Supplementary Information for

Ladder-Type Polymers and Ladder-Type Polyelectrolytes with On-Chain Dibenz[*a*,*h*]antracene Chromophores

Florian Trilling, Michelle-Kathrin Ausländer and Ullrich Scherf

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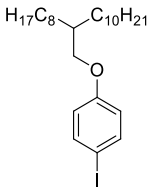
1. Materials and instruments:

All chemicals and solvents were purchased from suppliers (Sigma Aldrich, VWR, Fisher Scientific etc.) and used without further purification, if not mentioned separately.

^{1}H- and ^{13}C-NMR spectra were recorded on Bruker Avance 400 (basis frequencies: ^{1}H: 400 MHz; ^{13}C: 101 MHz) or Bruker Avance III 600 (basis frequencies: ^{1}H: 600 MHz; ^{13}C: 151 MHz) with tetramethylsilane (TMS) as an internal standard. Measurements were performed at 300 °K for deuterated chloroform and at 353 °K for deuterated tetrachloroethane. In the ^{13}C-NMR spectra only those signals were listed, differing from the background significantly. The coupling constants (*J*) are given in Hz and the multiplicity of signals is described as s (singlet), d (doublet), t (triplet), and m (multiplet). The measurement of the *m/z* ratios were carried out with three different setups. GC-MS-spectra were recorded on a Shimadzu GC 17A QP 5050 with Optima-1 Accent-0,25-column. High resolution APCI (atmospheric pressure chemical ionisation) mass spectra were measured on a Bruker Daltronic micrOTOF. High resolution FD (field desorption) mass spectra were recorded on a Jeol AccuTOF GCX. HOMO energy levels were determined by atmospheric pressure photoelectron spectroscopy using a RIKKEN KEIKI AC2 machine. The optical band gap was estimated from the onset of the absorption in solid state and correct by adding 0.3 eV for the exciton binding energy. LUMO levels were determined by subtracting HOMO and band gap energy. PL emission spectra were recorded on a HORIBA Scientific FluroMax-4 equipped with a Quanta-Phi integration sphere (used for photoluminescence quantum yield (PLQY) measurements in solution) and UV/VIS absorption spectra were determined on a JASCO V-670 spectrometer. The excitation wavelength is given as λ_{exc}. in nanometer. Wavelength in brackets correspond to shoulders of absorption/emission bands. Films of the polymers were spin coated from an 8 mg/ml solution in chloroform on a SÜSS MicroTec spin coater. Molecular weight distributions were determined by size exclusion chromatography (SEC) with a PSS SDV pre-column and two PSS SDV linear M columns in series with THF as eluent.

2. Synthesis of the Diethynyllinkers

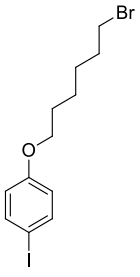
4-((2-Octyldodecyl)oxy)iodobenzene[1] (1a)



1a

In a flame dried two-neck round-bottom flask triphenylphosphine (14.31 g, 54.54 mmol), 4-iodophenol (10.00 g, 45.45 mmol) and 2-octyldodecanol (19.43 mL, 54.54 mmol) were dissolved in THF (140 mL) under an argon atmosphere. The solution was cooled to 0 °C, (E)-diisopropyl diazene-1,2-dicarboxylate (DIAD) (10.71 ml, 54.54 mmol) was added slowly and the solution was stirred in the cold for another 15 minutes. Afterwards the solution was warmed up to RT and stirred for 16 h. The reaction solution was diluted with water and extracted with hexane several times. The combined organic layers were washed with saturated, aqueous NaCl-solution, dried over $MgSO_4$ and the solvents removed under reduced pressure. The crude product was dissolved in hexane and passed through a silica pad (stationary phase: silica, eluent: hexane) to afford the product **1a** (20.20 g, 40.35 mmol, 89 %) as a colorless oil. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ [ppm] = 7.56 (d, *J* = 9.0 Hz, 2H), 6.70 (d, *J* = 9.0 Hz, 2H), 3.81 (d, *J* = 5.7 Hz, 2H), 1.83 – 1.71 (m, 1H), 1.50 – 1.23 (m, 32H), 0.91 (t, *J* = 6.8 Hz, 6H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 159.3, 138.1, 117.0, 82.3, 71.1, 37.9, 31.9, 31.9, 31.3, 29.9, 29.7, 29.6, 29.6, 29.6, 29.3, 29.3, 26.8, 22.7, 22.7, 14.1; **APCI**: calcd for *m/z* [M+H$^+$] 500.2510, found *m/z* [M+H$^+$] 500.2518

4-((6-Bromohexyl)oxy)iodobenzene[2] (1b)



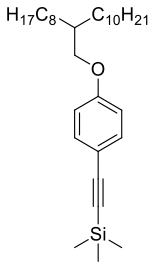
1b

4-Iodophenol (11.00 g, 50.00 mmol) was dissolved in Acetone (250 mL). Potassium carbonate (15.20 g, 110,00 mmol)) and 1,6-dibromohexyl (30.31 mL, 200,00 mmol) were added to the solution and the mixture was heated to reflux at 70 °C overnight. After cooling to RT the mixture was poured into water and extracted with MTBE three times. The combined organic layers were washed with 1 M aqueous NaOH-solution, water and dried over $MgSO_4$. The solvents were removed under reduced pressure and the crude product was purified by column chromatography (stationary phase: silica, eluent: hexane). The product **1b** (15.5 g, 40.4 mmol, 81 %) was obtained a white solid. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.57 (d, *J* = 9.0 Hz, 2H), 6.70 (d, *J* = 9.0 Hz, 2H), 3.95 (t, *J* = 6.4 Hz, 2H), 3.45 (t, *J* = 6.8 Hz, 2H), 1.95 – 1.88 (m, 2H), 1.86 – 1.78 (m, 2H), 1.58 – 1.48 (m, 4H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 158.9, 138.2, 116.9, 82.5, 67.8, 33.7, 32.6, 28.9, 27.9, 25.2; **APCI**: calcd for *m/z* [M+H$^+$] 381.9424, found *m/z* [M+H$^+$] 381.9411

General procedure for the synthesis of 1-(4-(Alkoxy)phenyl)-2-(trimethylsilyl)ethyne derivatives[3]

In a flame dried; three-neck round-bottom flask tetrabutylammonium bromide (0.03 eq), copper(I) iodide (0.05 eq), bis(triphenylphosphine)palladium dichloride (0.01 eq) and the 4-alkoxyiodobenzene (1 eq) were dissolved in a 1:1 mixture of toluene and diisopropylamine (0.5M) under an argon atmosphere. Trimethylsilylacetylene (1.05 eq) was added dropwise generating a noticeable amount of heat and the solution was stirred for one hour. Afterwards the reaction solution was diluted with hexane and washed with 2 M aqueous HCl-solution and water, dried over $MgSO_4$ and the solvents were removed *in vacuo*. Finally the crude product was passed through a silica pad (stationary phase: silica, eluent: hexane).

1-(4-(2-Octyldodecyloxy)phenyl)-2-(trimethylsilyl)ethyne (2a)

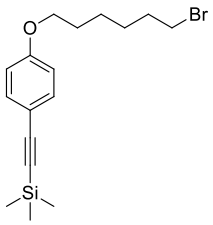


2a

According to the general procedure the reaction was carried out with **1a** (20.20 g, 40.36 mmol). The product **2a** (17.95 g, 38.10 mmol, 94 %) was obtained as an yellow oil. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ [ppm] = 7.41 (d, *J* = 8.8 Hz, 2H), 6.83 (d, *J* = 8.8 Hz, 2H), 3.84

(d, *J* = 5.7 Hz, 2H), 1.84 – 1.74 (m, 1H), 1.51 – 1.21 (m, 32H), 0.91 (t, *J* = 6.7 Hz, 6H), 0.26 (s, 9H); **^{13}C{H}-NMR** (101 MHz, $CDCl_3$) δ [ppm] = 159.6, 133.4, 114.4, 71.0, 37.9, 31.9, 31.9, 31.3, 29.9, 29.7, 29.6, 29.6, 29.6, 29.3, 29.3, 26.8, 22.7, 14.1, 0.1; **FD(MS)**: calcd for *m/z* [M^+] 470.3943, found *m/z* [M^+] 470.3819

1-(4-(6-Bromohexyloxy)phenyl)-2-(trimethylsilyl)ethyne (2b)



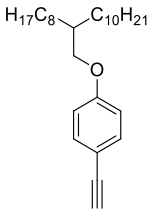
2b

Following the general procedure the reaction was carried out with **1b** (21.40 g, 55.87 mmol). The corresponding product **2b** (18.10 g, 51.22 mmol, 92 %) was isolated as a white solid. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.42 (d, *J* = 8.9 Hz, 2H), 6.83 (d, *J* = 8.9 Hz, 2H), 3.98 (t, *J* = 6.4 Hz, 2H), 3.45 (t, *J* = 6.8 Hz, 2H), 1.98 – 1.88 (m, 2H), 1.87 – 1.76 (m, 2H), 1.61 – 1.49 (m, 4H), 0.27 (s, *J* = 5.7 Hz, 9H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 159.2, 133.4, 115.1, 114.3, 105.3, 92.3, 67.7, 33.7, 32.6, 28.9, 27.9, 25.3, 0.1; **FD(MS)**: calcd for *m/z* [M^+] 352.0858, found *m/z* [M^+] 352.0766

General procedure for the synthesis of 4-(Alkoxy)ethynylbenzene derivatives[3]

In a round bottom flask the 1-(4-(alkoxy)phenyl)-2-(trimethylsilyl)ethyne derivative (1 eq) was dissolved in a 3:2 mixture of THF and Methanol (0.75 M) under an argon atmosphere. Afterwards a 40 % aqueous KOH-solution (0.1 eq) was added and the solution stirred at RT overnight. Finally the reaction solution was diluted with hexane, washed with water, dried over $MgSO_4$, concentrated *in vacuo* and passed through a silica pad with a given solvent.

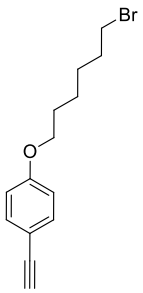
4-(2-Octyldodecyl)ethynylbenzene (3a)



3a

2a (17.95 g, 38.10 mmol) was used for the synthesis according to the general procedure. After purification through a silica pad (stationary phase: silica, eluent: hexane) the product **3a** (14.40 g, 36.12 mmol, 95 %) was obtained as a yellow oil. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.44 (d, *J* = 6.7 Hz, 2H), 6.86 (d, *J* = 6.7 Hz, 2H), 3.86 (d, *J* = 3.7 Hz, 2H), 3.01 (s, 1H), 1.80 (s, 1H), 1.52 – 1.12 (m, 32H), 0.91 (s, 6H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 159.8, 133.5, 114.5, 113.8, 83.8, 75.6, 71.1, 37.9, 31.9, 31.9, 31.4, 29.9, 29.7, 29.6, 29.6, 29.6, 29.3, 29.3, 26.8, 22.7, 14.1; **FD(MS)**: calcd for *m/z* [M^+] 398.3548, found *m/z* [M^+] 398.3584

4-(6-Bromohexyloxy)ethynylbenzene (3b)



3b

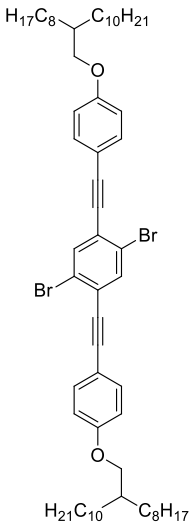
The reaction was carried out with **2b** (18.10 g, 51.22 mmol) according to the general procedure. Purification with a silica pad (stationary phase: silica, eluent: hexane/methylene chloride 1:1) resulted in the formation of **3b** (12.10 g, 43.03 mmol, 84 %) as a white solid. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.45 (d, *J* = 8.9 Hz, 2H), 6.86 (d, *J* = 8.9 Hz, 2H), 3.99 (t, *J* = 6.4 Hz, 2H), 3.45 (t, *J* = 6.8 Hz, 2H), 3.02 (s, 1H), 1.98 – 1.87 (m, 2H), 1.87 – 1.80 (m, 2H), 1.60 – 1.47 (m, 4H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 159.4, 133.6, 114.5, 114.0, 83.7, 75.7, 67.8, 33.7, 32.7, 28.9, 27.9, 25.3; **APCI**: calcd for *m/z* [$M+H^+$] 281.0536, found *m/z* [$M+H^+$] 281.0533

General procedure for the synthesis of 2,5-Dibromo-1,4-di(4-(alkoxy)phenyIethynyl)benzene derivatives[3]

In a flame dried, two-neck round-bottom flask containing a magnetic stir bar were placed: tetrabutylammonium bromide (0.06 eq), copper(I) iodide (0.1 eq), bis(triphenylphosphine)palladium dichloride (0.02 eq) and 1,4-dibromo-2,5-diiodobenzene (1 eq) under an argon atmosphere. The solids were dissolved in a 3:3:2 mixture of toluene, DIPA, and THF (0.2 M) and the 4-(Alkoxy)ethynylbenzene derivative (2.1 eq, dissolved in a small amount of THF) was slowly added over a period of 15 minutes. The reaction solution

became a little warm and was stirred for another two hours. Afterwards the solution was diluted with chloroform and washed with 2 M aqueous HCl-solution, water, 5 % aqueous ammonia-solution, water and saturated, aqueous NaCl-solution. The solution was dried over $MgSO_4$, the solvents removed under reduced pressure and the crude product purified by column chromatography in a given solvent.

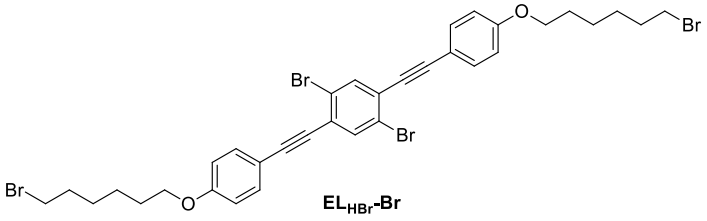
2,5-Dibromo-1,4-di(4-(2-octyldodecyloxy)phenyIethynyl)benzene (EL_{OD}-Br)



EL_{OD}-Br

Prepared from **3a** (3.43 g, 8.61 mmol) following the general procedure. After purification by column chromatography (stationary phase: silica, eluent: hexane/toluene 97:3) the product **EL_{OD}-Br** (3.75 g, 3.64 mmol, 89 %) was obtained as a white solid. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ [ppm] = 7.76 (s, 2H), 7.52 (d, *J* = 8.9 Hz, 4H), 6.91 (d, *J* = 8.9 Hz, 4H), 3.88 (d, *J* = 5.7 Hz, 4H), 1.87 – 1.73 (m, 2H), 1.53 – 1.23 (m, 64H), 0.91 (t, *J* = 6.8 Hz, 12H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 160.2, 135.7, 133.3, 126.4, 123.5, 114.7, 114.1, 97.0, 85.8, 71.1, 37.9, 31.9, 31.9, 31.4, 30.0, 29.7, 29.6, 29.6, 29.6, 29.4, 29.3, 26.8, 22.7, 22.7, 14.1; **APCI**: calcd for *m/z* [M+H$^+$] 1029.5520, found *m/z* [M+H$^+$] 1029.5526

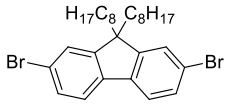
2,5-Dibromo-1,4-di(4-(6-bromhexyloxy)phenyIethynyl)benzene (EL_{HBr}-Br)



EL_{HBr}-Br

According to the general procedure the reaction was carried out with **3b** (3.27 g, 11.63 mmol). The crude product was purified by column chromatography (stationary phase: silica, eluent: hexane/ethyl acetate 9:1) and the product **EL$_{HBr}$-Br** (1.80 g, 2.27 mmol, 41 %) was obtained as a white solid. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.77 (s, 2H), 7.53 (d, *J* = 8.9 Hz, 4H), 6.91 (d, *J* = 8.9 Hz, 4H), 4.02 (t, *J* = 6.4 Hz, 4H), 3.46 (t, *J* = 6.8 Hz, 4H), 1.97 – 1.89 (m, 4H), 1.89 – 1.81 (m, 4H), 1.59 – 1.51 (m, 8H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 159.8, 135.7, 133.4, 126.4, 123.5, 114.7, 114.3, 96.9, 85.9, 67.9, 33.7, 32.7, 28.9, 27.9, 25.3; **APCI**: calcd for *m/z* [M+H$^+$] 790.9365, found *m/z* [M+H$^+$] 790.9474

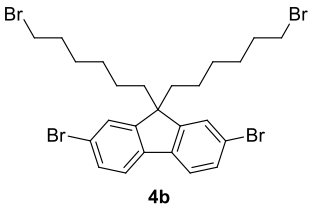
2,7-Dibromo-9,9-dioctylfluorene (4a)[4]



4a

In a three-neck round-bottom flask 2,7-dibromo-9*H*-fluorene (20.00 g, 61.73 mmol) and benzyltriethylammonium chloride (0.78 g, 3.39 mmol) were dissolved in DMSO (400 mL) under an argon atmosphere. A 50 % aqueous NaOH-solution (40 mL) and 1-bromooctane (25.76 mL, 148.15 mmol) were added and the solution was stirred at 80 °C for 6 h. Afterwards the solution was cooled to RT diluted with MTBE and washed with 2 M aqueous, HCl-solution, water and saturated, aqueous NaCl-solution. The solution was dried over $MgSO_4$, reduced *in vacuo* and purified by column chromatography (stationary phase: silica, eluent: hexane). The crude product was recrystallized from ethanol and the product **4a** (28.90 g, 52.70 mmol, 85 %) was obtained as white crystals. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.56 – 7.53 (m, 2H), 7.50 – 7.46 (m, 4H), 1.96 – 1.91 (m, 4H), 1.30 – 1.04 (m, 16H), 0.86 (t, *J* = 7.3 Hz, 6H), 0.66 – 0.58 (m, 4H); **GC(MS)**: calcd for *m/z* [M+H$^+$] 548.15, found *m/z* [M+H$^+$] 548.15

2,7-Dibromo-9,9-di(6-bromohexyl)fluorene (4b)[4]



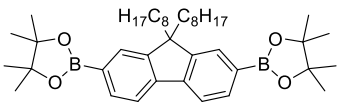
4b

2,7-Dibromo-9*H*-fluorene (15.00 g, 46.29 mmol) and tetrabutylammonium bromide (4.50 g, 13.96 mmol) were placed in a three-neck round-bottom flask under an argon atmosphere. A 50 % aqueous NaOH-solution (7.5 mL) and 1,6-dibromohexane (70.19 mL, 463.18 mmol) were added and the mixture was stirred at 80 °C for 3 H. After cooling down to RT, the mixture was diluted with water and diethyl ether and the phases were separated. The combined organic layers were washed with saturated, aqueous NaCl-solution, dried over $MgSO_4$ and the solvents removed under reduced pressure. The crude product was purified by column chromatography (stationary phase: silica, eluent: hexane/methylene chloride 9:1) and the product **4b** (10.80 g, 16.61 mmol, 36 %) was obtained as white crystals after recrystallization from ethanol. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.57 – 7.54 (m, 2H), 7.51 – 7.45 (m, 4H), 3.32 (t, *J* = 6.8 Hz, 2H), 1.99 – 1.92 (m, 4H), 1.74 – 1.66 (m, 4H), 1.27 – 1.20 (m, 4H), 1.15 – 1.08 (m, 4H), 0.66 – 0.58 (m, 4H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 152.2, 139.1, 130.3, 126.1, 121.6, 121.2, 55.6, 40.0, 33.8, 32.6, 28.9, 27.7, 23.5. **APCI**: calcd for *m/z* [M+H$^+$] 649.9037, found *m/z* [M+H$^+$] 649.9041

General procedure for the borylation of 2,7-dibromofluorenes[5]

In a flame dried three-neck-round-bottom flask a mixture of the 2,7-dibromofluorene derivative(1 eq), 4,4,4',4',5,5,5',5'-octamethyl-2,2'-bi(1,3,2-dioxaborolane) (2.6 eq), potassium acetate (4.5 eq) and [1,1'-bis(diphenylphosphino)ferrocene]palladium(II) dichloride (0.05 eq) were dissolved in dioxane (0.06 M) under an argon atmosphere. The solution was heated to 90 °C for 16 h, cooled down to RT, diluted with chloroform and water and the aqueous phase was extracted with chloroform. The combined organic layers were dried over $MgSO_4$ and the solvent removed *in vacuo*. The crude product was purified by column chromatography with a given solvent and recrystallized from ethanol.

