Supporting Information For:

Two-Dimensional, Acene-Containing Conjugated Polymers That Show Ratiometric Fluorescent Response to Singlet Oxygen

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1. General Considerations

All synthetic manipulations were performed under standard air-free conditions under an atmosphere of argon gas with magnetic stirring unless otherwise mentioned. Flash chromatography was performed using silica gel (230-400 mesh) as the stationary phase. NMR spectra were acquired on a Bruker Avance III 500 or Bruker DPX-300 spectrometer. Chemical shifts are reported relative to residual protonated solvent for $CHCl_3$. High-resolution mass spectra (HRMS) were obtained at the MIT Department of Chemistry Instrumentation Facility using a peak-matching protocol to determine the mass and error range of the molecular ion. Molecular weight distribution measurements of the polymers were conducted with a Shimadzu Gel Permeation Chromatography (GPC) system equipped with a Tosoh TSKgel GMHhr-M mixed-bed column and guard column using either UV or refractive index detectors. The column was calibrated with low polydispersity poly(styrene) standards (Tosoh, PSt Quick Kit) with THF as the mobile phase eluting at 0.75 mL/min. All reactants and solvents were purchased from commercial suppliers and used without further purification, unless otherwise noted.

2. Optical Experiments

All solution optical spectra were acquired of samples in quartz cuvettes (NSG Precision Cells). Electronic absorbance spectra were acquired with a Varian Cary-100 instrument in double-beam mode using a solvent-containing cuvette for background subtraction spectra. Fluorescence emission spectra were obtained by using a PTI Quantum Master 4 equipped with a 75 W Xe lamp. All fluorescence spectra are corrected for the output of the lamp and the dependence of detector response to the wavelength of emitted light. Fluorescence spectra were acquired using sample absorbances less than 0.1 OD. Fluorescence quantum yields were determined relative to either quinine sulfate in 0.1 N H_2SO_4 or Coumarin 6 in ethanol. Irradiation of the methylene blue photosensitizer to generate $^1O_2$ was performed with 200W Hg/Xe lamp (Newport-Oriel) equipped with either 1) a condensing lens, recirculating water, shutter, and 635 nm high-pass filters, or 2) a 635 nm laser diode (4.5 mW). Time-resolved fluorescence data was collected using a PTI time-correlated single-photon counting instrument with a pulsed LED operating at 403 nm. The instrumental response function (IRF) was determined using a diluted suspension of Ludox colloidal silica.

2a. Fluorescence response to singlet oxygen

A cuvette containing the test sample solution was irradiated for numerous timed intervals. Both the absorbance and fluorescence spectra were taken after each interval of irradiation. The absorbance for both methylene blue and samples was approximately 0.1 OD.

2b. Kinetics

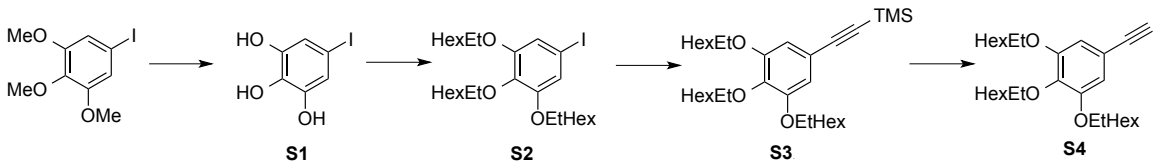
A stock solution of methylene blue was prepared in $CHCl_3$ to give an absorbance of ~1.0 at its peak. 9,10-diphenylanthracene (DPA) was used as a reference. DPA, **A2**, or **P2** was dissolved in 3.5 mL MB solution; the final concentration of the corresponding compound in the sample was 32 μM. The solution was irradiated for timed intervals, with

acquisition of an absorbance spectrum after each interval until the spectra stopped changing between intervals of irradiation. The wavelengths used for the analysis of kinetics were the peaks of the highest absorbance of the compounds.

3. Detailed synthetic procedures:

3a. Synthesis of P1 and P2:

Synthesis of 3,4,5-trialkoxyethynylbenzene



S1 S2 S3 S4

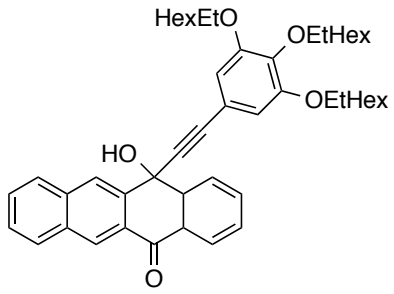
S1. Prepared following the established literature procedure.[1] JACS, 2008, 130 (8), 2535.

S2. Compound **S1** (562 mg, 2.23 mmol, 1.0 eq) and K_2CO_3 (2.5 g, 18 mmol, 8.0 eq) were dissolved in 12 mL of dry DMF at room temperature under argon. 2-ethylhexylbromide (1.8 mL, 10. mmol, 4.5 eq) was then added to this solution under an argon atmosphere. The mixture was heated to 95 °C and stirred for 4 days. The mixture was then cooled to room temperature and quenched with 10% aq NaOH. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.5:1) to yield **S2**. Yield: 1.05 g (80%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 6.86 (s, 2H), 3.84-3.78 (m, 6H), 1.77-1.73 (m, 2H), 1.71 -1.66 (m, 1H), 1.56-1.33 (m, 24H), 0.96-0.91 (m, 18H). ^{13}C NMR (125 MHz, $CDCl_3$): δ 154.2, 138.2, 115.6, 85.6, 75.9, 71.4, 40.6, 39.6, 30.5, 29.3, 29.1, 23.8, 23.7, 23.1, 23.0, 14.1, 14.1, 11.2, 11.01.

S3. A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (25 mg, 0.036 mmol, 0.02 eq) and CuI (14 mg, 0.072 mmol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, **S2**(1.05 g, 1.8 mmol, 1 eq) was dissolved in 63 mL of Et_3N:THF(1:3, v/v) and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. While stirring, trimethylsilylacetylene (0.31 mL, 2.2 mmol, 1.2 eq) was added dropwise to the flask. The reaction mixture was stirred for 2 days at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.5:1) to yield **S3**. Yield: 940 mg (94%). ^{1}H NMR (300 MHz, CDCl3): δ 6.65 (s, 2H), 3.81 (m, 6H), 1.72-1.64 (m, 3H), 1.5-1.31 (m, 24H), 0.92-0.88 (m, 18H), 0.23 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 153.2, 139.3, 117.5, 110.1, 105.8, 92.6, 76.1, 71.3, 40.8, 39.7, 30.7, 29.48, 29.47, 29.3, 23.97, 23.9, 23.3, 23.2, 14.29, 14.25, 11.37, 11.35, 11.2, 0.20.

S4. Compound **S3** (940 mg, 1.7 mmol, 1 eq) was dissolved in a mixture of MeOH (17 mL), Et_2O (17 mL) and 10% $NaOH_{(aq)}$ (7 mL). The reaction mixture was stirred overnight at room temperature. The reaction was stopped by acidification with 10% aq

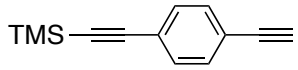
HCl. Organics were extracted twice with Et_2O, and combined organic phases were washed with brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.5:1) to yield **S4**. Yield: 652 g (79%). ^{1}H NMR (500 MHz, CDCl3): δ 6.71 (s, 2H), 3.88-3.81 (m, 6H), 3.02 (s, 1H), 1.79-1.67 (m, 3H), 1.55-1.28 (m, 24H), 0.96-0.91 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 153.2, 139.4, 116.3, 110.1, 84.2, 76, 75.7, 71.2, 40.6, 39.6, 30.5, 29.3, 29.1, 23.8, 23.7, 23.2, 23.1, 14.2, 14.1, 11.2, 11.1.



1

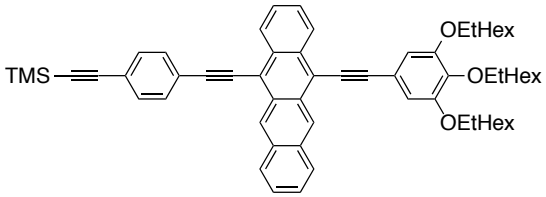
Compound 1.

Compound **3,4,5-triethylhexyloxyethynylbenzene** (195 mg, 0.4 mmol, 1eq) was dissolved in 2.1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.23 mL, 0.36 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing 5,12- naphthacenequinone (104 mg, 0.4 mmol, 1 eq), which was dissolved in 1.8 mL of dry THF and cooled to O °C, dropwisely via syringe. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction was quenched by addition of 10 mL of ice cold DI H_2O and then filtered via vacuum filtration by washing about 30 mL of THF:H_2O (1:1, v/v). Saturated NH_4Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **1**. Yield: 190 mg (63%). ^{1}H NMR (500 MHz, CDCl3): δ 8.71 (s, 1H), 8.66 (s, 1H), 8.28 (d, J=8 Hz, 1H), 8.2 (m, 1H), 7.97-7.94 (m, 2H), 7.75-7.72 (m, 1H), 7.63-7.6 (m, 1H), 7.57-7.54 (m, 1H), 7.5-7.47 (m, 1H), 6.63 (s, 2H), 3.84-3.74 (m, 6H), 1.74-1.57 (m, 3H), 1.54-1.28 (m, 24H), 0.96-0.89 (m, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 183.5, 153.1, 144.4, 139.6, 139.3, 135.9, 134.3, 132.7, 129.9, 129.8, 129.3, 129, 128.9, 128.2, 128.1, 127.7, 127.4, 127.2, 127.1, 116.2, 109.7, 89.9, 86.9, 76.1, 71.3, 67, 40.6, 39.6, 30.5, 29.31, 29.29, 29.1, 23.8, 23.7, 23.1, 23.06, 14.13, 14.1, 11.19, 11.18, 11.16, 11.07.

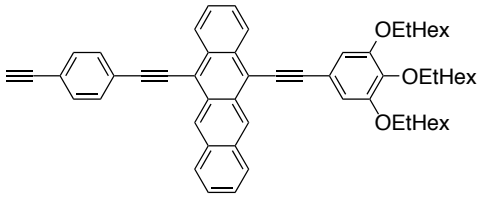


S5

S5. 1-Ethynyl-4`-trimethylsilylethynyl)benzene: Prepared following the established literature procedure.[2]



2a



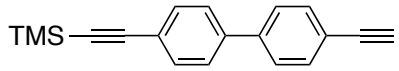
2

Compound 2.

Compound 2a. Compound **1-Ethynyl-4`-(trimethylsilylethynyl)benzene** (271 mg, 1.37 mmol, 4eq) was dissolved in 4.3 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.83 mL, 1.33 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 75 minutes and then transferred to the flask containing compound **1** (255 mg, 0.34 mmol, 1 eq), which was dissolved in 2.2 mL of dry THF and cooled to -78 °C, via cannula transfer. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction mixture was then treated with 10% HCl aqueous solution saturated with $SnCl_2$ dihydrate and left overnight stirring. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **2a**. Yield: 210 mg (67%). ^{1}H NMR (500 MHz, CDCl3): δ 9.33 (s, 1H), 9.3 (s, 1H), 8.72-8.68 (m, 2H), 8.16-8.13 (m, 2H), 7.84-7.8 (m, 2H), 7.65-7.61 (m, 4H), 7.53-7.51 (m, 2H), 7.05 (s, 2H), 4.02-3.95 (m, 6H), 1.87-1.83 (m, 2H), 1.8-1.74 (m, 1H), 1.68-1.28 (m, 24H), 1.02-0.94 (m, 18H), 0.33 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 153.5, 139.6, 132.5, 132.4, 132.34, 132.28, 132.26, 132.24, 132.17, 132.14, 131.6, 131.5, 129.9, 128.6, 128.5, 127.6, 127.3, 127.2, 126.83, 126.79, 126.58, 126.24, 126.14, 126.11, 126.05, 125.96, 125.93, 123.9, 123.6, 123.4, 122.3, 119.1, 118.9, 117.7, 117.6, 117.5, 110.1, 109.8, 104.7, 104.14, 104.1, 102.9, 102.6, 96.8, 89.2, 89.1, 85.7, 83.3, 79.3, 76.2, 71.5, 40.7, 39.7, 30.6, 30.5, 29.38, 29.36, 29.35, 29.18, 23.89, 23.75, 23.19, 23.13, 14.19, 14.14, 11.27, 11.25, 11.23, 11.19. HRMS (ESI) calcd for $C_{63}H_{76}O_3Si$ $(M+H)^+$, 909.5636, found, 909.5630.

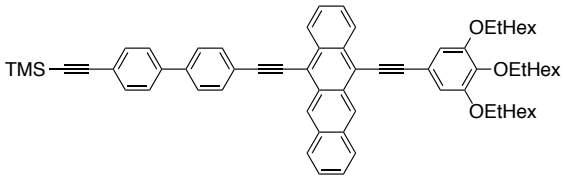
Compound **2a** (207 mg, 0.23 mmol, 1 eq) and K_2CO_3 (94 mg, 0.68 mmol, 3 eq) were dissolved in mixture of THF (4 mL), and MeOH (4 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 180 mg (94%). ^{1}H NMR (300 MHz, CDCl3): δ 9.29 (s, 1H), 9.26 (s, 1H), 8.67 (m, 2H), 8.12 (m, 2H), 7.80-7.78 (m, 2H),

7.62-7.60 (m, 4H), 7.5 (m, 2H), 7.01 (m, 2H), 3.97-3.93 (m, 6H), 3.24 (s, 1H), 1.82-1.74 (m, 3H), 1.54-1.24 (m, 24H), 0.99-0.92 (m, 18H).

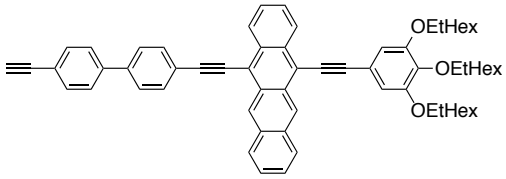


S6

S6. Ethynyl-4`-(trimethylsilylethynyl)biphenyl: Prepared following the established literature procedure.[3] *Eur. J. Org. Chem.* 2007, 5244–5249.



3a



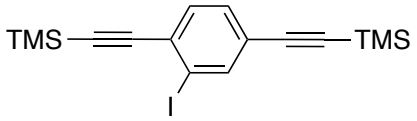
3

Compound 3.

Compound 3a. Compound **4-Ethynyl-4`-(trimethylsilylethynyl)biphenyl** (505 mg, 1.83 mmol, 7eq) was dissolved in 3.2 mL of dry THF, followed by dropwise addition of *n*-butyllithium (1.11 mL, 1.78 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 75 minutes and then transferred to the flask containing compound **1** (190 mg, 0.26 mmol, 1 eq), which was dissolved in 1.6 mL of dry THF and cooled to -78 °C, via cannula transfer. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction mixture was then treated with 10% HCl aqueous solution saturated with $SnCl_2$ dihydrate and left overnight stirring. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **3a**. Yield: 179 mg (70%). ^{1}H NMR (500 MHz, CDCl3): δ 9.29 (s, 2H), 8.70-8.69 (m, 2H), 8.13-8.12 (m, 2H), 7.92 (d, J=8 Hz, 2H), 7.74 (d, J=8 Hz, 2H), 7.66-7.56 (m, 6H), 7.52-7.49 (m, 2H), 7.07 (s, 2H), 4.04-3.98 (m, 6H), 1.89-1.78 (m, 3H), 1.68-1.41 (m, 24H), 1.04-0.96 (m, 18H), 0.34 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 153.5, 140.4, 140.3, 139.7, 132.8, 132.7, 132.6, 132.4, 132.3, 132.2, 132.1, 129.99, 129.97, 128.6, 128.56, 127.5, 127.4, 127.2, 127.1, 126.9, 126.89, 126.8, 126.7, 126.6, 126.2, 126, 125.9, 122.9, 122.6, 118.7, 117.9, 117.8, 109.9, 104.9, 104, 103.1, 95.4, 88.3, 85.8, 40.7, 39.8, 30.6, 30.5, 29.4, 29.2, 23.9, 23.8, 23.2, 23.15, 14.2, 14.1, 11.3, 11.2, 0.02.

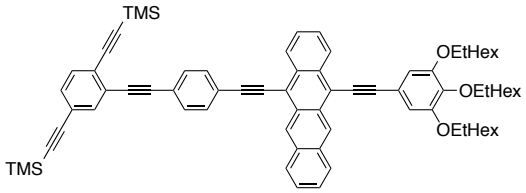
Compound **3a** (179 mg, 0.18 mmol, 1 eq) and K_2CO_3 (115 mg, 0.83 mmol, 3 eq) were dissolved in mixture of THF (1.5 mL), and MeOH (3 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 159 mg (94%). ^{1}H NMR (500 MHz,

CDCl3): δ 9.34 (s, 1H), 9.33 (s, 1H), 8.75-8.71 (m, 2H), 8.18-8.14 (m, 2H), 7.95 (d, J=8.5 Hz, 2H), 7.75 (d, J=8 Hz, 2H), 7.69-7.62 (m, 6H), 7.54-7.51 (m, 2H), 7.06 (s, 2H), 3.99-3.94 (m, 6H), 3.2 (s, 1H), 1.88-1.82 (m, 2H), 1.8-1.77 (m 1H), 1.68-1.23 (m, 24H), 1.02-0.94 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 153.6, 140.8, 140.6, 139.8, 132.9, 132.6, 132.5, 132.4, 132.37, 132.3, 130.2, 128.8, 128.7, 127.7, 127.5, 127.4, 127.1, 126.9, 126.7, 126.4, 126.2, 126.19, 123.1, 121.7, 118.9, 118.1, 117.9, 109.9, 104.2, 103.2, 88.4, 85.9, 83.6, 78.3, 76.4, 71.6, 40.8, 39.8, 30.7, 30.68, 29.5, 29.3, 24, 23.9, 23.3, 23.28, 14.33, 14.28, 11.39, 11.37, 11.34. HRMS (ESI) calcd for $C_{66}H_{72}O_3$ $(M+H)^+$, 913.5554, found, 913.5566

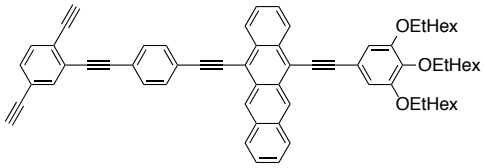


4

Compound 4. Prepared following the established literature procedure.[4]



5a



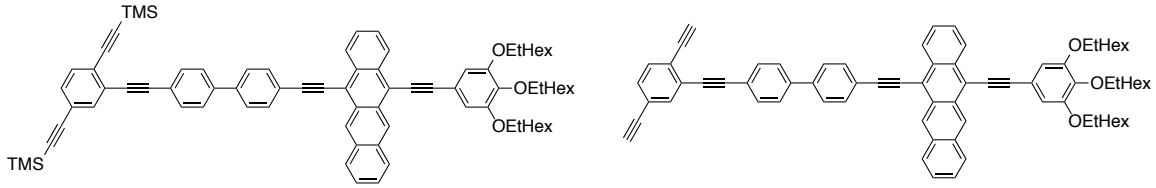
5

Compound 5.

Compound 5a. A round bottom flask was charged with **2** (180 mg, 0.22 mmol, 1 eq), **4** (196 mg, 0.49 mmol, 2.3 eq), $Pd(PPh_3)_2Cl_2$ (3 mg, 4.3 umol, 0.02 eq) and CuI (1.7 mg, 8.6 umol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, 11 mL of deoxygenated Et_3N:THF (1:3, v/v) was transferred to reaction flask. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **5a**. Yield: 135 mg (56%). ^{1}H NMR (500 MHz, CDCl3): δ 9.31 (s, 1H), 9.30 (s, 1H), 8.72-8.69 (m, 2H), 8.17-8.13 (m, 2H), 7.86 (d, J=8 Hz, 2H), 7.72-7.68 (m, 3H), 7.63-7.61 (m, 2H), 7.53-7.49 (m, 3H), 7.41-7.39 (m, 1H), 7.06 (s, 2H), 4.05-3.94 (m, 6H), 1.89-1.76 (m, 3H), 1.69-1.35 (m, 24H), 1.03-0.95 (m, 18H), 0.36 (s, 9H), 0.30 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 153.6, 141.8, 139.8, 135.3, 132.6, 132.4, 132.38, 132.28, 132.2, 132, 131.8, 131.5, 131.2, 130.1, 128.8, 128.7, 127.7, 127.5, 126.9, 126.7, 126.4, 126.3, 126.2, 126.1, 125.6, 123.8, 123.5, 123.4, 119.1, 117.9, 117.8, 109.9, 104.3, 103.8, 103.2, 103.1, 100.9, 97.2, 93.7, 89.8, 89.5, 85.9, 76.4, 71.6, 40.8, 39.8, 30.7, 30.6, 29.53, 29.51, 29.5, 29.3, 24, 23.9, 23.3, 23.28, 14.3, 14.28, 11.41, 11.40, 11.38, 11.34, 0.18, 0.02.

Compound **5a** (135 mg, 0.12 mmol, 1 eq) and K_2CO_3 (135 mg, 0.98 mmol, 8 eq) were dissolved in mixture of THF (2 mL), and MeOH (4 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and

brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.25:1) to yield **5**. Yield: 80 mg (68%). ^{1}H NMR (500 MHz, CDCl3): δ 9.34 (s, 1H), 9.32 (s, 1H), 8.73-8.70 (m, 2H), 8.18-8.14 (m, 2H), 7.87 (d, J=8.5 Hz, 2H), 7.74 (s, 1H), 7.71 (d, J=8.5, 2H), 7.64-7.62 (m, 2H), 7.56-7.52 (m, 3H), 7.46-7.44 (m, 1H), 7.08 (s, 2H), 4.04-3.93 (m, 6H), 3.52 (s, 1H), 3.24 (s, 1H), 1.90-1.73 (m, 3H), 1.66-1.37 (m, 24H), 1.02-0.89 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 153.5, 139.7, 135.3, 132.7, 132.5, 132.29, 132.27, 132.16, 132, 131.7, 131.6, 130, 128.6, 127.6, 127.3, 126.8, 126.6, 126.4, 126.3, 126.2, 126.1, 125.9, 124.9, 123.8, 123.1, 122.7, 119, 117.7, 117.6, 109.8, 104.2, 102.9, 93.9, 89.4, 89.1, 85.7, 83.1, 82.2, 81.7, 79.7, 76.2, 71.5, 40.7, 39.7, 30.6, 30.5, 29.4, 29.2, 23.9, 23.8, 23.2, 23.1, 14.2, 14.1, 11.25, 11.23, 11.2. HRMS (ESI) calcd for $C_{70}H_{72}O_3$ $(M+H)^+$, 961.5554, found, 961.5554.



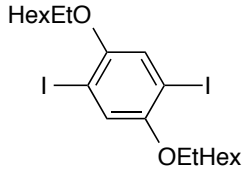
6a **6**

Compound 6.

Compound 6a. A round bottom flask was charged with **3** (159 mg, 0.17 mmol, 1 eq), **4** (165 mg, 0.42 mmol, 2.4 eq), $Pd(PPh_3)_2Cl_2$ (2.4 mg, 3.4 umol, 0.02 eq) and CuI (1.3 mg, 6.8 umol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, 10 mL of deoxygenated Et_3N:THF (1:3, v/v) was transferred to reaction flask. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **6a**. Yield: 110 mg (55%). ^{1}H NMR (500 MHz, CDCl3): δ 9.29 (s, 2H), 8.71-8.69 (m, 2H), 8.14-8.11 (m, 2H), 7.93 (d, J=8.5 Hz, 2H), 7.77 (d, J=8.5, 2H), 7.73-7.71 (m, 5H), 7.62-7.60 (m, 2H), 7.52-7.50 (m, 3H), 7.42-7.40 (m, 1H), 7.08 (s, 2H), 4.06-3.99 (m, 6H), 1.90-1.79 (m, 2H), 1.68-1.39 (m, 24H), 1.05-0.97 (m, 18H), 0.37 (s, 9H), 0.32 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 153.6, 140.5, 140.4, 139.8, 135.2, 132.5, 132.4, 132.36, 132.3, 132.25, 131.3, 130.1, 130, 128.7, 127.2, 127.1, 126.8, 126.6, 126.3, 126.29, 126.16, 126.13, 126.10, 125.6, 123.4, 123.1, 122.7, 118.8, 118.1, 117.9, 109.9, 104, 103.9, 103.3, 103.26, 100.9, 97.1, 93.9, 88.7, 88.5, 85.9, 76.4, 71.6, 40.8, 39.9, 30.8, 30.7, 29.54, 29.53, 29.51, 29.3, 24.1, 23.9, 23.4, 23.3, 14.33, 14.28, 11.43, 11.41, 11.39, 11.35, 0.18, 0.02.

Compound **6a** (105 mg, 0.09 mmol, 1 eq) and K_2CO_3 (104 mg, 0.75 mmol, 8.4 eq) were dissolved in mixture of THF (1.5 mL), and MeOH (3 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.75:1) to yield **5**. Yield: 78 mg (85%). ^{1}H NMR (500 MHz, CDCl3): δ 9.29 (s, 2H), 8.71-8.69 (m, 2H), 8.13-8.11 (m, 2H), 7.91 (d, J=8 Hz, 2H), 7.75-7.72 (m, 3H), 7.69 (s, 4H), 7.61-7.59 (m, 2H), 7.52-7.42 (m, 3H), 7.41-7.40 (m, 1H), 7.1 (s, 2H), 4.03-3.96 (m,

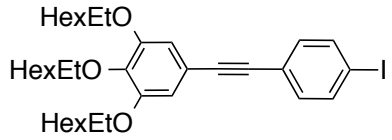
6H), 3.51 (s, 1H), 3.22 (s, 1H), 1.87-1.77 (m, 3H), 1.68-1.39 (m, 24H), 1.03-0.94 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 153.5, 140.5, 140.4, 139.7, 135.2, 132.6, 132.4, 132.39, 132.3, 132.25, 132.2, 132.1, 131.4, 130, 129.9, 128.6, 128.5, 127.2, 126.9, 126.7, 126.6, 126.5, 126.2, 126.04, 126, 124.9, 122.9, 122.7, 122.3, 118.7, 117.9, 117.8, 109.9, 104, 103, 94.1, 88.4, 88, 85.8, 82.9, 82.3, 81.8, 79.6, 76.3, 71.5, 40.7, 39.7, 30.62, 30.6, 29.41, 29.39, 29.38, 29.2, 23.9, 23.8, 23.2, 23.15, 14.2, 14.15, 11.29, 11.27, 11.25,11.21.



7

Compound 7. Prepared following the established literature procedure.[5]

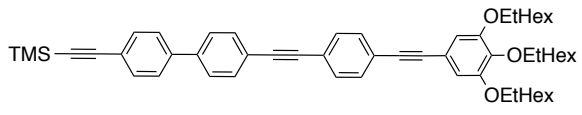
3b. Synthesis of P3:



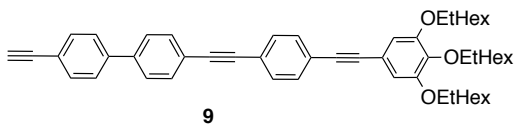
8

Compound 8.

A round bottom flask was charged with **3,4,5-triethylhexyloxyethynylbenzene** (652 mg, 1.34 mmol, 1 eq), **1,4-diiodobenzene** (1.33 g, 4 mmol, 3 eq), $Pd(PPh_3)_4$ (46 mg, 0.04 mmol, 0.03 eq) and CuI (15 mg, 0.08 mmol, 0.06eq) and evacuated and refilled with argon three times. In another flask, 51 mL of deoxygenated Et_3N:Toluene (1:5, v/v) was transferred to reaction flask. The reaction mixture was stirred for overnight at 40 ^{0}C. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.75:1) to yield **5a**. Yield: 230 mg (25%). ^{1}H NMR (500 MHz, CDCl3): δ 7.70 (d, J=9 Hz, 2H), 7.26 (d, J=10 Hz, 2H), 6.75 (s, 2H), 3.90-3.84 (m, 6H), 1.80-1.69 (m, 3H), 1.60-1.41 (m, 24 H), 0.97-0.92 (m, 18 H). ^{13}C NMR (125 MHz, CDCl3): δ 153.27, 137.5, 133, 122.9, 117.1, 110.4, 109.5, 93.8, 91.4, 87.1, 76, 71.3, 40.6, 39.6, 30.5, 29.3, 29.1, 23.82, 23.79, 23.71, 23.2, 23.1, 14.15, 14.11, 11.21, 11.19, 11.10.



9a

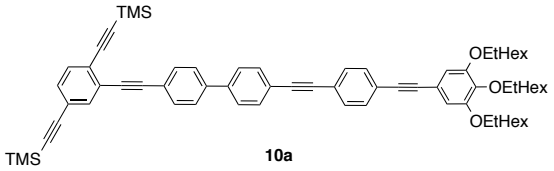


9

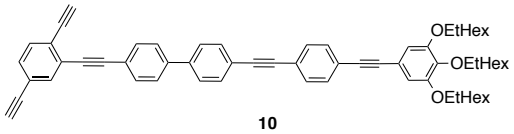
Compound 9.

Compound 9a. A round bottom flask was charged with **4-Ethynyl-4`-(trimethylsilylethynyl)biphenyl (S6)** (120 mg, 0.44 mmol, 1.3 eq), $Pd(PPh_3)_2Cl_2$ (5 mg, 6.8 umol, 0.02 eq) and CuI (2.6 mg, 13.6 umol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, **8** (230 mg, 0.34 mmol, 1 eq) was dissolved in 20 mL of Et_3N:THF (1:3, v/v) and this solution was added to flask containing catalysts and other starting material via cannula transfer after deoxygenating for 1 hour with argon. The reaction mixture was stirred for overweekend at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.75:1) to yield **9a**. Yield: 251 mg (90%). ^{1}H NMR (500 MHz, CDCl3): δ 7.62-7.54 (m, 12H), 6.78 (s, 2H), 3.93-3.84 (m, 6H), 1.82-1.70 (m, 3H), 1.61-1.35 (m, 24H), 0.99-0.93 (m, 18 H). ^{13}C NMR (125 MHz, CDCl3): δ 153.4, 140.4, 140.3, 139.4, 132.6, 132.3, 131.7, 131.6, 127.1, 126.9, 123.5, 122.9, 122.7, 122.5, 117.4, 109.8, 104.9, 95.4, 92.1, 91.2, 90.3, 87.9, 76.9, 76.2, 71.5, 40.8, 39.8, 30.7, 29.5, 29.49, 29.47, 29.3, 23.9, 23.88, 23.3, 23.2, 14.3, 14.25, 11.38, 11.37, 11.35, 11.25, 0.13.

Compound **9a** (251 mg, 0.3 mmol, 1 eq) and K_2CO_3 (120 mg, 0.9 mmol, 3 eq) were dissolved in mixture of THF (1.8 mL), and MeOH (3.6 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and ethylacetate (9:1) to yield **9**. Yield: 194 mg (84%). ^{1}H NMR (500 MHz, CDCl3): δ 7.65-7.62 (m, 4H), 7.60 (s, 4H), 7.56-7.52 (m, 4H), 6.77 (s, 2H), 3.92-3.86 (m, 6H), 3.17 (s, 1H), 1.81-1.70 (m, 3H), 1.60-1.35 (m, 24H), 0.98-0.92 (m, 18 H). ^{13}C NMR (125 MHz, CDCl3): δ 153.3, 140.6, 140.1, 139.2, 132.7, 132.1, 131.5, 131.4, 126.9, 126.8, 123.4, 122.8, 122.5, 121.5, 117.2, 109.6, 91.9, 90.9, 90.2, 87.8, 83.4, 78.1, 76.1, 71.3, 40.6, 39.6, 30.5, 29.34, 29.33, 29.32, 29.1, 23.8, 23.7, 23.1, 23.09, 14.13,14.09, 11.22, 11.20, 11.1. HRMS (ESI) calcd for $C_{54}H_{66}O3$ $(M+H)^+$, 763.5085, found, 763.5081.



10a



10

Compound 10.

Compound 10a. A round bottom flask was charged with **9** (194 mg, 0.25 mmol, 1 eq), **4** (131 mg, 0.33 mmol, 1.3 eq), $Pd(PPh_3)_2Cl_2$ (3.6 mg, 5.1 umol, 0.02 eq) and CuI (2 mg, 0.01 mmol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, 12 mL of deoxygenated Et_3N:THF (1:3, v/v) was transferred to reaction flask. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **10a**. Yield: 166 mg (63%). ^{1}H NMR (500 MHz, CDCl3): δ 7.68-7.63 (m, 9H), 7.56-7.53 (m, 4H), 7.48-7.46 (m, 2H), 7.38-7.36 (m, 2H), 6.78 (s, 2H), 3.92-3.87 (m, 6H), 1.82-1.70 (m, 3H), 1.60-1.36 (m, 24H), 1.01-0.90 (m, 18 H), 0.32 (s, 9H), 0.29 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 153.4, 140.4, 140.3, 139.4,

135.2, 132.4, 132.36, 132.29, 131.7, 131.6, 131.3, 127.1, 127, 126.3, 125.6, 123.5, 123.4, 122.9, 122.6, 117.4, 109.8, 103.9, 103.3, 100.8, 97.1, 93.9, 92.1, 91.2, 90.4, 88.6, 87.9, 76.2, 71.5, 40.8, 39.8, 30.7, 29.5, 29.3, 23.99, 23.88, 23.3, 23.25, 14.3, 14.2, 11.4, 11.3, 0.15, 0.01.

Compound **10a** (166 mg, 0.16 mmol, 1 eq) and K_2CO_3 (133 mg, 0.9 mmol, 8.4 eq) were dissolved in mixture of THF (1.8 mL), and MeOH (3.6 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 111 mg (78%). ^{1}H NMR (500 MHz, CDCl3): δ 7.71-7.70 (m, 1H), 7.68-7.64 (m, 8H), 7.56-7.52 (m, 5H), 7.43-7.41 (m, 1H), 6.77 (s, 2H), 3.92-3.86 (m, 6H), 3.5 (s, 1H), 3.22 (s, 1H), 1.81-1.70 (m, 3H), 1.61-1.35 (m, 24H), 0.98-0.92 (m, 18 H). ^{13}C NMR (125 MHz, CDCl3): δ 153.3, 140.5, 140.2, 139.2, 135.2, 132.6, 132.4, 132.2, 131.6, 131.5, 131.4, 126.97, 126.94, 126.6, 124.9, 123.4, 122.8, 122.7, 122.5, 122.2, 117.2, 109.6, 94, 91.9, 91, 90.2, 87.9, 87.8, 82.9, 82.3, 81.7, 79.6, 76.1, 71.3, 40.6, 39.6, 30.5, 29.3, 29.1, 23.8, 23.7, 23.2, 23.1, 14.16, 14.12, 11.24, 11.22, 11.11. HRMS (ESI) calcd for $C_{64}H_{70}O_3$ (M+H)+, 887.5398, found, 887.5418.

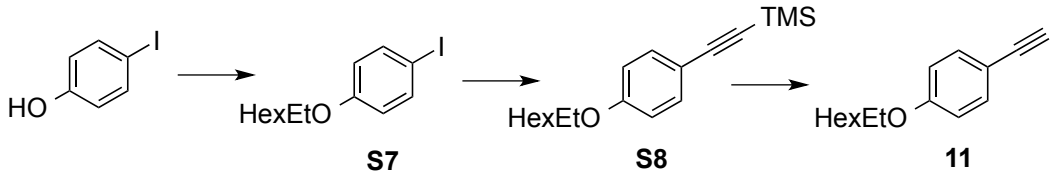
P1. A Schlenk tube was charged with <1 mg $Pd(PPh_3)_4$, and <1 mg CuI, and evacuated and refilled with argon three times. **5** (19.5 mg, 0.02 mmol, 1 eq) and **7** (12 mg, 0.02 mmol, 1 eq) was dissolved in 2.5 mL 4:1 (v:v) toluene:diisopropylamine and sparged with argon for 30 minutes. The solution was added to the reaction vessel and the mixture stirred for 72 hours at room tempareture. The reaction mixture was precipitated into 200 mL methanol and collected by centrifugation and decanting. The polymer was then dissolved in 2 mL of toluene and passed through a syringe filter to remove insoluble catalyst residues, reprecipitated into 100 mL of methanol and isolated by centrifugation and decanting. Mn [g/mol]: 26k, Mw [g/mol]: 47k. Yield: 20 mg (76%) ^{1}H NMR (500 MHz, CDCl3): δ 9.34-9.32 (m, 1H), 8.95 (m, 0.5H), 8.81 (m, 0.5H), 8.72 (m, 1H), 8.46 (m, 0.5H), 8.29 (m, 0.5H), 8.16 (m, 1H), 8.00 (m, 0.5), 7.89-7.80 (m, 2H), 7.75-7.68 (m, 3H), 7.65-7.37 (m, 6H), 7.13-7.02 (m, 3H), 4.02-3.76 (m, 10H), 1.89-1.75 (m, 5H), 1.67-1.28 (m, 40H), 1.08-0.79 (m, 30H).

P2. A Schlenk tube was charged with <1 mg $Pd(PPh_3)_4$, and <1 mg CuI, and evacuated and refilled with argon three times. **6** (18.3 mg, 0.016 mmol, 1 eq) and **7** (9.1 mg, 0.016 mmol, 1 eq) was dissolved in 2 mL 4:1 (v:v) toluene:diisopropylamine and sparged with argon for 30 minutes. The solution was added to the reaction vessel and the mixture stirred for 72 hours at room tempareture. The reaction mixture was precipitated into 200 mL methanol and collected by centrifugation and decanting. The polymer was then dissolved in 2 mL of toluene and passed through a syringe filter to remove insoluble catalyst residues, reprecipitated into 100 mL of methanol and isolated by centrifugation and decanting. Mn [g/mol]: 20k, Mw [g/mol]: 46k. Yield: 15 mg (71%) ^{1}H NMR (500 MHz, CDCl3): δ 9.34-9.3 (m, 1H), 9.22-9.18 (m, 1H), 8.72 (m, 1H), 8.64 (m, 1H), 8.15-8.07 (m, 2H), 7.97-7.88 (m, 2H), 7.82-7.70 (m, 7H), 7.63-7.49 (m, 6H), 7.17-7.03 (m, 4H), 4.02-3.88 (m, 10H), 1.86-1.76 (m, 5H), 1.65-1.29 (m, 40 H), 1.06-0.87 (m, 30H).

P3. A Schlenk tube was charged with <1 mg $Pd(PPh_3)_4$, and <1 mg CuI, and evacuated and refilled with argon three times. **10** (26 mg, 0.03 mmol, 1 eq) and **7** (17 mg, 0.03

mmol, 1 eq) was dissolved in 3.3 mL 4:1 (v:v) toluene:diisopropylamine and sparged with argon for 30 minutes. The solution was added to the reaction vessel and the mixture stirred for 72 hours at 60 °C. The reaction mixture was precipitated into 150 mL methanol and collected by centrifugation and decanting. The polymer was then dissolved in 2 mL of toluene and passed through a syringe filter to remove insoluble catalyst residues, reprecipitated into 100 mL of methanol and isolated by centrifugation and decanting. Mn [g/mol]: 31k, Mw [g/mol]: 58k. Yield: 25 mg (69%) ^{1}H NMR (500 MHz, CDCl3): δ 7.74 (m, 1H), 7.64-7.4 (m, 13H), 7.05-7.00 (m, 2H), 6.73 (m, 2H), 3.85 (m, 10H), 1.75 (m, 5H), 1.52-1.20 (m, 40H), 1.03-0.79 (m, 30H).

3c. Synthesis of A1, A2 and A3

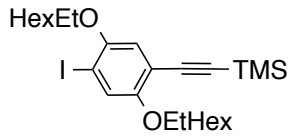


S7. 4-iodophenol (9 g, 0.04 mol, 1.0 eq), KOH (2.35 g, 0.04 mol, 1 eq) and KI (180 mg, 0.8 mmol, 0.02 eq) were dissolved in 102 mL of dry EtOH at room temperature under argon. 2-ethylhexylbromide (8.1 mL, 0.045 mmol, 1.1 eq) was then added to this solution under an argon atmosphere. The mixture was heated to 60 °C and stirred for overnight. The mixture was then cooled to room temperature. After precipitate (KBr) was collected, the solution was distilled off using rotavap and remaining residue was redissolved in CH_2Cl_2. Organic phase were washed with water and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was taken next step without further purification. Yield: 7.34 g (52%).

S8. A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (404 mg, 0.6 mmol, 0.04 eq) and CuI (195 mg, 1 mmol, 0.07 eq) and evacuated and refilled with argon three times. In another flask, **S5** (5 g, 14.4 mmol, 1 eq) was dissolved in 77 mL of Et_3N and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. While stirring, TMSA (2.4 mL, 16.7 mmol, 1.2 eq) were added dropwise to the flask. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.5:1) to yield **S8**. Yield: 3.23 mg (92%).

Compound 11. Compound **S8** (3.2 g, 10.6 mmol, 1 eq) was dissolved in mixture of MeOH (106 mL), Et_2O (106 mL) and 10% $NaOH_{(aq)}$ (44 mL). The reaction mixture was stirred overnight at room temperature. The reaction was stopped by acidification with 10% aq HCl. Organics were extracted twice with Et_2O, and combined organic phases were washed with brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.5:1) to yield **11**. Yield: 1.93 g (79%). ^{1}H and ^{13}C NMR is in good

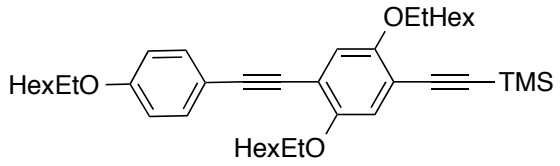
agreement with the same compound reported in the literature.[6] Macromol. Rapid Commun. 2015, 36, 31−37.



12

Compound 12.

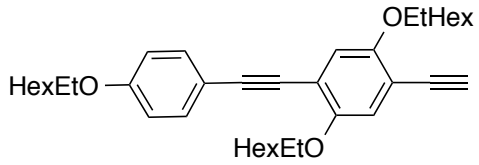
A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (39 mg, 0.06 mmol, 0.09 eq) and CuI (6 mg, 1 mmol, 0.05 eq) and evacuated and refilled with argon three times. In another flask, **XX** (1.11 g, 18.8 mmol, 1 eq) was dissolved in 15 mL of Et_3N and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. While stirring, TMSA (0.09 mL, 0.6 mmol, 1 eq) were added dropwise to the flask. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (7.5:1) to yield **12**. Yield: 350 mg (25%). ^1H and ^{13}C NMR is in good agreement with literature.[7]



13

Compound 13.

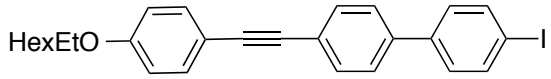
A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (7 mg, 0.01 mmol, 0.02 eq) and CuI (3.8 mg, 0.02 mmol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, **11** (112 mg, 0.49 mmol, 1 eq) and **12** (325 mg, 0.58 mmol, 1.2 eq) were dissolved in 20 mL of Et_3N:THF(1:3, v/v) and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (5:1) to yield **13**. Yield: 190 mg (59%). ^1H NMR (500 MHz, CDCl3): δ 7.46 (d, J=10 Hz, 2H), 6.97 (s, 1H), 6.96 (s, 1H), 6.89 (d, J=8.6 Hz, 2H), 3.94-3.85 (m, 6H), 1.82-1.73 (m, 3H), 1.64-1.34 (m, 24H), 0.99-0.89 (m, 18H), 0.28 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 159.6, 154.6, 153.6, 133.1, 117.2, 116.4, 115.5, 114.9, 114.7, 113.2, 101.5, 99.7, 95.2, 84.7, 72.2, 71.9, 70.7, 39.81, 39.80, 39.5, 30.8, 30.7, 29.32, 29.28, 29.2, 24.2, 24.1, 24, 23.24, 23.22, 23.19, 14.26, 14.23, 14.21, 11.44, 11.42, 11.26, 0.13.



14

Compound 14.

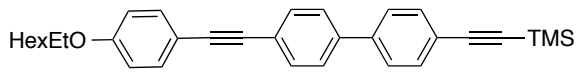
Compound **13** (190 mg, 0.3 mmol, 1 eq) and K_2CO_3 (120 mg, 0.9 mmol, 3 eq) were dissolved in mixture of THF (1 mL), and MeOH (2 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 154 mg (92%). ^{1}H NMR (500 MHz, CDCl3): δ 7.45 (d, J=8.8 Hz, 2H), 6.98 (s, 1H), 6.97 (s, 1H), 6.88 (d, J=8.8 Hz, 2H), 3.91-3.84 (m, 6H), 3.31 (s, 1H), 1.80-1.72 (m, 3H), 1.62-1.32 (m, 24H), 0.98-0.88 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 159.7, 154.7, 153.7, 133.1, 117.6, 116.8, 115.4, 115.3, 114.7, 112.2, 95.3, 84.5, 82.1, 80.3, 72.3, 72.2, 70.8, 39.8, 39.6, 39.5, 30.8, 30.7, 29.3, 29.24, 29.23, 24.2, 24.1, 24, 23.22, 23.20, 23.19, 14.23, 14.22, 11.4, 11.32, 11.26. HRMS (ESI) calcd for $C_{40}H_{58}O_3$ $(M+H)^+$, 587.4459, found, 587.4467.



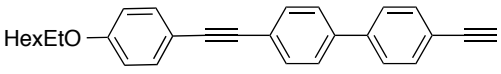
15

Compound 15.

A round bottom flask was charged with $Pd(PPh_3)_4$ (78 mg, 0.06 mmol, 0.03 eq) and CuI (26 mg, 0.12 mmol, 0.06 eq) and evacuated and refilled with argon three times. In another flask, **11** (500 mg, 2.18 mmol, 1 eq) and **4,4`-diiodophenyl** (2.64 g, 6.52 mmol, 3 eq) were dissolved in 80 mL of Et_3N:Toluene(1:5, v/v) and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. The reaction mixture was stirred for overnight at 40 ^{0}C. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (5:1) to yield **15**. Yield: 506 mg (46%). ^{1}H NMR (500 MHz, CDCl3): δ 7.8 (d, J=8.3 Hz, 2H), 7.59 (d, J= 8.5 Hz, 2H), 7.55(d, J=8 Hz, 2H), 7.49 (d, J=8.6 Hz, 2 H), 7.37 (d, J=8.3 Hz, 2H), 6.91 (d, J=8.6 Hz, 2H), 3.91-3.86 (m, 2H), 1.79-1.74 (m, 1H), 1.55-1.33 (m, 8H), 0.98-0.92 (m, 6H). ^{13}C NMR (125 MHz, CDCl3): δ 159.6, 139.9, 139.3, 137.9, 133, 131.9, 128.8, 126.7, 123.2, 114.9, 114.6, 93.3, 90.6, 87.7, 70.7, 39.4, 30.5, 29.1, 23.9, 23, 14.1, 11.1.



16a

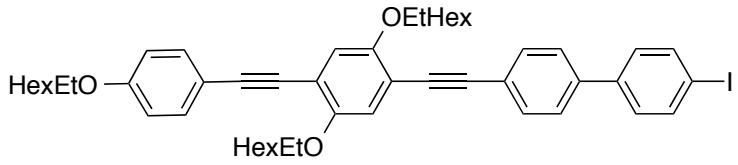


16

Compound 16.

Compound 16a. A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (5 mg, 0.006 mmol, 0.02 eq) and CuI (2.5 mg, 0.012 mmol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, **15** (170 mg, 0.33 mmol, 1 eq) was dissolved in 12 mL of Et_3N:THF(1:3, v/v) and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. While stirring, TMSA (57 uL, 0.4 mmol, 1.2 eq) were added dropwise to the flask. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (4:1) to yield **16a**. Yield: 160 mg (80%). ^{1}H NMR (300 MHz, CDCl3): δ 7.56-7.45 (m, 8H), 7.47(d, J=8.4 Hz) 6.88 (d, J=8.4 Hz), 3.85 (d, 2H), 1.75-1.69 (m, 1H), 1.50-1.25 (m, 8H), 0.95-0.88 (m, 6H), 0.27 (s, 9H). ^{13}C NMR (75 MHz, CDCl3): δ 159.7, 140.5, 139.7, 133.2, 132.6, 132.1, 126.9, 126.8, 123.2, 122.5, 115.1, 114.8, 105.1, 95.3, 90.7, 87.9, 70.8, 39.5, 30.7, 29.3, 24, 23.2, 14.2, 11.3, 0.14.

