

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 $^1\text{O}_2$ 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

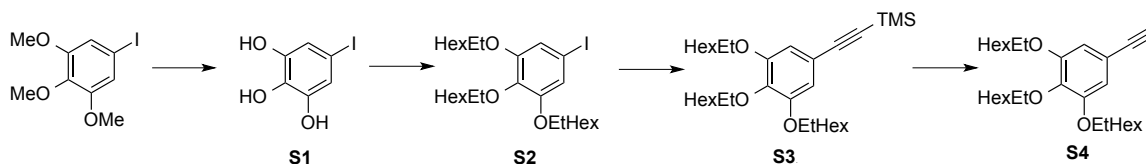
A stock solution of methylene blue was prepared in CHCl_3 to give an absorbance of ~ 1.0 at its peak. 9,10-diphenylanthracene (DPA) was used as a reference. DPA, **A2**, or **P2** was dissolved in 3.5 mL MB solution; the final concentration of the corresponding compound in the sample was 32 μM . The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



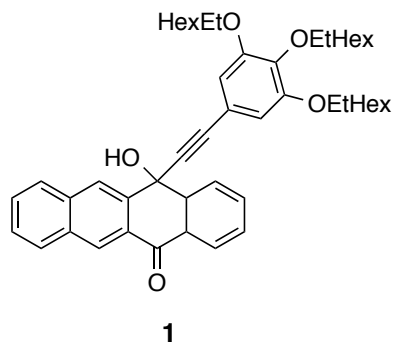
S1. Prepared following the established literature procedure.¹ JACS, 2008, 130 (8), 2535.

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%). 1H 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%). 1H NMR (300 MHz, $CDCl_3$): 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, $CDCl_3$): 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.

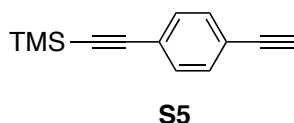
S4. Compound **S3** (940 mg, 1.7 mmol, 1 eq) was dissolved in a mixture of MeOH (17 mL), Et_2O (17 mL) and 10% $NaOH_{(aq)}$ (7 mL). The reaction mixture was stirred overnight at room temperature. The reaction was stopped by acidification with 10% aq

HCl. Organics were extracted twice with Et₂O, and combined organic phases were washed with brine, dried over MgSO₄, 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%). ¹H 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). ¹³C 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.

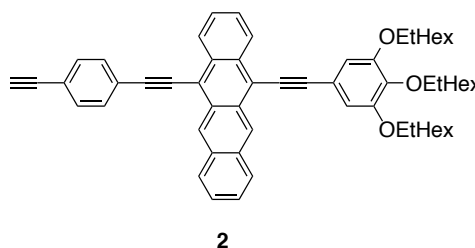
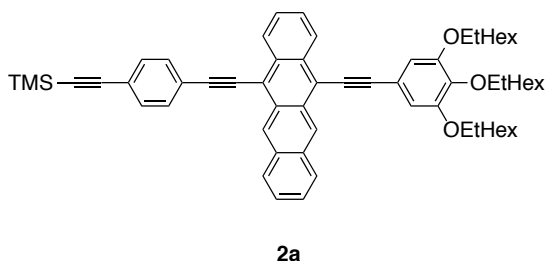


Compound 1.

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 0 °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 H₂O and then filtered via vacuum filtration by washing about 30 mL of THF:H₂O (1:1, v/v). Saturated NH₄Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **1**. Yield: 190 mg (63%). ¹H 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). ¹³C 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. 1-Ethynyl-4-(trimethylsilylethynyl)benzene: Prepared following the established literature procedure.²

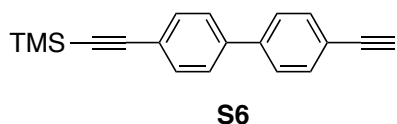


Compound 2.

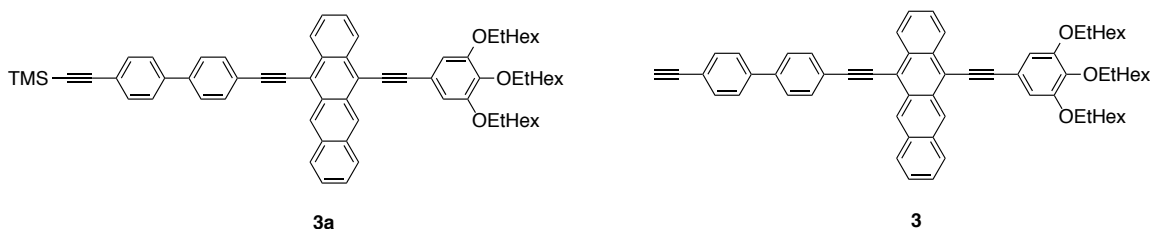
Compound 2a. Compound **1-Ethynyl-4-(trimethylsilylethynyl)benzene** (271 mg, 1.37 mmol, 4eq) was dissolved in 4.3 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.83 mL, 1.33 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 75 minutes and then transferred 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 SnCl₂ dihydrate and left overnight stirring. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, 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%). ¹H 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). ¹³C 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 C₆₃H₇₆O₃Si (M+H)⁺, 909.5636, found, 909.5630.

Compound **2a** (207 mg, 0.23 mmol, 1 eq) and K₂CO₃ (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 CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 180 mg (94%). ¹H 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. Ethynyl-4'-(trimethylsilylethynyl)biphenyl: Prepared following the established literature procedure.³ *Eur. J. Org. Chem.* 2007, 5244–5249.

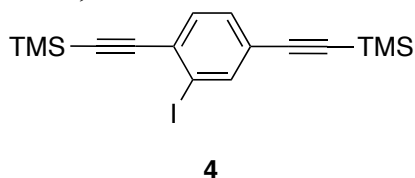


Compound 3.

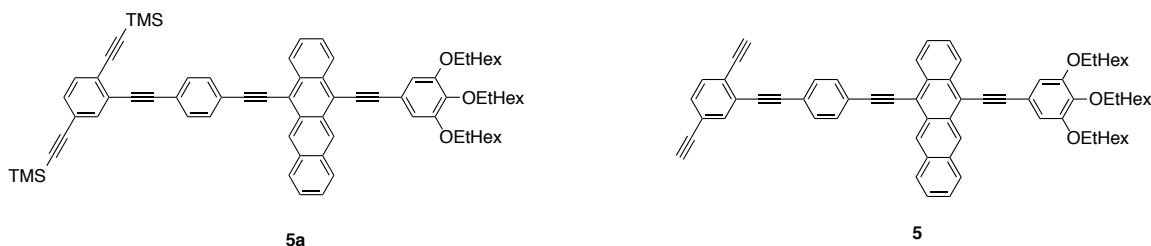
Compound 3a. Compound **4-Ethynyl-4'-(trimethylsilylethynyl)biphenyl** (505 mg, 1.83 mmol, 7eq) was dissolved in 3.2 mL of dry THF, followed by dropwise addition of *n*-butyllithium (1.11 mL, 1.78 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 75 minutes and then transferred 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 SnCl₂ dihydrate and left overnight stirring. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, 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%). ¹H 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). ¹³C 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 K₂CO₃ (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 CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was used without further purification. Yield: 159 mg (94%). ¹H 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). ¹³C 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 C₆₆H₇₂O₃ (M+H)⁺, 913.5554, found, 913.5566



Compound 4. Prepared following the established literature procedure.⁴

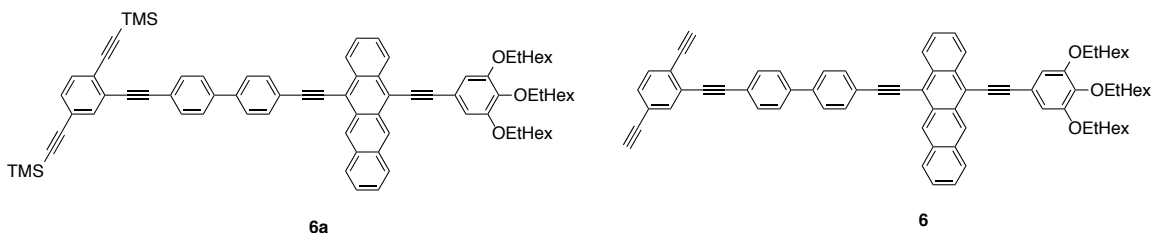


Compound 5.

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(PPh₃)₂Cl₂ (3 mg, 4.3 μ mol, 0.02 eq) and CuI (1.7 mg, 8.6 μ mol, 0.04 eq) and evacuated and refilled with argon three times. In another flask, 11 mL of deoxygenated Et₃N: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%). ¹H 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). ¹³C 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 K₂CO₃ (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 CH₂Cl₂, and combined organic phases were washed with H₂O 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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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 $\text{C}_{70}\text{H}_{72}\text{O}_3$ ($\text{M}+\text{H}$) $^+$, 961.5554, found, 961.5554.

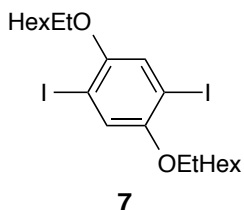


Compound 6.

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), $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (2.4 mg, 3.4 μmol , 0.02 eq) and CuI (1.3 mg, 6.8 μmol , 0.04 eq) and evacuated and refilled with argon three times. In another flask, 10 mL of deoxygenated $\text{Et}_3\text{N}:\text{THF}$ (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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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.

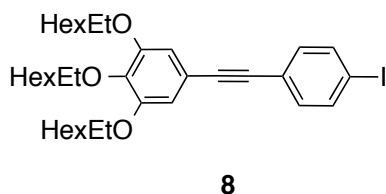
Compound **6a** (105 mg, 0.09 mmol, 1 eq) and K_2CO_3 (104 mg, 0.75 mmol, 8.4 eq) were dissolved in mixture of THF (1.5 mL), and MeOH (3 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2 , and combined 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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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.



Compound 7. Prepared following the established literature procedure.⁵

3b. Synthesis of P3:



Compound 8.

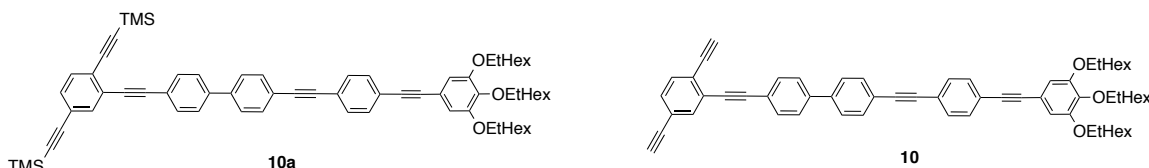
A round bottom flask was charged with **3,4,5-triethylhexyloxyethynylbenzene** (652 mg, 1.34 mmol, 1 eq), **1,4-diiodobenzene** (1.33 g, 4 mmol, 3 eq), $\text{Pd}(\text{PPh}_3)_4$ (46 mg, 0.04 mmol, 0.03 eq) and CuI (15 mg, 0.08 mmol, 0.06eq) and evacuated and refilled with argon three times. In another 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°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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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.



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(PPh₃)₂Cl₂ (5 mg, 6.8 μ mol, 0.02 eq) and CuI (2.6 mg, 13.6 μ mol, 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 Et₃N: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%). ¹H 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). ¹³C 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 K₂CO₃ (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 CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, 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%). ¹H 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). ¹³C 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 C₅₄H₆₆O₃ (M+H)⁺, 763.5085, found, 763.5081.



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(PPh₃)₂Cl₂ (3.6 mg, 5.1 μ mol, 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 Et₃N: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%). ¹H 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). ¹³C 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%). 1H NMR (500 MHz, $CDCl_3$): 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, $CDCl_3$): 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.

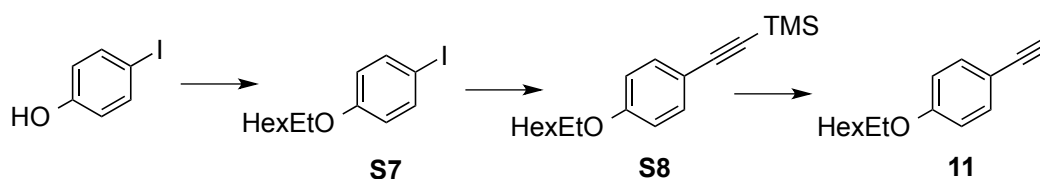
P1. A Schlenk tube was charged with <1 mg $Pd(PPh_3)_4$, and <1 mg CuI, and evacuated and refilled with argon three times. **5** (19.5 mg, 0.02 mmol, 1 eq) and **7** (12 mg, 0.02 mmol, 1 eq) was dissolved in 2.5 mL 4:1 (v:v) toluene:diisopropylamine and sparged with argon for 30 minutes. The solution was added to the reaction vessel and the mixture stirred for 72 hours at room temperature. 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%) 1H NMR (500 MHz, $CDCl_3$): 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 temperature. 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%) 1H NMR (500 MHz, $CDCl_3$): 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%) ¹H 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

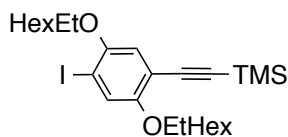


S7. 4-iodophenol (9 g, 0.04 mol, 1.0 eq), KOH (2.35 g, 0.04 mol, 1 eq) and KI (180 mg, 0.8 mmol, 0.02 eq) were dissolved in 102 mL of dry EtOH at room temperature under argon. 2-ethylhexylbromide (8.1 mL, 0.045 mmol, 1.1 eq) was then added to this solution under an argon atmosphere. The mixture was heated 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 CH₂Cl₂. Organic phase were washed with water and brine, dried over MgSO₄, 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(PPh₃)₂Cl₂ (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 Et₃N 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), Et₂O (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 Et₂O, and combined organic phases were washed with brine, dried over MgSO₄, 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%). ¹H and ¹³C NMR is in good

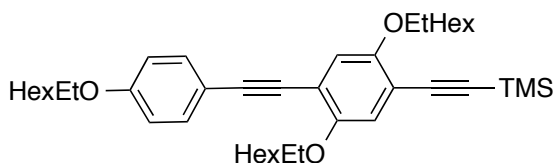
agreement with the same compound reported in the literature.⁶ *Macromol. Rapid Commun.* 2015, 36, 31–37.



12

Compound 12.