9,9-Dioctyl-fluorene-2,7-diboronic acid bis(pinacol) ester (F8-BPin)

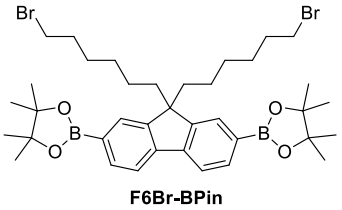


F8-BPin

Prepared from **4a** (10.00 g, 18.23 mmol) according to the general procedure. The crude product was purified by column chromatography (stationary phase: silica, eluent: hexane/methylene chloride 4:1) and the product **F8-BPin** (8.00 g, 12.45 mmol, 68 %) was obtained as a white solid. **^{1}H-NMR** (400 MHz, $CDCl_3$) δ [ppm] = 7.83 (dd, *J* = 7.5 Hz, 0.9 Hz, 2H), 7.79 – 7.72 (m, 4H), 2.06 – 1.98 (m, 4H), 1.41 (s, 24H), 1.25 – 0.98 (m, 20H), 0.83

(t, *J* = 7.1 Hz, 6H), 0.63 – 0.52 (m, 4H); **^{13}C{H}-NMR** (101 MHz, $CDCl_3$) δ [ppm] = 150.5, 143.9, 133.7, 128.9, 119.4, 83.7, 55.2, 40.1, 31.8, 29.9, 29.2, 29.1, 24.9, 23.6, 22.6, 14.0; **APCI**: calcd for *m/z* [M+H$^+$] 642.4999, found *m/z* [M+H$^+$] 642.4993

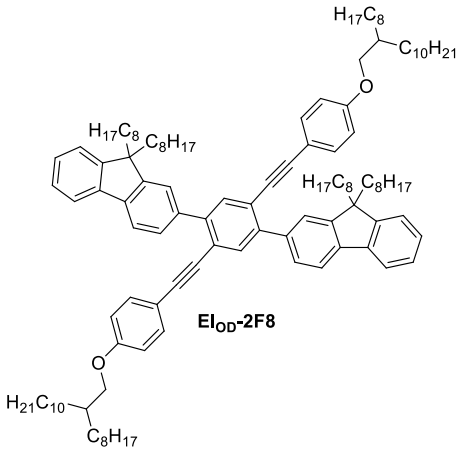
9,9-Di(6-bromohexyl)fluorene-2,7-diboronic acid bis(pinacol) ester (F6$_{Br}$-BPin)



F6Br-BPin

Following the general procedure the reaction was carried out with **4b** (3.00 g, 4.61 mmol). The crude product was purified by column chromatography (stationary phase: silica, eluent: hexane/methylene chloride 3:2) and the product **F6$_{Br}$-BPin** (2.70 g, 3.63 mmol, 79 %) was isolated as a white solid. **^{1}H-NMR** (600 MHz, $CDCl_3$) δ [ppm] = 7.84 (dd, *J* = 7.5 Hz, 0.8 Hz, 2H), 7.78 – 7.73 (m, 4H), 3.28 (t, *J* = 6.9 Hz, 4H), 2.07 – 2.00 (m, 4H), 1.69 – 1.60 (m, 4H), 1.42 (s, 24H), 1.22 – 1.14 (m, 4H), 1.11 – 1.02 (m, 4H), 0.63 – 0.54 (m, 4H); **^{13}C{H}-NMR** (151 MHz, $CDCl_3$) δ [ppm] = 150.1, 143.9, 133.8, 128.8, 119.5, 83.8, 55.1, 39.9, 33.9, 32.7, 28.9, 27.7, 24.9, 23.4. **APCI**: calcd for *m/z* [M+H$^+$] 744.2565, found *m/z* [M+H$^+$] 744.2548

El$_{OD}$-2F8

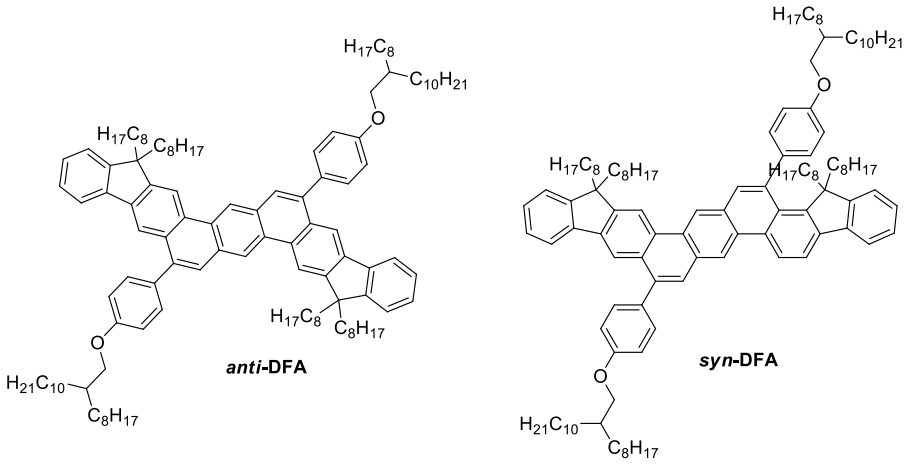


EI$_{OD}$-2F8

In a microwave vessel **EL$_{OD}$-Br** (0.50 g, 0.49 mmol; containing additional 5 % non-reactive Glaser coupling product (see S27)), **F8-mPin** (0.53 g, 1.02 mmol), potassium carbonate (0.64 g, 4.62 mmol) and tetrakis(triphenylphosphine)palladium(0) (56 mg, 49 µmol) were dissolved in mixture of THF (15 mL) and water (5 mL) under an argon atmosphere and the mixture was heated at 80 °C for 16 h in the abstinence of light. Subsequently, the mixture was diluted with water and extracted with chloroform. The combined organic layers were washed

with water and brine, dried over $MgSO_4$ and the solvent was removed *in vacuo*. The crude product was purified by column chromatography (stationary phase: silica, eluent: hexane/methylene chloride 8:2) and the product **ELOD-2F8** (0.31 g, 0.19 mmol, 39 %) was obtained as a yellow oil. **^{1}H-NMR** (600 MHz, $C_2D_2Cl_4$) δ [ppm] = 7.80 – 7.77 (m, 2H), 7.74 (d, *J* = 7.6 Hz, 4H), 7.70 – 7.66 (m, 4H), 7.38 – 7.27 (m, 6H), 7.24 (d, *J* = 8.7 Hz, 4H), 6.77 (d, *J* = 8.8 Hz, 4H), 3.75 (d, *J* = 5.7 Hz, 4H), 2.03 – 1.83 (m, 8H), 1.75 – 1.68 (m, 2H), 1.41 – 0.90 (m, 104H), 0.85 (t, *J* = 6.7 Hz, 12H), 0.80 – 0.62 (m, 20H). **^{13}C{H}-NMR** (151 MHz, $C_2D_2Cl_4$) δ [ppm] = 159.9, 151.5, 151.1, 142.8, 141.0, 140.7, 138.7, 133.2, 128.2, 126.9, 123.5, 121.9, 114.9, 99.8, 94.4, 88.3, 71.4, 55.3, 40.3, 38.1, 32.2, 32.2, 32.1, 31.6, 30.4, 30.3, 29.9, 29.9, 29.9, 29.9, 29.6, 29.6, 29.6, 27.1, 24.3, 23.0, 23.0, 22.9, 14.5, 14.5 **FD(MS)**: calcd for *m/z* [M^+] 1647.3514, found *m/z* [M^+] 1647.3299

***anti*-DFA / *syn*-DFA**



In a one-neck round-bottom flask **ElOD-2F8** (150 mg, 91 µmol) was dissolved in methylene chloride (54 mL) under an argon atmosphere. An Excess of trifluoroacetic acid (TFA, 3 mL, 39 mmol) was added and the mixture was stirred at RT for 3 h. Subsequently the acid was quenched by addition of DIPA (6 mL) and the solution was diluted with chloroform and washed with water. The solvents were evaporated under reduced pressure and the crude polymer was purified by column chromatography (stationary phase: silica, eluent: hexane/methylene chloride 7:3 -> 3:2) and the two isomers (143 mg, 87 µmol, 95 %; *anti*: 95.8 mg, 58.3 µmol, 67 %; *syn*: 47.2 mg, 28.7 µmol, 33 %) were obtained as yellow oils.

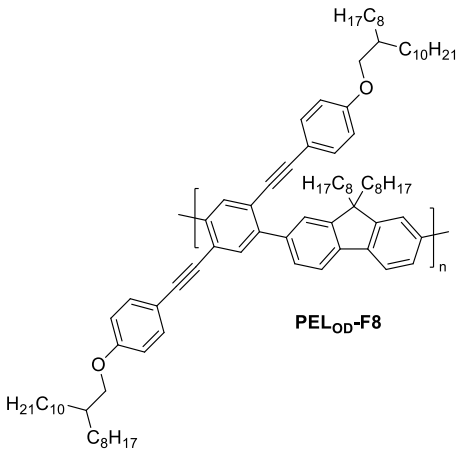
Anti: **^{1}H-NMR** (400 MHz, $C_2D_2Cl_4$) δ [ppm] = 9.23 (s, 2H), 8.85 (s, 2H), 8.30 (s, 2H), 7.98 (s, 2H), 7.77 – 7.72 (m, 2H), 7.65 (d, *J* = 8.5 Hz, 4H), 7.42 (s, 2H), 7.39 – 7.30 (m, 4H), 7.15 (d, *J* = 8.5 Hz, 4H), 4.01 (d, *J* = 5.6 Hz, 4H), 2.29 – 2.07 (m, 8H), 1.95 – 1.82 (m, 2H), 1.62 – 1.00 (m, 112H), 0.96 – 0.81 (m, 12H), 0.76 (t, *J* = 7.0 Hz, 12H); **APCI**: calcd for *m/z* [M+H$^+$] 1649.3621, found *m/z* [M+H$^+$] 1649.3443; *Syn*: **^{1}H-NMR** (400 MHz, $C_2D_2Cl_4$) δ [ppm] = 9.30 (s, 1H), 9.24 (d, *J* = 7.0 Hz, 2H), 8.87 (s, 1H), 8.32 (s, 1H), 8.08 (d, *J* = 7.4 Hz, 1H), 7.99 (d, *J* = 6.5 Hz, 3H), 7.76 (dd, *J* = 5.8 Hz, 2.7 Hz, 1H), 7.65 (dd, *J* = 23.9, 8.5 Hz, 4H), 7.49 – 7.30 (m, 6H), 7.15 (dd, *J* = 14.9 Hz, 8.6 Hz, 4H), 4.01 (t, *J* = 6.1 Hz, 4H), 2.27 – 2.07 (m, 4H), 2.06 – 1.85 (m, 6H), 1.64 – 1.00 (m, 112H), 0.99 – 0.66 (m, 24H). **APCI**: calcd for *m/z* [M+H$^+$] 1649.3621, found *m/z* [M+H$^+$] 1649.3961

3. Polymer Synthesis

General procedure for copolymerization and coupling reactions *via* Suzuki coupling

In a microwave vessel were placed the dibrominated ethynyl linker (1 eq), the diborylated fluorene derivative (1 eq), potassium carbonate (9.5 eq) and tetrakis(triphenylphosphine)palladium(0) (0.1 eq) under an argon atmosphere. The solids were dissolved in a mixture of THF (15 mL) and degassed water (5 mL) and stirred at 80 °C for 72 h. Afterwards the solution was cooled down, diluted with chloroform and washed with aqueous 2M HCl-solution, water, saturated aqueous EDTA-solution and brine. Subsequently, the crude polymer was dissolved in a small amount of chloroform, precipitated into cold methanol and purified by Soxhlet extraction (methanol, acetone, chloroform).

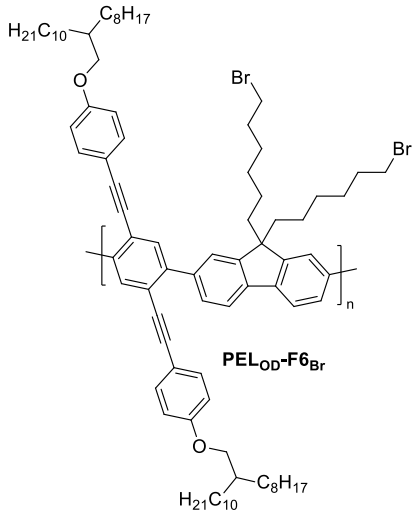
PEL$_{OD}$-F8



PEL$_{OD}$-F8 was prepared from **EL$_{OD}$-Br** (500 mg, 486 µmol; containing additional 5 % non-reactive Glaser coupling product (see S27)) and **F8-BPin** (312 mg, 486 µmol) according to the general procedure and obtained as a yellowish solid. **^{1}H-NMR** (600 MHz, $C_2D_2Cl_4$) δ [ppm] = 7.92 – 7.67 (m, 8H), 7.35 – 7.24 (m, 4H), 6.88 – 6.73 (m, 4H), 3.88 – 3.76 (m, 4H), 2.06 (s, 4H), 1.77 (s, 2H), 1.48 – 0.76 (m, 106H); **^{13}C{H}-NMR** (151 MHz, $C_2D_2Cl_4$) δ [ppm] = 160.0, 151.7, 142.9, 140.6, 139.1, 134.4, 133.2, 128.4, 124.2, 122.2, 119.5, 115.5, 115.2, 99.9, 94.7, 88.5, 83.9, 71.9, 55.7, 40.3, 38.4, 32.1, 32.1, 31.9, 31.8, 30.3, 30.2, 29.8, 29.8, 29.7, 29.7, 29.5, 29.4, 29.4, 29.3, 29.3, 27.1, 25.2, 24.4, 22.8, 22.8, 22.7, 14.2, 14.2, 14.2; **IR** ν [cm^{-1}] = 2920, 2852 (s, aliph. -C-H stretch); 2210 (w, -C≡C stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (368), 336; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 320 nm) = 414; **E_{HOMO}** [eV] = - 5.67; **E_{LUMO}** [eV] = - 2.28; **E_g** [eV] = 3.39.

Fraction	M_n [g/mol]	M_w [g/mol]	M_w/M_n	Yield [mg]	Yield [%]
Chloroform	10,000	16,400	1.64	450	72

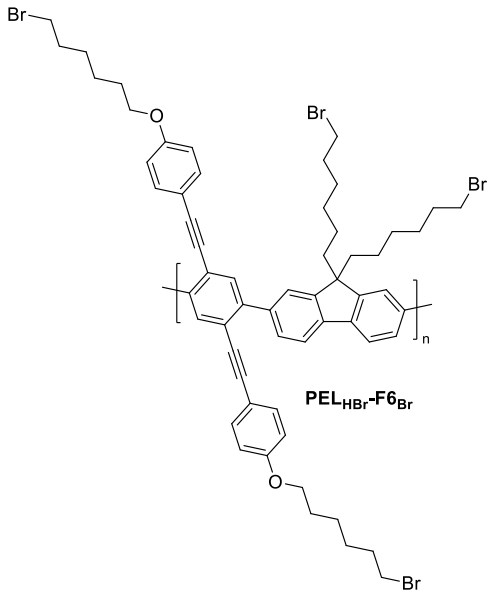
PEL_{OD}-$F6_{Br}$



PEL_{OD}-$F6_{Br}$ was prepared from **EL_{OD}-Br** (500 mg, 486 µmol; containing additional 5 % non-reactive Glaser coupling product (see S27)) and **$F6_{Br}$-BPin** (362 mg, 486 µmol) according to the general procedure and obtained as a yellowish solid. **^{1}H-NMR** (600 MHz, $C_2D_2Cl_4$) δ [ppm] = 7.96 – 7.65 (m, 8H), 7.31 (s, 4H), 6.83 (s, 4H), 3.85 (s, 4H), 3.20 (s, 4H), 2.07 (s, 4H), 1.79 (s, 2H), 1.61 (s, 4H), 1.51 – 0.75 (m, 88H); **^{13}C{H}-NMR** (151 MHz, $C_2D_2Cl_4$) δ [ppm] = 160.2, 151.3, 140.7, 134.4, 133.2, 128.7, 124.1, 122.3, 120.6, 119.5, 115.5, 115.3, 98.9, 94.7, 88.5, 72.1, 55.6, 40.2, 38.4, 33.7, 32.9, 32.0, 31.8, 30.2, 29.8, 29.7, 29.7, 29.7, 29.4, 29.4, 29.3, 28.1, 27.1, 24.2, 22.7, 14.1; **IR** ν [cm^{-1}] = 2958, 2927, 2858 (s, aliph. -C-H stretch); 2218 (w, -C≡C stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (370), 338; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 320 nm) = 415; E_{HOMO} [eV] = - 5.70; E_{LUMO} [eV] = - 2.27; E_g [eV] = 3.43

Fraction	M_n [g/mol]	M_w [g/mol]	M_w/M_n	Yield [mg]	Yield [%]
Chloroform	21,500	58,900	2.73	270	40

PEL_{HBr}-$F6_{Br}$



PEL_{HBr}-$F6_{Br}$ was prepared from **EL_{HBr}-Br** (500 mg, 630 µmol; containing additional 29 % non-reactive Glaser coupling product (see S27)) and **$F6_{Br}$-BPin** (469 mg, 630 µmol) according to the general procedure and obtained as a yellowish solid. **^{1}H-NMR** (400 MHz, $C_2D_2Cl_4$) δ [ppm] = 7.96 – 7.66 (m, 8H), 7.42 – 7.25 (m, 4H), 6.95 – 6.75 (m, 4H), 3.99 (s, 4H), 3.51 – 3.38 (m, 4H), 3.32 – 3.14 (m, 4H), 2.21 – 0.74 (m, 36H); **^{13}C{H}-NMR** (101 MHz, $C_2D_2Cl_4$) δ [ppm] = 159.7, 151.3, 142.9, 140.6, 139.1, 138.7, 134.4, 133.2, 128.6, 124.2, 122.2, 119.6, 115.6, 115.2, 114.9, 94.6, 88.5, 83.9, 68.4, 55.5, 40.2, 34.0, 33.9, 33.5, 33.0, 32.9, 30.9, 29.9, 29.3, 28.9, 28.2, 28.1, 25.6, 25.5, 25.2, 24.2; **IR** ν [cm^{-1}] = 2929, 2844 (s, aliph. -C-H stretch); 2212 (w, -C≡C stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (370), 335; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 320 nm) = 412; **E_{HOMO}** [eV] = - 5.79; **E_{LUMO}** [eV] = - 2.39; **E_g** [eV] = 3.40

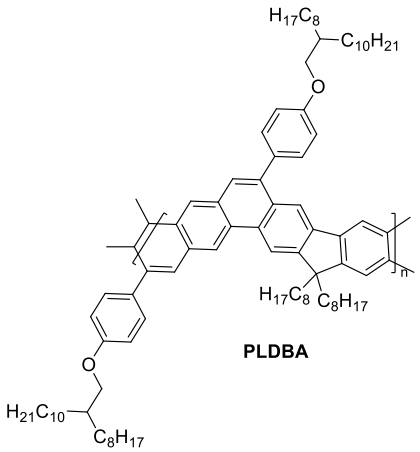
Fraction	M_n [g/mol]	M_w [g/mol]	M_w/M_n	Yield [mg]	Yield [%]
Chloroform	13,000	52,300	4.09	220	30

General procedure for polymer analogous ladderization *via* electrophile induced cyclization[3]

In a microwave vessel 50 mg of the corresponding precursorpolymer was dissolved in methylene chloride (18 mL) under an argon atmosphere. An Excess of trifluoroacetic acid (TFA, 1 mL) was added and the mixture was stirred at RT for 3 h. Subsequently the acid was quenched by addition of DIPA (2 mL) and the solution was diluted with chloroform and

washed with water. The solvents were evaporated under reduced pressure and the crude polymer was dissolved in a small amount of chloroform, precipitated into cold methanol and dried under HV.

PLDBA

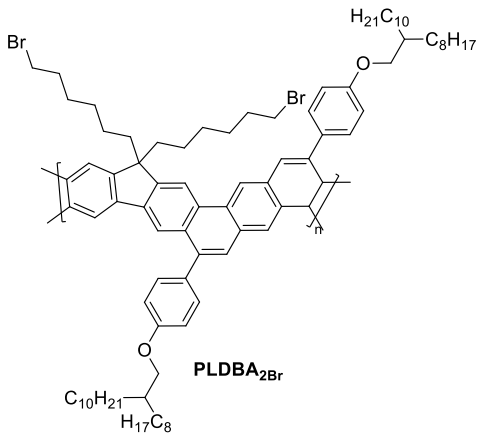


PLDBA

PLDBA was prepared from **PEL$_{OD}$-F8** according to the general procedure and obtained as a yellow solid in a nearly quantitative yield. **^{1}H-NMR** (600 MHz, $C_2D_2Cl_4$) δ [ppm] = 9.27 (s, 2H), 9.03 – 8.82 (m, 2H), 8.43 (s, 2H), 8.10 – 7.92 (m, 2H), 7.84 – 7.56 (m, 4H), 7.33 – 7.09 (m, 4H), 4.09 (s, 4H), 2.64 – 1.81 (m, 6H), 1.77 – 0.52 (m, 106H); **^{13}C{H}-NMR** (151 MHz, $C_2D_2Cl_4$) δ [ppm] = 159.7, 150.6, 140.6, 139.5, 129.7, 127.9, 122.3, 118.3, 117.6, 115.2, 99.9, 72.2, 55.7, 55.3, 41.8, 38.6, 32.2, 32.1, 31.9, 31.9, 30.5, 30.4, 30.3, 30.0, 29.9, 29.9, 29.9, 29.8, 29.6, 29.6, 29.5, 29.4, 29.4, 29.3, 27.3, 27.3, 24.6, 22.9, 22.7, 14.2, 14.1, 14.0; **IR** ν [cm^{-1}] = 2921, 2852 (s, aliph. -C-H stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (436), 419, 395; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 380 nm) = 441, (470), (507); **PLQY** (Chloroform) = 27 %; **E$_{HOMO}$** [eV] = - 5.64; **E$_{LUMO}$** [eV] = - 2.58; **E$_g$** [eV] = 3.06

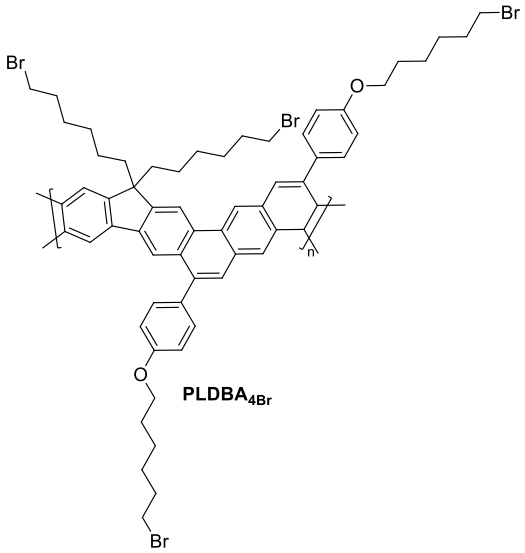
Fraction	M_n [g/mol]	M_w [g/mol]	M_w/M_n	Yield [mg]	Yield [%]
Chloroform	14,400	20,500	1.64	50	100

PLDBA$_{2Br}$



PLDBA$_{2Br}$ was prepared from **PEL$_{OD}$-F6$_{Br}$** according to the general procedure and obtained as a yellow solid in a nearly quantitative yield. **^{1}H-NMR** (600 MHz, $C_2D_2Cl_4$) δ [ppm] = 9.28 (s, 2H), 8.95 (s, 2H), 8.45 (s, 2H), 8.03 (s, 2H), 7.83 – 7.57 (m, 4H), 7.16 (s, 4H), 4.09 (s, 4H), 3.21 (s, 4H), 2.50 – 1.90 (m, 6H), 1.77 – 1.09 (m, 80H), 1.06 – 0.74 (m, 12H); **IR** ν [cm^{-1}] = 2920, 2848 (s, aliph. -C-H stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (438), 420, 395; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 380 nm) = 441, (471), 504; **E$_{HOMO}$** [eV] = - 5.70; **E$_{LUMO}$** [eV] = - 2.64; **E$_g$** [eV] = 3.06

PLDBA$_{4Br}$



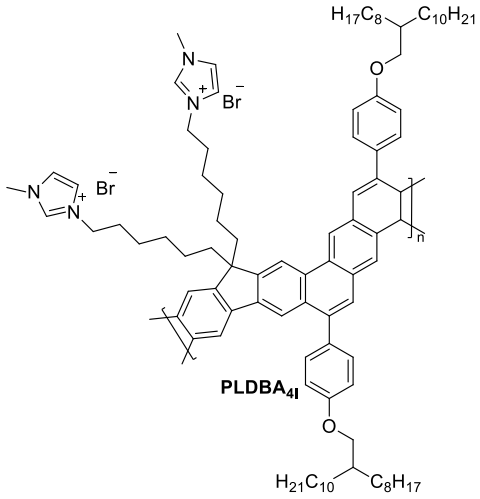
LP3 was prepared from **precursorpolymer 3** according to the general procedure and obtained as a yellow solid in a nearly quantitative yield. **^{1}H-NMR** (600 MHz, $C_2D_2Cl_4$) δ [ppm] = 9.28 (s, 2H), 8.94 (s, 2H), 8.44 – 8.28 (m, 2H), 8.03 (s, 2H), 7.91 – 7.51 (m, 4H), 7.15 (s, 4H), 4.20 (s, 4H), 3.60 – 3.40 (m, 4H), 3.34 – 3.14 (m, 4H), 2.52 – 0.64 (m, 36H); **IR**

ν [cm^{-1}] = 2924, 2848 (s, aliph. -C-H stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (438), 420, 395; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 380 nm) = 441, (471), (504); $\mathbf{E_{HOMO}}$ [eV] = - 5.70; $\mathbf{E_{LUMO}}$ [eV] = - 2.62; $\mathbf{E_g}$ [eV] = 3.08

General procedure for polymer analogous synthesis of cLPEs

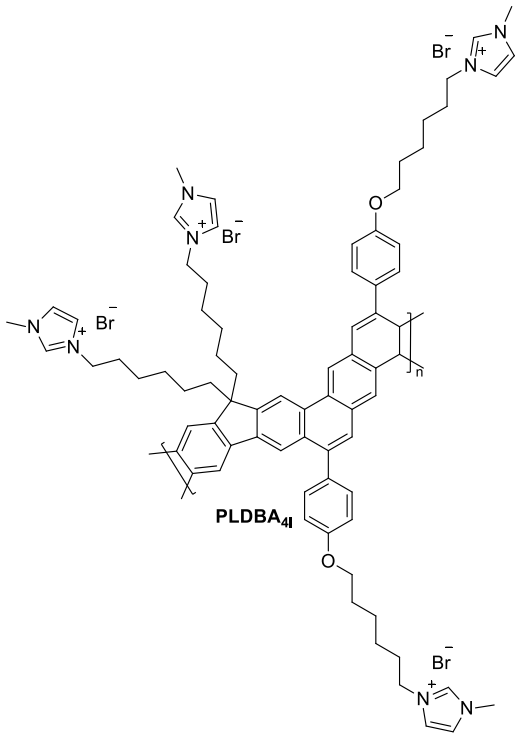
In a microwave vessel 50 mg of the ladder type polymer (bearing bromo-functionalized sidechains) were dissolved in THF (10 mL). After addition of an excess of 1-methylimidazole (1 mL) the reaction was stirred at 80 °C overnight. During this time the PCE started precipitate from the solution. Subsequently, the cLPE was filtered of, washed with THF and solved in a given solvent. The solution was filled into a dialysis tube (cutoff limit: 3.5 kDa) and purified *via* dialysis against a given solvent for three days. Afterwards the solvent was removed under reduced pressure.

