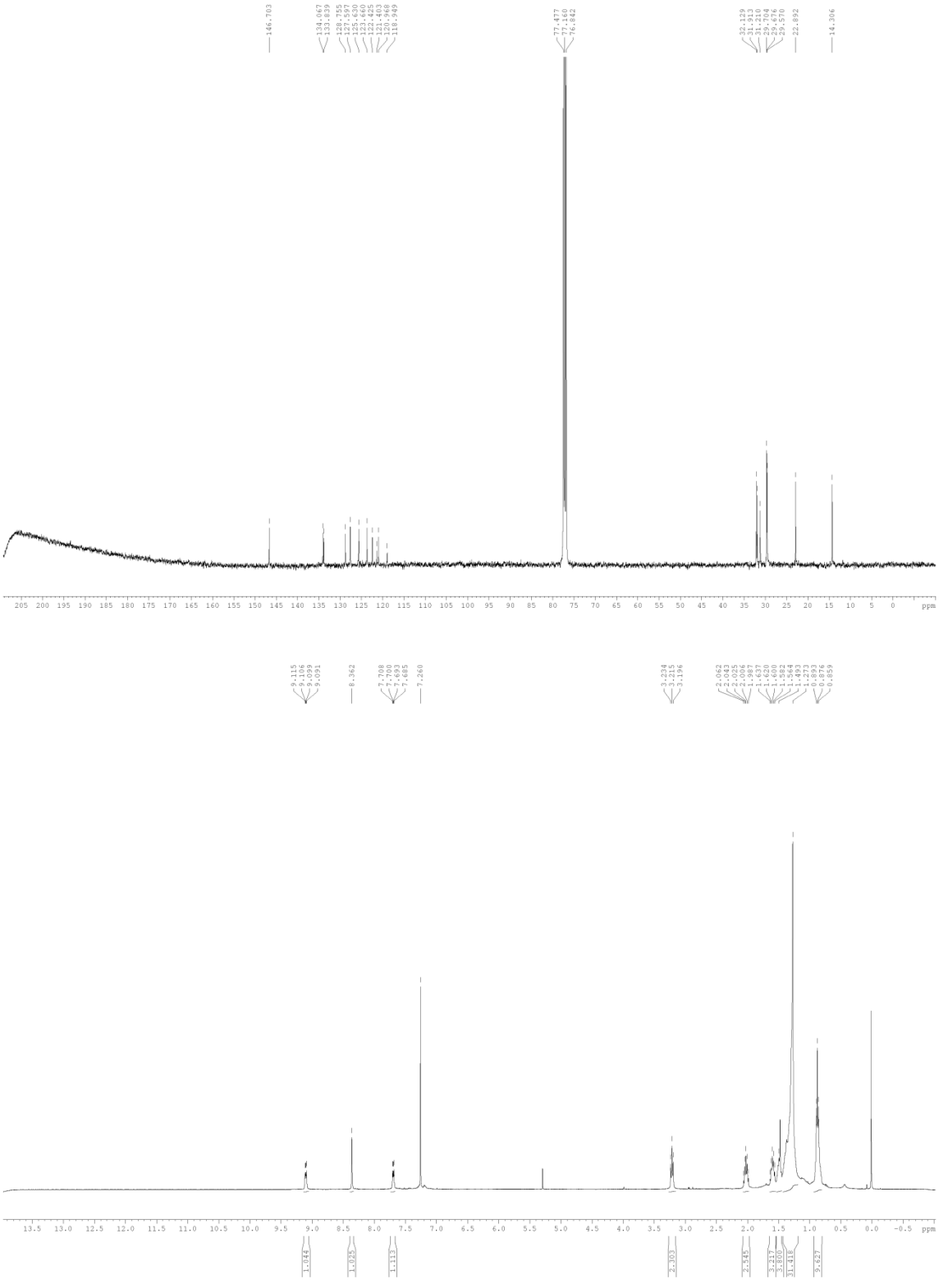


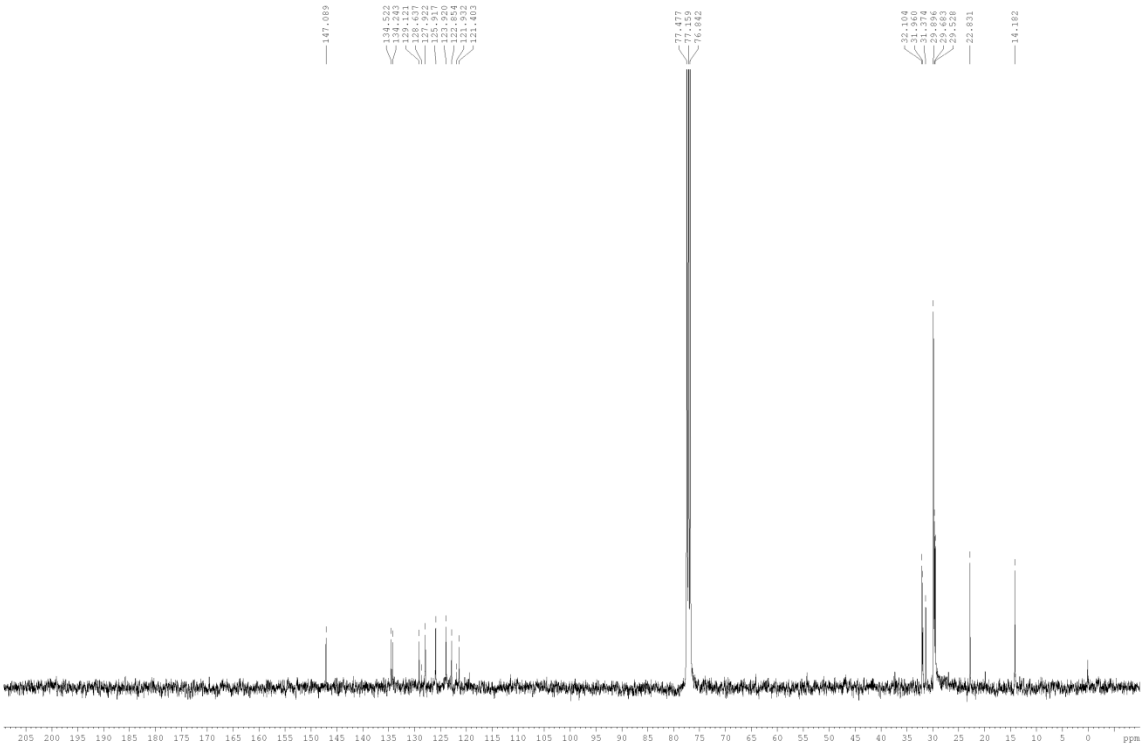


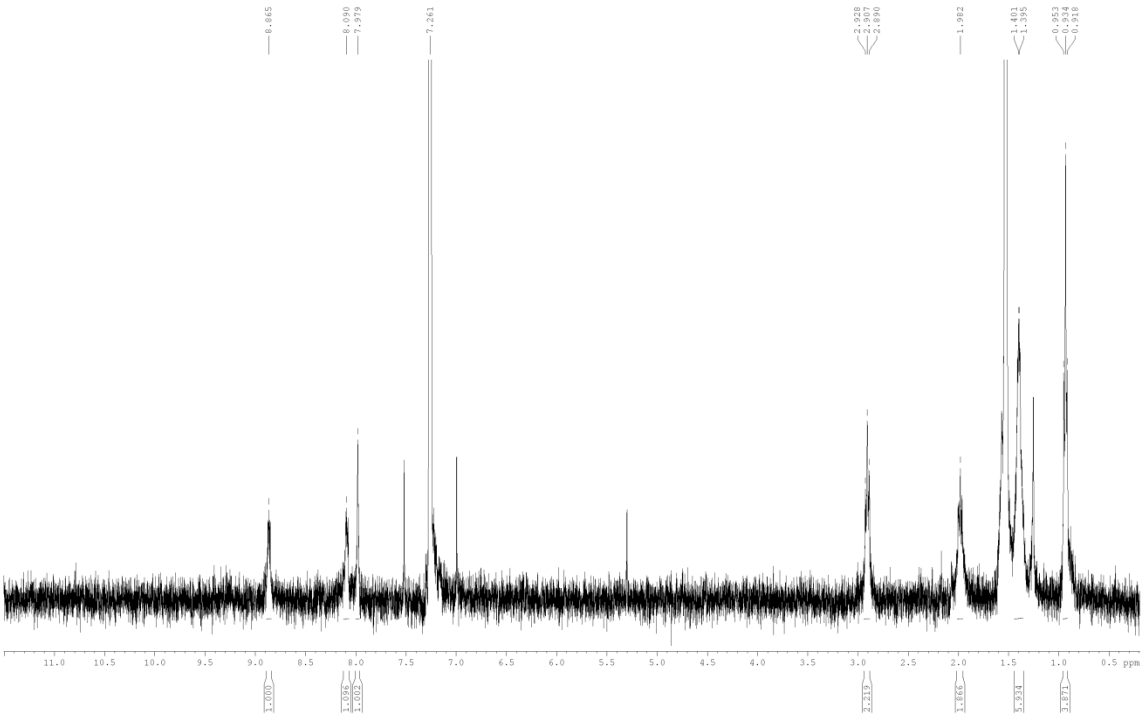

146.866
134.199
133.430
128.842
127.766
127.111
125.792
123.757
123.351