Compound **16a** (129 mg, 0.26 mmol, 1 eq) and K_2CO_3 (106 mg, 0.77 mmol, 3 eq) were dissolved in mixture of THF (1 mL), and MeOH (2 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 106 mg (95%). ^{1}H NMR (500 MHz, CDCl3): δ 7.62-7.58 (m, 8H), 7.5 (d, J=8.6 Hz, 2H), 6.91 (d, J=8.6 Hz, 2H), 3.89-3.88 (m, 2H), 3.17 (s, 1H), 1.79-1.74 (m, 1H), 1.56-1.34 (m, 8H), 0.98-0.93 (m, 6H). ^{13}C NMR (125 MHz, CDCl3): δ 159.6, 140.8, 139.5, 133.1, 132.6, 131.9, 126.9, 126.8, 123.2, 121.3, 114.9, 114.6, 90.7, 87.8, 83.5, 77.9, 70.6, 39.4, 30.5, 29.1, 23.9, 23.1, 14.1, 11.1. HRMS (ESI) calcd for $C_{30}H_{30}O$ $(M+H)^+$, 407.2369, found, 407.2367.

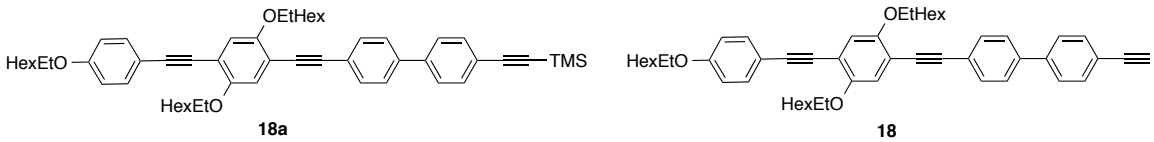


17

Compound 17.

A round bottom flask was charged with $Pd(PPh_3)_4$ (9 mg, 7.9 umol, 0.03 eq) and CuI (3 mg, 15.8 mmol, 0.06 eq) and evacuated and refilled with argon three times. In another flask, **14** (154 mg, 0.26 mmol, 1 eq) and **4,4`-diiodophenyl** (320 mg, 0.79 mmol, 3 eq) were dissolved in 12 mL of Et_3N:Toluene(1:5, v/v) and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. The reaction mixture was stirred for overnight at 40 ^{0}C. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (4:1) to yield **17**. Yield: 140 mg (62%). ^{1}H NMR (500 MHz, CDCl3): δ 7.8 (d, J=8 Hz, 2H), 7.61 (d, J=8 Hz, 2H), 7.57 (d, J=8 Hz, 2H), 7.48 (d, J=8 Hz, 2H), 7.38 (d, J=8 Hz, 2H), 7.04 (s, 1H), 7.03 (s, 1H), 6.90 (d, J=8.5 Hz, 2H), 3.97-3.94 (m, 4H), 3.89-3.88 (m, 2H), 1.84-1.82 (m, 2H), 1.79-1.73 (m, 1H), 1.67-1.29 (m, 24H), 1.02-

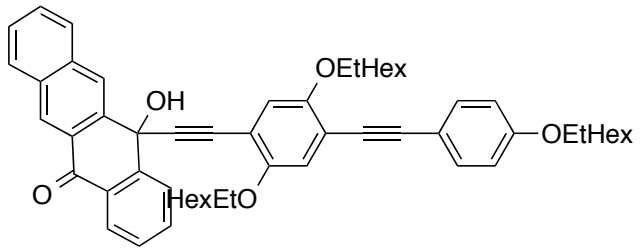
0.91 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 159.5, 153.9, 153.7, 139.9, 139.6, 137.9, 132.9, 132, 128.8, 126.7, 123.1, 116.7, 116.5, 115.4, 114.7, 114.6, 113.3, 95.2, 94.3, 93.4, 87.3, 84.6, 72.1, 72, 70.6, 39.7, 39.4, 30.71, 30.69, 30.53, 29.2, 29.1, 24.06, 24.04, 23.88, 23.09, 23.04, 14.09, 14.06, 11.29, 11.11.



Compound 18.

Compound 18a. A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (2 mg, 3.2 umol, 0.02 eq) and CuI (1 mg, 6.4 umol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, **17** (140 mg, 0.16 mmol, 1 eq) was dissolved in 6 mL of Et_3N:THF(1:3, v/v) and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. While stirring, TMSA (40 uL, 0.28 mmol, 1.8 eq) were added dropwise to the flask. The reaction mixture was stirred for 2 days at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **18a**. Yield: 121 mg (90%). ^{1}H NMR (500 MHz, CDCl3): δ 7.61-7.56 (m, 8H), 7.48 (d, J=8.7 Hz, 2H), 7.04 (s, 1H), 7.03 (s, 1H), 6.9 (d, J=8.7 Hz, 2H), 3.98-3.91 (m, 4H), 3.89-3.88 (m, 2H), 1.86-1.81 (m, 2H), 1.78-1.74 (m, 1H), 1.67-1.28 (m, 24), 1.02-0.9 (m, 18H), 0.3 (s, 9H). ^{13}C NMR (125 MHz, CDCl3): δ 159.7, 154.2, 153.9, 140.5, 140, 133.2, 132.7, 132.2, 127.1, 126.9, 123.2, 122.6, 116.8, 116.7, 115.6, 114.8, 113.5, 105.1, 95.4, 95.3, 94.6, 87.5, 84.9, 72.3, 72.2, 70.8, 39.9, 39.6, 30.9, 30.7, 29.4, 29.3, 24.27, 24.25, 24.09, 23.31, 23.26, 14.32, 14.29, 11.53, 11.52, 11.33, 0.21.

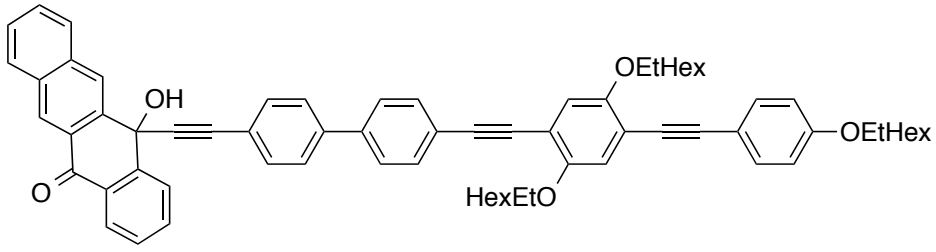
Compound **18a** (121 mg, 0.15 mmol, 1 eq) and K_2CO_3 (60 mg, 0.45 mmol, 3 eq) were dissolved in mixture of THF (1 mL), and MeOH (2 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 100mg (>99%). ^{1}H NMR (500 MHz, CDCl3): δ 7.64-7.59 (m, 8H), 7.48 (d, J=8.6 Hz, 2H), 7.05 (s, 1H), 7.03 (s, 1H), 6.9 (d, J=8.6 Hz, 2H), 3.99-3.92 (m, 4H), 3.89-3.86 (m, 2H), 3.17 (s, 1H), 1.86-1.81 (m, 2H), 1.79-1.74 (m, 1H), 1.68-1.28 (m, 24H), 1.02-0.91 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 159.7, 154.2, 153.9, 140.9, 139.9, 133.2, 132.9, 132.2, 127.1, 127.06, 123.3, 121.5, 116.8, 116.7, 115.6, 114.8, 114.77, 113.5, 95.4, 94.6, 87.5, 84.9, 83.7, 78.2, 72.3, 72.2, 70.8, 39.9, 39.6, 30.92, 30.9, 30.7, 29.4, 29.3, 24.27, 24.25, 24.1, 23.3, 23.26, 14.32, 14.29, 11.52, 11.33. HRMS (ESI) calcd for $C_{54}H_{66}O_3$ $(M+H)^+$, 763.5085, found, 763.5096.



19

Compound 19.

Compound **14** (149 mg, 0.25 mmol, 1eq) was dissolved in 1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.14 mL, 0.23 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing 5,12- naphthacenequinone (66 mg, 0.25 mmol, 1 eq), which was dissolved in 1 mL of dry THF and cooled to O °C, dropwisely via syringe. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction was quenched by addition of 5 mL of ice cold DI H_2O and then filtered via vacuum filtration by washing about 20 mL of THF:H_2O (1:1, v/v). Saturated NH_4Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **19**. Yield: 117 mg (54%). ^{1}H NMR (500 MHz, CDCl3): δ 8.8 (s, 1H), 8.69 (s, 1H), 8.32-8.28 (m, 2H), 8.02 (d, J=8.1 Hz, 1H), 7.97 (d, J=8.2, 1H), 7.77-7.73 (m, 1H), 7.65-7.62 (m, 1H), 7.59-7.53 (m, 2H), 7.45 (d, J=8.7 Hz, 2H), 6.90-6.88 (m, 4H), 3.90-3.73 (m, 6H), 3.71 (s, 1H), 1.8-1.73 (m, 3H), 1.62-1.14 (m, 24H), 0.97-0.88 (m, 12H), 0.84-0.79 (m, 3H), 0.77-0.72 (m, 3H). ^{13}C NMR (125 MHz, CDCl3): δ 183.5, 159.6, 154.1, 153.4, 144.2, 139.5, 135.9, 134.2, 132.9, 132.7, 130, 129.8, 129.3, 129, 128.8, 128.3, 128.1, 127.7, 127.4, 127.3, 127.2, 116.9, 116, 115.2, 115.1, 114.6, 111.7, 96.1, 95.3, 84.5, 83.4, 72.1, 71.3, 70.6, 67.2, 39.6, 39.4, 39.33, 39.31, 30.6, 30.5, 30.2, 30.1, 29.2, 29.1, 28.9, 28.8, 23.9, 23.8, 23.7, 23.6, 23.07, 23.04, 22.94, 22.93, 14.09, 14.08, 14.06, 11.3, 11.1, 10.96, 10.92.

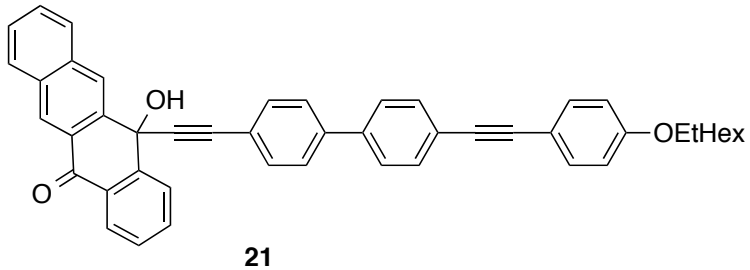


20

Compound 20.

Compound **18** (202 mg, 0.27 mmol, 1eq) was dissolved in 1.4 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.15 mL, 0.24 mmol, 1.6 M in hexanes) at -78

°C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing 5,12- naphthacenequinone (69 mg, 0.27 mmol, 1 eq), which was dissolved in 1.2 mL of dry THF and cooled to O °C, dropwisely via syringe. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction was quenched by addition of 5 mL of ice cold DI H_2O and then filtered via vacuum filtration by washing about 30 mL of THF:H_2O (1:1, v/v). Saturated NH_4Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **20**. Yield: 150 mg (55%). ^{1}H NMR (500 MHz, CDCl3): δ 8.9 (s, 1H), 8.7 (s, 1H), 8.38-8.36 (m, 1H), 8.31-8.29 (m, 1H), 8.1-8.09 (m, 1H), 8.05-8.03 (m, 1H), 7.83-7.79 (m, 1H), 7.7-7.67 (m, 1H), 7.64-7.54 (m, 10H), 7.47 (d, J= 8.8 Hz, 2H), 7.03 (s, 1H), 7.02 (s, 1H), 6.9 (d, J=8.8 Hz, 2H), 3.98-3.91 (m, 4H), 3.89-3.86 (m, 2H), 3.18 (s, 1H), 1.85-1.80 (m, 2H), 1.78-1.73 (m, 1H), 1.66-1.35 (m, 24H), 1.01-0.89 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 183.5, 159.7, 154.1, 153.8, 144.1, 140.9, 139.8, 139.4, 136, 134.5, 133.1, 132.9, 132.4, 132.1, 130.3, 130, 129.7, 129.4, 129.1, 128.4, 128.1, 127.8, 127.7, 127.6, 127.4, 127, 126.9, 123.3, 121.3, 116.7, 116.6, 115.5, 114.8, 114.7, 113.3, 95.3, 94.5, 92.1, 87.5, 86.7, 84.8, 72.2, 72.1, 70.7, 67.4, 39.8, 39.5, 30.8, 30.7, 29.3, 29.2, 24.18, 24.16, 24, 23.23, 23.18, 14.3, 14.2, 11.4, 11.3.

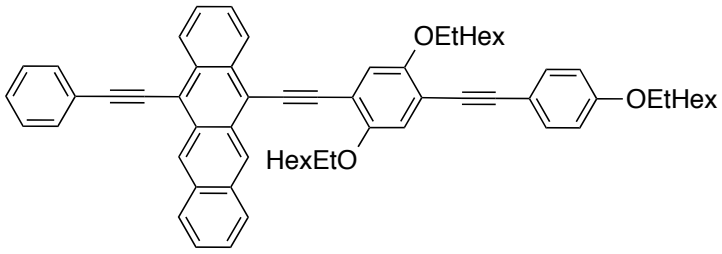


21

Compound 21.

Compound **16** (135 mg, 0.33 mmol, 1eq) was dissolved in 1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.18 mL, 0.29 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing 5,12- naphthacenequinone (86 mg, 0.33 mmol, 1 eq), which was dissolved in 1.5 mL of dry THF and cooled to O °C, dropwisely via syringe. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction was quenched by addition of 5 mL of ice cold DI H_2O and then filtered via vacuum filtration by washing about 20 mL of THF:H_2O (1:1, v/v). Saturated NH_4Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **21**. Yield: 100 mg (45%). ^{1}H NMR (500 MHz, CDCl3): δ 8.77 (s, 1H), 8.67 (s, 1H), 8.29-8.25 (m, 2H), 8.01-7.98 (m, 2H), 7.78-7.75 (m, 1H), 7.65-7.63 (m, 1H), 7.59-7.48 (m,

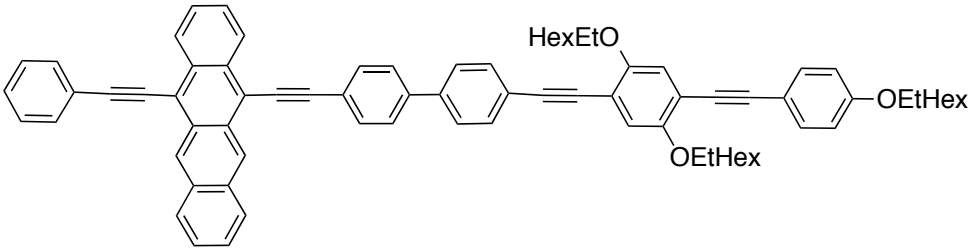
12H), 6.9 (d, J=8.8 Hz, 2H), 3.89-3.87 (m, 2H), 3.61 (s, 1H), 1.78-1.73 (m, 1H), 1.56-1.29 (m, 8H), 0.98-0.93 (m, 6H). ^{13}C NMR (125 MHz, CDCl3): δ 183.7, 159.8, 144.3, 140.9, 139.5, 136.1, 134.5, 133.2, 132.9, 132.5, 132.1, 130.2, 130, 129.7, 129.4, 129.1, 128.4, 128.3, 127.9, 127.7, 127.5, 127.4, 127, 126.9, 123.4, 121.3, 115.1, 114.8, 92.3, 90.9, 87.9, 86.6, 70.8, 67.4, 39.5, 30.7, 29.3, 24, 23.2, 14.3, 11.3.



A1

A1.

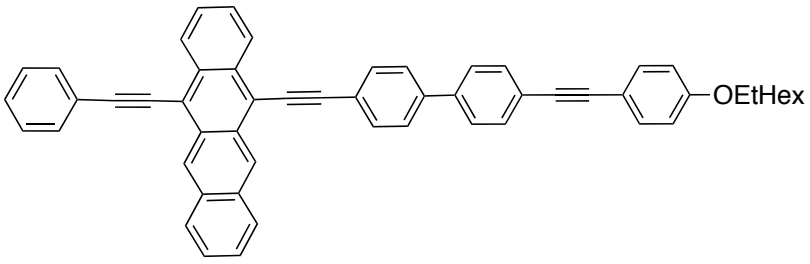
Phenylacethylene (51 mg, 0.50 mmol, 4 eq) was dissolved in 1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.3 mL, 0.48 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing **20** (105 mg, 0.12 mmol, 1 eq), which was dissolved in 0.6 mL of dry THF and cooled to -78 °C, dropwisely via cannula. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction mixture was then treated with 15 mL of 10% HCl aqueous solution saturated with $SnCl_2$ dihydrate and left overnight stirring. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3.5:1) to yield **A1**. Yield: 56 mg (50%). ^{1}H NMR (500 MHz, CDCl3): δ 9.41 (s, 1H), 9.33 (s, 1H), 8.86-8.84 (m, 1H), 8.73-8.71 (m, 1H), 8.16-8.14 (m, 2H), 7.89-7.87 (m, 2H), 7.63-7.58 (m, 2H), 7.55-7.47 (m, 7H), 7.32 (s, 1H), 7.16 (s, 1H), 6.95-6.92 (m, 2H), 4.13-4.07 (m, 4H), 3.93-3.90 (m, 2H), 2.06-1.98 (m, 1H), 1.95-1.88 (m, 1H), 1.8-1.76 (m, 1H), 1.73-1.21 (m, 24H), 1.07 (t, 3H), 0.99-0.93 (m, 12H), 0.79 (t, 3H). ^{13}C NMR (125 MHz, CDCl3): δ 159.6, 154.1, 153.8, 133, 132.4, 132.3, 132.2, 132.1, 131.8, 130.1, 129.9, 128.7, 128.6, 127.9, 127.3, 126.7, 126.5, 126.4, 126, 125.9, 125.8, 123.6, 118.9, 118.1, 116.9, 116.1, 115.3, 115.2, 114.6, 113.4, 103.3, 100.5, 95.6, 92.5, 87.3, 84.9, 72.3, 71.9, 70.6, 39.8, 39.5, 39.4, 30.8, 30.5, 30.4, 29.3, 29.1, 29, 24.1, 23.9, 23.8, 23.1, 23.06, 23, 14.2, 14.1, 13.9, 11.4, 11.1, 10.95. HRMS (ESI) calcd for $C_{66}H_{72}O_3$ (M^+), 912.5476, found, 912.5493.



A2

A2.

Phenylacethylene (59 mg, 0.58 mmol, 4 eq) was dissolved in 1.1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.35 mL, 0.56 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing **20** (148 mg, 0.15 mmol, 1 eq), which was dissolved in 0.5 mL of dry THF and cooled to -78 °C, dropwisely via cannula. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction mixture was then treated with 15 mL of 10% HCl aqueous solution saturated with $SnCl_2$ dihydrate and left overnight stirring. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.75:1) to yield **A2**. ^{1}H NMR (500 MHz, CDCl3): δ 9.29 (s, 2H), 8.7-8.68 (m, 2H), 8.14-8.12 (m, 2H), 7.94-7.93 (m, 2H), 7.89-7.87 (m, 2H), 7.78-7.76 (m, 2H), 7.72-7.67 (m, 4H), 7.61-7.59 (m, 2H), 7.55-7.49 (m, 7H), 7.08 (s, 1H), 7.06 (s, 1H), 6.91 (d, J= 9 Hz, 2H), 3.99-3.96 (m, 4H), 3.9-3.89 (m, 2H), 1.89-1.83 (m, 2H), 1.79-1.74 (m, 1H), 1.71-1.30 (m, 24H), 1.05-0.92 (m, 18H). ^{13}C NMR (125 MHz, CDCl3): δ 159.5, 153.9, 153.7, 140.5, 139.8, 132.9, 132.3, 132.25, 132.18, 132.1, 131.8, 129.94, 129.92, 128.8, 126.7, 128.6, 127.4, 127.1, 126.9, 126.7, 126.6, 126.1, 126, 123.6, 123.2, 122.8, 118.4, 118.3, 116.6, 116.5, 115.4, 114.63, 114.57, 113.3, 103.4, 103.3, 95.2, 87.4, 87.2, 84.7, 72.1, 72, 70.6, 39.7, 39.4, 30.74, 30.71, 30.5, 29.23, 29.22, 29.1, 24.09, 24.06, 23.9, 23.14, 23.12, 23.06, 14.16, 14.14, 14.10, 11.35, 11.33, 11.13. HRMS calcd for $C_{80}H_{80}O_3$ $(M+H)^+$, 1089.6180, found, 1089.6184



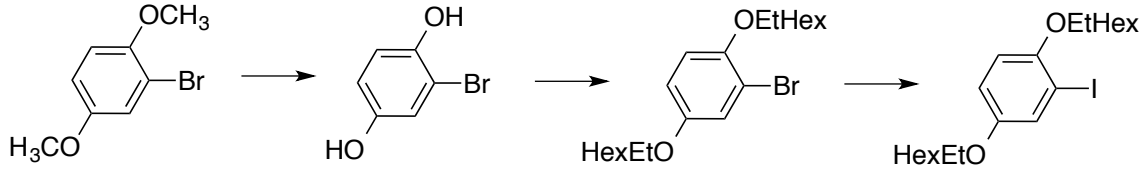
A3

A3.

Phenylacethylene (48 mg, 0.47 mmol, 4 eq) was dissolved in 1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.29 mL, 0.45 mmol, 1.6 M in hexanes) at -78

°C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing **21** (78 mg, 0.12 mmol, 1 eq), which was dissolved in 0.5 mL of dry THF and cooled to -78 °C, dropwisely via cannula. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction mixture was then treated with 15 mL of 10% HCl aqueous solution saturated with $SnCl_2$ dihydrate and left overnight stirring. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (3:1) to yield **A3**. Yield: 45 mg (53%). ^{1}H NMR (500 MHz, CDCl3): δ 9.35 (s, 1H), 9.34 (s, 1H), 8.75-8.72 (m, 2H), 8.18-8.15 (m, 2H), 7.95 (d, J=8.5 Hz, 2H), 7.89-7.88 (m, 2H), 7.78 (d, J=8.5 Hz, 2H), 7.70 (d, J=8.4 Hz, 2H), 7.66 (d, J=8.4 Hz, 2H), 7.64-7.61 (m, 2H), 7.55-7.48 (m, 7H), 6.93 (d, J=8.7 Hz, 2H), 3.91-3.89 (m, 2H), 1.79-1.75 (m, 1H), 1.56-1.28 (m, 8H), 0.98-0.93 (m, 6H). ^{13}C NMR (125 MHz, CDCl3): δ 159.6, 140.6, 139.6, 133.1, 132.35, 132.34, 132.25, 132.2, 132, 131.8, 129.98, 129.97, 128.8, 128.7, 128.6, 127.5, 127.4, 127.1, 126.9, 126.7, 126.6, 126.1, 126.08, 123.5, 123.2, 122.7, 118.4, 118.3, 114.9, 114.6, 103.4, 103.3, 90.7, 88.2, 87.8, 87.1, 70.6, 39.4, 30.5, 29.1, 23.9, 23.1, 14.1, 11.1. HRMS calcd for $C_{56}H_{44}O$ $(M)^+$, 732.3387, found, 732.3377

3d. Synthesis of Compound 22



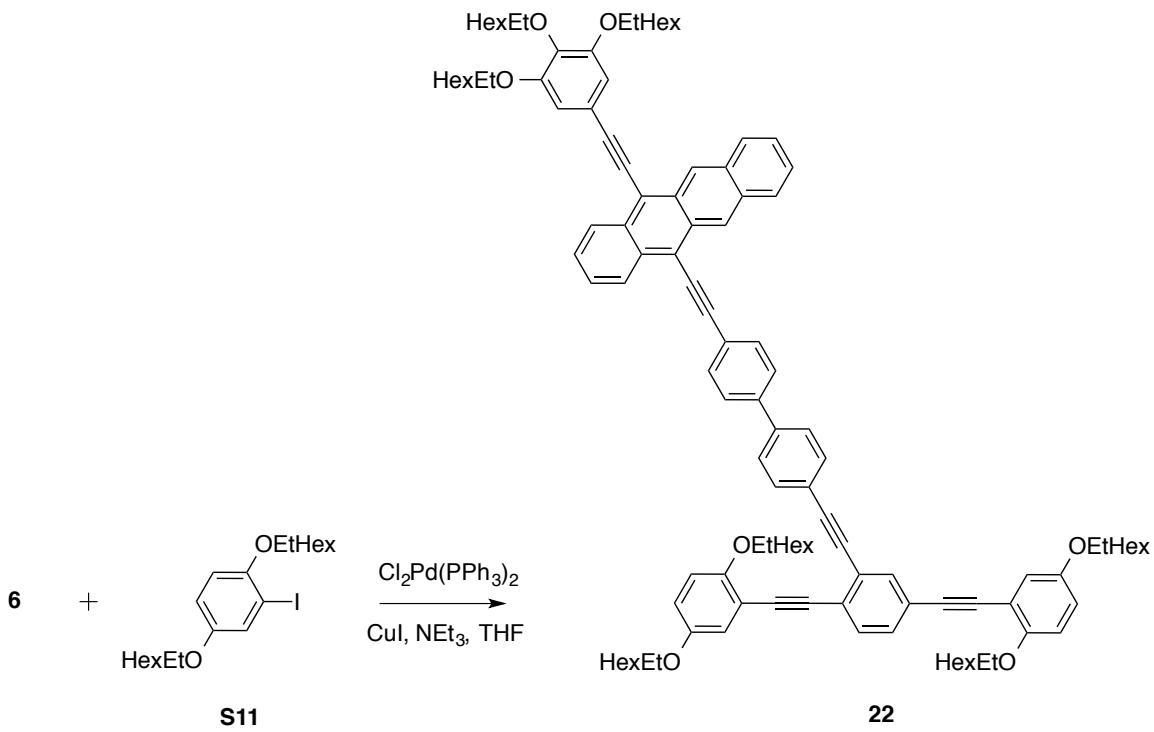
S9 **S10** **S11**

S9. Compound **1-bromo-2,5-dimethoxybenzene** (800 mg, 3.7 mmol, 1.0 eq) was suspended in 4 mL of dry CH_2Cl_2, followed by the addition of BBr_3 (11 mL, 1.0 M in CH_2Cl_2, 11 mmol, 3 eq) at -78 °C under argon and stirred overnight at room temperature. The reaction was stopped by pouring the reaction mixture onto ice. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with brine, dried over MgSO4, and filtered. Removal of solvent *in vacuo* yielded 650 mg of **S9** (94%) that was taken to the next step immediately without further purification. ^{1}H NMR (500 MHz, D-THF): δ 7.86 (s, 2H), 6.85-6.84 (m, 1H), 6.67-6.66 (m, 1H), 6.56-6.54 (m, 1H).

S10. Compound **S9** (639 mg, 3.4 mmol, 1.0 eq) and K_2CO_3 (1.9 g, 13.5 mmol, 4.0 eq) were dissolved in 22.5 mL of dry DMF at room temperature under argon. 2-ethylhexylbromide (1.3 mL, 7.4 mmol, 2.2 eq) was then added to this solution under an argon atmosphere. The mixture was heated to 70 °C and stirred for overnight. The mixture was then cooled to room temperature. The reaction was stopped by quenching with 10% aq NaOH. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with brine, dried over $MgSO_4$, filtered and concentrated using rotary

evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (9:1) to yield **S10**. Yield: 812 mg (58%). ^{1}H NMR (500 MHz, CDCl3): δ 7.14 (m, 1H), 6.85-6.8 (m, 2H), 3.87-3.85 (m, 2H), 3.81-3.79 (m, 2H), 1.78-1.69 (m, 1H), 1.61-1.58 (m, 1H), 1.56-1.33 (m, 16H), 0.98-0.92 (m, 12H). ^{13}C NMR (125 MHz, CDCl3): δ 153.8, 149.9, 119.5, 114.34, 114.29, 112.7, 72.5, 71.3, 39.5, 39.4, 30.5, 29.09, 29.08, 23.89, 23.83, 23.1, 14.1, 11.2, 11.1.

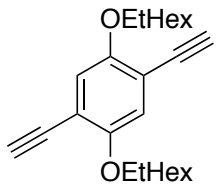
S11. Compound **S10** (658.8 mg, 1.66 mmol, 1eq) was dissolved in 12 mL of dry THF, followed by dropwise addition of *n*-butyllithium (2.6 mL, 4.2 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then I_2 (969 mg, 3.8 mmol, 2.3 eq) which was dissolved in 7 mL of dry THF was added to the solution containing S10 via syringe. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction was quenched by addition of aqueous $Na_2S_2O_3$. Organics were extracted twice with CH_2Cl_2, and combined organic phases were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (9:1) to yield **S11**. Yield: 714 mg (93%). ^{1}H NMR (500 MHz, CDCl3): δ 7.36-7.35 (m, 1H), 6.88-6.85 (m, 1H), 6.75-6.73 (m, 1H), 3.86-3.85 (m, 2H), 3.79-3.78 (m, 2H), 1.78-1.75 (m, 1H), 1.72-1.68 (m, 1H), 1.61-1.34 (m, 16H), 0.98-0.97 (m, 12H). ^{13}C NMR (125 MHz, CDCl3): δ 153.9, 152.2, 125.4, 115.3, 112.6, 86.8, 72.2, 71.3, 39.5, 39.4, 30.6, 30.5, 29.11, 29.08, 23.9, 23.8, 23.1, 14.14, 14.11, 11.2, 11.1.



S11 **22**

A round bottom flask was charged with $Pd(PPh_3)_2Cl_2$ (0.5 mg, 0.67 umol, 0.02 eq), CuI (0.3 mg, 1.4 umol, 0.04 eq) and **6** (35 mg, 33.7 umol, 1 eq) was placed in a 25 mL two necks flask and evacuated and refilled with argon three times. In another flask, **S9** (60 mg, 0.1 mmol, 3.9 eq) was dissolved in 1.2 mL of Et_3N:THF (1:3) mixture and this solution was added to flask containing catalysts and **6** via cannula transfer after deoxygenating for 1 hour with argon. The reaction mixture was stirred for overnight at room temperature. The solvent was removed *in vacuo*. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.5:1) to yield **22**. Yield: 20 mg (35%). ^{1}H NMR (500 MHz, CDCl3): δ 9.36 (s, 1H), 9.34 (s, 1H), 8.76-8.72 (m, 2H), 8.19-8.15 (m, 2H), 7.95 (d, J=8.3 Hz, 2H), 7.78-7.76 (m, 3H), 7.75-7.68 (m, 4H), 7.64-7.63 (m, 2H), 7.56-7.52 (m, 3H), 7.48-7.46 (m, 1H), 7.14-7.13 (m, 1H), 7.07-7.06 (m, 3H), 6.93-6.87 (m, 4H), 4.05-3.90 (m, 10H), 3.86-3.84 (m, 2H), 3.79-3.77 (m, 2H), 1.88-1.73 (m, 7H), 1.70-1.28 (m, 56 H), 1.04-0.89 (m, 42 H). ^{13}C NMR (125 MHz, CDCl3): δ 154.7, 153.7, 153.3, 153.2, 140.7, 140.3, 139.8, 134.7, 132.59, 132.56, 132.5, 132.4, 132.3, 131.8, 130.9, 130.2, 128.8, 128.7, 127.7, 127.6, 127.3, 127.1, 126.9, 126.7, 126.4, 126.23, 126.19, 125.95, 125.93, 123.6, 123, 118.9, 118.59, 118.58, 118.2, 117.9, 117.3, 117.1, 114.3, 113.9, 113.7, 113.4, 109.9, 104.2, 103.3, 93.8, 92.41, 92.38, 92.1, 89.2, 88.6, 88.4, 85.9, 76.4, 72.7, 72.4, 71.7, 71.5, 71.3, 40.9, 39.9, 39.86, 39.8, 39.7, 39.6, 30.9, 30.85, 30.75, 30.70, 29.9, 29.5, 29.39, 29.36, 29.33, 29.3, 24.2, 24.14, 24.06, 24, 23.9, 23.33, 23.28, 23.22, 23.2, 14.32, 14.27, 14.26, 14.25, 14.23, 11.5, 11.4, 11.33, 11.29, 11.28. HRMS calcd for $C_{120}H_{148}O_7$ (M^+), 1702.1298, found, 1702.1223

3e. Synthesis of P2-25



S12

S12. Prepared following the established literature procedure.[5]

P2-25. A Schlenk tube was charged with <1 mg $Pd(PPh_3)_4$, and <1 mg CuI, and evacuated and refilled with argon three times. **6** (15 mg, 0.014 mmol, 1 eq), **7** (34 mg, 0.058 mmol, 4 eq), and **S12** was dissolved in 3 mL 4:1 (v:v) toluene:diisopropylamine and sparged with argon for 30 minutes. The solution was added to the reaction vessel and the mixture stirred for 72 hours at room tempareture. The reaction mixture was precipitated into 200 mL methanol and collected by centrifugation and decanting. The polymer was then dissolved in 2 mL of toluene and passed through a syringe filter to remove insoluble catalyst residues, reprecipitated into 100 mL of methanol and isolated by centrifugation and decanting. Mn [g/mol]: 68k, Mw [g/mol]: 176k. ^{1}H NMR (500 MHz, CDCl3): δ 9.37-9.35 (m, 0.5H), 8.75 (m, 0.5H), 8.17 (m, 0.5), 7.98-7.96 (m, 0.5H), 7.80-7.70 (m, 4H), 7.63 (m, 1H), 7.11-7.02 (m, 8H), 4.02-3.91 (m, 18H), 1.8 (m, 9H), 1.65-1.28 (m, 72H), 1.00-0.91 (m, 54H).

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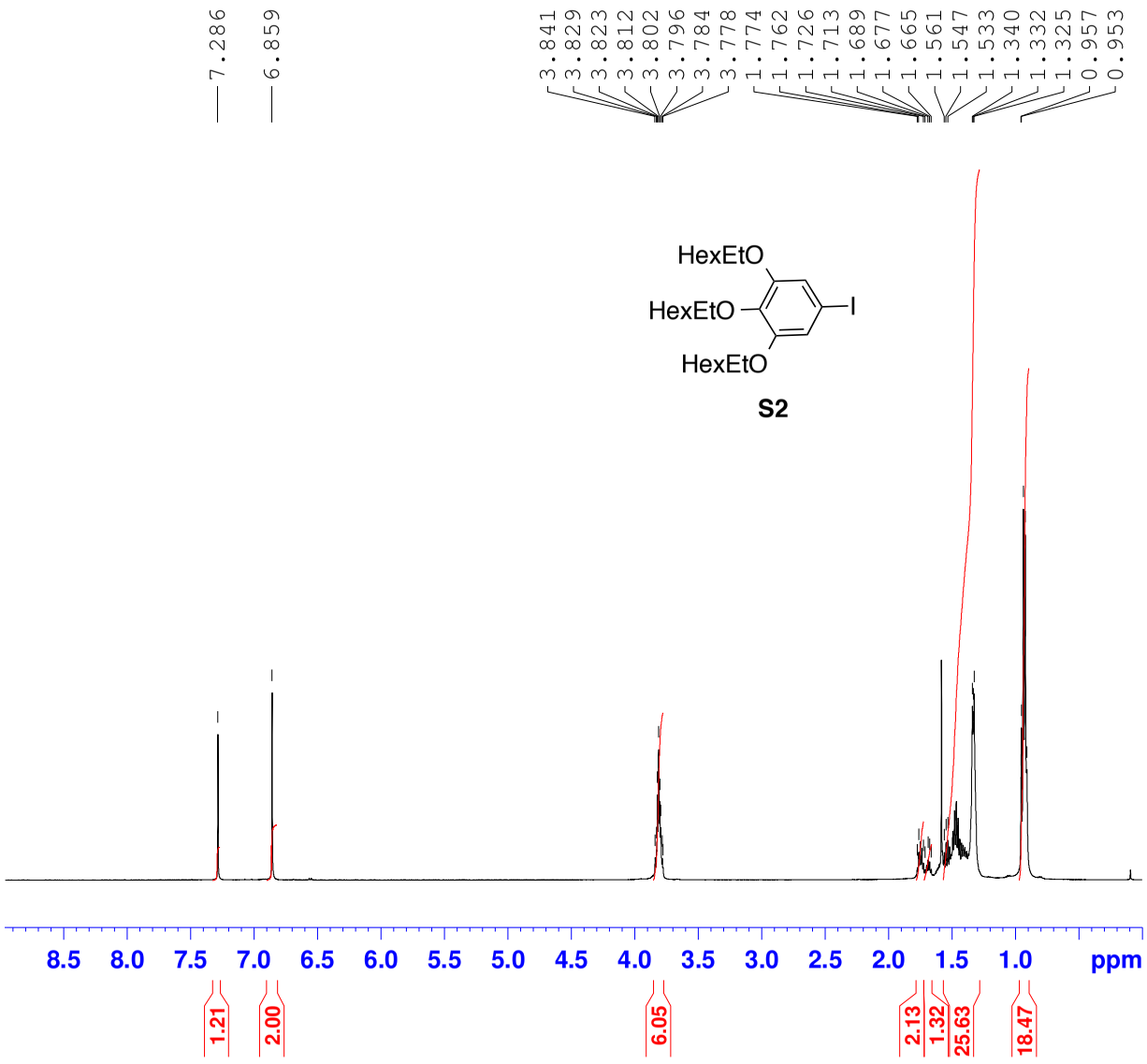

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TE                   290.6 K
D1                0.50000000 sec
TD0                       1

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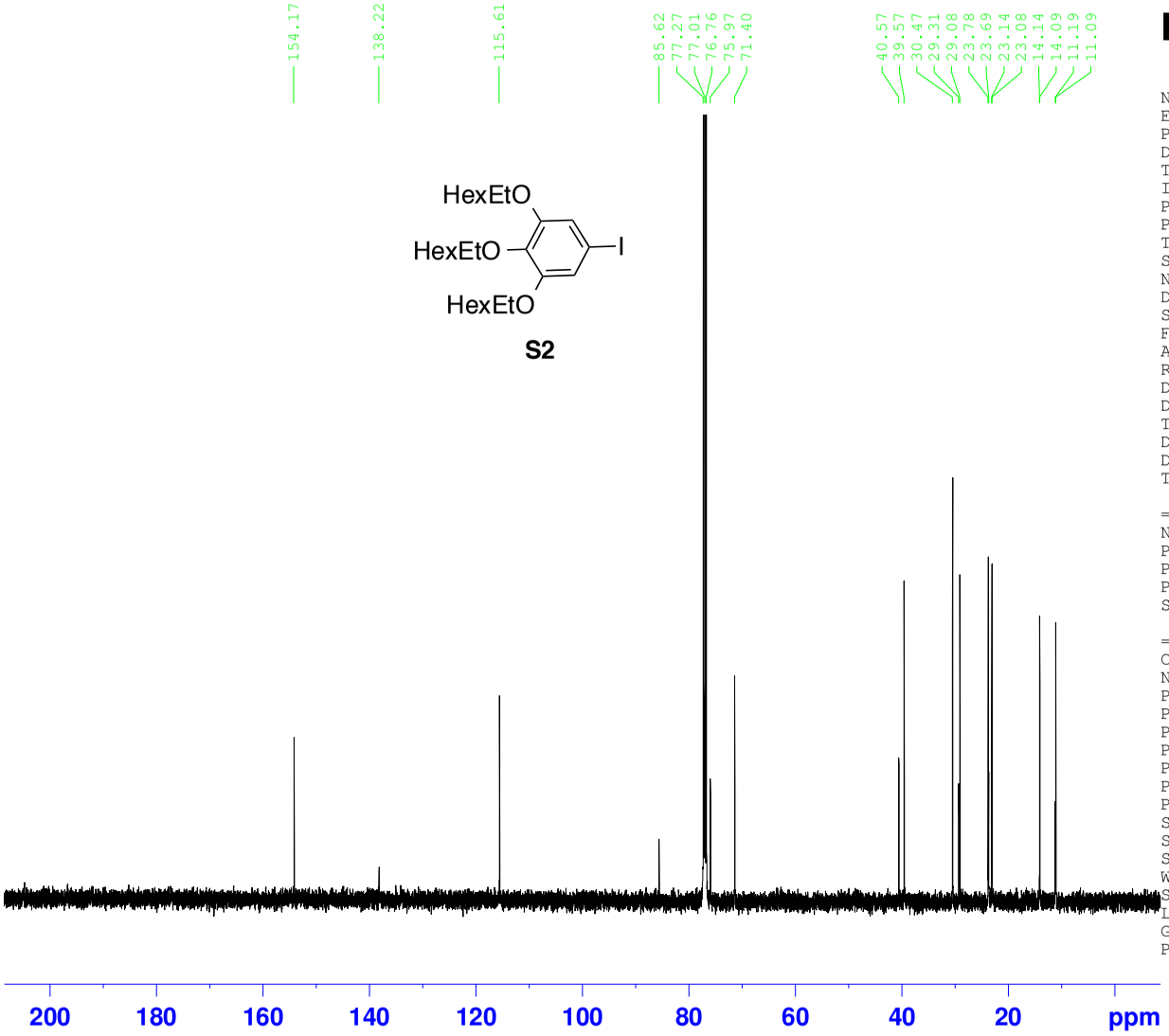

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PL13	16.80 dB
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PL12W	1.11017132 W
PL13W	0.46707872 W
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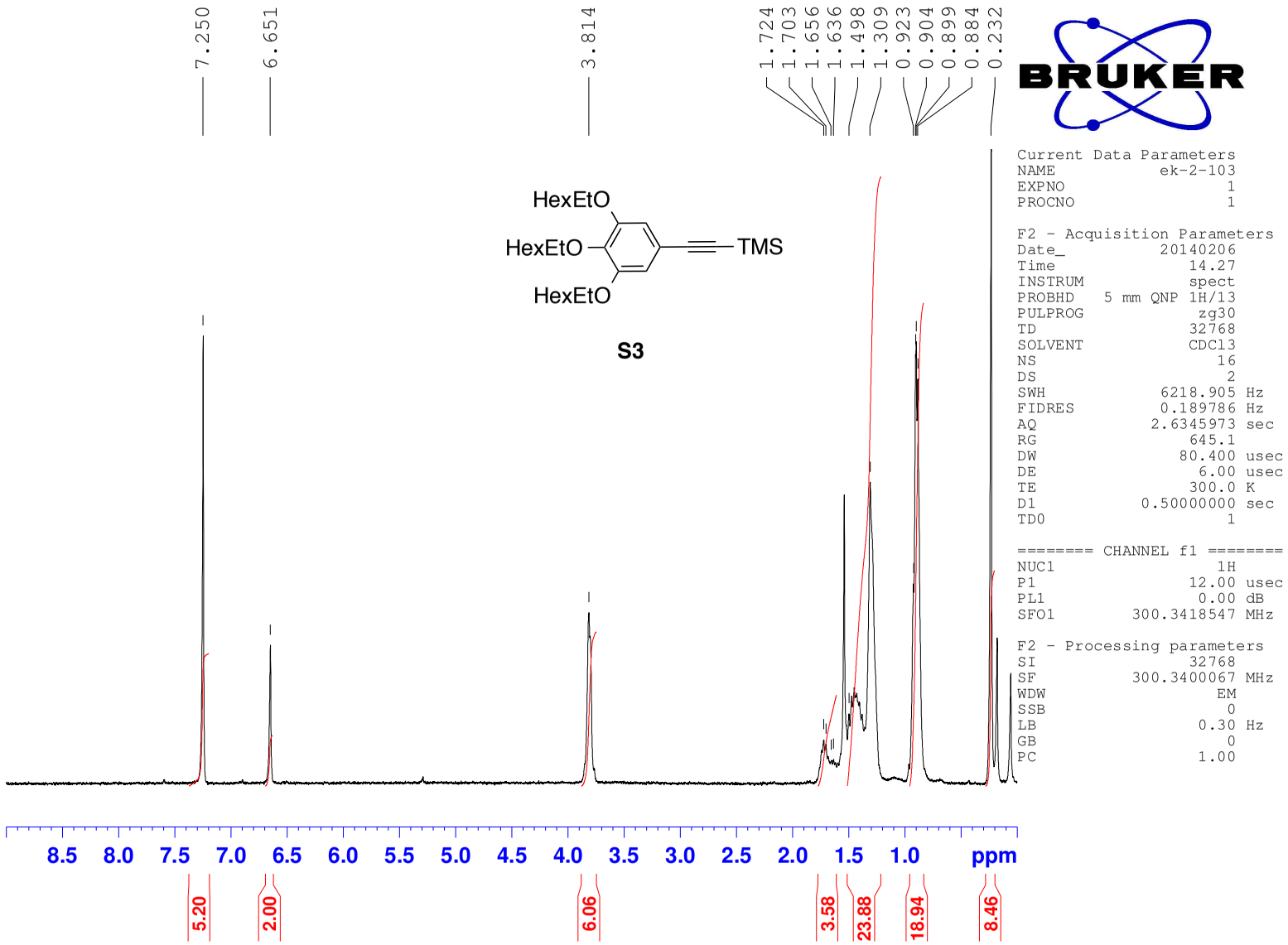


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F2 - Processing parameters
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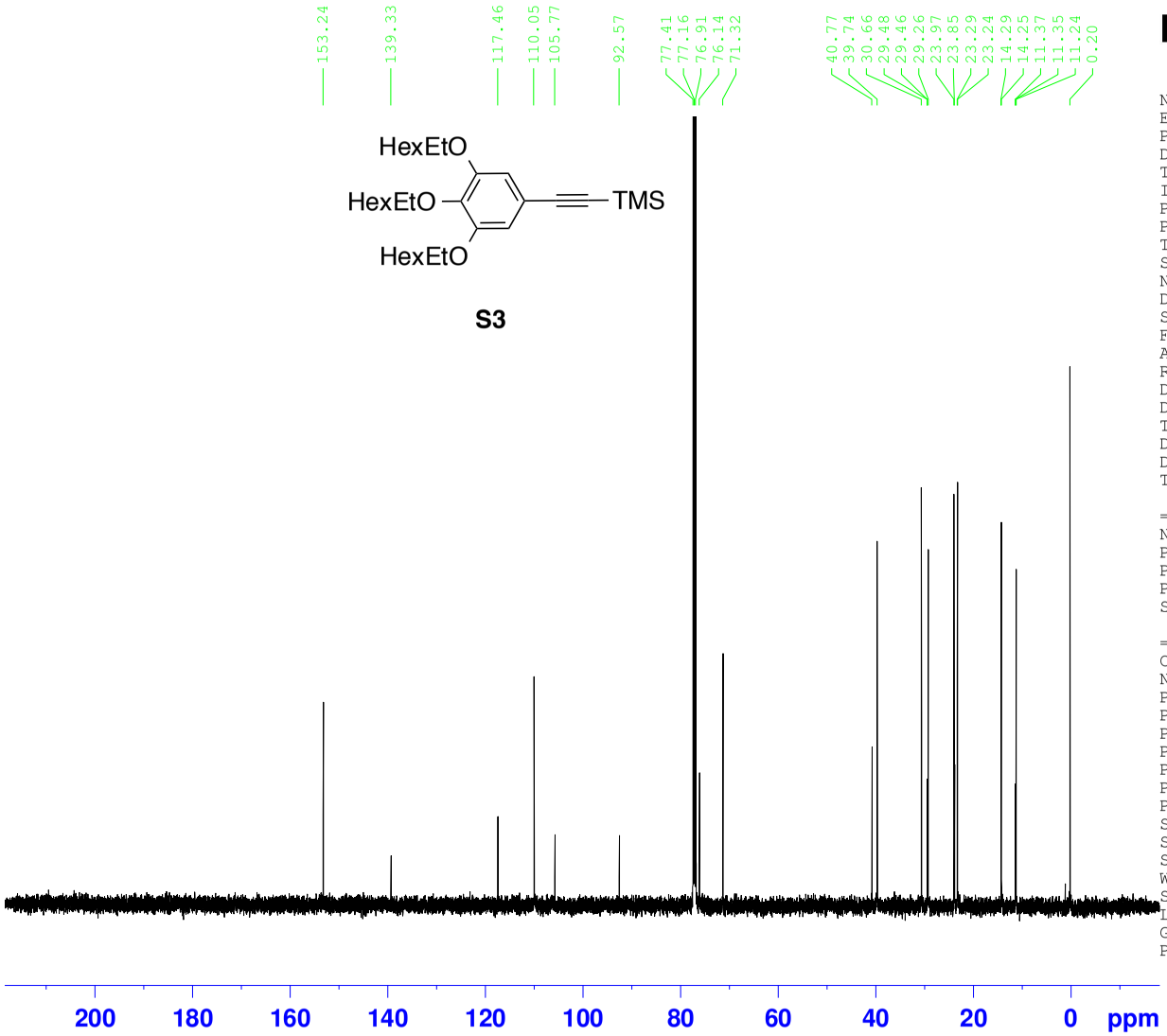