$PLDBA_{2I}$



$PLDBA_{2I}$ was prepared from **$PLDBA_{2Br}$** according to the general procedure, purified *via* dialysis against a 1:1 mixture of methanol, and chloroform and obtained as a yellow solid in a nearly quantitative yield. **^{1}H-NMR** (600 MHz, MeOD/$CDCl_3$ 1:1) δ [ppm] = 9.41 (s, 2H), 9.04 (s, 2H), 8.46 (s, 2H), 8.11 (s, 4H), 7.89 – 7.60 (m, 4H), 7.45 – 6.99 (m, 8H), 4.17 (s, 4H), 4.11 – 3.91 (m, 6H), 3.89 – 3.66 (m, 4H), 2.09 – 1.85 (m, 2H), 1.87 – 0.54 (m, 96H); **IR** ν [cm^{-1}] = 3367, 3048 (sbr, aromatic -C-H stretch (imidazole)); 2923, 2853 (s, aliph. -C-H stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (438), 420, 395; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 380 nm) = 441, (471), 504; $\mathbf{E_{HOMO}}$ [eV] = - 5.70; $\mathbf{E_{LUMO}}$ [eV] = - 2.66; $\mathbf{E_g}$ [eV] = 3.04

PLDBA$_{4I}$



PLDBA$_{4I}$ was prepared from **PLDBA$_{4Br}$** according to the general procedure, purified *via* dialysis against methanol and obtained as a yellow solid in a nearly quantitative yield. **^{1}H-NMR** (600 MHz, MeOD) δ [ppm] = 9.57 (s, 2H), 9.24 (s, 2H), 8.45 – 7.97 (m, 4H), 7.83 – 7.49 (m, 8H), 7.48 – 7.17 (m, 8H), 4.01 (s, 12H), 3.83 – 3.68 (m, 8H), 2.68 – 0.61 (m, 40H); **IR** ν [cm^{-1}] = 3375, 3071 (sbr, aromatic -C-H stretch (imidazole)); 2932, 2855 (s, aliph. -C-H stretch); **UV/Vis** $\lambda_{max.abs.}$ [nm] = (438), 420, 395; **PL** $\lambda_{max.em.}$ [nm] ($\lambda_{exc.}$ = 380 nm) = 442, (471), 504; $\mathbf{E_{HOMO}}$ [eV] = - 5.50; $\mathbf{E_{LUMO}}$ [eV] = - 2.47; $\mathbf{E_g}$ [eV] = 3.03

4. Literature

(1) Manhas, M. S.; Hoffman, W. H.; Lal, B.; Bose, A. K. Steroids. Part X. A Convenient Synthesis of Alkyl Aryl Ethers. *J. Chem. Soc., Perkin Trans. 1* **1975**, *5*, 461–463.

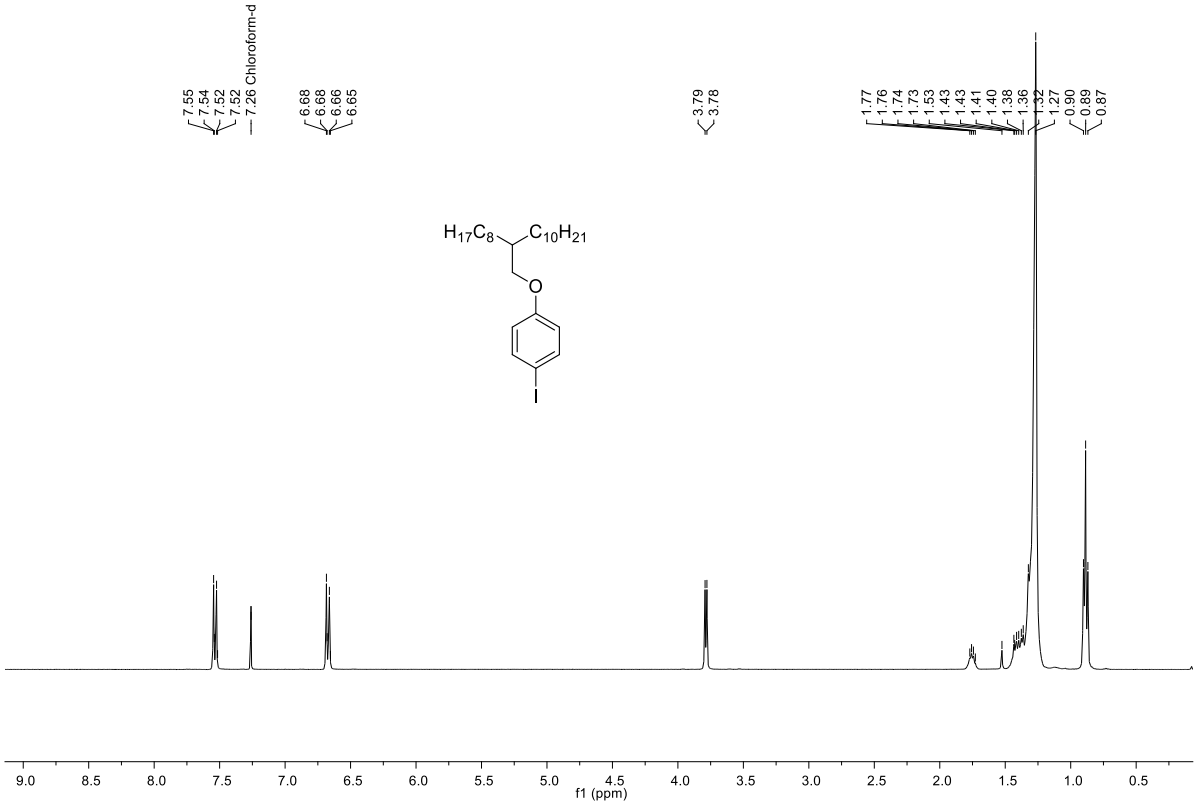
(2) Persigehl, P.; Jordan, R.; Nuyken, O. Functionalization of Amphiphilic Poly(2-oxazoline) Block Copolymers: A Novel Class of Macroligands for Micellar Catalysis †. *Macromolecules* **2000**, *33*, 6977–6981.

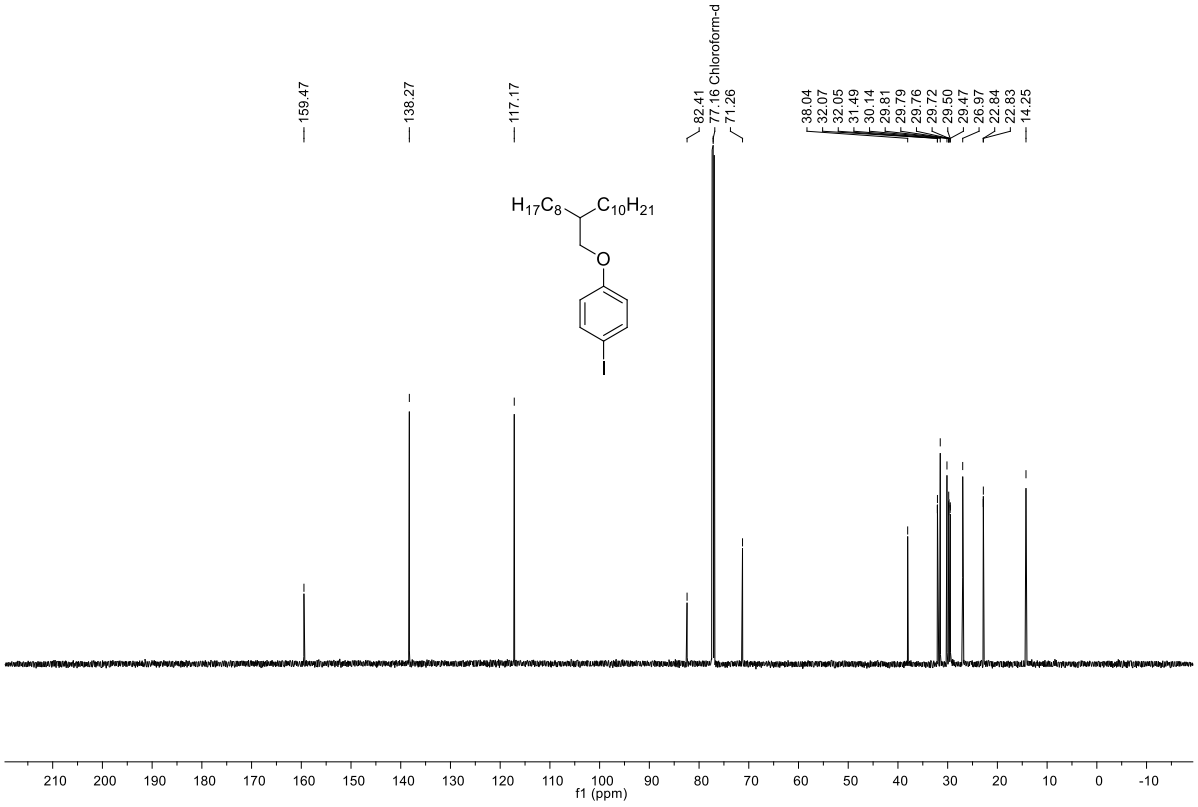
(3) Goldfinger, M. B.; Swager, T. M. Fused Polycyclic Aromatics via Electrophile-Induced Cyclization Reactions: Application to the Synthesis of Graphite Ribbons. *J. Am. Chem. Soc.* **1994**, *116*, 7895–7896.

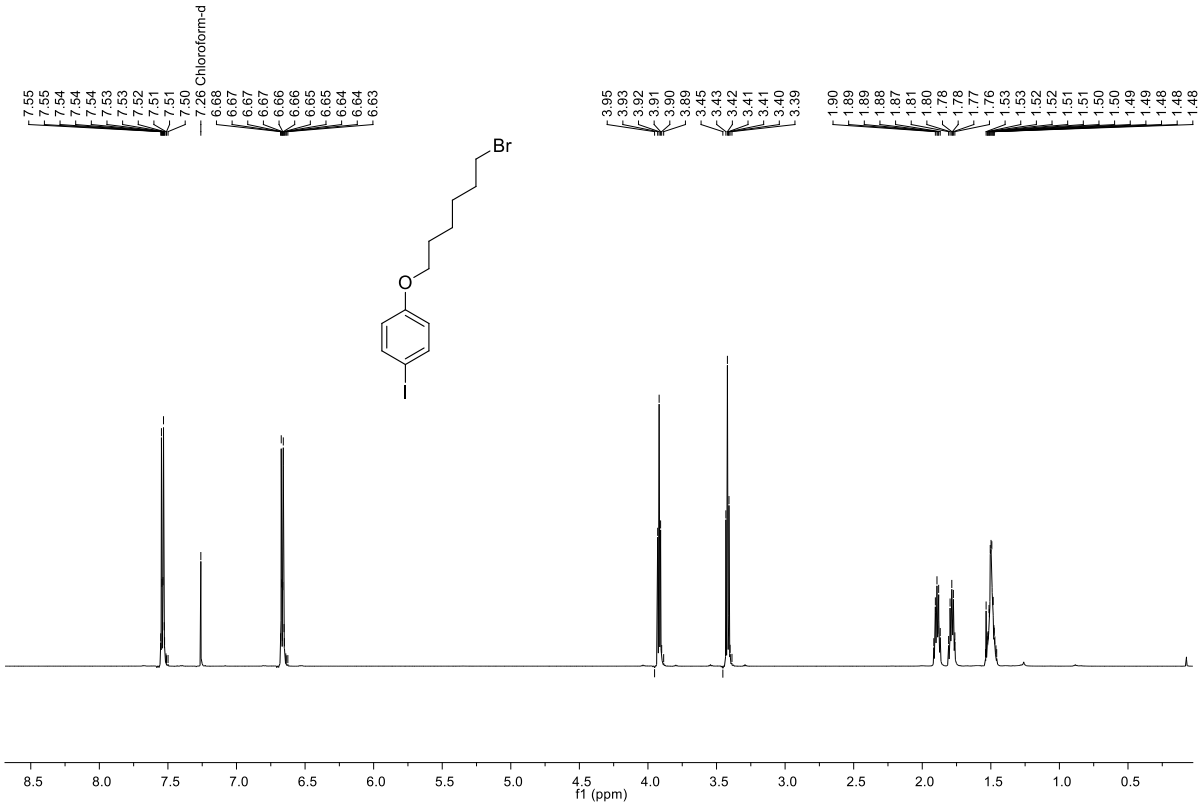
(4) Belfield, K. D.; Schafer, K. J.; Mourad, W.; Reinhardt, B. A. Synthesis of New Two-Photon Absorbing Fluorene Derivatives via Cu-Mediated Ullmann Condensations. *J. Org. Chem.* **2000**, 4475–4482.

(5) Tsao, H. N.; Cho, D.; Andreasen, J. W.; Rouhanipour, A.; Breiby, D. W.; Pisula, W.; Müllen, K. The Influence of Morphology on High-Performance Polymer Field-Effect Transistors. *Adv. Mater.* **2009**, *21*, 209–212.

5. Spectral Data



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7.50
7.26 Chloroform-d
6.68
6.67
6.67
6.67
6.66
6.66
6.66
6.65
6.65
6.64
6.64
6.63
3.95
3.93
3.92
3.91
3.90
3.89
3.45
3.43
3.42
3.41
3.41
3.40
3.39
1.90
1.89
1.89
1.88
1.87
1.81
1.80
1.78
1.78
1.77
1.76
1.53
1.53
1.52
1.52
1.51
1.51
1.50
1.50
1.49
1.49
1.48
1.48
Br
O
I
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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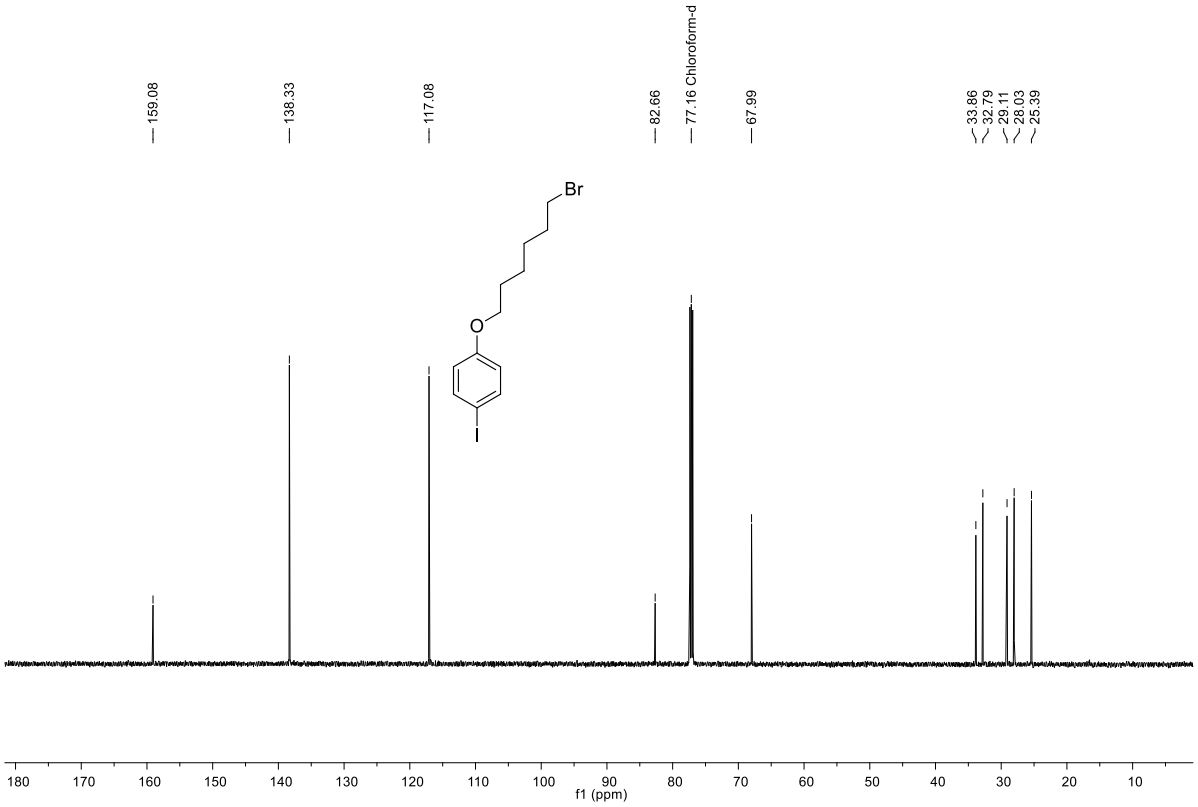
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)


159.08
138.33
117.08
82.66
77.16 Chloroform-d
67.99
33.86
32.79
29.11
28.03
25.39
Br
O
I
180
170
160
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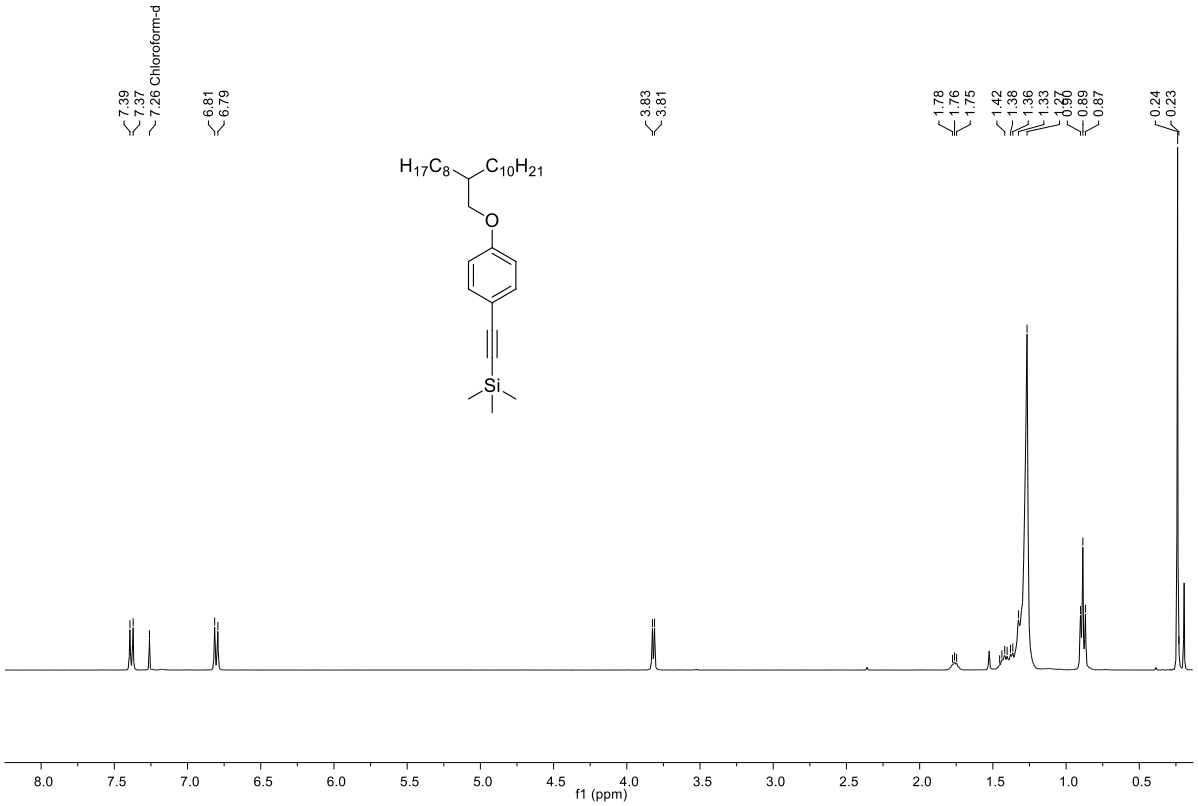
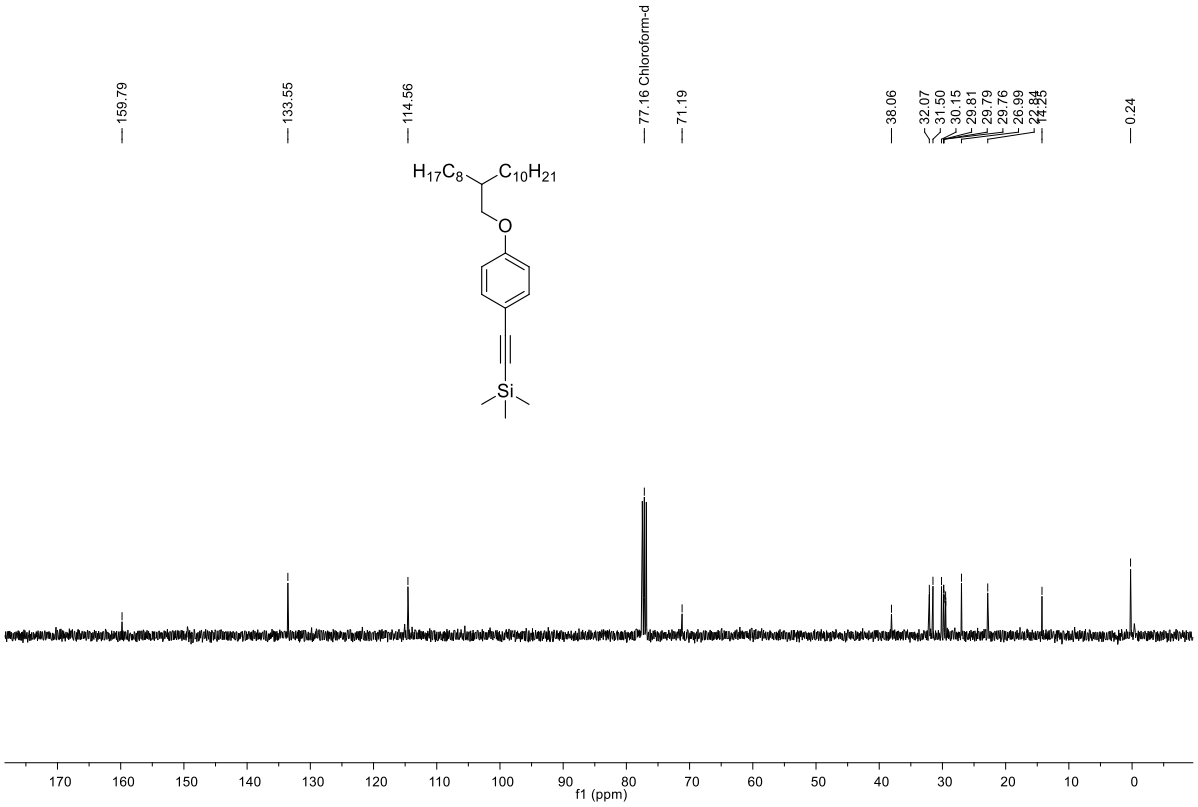
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.39
7.37
7.26 Chloroform-d
6.81
6.79
3.83
3.81
1.78
1.76
1.75
1.42
1.38
1.36
1.33
0.90
0.89
0.87
0.24
0.23
H17C8
C10H21
O
Si
f1 (ppm)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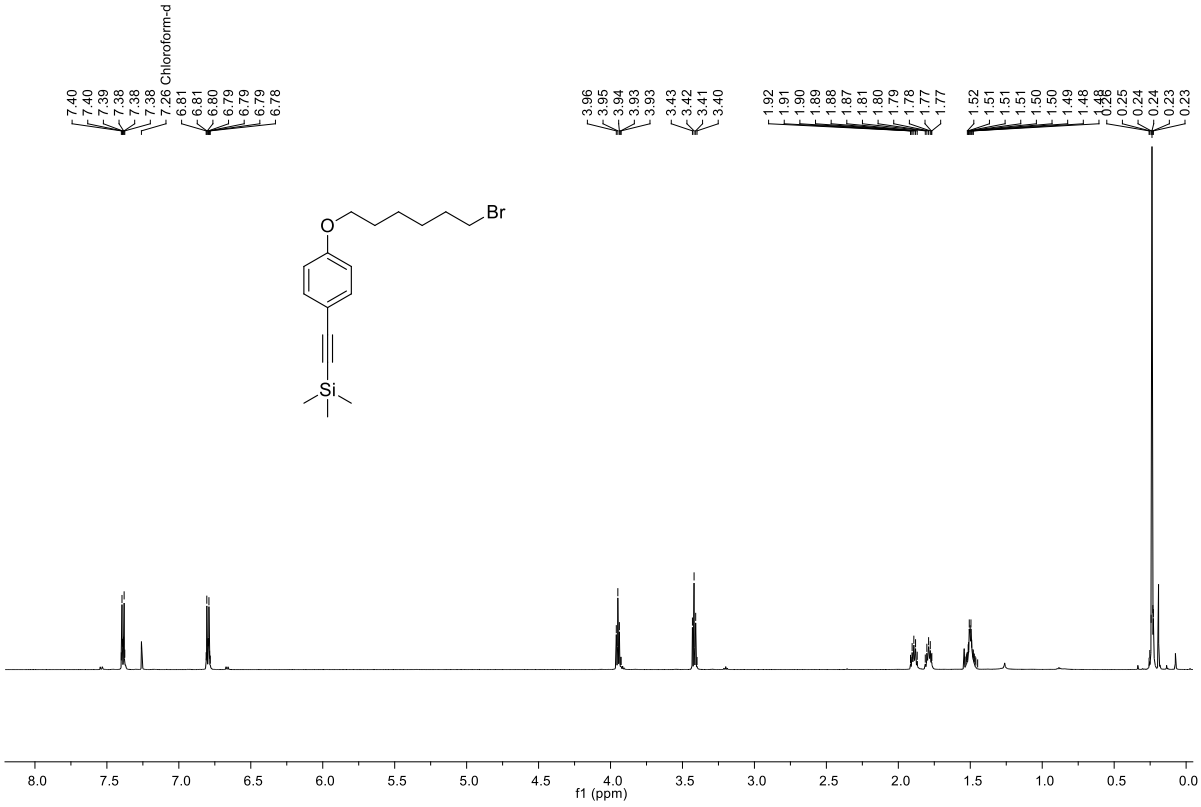
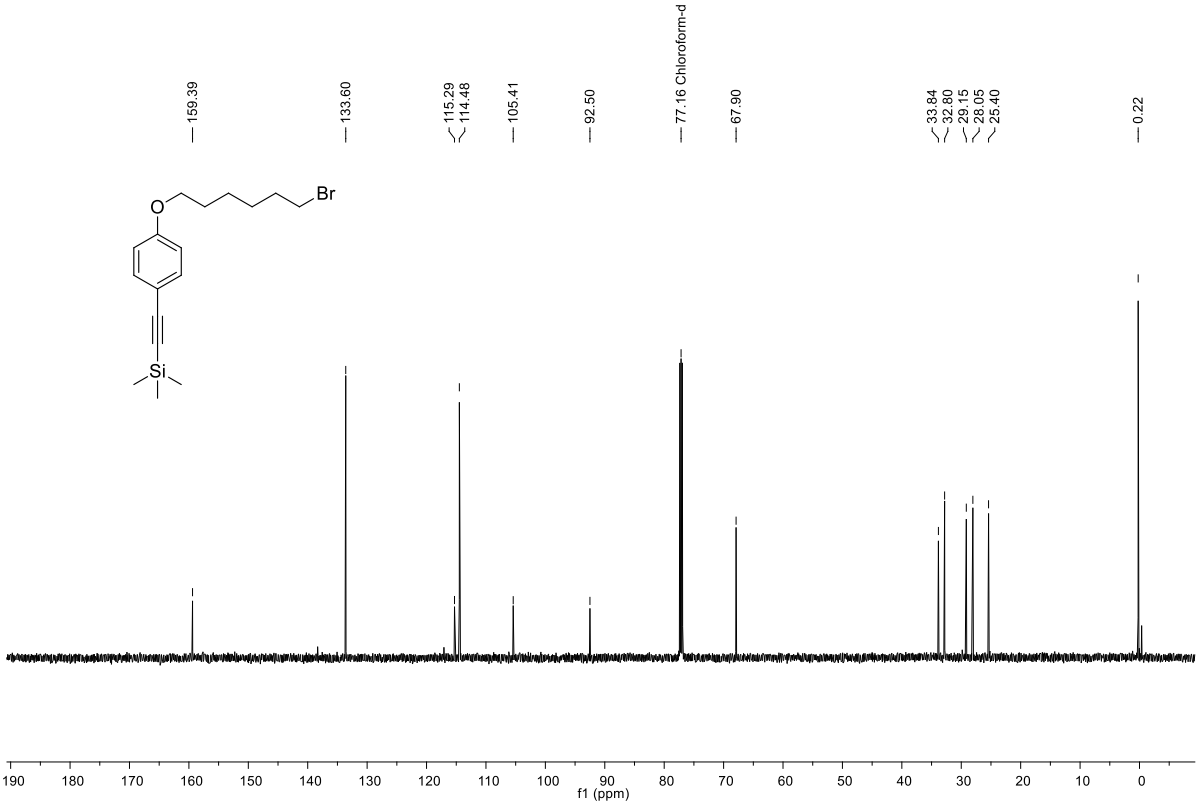
133.55
114.56
77.16 Chloroform-d
71.19
38.06
32.07
31.50
30.15
29.81
29.79
29.76
26.99
22.84
14.25
0.24
H17C8
C10H21
O
Si
f1 (ppm)