121.097
118.982
77.582
77.369
76.736
24.018
30.953
22.735
14.144
270 260 250 240 230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 ppm

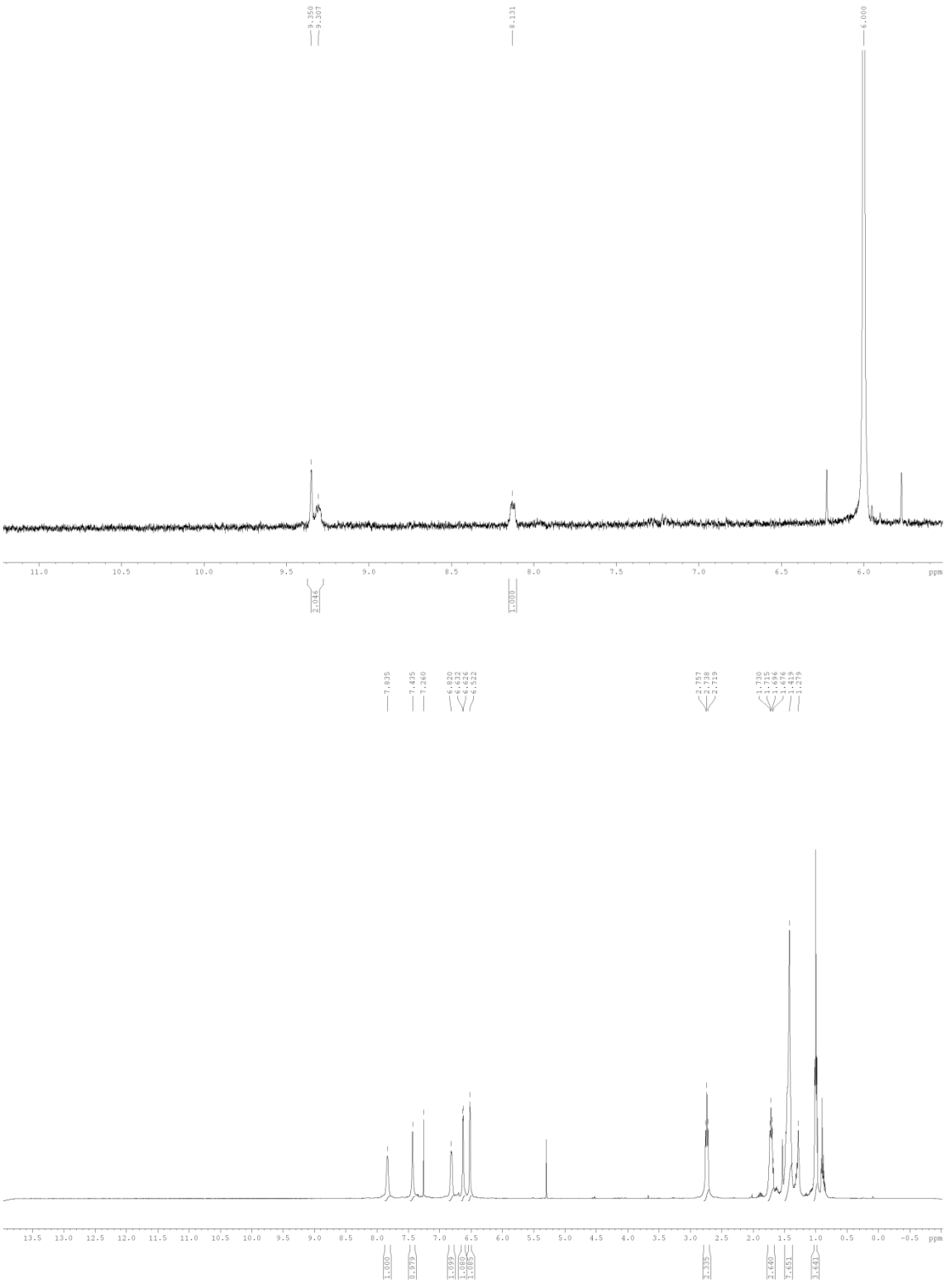

8.912
8.171
7.579
7.260
3.120
3.101
3.082
1.988
1.969
1.951
1.555
1.538
1.458
1.425
1.004
0.986
0.969
13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 ppm
1.0000
1.0007
1.0022
2.1240
2.1690
2.0446
4.4657
3.2680