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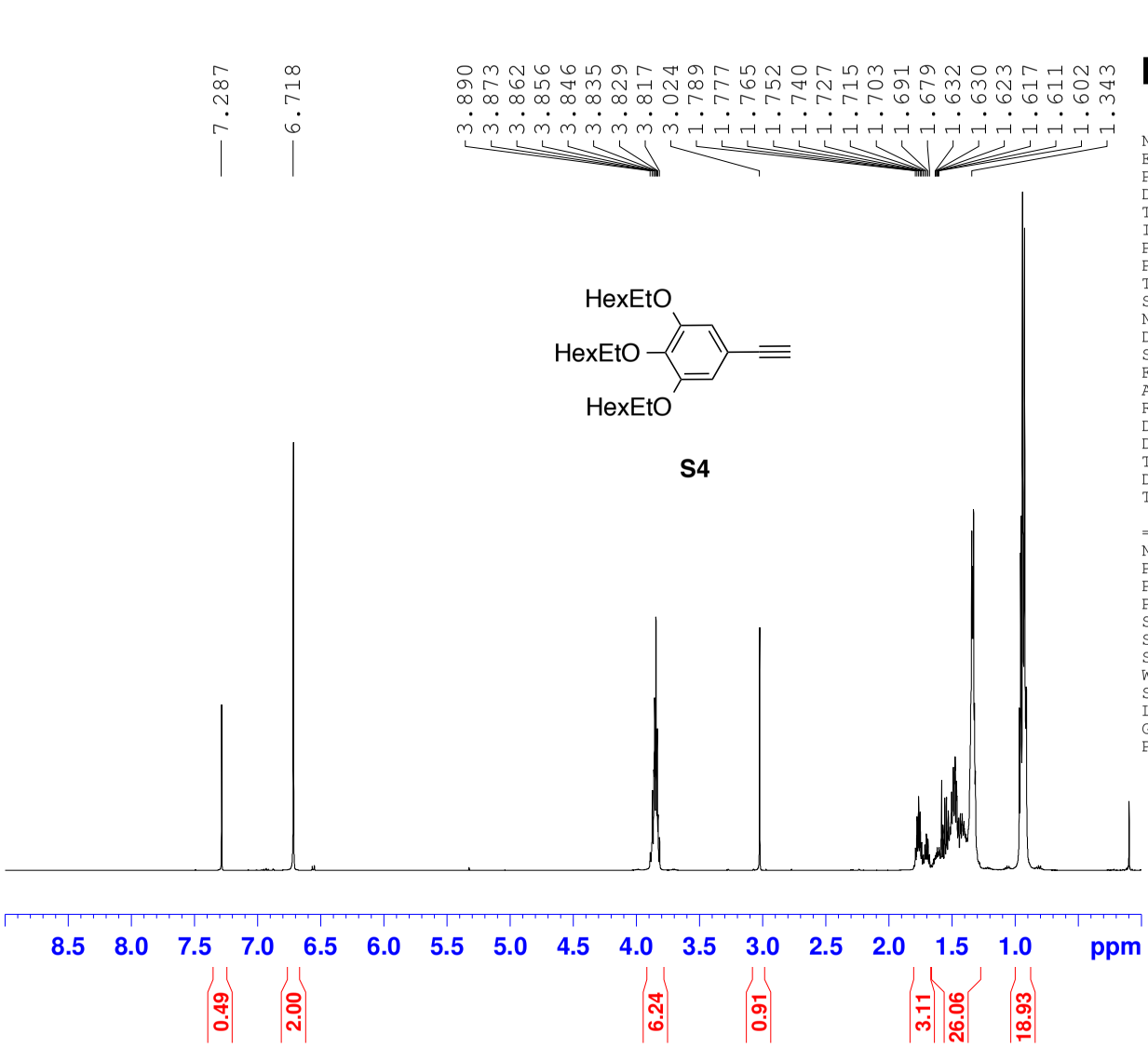

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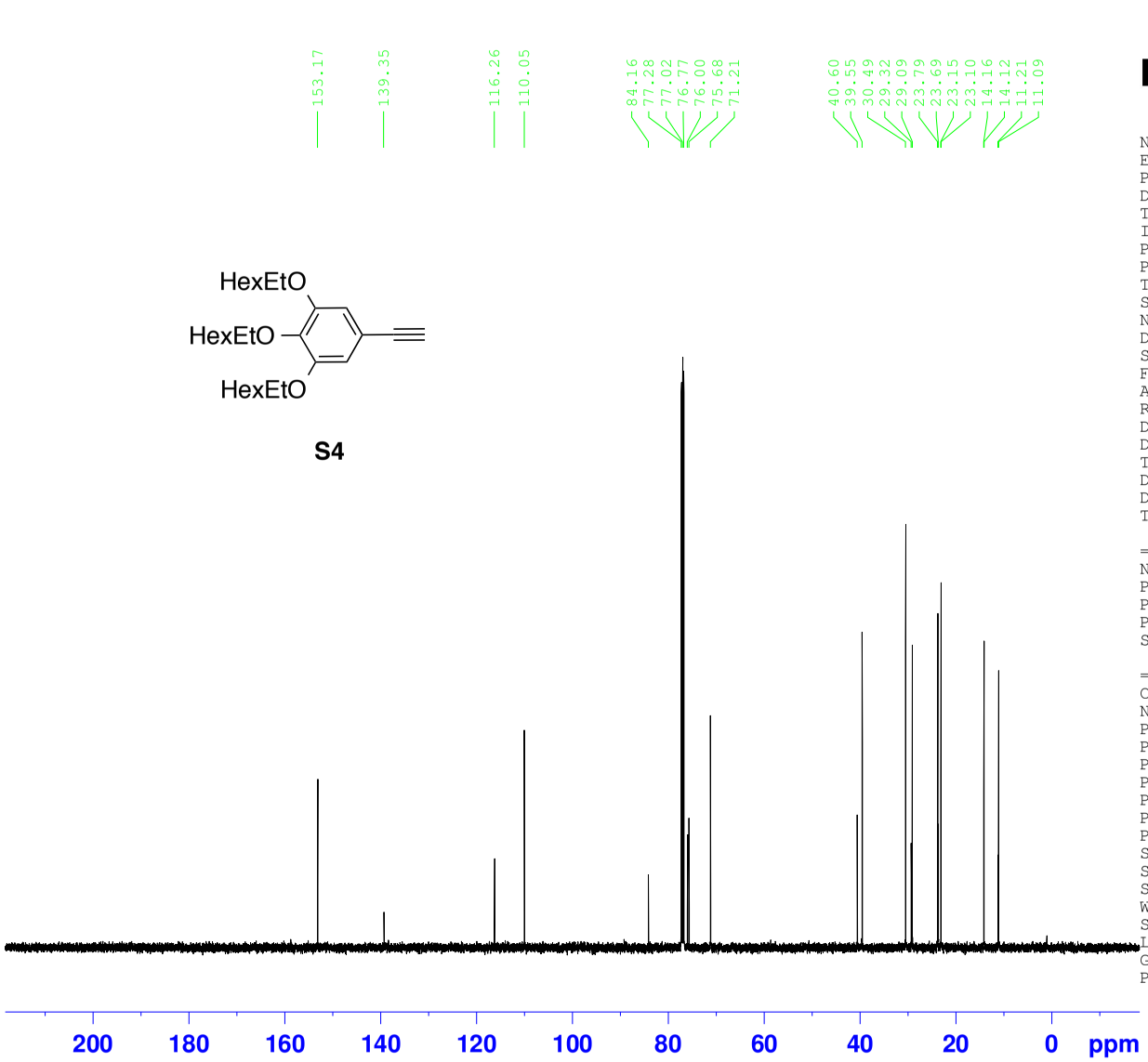


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D1              0.50000000 sec
D11             0.03000000 sec
TD0                        1

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PL1W           89.92553711 W
SFO1          125.7703643 MHz

======== CHANNEL f2 ========
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PL2                    1.00 dB
PL12                  13.04 dB
PL13                  16.80 dB
PL2W           17.75783539 W
PL12W           1.11017132 W
PL13W           0.46707872 W
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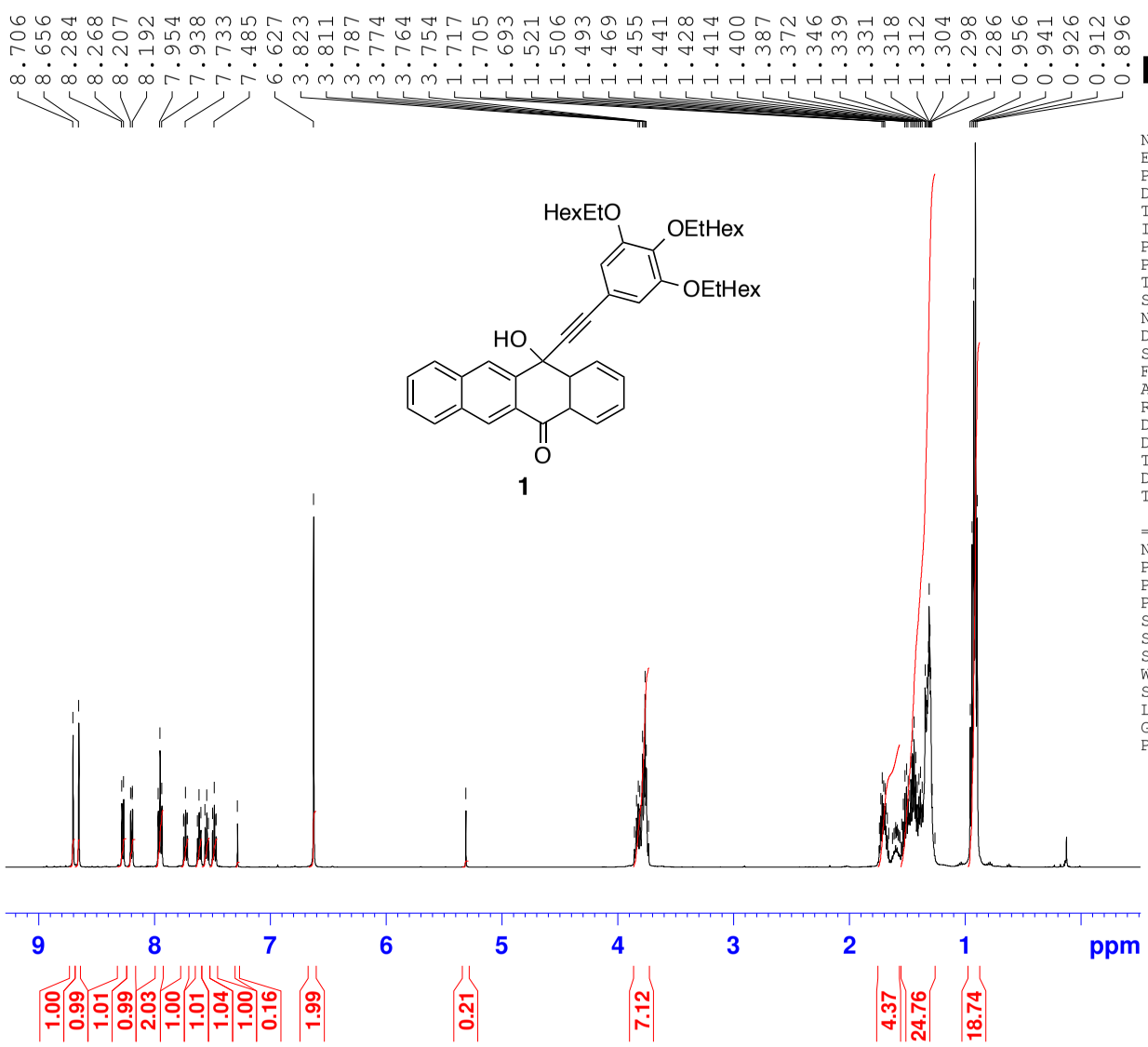

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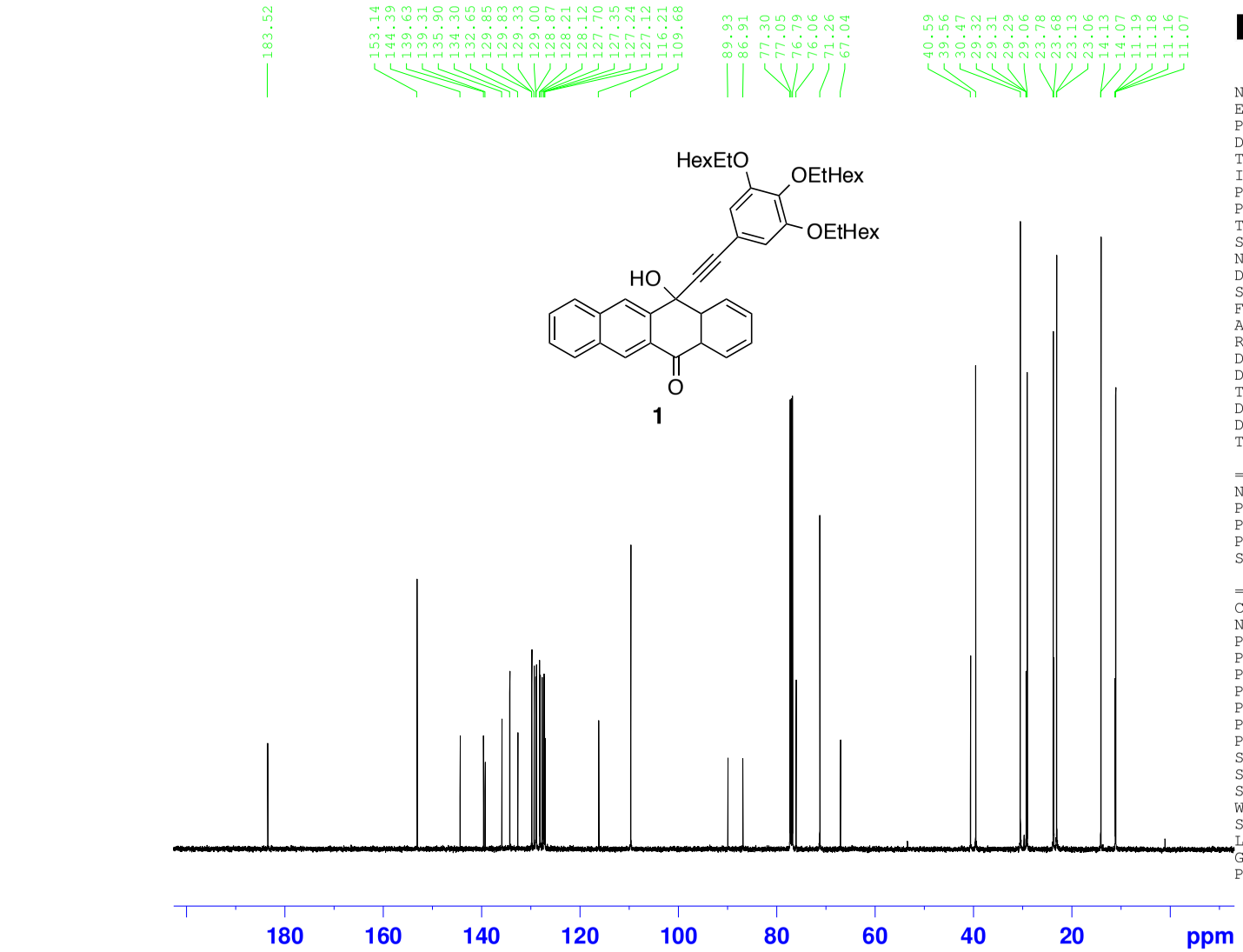
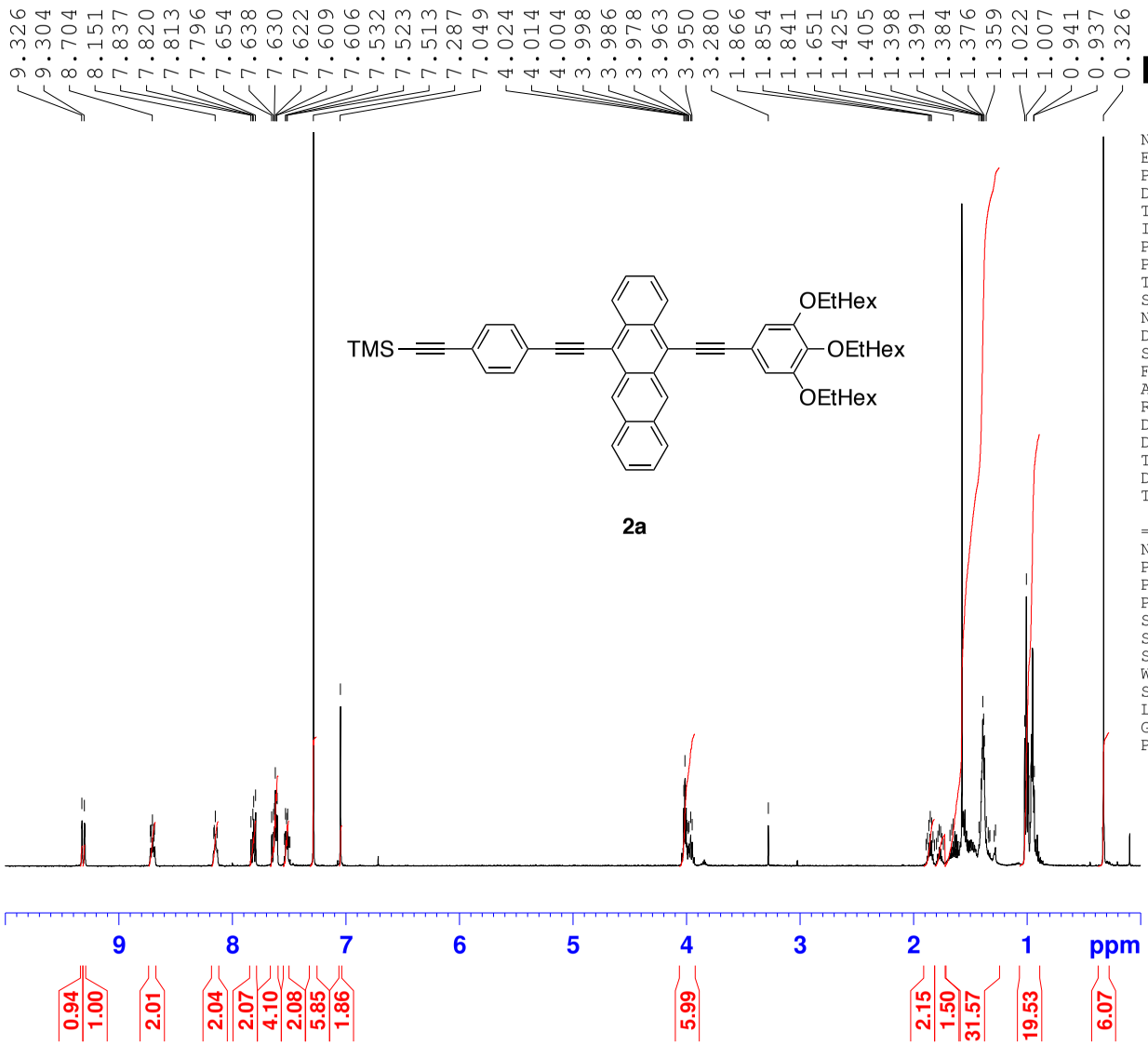
LB	0.30 Hz
GB	0
PC	1.00



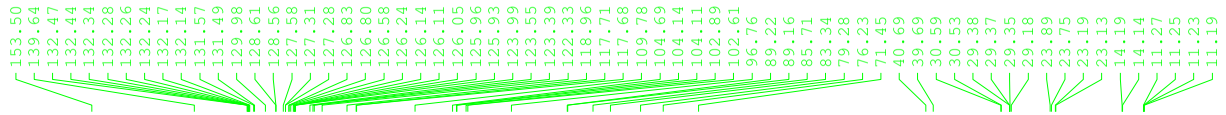
BRUKER

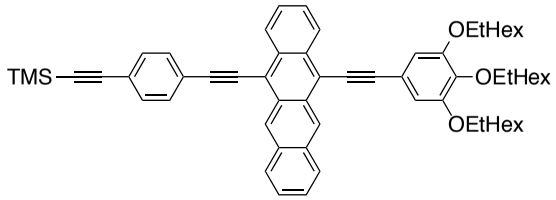
NAME	ek-2-050
EXPNO	4
PROCNO	1
Date_	20131101
Time	15.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.1 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



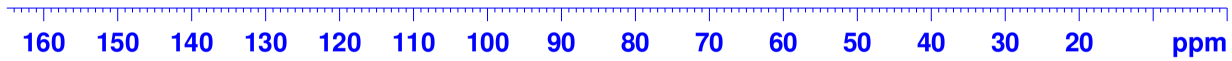
BRUKER

NAME	ek-2-124
EXPNO	2
PROCNO	1
Date_	20140312
Time	16.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	293.6 K
D1	0.50000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





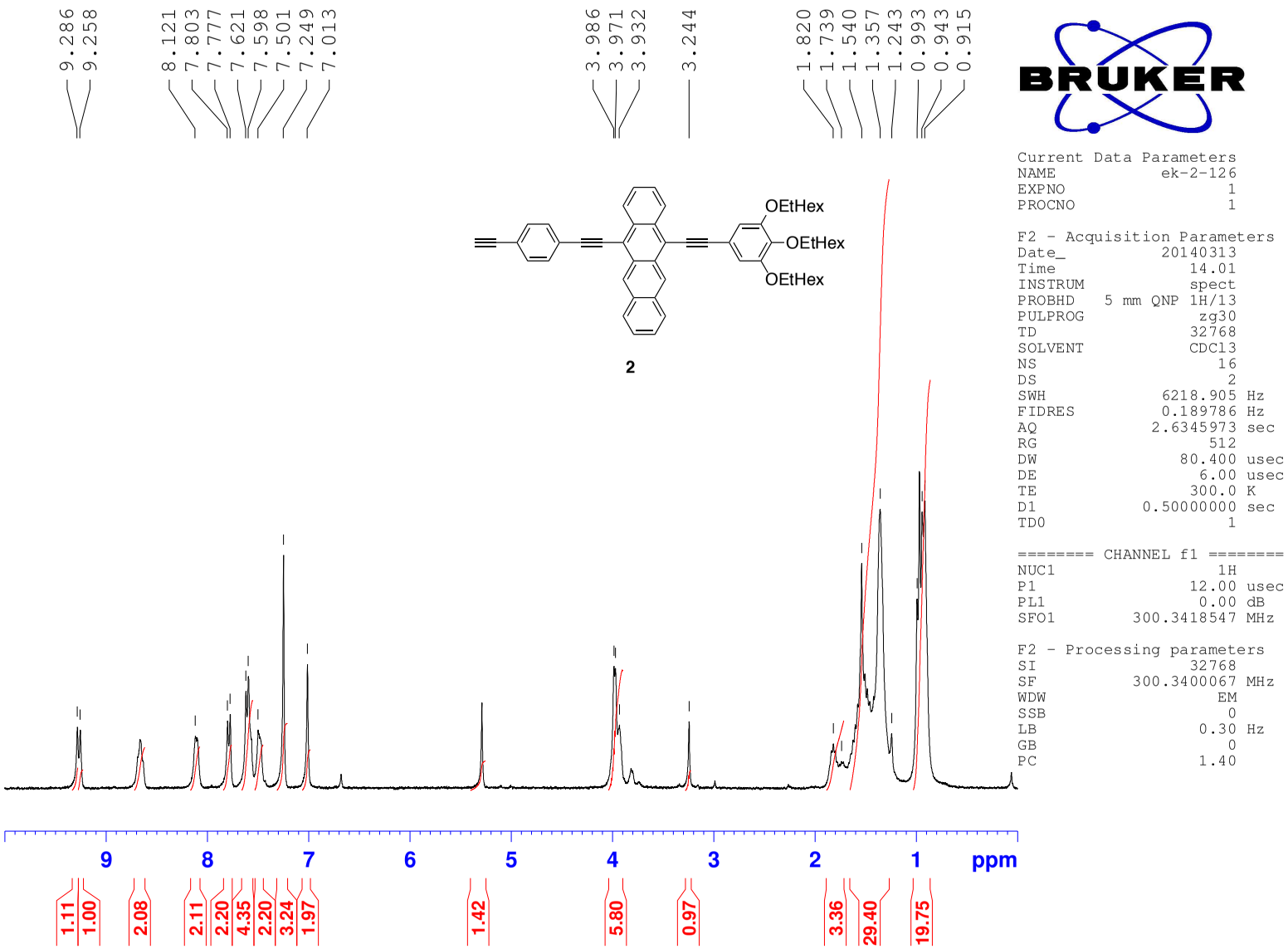
2a




```
NAME                ek-2-124
EXPNO                      4
PROCNO                     1
Date_               20140312
Time                   19.34
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                      16384
DS                          4
SWH                 29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010548 sec
RG                        203
DW                     16.800 usec
DE                      6.50 usec
TE                     293.8 K
D1                  0.50000000 sec
D11                 0.03000000 sec
TD0                       100

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.50 usec
PL1                      0.00 dB
PL1W               89.92553711 W
SFO1               125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      1.00 dB
PL12                    13.04 dB
PL13                    16.80 dB
PL2W               17.75783539 W
PL12W               1.11017132 W
PL13W               0.46707872 W
SFO2               500.1320005 MHz
SI                      65536
SF                 125.7577890 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

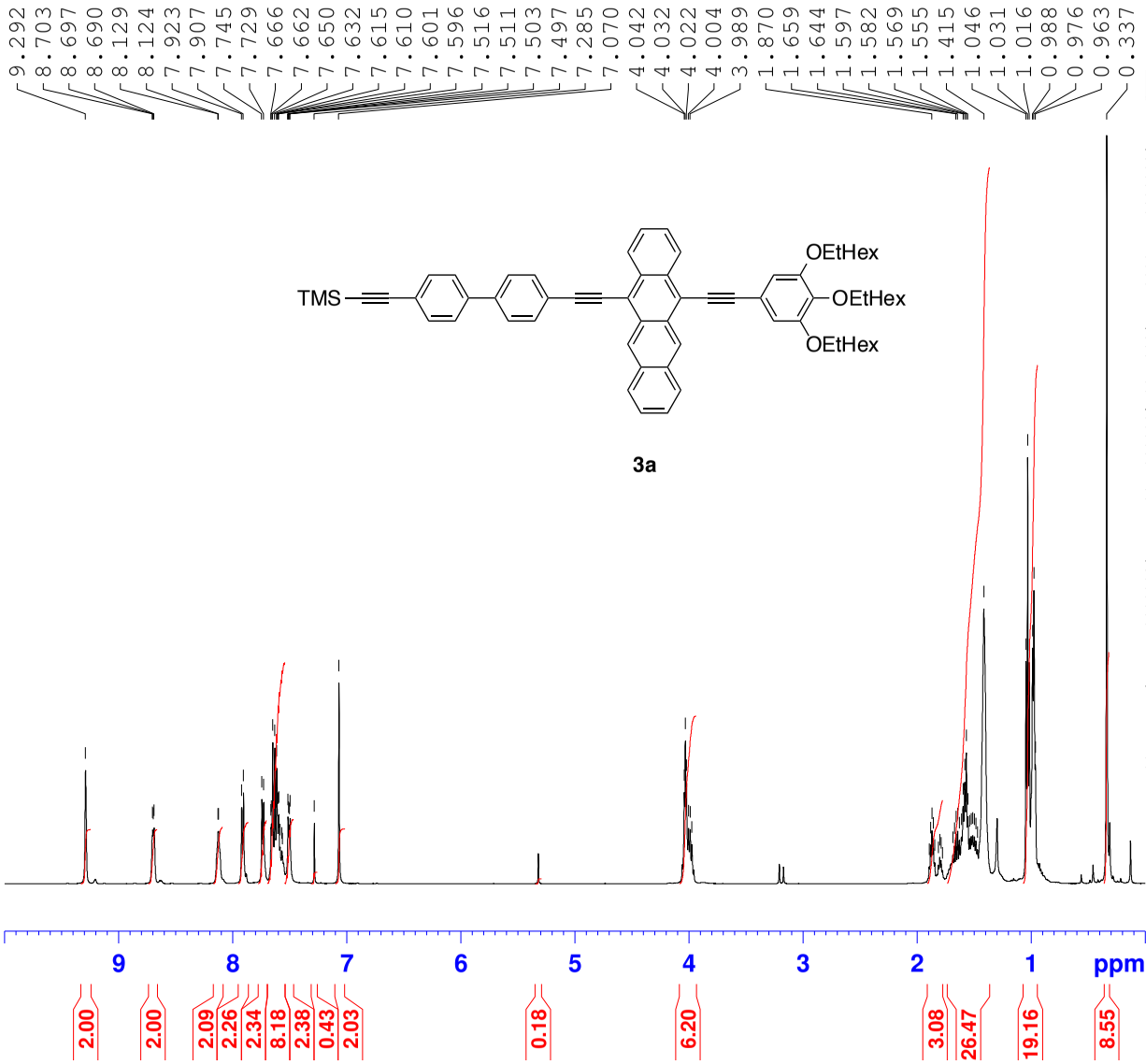


Current Data Parameters
NAME ek-2-126
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140313
Time 14.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 6218.905 Hz
FIDRES 0.189786 Hz
AQ 2.6345973 sec
RG 512
DW 80.400 usec
DE 6.00 usec
TE 300.0 K
D1 0.50000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 12.00 usec
PL1 0.00 dB
SFO1 300.3418547 MHz

F2 - Processing parameters
SI 32768
SF 300.3400067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

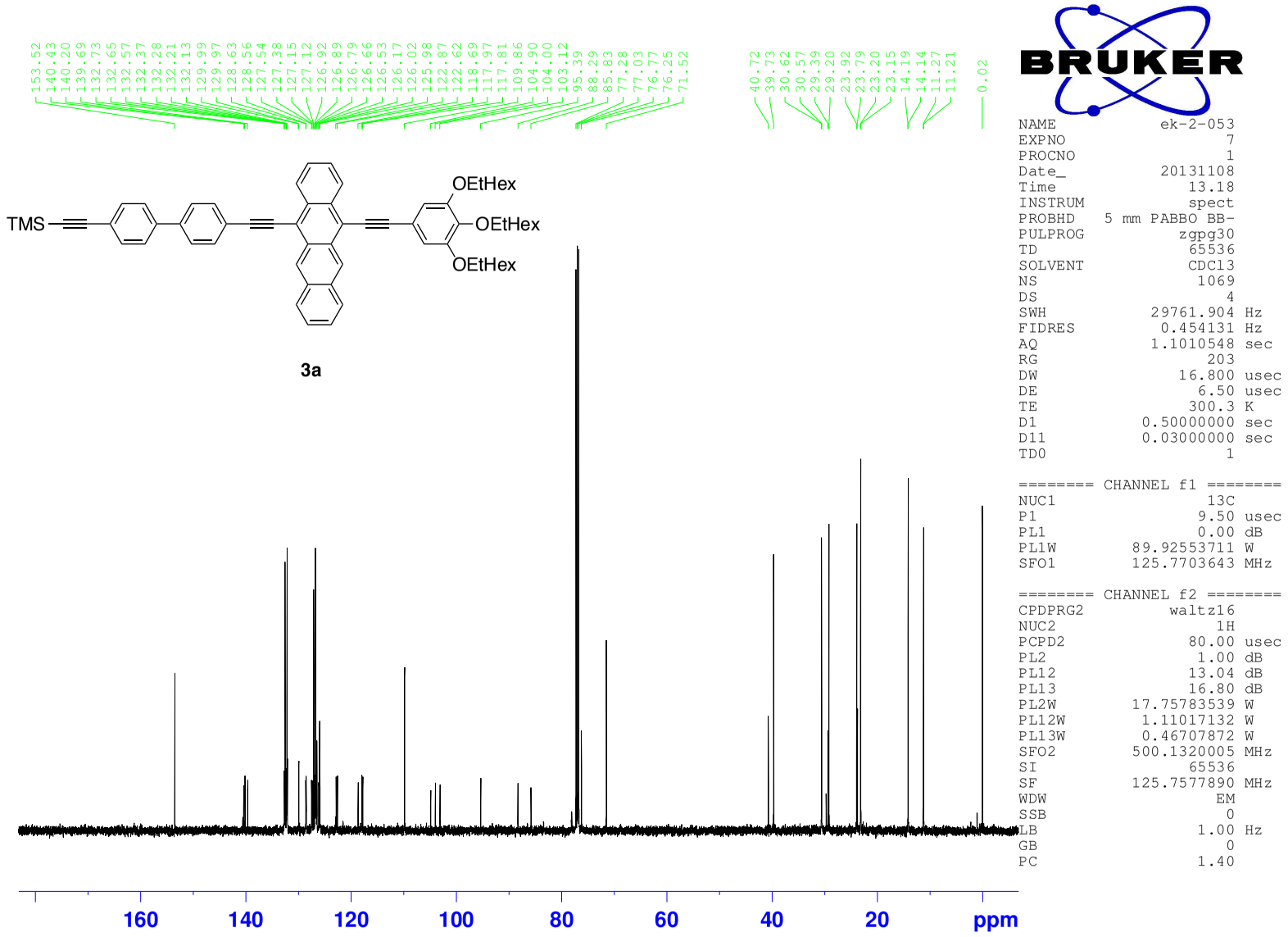


BRUKER

NAME	ek-2-053
EXPNO	6
PROCNO	1
Date_	20131108
Time	13.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	71.8
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	5.00000000 sec
TD0	1

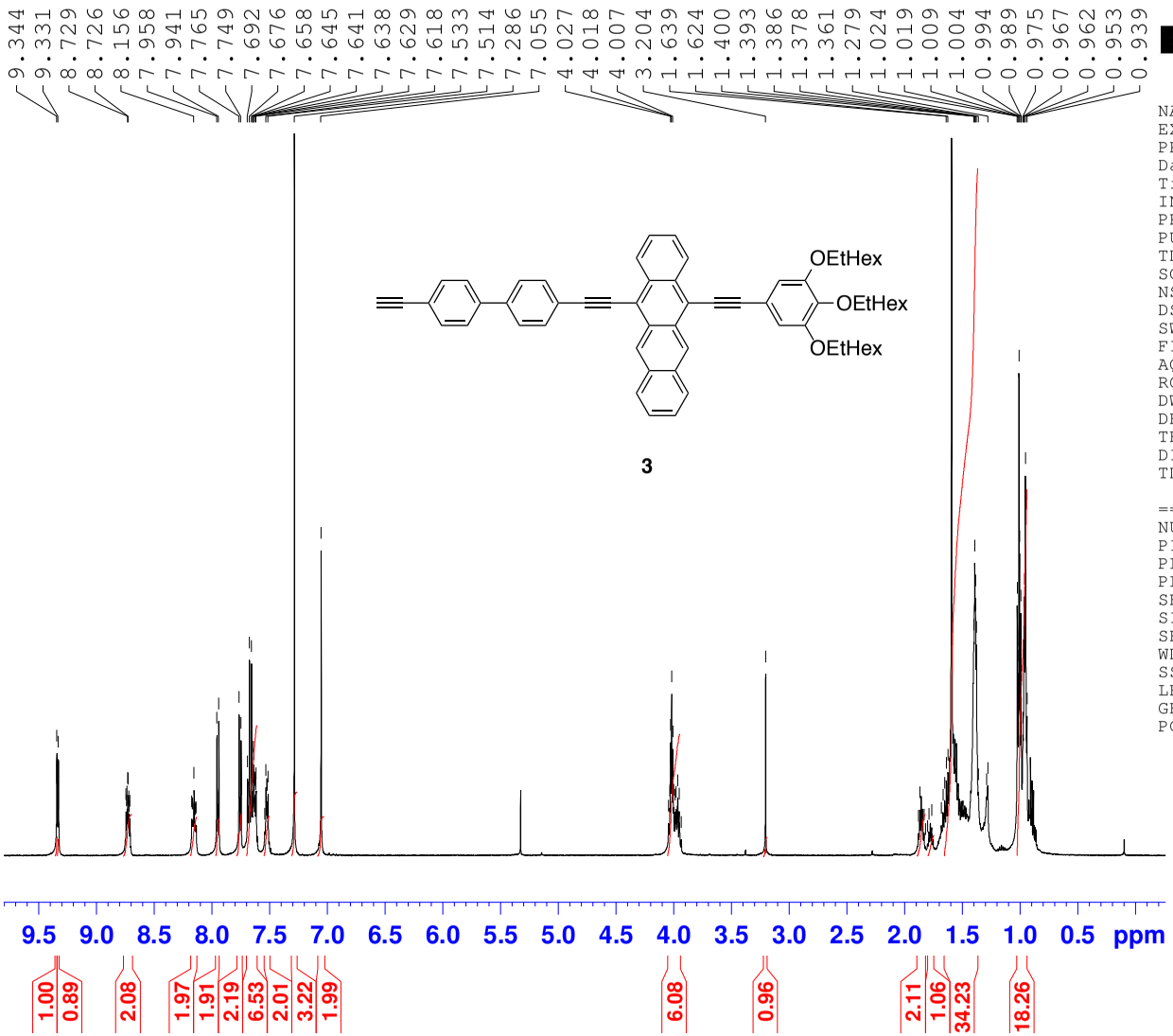
======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



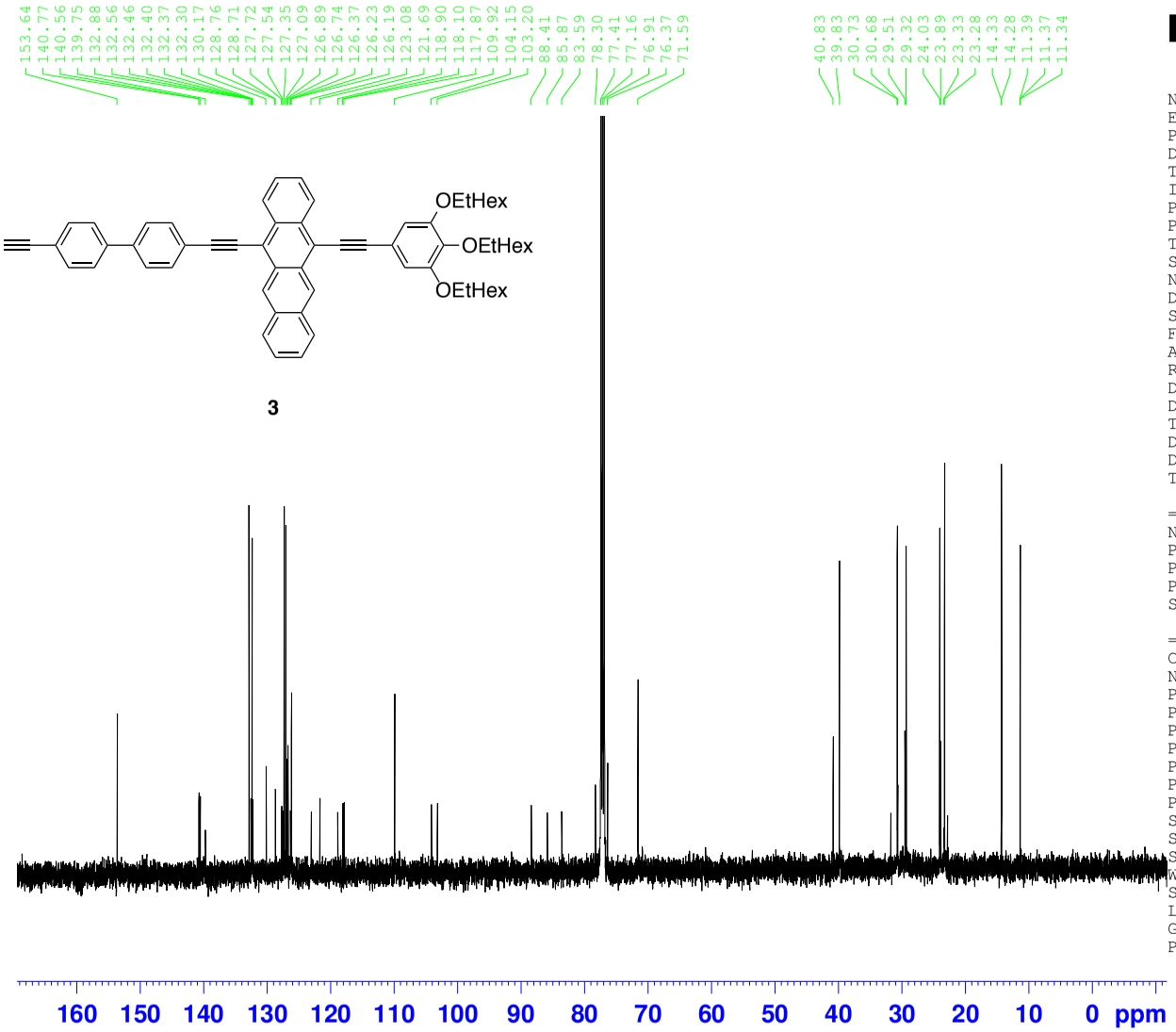
BRUKER

NAME	ek-2-053
EXPNO	7
PROCNO	1
Date_	20131108
Time	13.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1069
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.3 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

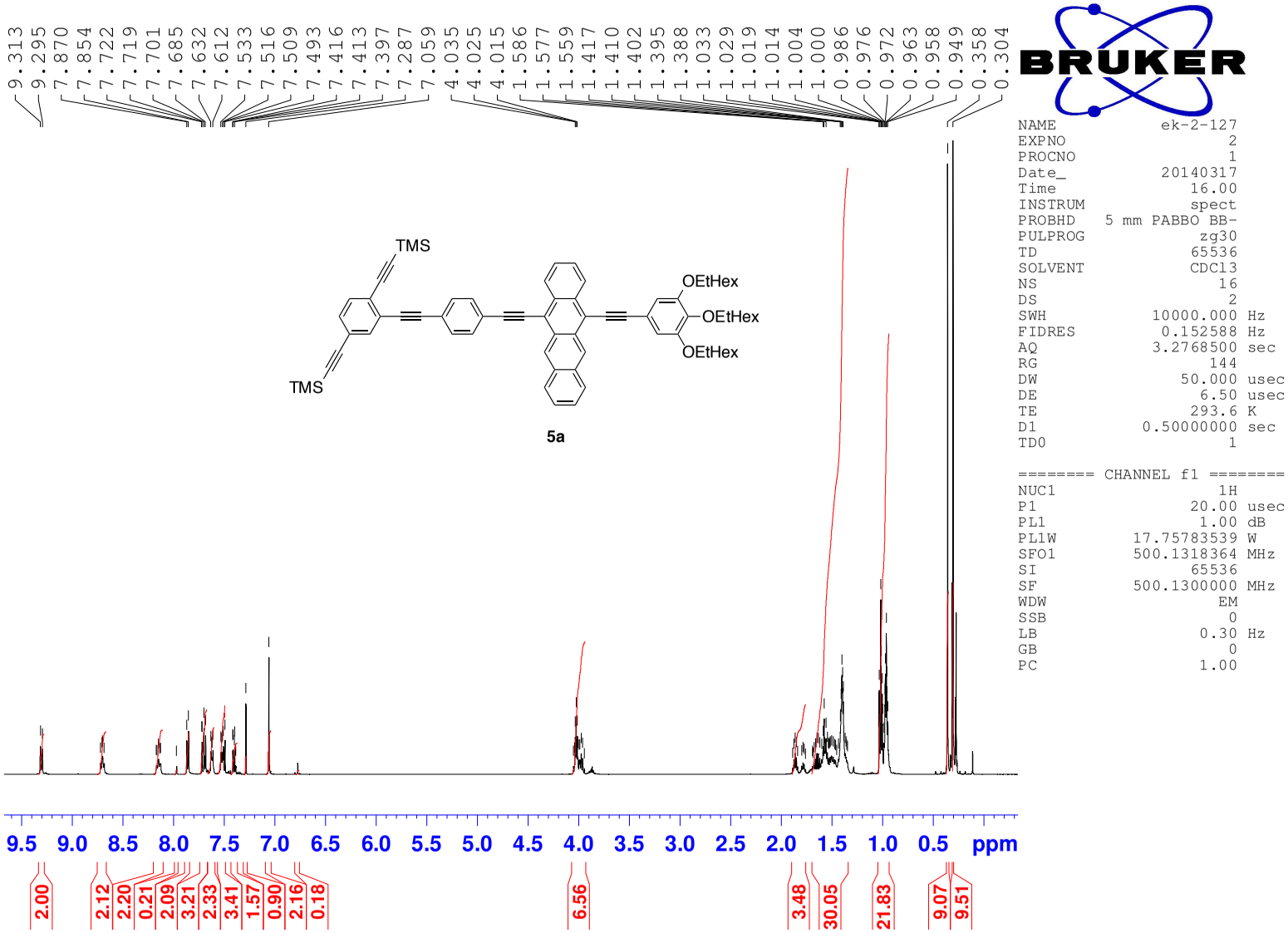



```
NAME                ek-2-112
EXPNO                      5
PROCNO                     1
Date_               20150512
Time                   15.40
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2768500 sec
RG                       203
DW                  50.000 usec
DE                   6.50 usec
TE                   290.6 K
D1               0.50000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    20.00 usec
PL1                    1.00 dB
PL1W          17.75783539 W
SFO1          500.1318364 MHz
SI                     65536
SF            500.1300000 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```