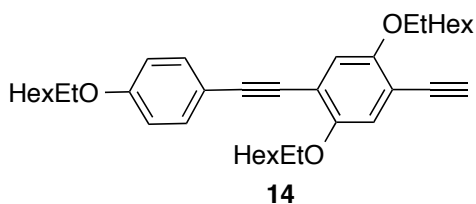
A round bottom flask was charged with $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (39 mg, 0.06 mmol, 0.09 eq) and CuI (6 mg, 1 mmol, 0.05 eq) and evacuated and refilled with argon three times. In another flask, **XX** (1.11 g, 18.8 mmol, 1 eq) was dissolved in 15 mL of Et_3N and this solution was added to 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

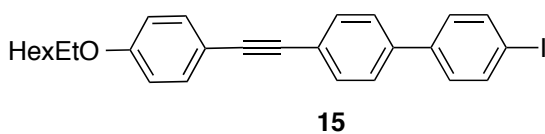
Compound 13.

A round bottom flask was charged with $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (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 $\text{Et}_3\text{N}:\text{THF}$ (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, CDCl_3): 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, CDCl_3): 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.



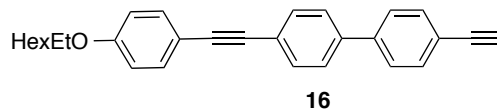
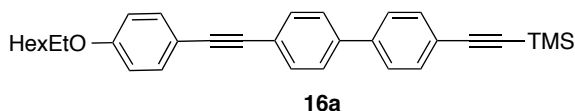
Compound 14.

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%). 1H NMR (500 MHz, $CDCl_3$): 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, $CDCl_3$): 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.



Compound 15.

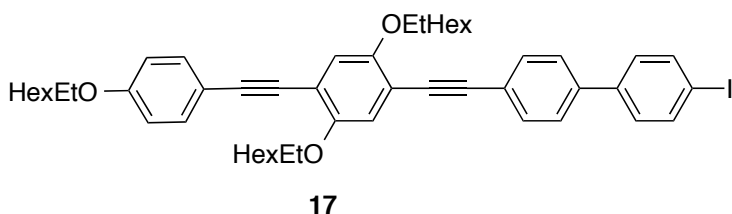
A round bottom flask was charged with $Pd(PPh_3)_4$ (78 mg, 0.06 mmol, 0.03 eq) and CuI (26 mg, 0.12 mmol, 0.06 eq) and evacuated and refilled with argon three times. In another flask, **11** (500 mg, 2.18 mmol, 1 eq) and 4,4'-diiodophenyl (2.64 g, 6.52 mmol, 3 eq) were dissolved in 80 mL of Et_3N :Toluene(1:5, 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 $^{\circ}C$. 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%). 1H NMR (500 MHz, $CDCl_3$): 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, 2H), 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, $CDCl_3$): 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.



Compound 16.

Compound 16a. A round bottom flask was charged with $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (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 $\text{Et}_3\text{N}:\text{THF}$ (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 μL , 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%). ^1H NMR (300 MHz, CDCl_3): 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, CDCl_3): 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.

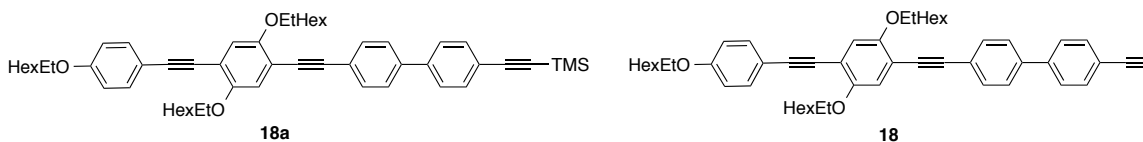
Compound **16a** (129 mg, 0.26 mmol, 1 eq) and K_2CO_3 (106 mg, 0.77 mmol, 3 eq) were dissolved in mixture of THF (1 mL), and MeOH (2 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2 , and combined organic 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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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 $\text{C}_{30}\text{H}_{30}\text{O}$ ($\text{M}+\text{H}$) $^+$, 407.2369, found, 407.2367.



Compound 17.

A round bottom flask was charged with $\text{Pd}(\text{PPh}_3)_4$ (9 mg, 7.9 μmol , 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 $\text{Et}_3\text{N}:\text{Toluene}$ (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 $^\circ\text{C}$. 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%). ^1H NMR (500 MHz, CDCl_3): 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-

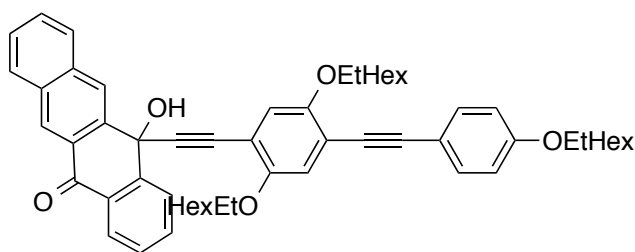
0.91 (m, 18H). ^{13}C NMR (125 MHz, CDCl_3): δ 159.5, 153.9, 153.7, 139.9, 139.6, 137.9, 132.9, 132, 128.8, 126.7, 123.1, 116.7, 116.5, 115.4, 114.7, 114.6, 113.3, 95.2, 94.3, 93.4, 87.3, 84.6, 72.1, 72, 70.6, 39.7, 39.4, 30.71, 30.69, 30.53, 29.2, 29.1, 24.06, 24.04, 23.88, 23.09, 23.04, 14.09, 14.06, 11.29, 11.11.



Compound 18.

Compound 18a. A round bottom flask was charged with $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (2 mg, 3.2 μmol , 0.02 eq) and CuI (1 mg, 6.4 μmol , 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 $\text{Et}_3\text{N}:\text{THF}(1:3, \text{v/v})$ and this solution was added to flask containing catalysts via cannula transfer after deoxygenating for 1 hour with argon. While stirring, TMSA (40 μL , 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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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.

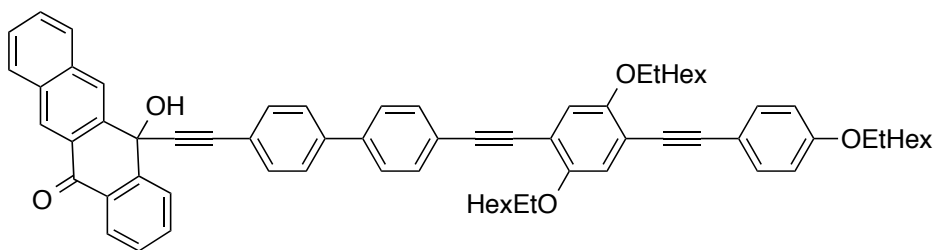
Compound **18a** (121 mg, 0.15 mmol, 1 eq) and K_2CO_3 (60 mg, 0.45 mmol, 3 eq) were dissolved in mixture of THF (1 mL), and MeOH (2 mL). The reaction mixture was stirred overnight at room temperature. The solvent was removed *in vacuo*. Organics were extracted twice with CH_2Cl_2 , and combined organic 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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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 $\text{C}_{54}\text{H}_{66}\text{O}_3$ ($\text{M}+\text{H}$) $^+$, 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 0 °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 H₂O and then filtered via vacuum filtration by washing about 20 mL of THF:H₂O (1:1, v/v). Saturated NH₄Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **19**. Yield: 117 mg (54%). ¹H 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). ¹³C 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.

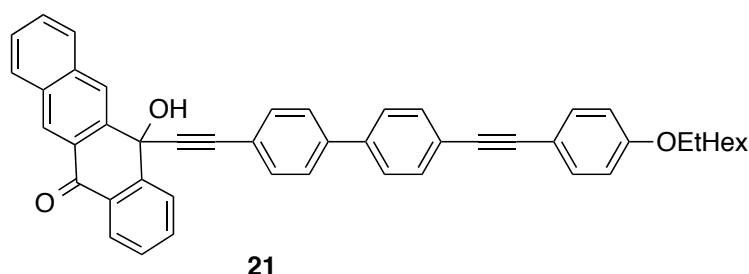


20

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

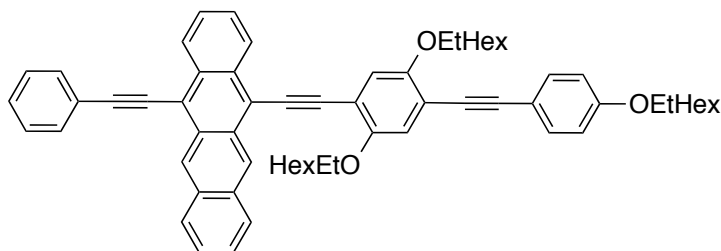
°C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing 5,12- naphthacenequinone (69 mg, 0.27 mmol, 1 eq), which was dissolved in 1.2 mL of dry THF and cooled to 0 °C, dropwisely via syringe. Upon completion of transfer, the reaction mixture was allowed to warm to room temperature and stirred overnight under argon. The reaction was quenched by addition of 5 mL of ice cold DI H₂O and then filtered via vacuum filtration by washing about 30 mL of THF:H₂O (1:1, v/v). Saturated NH₄Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **20**. Yield: 150 mg (55%). ¹H 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). ¹³C 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.



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 0 °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 H₂O and then filtered via vacuum filtration by washing about 20 mL of THF:H₂O (1:1, v/v). Saturated NH₄Cl was added to filtrate and let it stir for 30 min. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using pure dichloromethane to yield **21**. Yield: 100 mg (45%). ¹H 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,

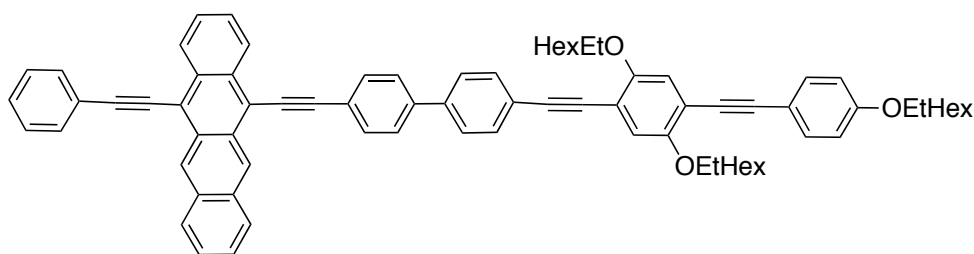
12H), 6.9 (d, $J=8.8$ Hz, 2H), 3.89-3.87 (m, 2H), 3.61 (s, 1H), 1.78-1.73 (m, 1H), 1.56-1.29 (m, 8H), 0.98-0.93 (m, 6H). ^{13}C NMR (125 MHz, CDCl_3): δ 183.7, 159.8, 144.3, 140.9, 139.5, 136.1, 134.5, 133.2, 132.9, 132.5, 132.1, 130.2, 130, 129.7, 129.4, 129.1, 128.4, 128.3, 127.9, 127.7, 127.5, 127.4, 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.

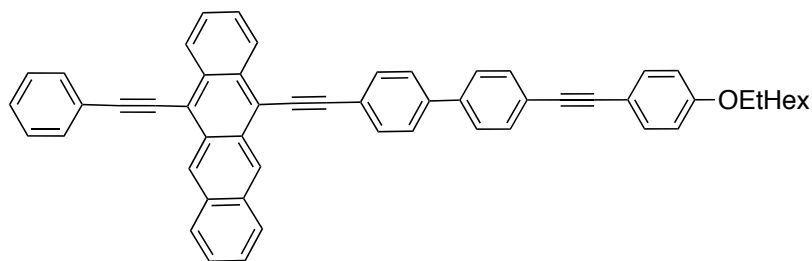
Phenylacetylene (51 mg, 0.50 mmol, 4 eq) was dissolved in 1 mL of dry THF, followed by dropwise addition of *n*-butyllithium (0.3 mL, 0.48 mmol, 1.6 M in hexanes) at -78 °C. The reaction mixture was stirred at -78 °C for 1 hour and then transferred to the flask containing **20** (105 mg, 0.12 mmol, 1 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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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 $\text{C}_{66}\text{H}_{72}\text{O}_3$ (M^+), 912.5476, found, 912.5493.



A2

A2.

Phenylacetylene (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 SnCl₂ dihydrate and left overnight stirring. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, filtered and concentrated using rotary evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (2.75:1) to yield **A2**. ¹H 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). ¹³C 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 C₈₀H₈₀O₃ (M+H)⁺, 1089.6180, found, 1089.6184



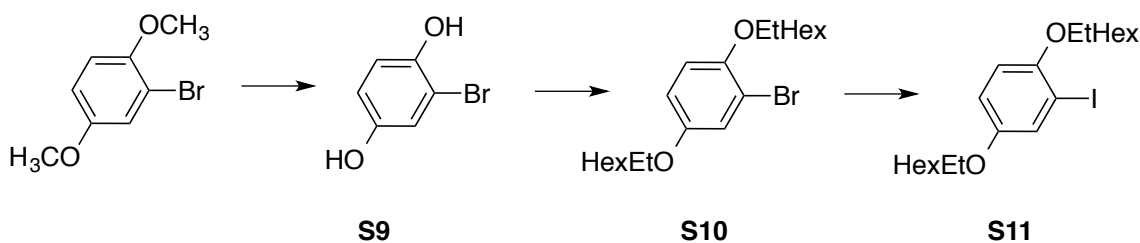
A3

A3.