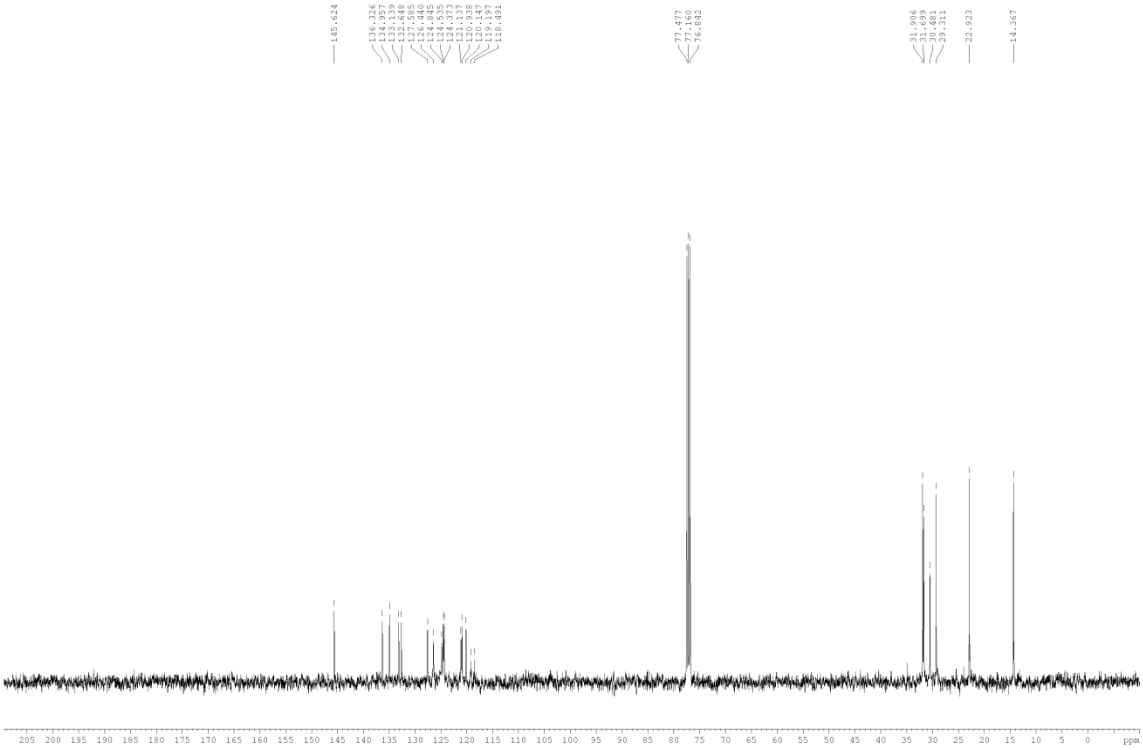





147.089
134.532
134.243
129.121
128.677
127.922
125.917
123.820
123.584
121.932
121.403
77.477
77.159
76.842
32.104
31.960
31.374
29.966
29.685
29.520
22.831
14.182
ppm


8.865
8.090
7.959
7.261
2.928
2.907
2.890
1.982
1.401
1.395
0.953
0.934
0.918
ppm
1.000
1.106
1.100
2.213
1.866
5.934
3.871


9.350
9.307
8.131
6.000
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
ppm
2.046
1.000
7.835
7.435
7.260
6.830
6.632
6.626
6.522
2.757
2.738
2.719
1.730
1.715
1.696
1.676
1.419
1.279
13.5
13.0
12.5
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
1.000
0.970
1.099
1.080
1.080
1.085
2.335
2.640
7.451
3.641


145.624
136.326
134.957
133.139
132.648
132.085
126.440
124.845
124.435
124.373
121.137
120.038
120.047
119.197
118.491
77.477
77.160
76.842
31.906
31.699
30.481
29.311
22.923
14.367
205 200 195 190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 ppm