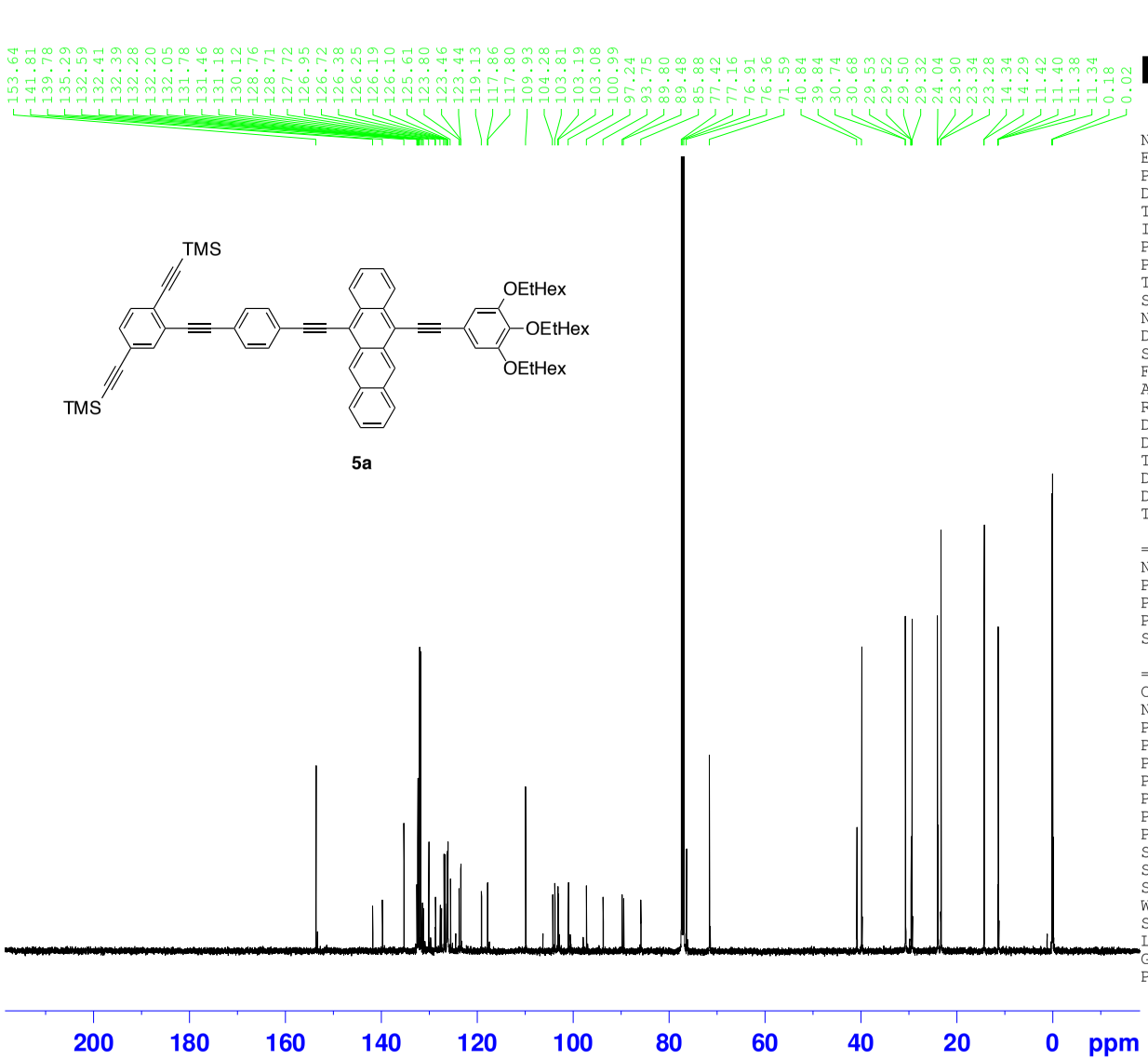


NAME	ek-2-112
EXPNO	6
PROCNO	1
Date_	20150512
Time	15.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	5789
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	292.0 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577712 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	0.50



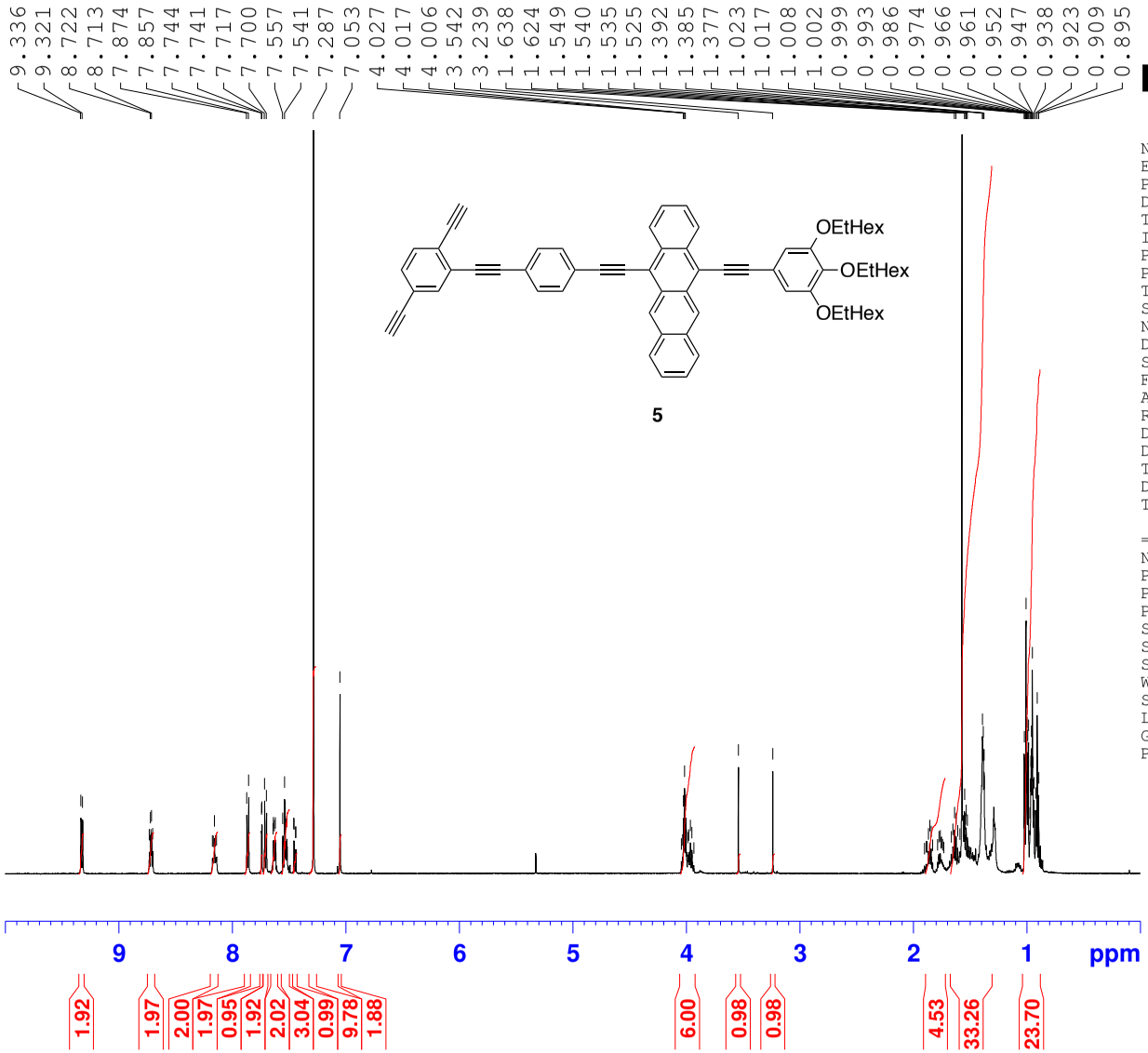

```
NAME                ek-2-127
EXPNO                      2
PROCNO                     1
Date_               20140317
Time                   16.00
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2768500 sec
RG                       144
DW                    50.000 usec
DE                     6.50 usec
TE                    293.6 K
D1                 0.50000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     20.00 usec
PL1                     1.00 dB
PL1W           17.75783539 W
SFO1           500.1318364 MHz
SI                    65536
SF             500.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



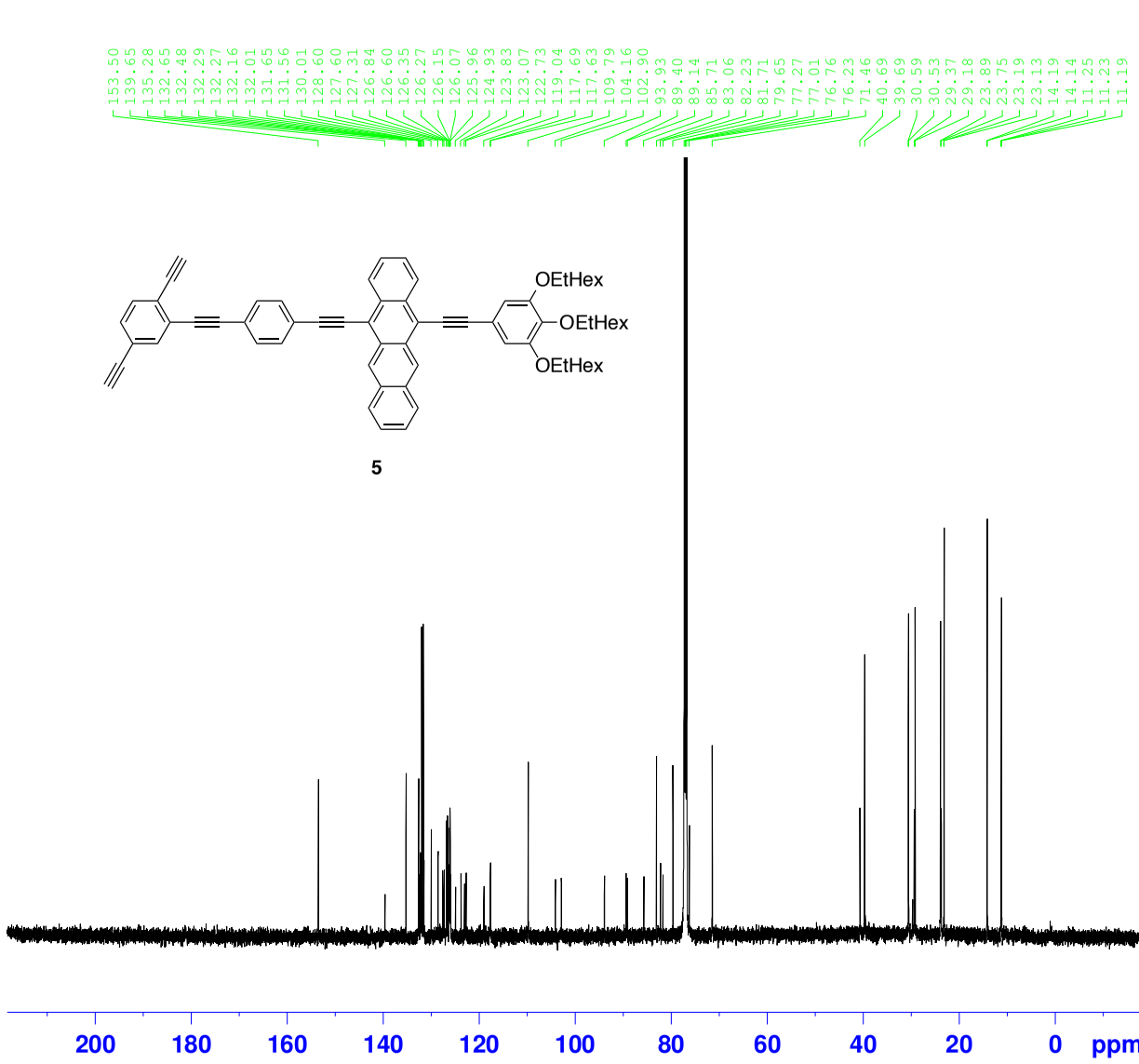
BRUKER

NAME	ek-2-127	
EXPNO	3	
PROCNO	1	
Date_	20140317	
Time	16.04	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	6382	
DS	4	
SWH	29761.904	Hz
FIDRES	0.454131	Hz
AQ	1.1010548	sec
RG	203	
DW	16.800	usec
DE	6.50	usec
TE	293.6	K
D1	0.50000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.50	usec
PL1	0.00	dB
PL1W	89.92553711	W
SFO1	125.7703643	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	1.00	dB
PL12	13.04	dB
PL13	16.80	dB
PL2W	17.75783539	W
PL12W	1.11017132	W
PL13W	0.46707872	W
SFO2	500.1320005	MHz
SI	65536	
SF	125.7577719	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



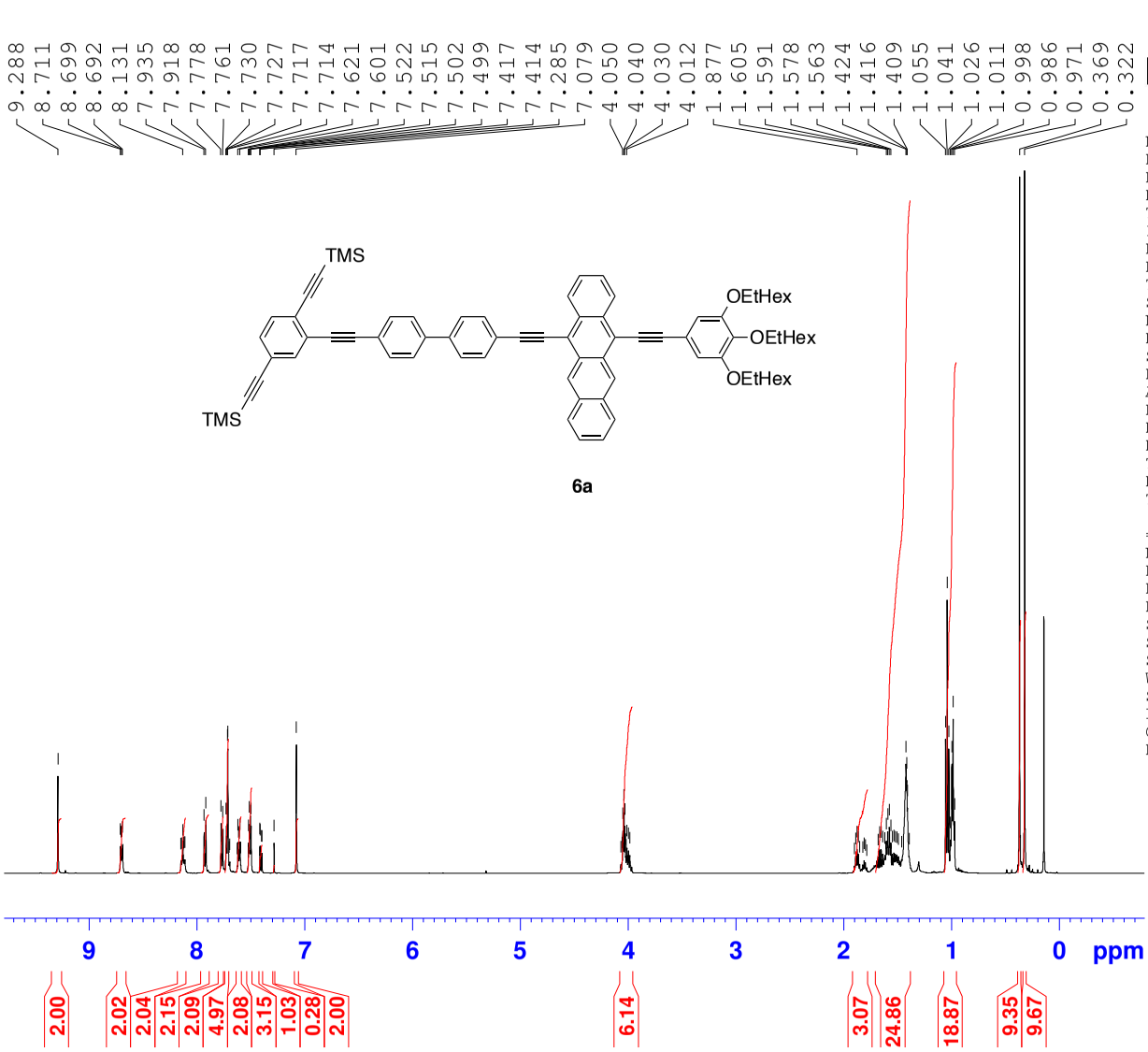

```
NAME                ek-2-128
EXPNO                      1
PROCNO                     1
Date_               20140318
Time                   16.08
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        32
DS                         2
SWH             10000.000 Hz
FIDRES              0.152588 Hz
AQ              3.2768500 sec
RG                       203
DW                  50.000 usec
DE                   6.50 usec
TE                   293.6 K
D1              5.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    20.00 usec
PL1                    1.00 dB
PL1W          17.75783539 W
SFO1          500.1318364 MHz
SI                     65536
SF            500.1300000 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```



BRUKER

NAME	ek-2-128
EXPNO	7
PROCNO	1
Date_	20140320
Time	18.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	30977
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	294.0 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	100
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

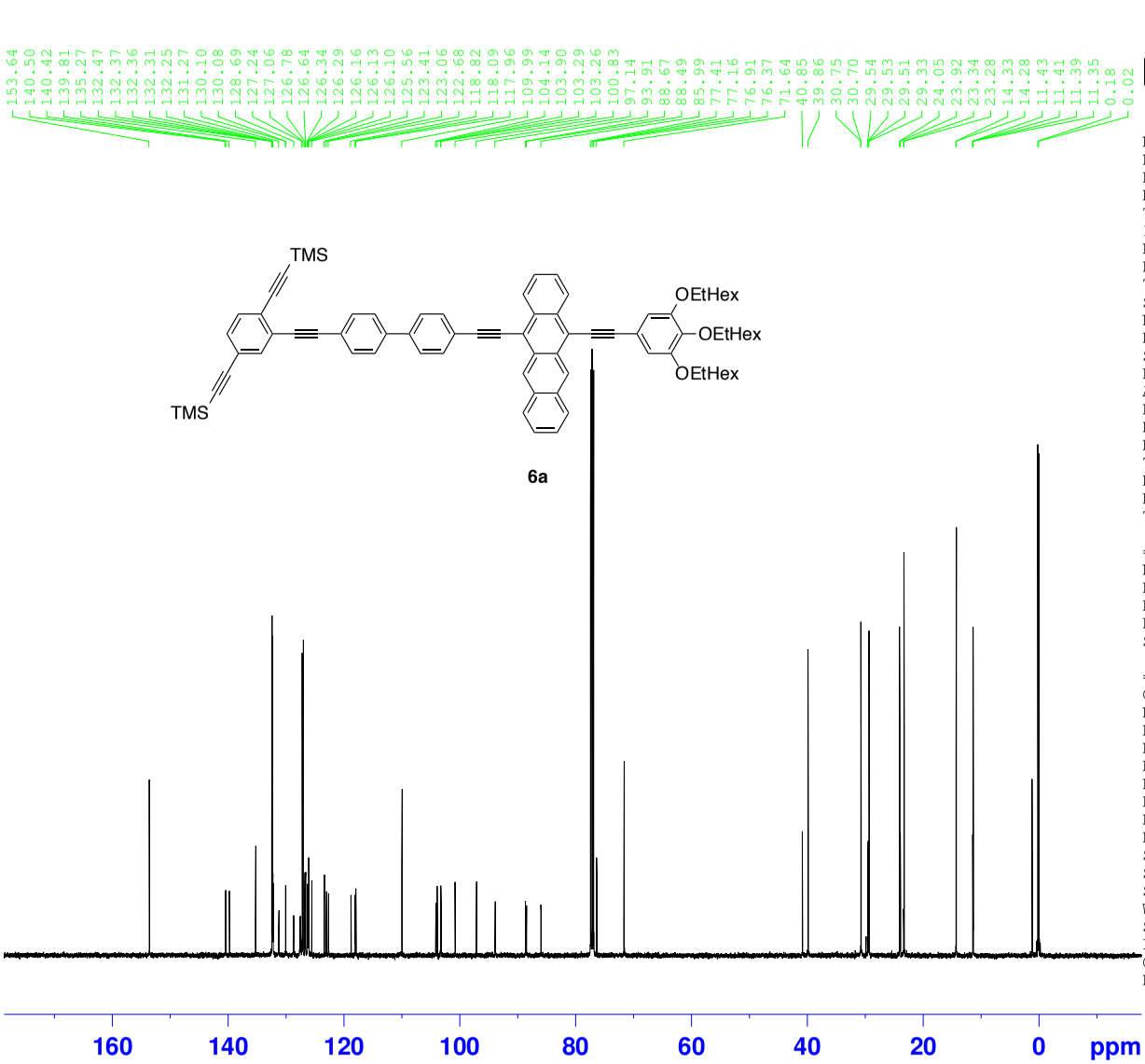


BRUKER

NAME	ek-2-057
EXPNO	3
PROCNO	1
Date_	20131113
Time	14.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	50.8
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	5.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

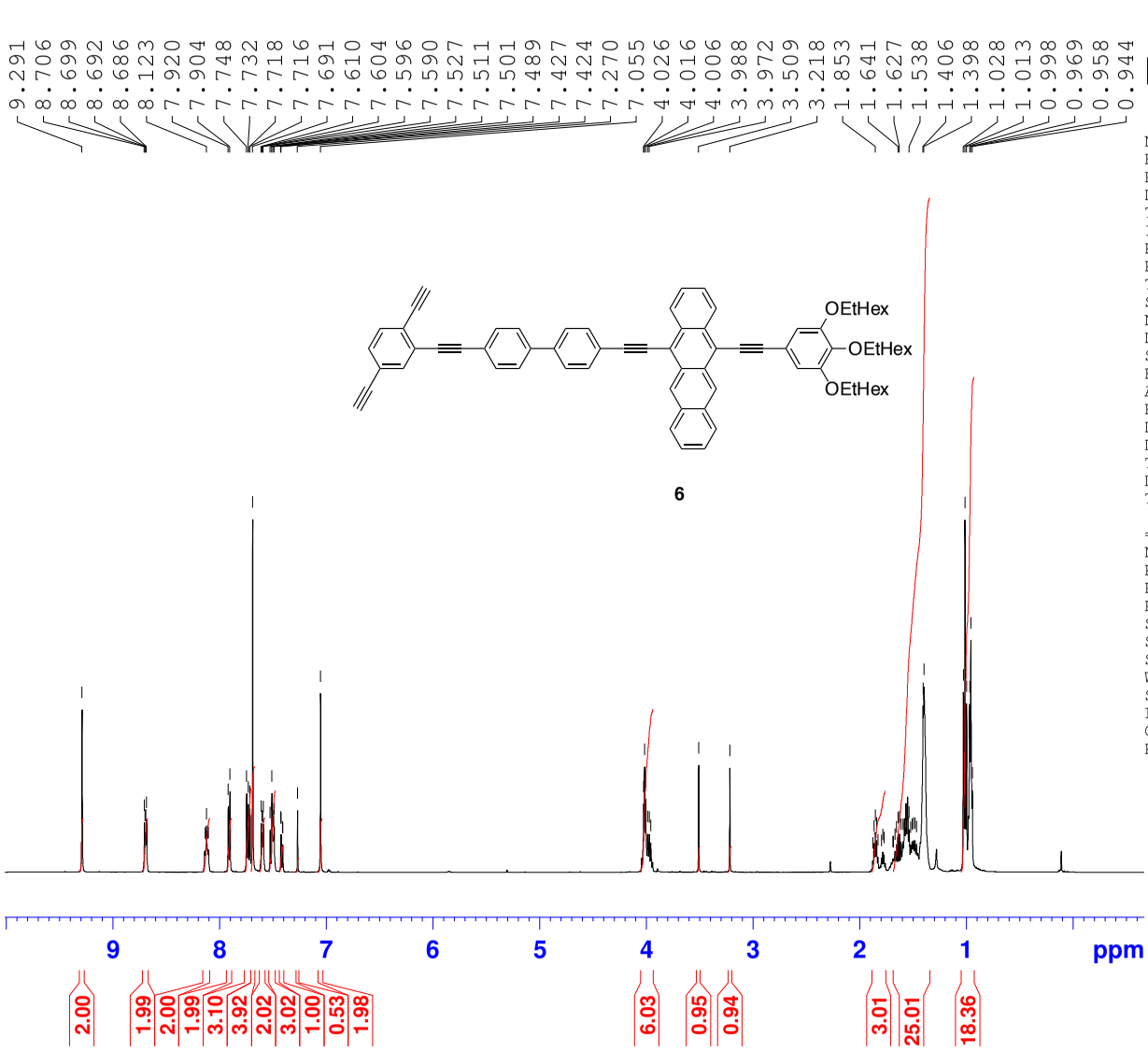


BRUKER

```
NAME                ek-2-057
EXPNO                      5
PROCNO                     1
Date_               20131113
Time                   14.44
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDC13
NS                       1540
DS                          4
SWH                 29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010548 sec
RG                        203
DW                     16.800 usec
DE                      6.50 usec
TE                     300.6 K
D1                  0.50000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                     0.00 dB
PL1W             89.92553711 W
SFO1            125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     1.00 dB
PL12                   13.04 dB
PL13                   16.80 dB
PL2W             17.75783539 W
PL12W             1.11017132 W
PL13W             0.46707872 W
SFO2            500.1320005 MHz
SI                      65536
SF              125.7577741 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.40
```

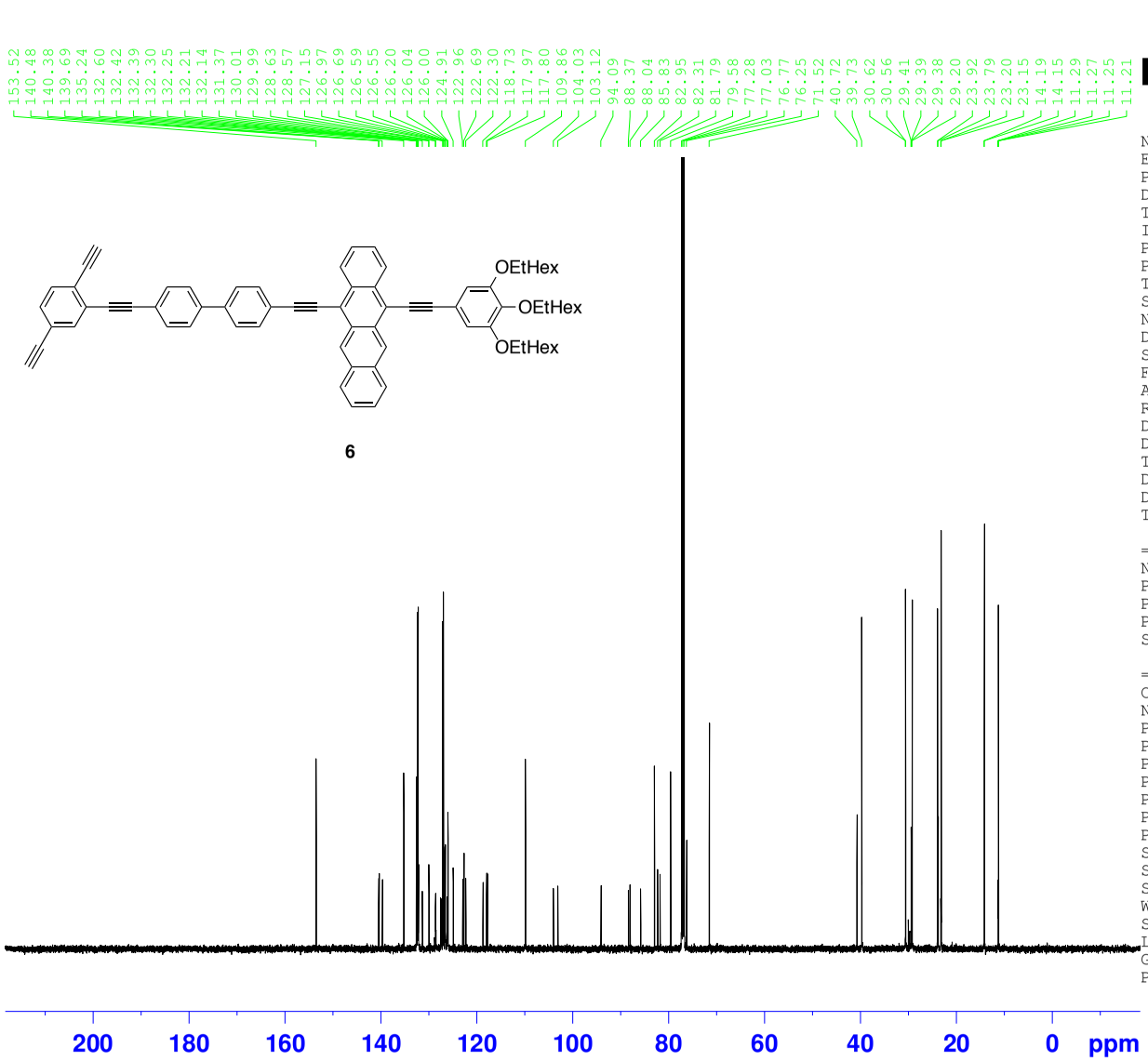


BRUKER

NAME	ek-2-053
EXPNO	10
PROCNO	1
Date_	20131119
Time	9.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	71.8
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	5.00000000 sec
TD0	1

======== CHANNEL f1 ========

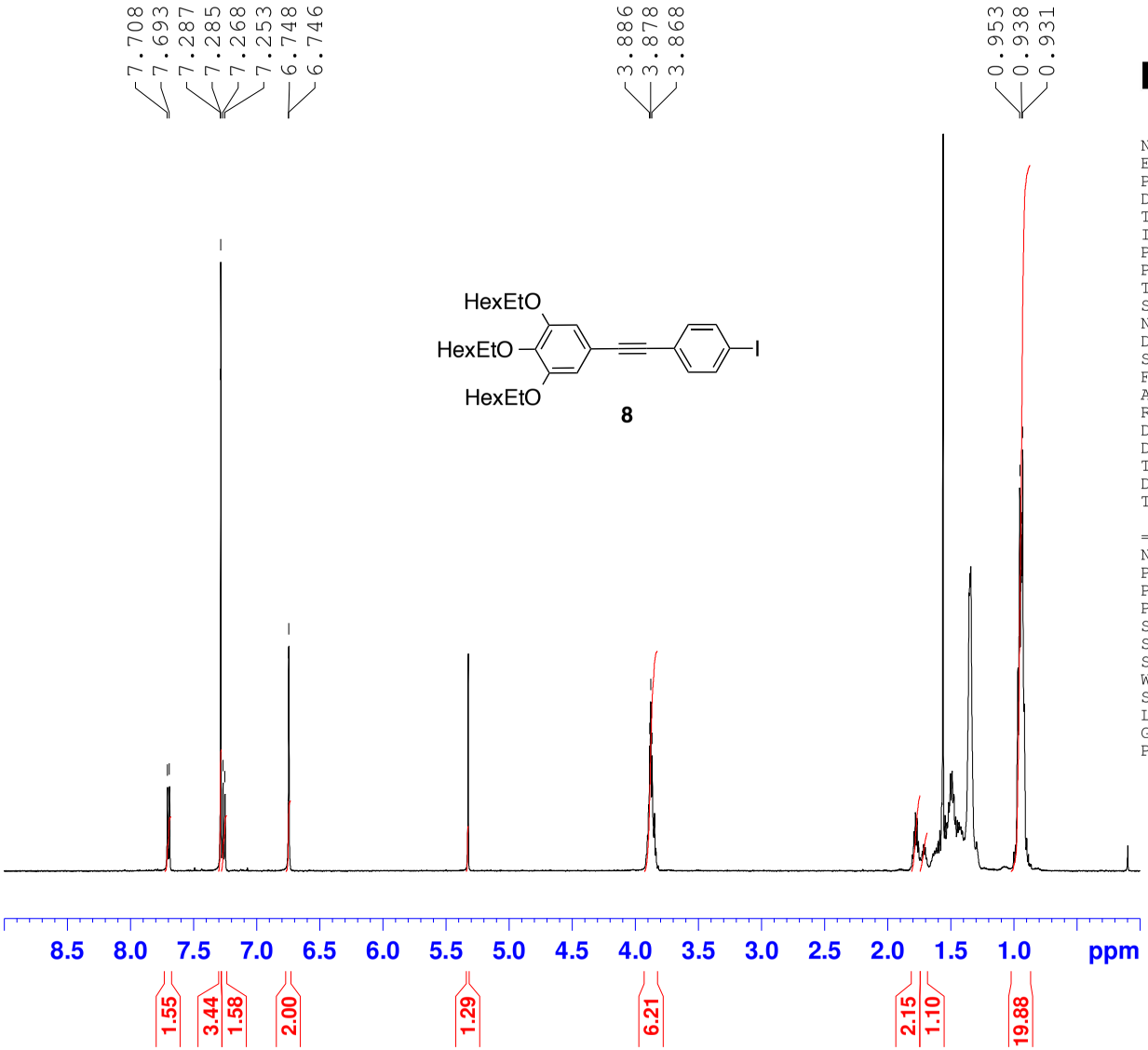
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300078 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



6

BRUKER

NAME	ek-2-053
EXPNO	12
PROCNO	1
Date_	20131119
Time	9.57
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2034
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.1 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

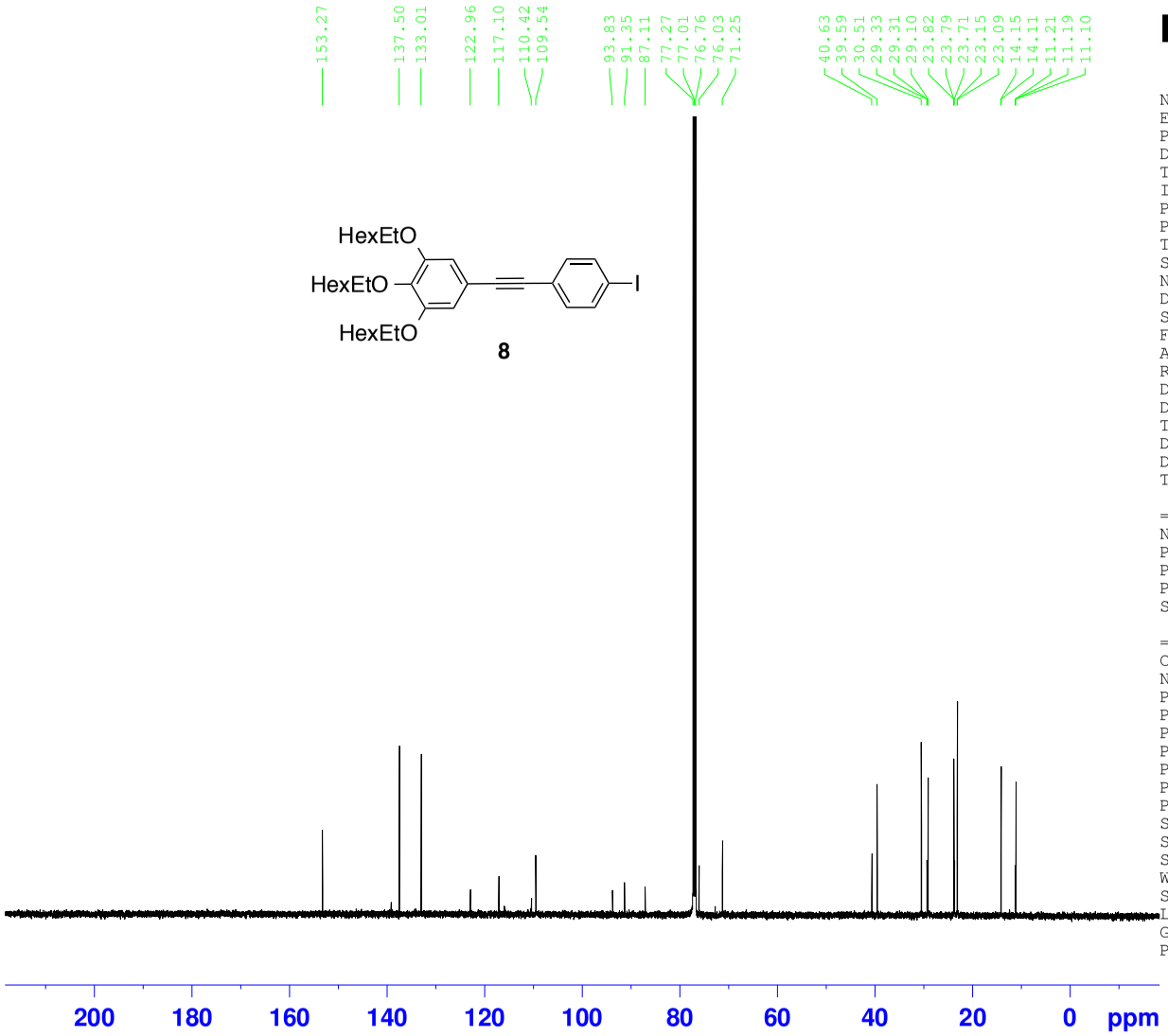


BRUKER

NAME	ek-2-087
EXPNO	4
PROCNO	1
Date_	20140115
Time	14.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	0.50000000 sec
TD0	1

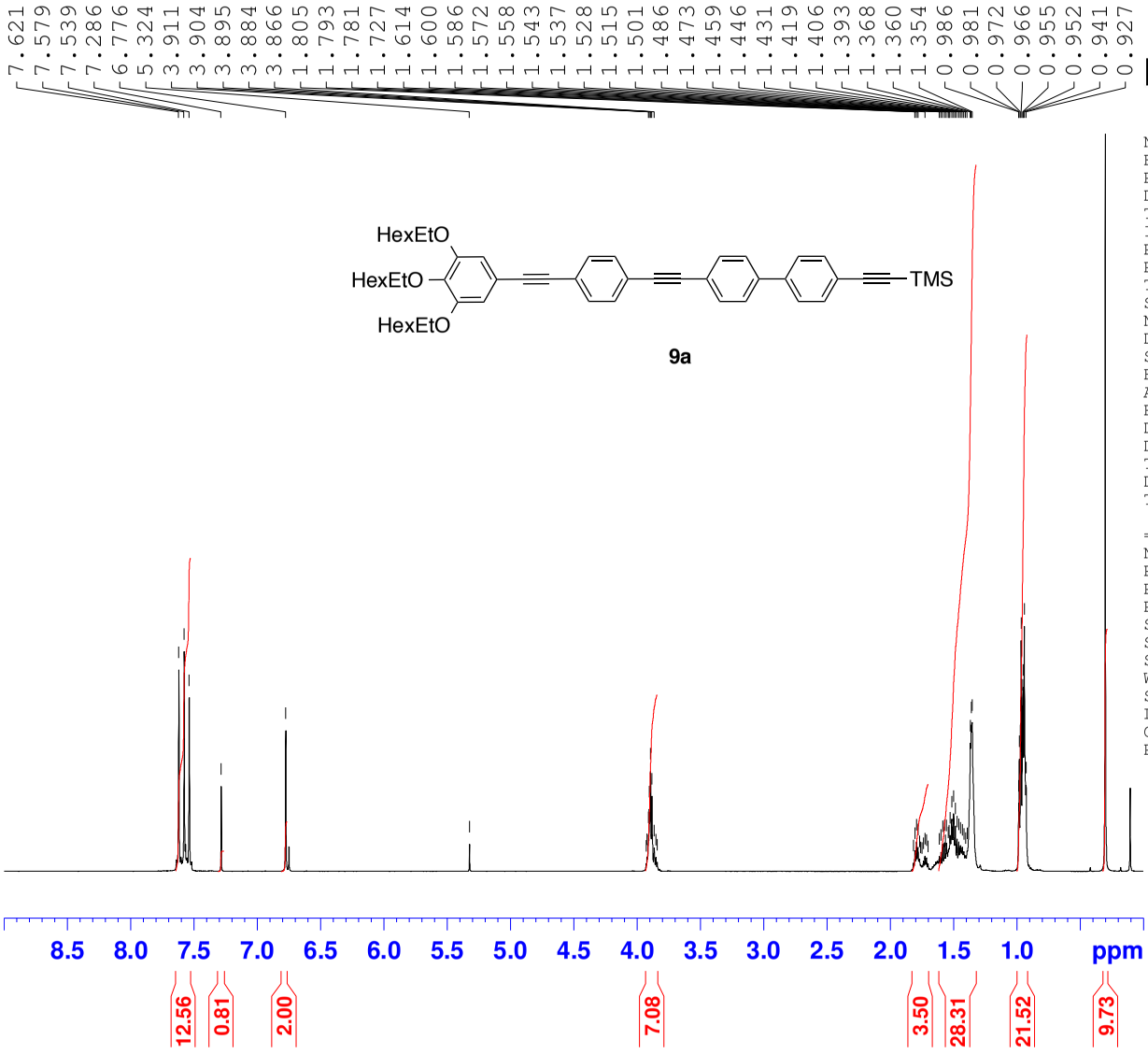
======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



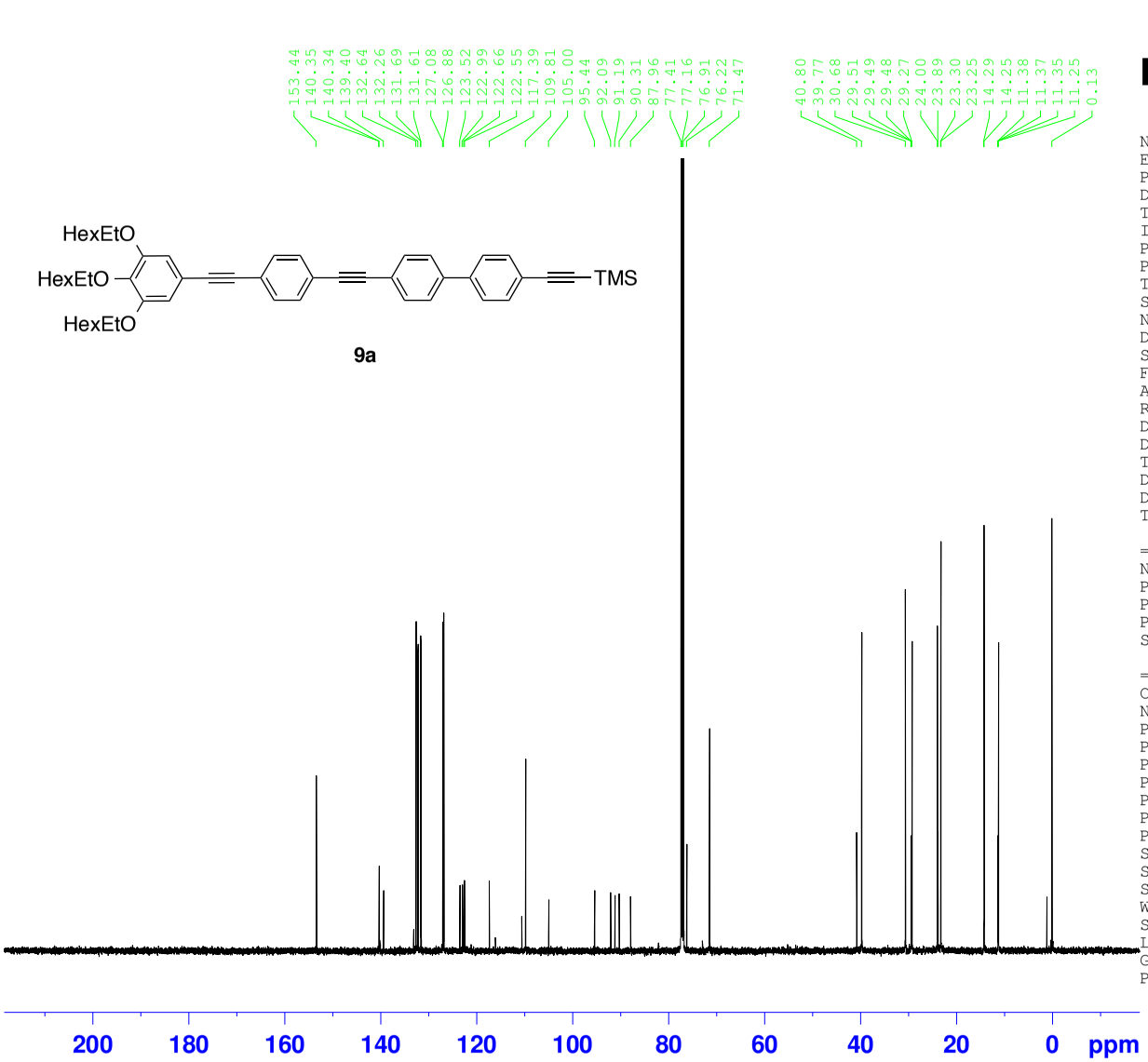
BRUKER

NAME	ek-2-87
EXPNO	15
PROCNO	1
Date_	20150507
Time	16.37
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	9160
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	292.5 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



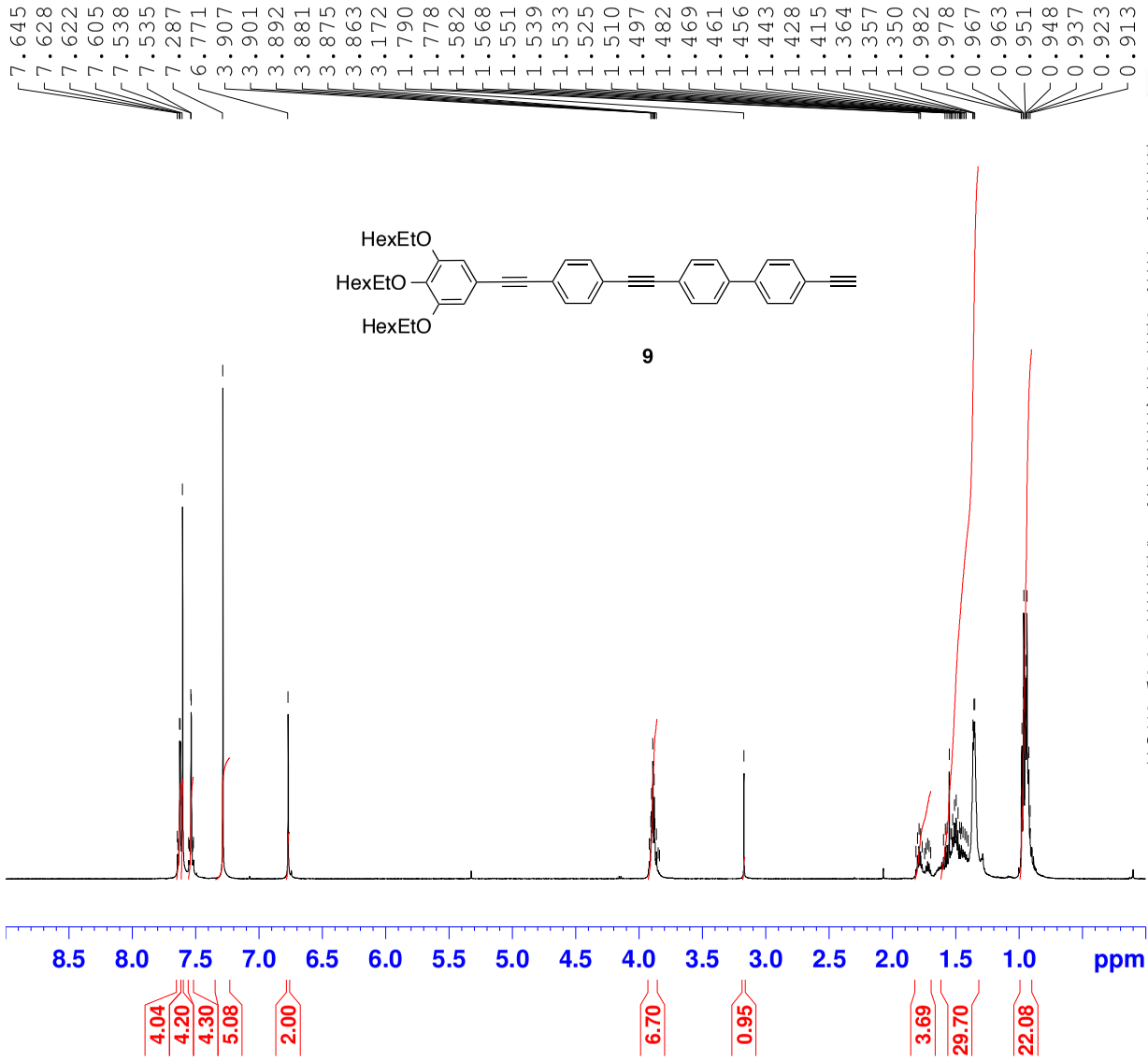
BRUKER

NAME	ek-2-090
EXPNO	3
PROCNO	1
Date_	20140121
Time	13.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	128
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	0.50000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

NAME	ek-2-090
EXPNO	34
PROCNO	1
Date_	20140121
Time	13.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4190
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.1 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577699 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