Phenylacetylene (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 SnCl₂ dihydrate and left overnight stirring. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, 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%). ¹H 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). ¹³C 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 C₅₆H₄₄O (M)⁺, 732.3387, found, 732.3377

3d. Synthesis of Compound 22

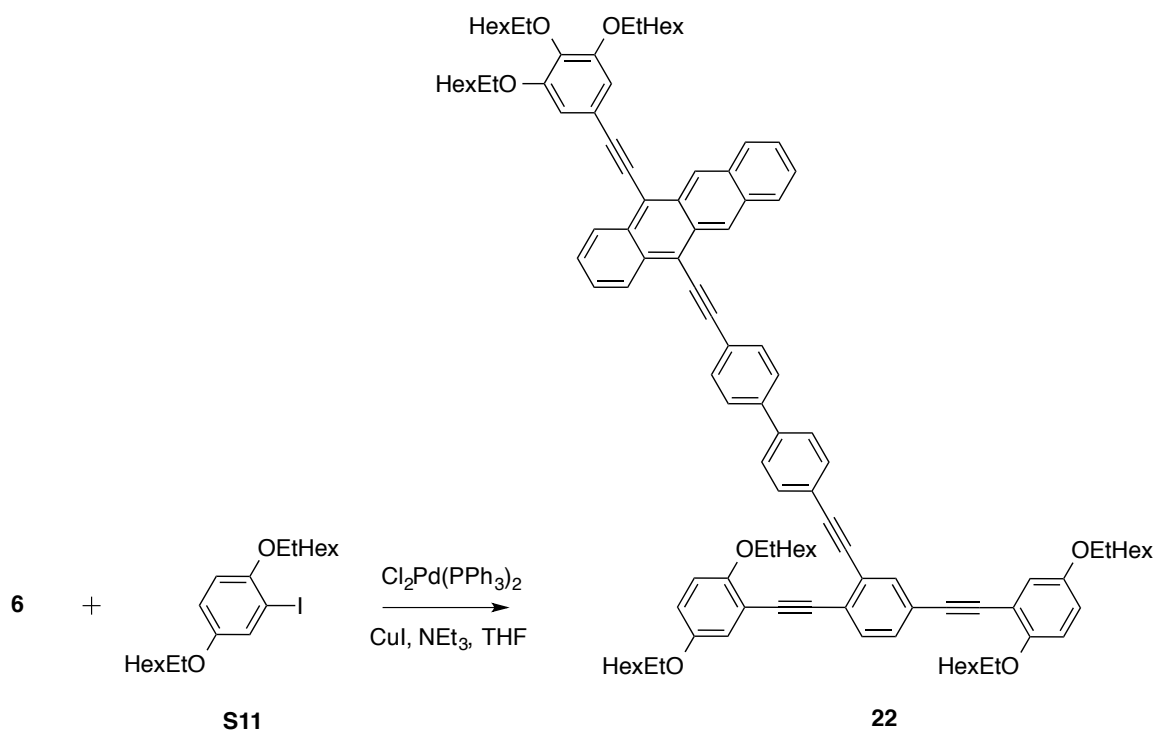


S9. Compound **1-bromo-2,5-dimethoxybenzene** (800 mg, 3.7 mmol, 1.0 eq) was suspended in 4 mL of dry CH₂Cl₂, followed by the addition of BBr₃ (11 mL, 1.0 M in CH₂Cl₂, 11 mmol, 3 eq) at -78 °C under argon and stirred overnight at room temperature. The reaction was stopped by pouring the reaction mixture onto ice. Organics were extracted twice with CH₂Cl₂, 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. ¹H 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 K₂CO₃ (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 CH₂Cl₂, and combined organic phases were washed with brine, dried over MgSO₄, filtered and concentrated using rotary

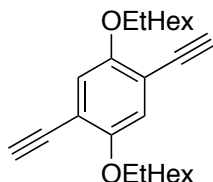
evaporation. The crude product was purified *via* flash chromatography using hexanes and dichloromethane (9:1) to yield **S10**. Yield: 812 mg (58%). ¹H NMR (500 MHz, CDCl₃): δ 7.14 (m, 1H), 6.85-6.8 (m, 2H), 3.87-3.85 (m, 2H), 3.81-3.79 (m, 2H), 1.78-1.69 (m, 1H), 1.61-1.58 (m, 1H), 1.56-1.33 (m, 16H), 0.98-0.92 (m, 12H). ¹³C 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 I₂ (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 Na₂S₂O₃. Organics were extracted twice with CH₂Cl₂, and combined organic phases were washed with H₂O and brine, dried over MgSO₄, 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%). ¹H 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). ¹³C 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.



A round bottom flask was charged with $\text{Pd}(\text{PPh}_3)_2\text{Cl}_2$ (0.5 mg, 0.67 μmol , 0.02 eq), CuI (0.3 mg, 1.4 μmol , 0.04 eq) and **6** (35 mg, 33.7 μmol , 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 $\text{Et}_3\text{N}:\text{THF}$ (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%). ^1H NMR (500 MHz, CDCl_3): 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, CDCl_3): 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 $\text{C}_{120}\text{H}_{148}\text{O}_7$ (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(PPh₃)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 temperature. 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. ¹H 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).

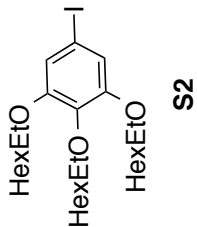
References:

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7. Nojima, M.; Ohta, Y.; Yokozawa, T. *Journal of Polymer Science, Part A: Polymer Chemistry*, 2014, *52*, 2643-2653.

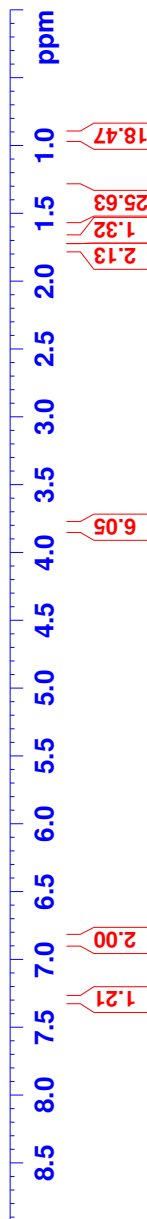


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FIDRES 0.152588 Hz
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RG 203
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NAME ek-2-100

EXPNO 11

PROCNO 1

Date_ 20150508

Time_ 13.31

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PULPROG zgpg30

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SOLVENT CDCl3

NS 2398

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FIDRES 0.454131 Hz

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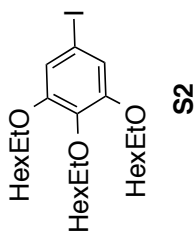
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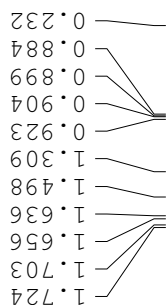
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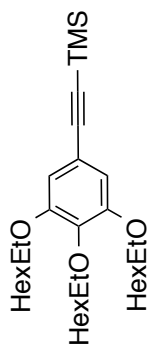


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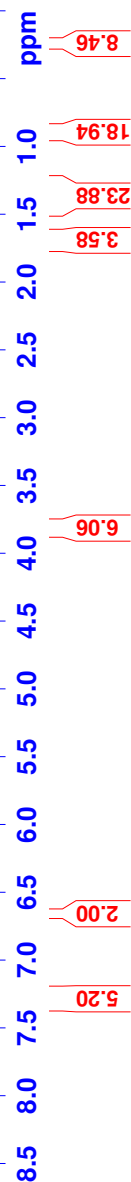
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S3





NAME
ek-2-040

EXPNO
2

PROCNO
1

Date_
20131021

Time
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spect

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TD
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AQ
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RG
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DW
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DE
6.50 usec

TE
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D1
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D11
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TD0
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P1
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PL1
0.00 dB

PL1W
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SFO1
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waltz16

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1H

PCPD2
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P12
1.00 dB

PL12
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PL13
16.80 dB

PL12W
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PL12W
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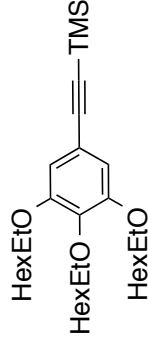
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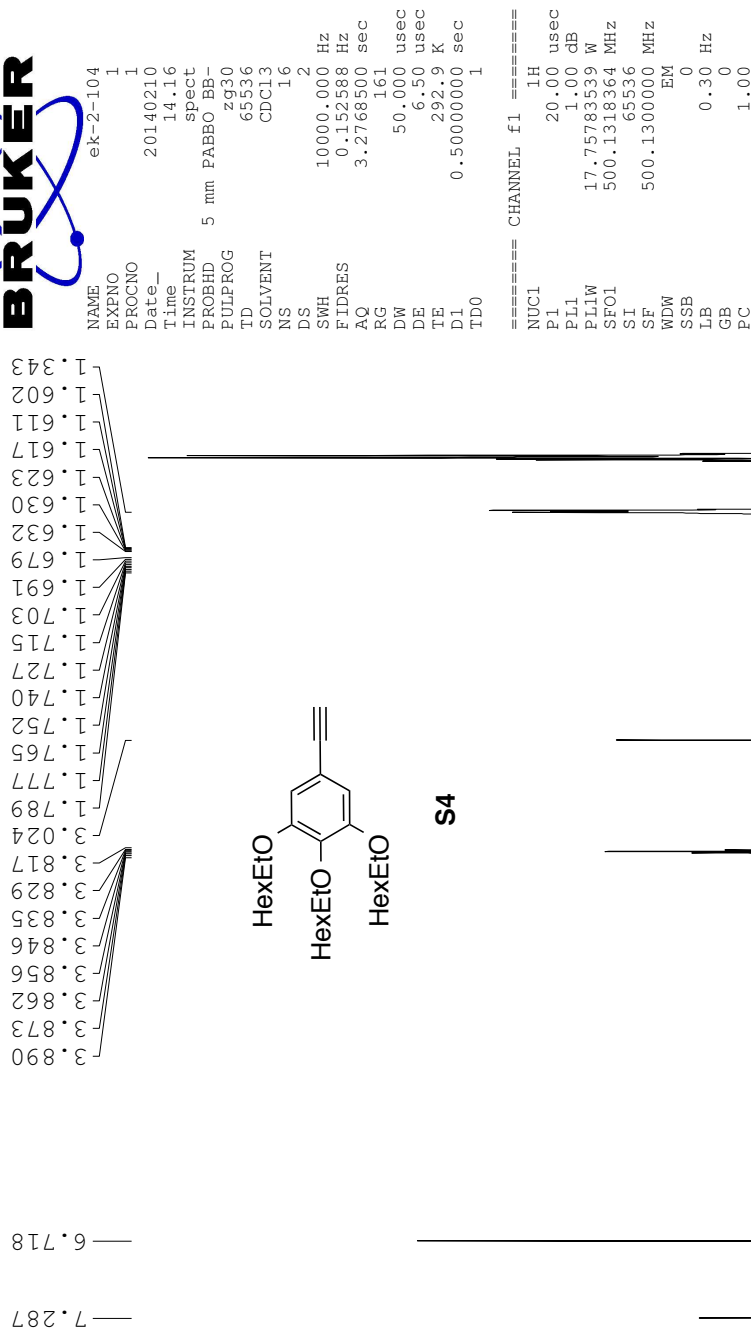
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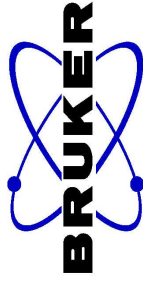
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S3

ppm





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PROCNO 1
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FIDRES 0.454131 Hz
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D11 0.03000000 sec
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SFO1 125.7703643 MHz

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PL12W 17.75783539 W
PL12W 1.11017132 W
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GB 0
PC 1.40

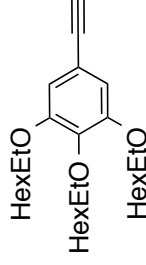
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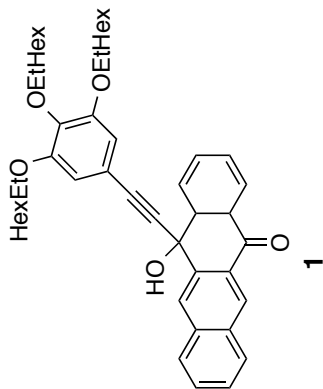


S4

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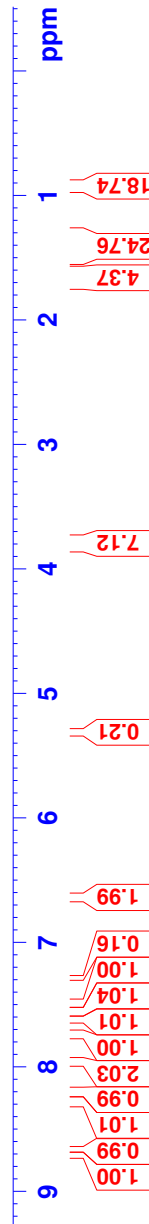


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PROCNO 1
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PULPROG zg30
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SOLVENT CDCl3
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TD0 1

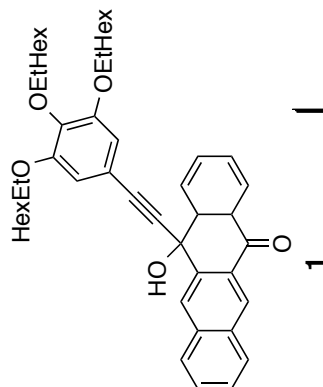
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PROCNO 1
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PL13 16.80 dB
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PL12W 1.11017132 W
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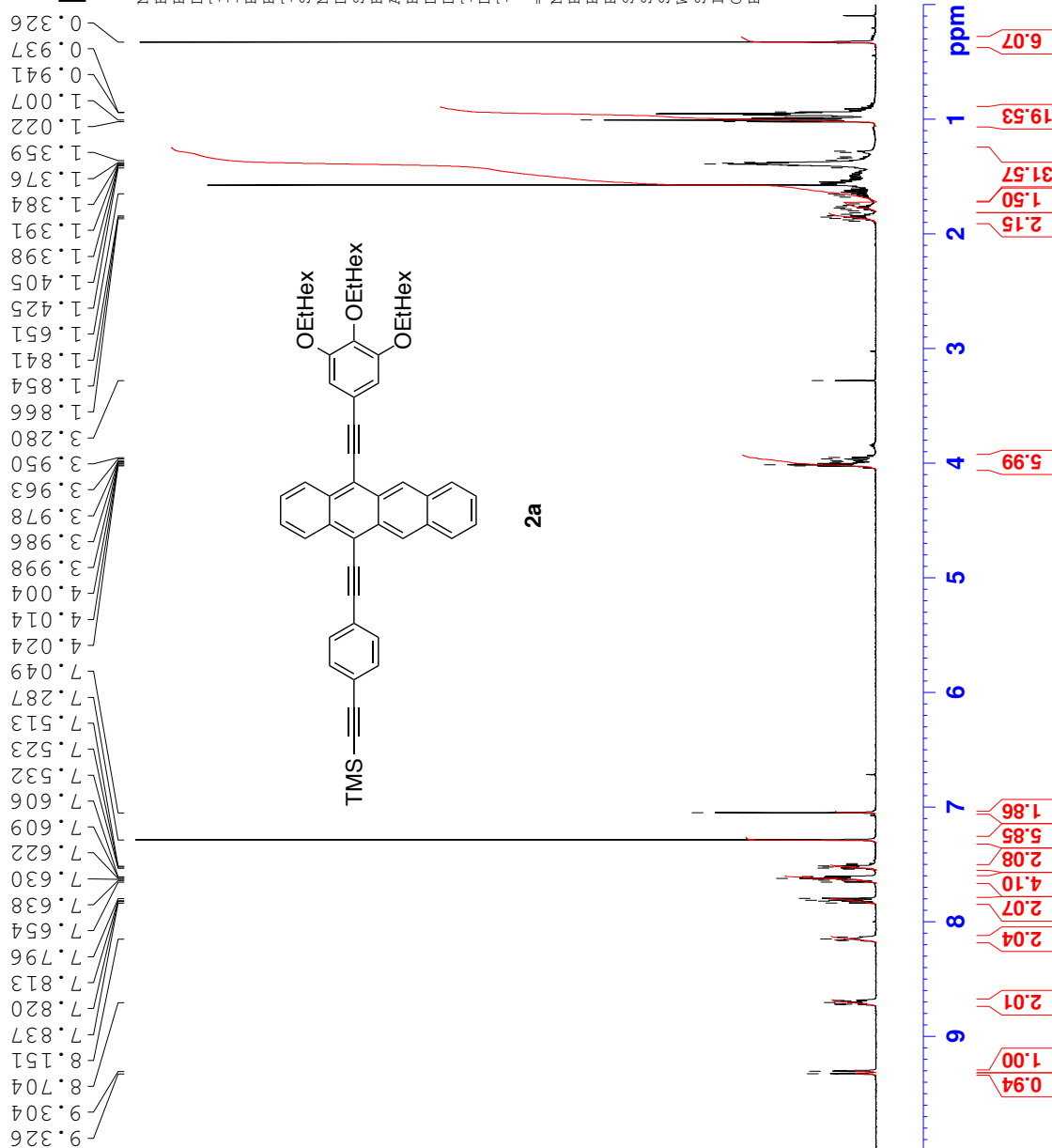
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11.16
11.07