7.40
7.40
7.39
7.38
7.38
7.38
7.26 Chloroform-d
6.81
6.80
6.79
6.79
6.79
6.78
3.96
3.95
3.94
3.93
3.93
3.43
3.42
3.41
3.40
1.92
1.91
1.90
1.89
1.88
1.87
1.81
1.80
1.79
1.78
1.77
1.77
1.52
1.51
1.51
1.51
1.50
1.50
1.49
1.48
0.25
0.24
0.24
0.23
0.23
O
Br
Si
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
f1 (ppm)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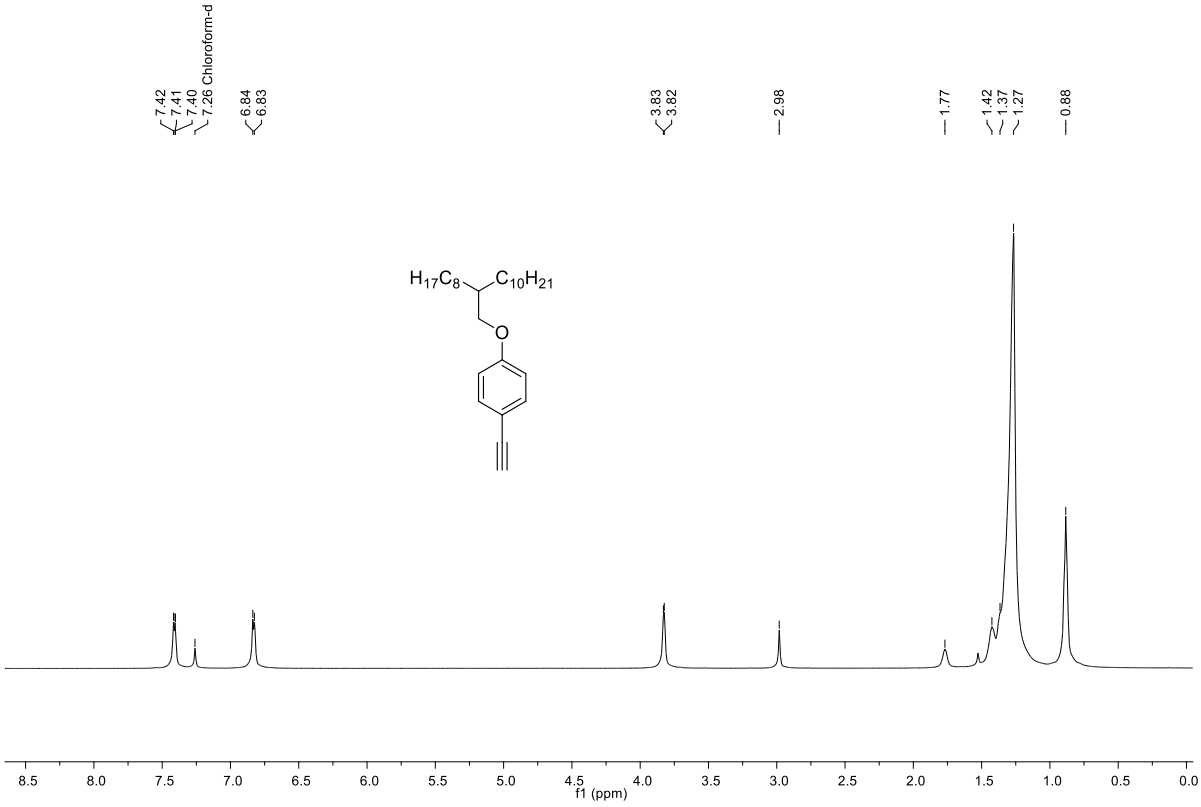
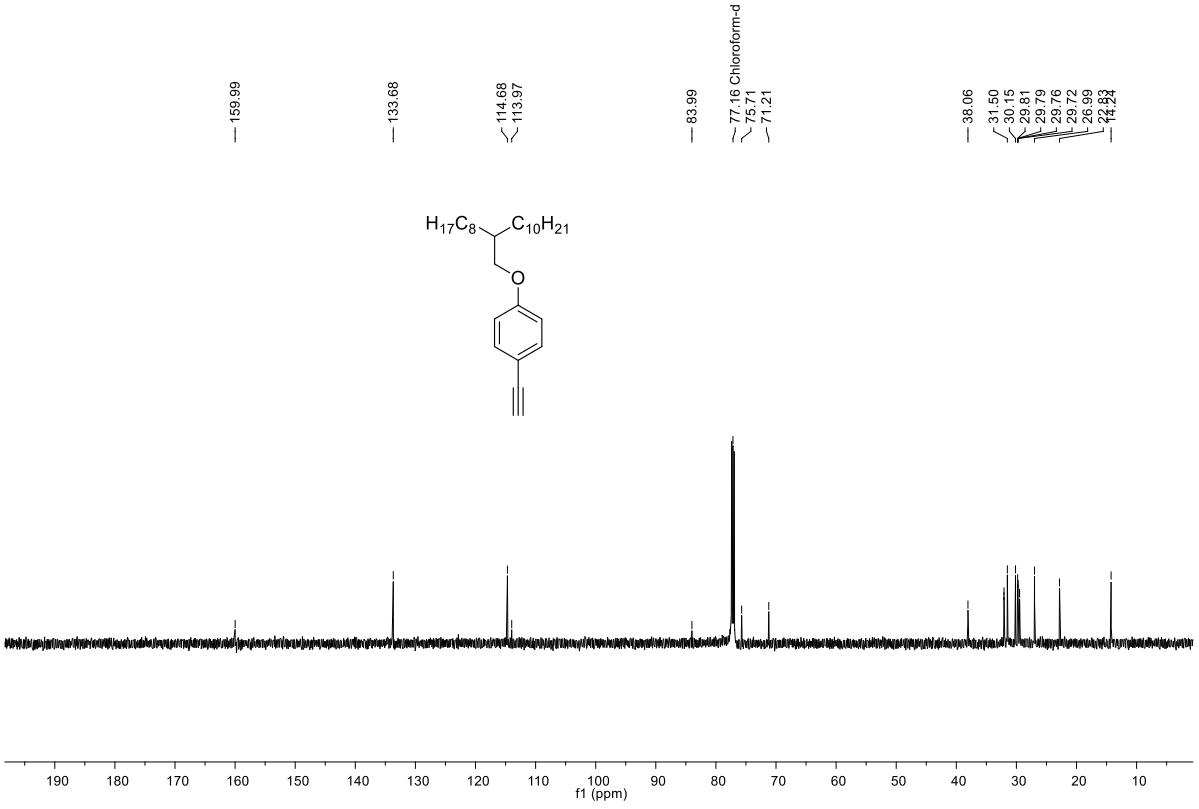
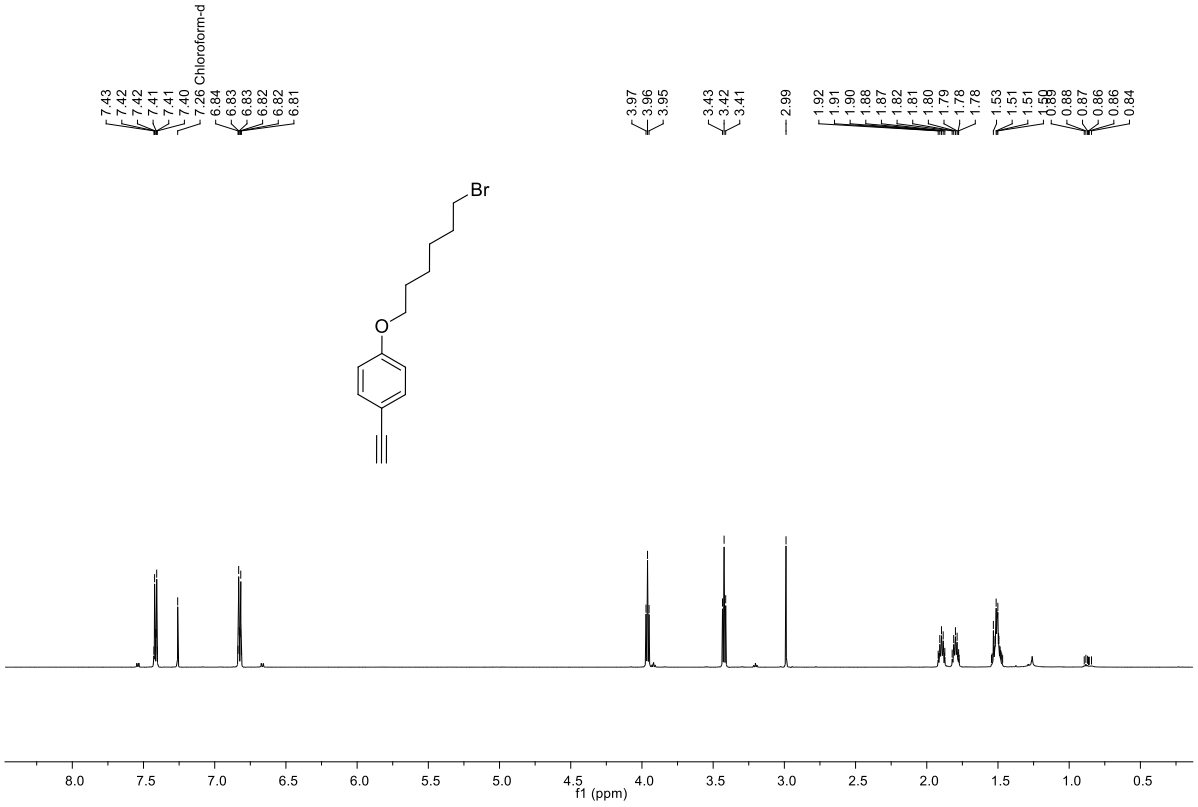
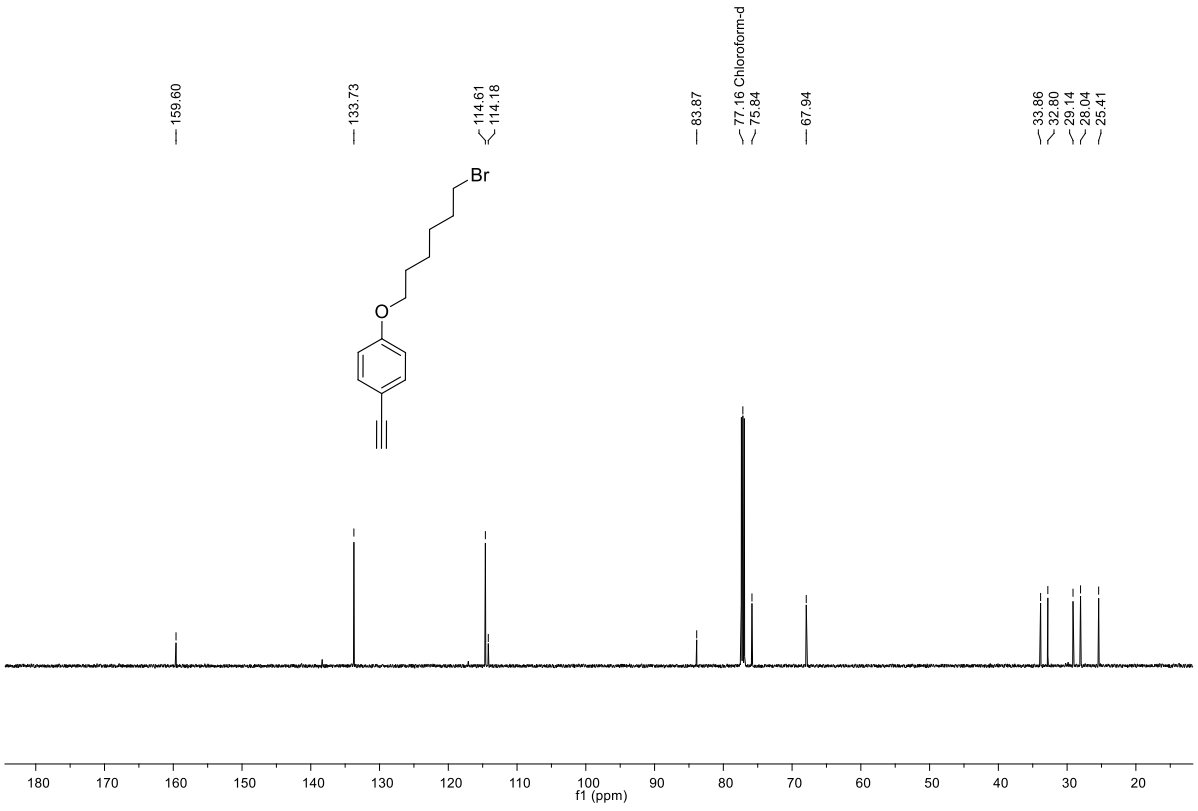
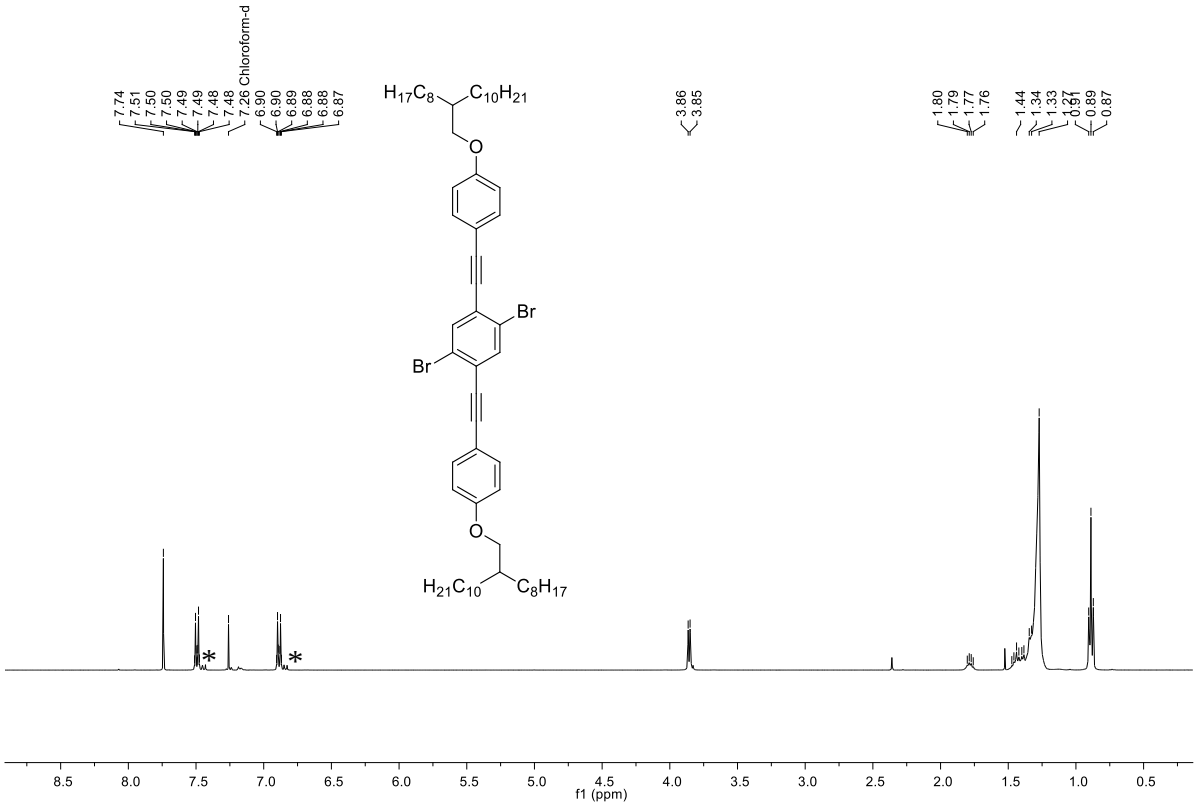
133.60
115.29
114.48
105.41
92.50
77.16 Chloroform-d
67.90
33.84
32.80
29.15
28.05
25.40
0.22
O
Br
Si
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.42
7.41
7.40
7.26 Chloroform-d
6.84
6.83
3.83
3.82
2.98
1.77
1.42
1.37
1.27
0.88
H17C8
C10H21
O
f1 (ppm)


159.99
133.68
114.68
113.97
83.99
77.16 Chloroform-d
75.71
71.21
38.06
31.50
30.15
29.81
29.79
29.76
29.72
26.99
22.83
14.24
H17C8
C10H21
O
f1 (ppm)

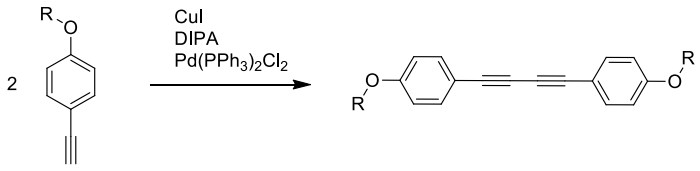

7.43
7.42
7.42
7.41
7.41
7.40
7.26 Chloroform-d
6.84
6.83
6.83
6.82
6.82
6.81
3.97
3.96
3.95
3.43
3.42
3.41
2.99
1.92
1.91
1.90
1.88
1.87
1.82
1.81
1.80
1.79
1.78
1.78
1.53
1.51
1.51
0.88
0.87
0.86
0.86
0.84
Br
O
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