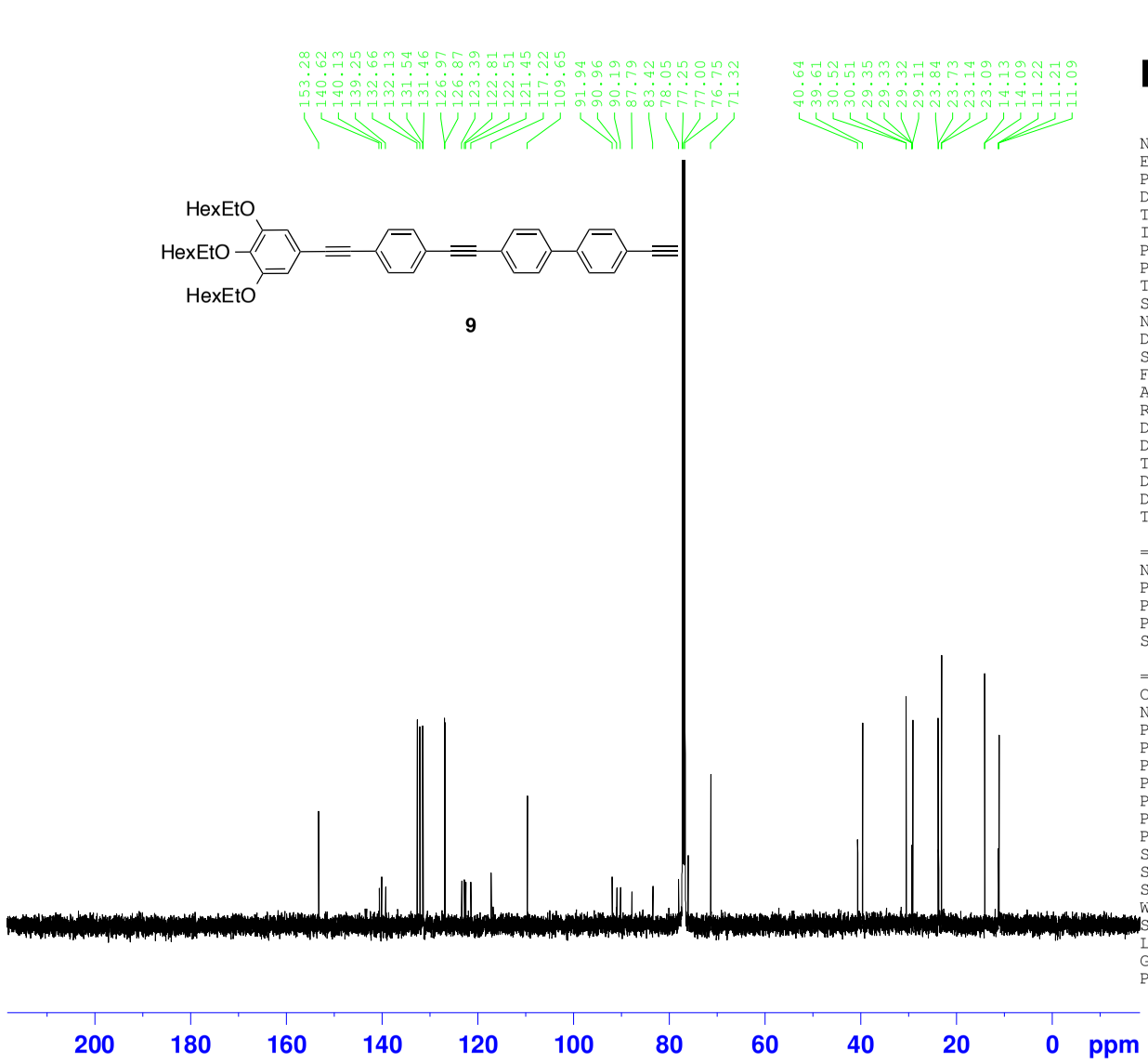


BRUKER

NAME	ek-2-091
EXPNO	4
PROCNO	1
Date_	20140122
Time	15.50
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	5.00000000 sec
TD0	1

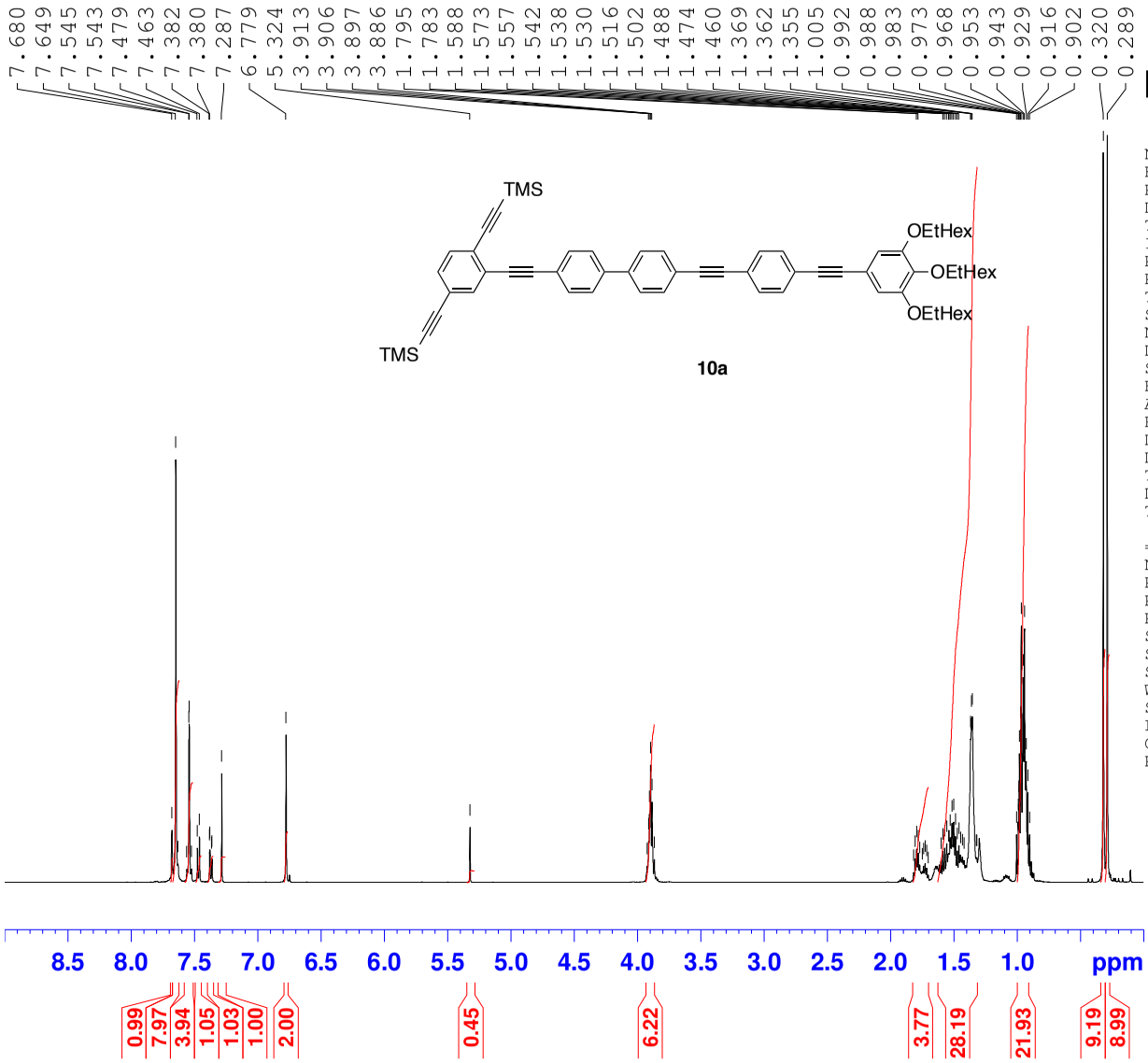
======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



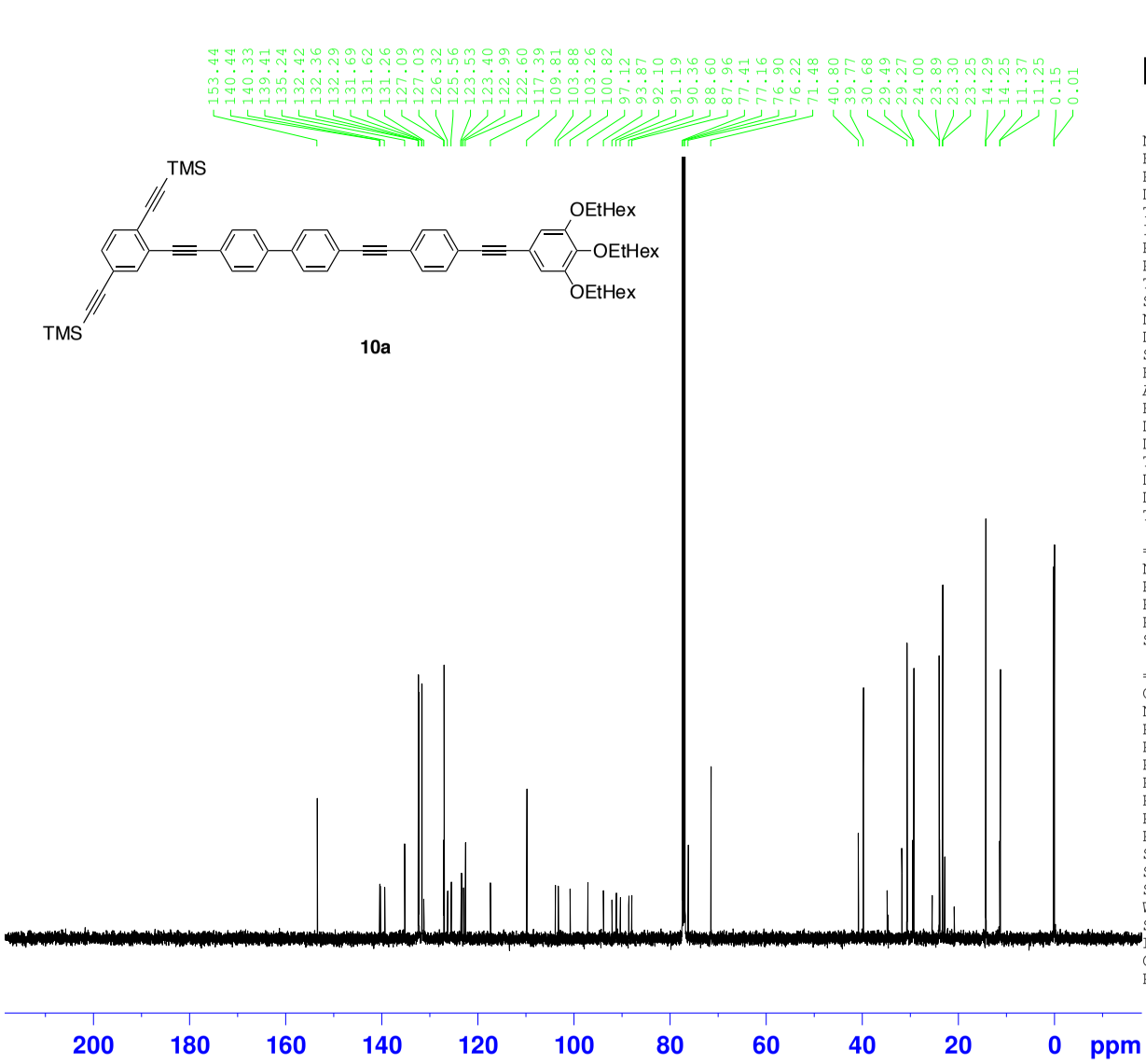
BRUKER

NAME	ek-2-091	
EXPNO	5	
PROCNO	1	
Date_	20140122	
Time	15.54	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	5362	
DS	4	
SWH	29761.904	Hz
FIDRES	0.454131	Hz
AQ	1.1010548	sec
RG	203	
DW	16.800	usec
DE	6.50	usec
TE	300.1	K
D1	0.50000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.50	usec
PL1	0.00	dB
PL1W	89.92553711	W
SFO1	125.7703643	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	1.00	dB
PL12	13.04	dB
PL13	16.80	dB
PL2W	17.75783539	W
PL12W	1.11017132	W
PL13W	0.46707872	W
SFO2	500.1320005	MHz
SI	65536	
SF	125.7577890	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	0.20	



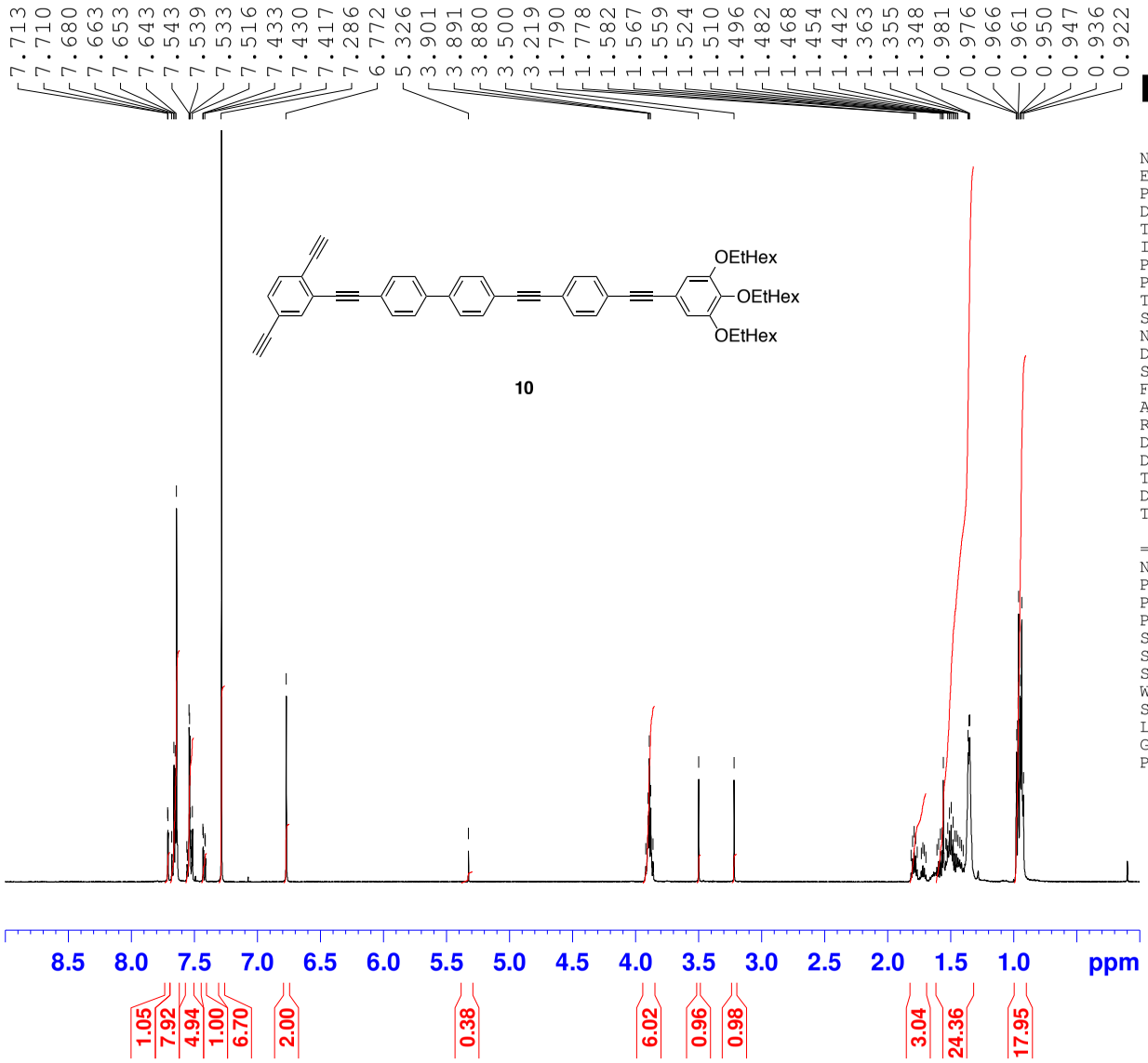
BRUKER

NAME	ek-2-092	
EXPNO	3	
PROCNO	1	
Date_	20140123	
Time	16.03	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	10000.000	Hz
FIDRES	0.152588	Hz
AQ	3.2768500	sec
RG	144	
DW	50.000	usec
DE	6.50	usec
TE	300.0	K
D1	0.50000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	20.00	usec
PL1	1.00	dB
PL1W	17.75783539	W
SFO1	500.1318364	MHz
SI	65536	
SF	500.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



BRUKER

NAME	ek-2-092
EXPNO	4
PROCNO	1
Date_	20140123
Time	16.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1295
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.0 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577699 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

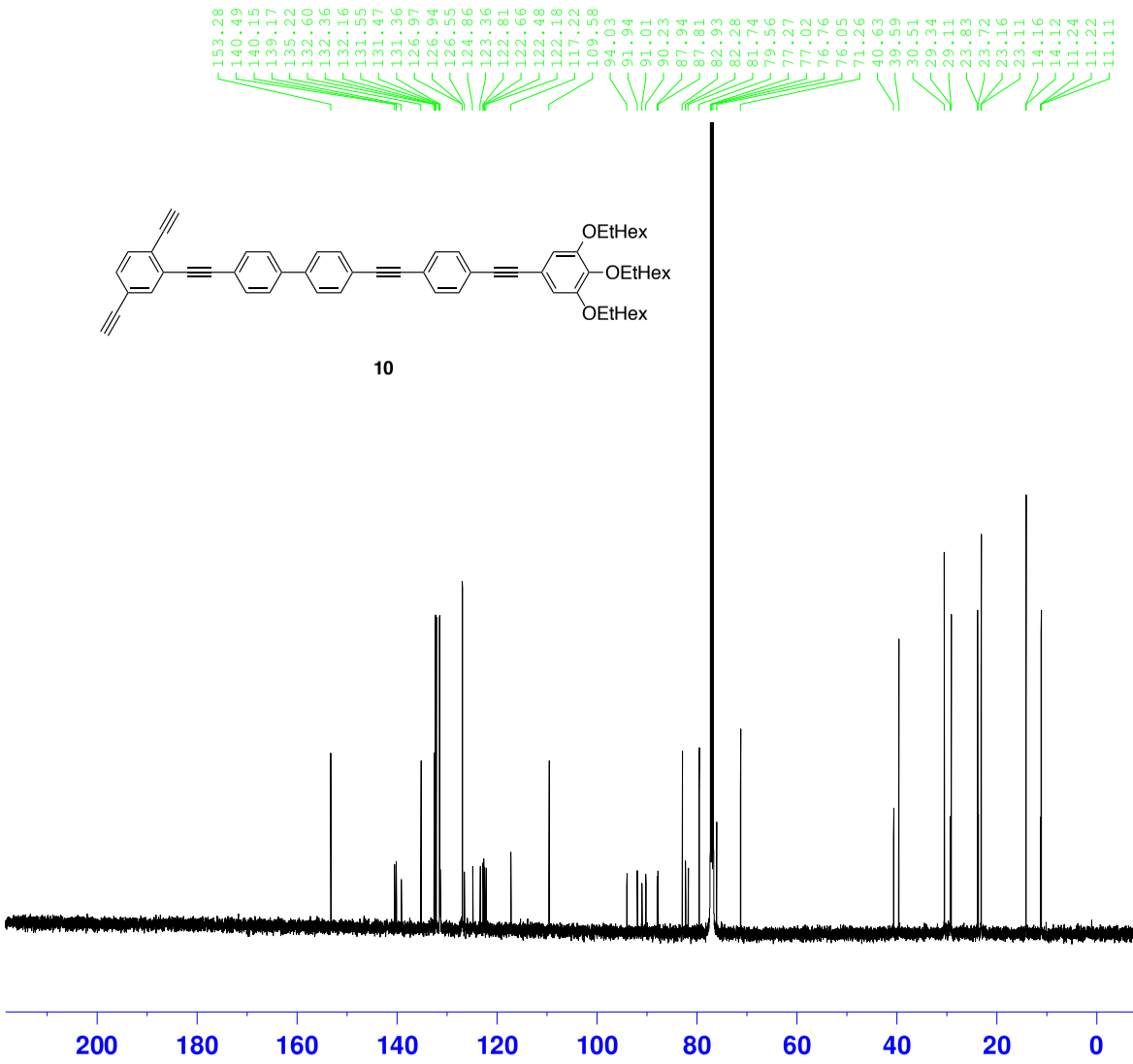


BRUKER

NAME	ek-2-093
EXPNO	2
PROCNO	1
Date_	20140124
Time	14.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	296.0 K
D1	5.00000000 sec
TD0	1

======== CHANNEL f1 ========

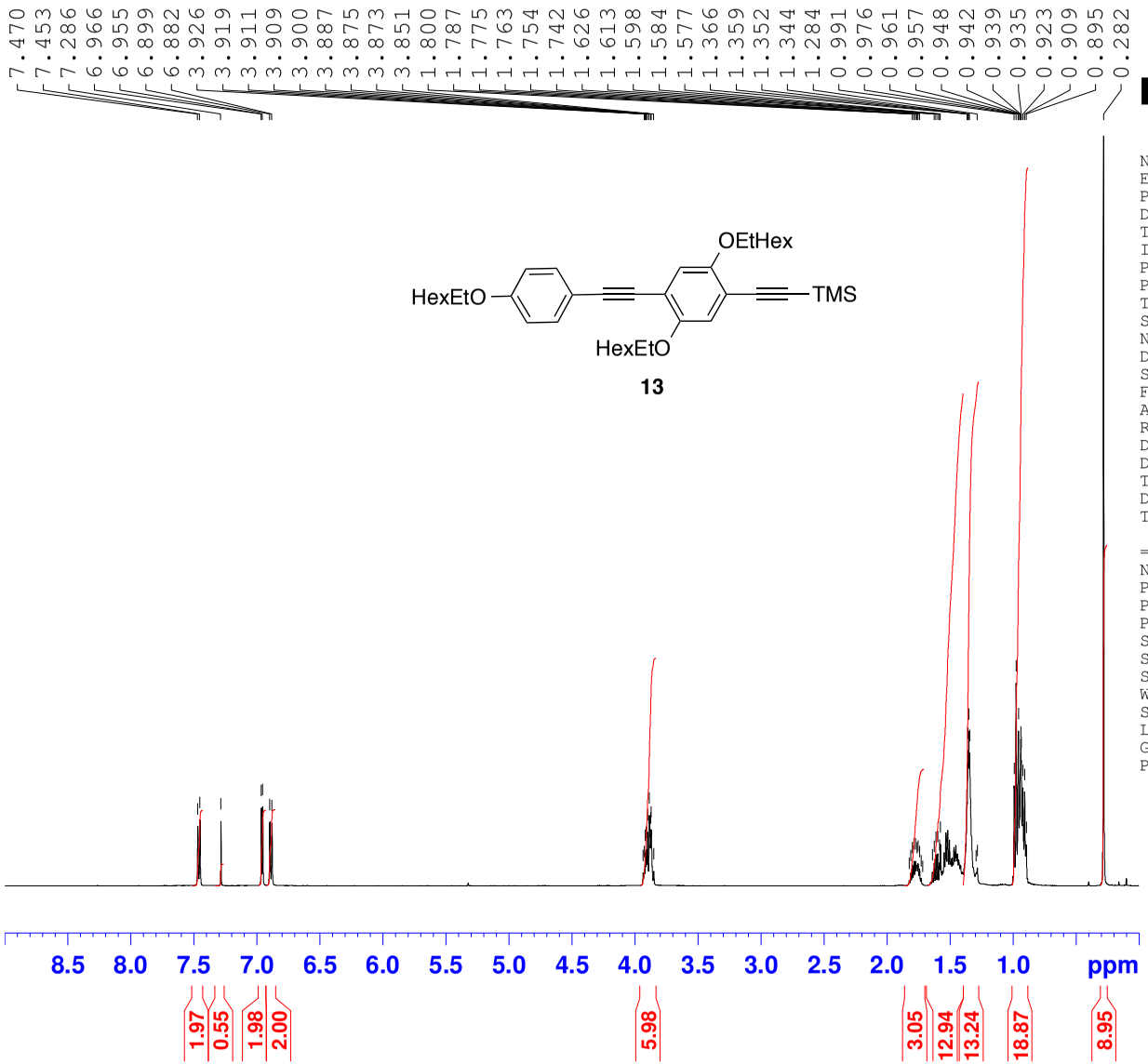
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
NAME                ek-2-93
EXPNO                    11
PROCNO                    1
Date_              20150507
Time                  21.47
INSTRUM               spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT                CDCl3
NS                    24025
DS                        4
SWH               29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010548 sec
RG                      203
DW                   16.800 usec
DE                    6.50 usec
TE                   291.5 K
D1                0.50000000 sec
D11               0.03000000 sec
TD0                       1

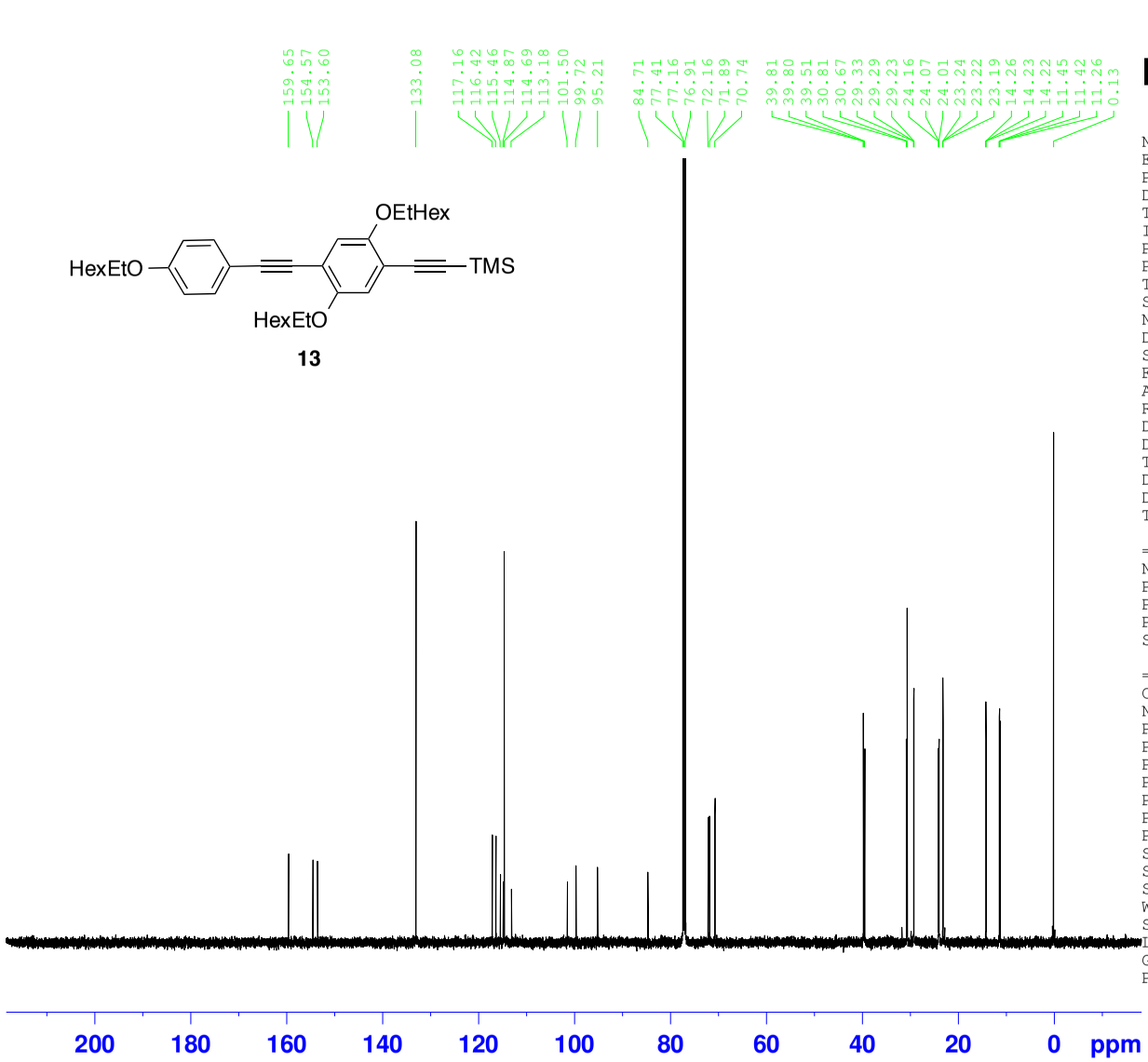
======== CHANNEL f1 ========
NUC1                    13C
P1                     9.50 usec
PL1                    0.00 dB
PL1W            89.92553711 W
SFO1           125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2                 80.00 usec
PL2                    1.00 dB
PL12                  13.04 dB
PL13                  16.80 dB
PL2W            17.75783539 W
PL12W            1.11017132 W
PL13W            0.46707872 W
SFO2           500.1320005 MHz
SI                    65536
SF             125.7577890 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```




```
NAME                ek-2-019
EXPNO                      1
PROCNO                     1
Date_               20130910
Time                    9.55
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        27
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2768500 sec
RG                      71.8
DW                    50.000 usec
DE                     6.50 usec
TE                    295.2 K
D1                 5.00000000 sec
TD0                        1

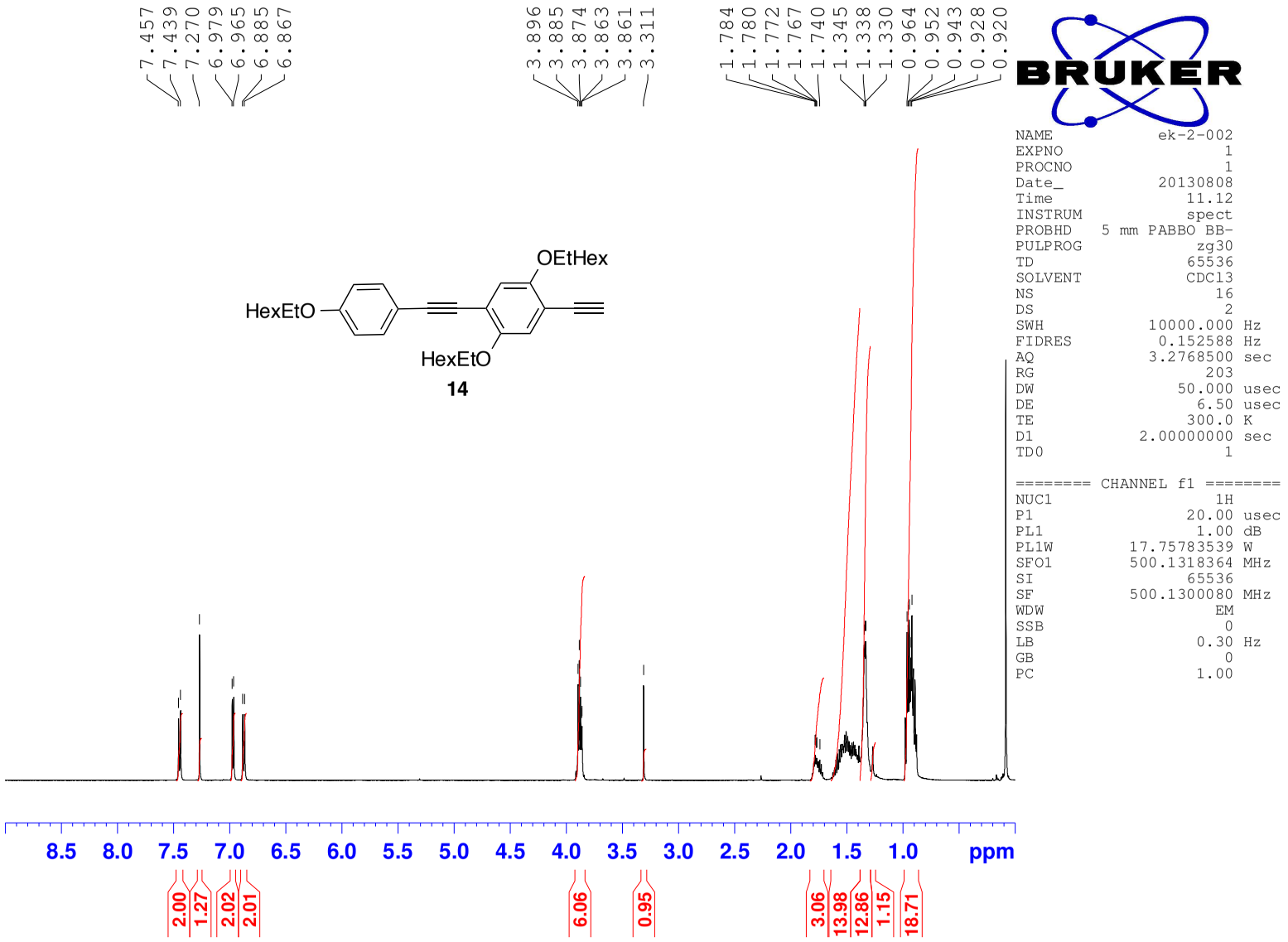
======== CHANNEL f1 ========
NUC1                      1H
P1                     20.00 usec
PL1                     1.00 dB
PL1W            17.75783539 W
SFO1            500.1318364 MHz
SI                     65536
SF              500.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```




```
NAME                ek-2-019
EXPNO                      2
PROCNO                     1
Date_               20130910
Time                    9.59
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                      65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                       203
DW                    16.800 usec
DE                     6.50 usec
TE                    295.4 K
D1                 0.50000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      9.50 usec
PL1                     0.00 dB
PL1W              89.92553711 W
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2               waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                     1.00 dB
PL12                   13.04 dB
PL13                   16.80 dB
PL2W              17.75783539 W
PL12W              1.11017132 W
PL13W              0.46707872 W
SFO2             500.1320005 MHz
SI                      65536
SF               125.7577706 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```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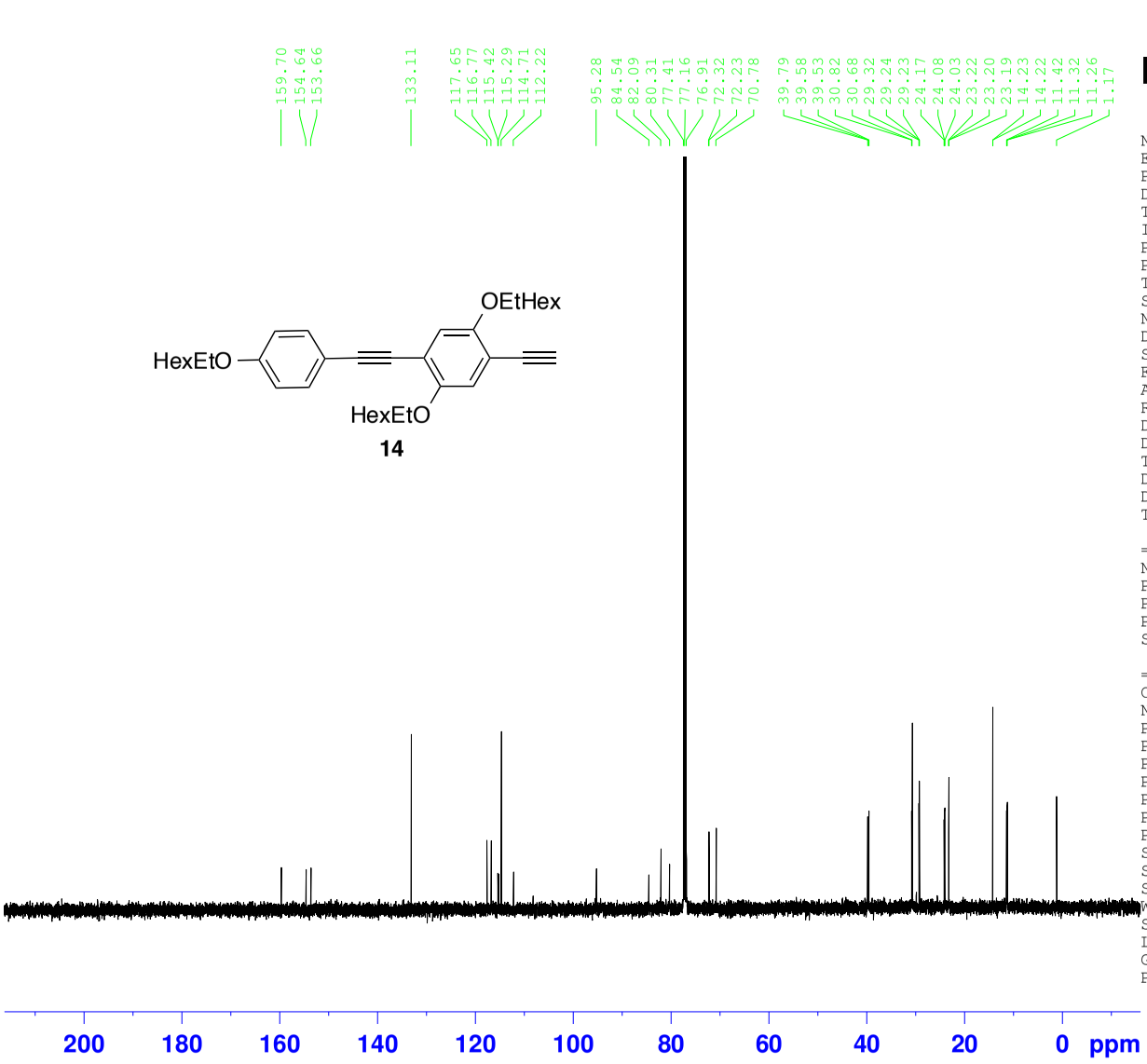
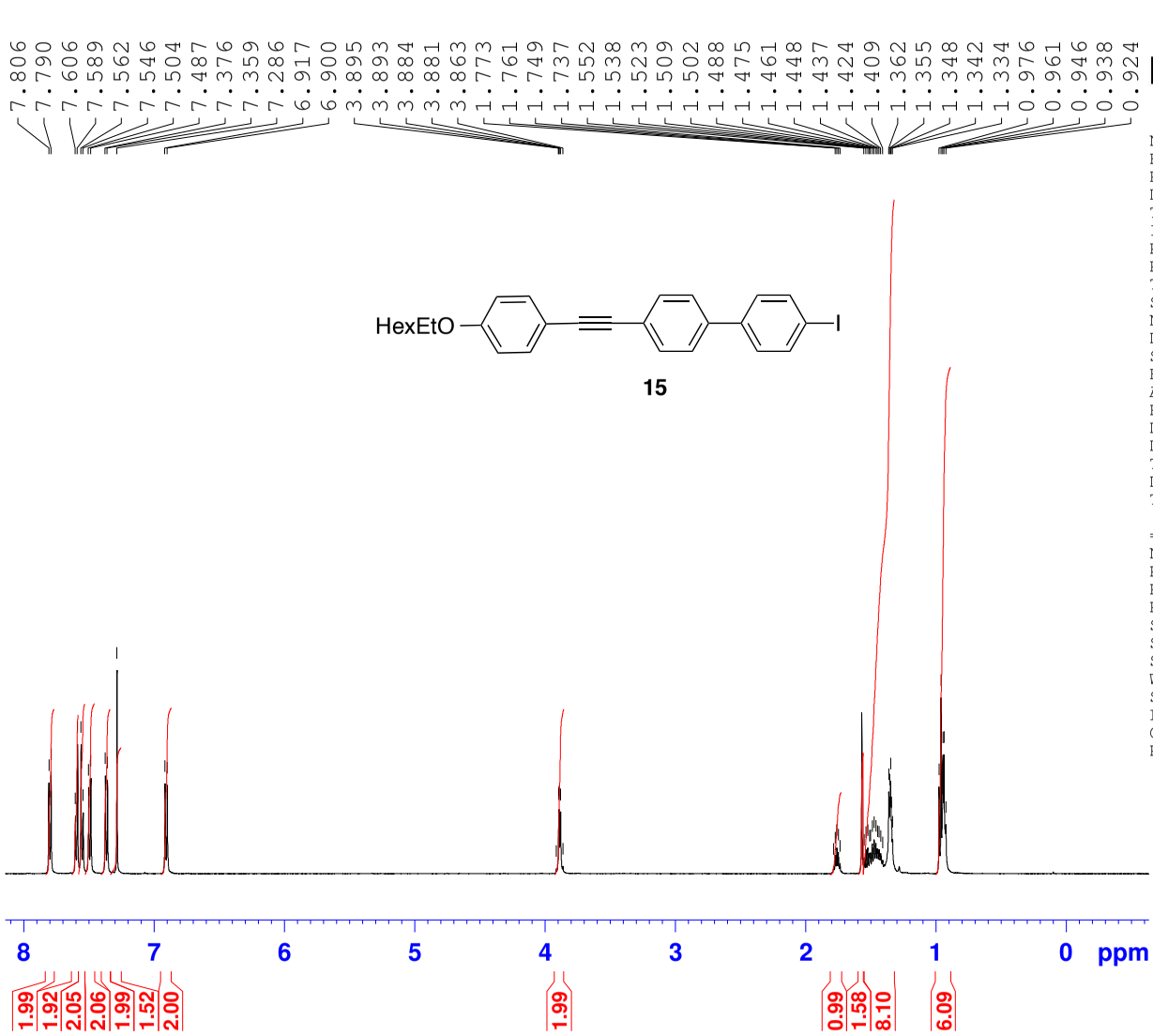
7.270
6.979
6.965
6.885
6.867
3.896
3.885
3.874
3.863
3.861
3.311
1.784
1.780
1.772
1.767
1.740
1.345
1.338
1.330
0.964
0.952
0.943
0.928
0.920
BRUKER
OEtHex
HexEtO
HexEtO
14
NAME ek-2-002
EXPNO 1
PROCNO 1
Date_ 20130808
Time 11.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 20.00 usec
PL1 1.00 dB
PL1W 17.75783539 W
SFO1 500.1318364 MHz
SI 65536
SF 500.1300080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
2.00
1.27
2.02
2.01
6.06
0.95
3.06
13.98
12.86
1.15
18.71




```
NAME                ek-2-002
EXPNO                      2
PROCNO                     1
Date_               20130808
Time                   11.17
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDC13
NS                        892
DS                          4
SWH                 29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010548 sec
RG                        203
DW                     16.800 usec
DE                      6.50 usec
TE                     300.0 K
D1                  0.50000000 sec
D11                 0.03000000 sec
TD0                        1

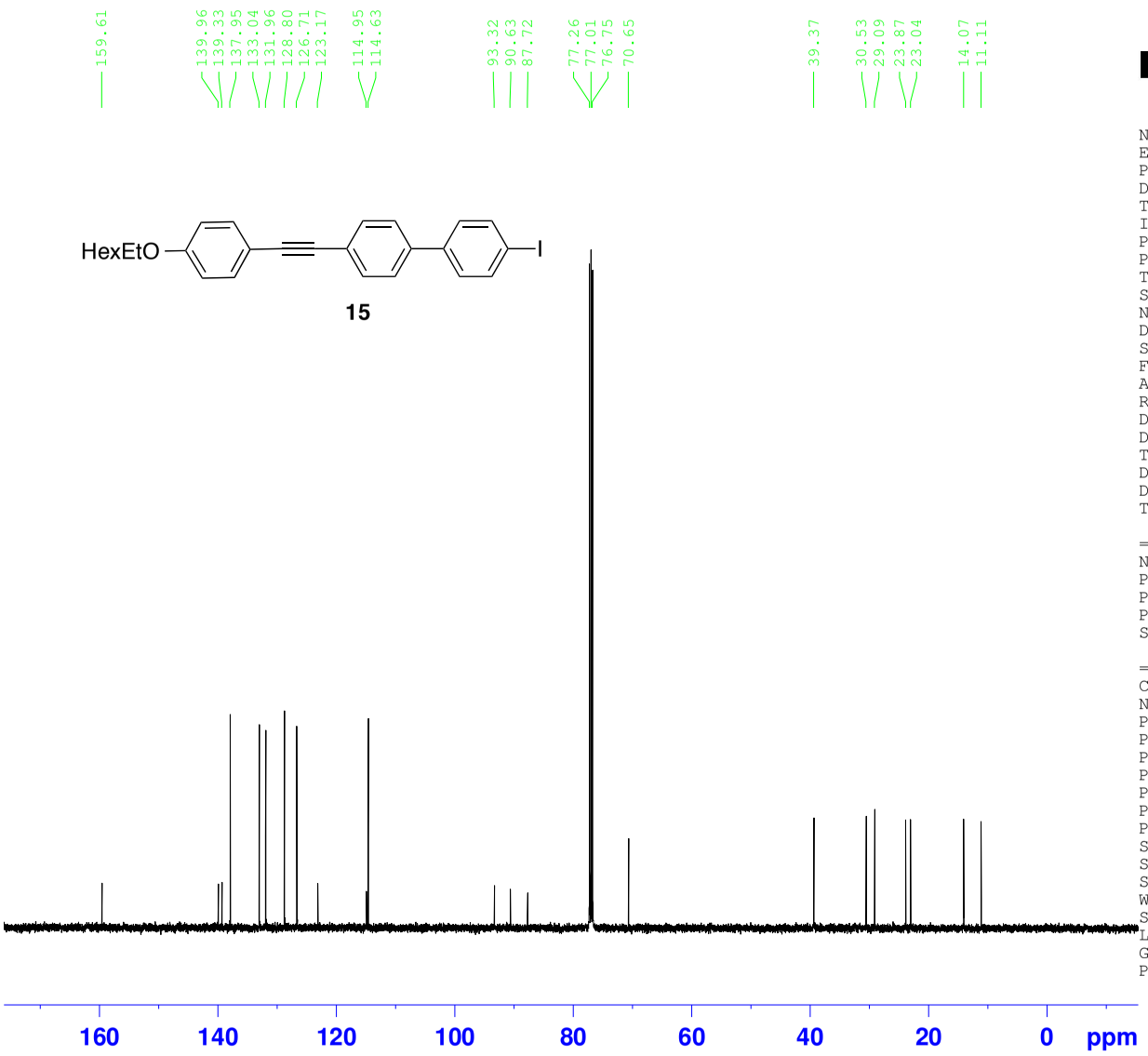
======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                     0.00 dB
PL1W               89.92553711 W
SFO1              125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                     1.00 dB
PL12                   13.04 dB
PL13                   16.80 dB
PL2W               17.75783539 W
PL12W               1.11017132 W
PL13W               0.46707872 W
SFO2              500.1320005 MHz
SI                      65536
SF                125.7577691 MHz
WDW                        EM
SSB                         0
LB                      1.00 Hz
GB                          0
PC                      1.00
```



BRUKER

NAME	ek-2-011
EXPNO	1
PROCNO	1
Date_	20130822
Time	13.51
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	9
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	295.8 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