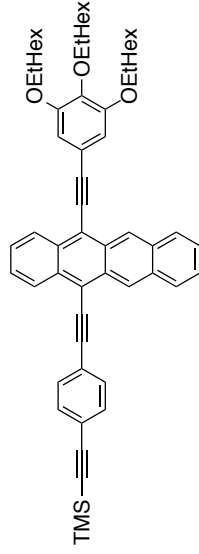
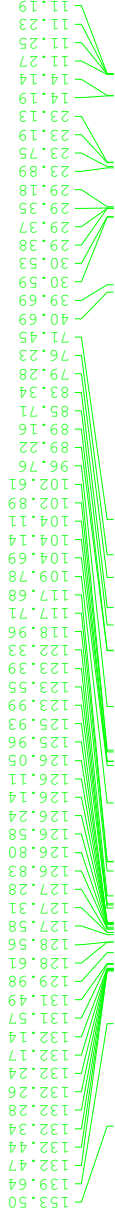
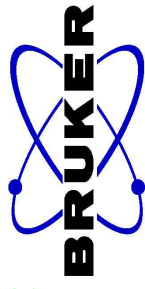


ppm



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 0.5000000 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
PL12W 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
DE 80.400 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

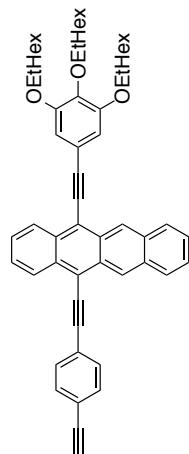
F2 - Processing parameters
SI 32768
SF 300.3400067 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

0.915
0.943
0.993
1.243
1.357
1.540
1.739
1.820

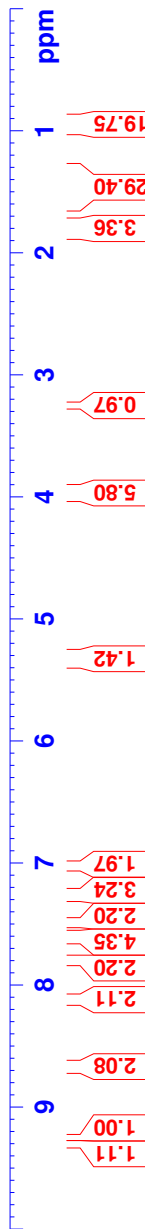
3.244
3.932
3.971
3.986

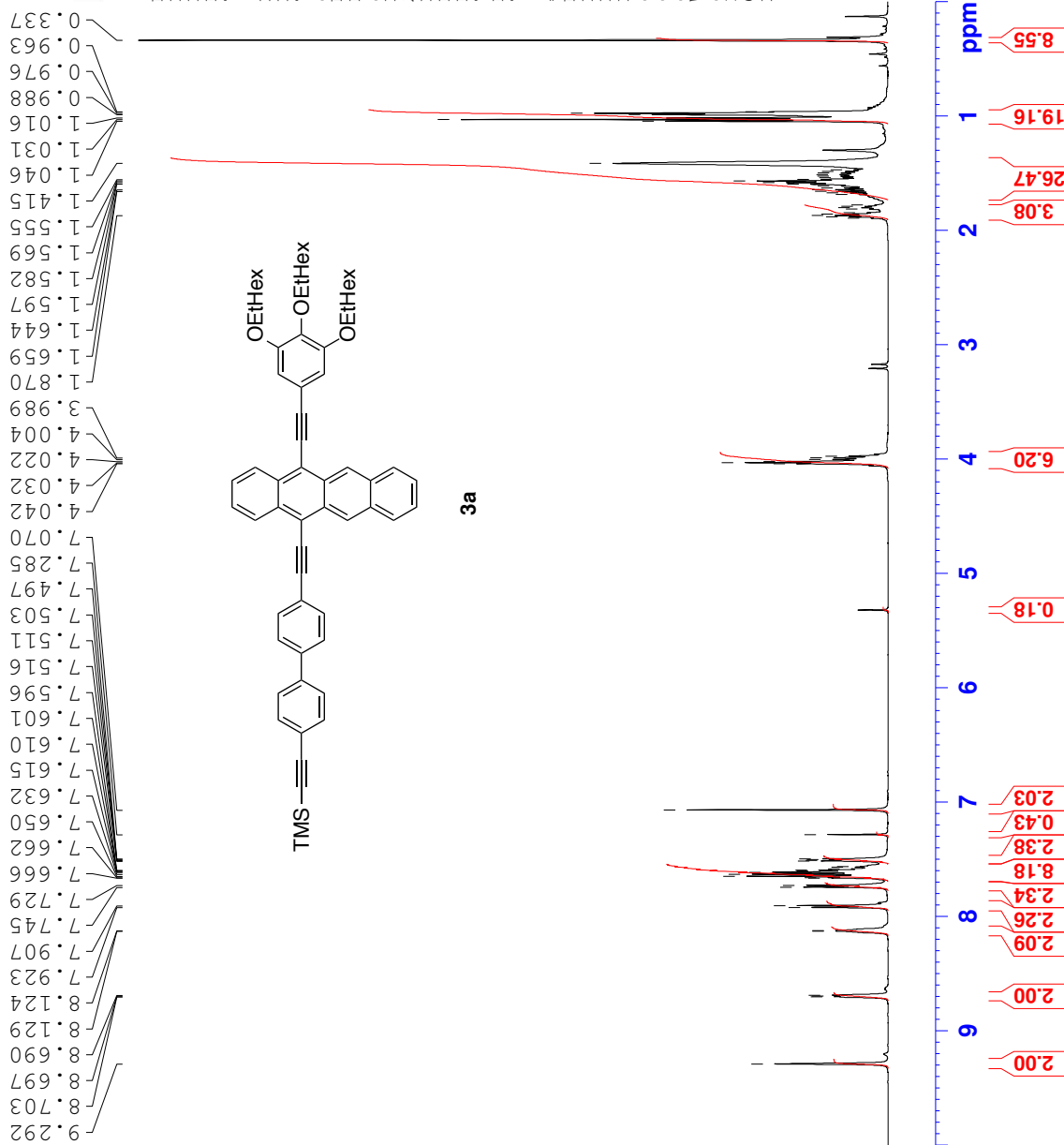
7.013
7.249
7.501
7.598
7.621
7.777
7.803
8.121

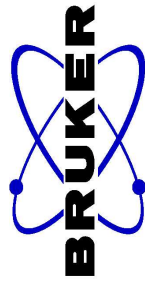
9.286
9.258



2



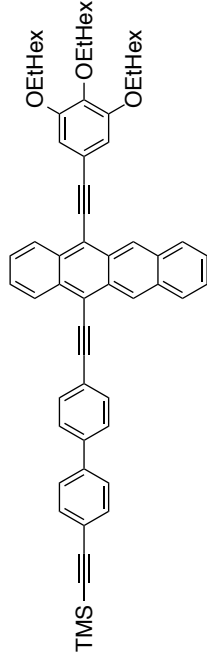




NAME ek-2-053
EXPNO 7
PROCNO 1
Date_ 20131108
Time 13.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1069
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.3 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 0.00 dB
PL1W 89.92553711 W
SF01 125.7703643 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
P12 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL1W 17.75783539 W
PL12W 1.11017132 W
PL13W 0.46707872 W
SF02 500.1320005 MHz
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

40.72
39.73
30.62
30.57
29.39
29.20
23.92
23.79
23.20
23.15
14.19
14.14
11.27
11.21
0.02

153.52
140.43
140.20
139.69
132.73
132.65
132.57
132.37
132.28
132.21
132.13
129.99
129.97
128.63
128.56
127.54
127.38
127.15
127.12
126.92
126.89
126.79
126.66
126.53
126.17
126.02
125.98
122.87
122.62
118.69
117.97
117.81
109.86
104.90
104.00
103.12
95.39
88.29
85.83
77.28
77.03
76.77
76.25
71.52



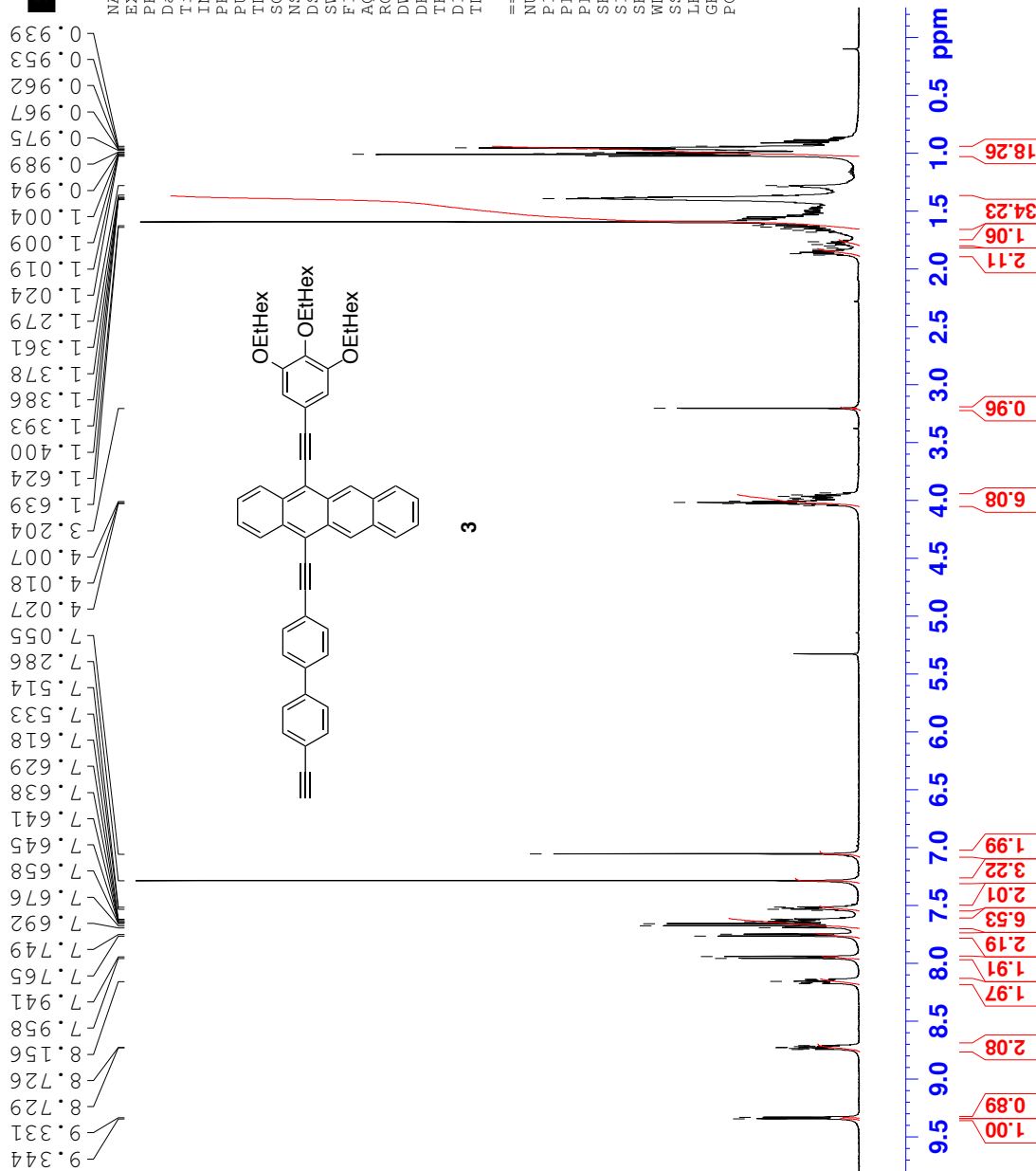
3a

ppm



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 0.5000000 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
EM 0
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





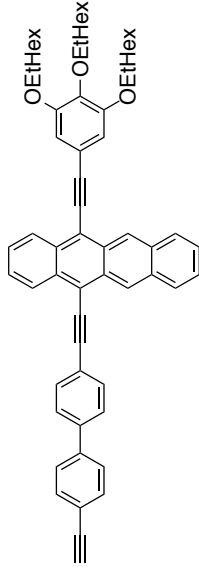
NAME ek-2-112
EXPNO 6
PROCNO 1
Date_ 20150512
Time 15.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 5789
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 292.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

===== 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
P2 1.00 dB
PL2 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

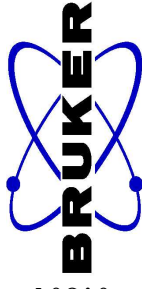
40.83
39.83
30.73
30.68
29.51
29.32
24.03
23.89
23.33
23.28
14.33
14.28
11.39
11.37
11.34

153.64
140.77
140.56
139.75
132.88
132.56
132.46
132.40
132.37
132.30
130.17
128.76
128.71
127.72
127.54
127.35
127.09
126.89
126.74
126.37
126.23
126.19
123.08
121.69
118.90
118.10
117.87
109.92
104.15
103.20
88.41
85.87
83.59
78.30
77.41
77.16
76.91
76.37
71.59