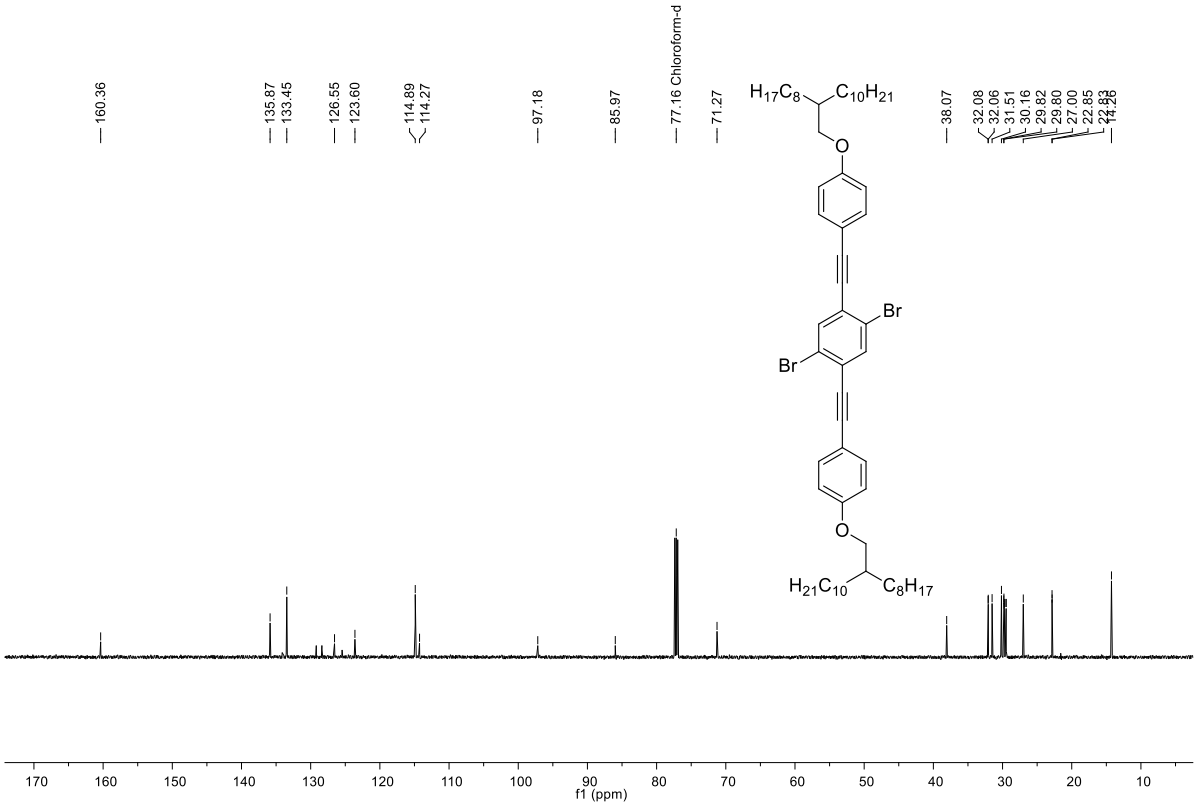

159.60
133.73
114.61
114.18
83.87
77.16 Chloroform-d
75.84
67.94
33.86
32.80
29.14
28.04
25.41
Br
O
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

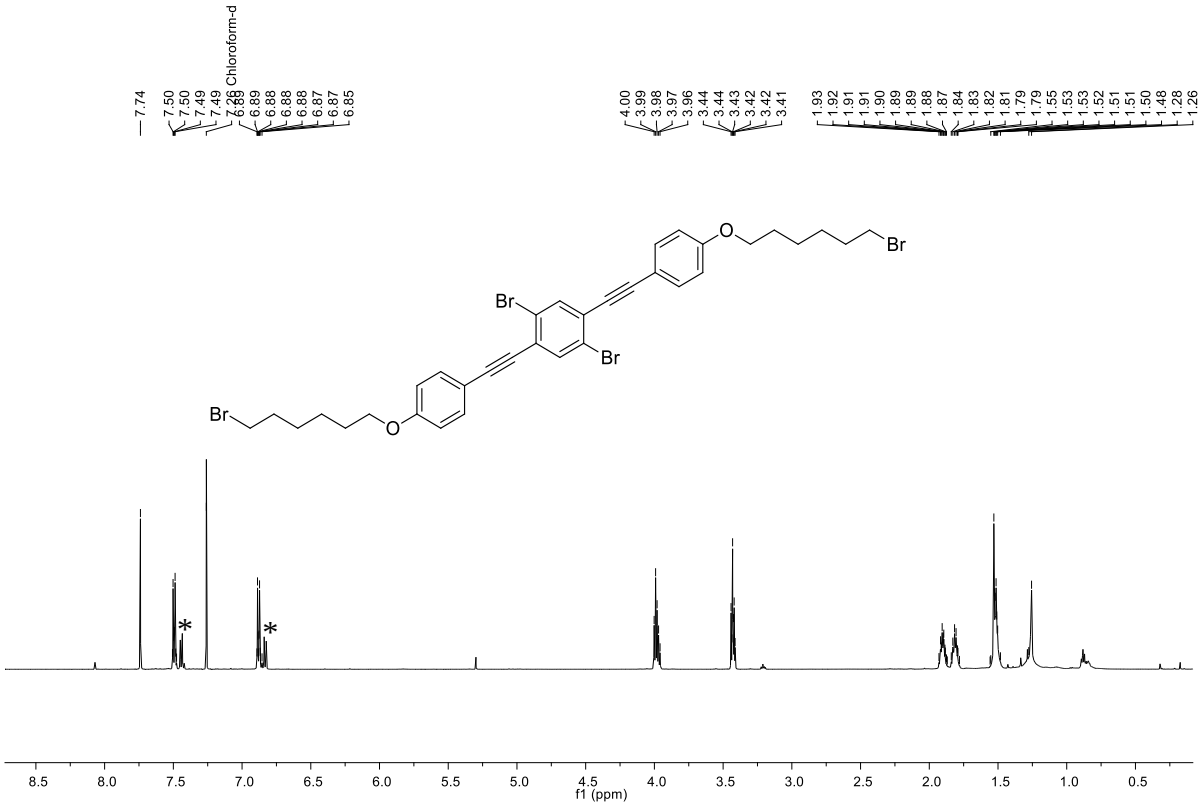


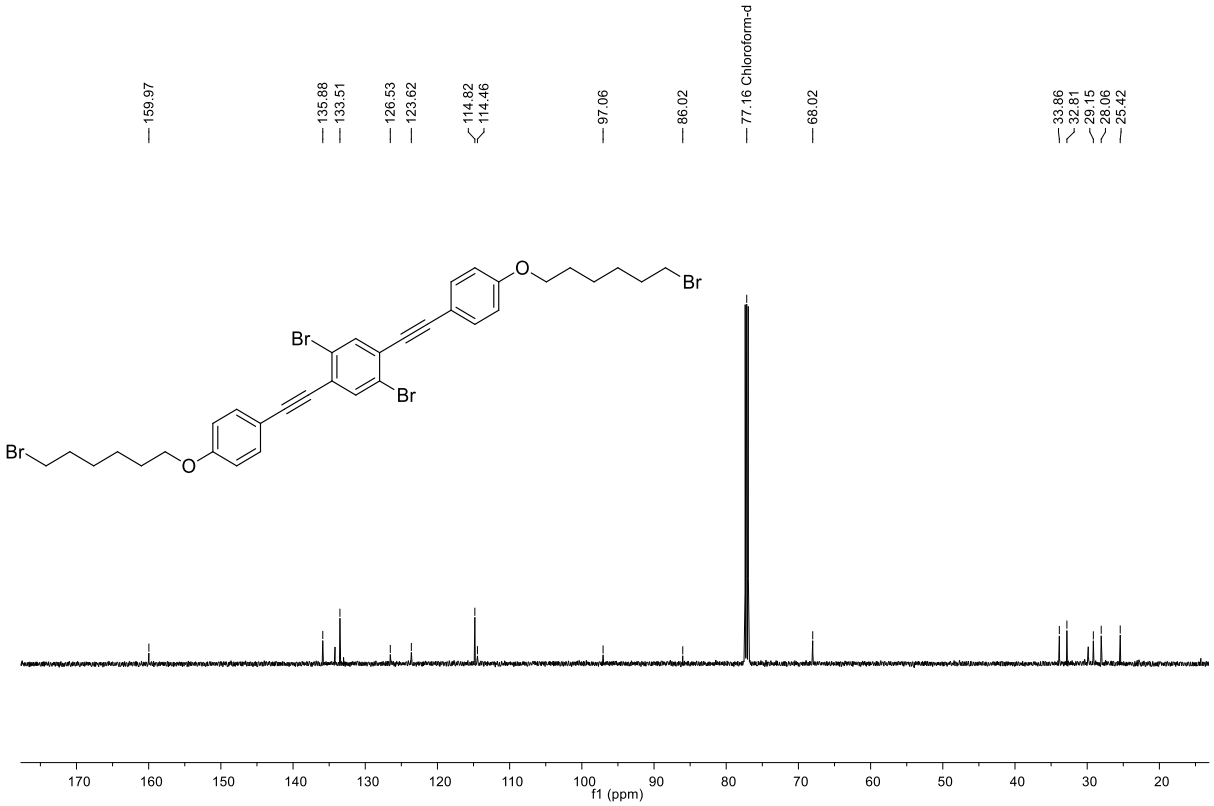
The small shielded doublets in the spectra of **EL$_{OD}$-Br** and **EL$_{HBr}$-Br** can be assigned to diacetylene byproducts resulting from a Glaser-type homocoupling of the alkynyl species and could be removed after polycondensation during the purification (Soxhlet-extraction) of the corresponding precursor polymers. The educt mass used in the polymerization reaction have been corrected based on the portion of present, but not reactive Glaser coupling product (*, represents signals of the byproduct)

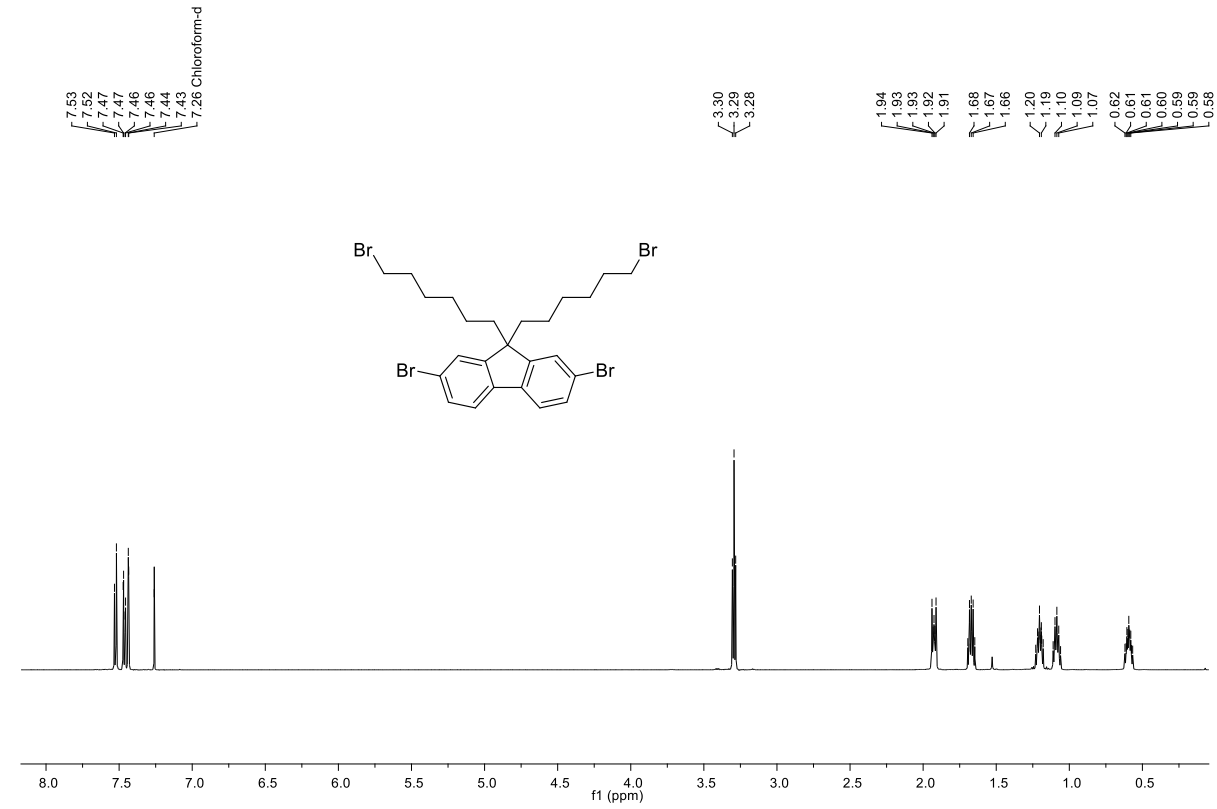
Glaser-type coupling byproduct

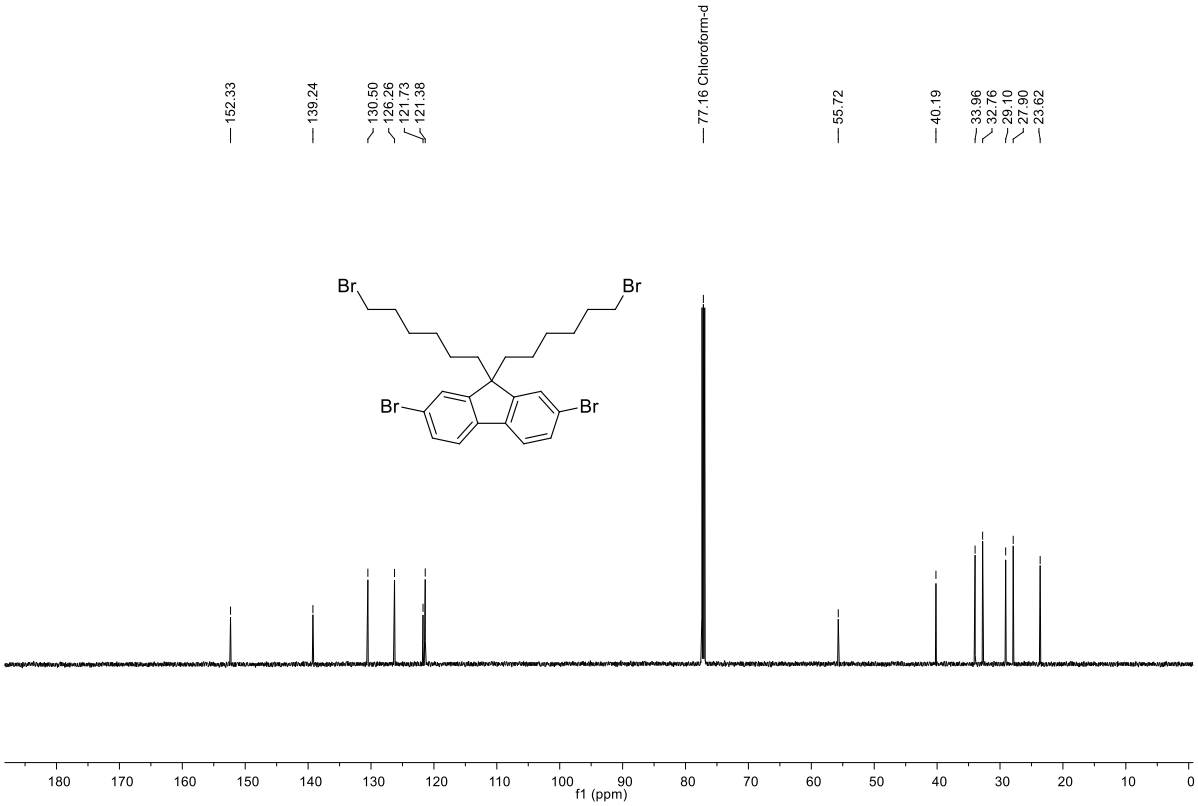


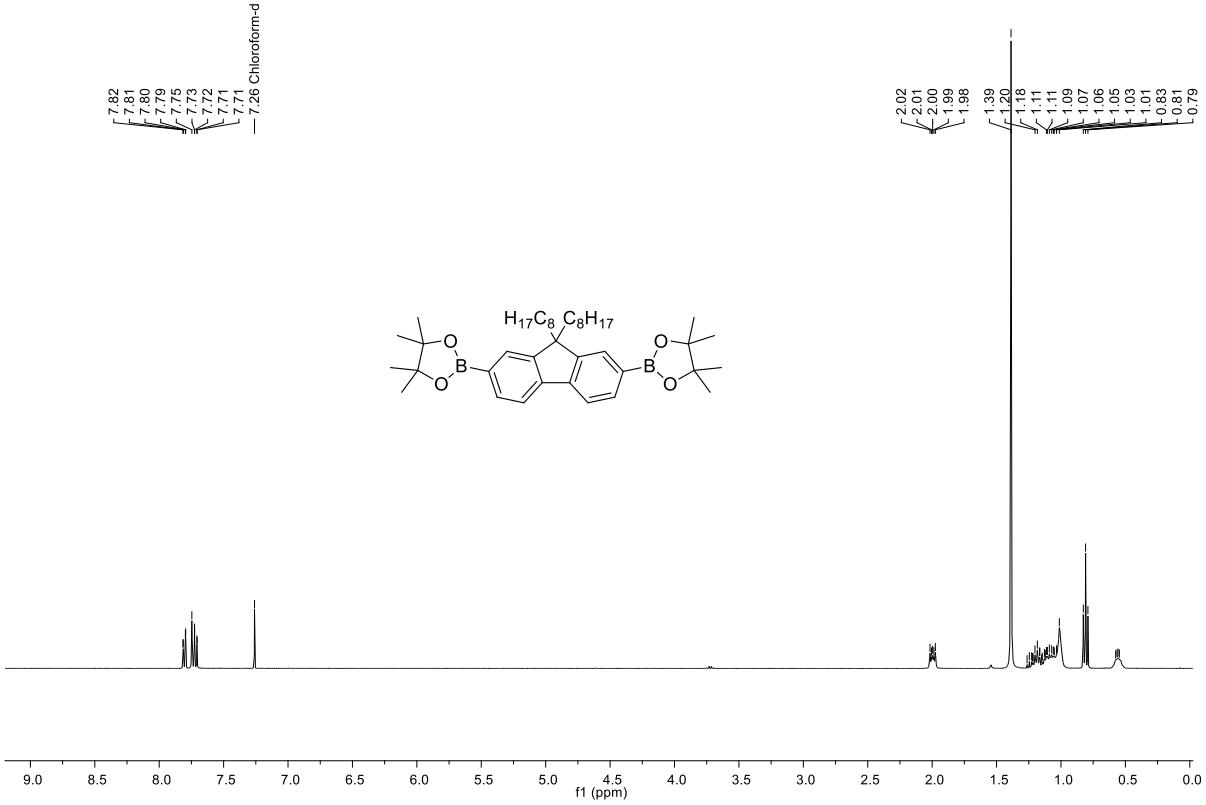

160.36
135.87
133.45
126.55
123.60
114.89
114.27
97.18
85.97
77.16 Chloroform-d
71.27
38.07
32.08
32.06
31.51
30.16
29.82
29.80
27.00
22.85
22.83
14.26
14.26
H17C8
C10H21
O
Br
Br
O
H21C10
C8H17
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

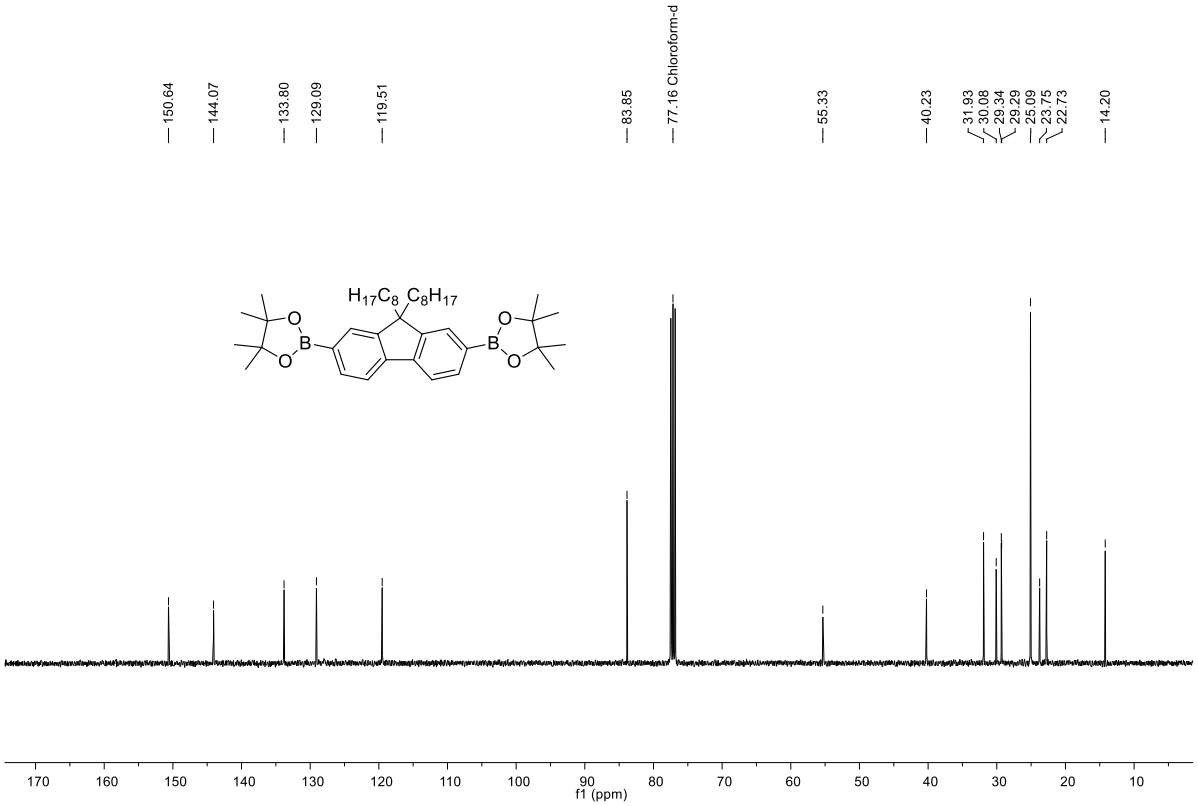

7.74
7.50
7.50
7.49
7.49
7.26 Chloroform-d
6.89
6.88
6.88
6.88
6.87
6.87
6.85
4.00
3.99
3.98
3.97
3.96
3.44
3.43
3.42
3.42
3.41
1.93
1.92
1.91
1.91
1.90
1.89
1.89
1.88
1.87
1.84
1.83
1.82
1.81
1.79
1.79
1.55
1.53
1.53
1.52
1.51
1.51
1.50
1.48
1.28
1.26
O
Br
Br
Br
Br
O
*
*
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

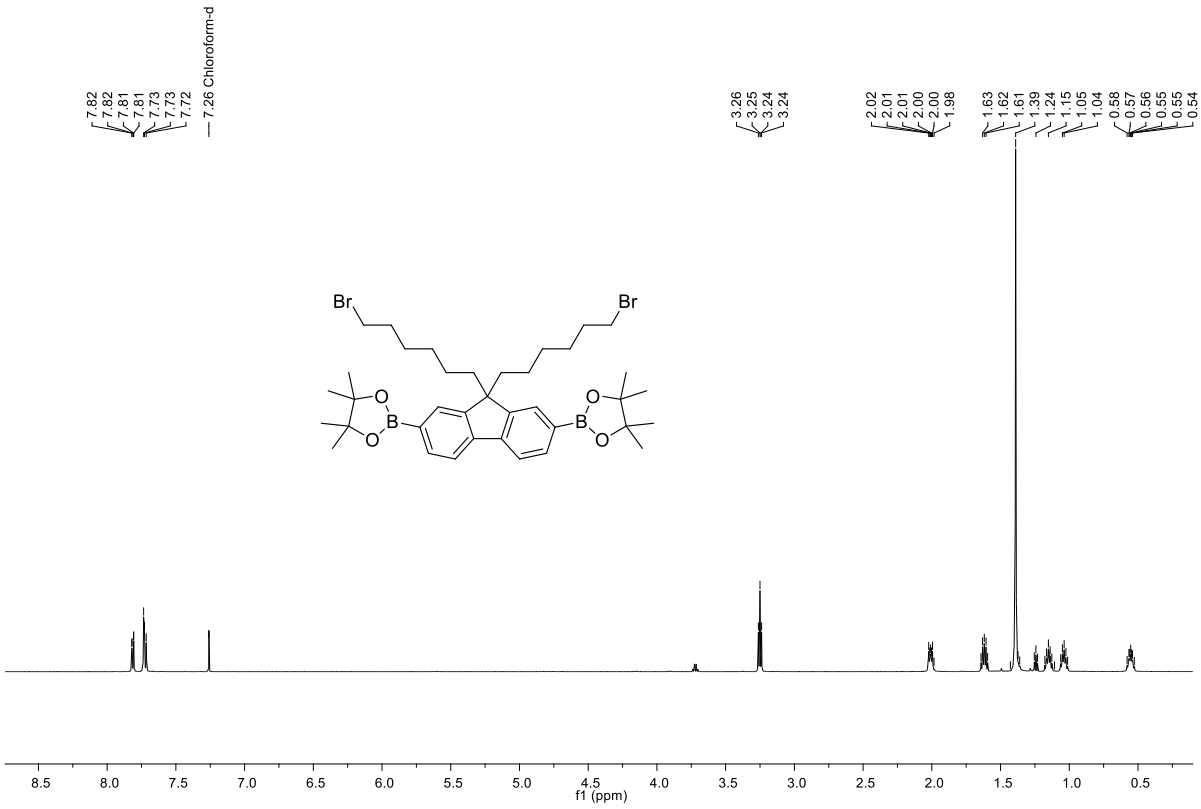

159.97
135.88
133.51
126.53
123.62
114.82
114.46
97.06
86.02
77.16 Chloroform-d
68.02
33.86
32.81
29.15
28.06
25.42
Br
Br
Br
O
O
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