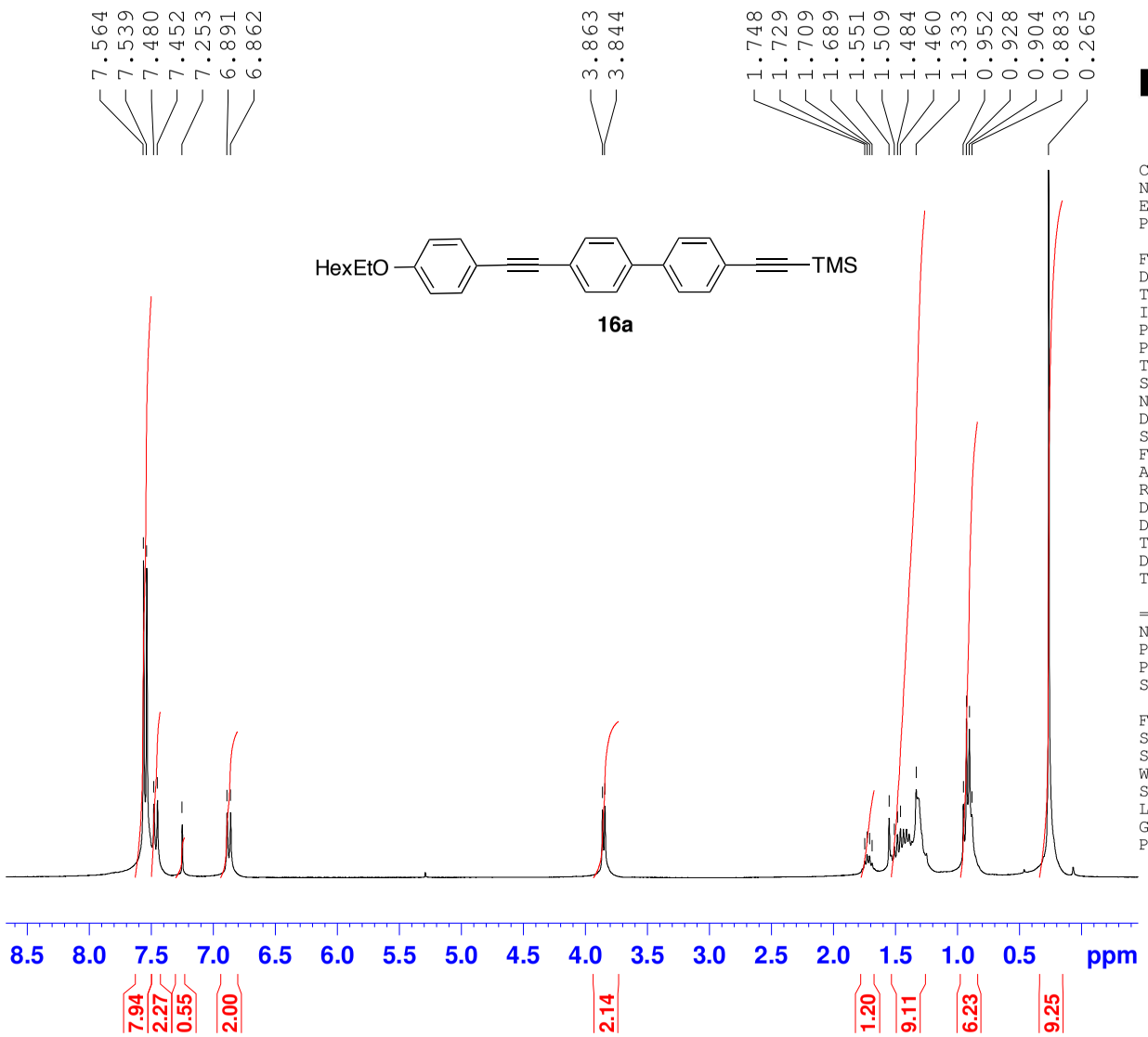


BRUKER

```
NAME                ek-2-006
EXPNO                      2
PROCNO                     1
Date_               20130815
Time                   16.46
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        810
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                        203
DW                    16.800 usec
DE                     6.50 usec
TE                     300.5 K
D1                 0.50000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      9.50 usec
PL1                     0.00 dB
PL1W             89.92553711 W
SFO1            125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  80.00 usec
PL2                     1.00 dB
PL12                   13.04 dB
PL13                   16.80 dB
PL2W             17.75783539 W
PL12W             1.11017132 W
PL13W             0.46707872 W
SFO2            500.1320005 MHz
SI                      65536
SF              125.7577890 MHz
WDW                        EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```



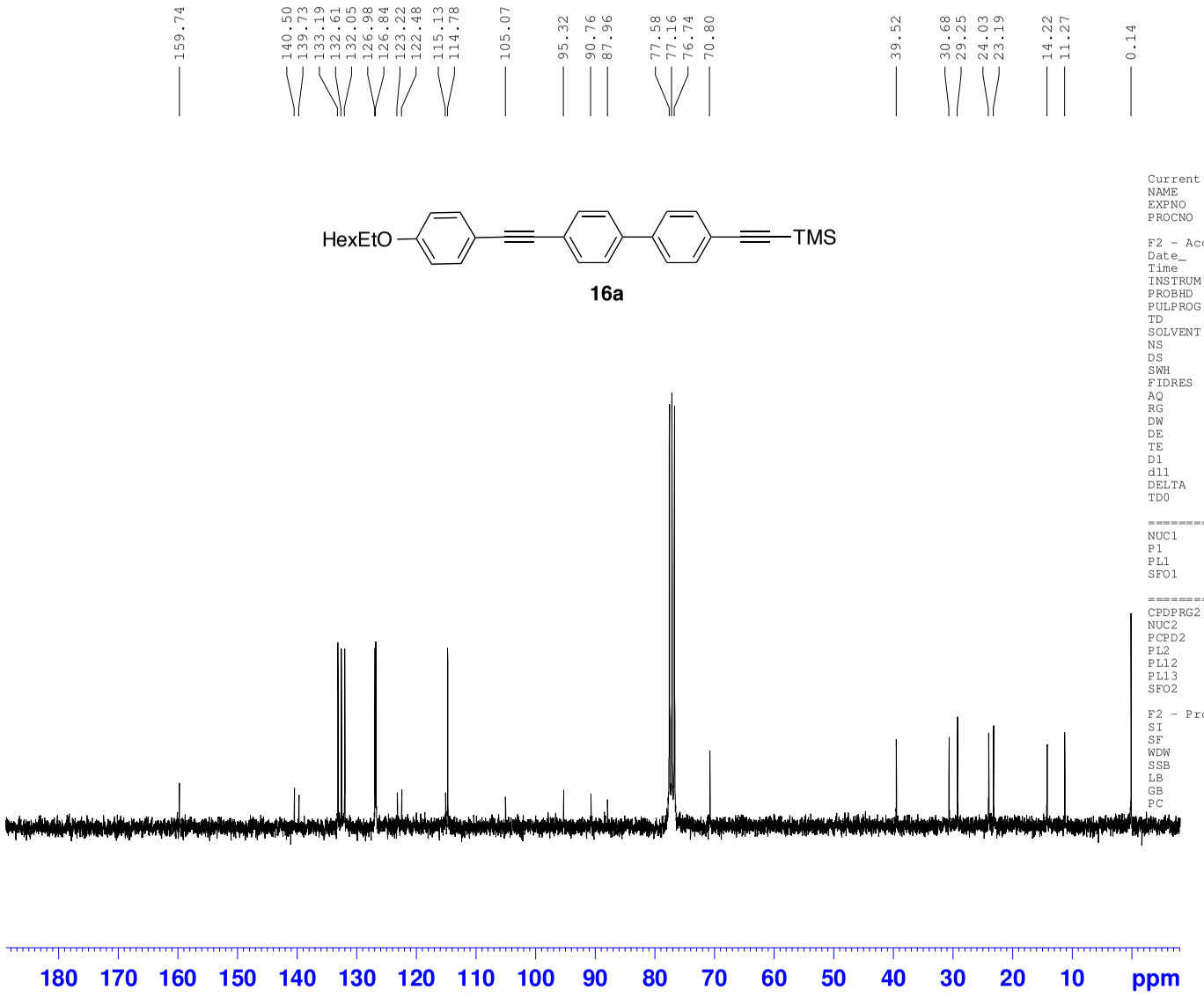
BRUKER

```
Current Data Parameters
NAME                 ek-2-008
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20130819
Time                   13.08
INSTRUM                spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       46
DS                        2
SWH                6218.905 Hz
FIDRES            0.189786 Hz
AQ                2.6345973 sec
RG                    322.5
DW                   80.400 usec
DE                    6.00 usec
TE                   300.0 K
D1                2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.00 usec
PL1                      0.00 dB
SFO1             300.3418547 MHz

F2 - Processing parameters
SI                         32768
SF               300.3400067 MHz
WDW                           EM
SSB                            0
LB                        0.30 Hz
GB                             0
PC                         1.50
```



Current Data Parameters

NAME	ek-2-008
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20130819
Time	13.15
INSTRUM	spect
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
SOLVENT	CDCl3
NS	1605
DS	4
SWH	18115.941 Hz
FIDRES	0.552855 Hz
AQ	0.9044468 sec
RG	7298.2
DW	27.600 usec
DE	6.00 usec
TE	300.0 K
D1	0.50000000 sec
d11	0.03000000 sec
DELTA	0.40000001 sec
TD0	1

======== CHANNEL f1 ========

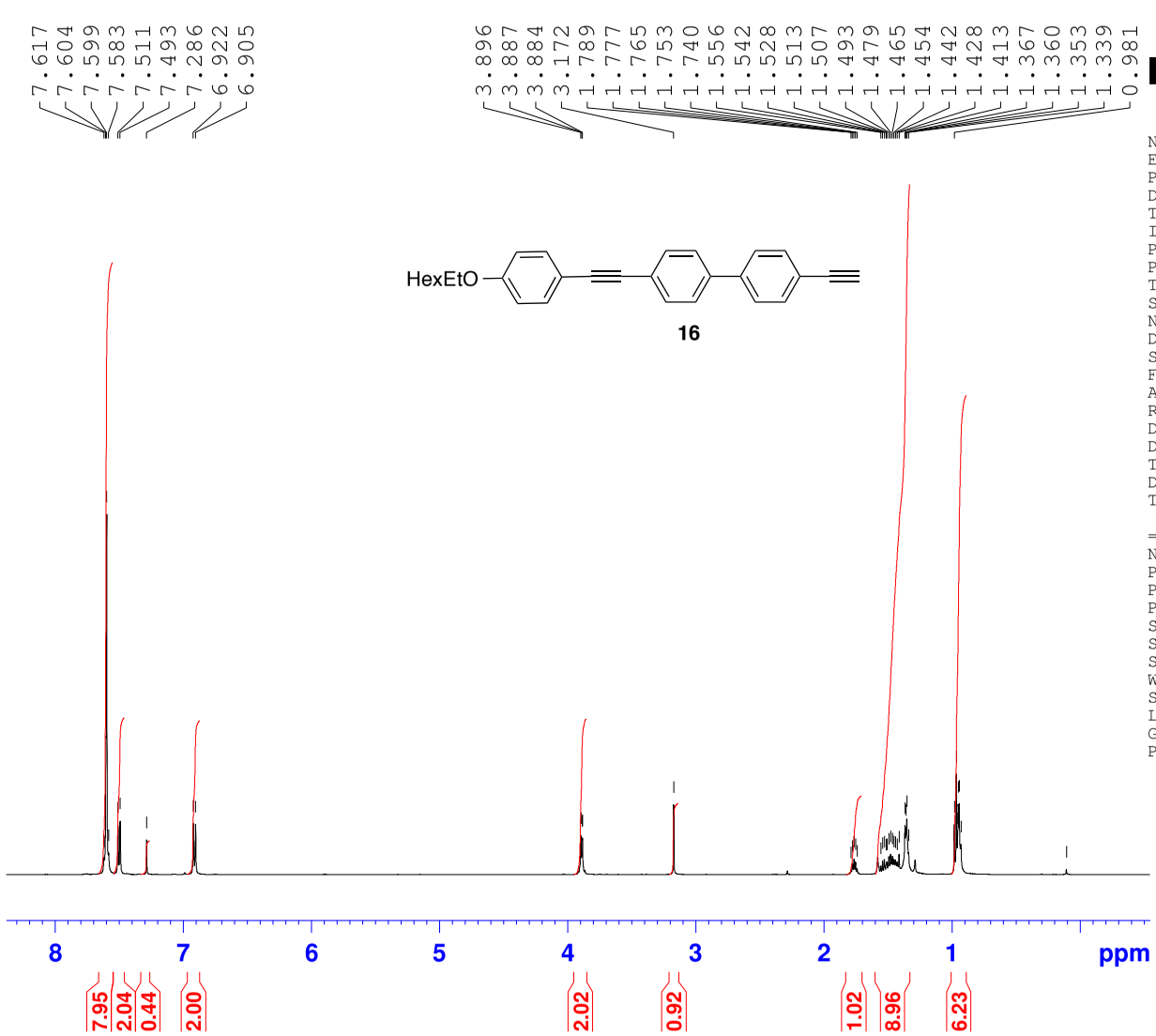
NUC1	13C
P1	9.00 usec
PL1	0.00 dB
SFO1	75.5281051 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.30 dB
PL13	17.30 dB
SFO2	300.3412014 MHz

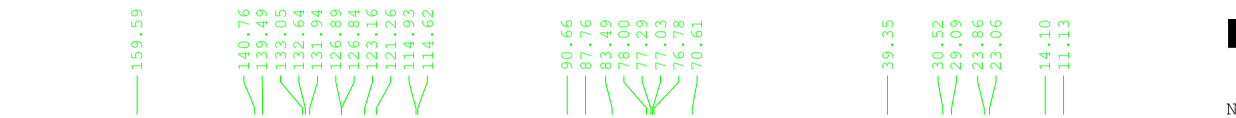
F2 - Processing parameters

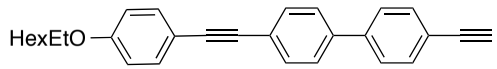
SI	32768
SF	75.5205409 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	ek-2-010
EXPNO	1
PROCNO	1
Date_	20130820
Time	13.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	295.7 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





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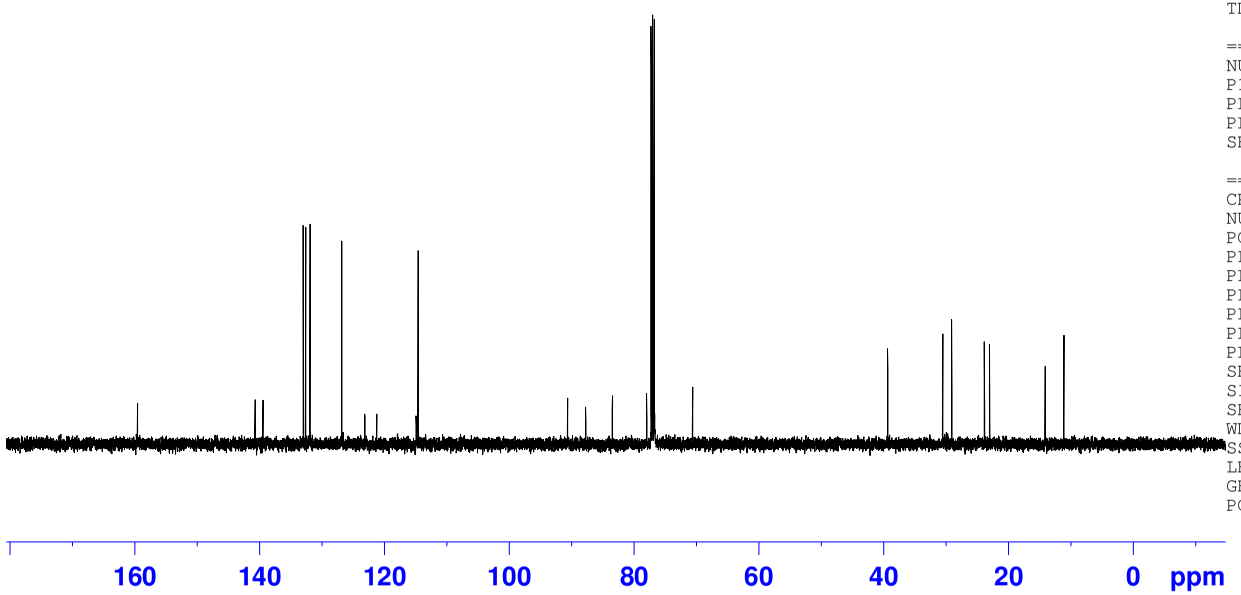
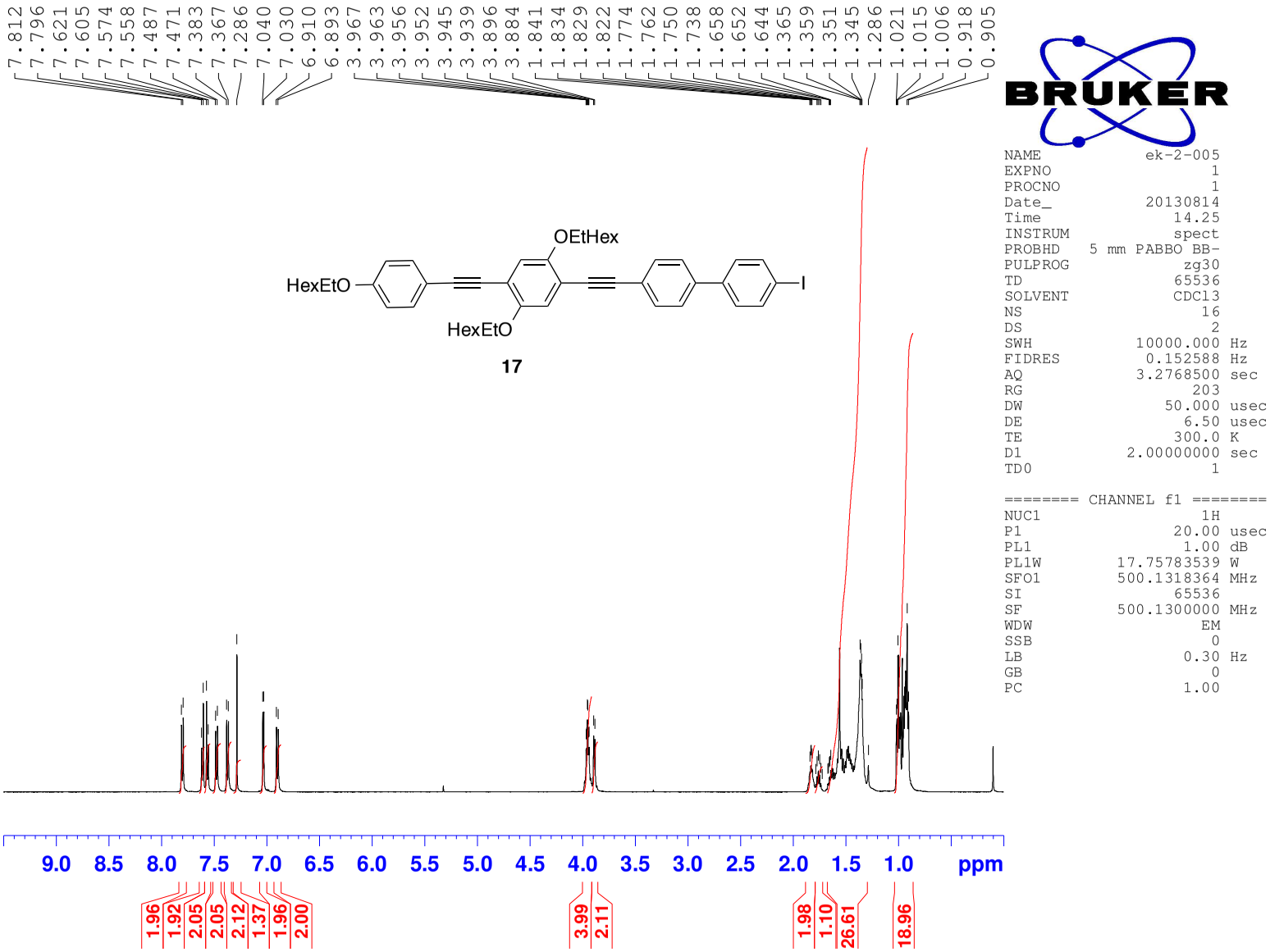


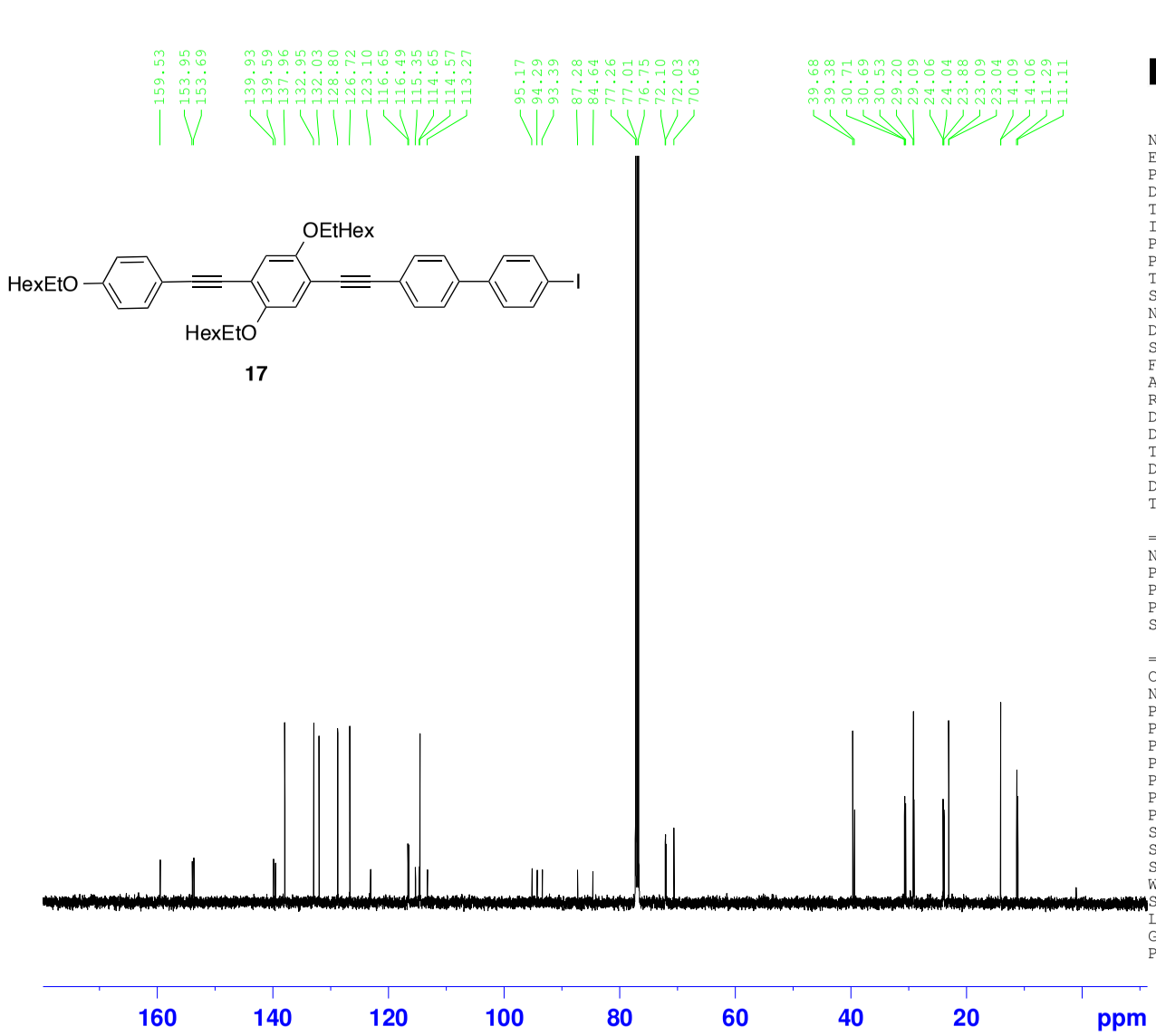
BRUKER

NAME	ek-2-010
EXPNO	2
PROCNO	1
Date_	20130820
Time	13.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	175
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	296.3 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	ek-2-005
EXPNO	1
PROCNO	1
Date_	20130814
Time	14.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



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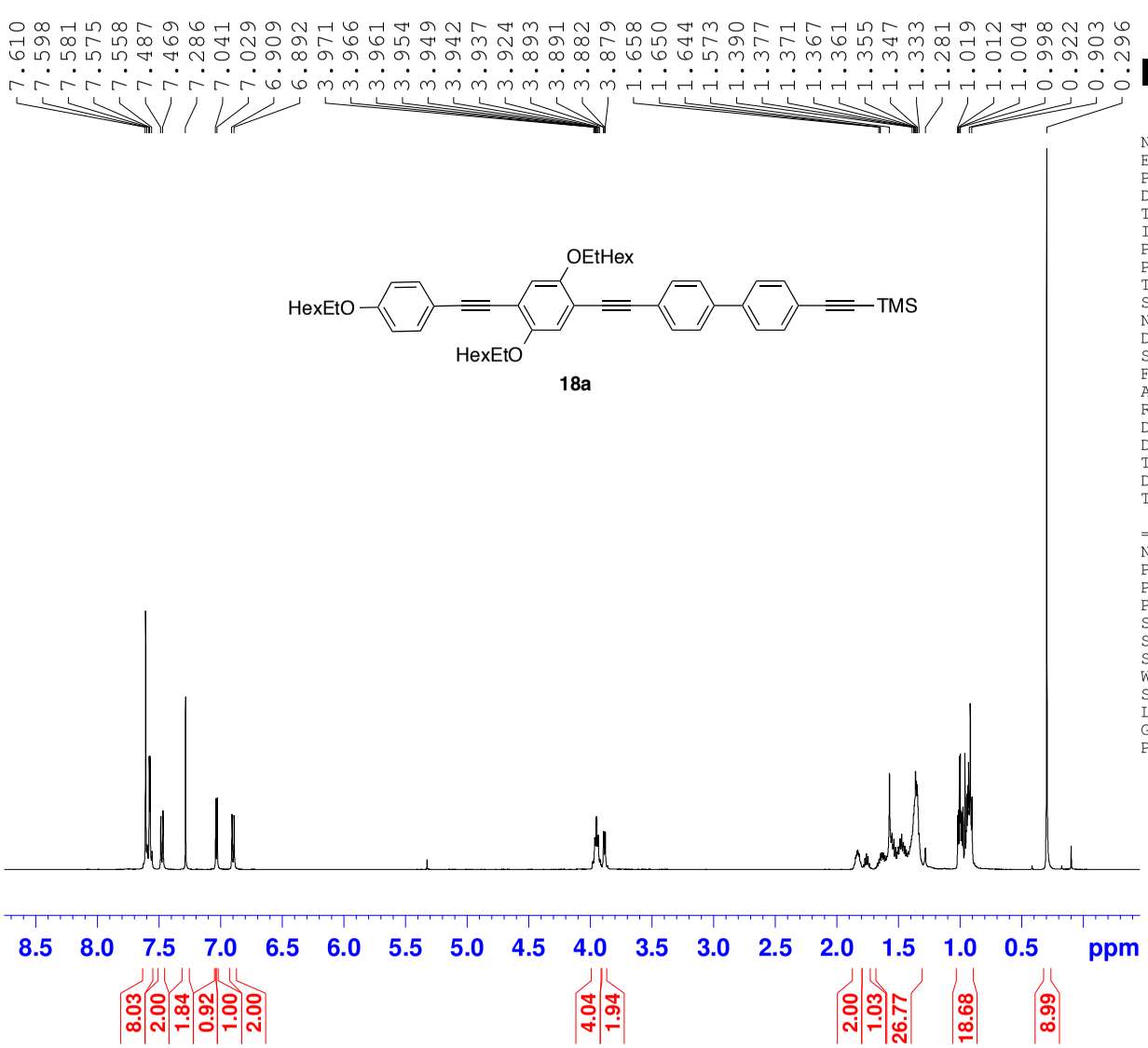
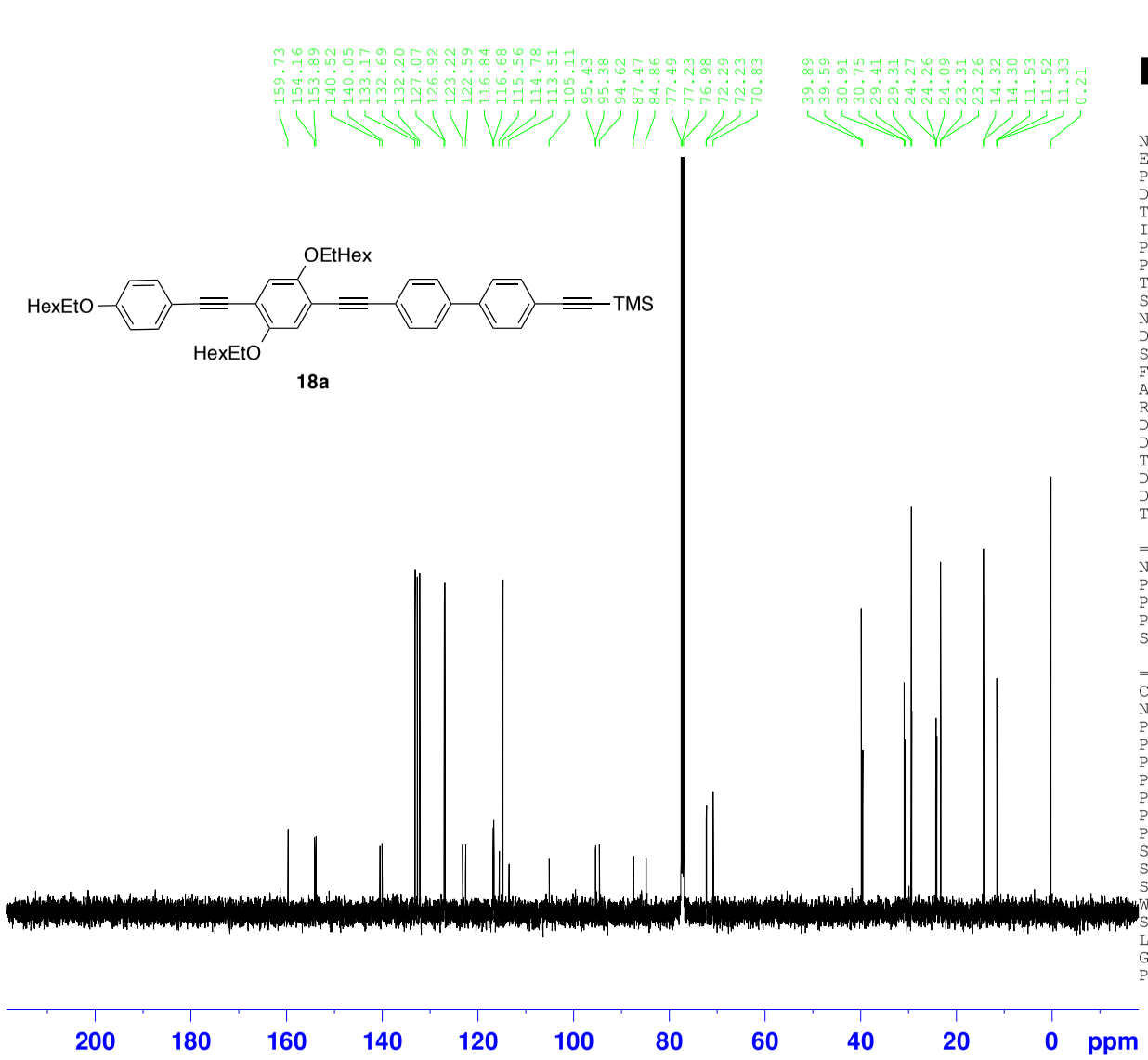
BRUKER

NAME	ek-2-005
EXPNO	3
PROCNO	1
Date_	20130814
Time	14.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1041
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.2 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	ek-2-007
EXPNO	2
PROCNO	1
Date_	20130816
Time	13.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	294.9 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

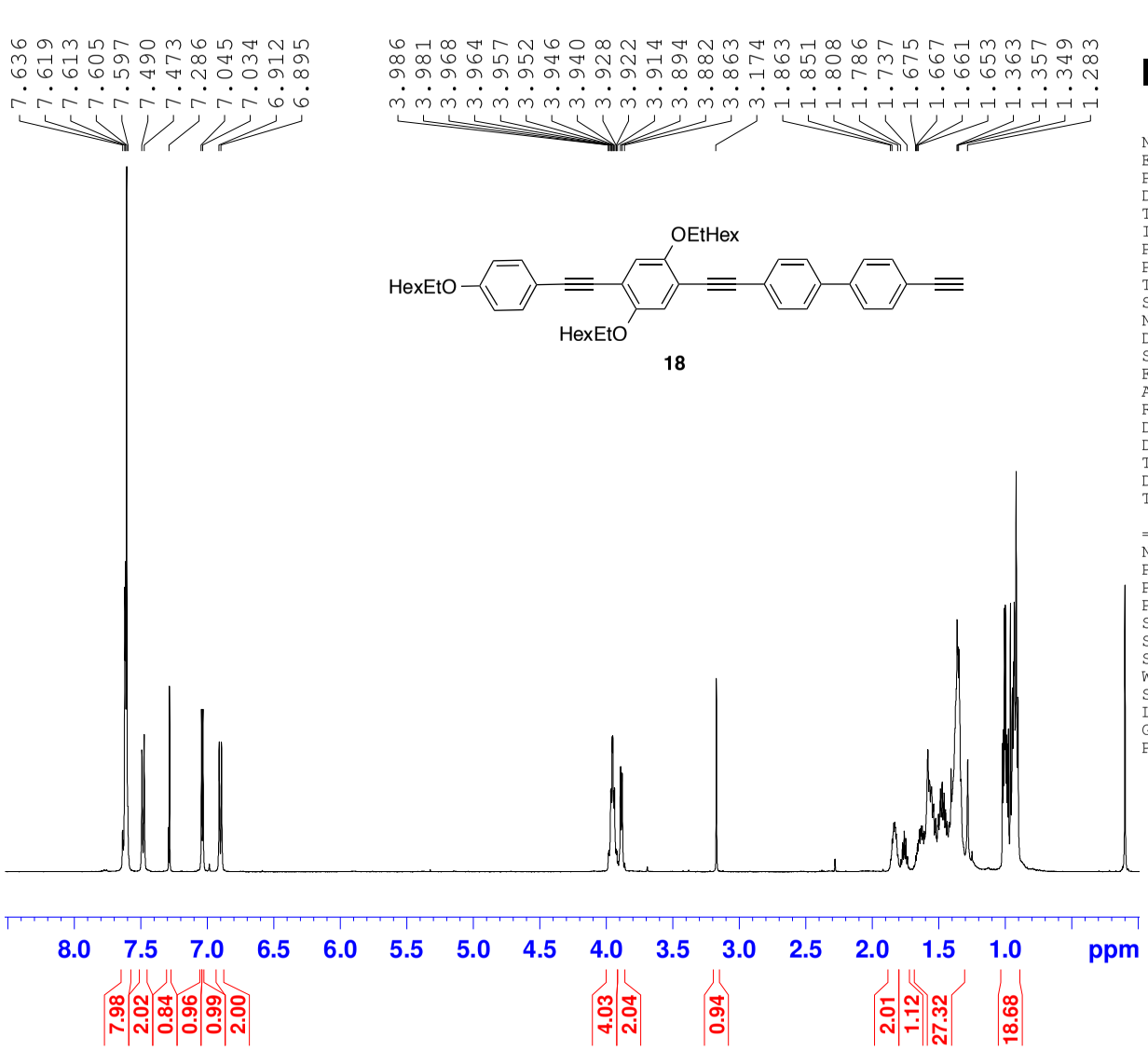


BRUKER

```
NAME                ek-2-007
EXPNO                      3
PROCNO                     1
Date_               20130816
Time                   13.53
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1689
DS                          4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010548 sec
RG                       203
DW                    16.800 usec
DE                     6.50 usec
TE                    296.0 K
D1                 0.50000000 sec
D11                0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.50 usec
PL1                      0.00 dB
PL1W              89.92553711 W
SFO1             125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      1.00 dB
PL12                    13.04 dB
PL13                    16.80 dB
PL2W              17.75783539 W
PL12W              1.11017132 W
PL13W              0.46707872 W
SFO2             500.1320005 MHz
SI                      65536
SF               125.7577613 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```



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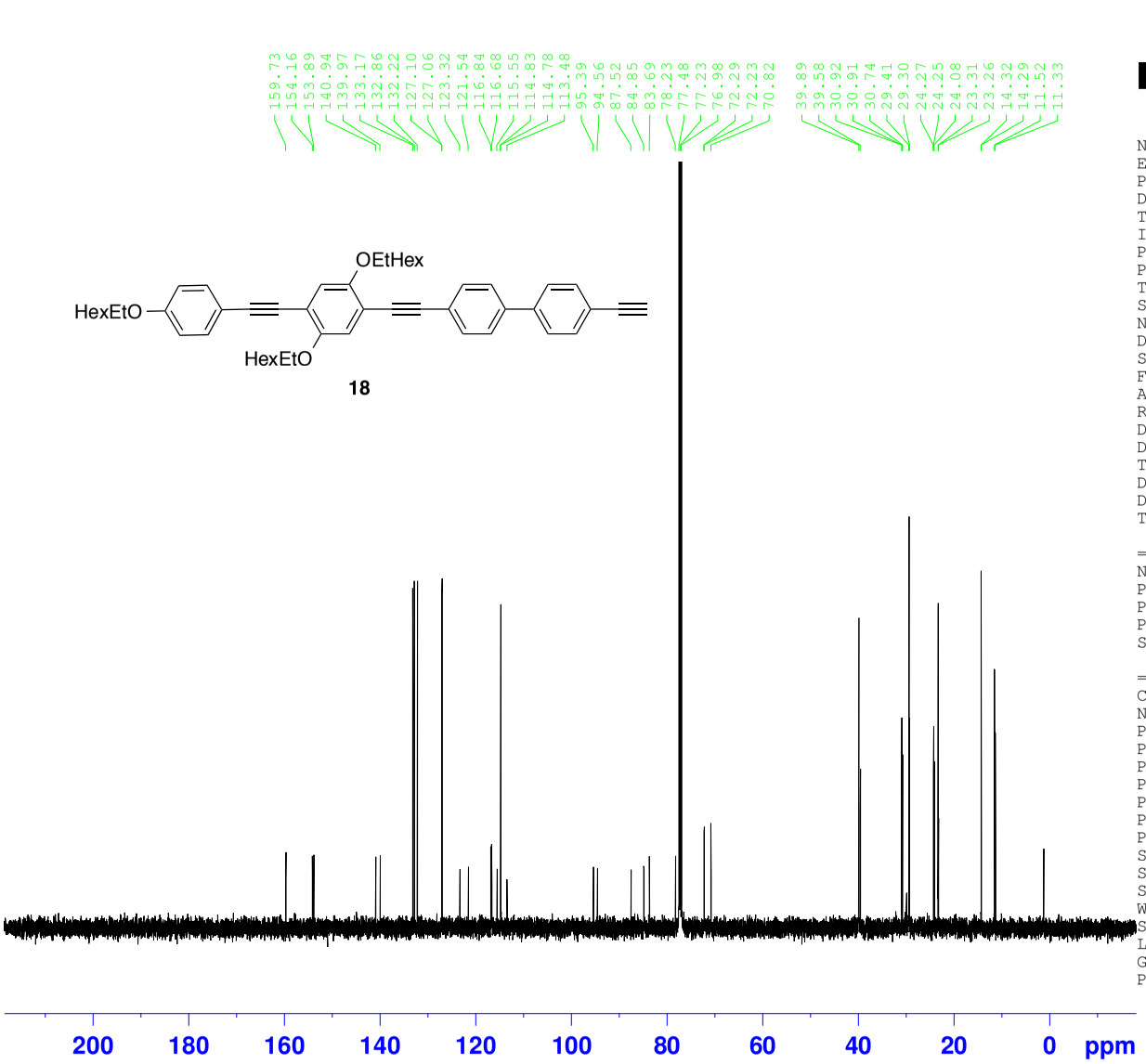
BRUKER

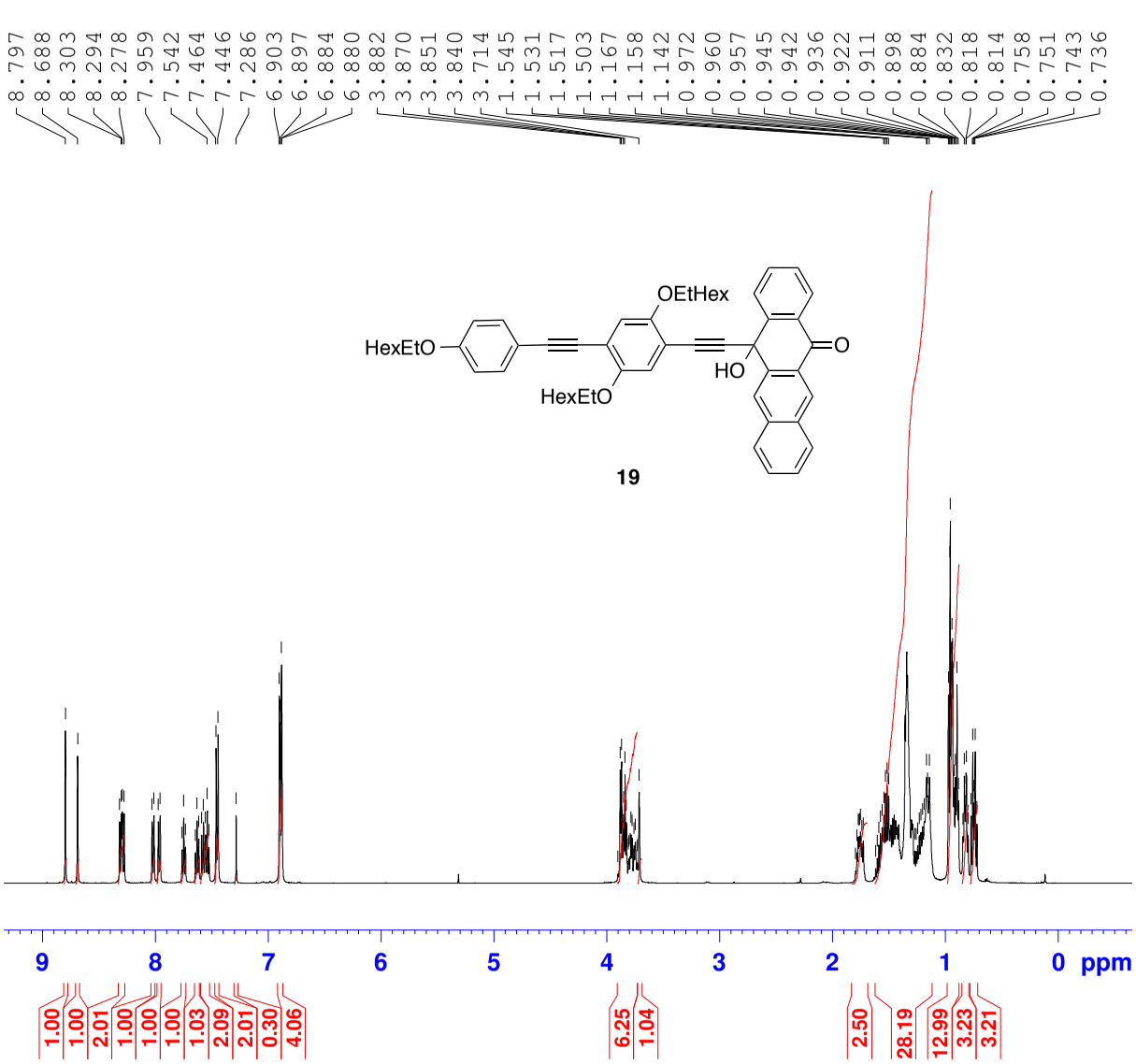
```
NAME                ek-2-009
EXPNO                      1
PROCNO                     1
Date_               20130820
Time                   13.00
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                10000.000 Hz
FIDRES             0.152588 Hz
AQ                 3.2768500 sec
RG                       181
DW                    50.000 usec
DE                     6.50 usec
TE                    295.0 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    20.00 usec
PL1                    1.00 dB
PL1W             17.75783539 W
SFO1             500.1318364 MHz
SI                     65536
SF               500.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                     1.00
```



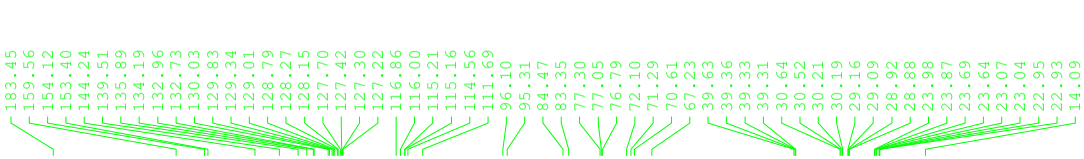
BRUKER

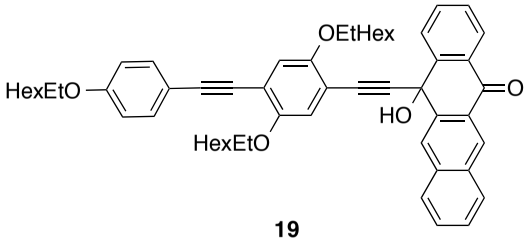
NAME	ek-2-009	
EXPNO	2	
PROCNO	1	
Date_	20130820	
Time	13.06	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	871	
DS	4	
SWH	29761.904	Hz
FIDRES	0.454131	Hz
AQ	1.1010548	sec
RG	203	
DW	16.800	usec
DE	6.50	usec
TE	296.0	K
D1	0.50000000	sec
D11	0.03000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	13C	
P1	9.50	usec
PL1	0.00	dB
PL1W	89.92553711	W
SFO1	125.7703643	MHz
======== CHANNEL f2 ========		
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00	usec
PL2	1.00	dB
PL12	13.04	dB
PL13	16.80	dB
PL2W	17.75783539	W
PL12W	1.11017132	W
PL13W	0.46707872	W
SFO2	500.1320005	MHz
SI	65536	
SF	125.7577621	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	



BRUKER

NAME	ek-2-021
EXPNO	5
PROCNO	1
Date_	20130916
Time	9.20
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	26
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	71.8
DW	50.000 usec
DE	6.50 usec
TE	295.2 K
D1	5.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