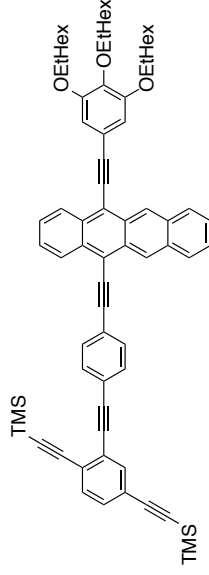
3

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



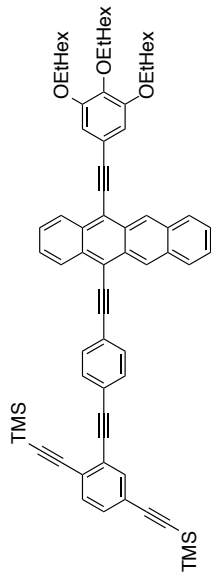
NAME ek-2-127
EXPNO 2
PROCNO 1
Date_ 20140317
Time_ 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 144
DW 50.000 usec
DE 6.50 usec
TE 293.6 K
D1 0.50000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 20.00 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

9.313
9.295
7.870
7.854
7.722
7.719
7.701
7.685
7.632
7.612
7.533
7.516
7.509
7.493
7.416
7.413
7.397
7.287
7.059
4.035
4.025
4.015
1.586
1.577
1.559
1.417
1.410
1.402
1.395
1.388
1.033
1.029
1.019
1.014
1.004
1.000
0.986
0.976
0.972
0.963
0.958
0.949
0.358
0.304

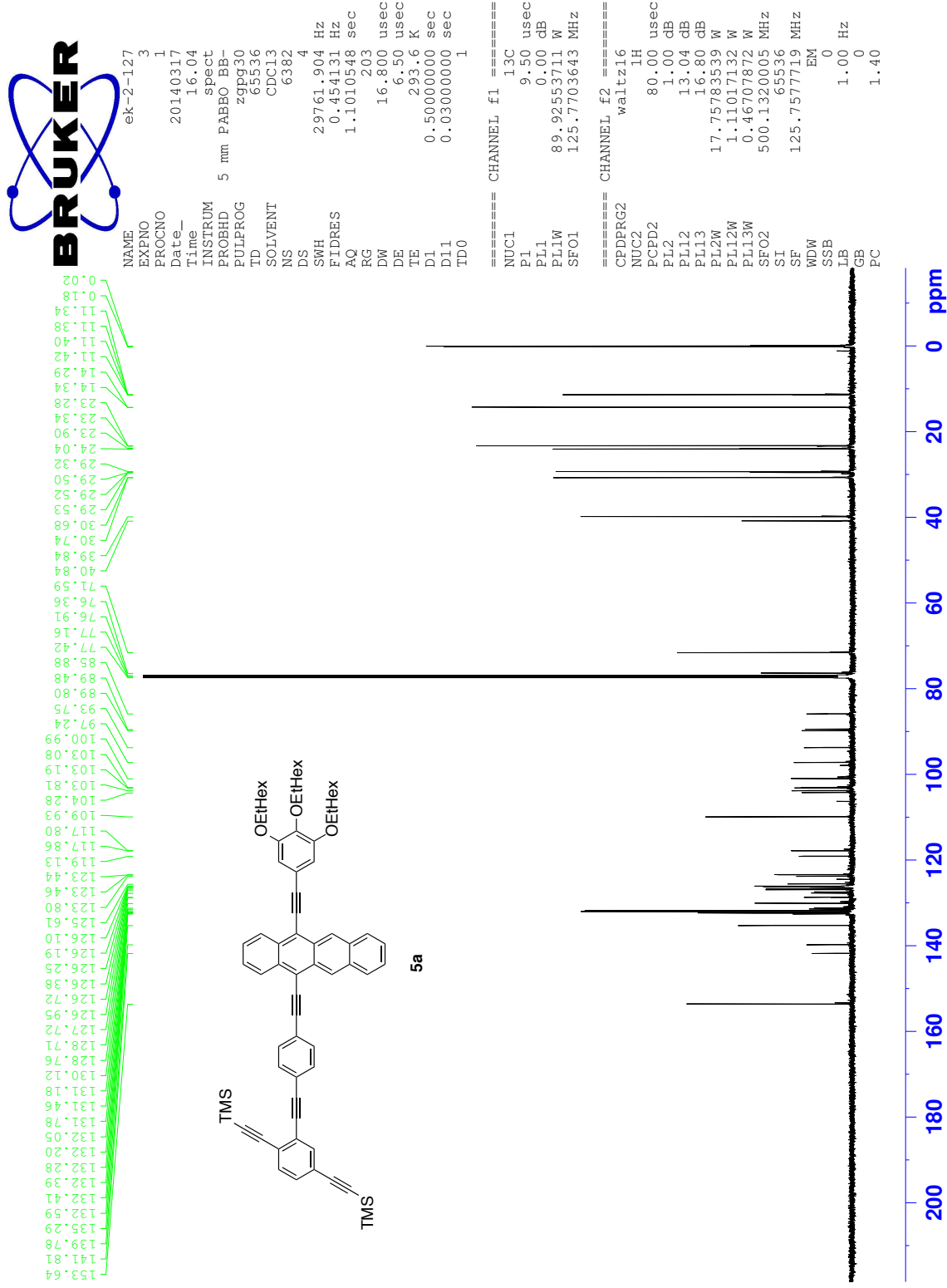


5a



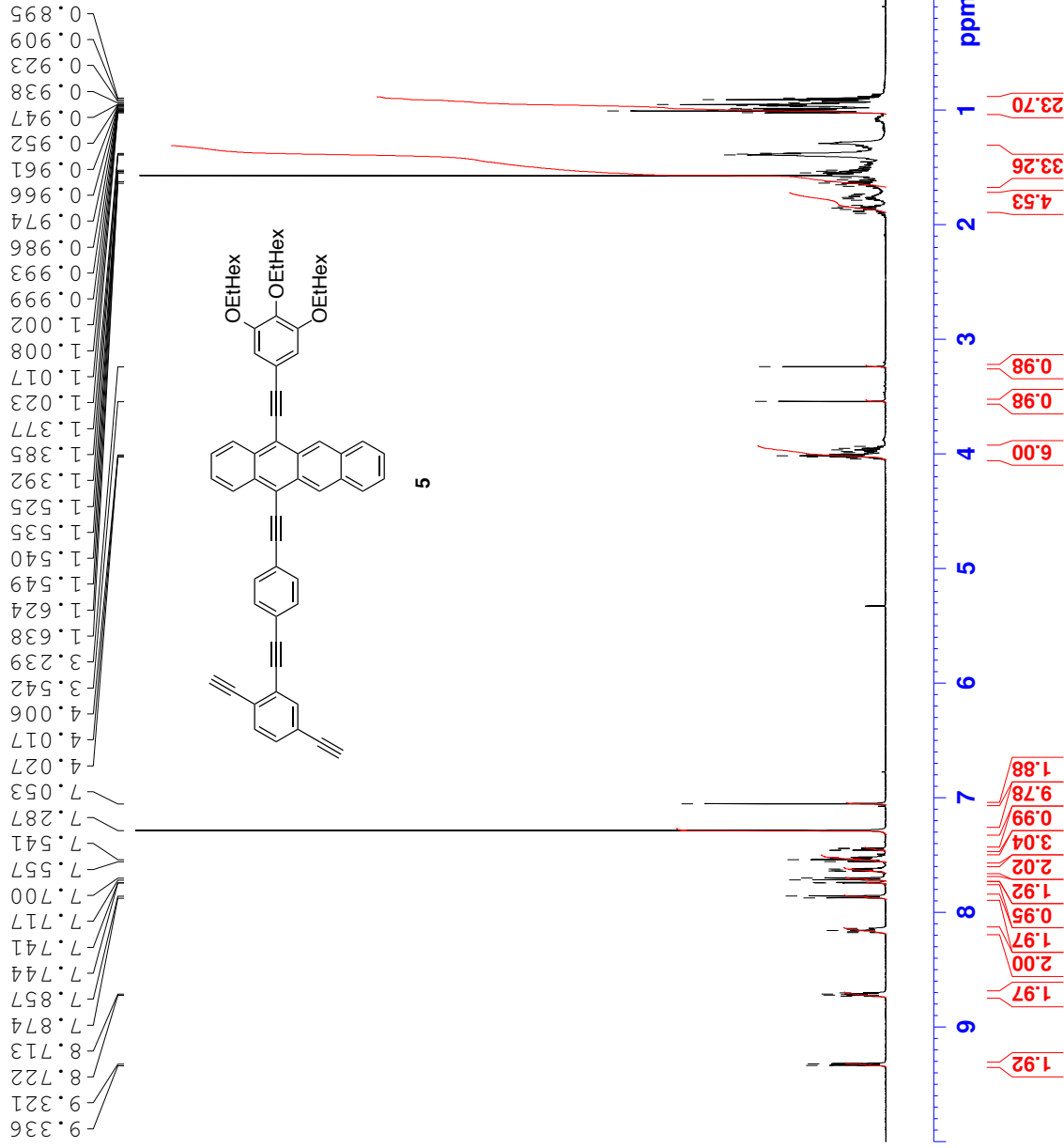


5a





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 CDC13
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 5.0000000 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-2-128

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

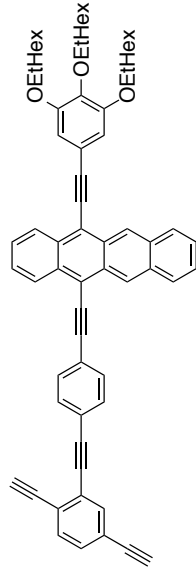
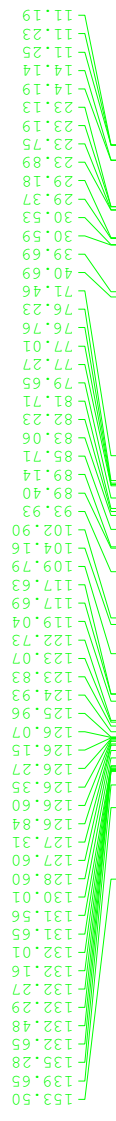
SF 125.7577890 MHz

WDW EM

SSB 0

GB 1.00 Hz

PC 1.40



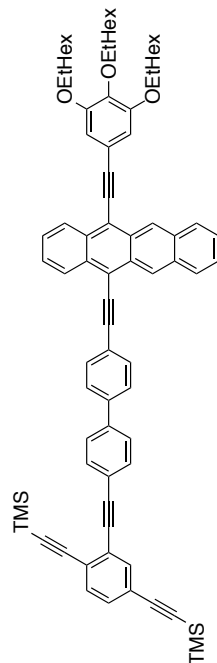
5

200 180 160 140 120 100 80 60 40 20 0 ppm

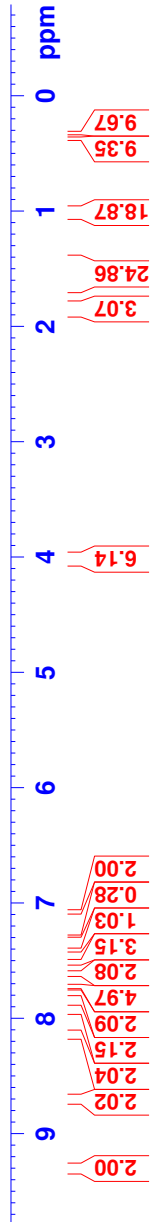


NAME ek-2-057
EXPNO 3
PROCNO 1
Date_ 20131113
Time 14.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 50.8
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 5.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 20.00 usec
PL1 1.00 dB
PL1W 17.75783539 W
SF01 500.1318364 MHz
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

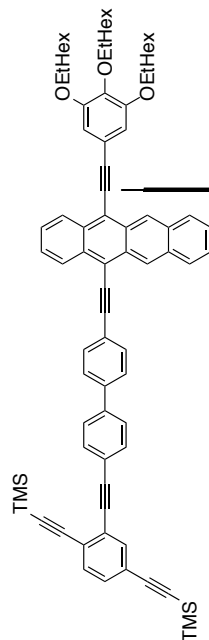


6a





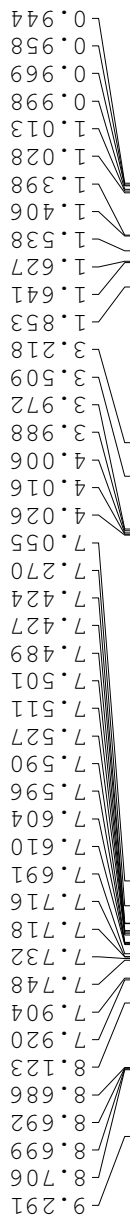
153.64
140.50
140.42
139.81
135.27
132.47
132.37
132.36
132.31
132.25
131.27
130.10
130.08
128.69
127.24
127.06
126.78
126.64
126.34
126.29
126.16
126.13
126.10
125.56
123.41
123.06
122.68
118.82
117.96
109.99
104.14
103.90
103.29
103.26
100.83
97.14
93.91
88.67
88.49
85.99
77.41
77.16
76.91
76.37
71.64
40.85
39.86
30.75
30.70
29.54
29.53
29.51
24.05
23.92
23.34
23.28
14.28
14.33
11.43
11.41
11.39
11.35
11.01
0.18
0.20



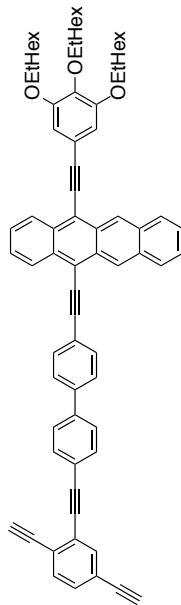
6a

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 CDCl3
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
PL12W 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

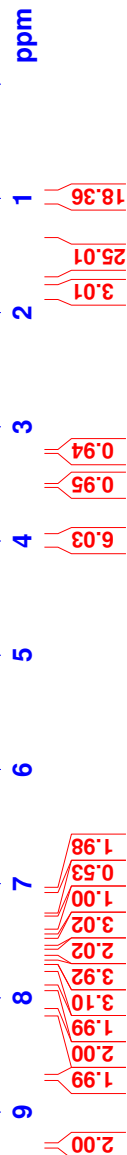
160 120 80 40 0 ppm

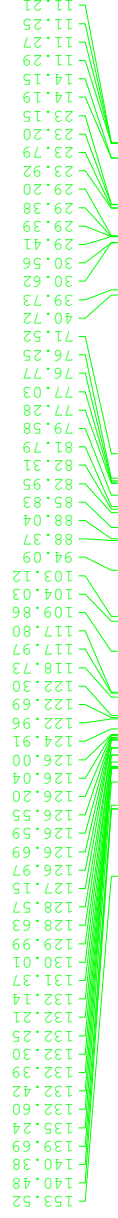
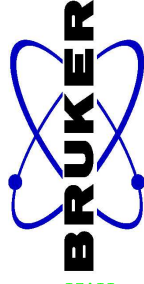