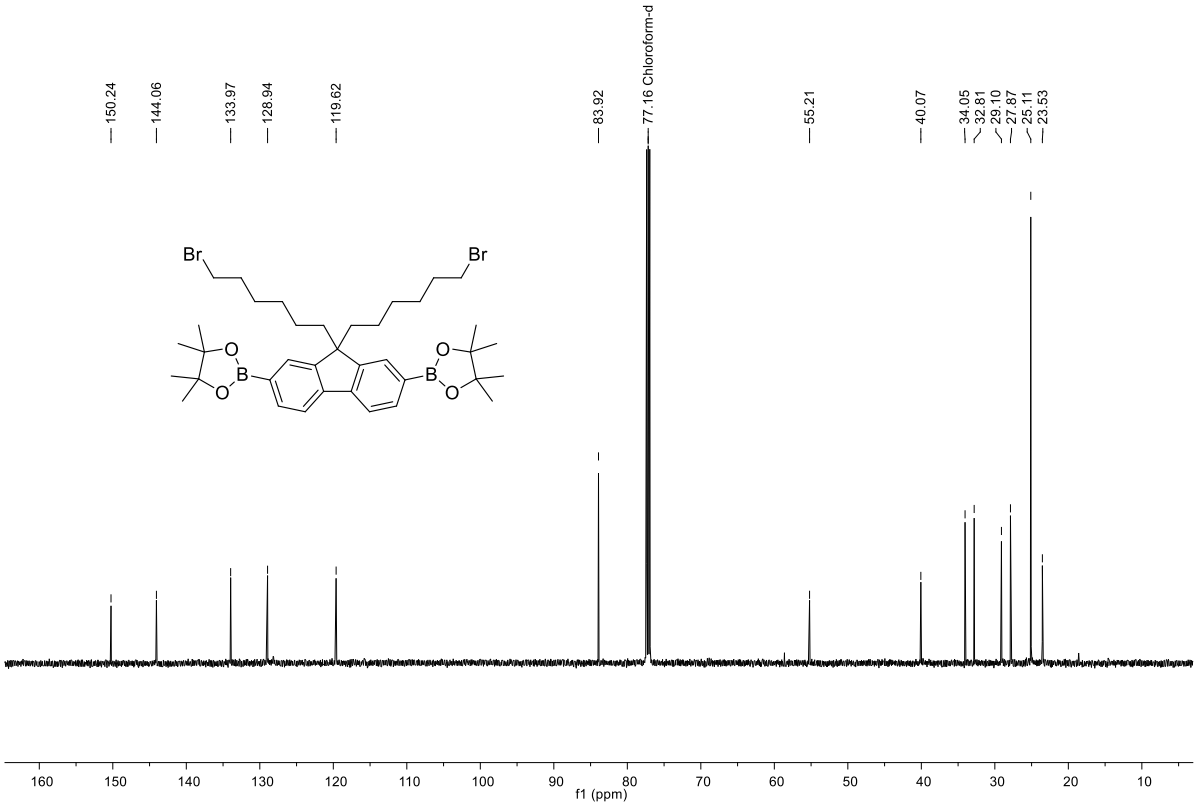

7.53
7.52
7.47
7.47
7.46
7.46
7.44
7.43
7.26 Chloroform-d
3.30
3.29
3.28
1.94
1.93
1.93
1.92
1.91
1.68
1.67
1.66
1.20
1.19
1.10
1.09
1.07
0.62
0.61
0.61
0.60
0.59
0.59
0.58
Br
Br
Br
Br
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

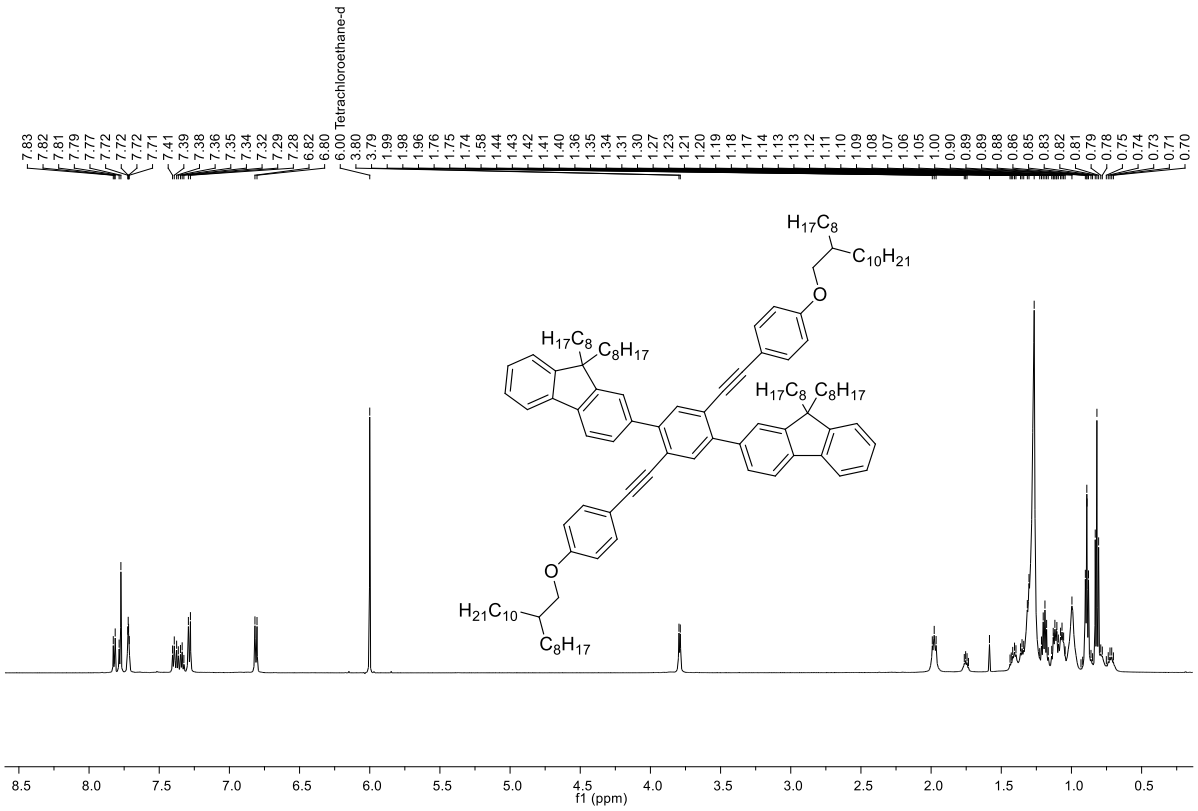

152.33
139.24
130.50
126.26
121.73
121.38
77.16 Chloroform-d
55.72
40.19
33.96
32.76
29.10
27.90
23.62
Br
Br
Br
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

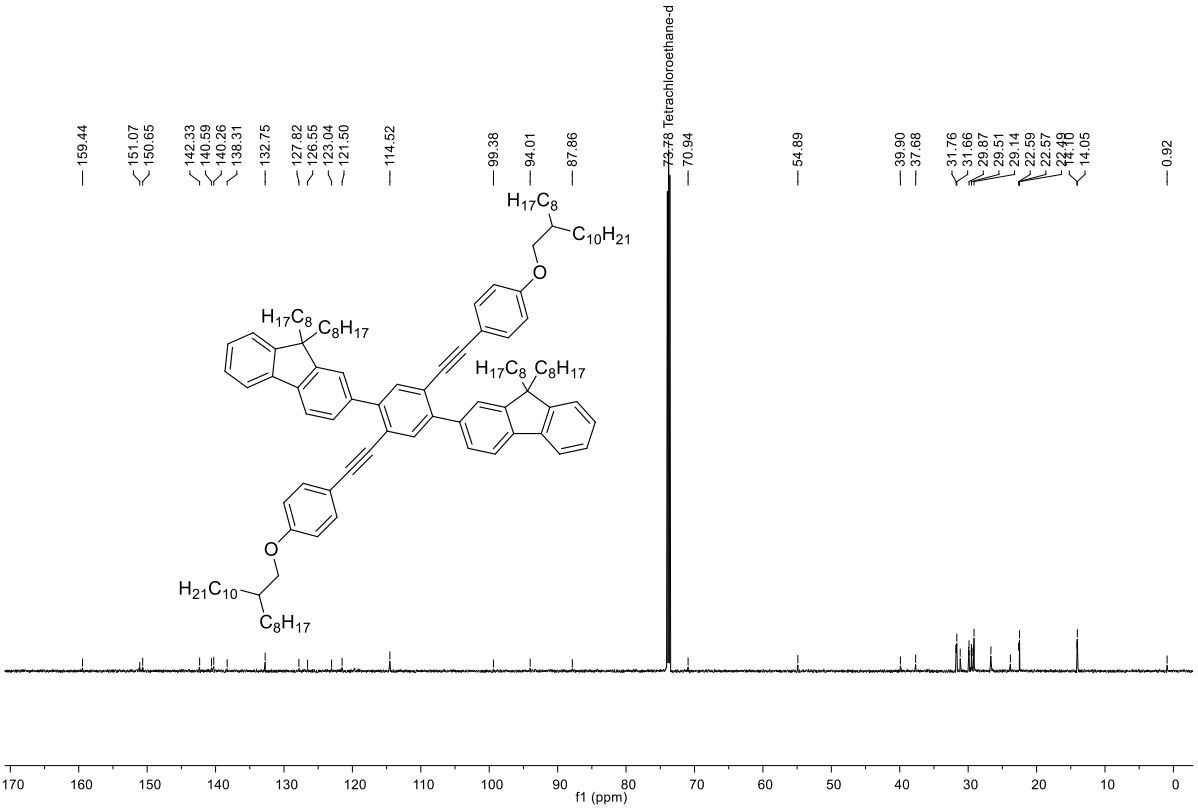

7.82
7.81
7.80
7.79
7.75
7.73
7.72
7.71
7.71
7.26 Chloroform-d
2.02
2.01
2.00
1.99
1.98
1.39
1.20
1.18
1.11
1.11
1.09
1.07
1.06
1.05
1.03
1.01
0.83
0.81
0.79
H17C8 C8H17
O
B
O
O
B
O
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

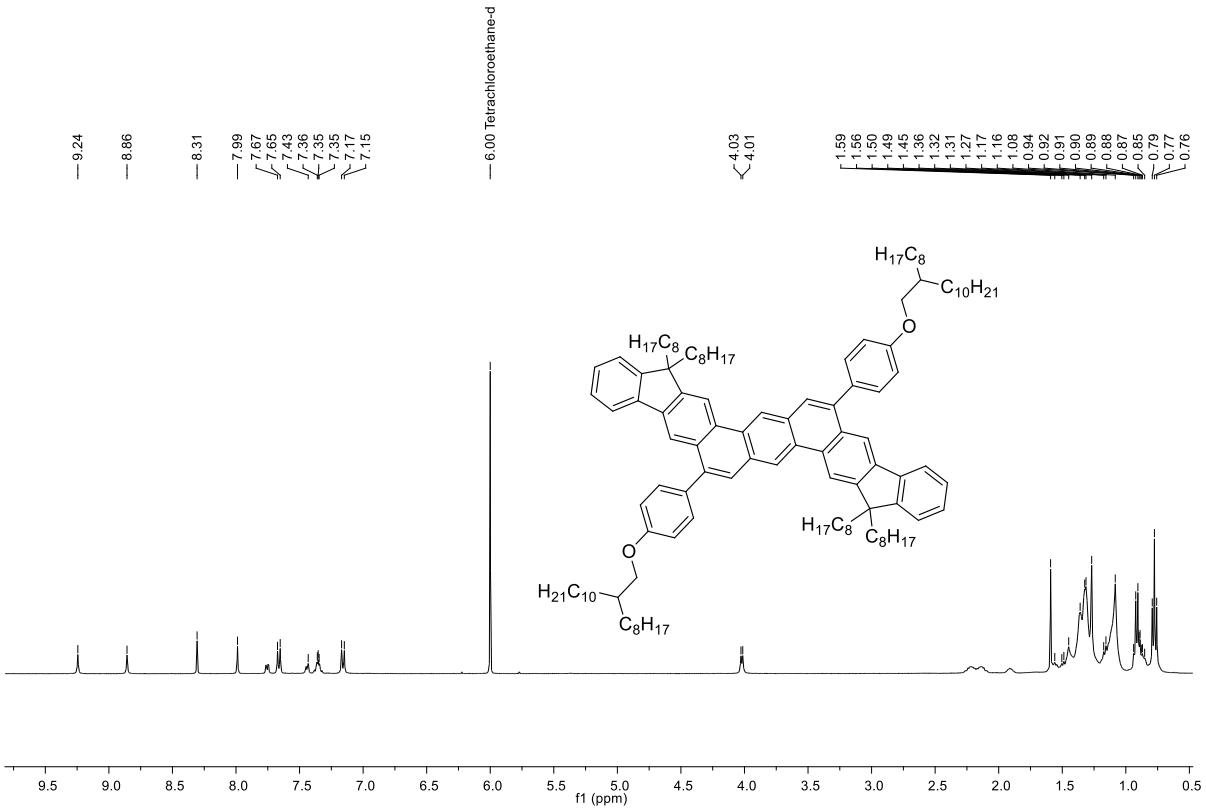

150.64
144.07
133.80
129.09
119.51
83.85
77.16 Chloroform-d
55.33
40.23
31.93
30.08
29.34
29.29
25.09
23.75
22.73
14.20
$H_{17}C_8$ C_8H_{17}
f1 (ppm)

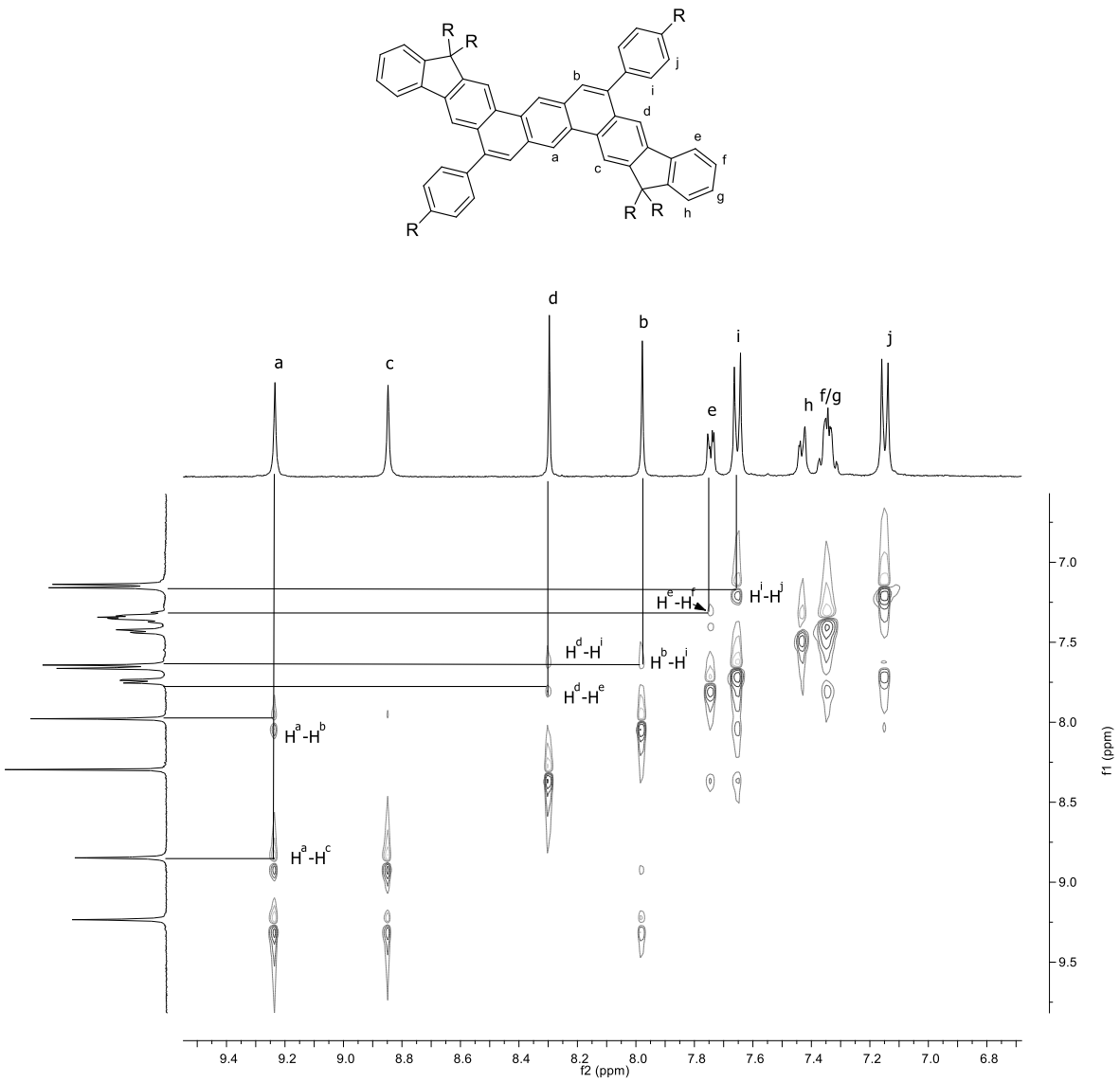

7.82
7.82
7.81
7.81
7.73
7.73
7.72
7.26 Chloroform-d
3.26
3.25
3.24
3.24
2.02
2.01
2.01
2.00
2.00
1.98
1.63
1.62
1.61
1.39
1.24
1.15
1.05
1.04
0.58
0.57
0.56
0.55
0.55
0.54
Br
Br
f1 (ppm)

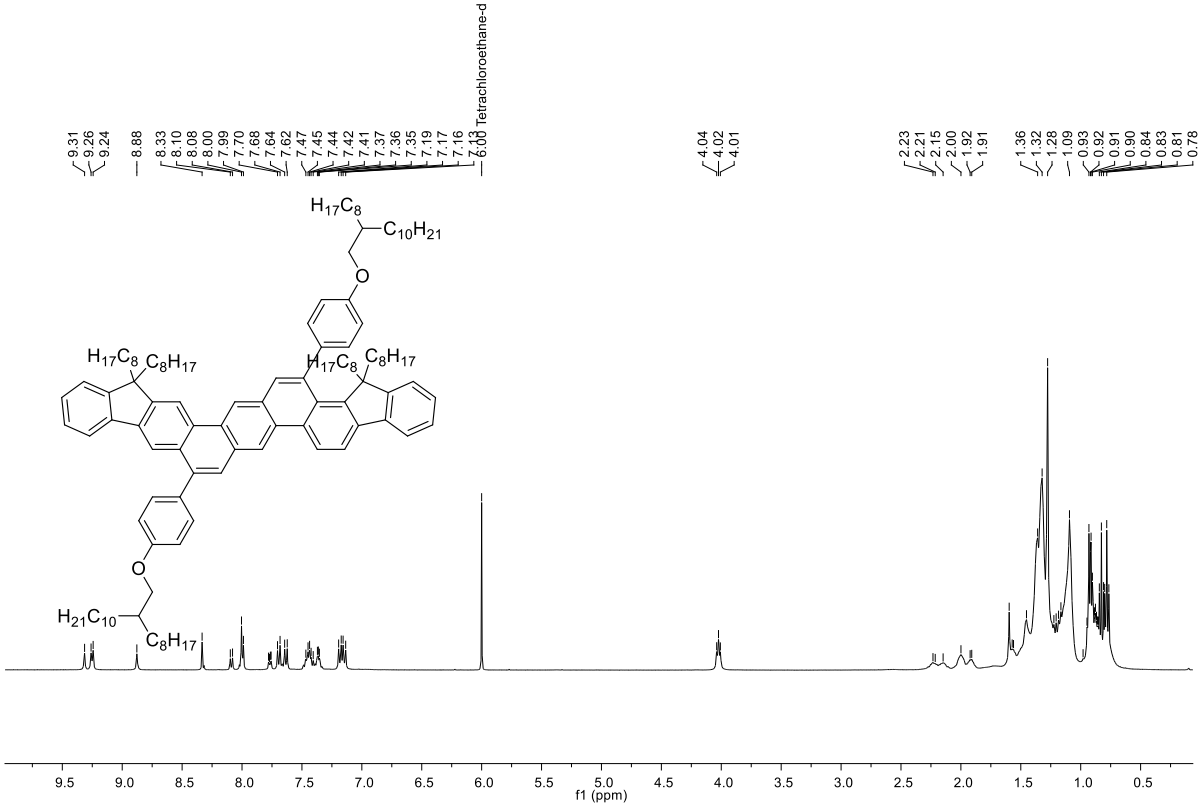

150.24
144.06
133.97
128.94
119.62
83.92
77.16 Chloroform-d
55.21
40.07
34.05
32.81
29.10
27.87
25.11
23.53
Br
Br
O
B
O
O
B
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.83
7.82
7.81
7.79
7.77
7.72
7.72
7.72
7.71
7.41
7.39
7.38
7.36
7.35
7.34
7.32
7.29
7.28
6.82
6.80
6.00 Tetrachloroethane-d
3.80
3.79
1.99
1.98
1.96
1.76
1.75
1.74
1.58
1.44
1.43
1.42
1.41
1.40
1.36
1.35
1.34
1.31
1.30
1.27
1.23
1.21
1.20
1.19
1.18
1.17
1.14
1.13
1.13
1.12
1.11
1.10
1.09
1.08
1.07
1.06
1.05
1.00
0.90
0.89
0.89
0.88
0.86
0.85
0.83
0.82
0.81
0.79
0.78
0.75
0.74
0.73
0.71
0.70
H17C8
C10H21
O
H17C8 C8H17
H17C8 C8H17
O
H21C10
C8H17
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
f1 (ppm)


159.44
151.07
150.65
142.33
140.59
140.26
138.31
132.75
127.82
126.55
123.04
121.50
114.52
99.38
94.01
87.86
73.78 Tetrachloroethane-d
70.94
54.89
39.90
37.68
31.76
31.66
29.87
29.51
29.14
22.59
22.57
22.49
14.10
14.05
0.92
f1 (ppm)


9.24
8.86
8.31
7.99
7.67
7.65
7.43
7.36
7.35
7.35
7.17
7.15
6.00 Tetrachloroethane-d
4.03
4.01
1.59
1.56
1.50
1.49
1.45
1.36
1.32
1.31
1.27
1.17
1.16
1.08
0.94
0.92
0.91
0.90
0.89
0.88
0.87
0.85
0.79
0.77
0.76
f1 (ppm)