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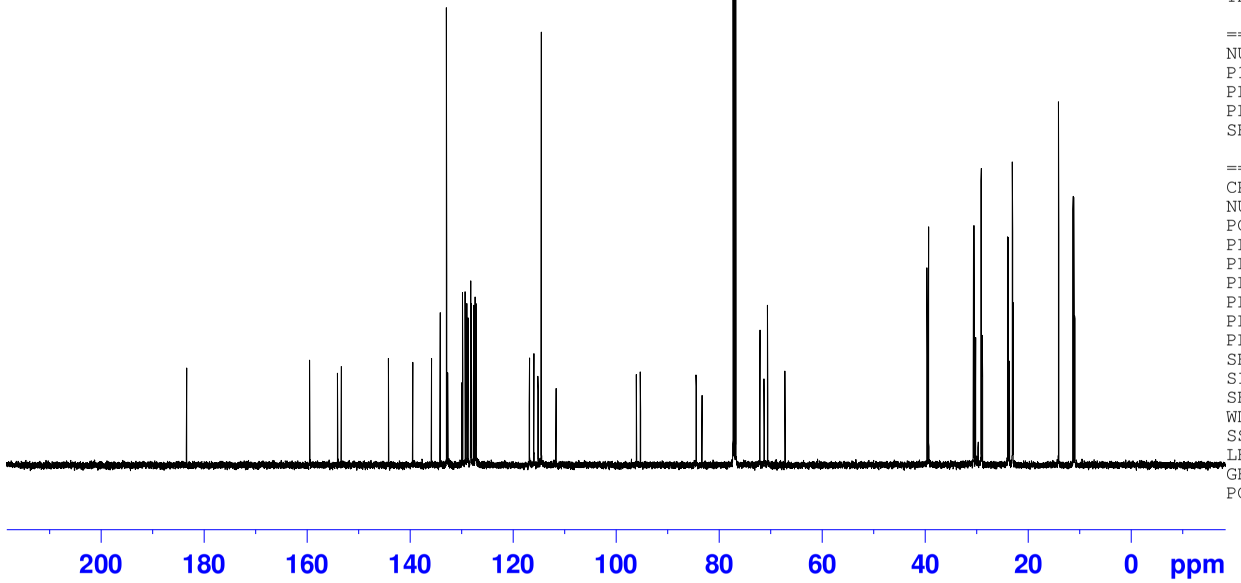
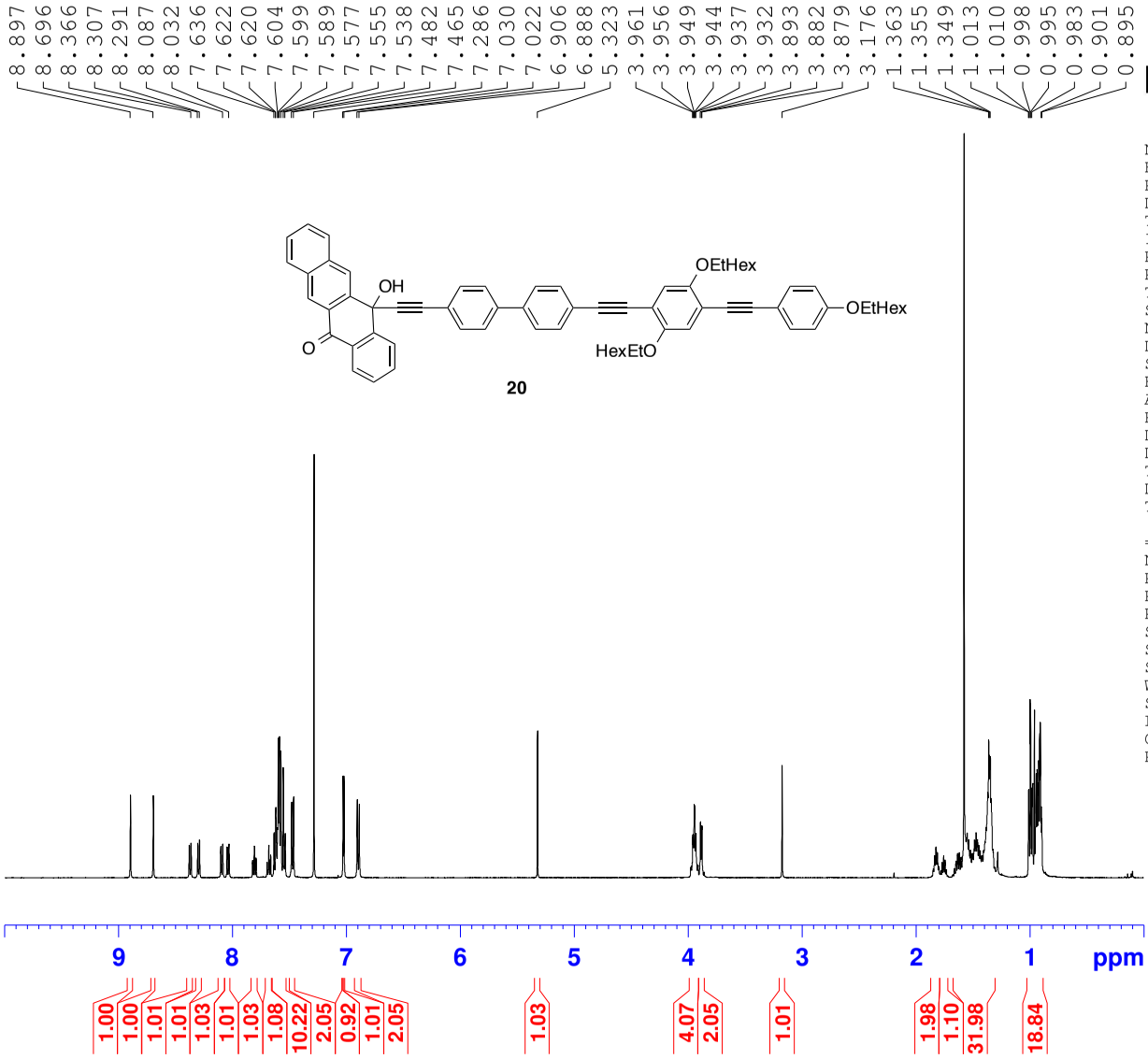



```
NAME                ek-2-021
EXPNO                      6
PROCNO                     1
Date_               20130916
Time                    9.25
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1338
DS                          4
SWH                29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010548 sec
RG                        203
DW                     16.800 usec
DE                      6.50 usec
TE                     295.2 K
D1                 0.50000000 sec
D11                0.03000000 sec
TD0                        1

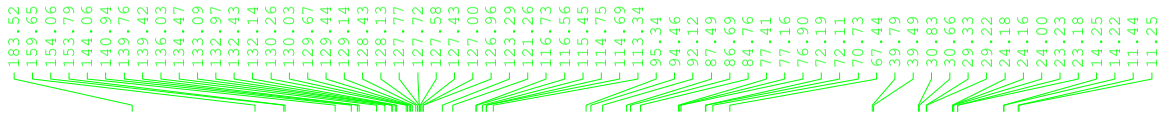
======== CHANNEL f1 ========
NUC1                      13C
P1                       9.50 usec
PL1                      0.00 dB
PL1W              89.92553711 W
SFO1             125.7703643 MHz

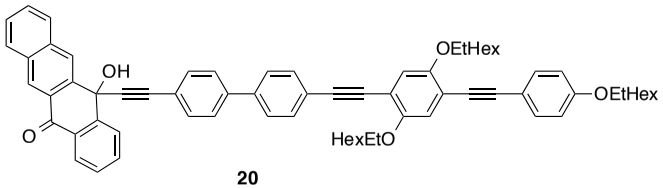
======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      1.00 dB
PL12                    13.04 dB
PL13                    16.80 dB
PL2W              17.75783539 W
PL12W              1.11017132 W
PL13W              0.46707872 W
SFO2             500.1320005 MHz
SI                       65536
SF               125.7577890 MHz
WDW                         EM
SSB                          0
LB                       1.00 Hz
GB                           0
PC                       1.40
```



BRUKER

NAME	ek-2-034
EXPNO	2
PROCNO	1
Date_	20131004
Time	15.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	5.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





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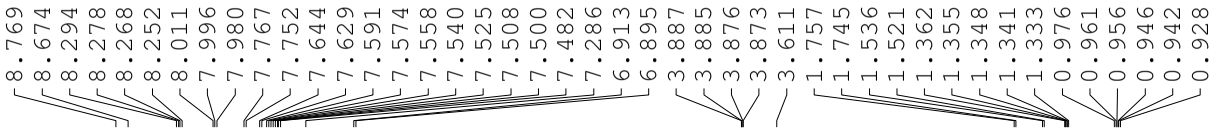
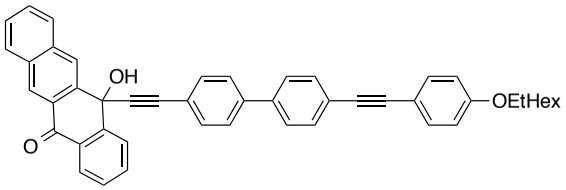
BRUKER

NAME	ek-2-034
EXPNO	6
PROCNO	1
Date_	20150511
Time	16.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	33611
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	290.4 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577718 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40





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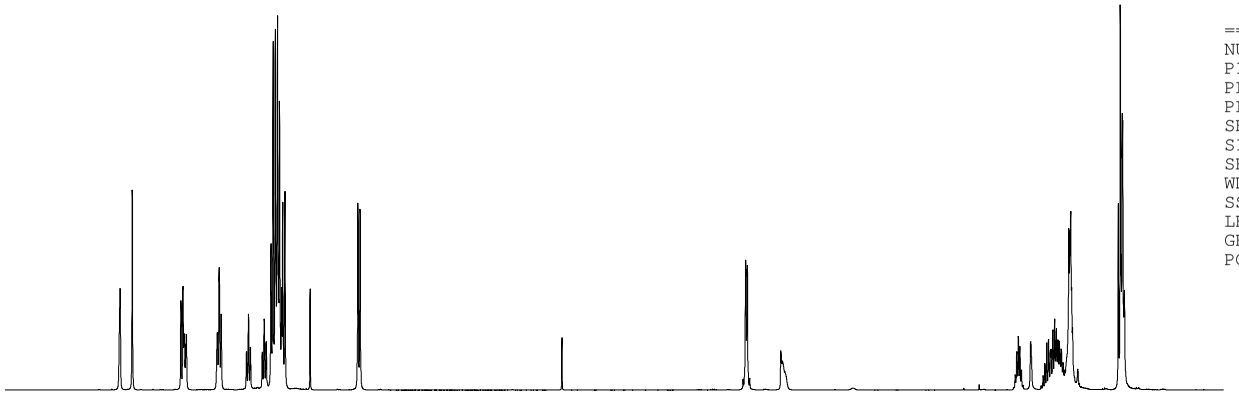
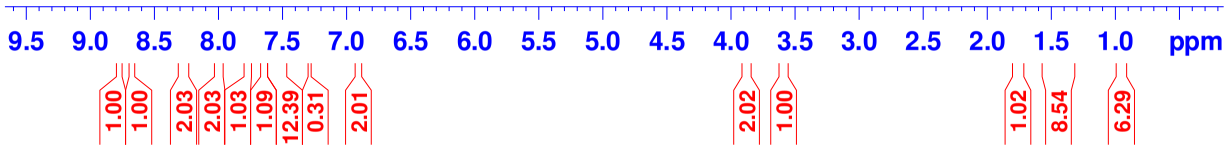
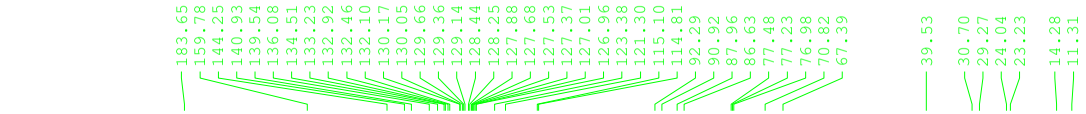
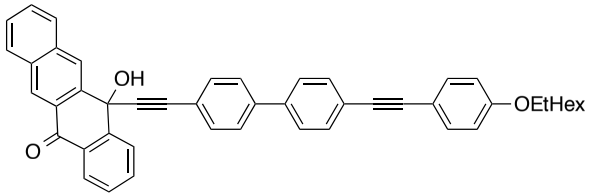





```
NAME                ek-2-016
EXPNO                      3
PROCNO                     1
Date_               20130904
Time                   15.49
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        24
DS                         2
SWH             10000.000 Hz
FIDRES              0.152588 Hz
AQ              3.2768500 sec
RG                       114
DW                  50.000 usec
DE                   6.50 usec
TE                  295.2 K
D1              5.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    20.00 usec
PL1                    1.00 dB
PL1W          17.75783539 W
SFO1          500.1318364 MHz
SI                     65536
SF            500.1300000 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                     1.00
```





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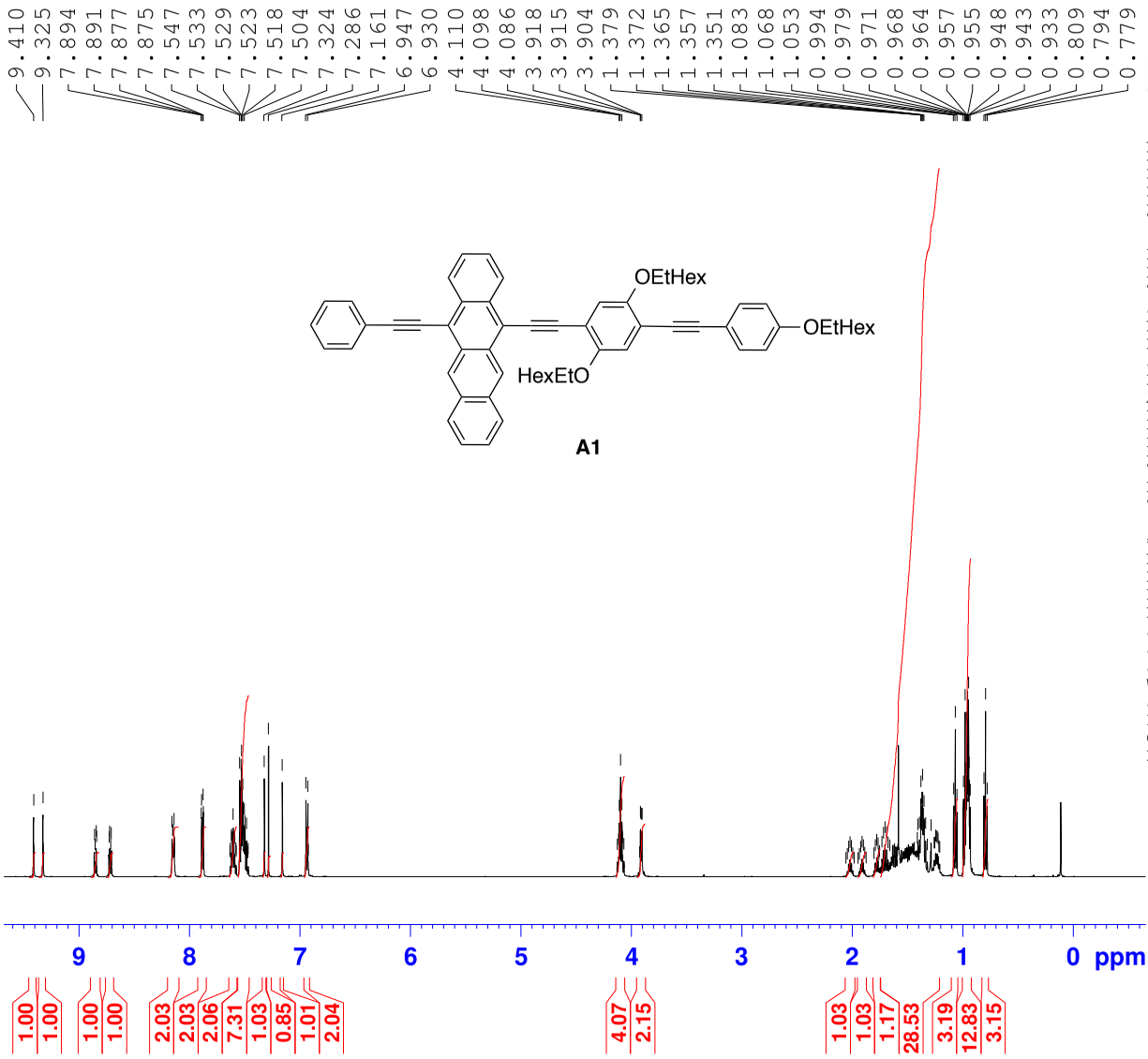
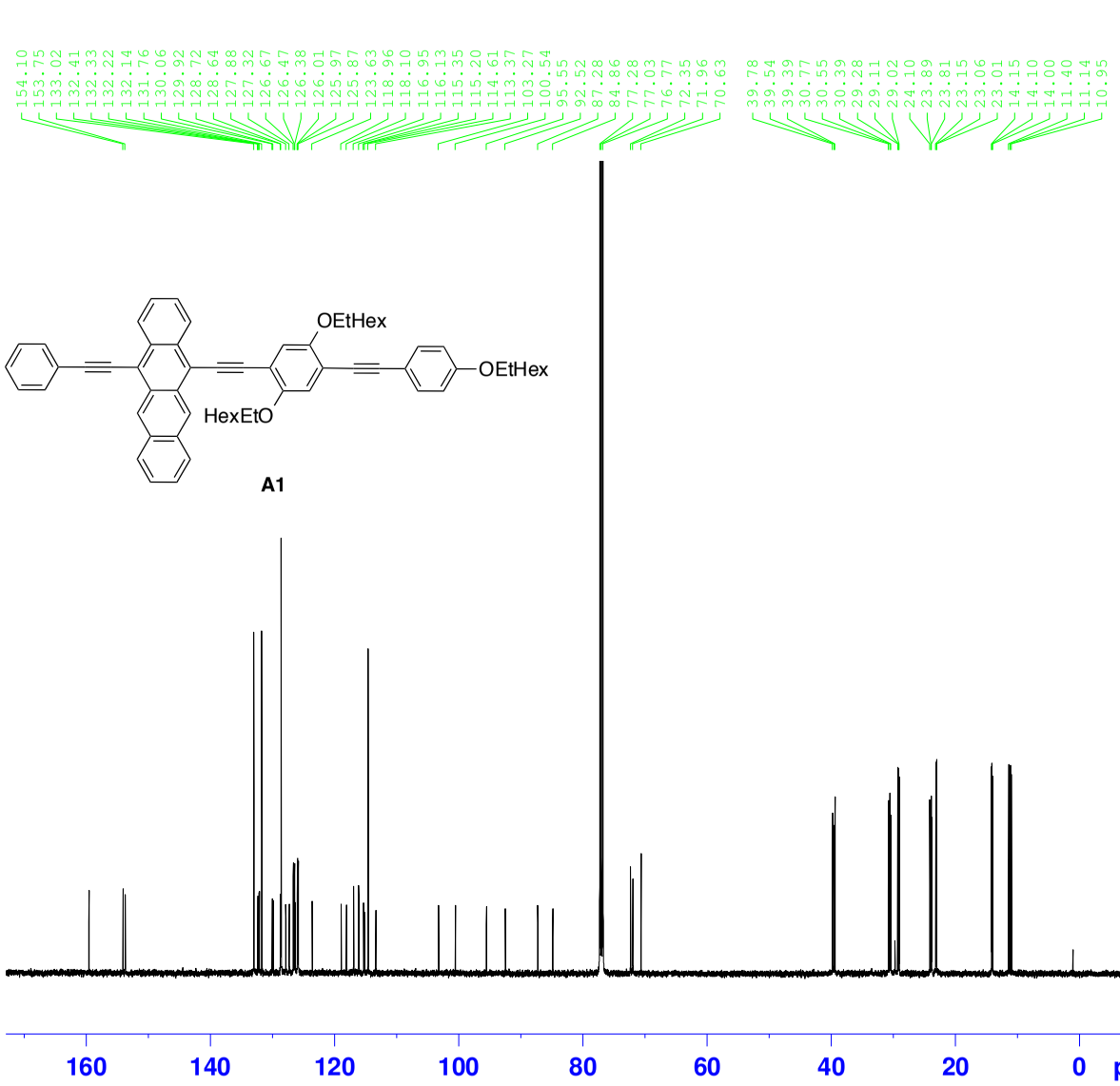
BRUKER

NAME	ek-2-016
EXPNO	4
PROCNO	1
Date_	20130904
Time	15.53
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	560
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	295.4 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577663 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



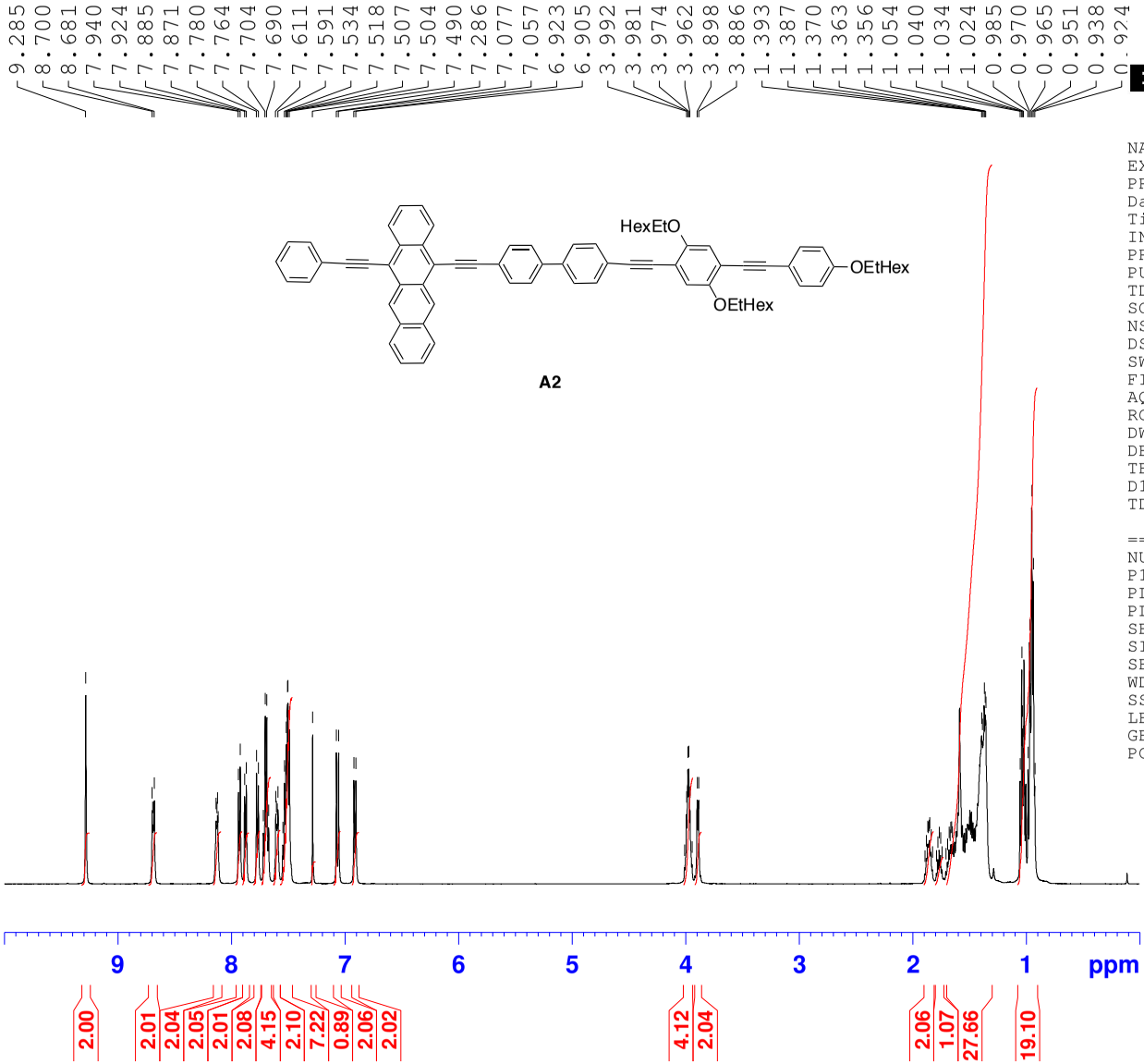
BRUKER

NAME	ek-2-023
EXPNO	2
PROCNO	1
Date_	20130924
Time	9.18
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	19
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	144
DW	50.000 usec
DE	6.50 usec
TE	294.8 K
D1	5.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



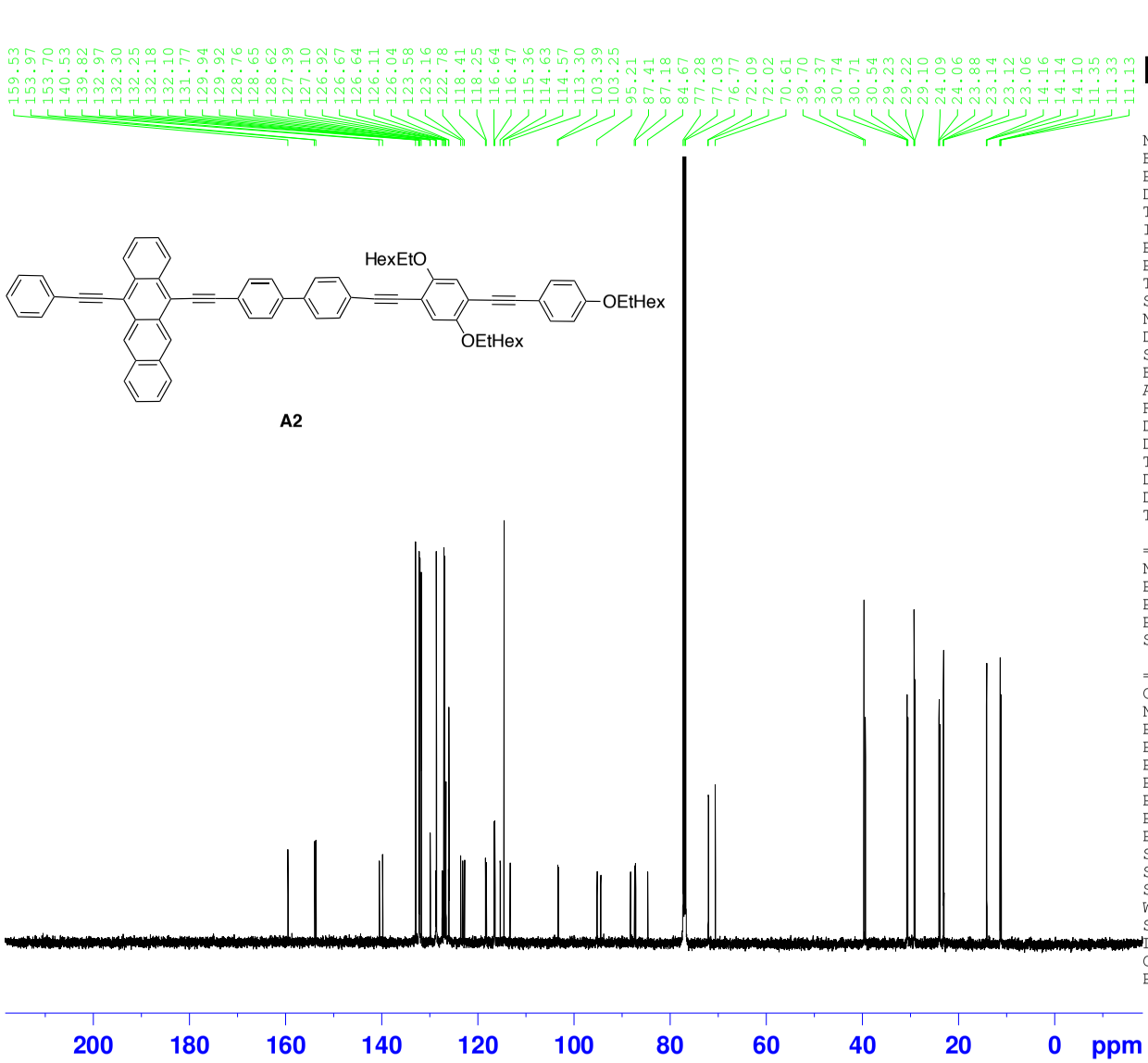
BRUKER

NAME	ek-2-023
EXPNO	8
PROCNO	1
Date_	20130924
Time	10.59
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4475
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	295.0 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

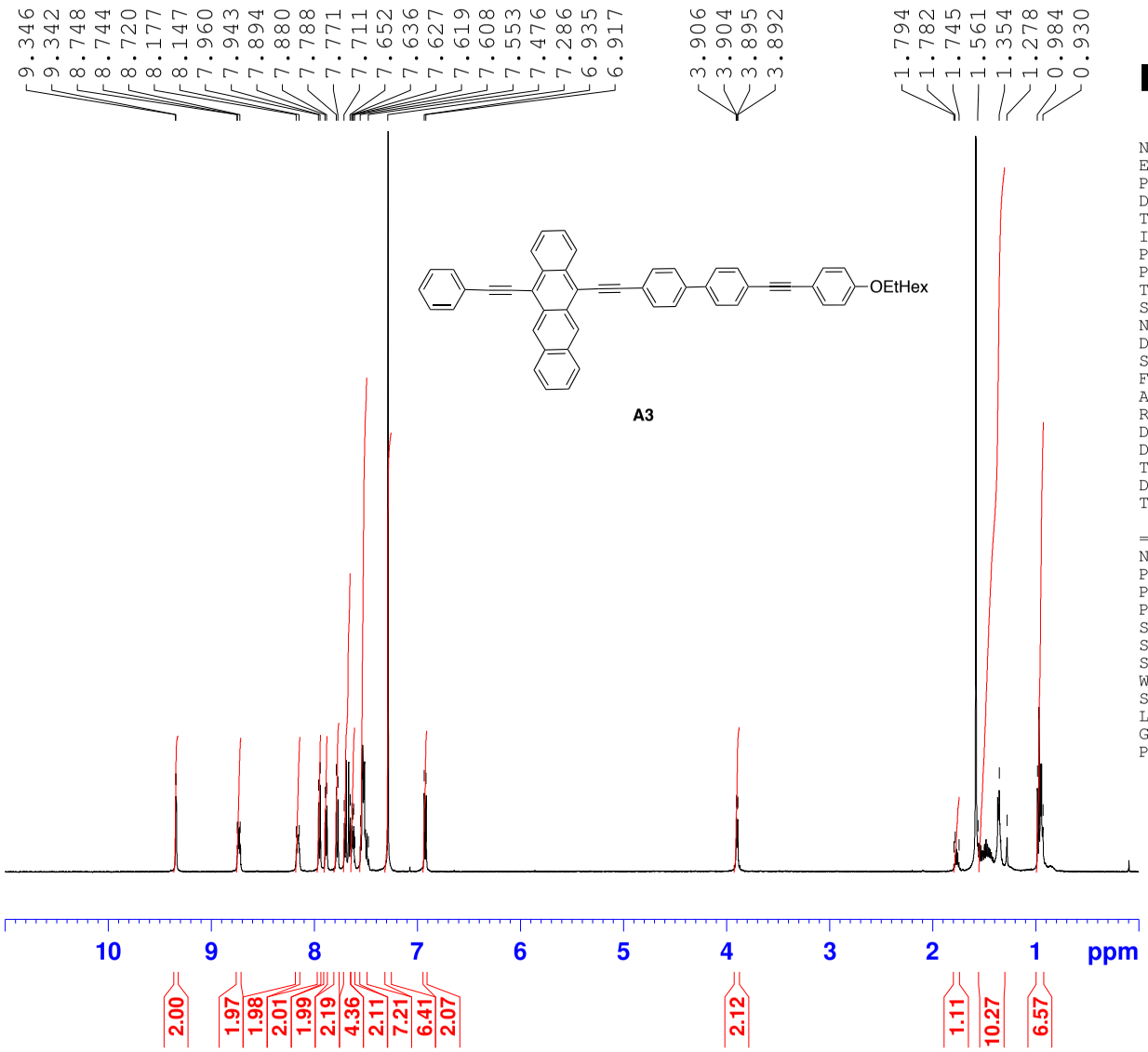


BRUKER

NAME	ek-2-035
EXPNO	20
PROCNO	1
Date_	20150516
Time	12.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	181
DW	50.000 usec
DE	6.50 usec
TE	291.1 K
D1	0.50000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

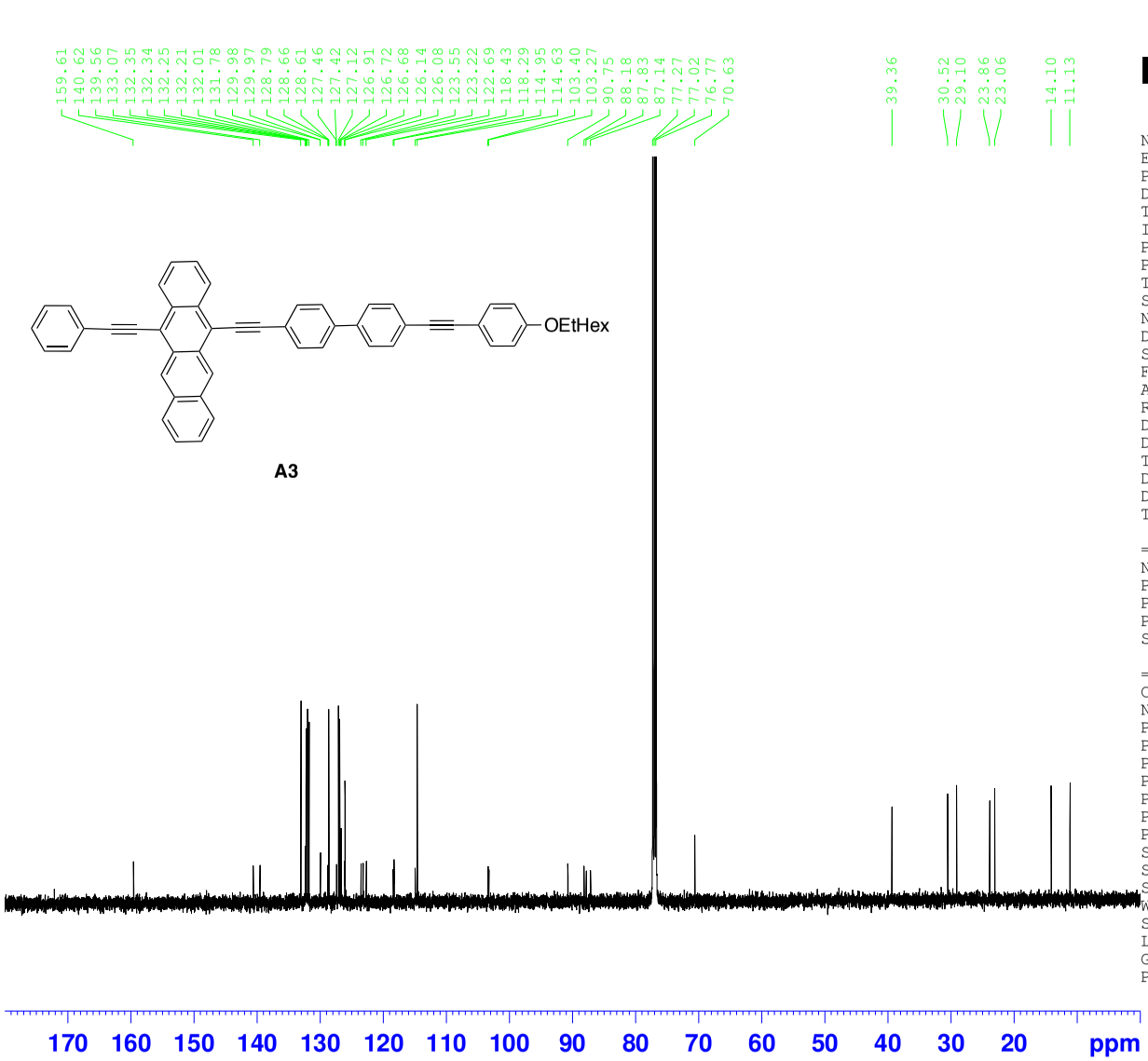


NAME	ek-2-035
EXPNO	21
PROCNO	1
Date_	20150516
Time	12.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	6673
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	291.3 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	0.50



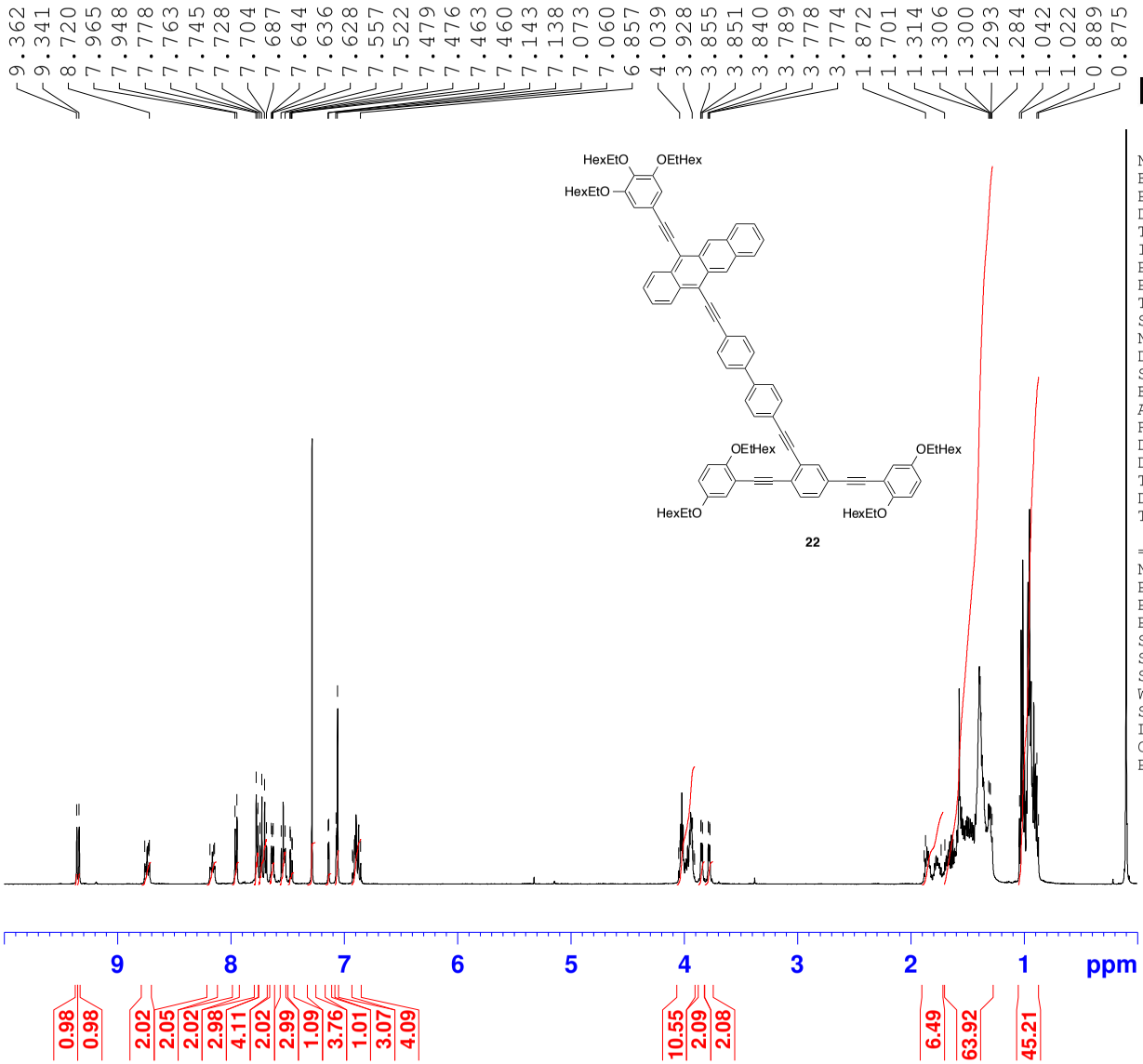
BRUKER

NAME	ek-2-018	
EXPNO	15	
PROCNO	1	
Date_	20150514	
Time	14.21	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	CDCl3	
NS	16	
DS	2	
SWH	10000.000	Hz
FIDRES	0.152588	Hz
AQ	3.2768500	sec
RG	203	
DW	50.000	usec
DE	6.50	usec
TE	291.0	K
D1	0.50000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	20.00	usec
PL1	1.00	dB
PL1W	17.75783539	W
SFO1	500.1318364	MHz
SI	65536	
SF	500.1300000	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	



BRUKER

NAME	ek-2-018
EXPNO	17
PROCNO	1
Date_	20150514
Time	14.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3993
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	292.2 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	0.10

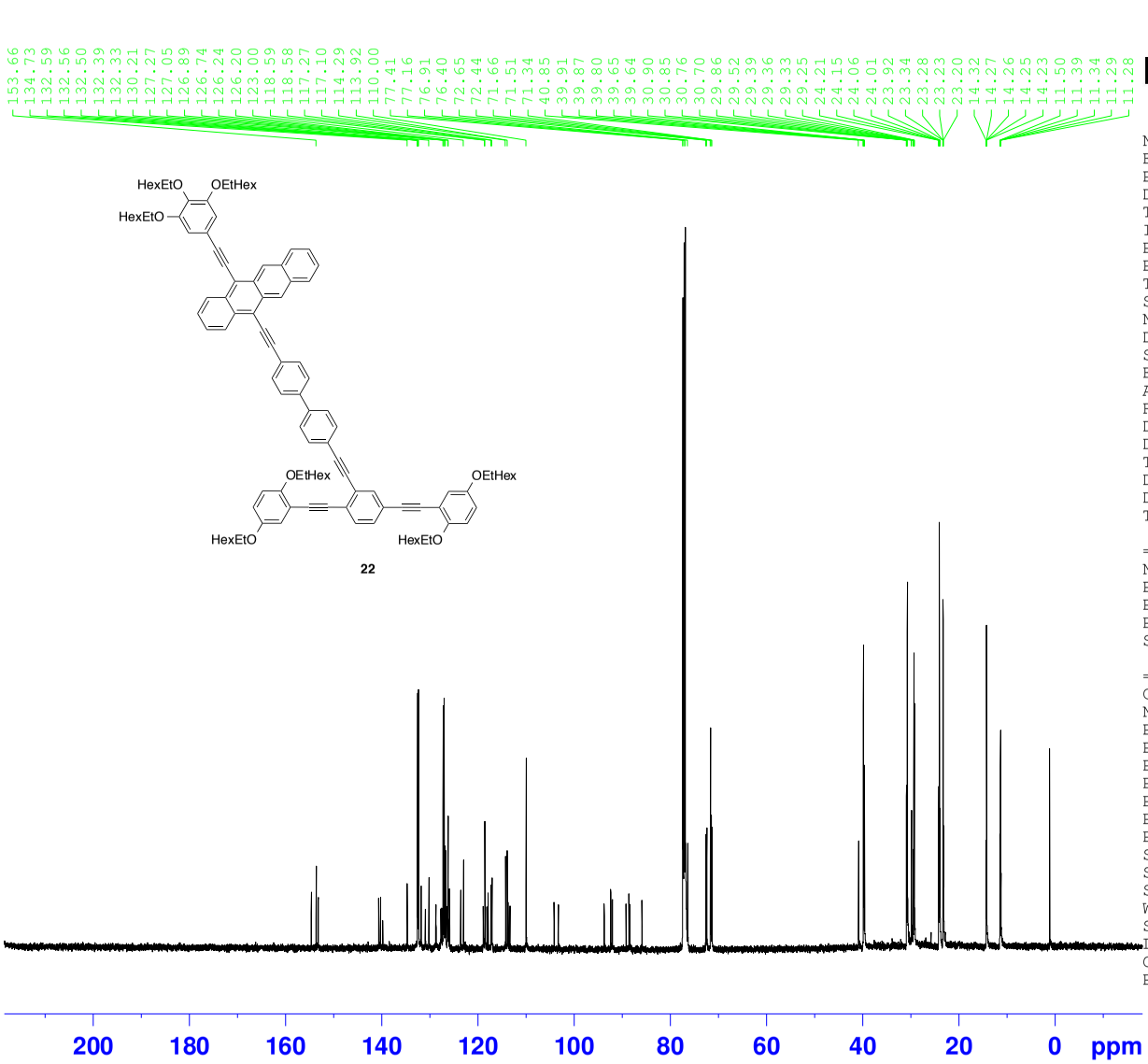


BRUKER

NAME	ek-2-115
EXPNO	2
PROCNO	1
Date_	20140225
Time	14.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	293.8 K
D1	5.00000000 sec
TD0	1

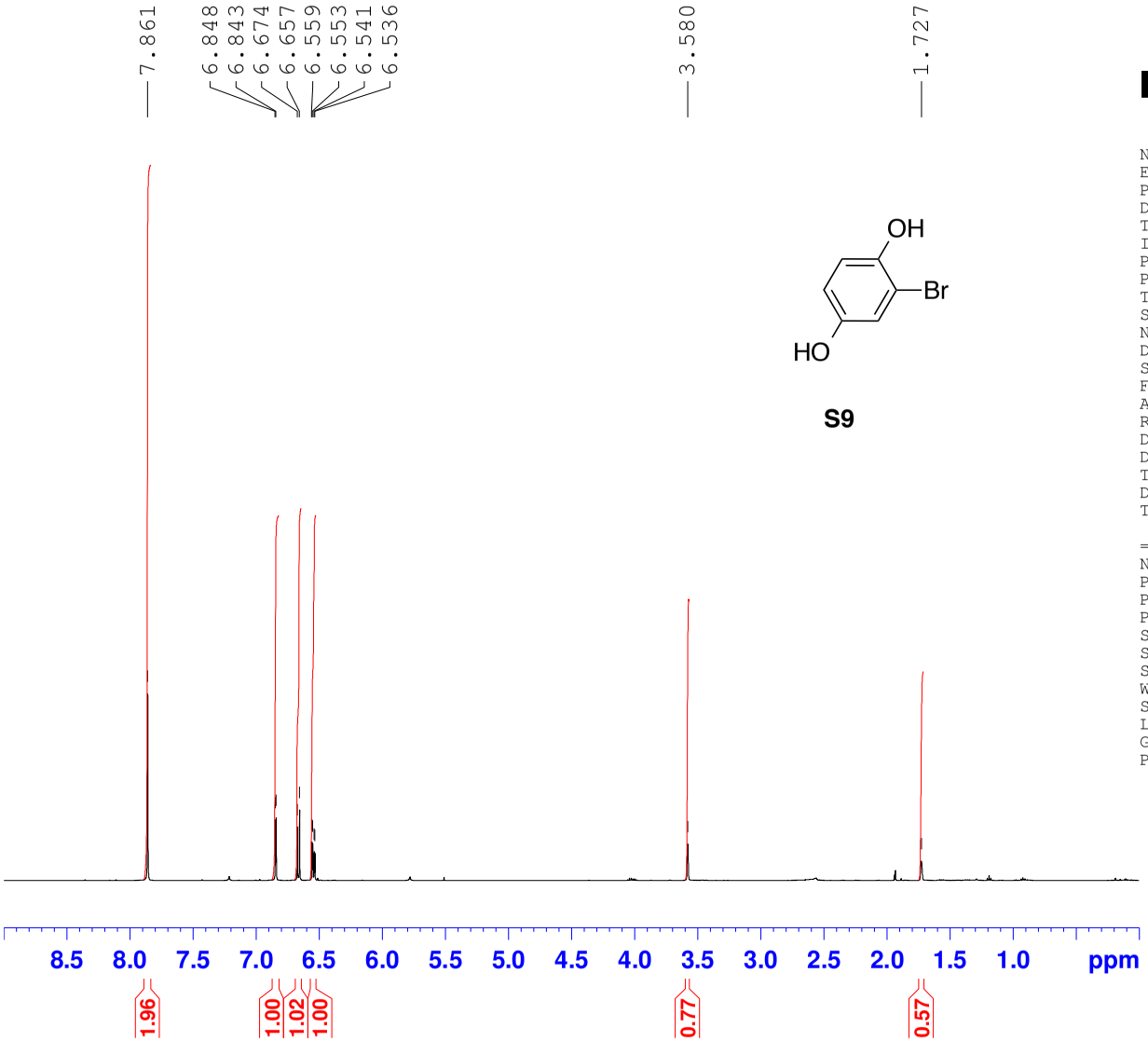
======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