NAME ek-2-053
EXPNO 10
PROCNO 1
Date_ 20131119
Time 9.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
DS 16
NS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 71.8
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 20.00 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





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 CDC13

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

PL1W 17.75783539 W

PL12W 1.11017132 W

PL13W 0.46707872 W

SFO2 500.1320005 MHz

SI 65536

SF 125.7577890 MHz

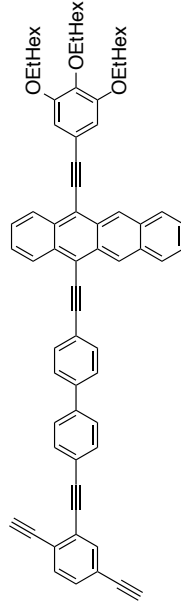
WDW EM

SSB 0

LB 1.00 Hz

GB 0

PC 1.40

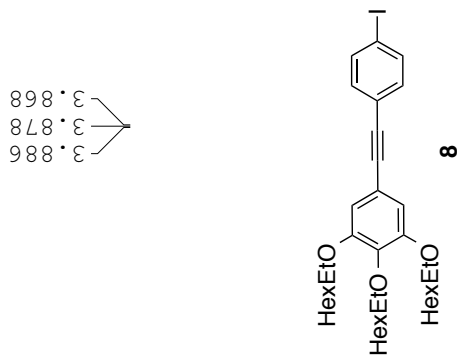


6

200 180 160 140 120 100 80 60 40 20 0 ppm



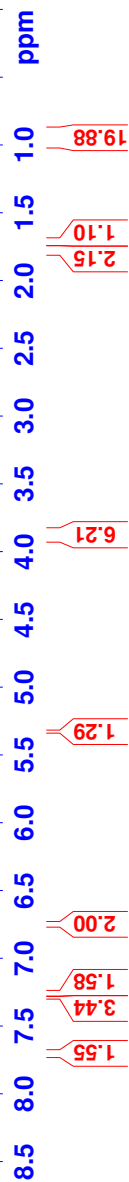
NAME ek-2-087
EXPNO 4
PROCNO 1
Date_ 20140115
Time 14.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 0.50000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 20.00 usec
PL1 1.00 dB
PL1W 17.75783539 W
SF01 500.1318364 MHz
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



7.708
7.693
7.287
7.285
7.268
7.253
6.748
6.746

3.886
3.878
3.868

0.953
0.938
0.931

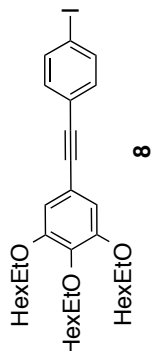




NAME ek-2-87
EXPNO 15
PROCNO 1
Date_ 20150507
Time 16.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65336
SOLVENT CDCl3
NS 9160
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 292.5 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

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

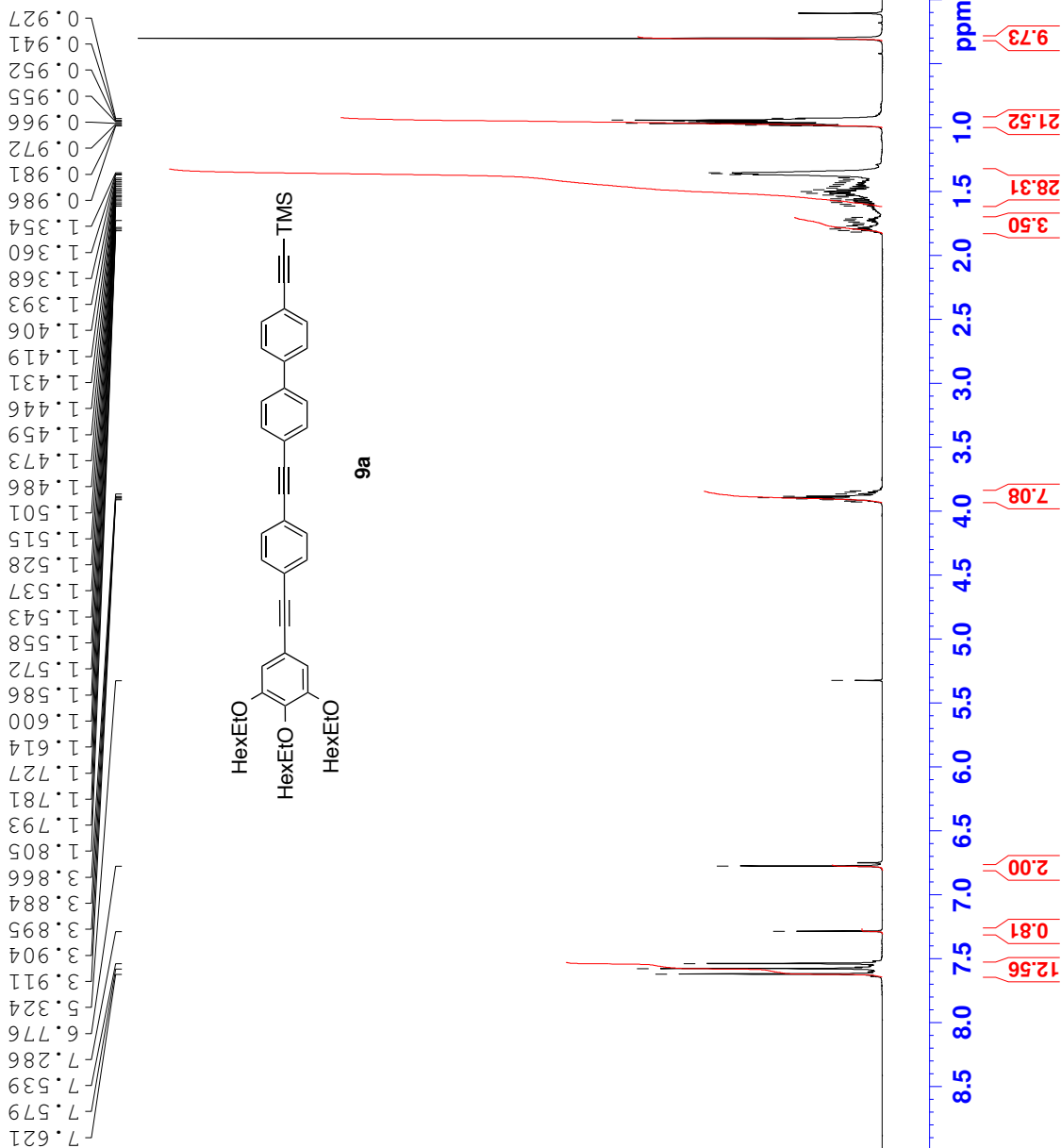
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL2W 17.75783539 W
PL12W 1.11017132 W
PL13W 0.46707872 W
SFO2 500.1320005 MHz
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

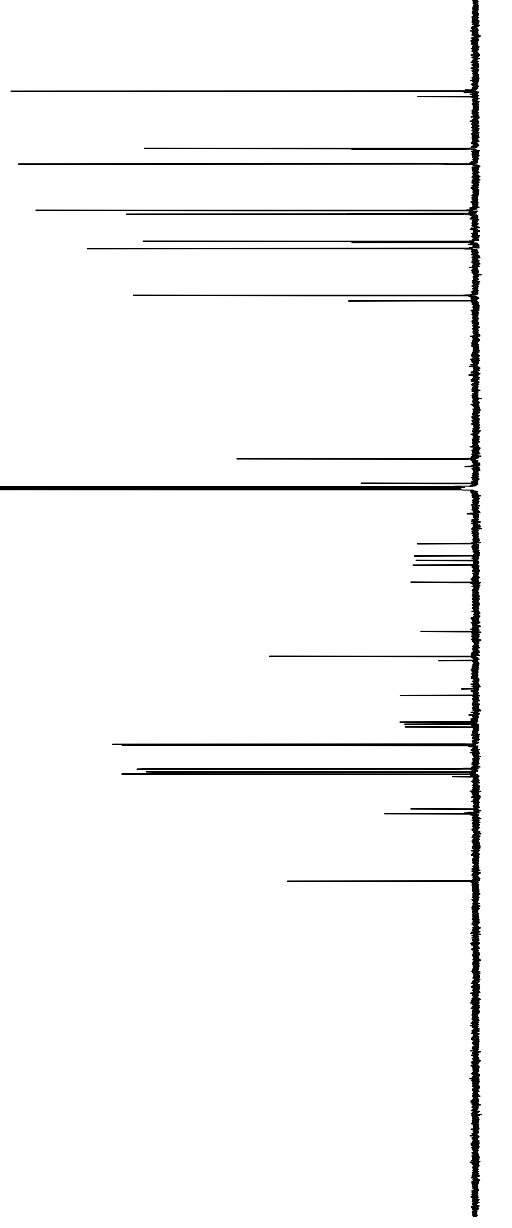
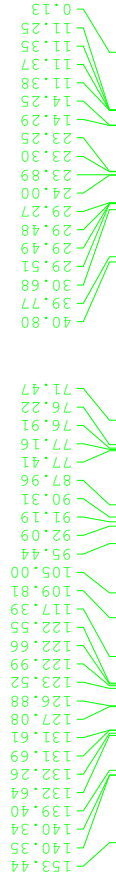
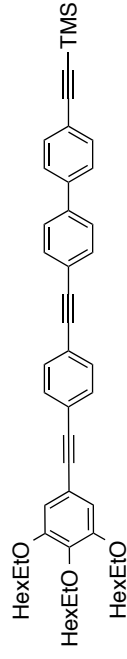


200 180 160 140 120 100 80 60 40 20 0 ppm



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
SF01 500.1318364 MHz
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





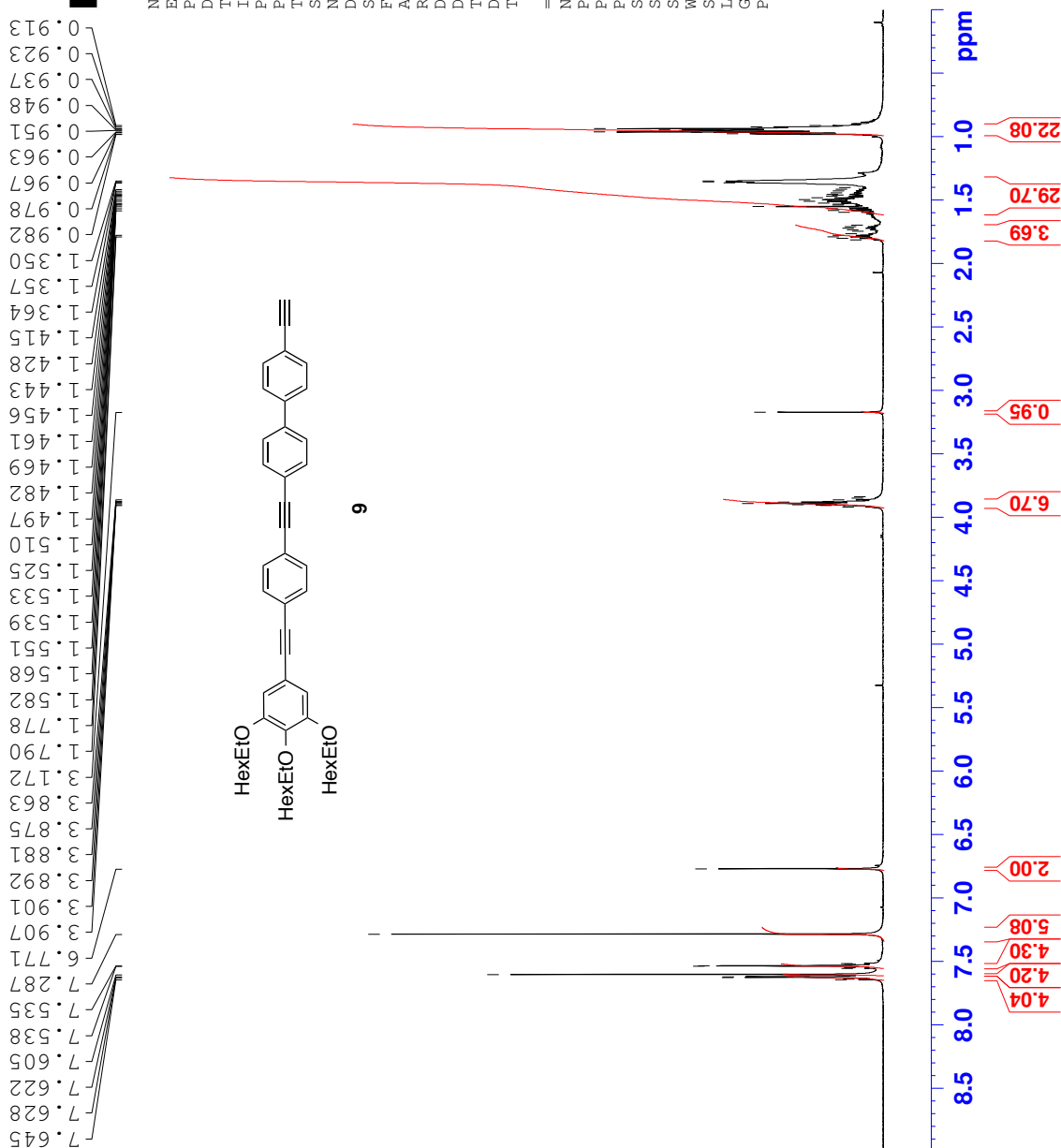
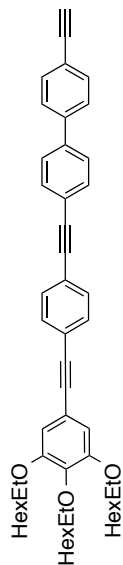
NAME	ek-2-090
EXPNO	34
PROCNO	1
Date_	20140121
Time	13.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	4190
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	300.1 K
D1	0.5000000 sec
D11	0.03000000 sec
TD0	1
=====	CHANNEL f1 =====
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



```

===== CHANNEL f1 =====
NUC1      1H
P1         20.00 usec
P1L        1.00 dB
P1LW       17.75783539 W
SF01       500.1318364 MHz
SI         65536
SF         500.1300000 MHz
WDW        EM
M          0
LB         0.30 Hz
GB         0
PC         1.00