R
R
R
R
R
R
a
b
c
d
e
f
g
h
i
j
a
c
d
b
e
i
h
f/g
j
H^a-H^b
H^a-H^c
H^d-H^e
H^d-H^i
H^b-H^i
H^e-H^f
H^i-H^j
9.4
9.2
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
f2 (ppm)
7.0
7.5
8.0
8.5
9.0
9.5
f1 (ppm)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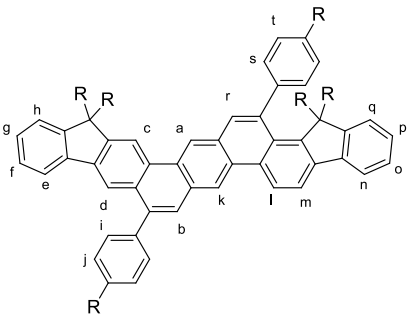
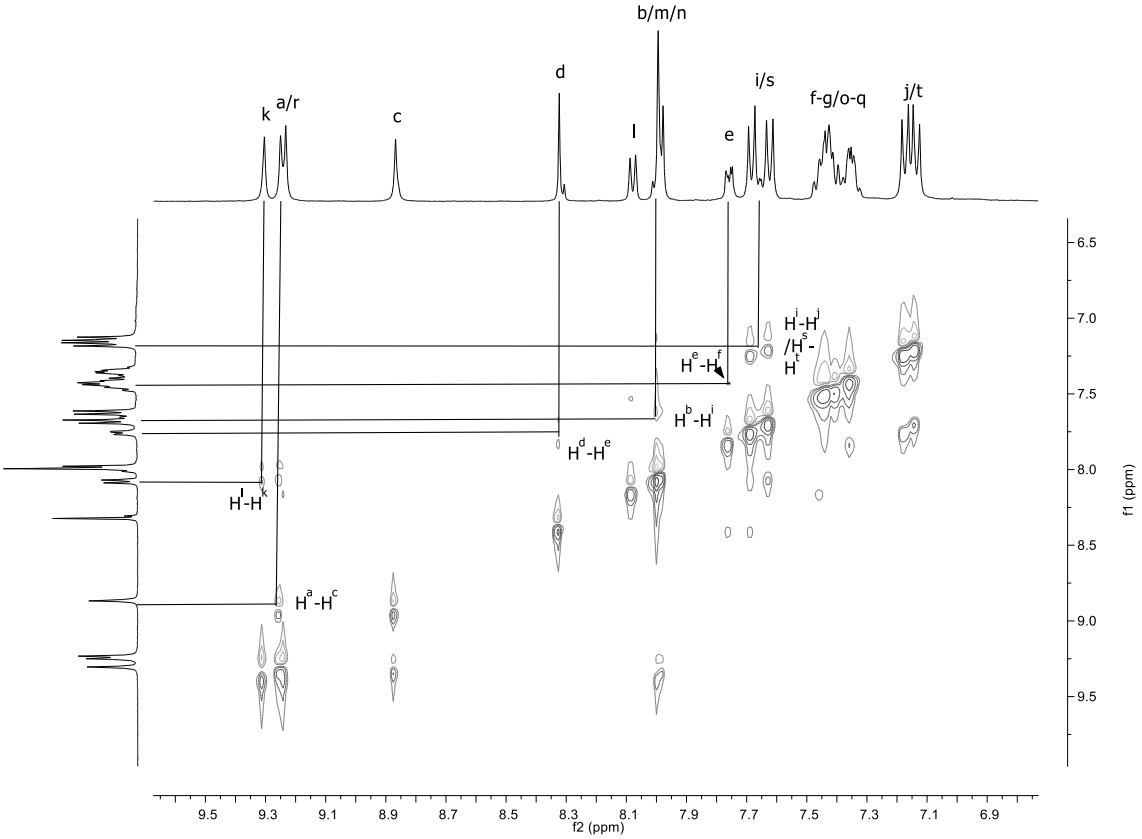
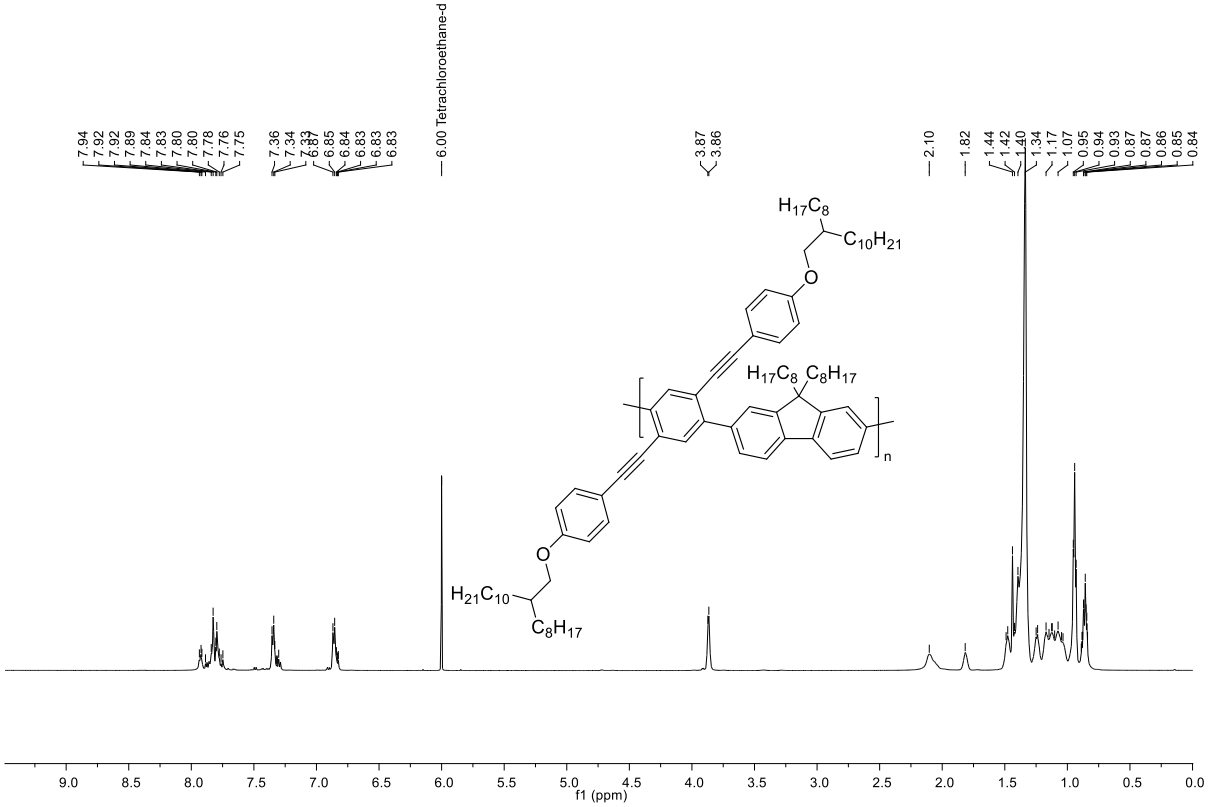
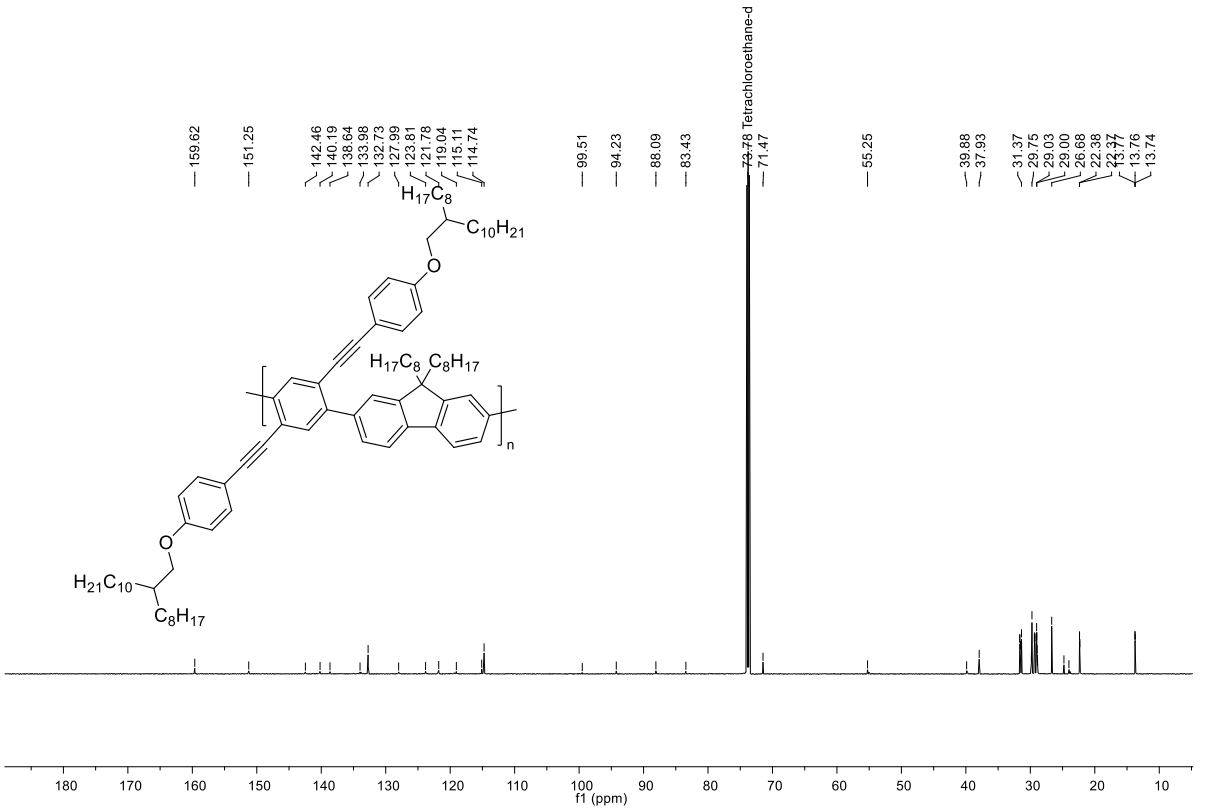
9.26
9.24
8.88
8.33
8.10
8.08
8.00
7.99
7.70
7.68
7.64
7.62
7.47
7.45
7.44
7.42
7.41
7.37
7.36
7.35
7.19
7.17
7.16
7.13
6.00 Tetrachloroethane-d
4.04
4.02
4.01
2.23
2.21
2.15
2.00
1.92
1.91
1.36
1.32
1.28
1.09
0.93
0.92
0.91
0.90
0.84
0.83
0.81
0.78
H17C8
C10H21
O
H17C8 C8H17
H17C8 C8H17
O
H21C10
C8H17
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
f1 (ppm)


R
R
R
R
R
t
s
r
q
p
o
n
m
l
k
d
i
b
j
h
g
f
e
c
a


b/m/n
d
i/s
f-g/o-q
j/t
k
a/r
c
l
e
H^l-H^k
H^a-H^c
H^d-H^e
H^b-H^j
H^e-H^f
H^j-H^j
/H^s-
H^t
f2 (ppm)
f1 (ppm)


7.94
7.92
7.92
7.89
7.84
7.83
7.80
7.80
7.78
7.76
7.75
7.36
7.34
7.33
6.87
6.85
6.84
6.83
6.83
6.83
6.00 Tetrachloroethane-d
3.87
3.86
2.10
1.82
1.44
1.42
1.40
1.34
1.17
1.07
0.95
0.94
0.93
0.87
0.87
0.86
0.85
0.84
H17C8
C10H21
O
H17C8 C8H17
n
O
H21C10
C8H17
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
f1 (ppm)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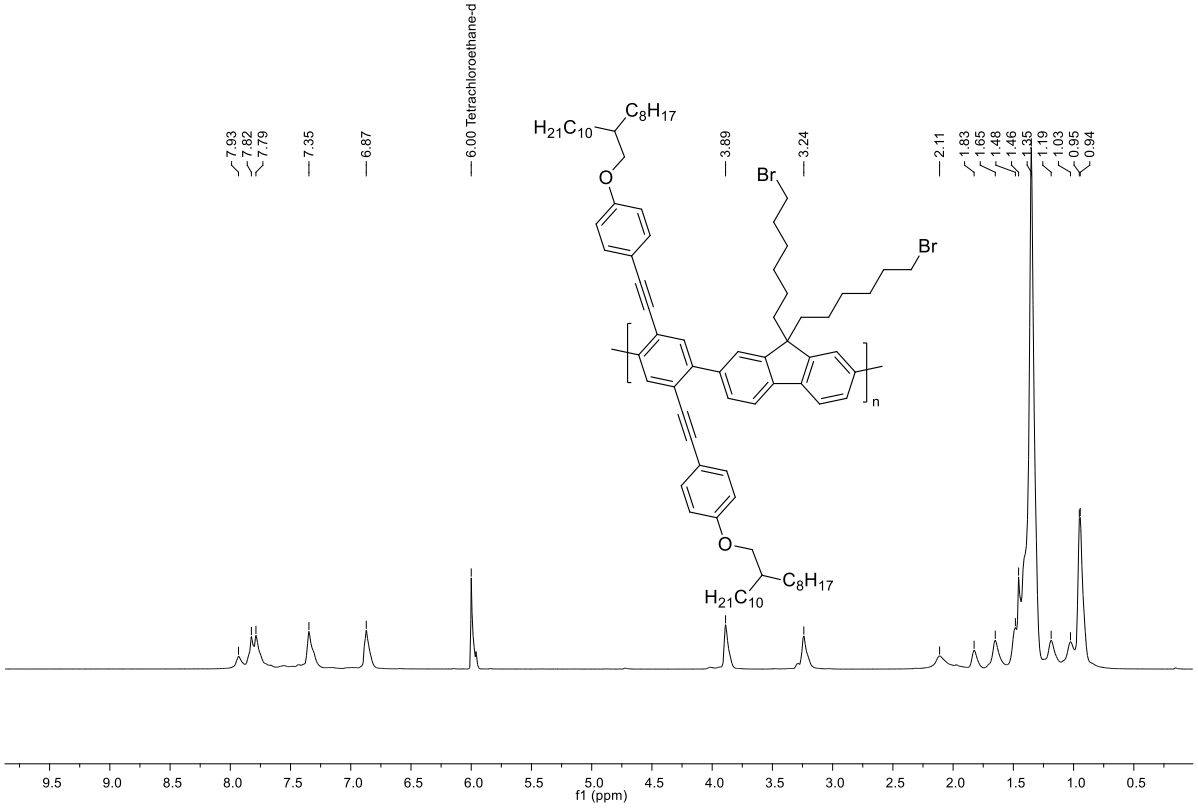
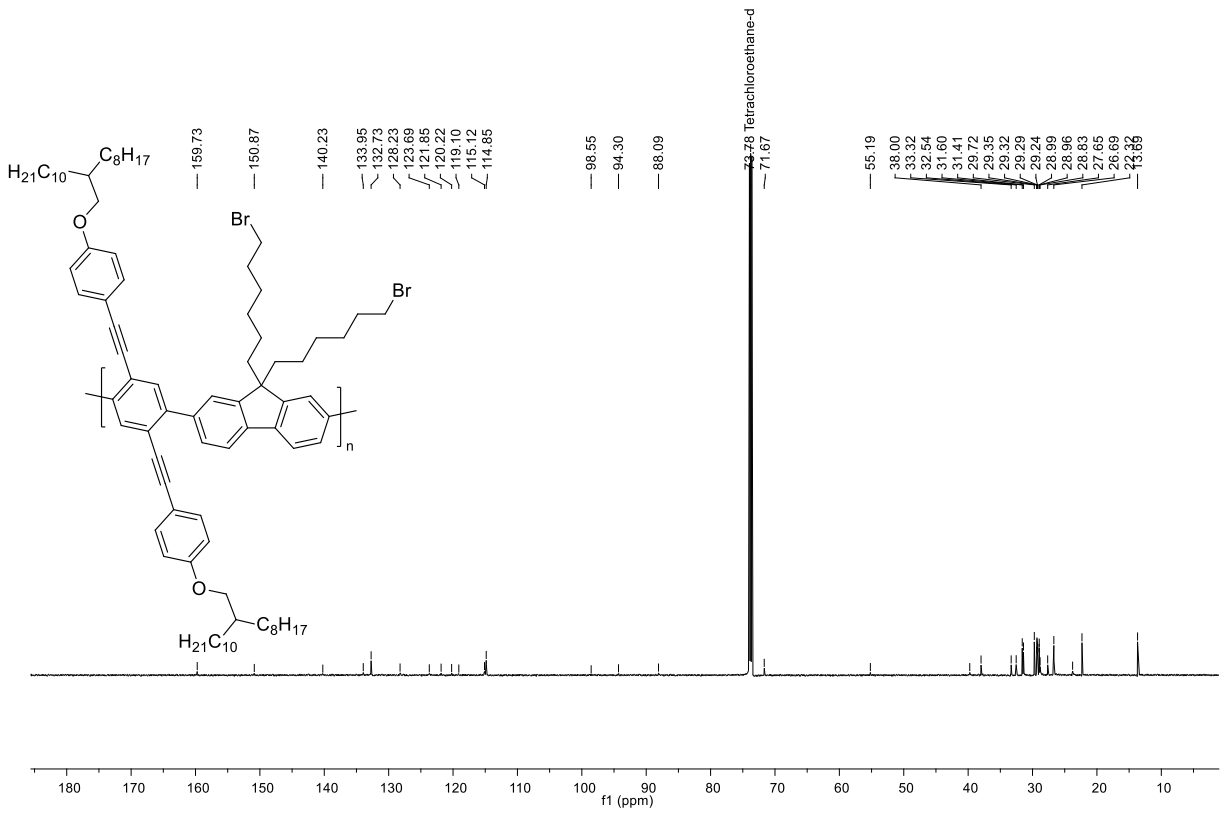
151.25
142.46
140.19
138.64
133.98
132.73
127.99
123.81
121.78
119.04
115.11
114.74
99.51
94.23
88.09
83.43
73.78 Tetrachloroethane-d
71.47
55.25
39.88
37.93
31.37
29.75
29.03
29.00
26.68
22.38
13.76
13.74
H17C8
C10H21
O
H17C8 C8H17
n
O
H21C10
C8H17
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