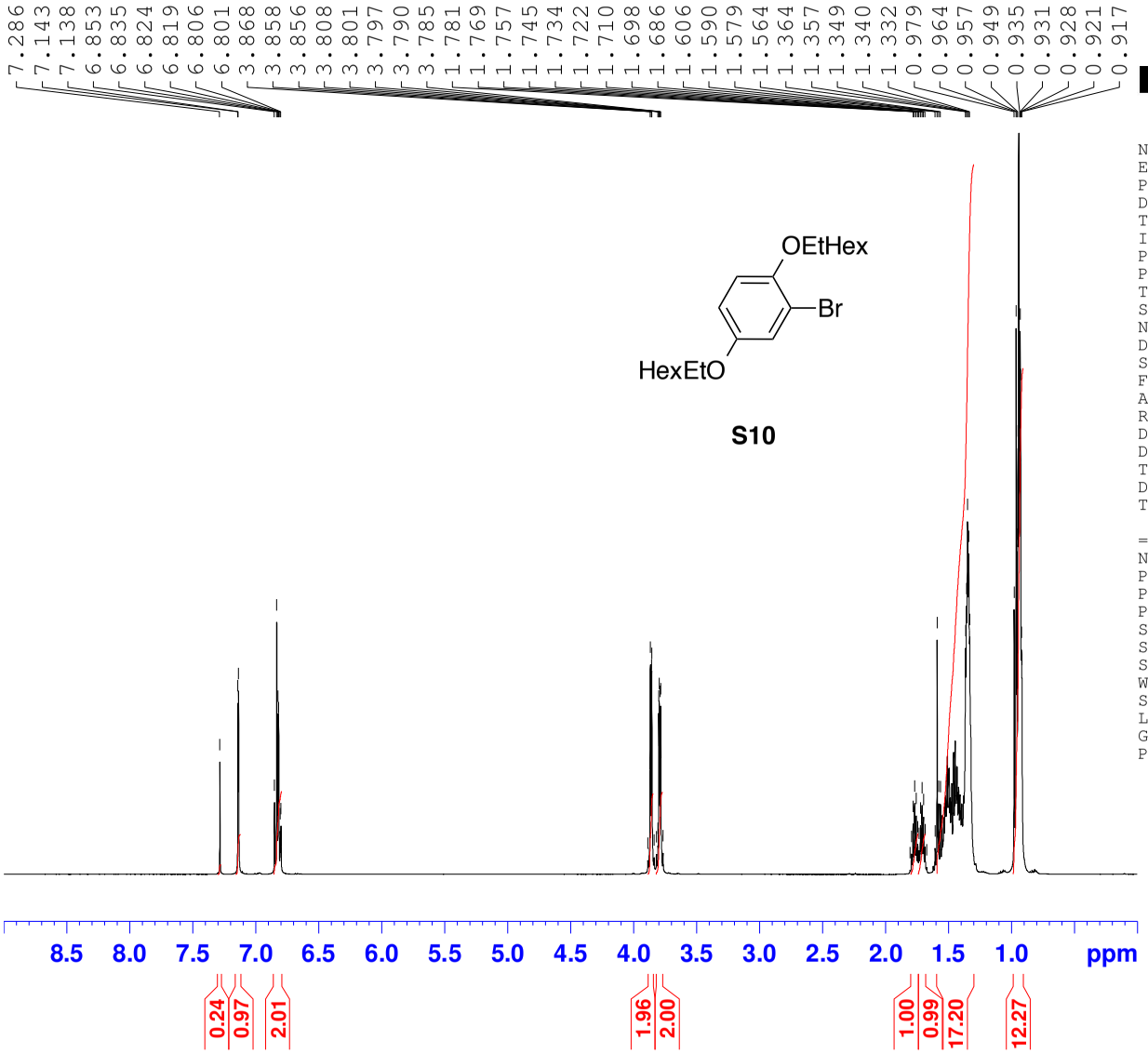
BRUKER

NAME	ek-2-115
EXPNO	7
PROCNO	1
Date_	20140415
Time	17.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg
TD	65536
SOLVENT	CDCl3
NS	33378
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.3 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	40
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577694 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40




```
NAME                ek-2-076
EXPNO                      1
PROCNO                     1
Date_               20131211
Time                   11.45
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                 THF
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2768500 sec
RG                      203
DW                   50.000 usec
DE                    6.50 usec
TE                   293.8 K
D1               0.50000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    20.00 usec
PL1                    1.00 dB
PL1W           17.75783539 W
SFO1           500.1318364 MHz
SI                    65536
SF             500.1300185 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```

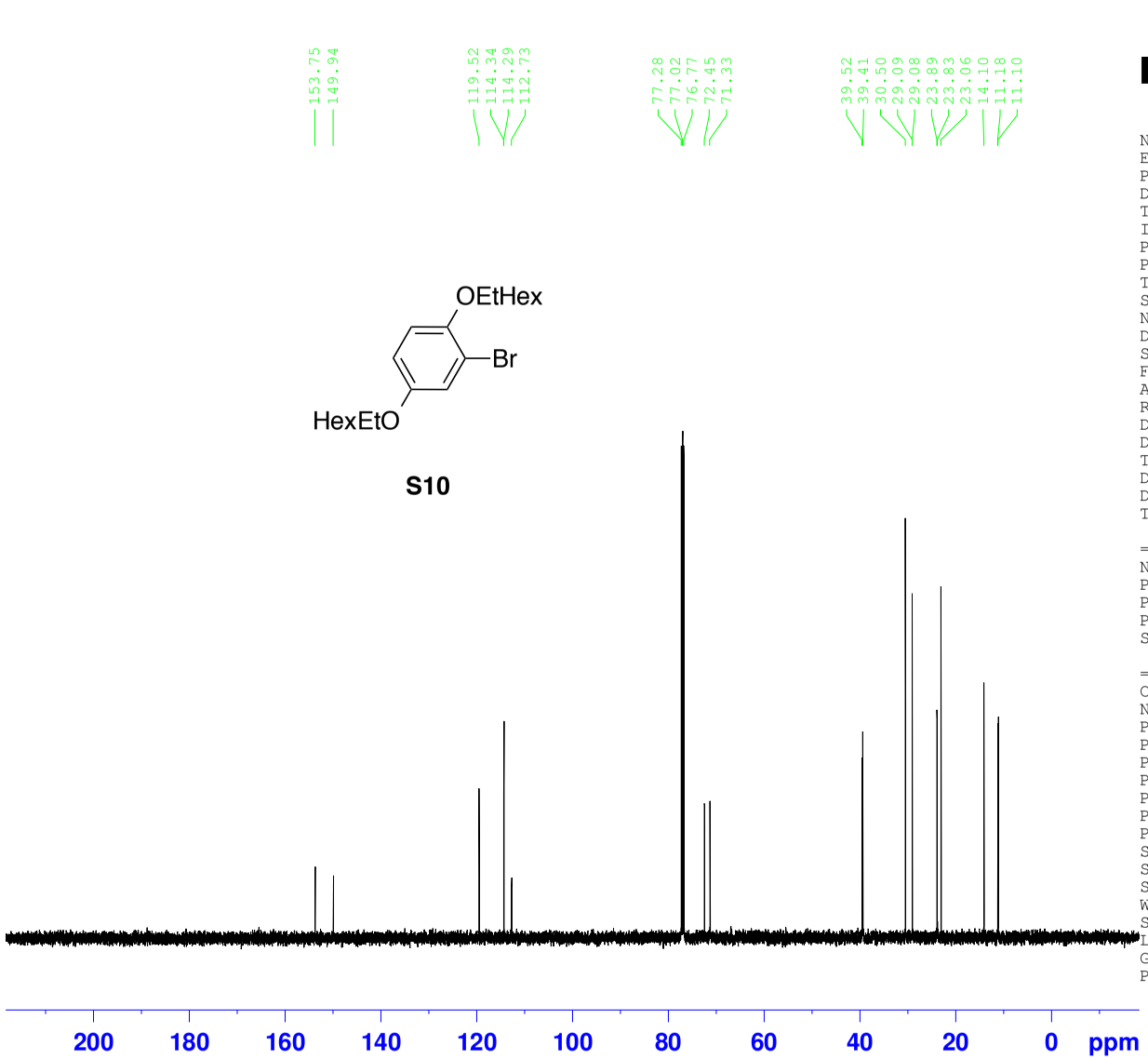


BRUKER

NAME	ek-2-077
EXPNO	5
PROCNO	1
Date_	20150512
Time	8.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	71.8
DW	50.000 usec
DE	6.50 usec
TE	291.2 K
D1	0.50000000 sec
TD0	1

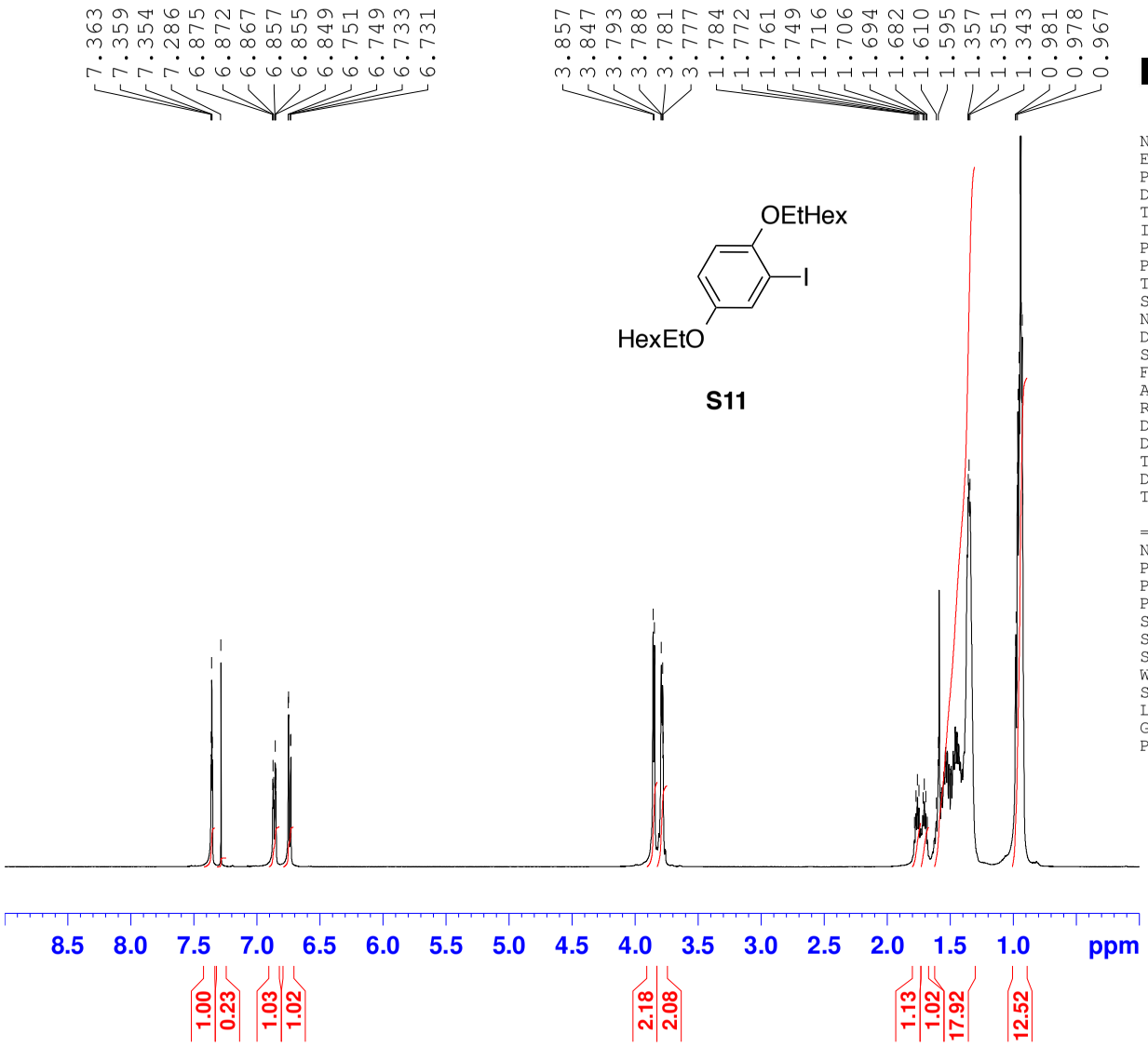
======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



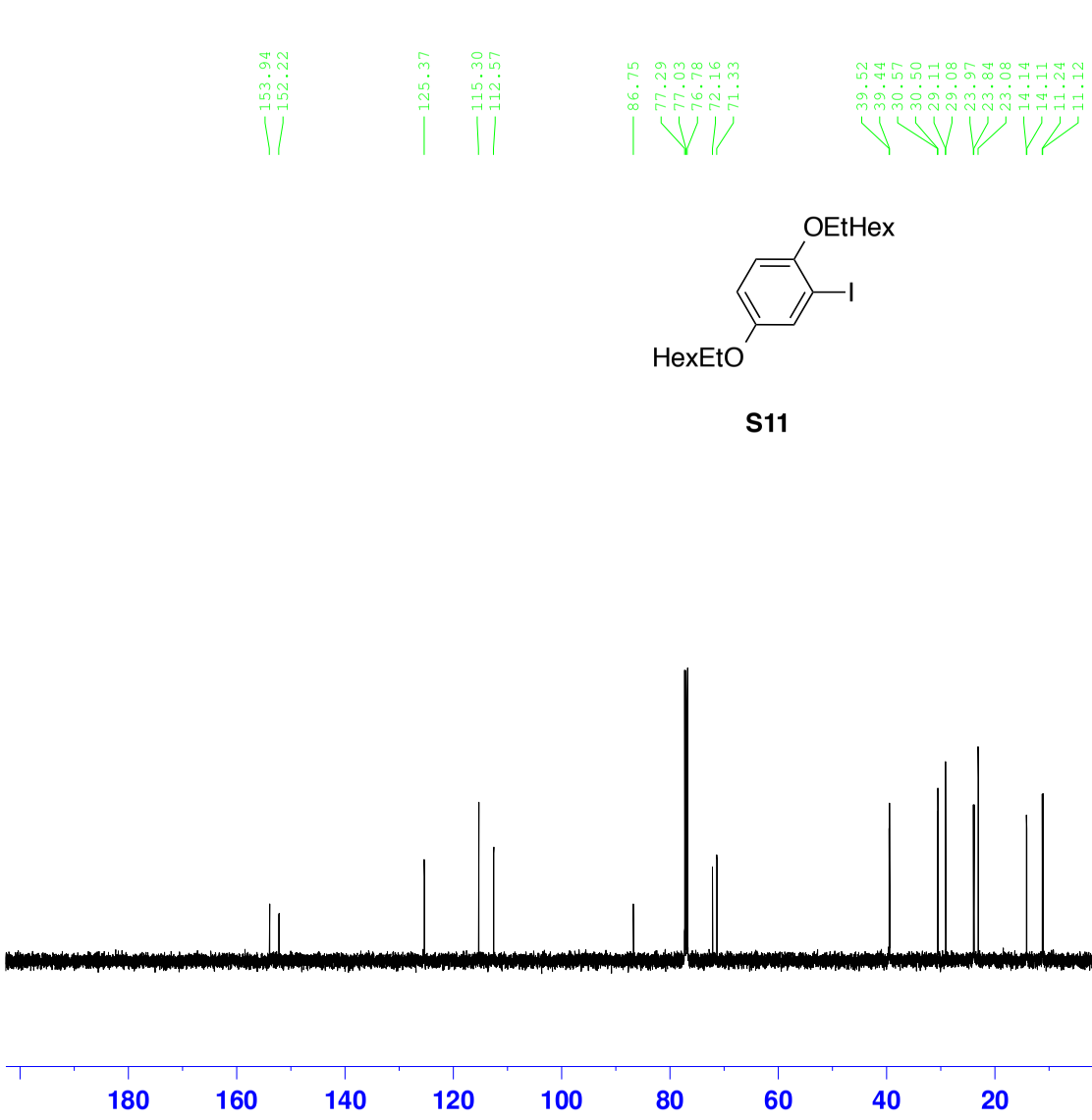
BRUKER

NAME	ek-2-077
EXPNO	6
PROCNO	1
Date_	20150512
Time	9.01
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	242
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	291.6 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



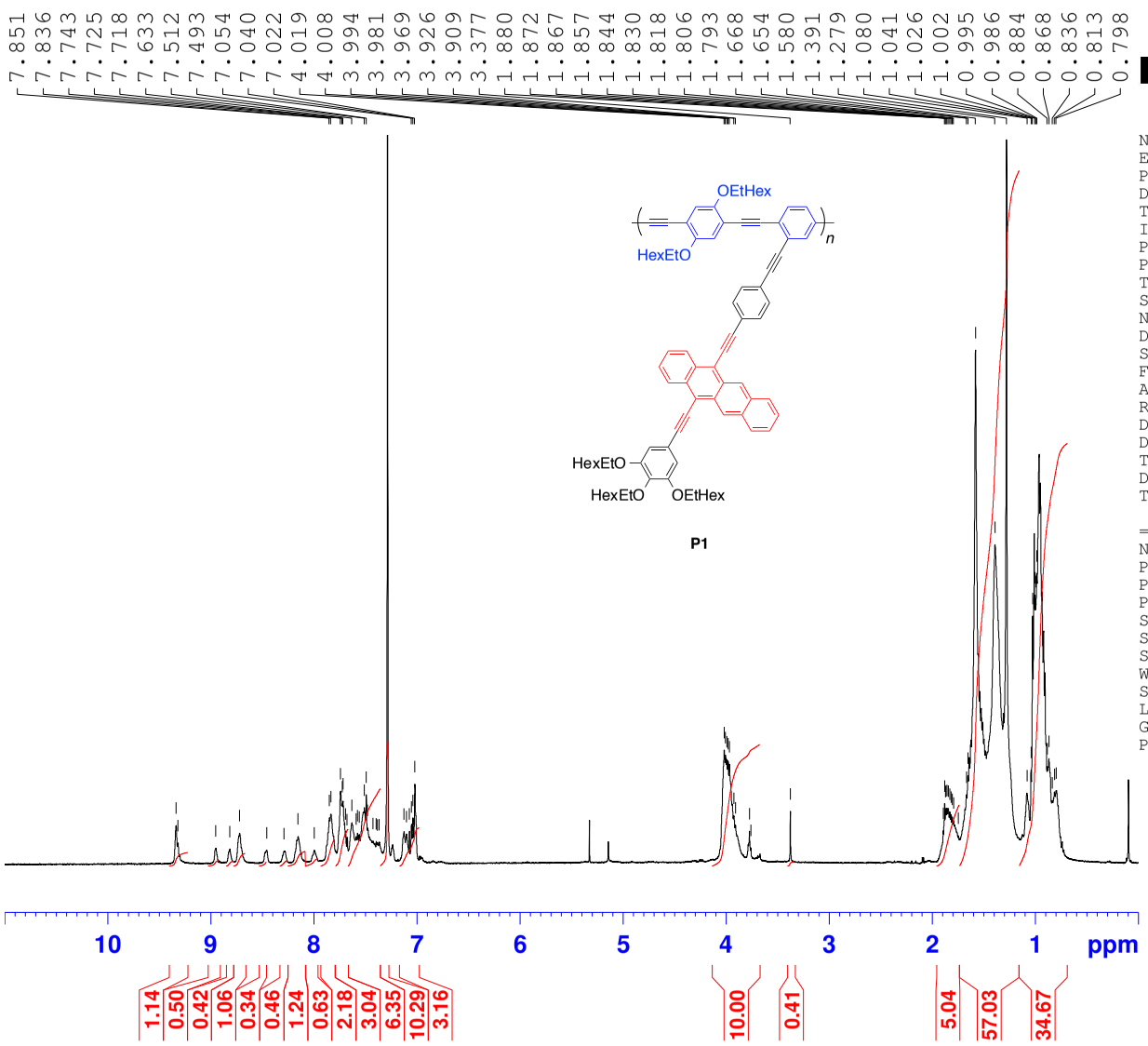
BRUKER

NAME	ek-2-078
EXPNO	5
PROCNO	1
Date_	20150512
Time	9.13
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	71.8
DW	50.000 usec
DE	6.50 usec
TE	291.1 K
D1	0.50000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



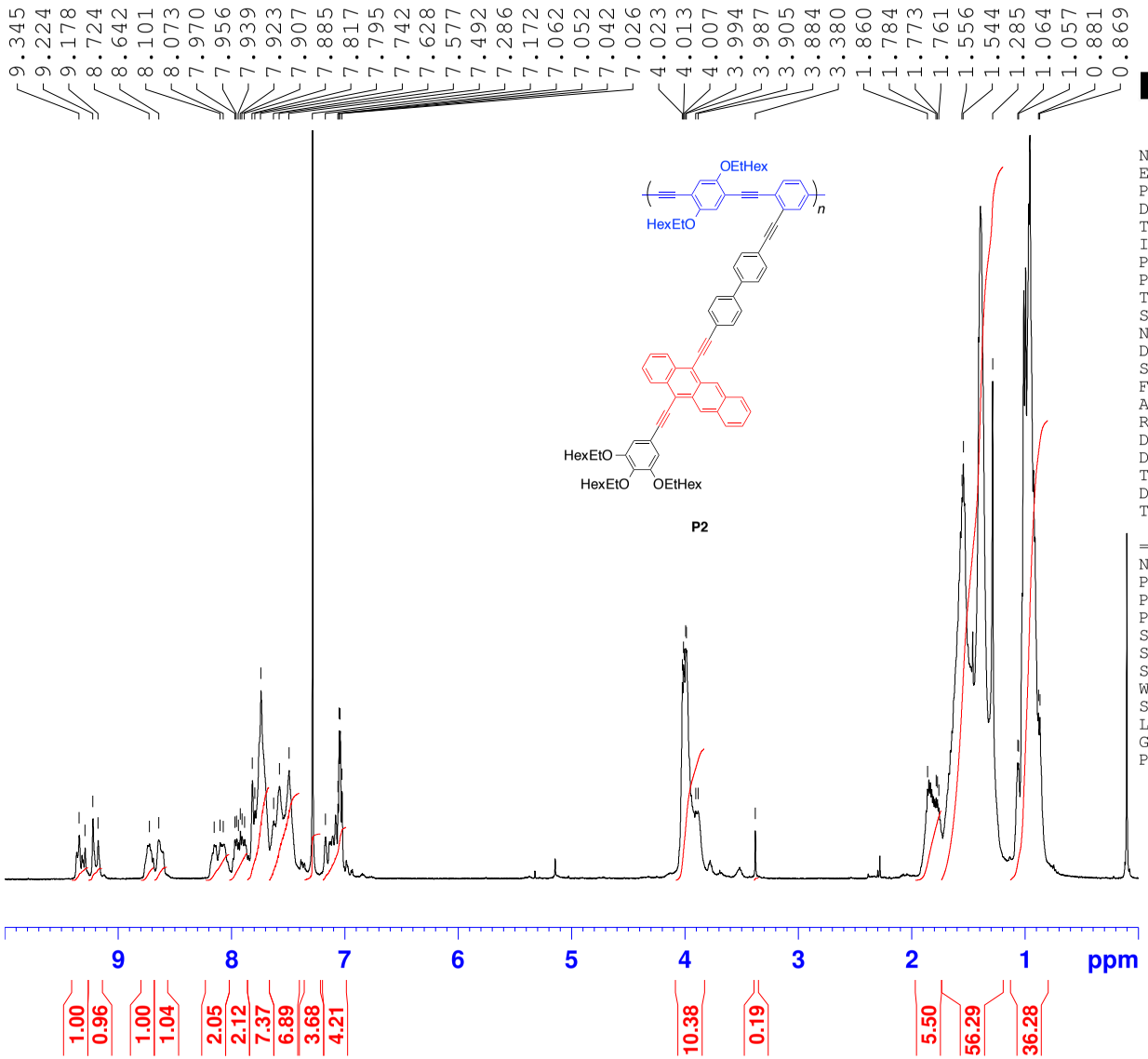
BRUKER

NAME	ek-2-078
EXPNO	6
PROCNO	1
Date_	20150512
Time	9.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	119
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	291.9 K
D1	0.50000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.50 usec
PL1	0.00 dB
PL1W	89.92553711 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	13.04 dB
PL13	16.80 dB
PL2W	17.75783539 W
PL12W	1.11017132 W
PL13W	0.46707872 W
SFO2	500.1320005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	ek-2-129
EXPNO	1
PROCNO	1
Date_	20140403
Time	13.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	254
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	293.6 K
D1	5.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

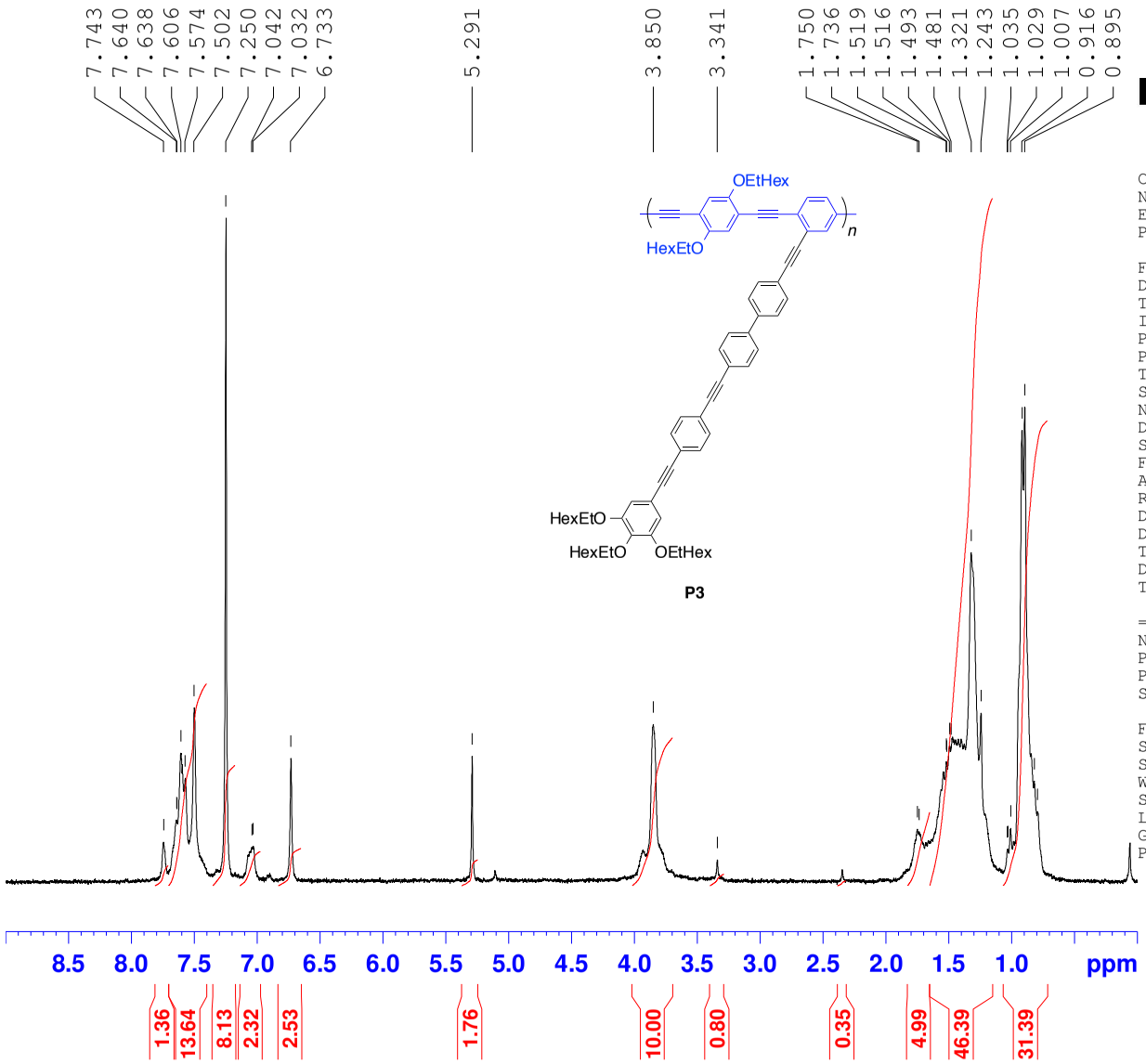


BRUKER

NAME	PPE-TET
EXPNO	1
PROCNO	1
Date_	20131205
Time	15.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	67
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	300.0 K
D1	5.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00




```
Current Data Parameters
NAME                  ek-2-094
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20140127
Time                     15.09
INSTRUM                  spect
PROBHD    5 mm QNP 1H/13
PULPROG                  zg30
TD                      32768
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  6218.905 Hz
FIDRES               0.189786 Hz
AQ                  2.6345973 sec
RG                       574.7
DW                      80.400 usec
DE                       6.00 usec
TE                      300.0 K
D1                 5.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       12.00 usec
PL1                       0.00 dB
SFO1               300.3418547 MHz

F2 - Processing parameters
SI                          32768
SF                 300.3400067 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         0.20
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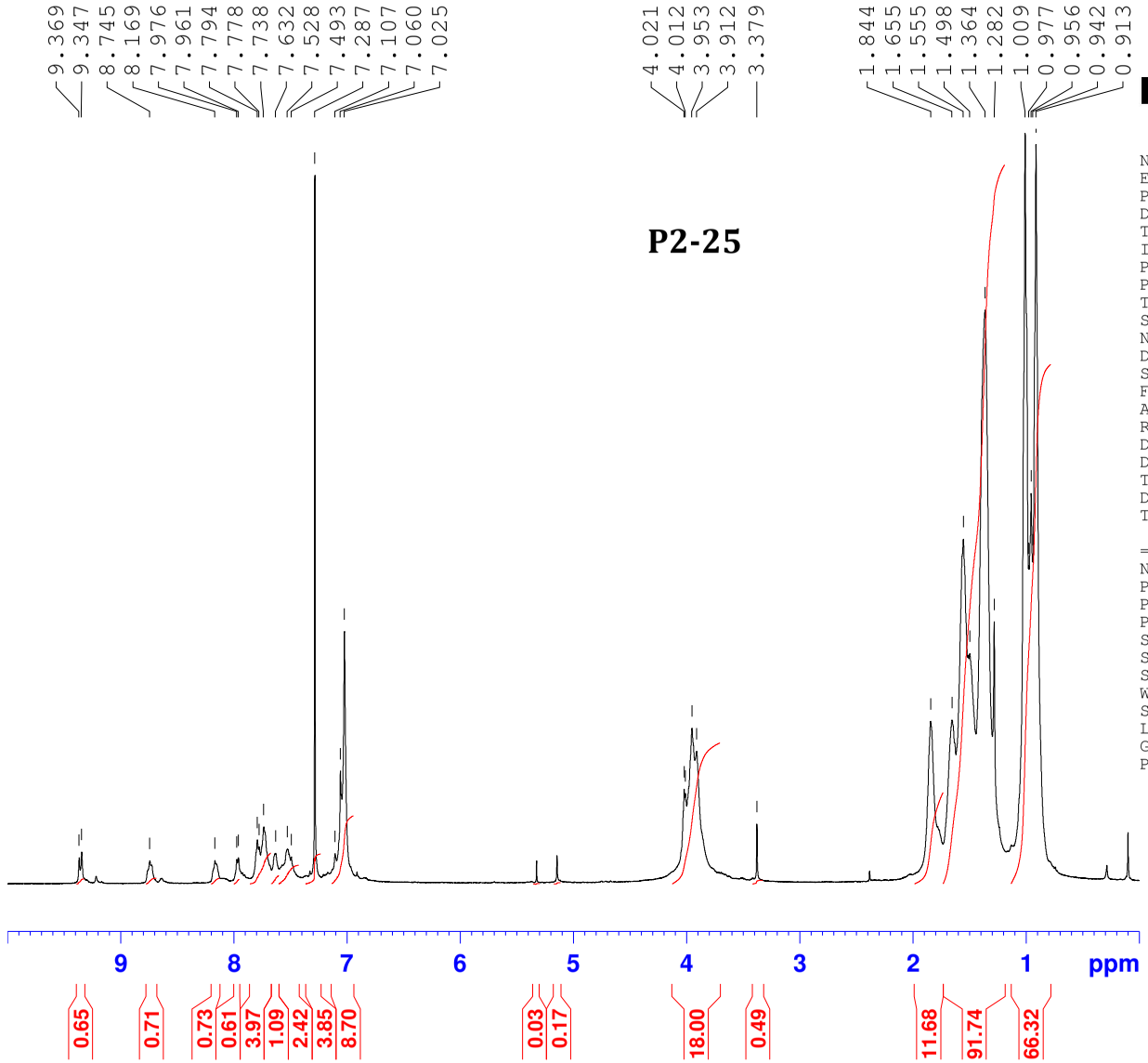


BRUKER

NAME	ek-2-116
EXPNO	2
PROCNO	1
Date_	20140228
Time	13.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	293.6 K
D1	5.00000000 sec
TD0	1

======== CHANNEL f1 ========

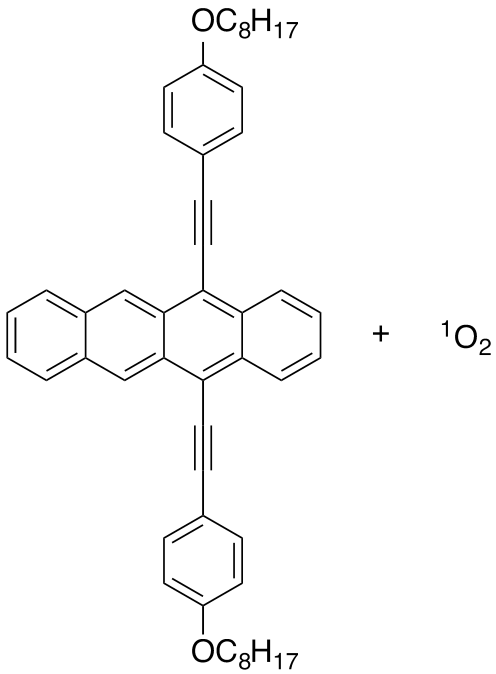
NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

ek-1-296 t=3 h MB removed

7.891 7.797 7.780 7.639 7.622 7.534 7.517 7.480 7.474 7.469 7.463 7.435 7.428 7.423 7.417 6.934 6.931 6.925 6.917 6.911 6.907 6.645

4.740

4.285 4.030 4.017 4.011 4.004



+ $^1O_2$

NAME	ek-1-296
EXPNO	25
PROCNO	1
Date_	20130710
Time	15.17
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	10000.000 Hz
FIDRES	0.152588 Hz
AQ	3.2768500 sec
RG	203
DW	50.000 usec
DE	6.50 usec
TE	295.9 K
D1	5.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	20.00 usec
PL1	1.00 dB
PL1W	17.75783539 W
SFO1	500.1318364 MHz
SI	65536
SF	500.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
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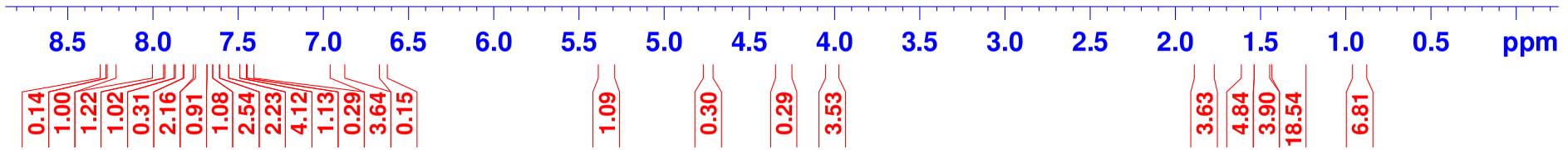


0.14 1.00 1.22 1.02 0.31 2.16 0.91 1.08 2.54 2.23 4.12 1.13 0.29 3.64 0.15

1.09

0.30

0.29

3.53

3.63 4.84 3.90 18.54

6.81

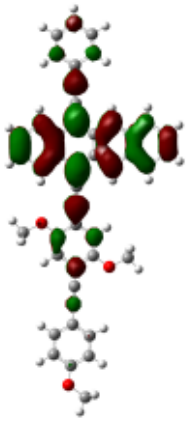
DFT Calculations

Molecular geometries of each molecule studied were determined using sequential geometry optimizations. Within the B3LYP function, the three levels of theory used were 6-31G(d,p), 6-311G(d,p), and 6-311+G(d,p). All geometry optimizations were run in the chloroform PCM with the SCRF method. All molecular orbital and energy calculations were also carried out at the same three levels of theory. All time dependent calculations were carried out with the Tamm-Dancoff approximation, B3LYP functional and 6-31G(d,p) basis set. The calculations resulted in the first 40 electronic transitions of each molecule, starting at long wavelengths. The tables includes only transitions with an oscillator strength (*f*) greater than 0.2. Also, the orbital transitions were only included if they contributed to at least 20 % of the electronic transition. All DFT calculations were carried out in Gaussian 09.

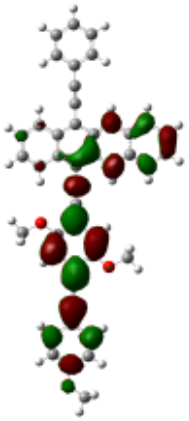
Gaussian 09, R. D., Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

A1

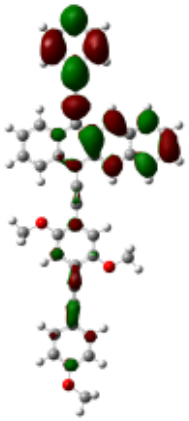
LUMO (163)
E= -2.98983 eV



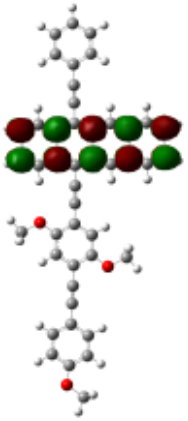
LUMO+1 (164)
E= -1.86249 eV



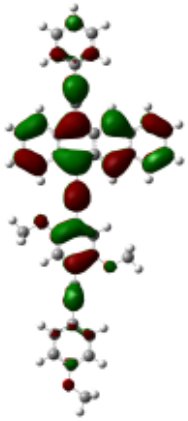
LUMO+2 (165)
E= -1.40132 eV



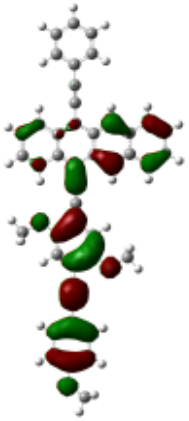
LUMO+3 (166)
E= -0.95482 eV



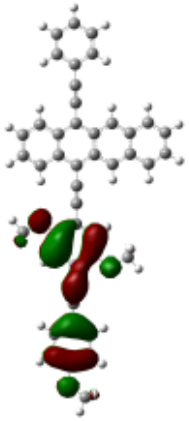
HOMO (162)
E= -5.05975 eV



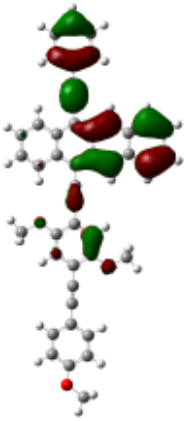
HOMO-1 (161)
E= -5.70856 eV



HOMO-2 (160)
E= -6.32548 eV



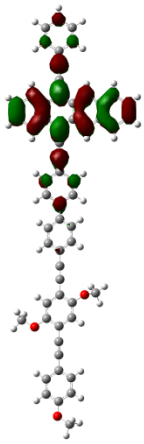
HOMO-3 (159)
E= -6.45909 eV



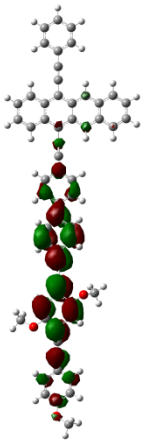
Excited State	Transition	*f*	λ (nm)	E (eV)
1	162→163 (94 %)	1.5942	624.53	1.9852
3	162→164 (79 %)	0.4557	423.61	2.9269
4	159→163 (54 %), 160→163 (25 %)	0.271	409.33	3.0289
5	160→163 (72 %), 159→163 (23 %)	0.2062	407.37	3.0435
7	162→165 (66 %)	0.3056	365.13	3.3956
9	161→164 (58 %), 156→163 (20 %)	0.3148	342.94	3.6153
19	162→166 (35 %), 157→163 (20 %)	0.8129	295.94	4.1895
25	161→166 (59 %)	0.4014	276.14	4.4899
34	157→164 (31 %)	0.848	255.57	4.8512

A2

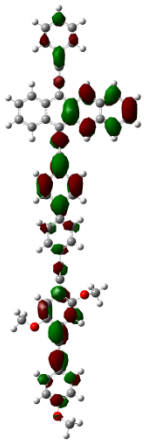
LUMO (209)
E= -3.02202 eV



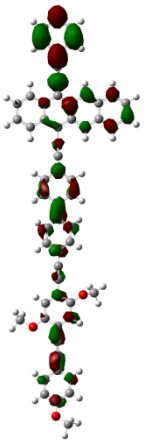
LUMO+1 (210)
E= -2.23998 eV



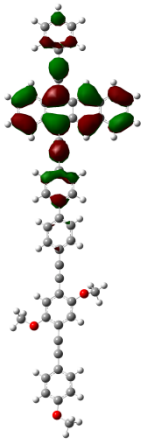
LUMO+2 (211)
E= -1.6287 eV



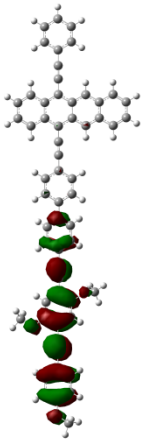
LUMO+3 (212)
E= -1.37803 eV



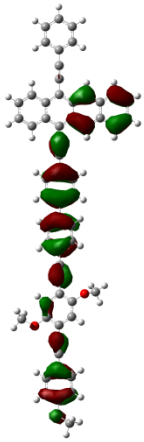
HOMO (208)
E= -5.16429 eV



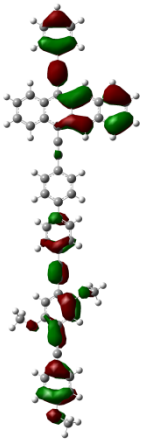
HOMO-1 (207)
E= -5.58023 eV



HOMO-2 (206)
E= -6.26396 eV



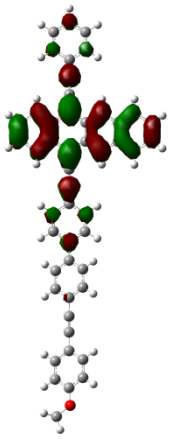
HOMO-3 (205)
E= -6.49949 eV



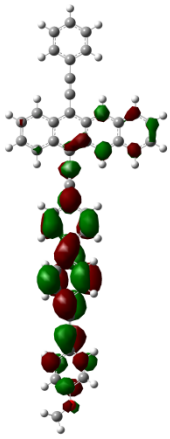
Excited State	Transition	*f*	λ (nm)	E (eV)
1	208→209 (94 %)	1.602	597.68	2.0744
3	208→210 (91 %)	0.2803	454.81	2.7261
4	206→209 (68 %)	0.7195	431.53	2.8731
5	207→210 (62 %)	1.3442	401.64	3.087
6	205→209 (34 %), 207→210 (27 %)	0.3251	392.68	3.1574
13	207→211 (48 %), 206→210 (42 %)	0.3195	331.95	3.735
26	208→217 (33 %), 200→209 (26 %)	0.2772	292.24	4.2426
28	200→209 (30 %), 196→209 (21 %)	0.5375	289.67	4.2802
30	196→209 (43 %)	0.3499	286.38	4.3293
32	203→210 (44 %), 206→211 (30 %)	0.2118	281.13	4.4102

A3

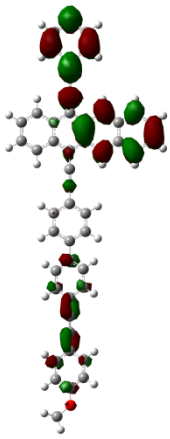
LUMO (167)
E= -3.00934 eV



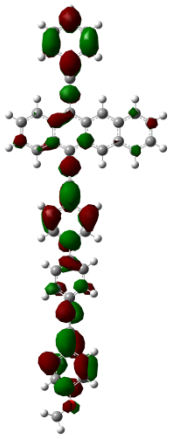
LUMO+1 (168)
E= -1.95686 eV



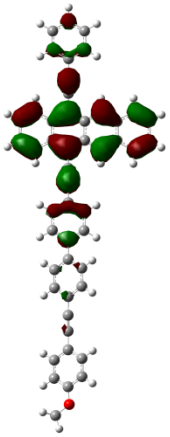
LUMO+2 (169)
E= -1.47637 eV



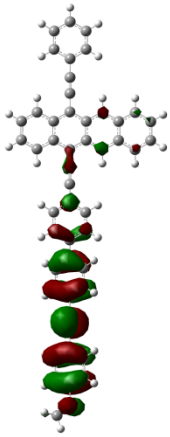
LUMO+3 (170)
E= -1.08301 eV



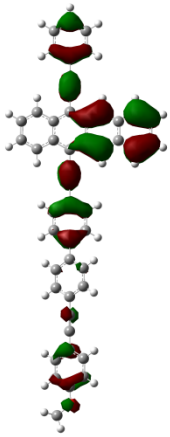
HOMO (166)
E= -5.15403 eV



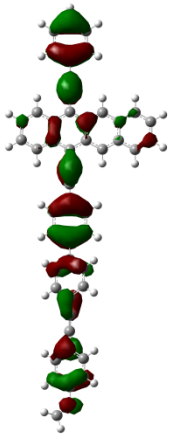
HOMO-1 (165)
E= -5.79109 eV



HOMO-2 (164)
E= -6.39411 eV



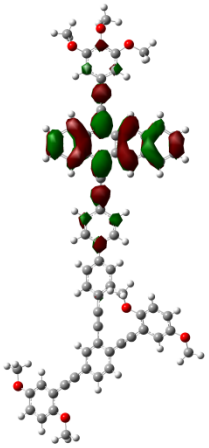
HOMO-3 (163)
E= -6.71247 eV



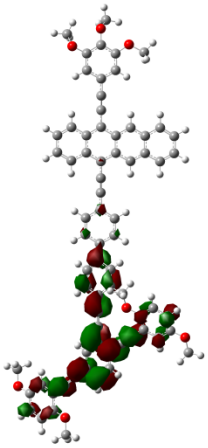
Excited State	Transition	*f*	λ (nm)	E (eV)
1	166→167 (95 %)	1.4116	594.73	2.0847
4	164→167 (50 %), 166→168 (41 %)	0.7166	413.59	2.9978
5	163→167 (58 %), 166→169 (21 %)	0.2786	374.78	3.3082
7	166→169 (58 %), 163→167 (30 %)	0.2782	358.56	3.4579
9	165→168 (86 %)	0.7378	342.65	3.6184
20	164→168 (47 %), 165→169 (21 %)	0.2141	293.23	4.2282
23	166→171 (40 %), 162→167 (27 %)	1.3052	287.33	4.3151
33	164→169 (72 %)	0.3093	265.91	4.6627
38	162→168 (42 %)	0.4421	257.38	4.8171

22

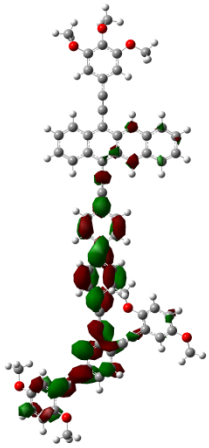
LUMO (267)
E= -3.00398 eV



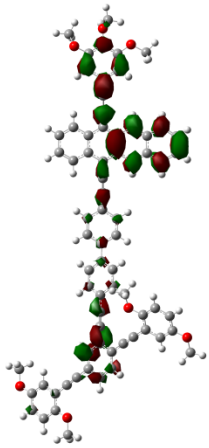
LUMO+1 (268)
E= -2.31827 eV



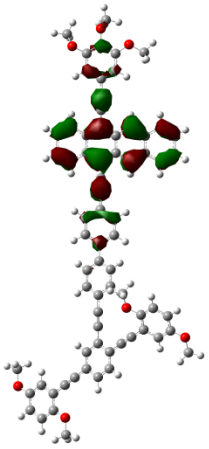
LUMO+2 (269)
E= -1.90336 eV



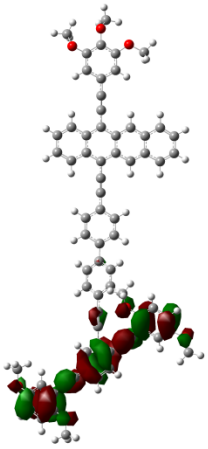
LUMO+3 (270)
E= -1.46339 eV



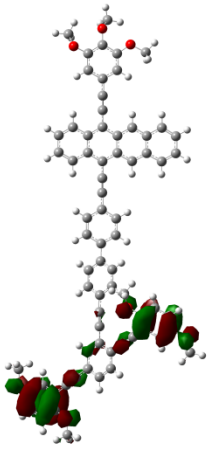
HOMO (266)
E= -5.13444 eV



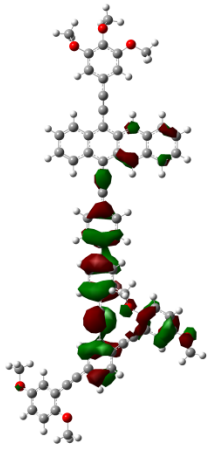
HOMO-1 (265)
E= -5.56864 eV



HOMO-2 (264)
E= -5.88633 eV



HOMO-3 (263)
E= -6.07917 eV



Excited State	Transition	*f*	λ (nm)	E (eV)
1	266→267 (95 %)	1.5128	600.53	2.0646
5	263→267 (51 %), 262→267 (27 %)	0.2657	445.55	2.7827
7	265→268 (91 %)	0.7244	419.04	2.9588
8	266→269 (80 %)	0.6743	409.29	3.0292
13	265→269 (50 %)	0.3836	370.23	3.3488
15	266→270 (47 %), 259→267 (22 %)	0.6439	362.48	3.4204
16	263→268 (61 %)	0.2381	355.22	3.4904
20	261→268 (60 %)	0.3415	328.27	3.7769
23	266→272 (24 %), 263→269 (21 %)	0.2414	318.73	3.8899
24	266→272 (28 %), 265→270 (21 %)	0.3424	317.17	3.909
38	261→269 (30 %), 264→270 (20 %)	0.3382	291.61	4.2518
39	264→270 (64 %)	0.2248	290.1	4.2738