```





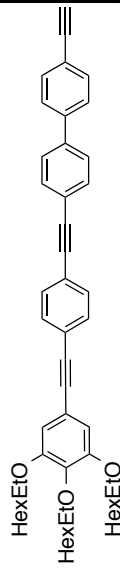
NAME ek-2-091
EXPNO 5
PROCNO 1
Date_ 20140122
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5362
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.1 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

==== 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

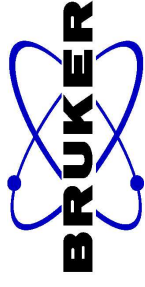
40.64
39.61
30.52
30.51
29.35
29.33
29.32
29.11
23.84
23.73
23.14
23.09
14.13
14.09
11.22
11.21
11.09

153.28
140.62
140.13
139.25
132.66
132.13
131.54
131.46
126.97
126.87
123.39
122.81
122.51
121.45
117.22
109.65
91.94
90.96
90.19
87.79
83.42
78.05
77.25
77.00
76.75
71.32



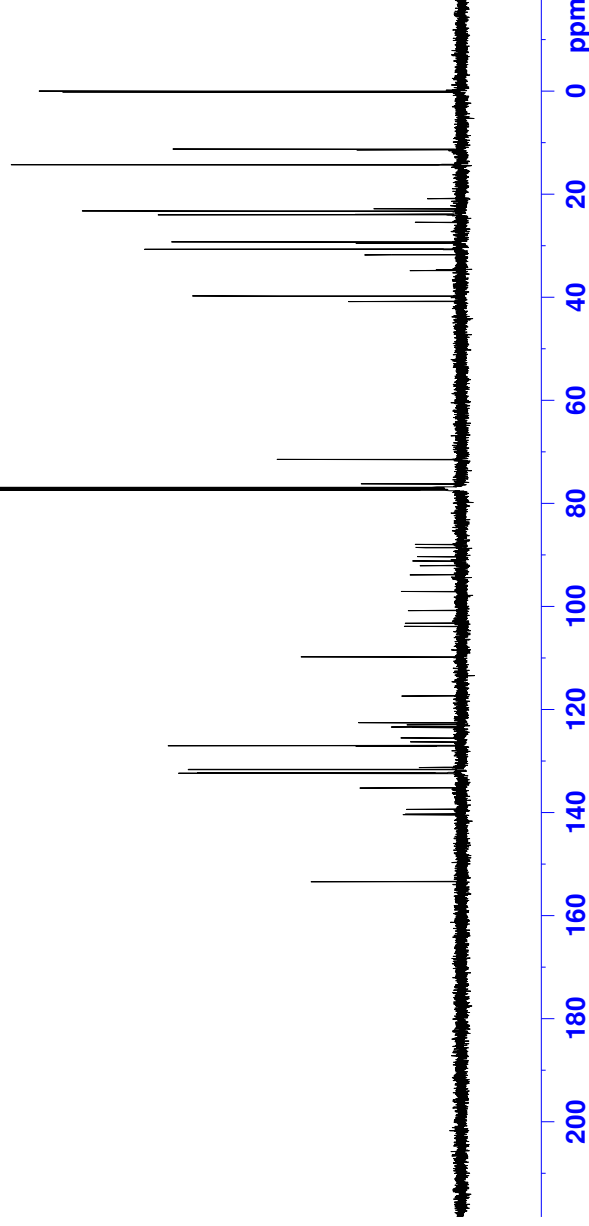
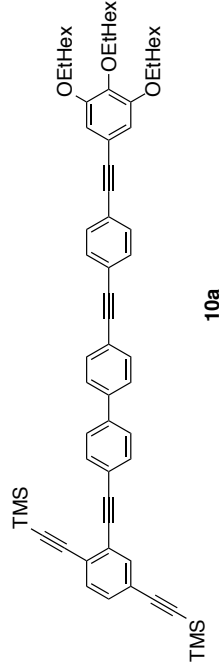
9

ppm



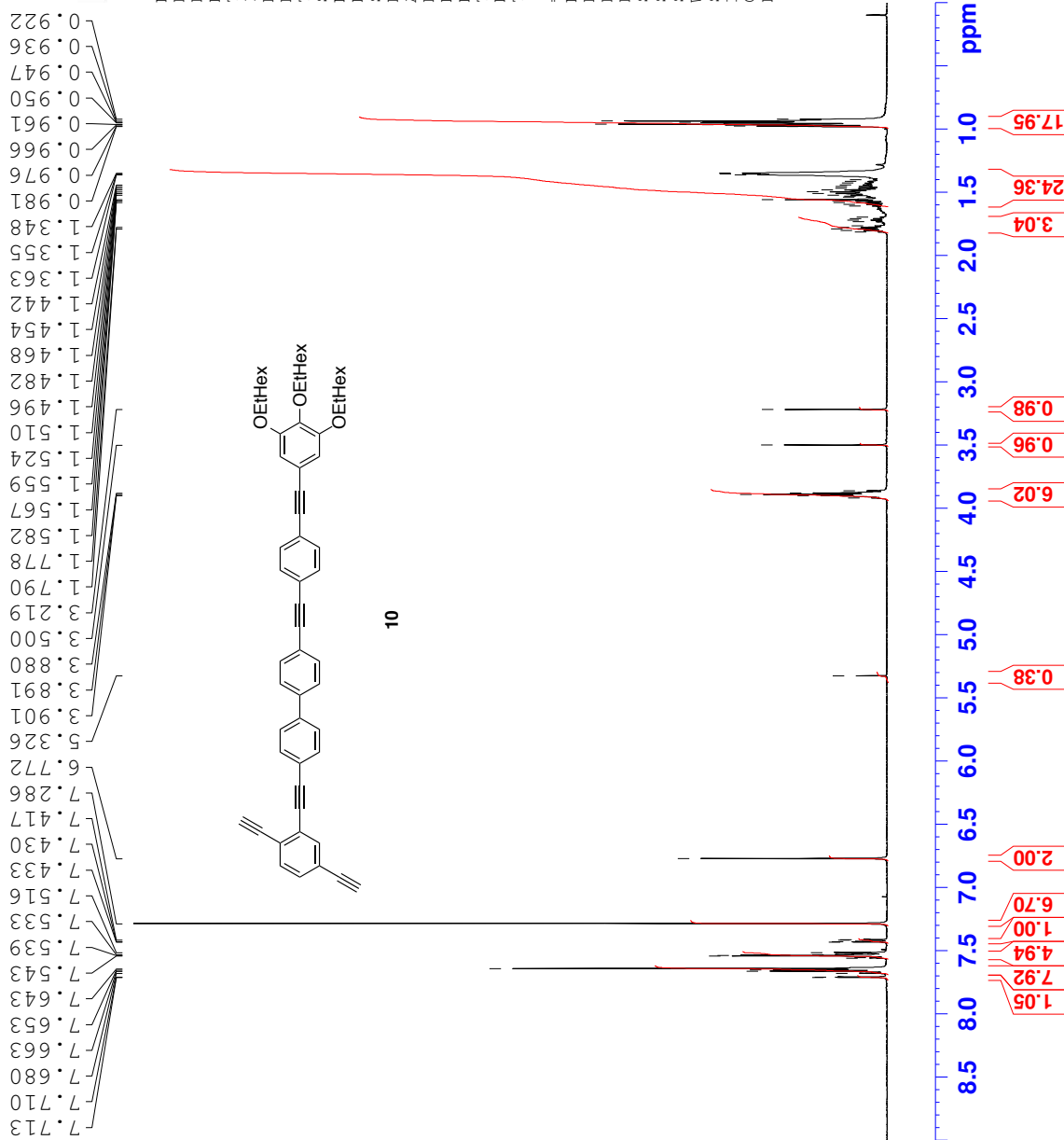
NAME ek-2-092
EXPNO 4
PROCNO 1
Date_ 20140123
Time_ 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1295
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL 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
PL1W 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

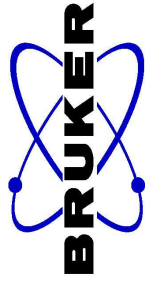
153.44
140.44
140.33
139.41
135.24
132.42
132.36
132.29
131.69
131.62
131.26
127.09
127.03
126.32
125.56
123.53
123.40
122.99
122.60
117.39
109.81
103.88
103.26
100.82
97.12
93.87
92.10
91.19
90.36
88.60
87.96
77.41
77.16
76.90
76.22
71.48
40.80
39.77
30.68
29.49
29.27
24.00
23.89
23.30
23.25
14.29
14.25
11.37
11.25
11.15
10.10





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
PL 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



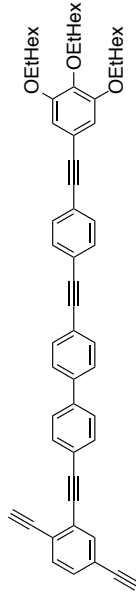


NAME ek-2-93
EXPNO 11
PROCNO 1
Date_ 20150507
Time 21.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 24025
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 291.5 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

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

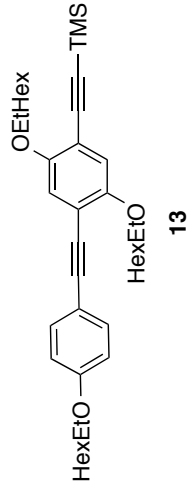
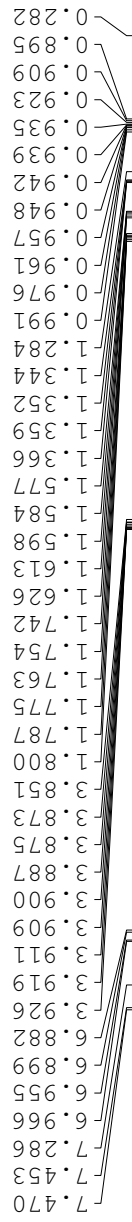
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL2W 17.75783539 W
PL12W 1.11017132 W
PL13W 0.46707872 W
SFO2 500.1320005 MHz
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

153.28
140.49
139.17
135.22
132.60
132.36
132.16
131.55
131.47
131.36
126.97
126.94
126.55
124.86
123.36
122.81
122.48
122.18
117.22
109.58
94.03
91.94
91.01
90.23
87.94
87.81
82.93
82.28
81.74
79.56
77.27
77.02
76.76
76.05
71.26
40.63
39.59
30.51
29.34
29.11
23.72
23.16
23.11
14.16
14.12
11.24
11.22
11.11



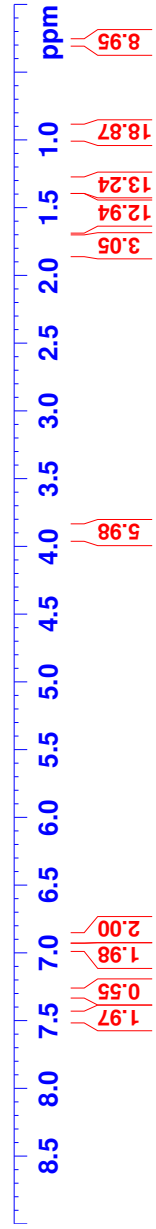
10

ppm



NAME	ek-2-019
EXPNO	1
PROCNO	1
Date_	20130910
Time	9.55
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
ID	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
P1L       1.00 dB
P1LW      17.75793539 W
SF01      500.1318364 MHz
SI        65536
ST        500.1300000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```

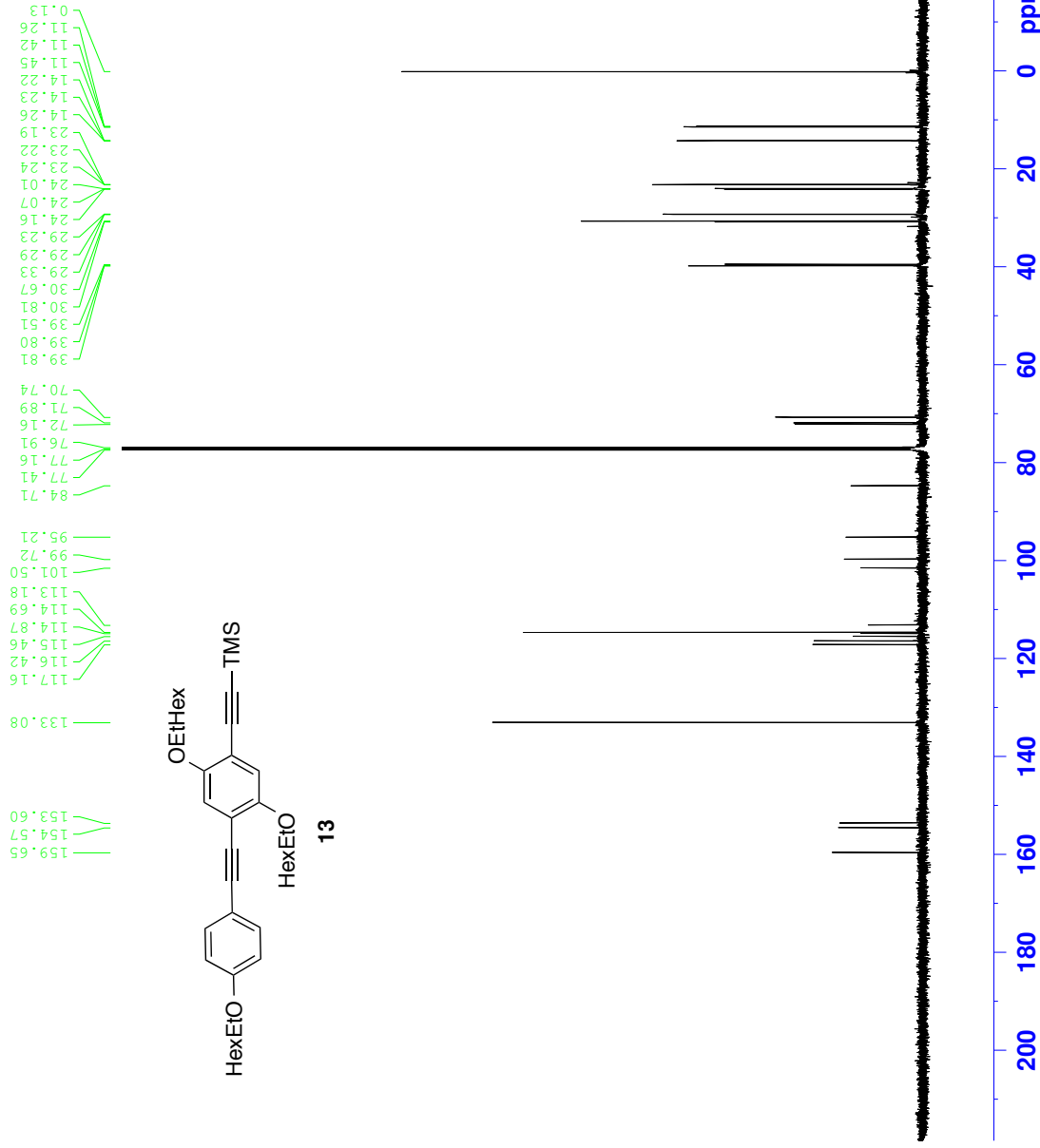


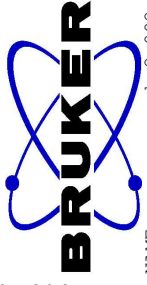


NAME ek-2-019
EXPNO 2
PROCNO 1
Date_ 20130910
Time 9.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