7.93
7.82
7.79
7.35
6.87
6.00 Tetrachloroethane-d
3.89
3.24
2.11
1.83
1.65
1.48
1.46
1.35
1.19
1.03
0.95
0.94
Br
Br
n
O
O
$H_{21}C_{10}$
C_8H_{17}
$H_{21}C_{10}$
C_8H_{17}
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
f1 (ppm)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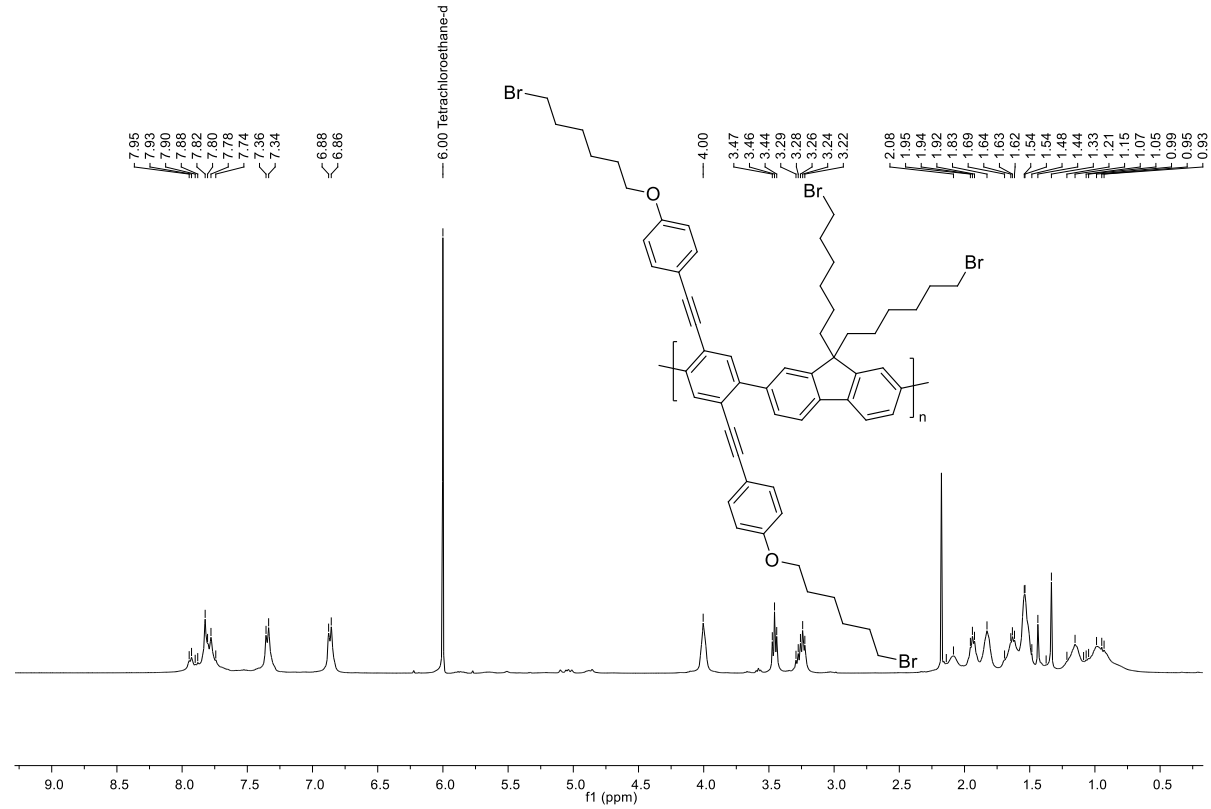
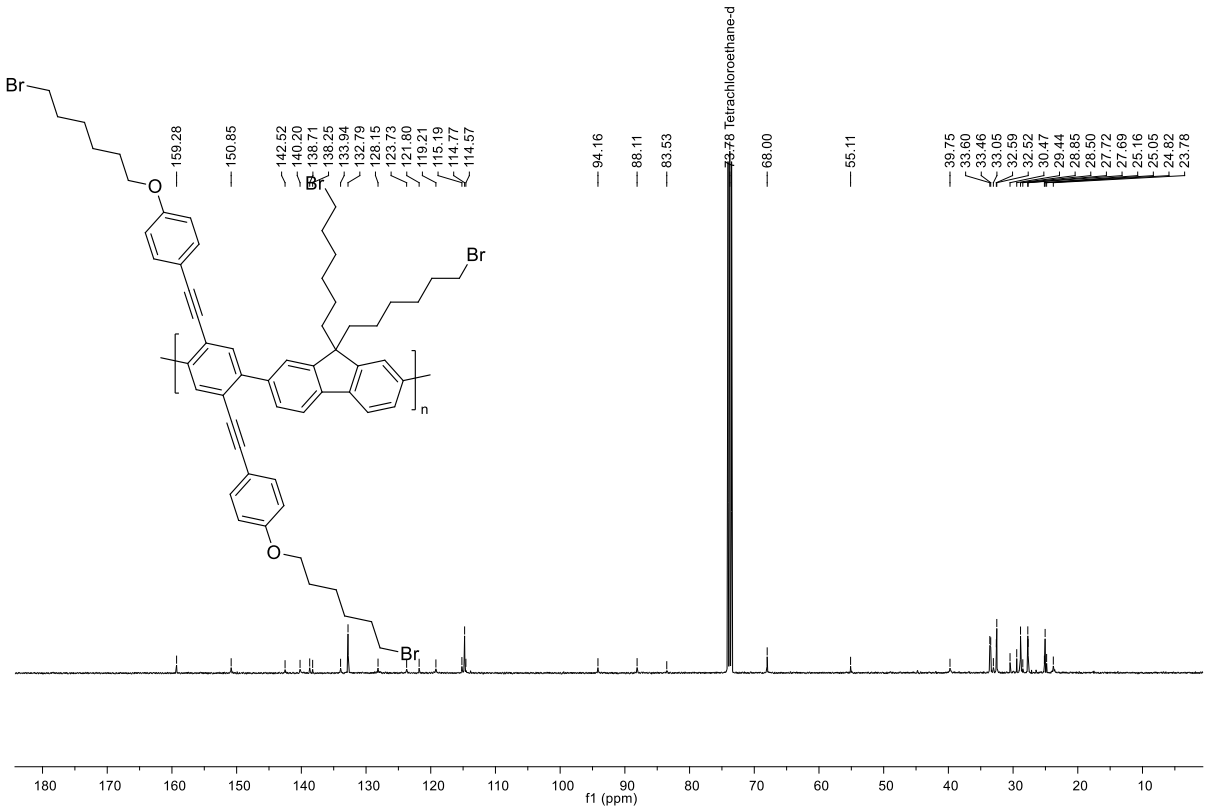
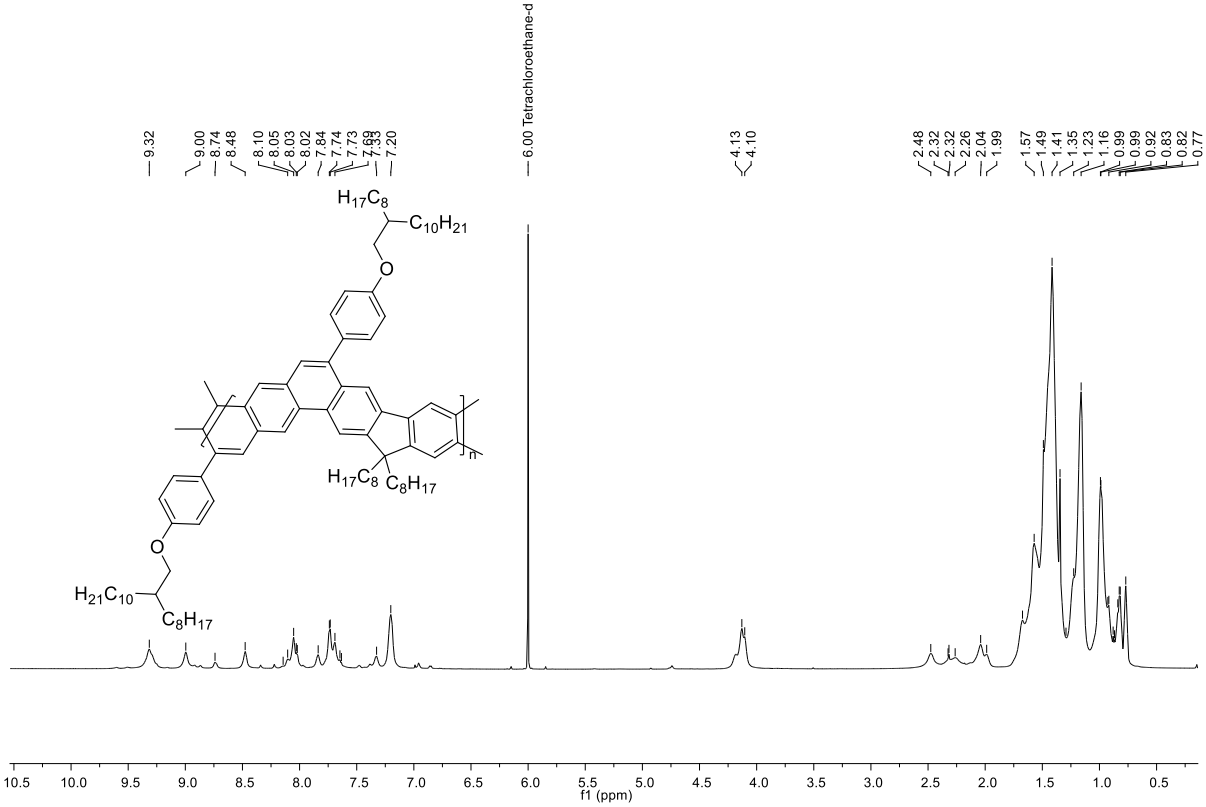
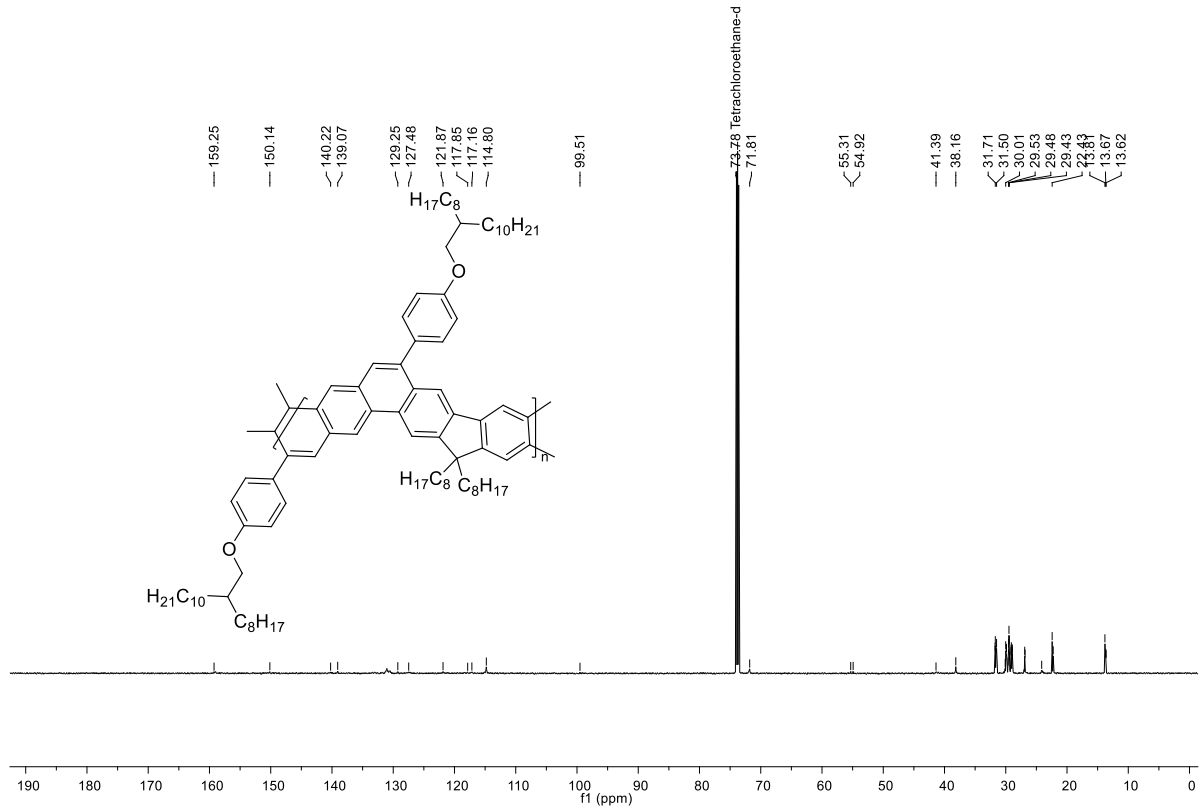
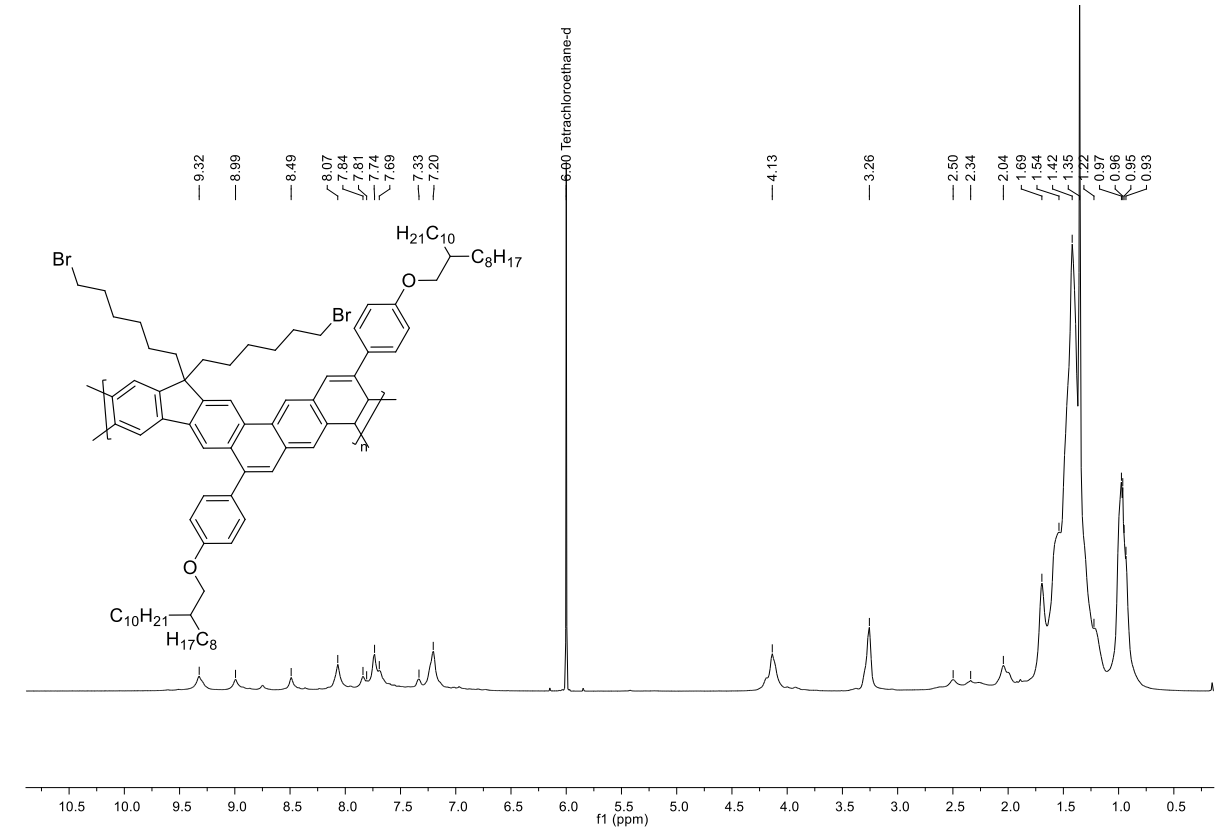
150.87
140.23
133.95
132.73
128.23
123.69
121.85
120.22
119.10
115.12
114.85
98.55
94.30
88.09
73.78 Tetrachloroethane-d
71.67
55.19
38.00
33.32
32.54
31.60
31.41
29.72
29.35
29.32
29.29
29.24
28.99
28.96
28.83
27.65
26.69
22.32
13.69
$H_{21}C_{10}$
C_8H_{17}
Br
Br
n
O
O
$H_{21}C_{10}$
C_8H_{17}
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

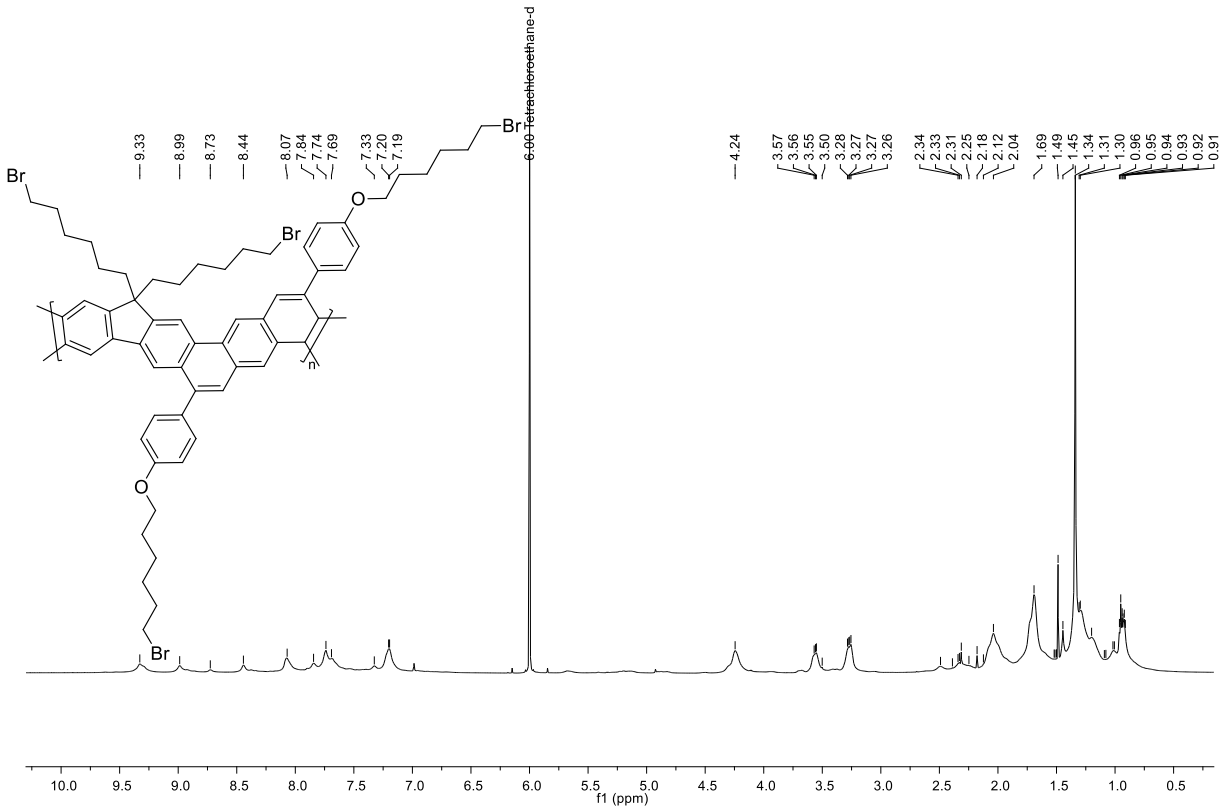

7.95
7.93
7.90
7.88
7.82
7.80
7.78
7.74
7.36
7.34
6.88
6.86
6.00 Tetrachloroethane-d
4.00
3.47
3.46
3.44
3.29
3.28
3.26
3.24
3.22
2.08
1.95
1.94
1.92
1.83
1.69
1.64
1.63
1.62
1.54
1.54
1.48
1.44
1.33
1.21
1.15
1.07
1.05
0.99
0.95
0.93
Br
O
Br
Br
n
O
Br
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

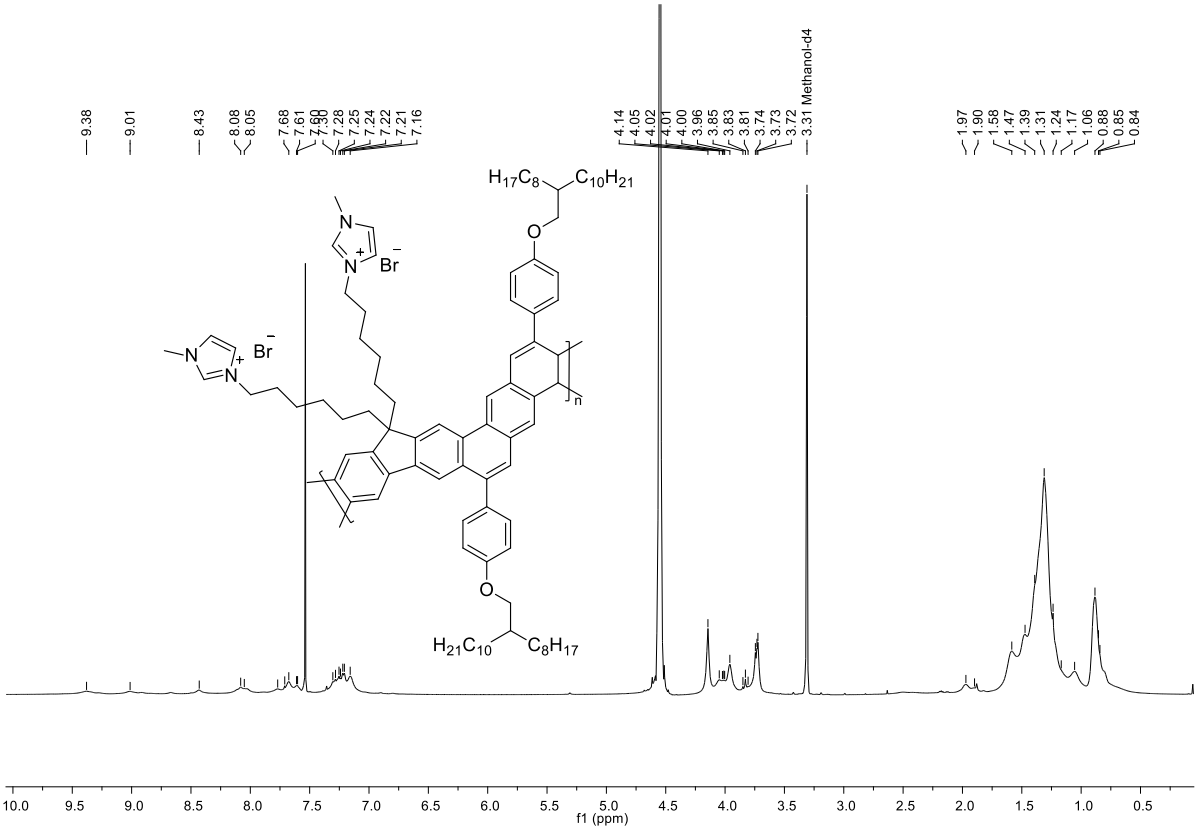

Br
O
159.28
150.85
142.52
140.20
138.71
138.25
133.94
132.79
128.15
123.73
121.80
119.21
115.19
114.77
114.57
94.16
88.11
83.53
Br
Br
n
O
Br
77.78 Tetrachloroethane-d
68.00
55.11
39.75
33.60
33.46
33.05
32.59
32.52
30.47
29.44
28.85
28.50
27.72
27.69
25.16
25.05
24.82
23.78
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


9.32
9.00
8.74
8.48
8.10
8.05
8.03
8.02
7.84
7.74
7.73
7.69
7.33
7.20
6.00 Tetrachloroethane-d
4.13
4.10
2.48
2.32
2.32
2.26
2.04
1.99
1.57
1.49
1.41
1.35
1.23
1.16
0.99
0.99
0.92
0.83
0.82
0.77
H17C8
C10H21
O
H17C8 C8H17
O
H21C10
C8H17
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
f1 (ppm)


159.25
150.14
140.22
139.07
129.25
127.48
121.87
117.85
117.16
114.80
99.51
73.78 Tetrachloroethane-d
71.81
55.31
54.92
41.39
38.16
31.71
31.50
30.01
29.53
29.48
29.43
22.43
13.81
13.67
13.62
H17C8
C10H21
O
H17C8 C8H17
O
H21C10
C8H17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.32
8.99
8.49
8.07
7.84
7.81
7.74
7.69
7.33
7.20
6.00 Tetrachloroethane-d
4.13
3.26
2.50
2.34
2.04
1.69
1.54
1.42
1.35
1.22
0.97
0.96
0.95
0.93
Br
Br
O
O
n
$H_{21}C_{10}$
C_8H_{17}
$C_{10}H_{21}$
$H_{17}C_8$
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
f1 (ppm)


9.33
8.99
8.73
8.44
8.07
7.84
7.74
7.69
7.33
7.20
7.19
6.00 Tetrachloroethane-d
4.24
3.57
3.56
3.55
3.50
3.28
3.27
3.27
3.26
2.34
2.33
2.31
2.25
2.18
2.12
2.04
1.69
1.49
1.45
1.34
1.31
1.30
0.96
0.95
0.94
0.93
0.92
0.91
Br
Br
Br
Br
O
O
n
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
f1 (ppm)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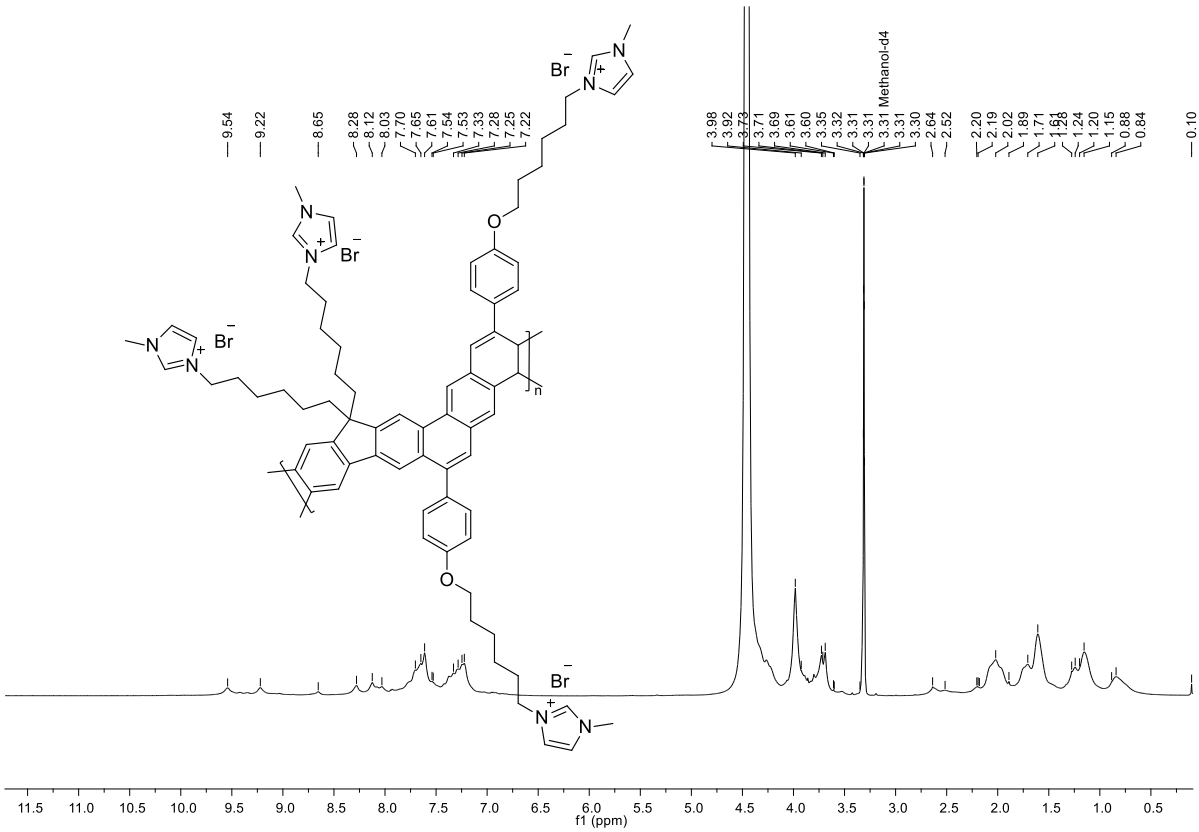
9.01
8.43
8.08
8.05
7.68
7.61
7.28
7.25
7.24
7.22
7.21
7.16
4.14
4.05
4.02
4.01
4.00
3.96
3.85
3.83
3.81
3.74
3.73
3.72
3.31 Methanol-d4
1.97
1.90
1.58
1.47
1.39
1.31
1.24
1.17
1.06
0.88
0.85
0.84
H17C8
C10H21
H21C10
C8H17
Br
n
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)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8.65
8.28
8.12
8.03
7.70
7.65
7.61
7.54
7.53
7.33
7.28
7.25
7.22
3.98
3.92
3.73
3.71
3.69
3.61
3.60
3.35
3.32
3.31
3.31 Methanol-d4
3.31
3.30
2.64
2.52
2.20
2.19
2.02
1.89
1.71
1.24
1.20
1.15
0.88
0.84
0.10
Br
n
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
f1 (ppm)