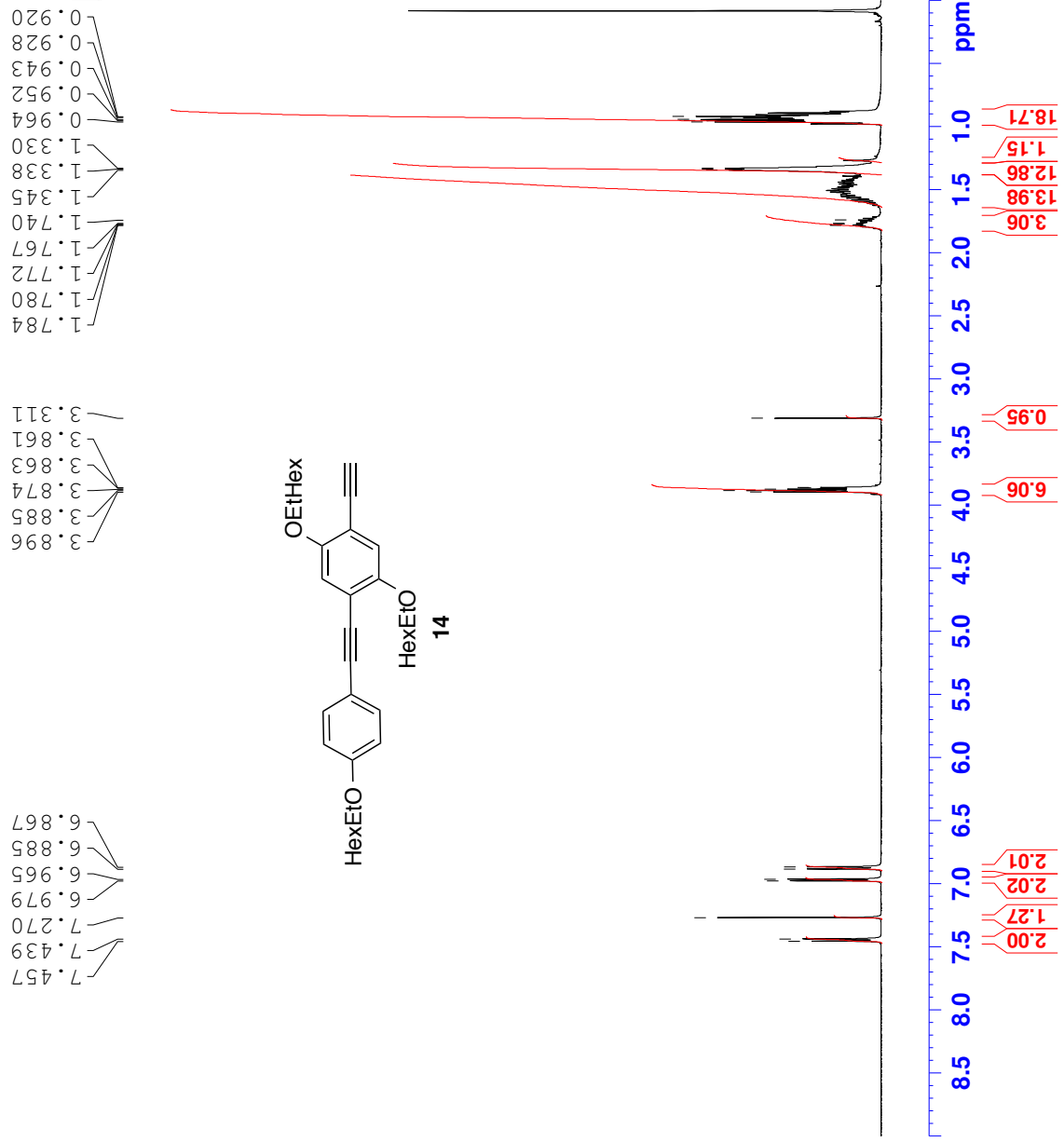
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 0.00 dB
PL1W 89.92553711 W
SFO1 125.7703643 MHz

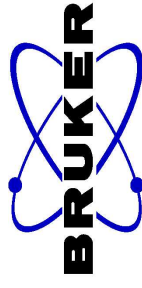
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL2W 17.75783539 W
PL12W 1.11017132 W
PL13W 0.46707872 W
SFO2 500.1320005 MHz
SI 65536
SF 125.7577706 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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





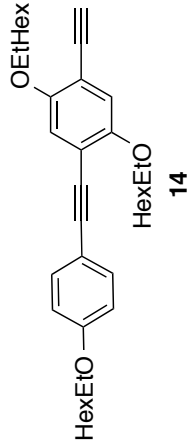
NAME ek-2-002
EXPNO 2
PROCNO 1
Date_ 20130808
Time 11.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 892
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.5000000 sec
D11 0.0300000 sec
TD0 1

===== 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
EM 0
SSB 1.00 Hz
LB 0
GB 0
PC 1.00

95.28
84.54
82.09
80.31
77.41
77.16
72.32
72.23
70.78
39.79
39.58
39.53
30.82
30.68
29.22
29.24
29.23
24.17
24.08
24.03
23.22
23.20
23.19
14.23
14.22
11.42
11.32
11.26
1.17

159.70
154.64
153.66
133.11
117.65
116.77
115.42
115.29
114.71
112.22



200 180 160 140 120 100 80 60 40 20 0 ppm

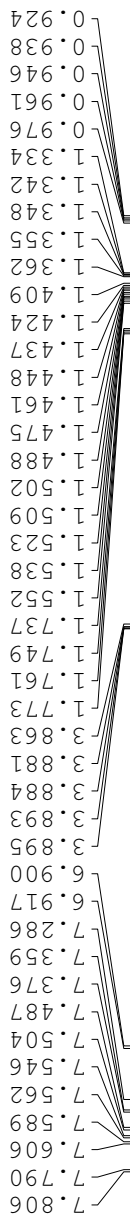
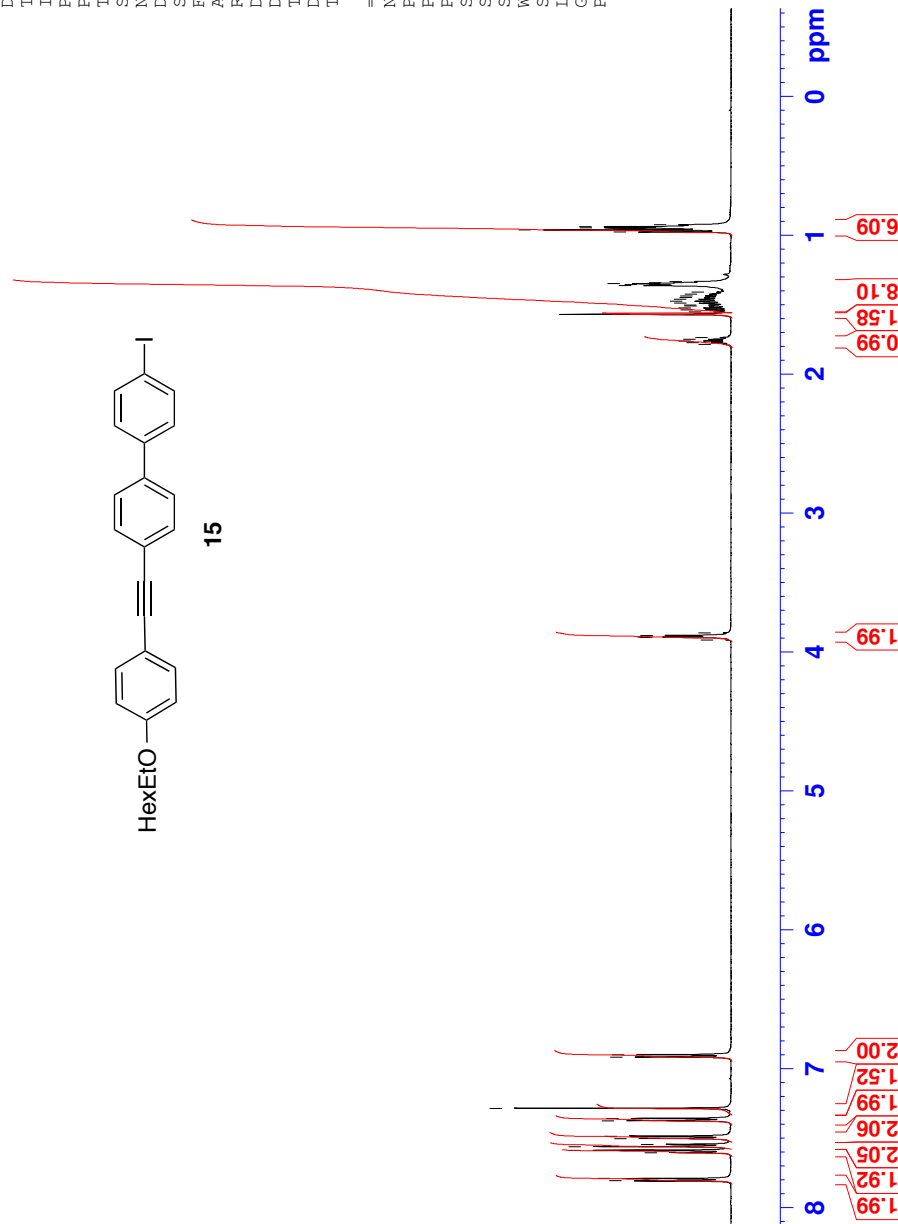
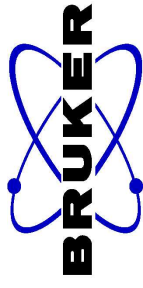


Figure 1 is a line graph showing the evolution of the average number of nodes per cluster, N_c , as a function of the number of nodes, N . The x-axis is logarithmic, ranging from 10^1 to 10^4 . The y-axis is linear, ranging from 0 to 10. Multiple lines represent different values of the parameter α , ranging from 0.924 to 0.998. All lines show a sharp increase in N_c as N increases, with the rate of increase being higher for larger α values.

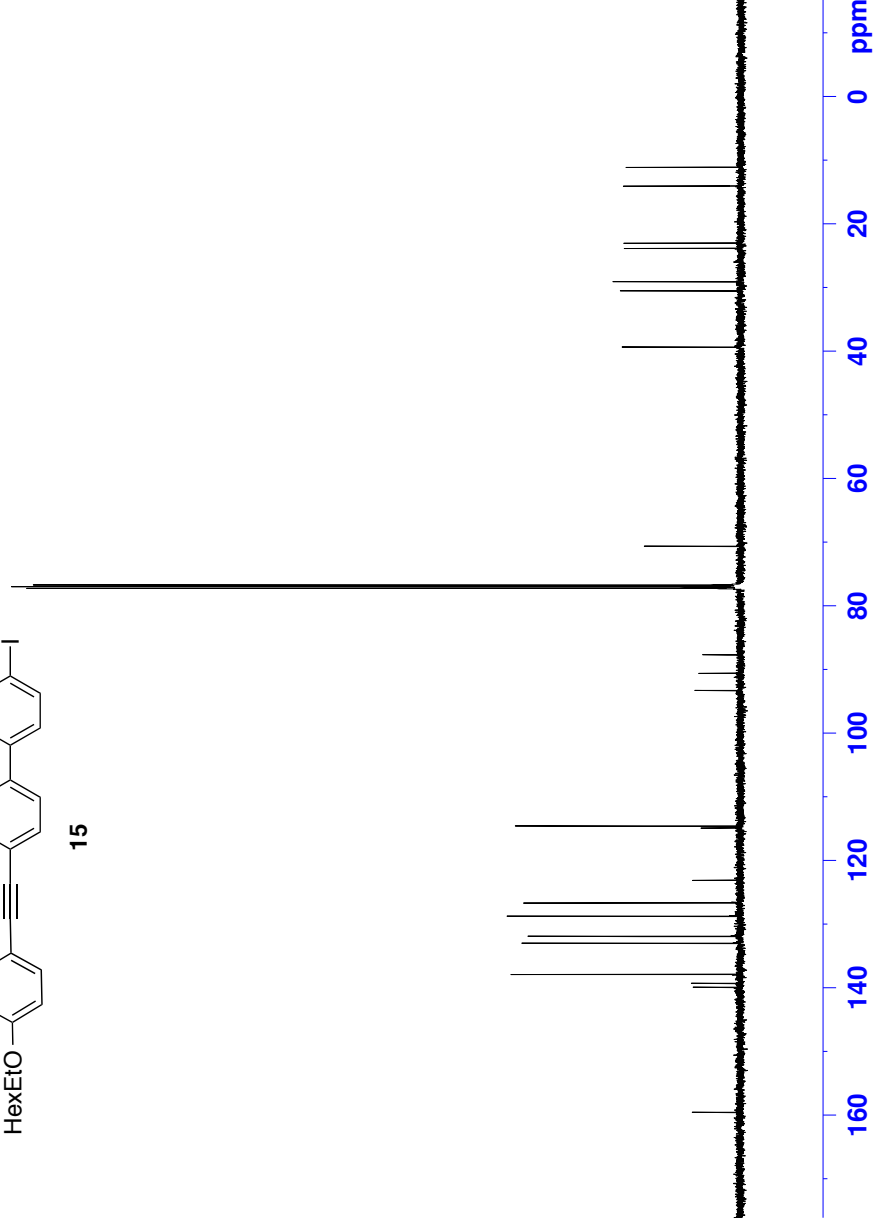
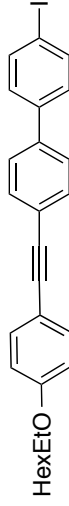
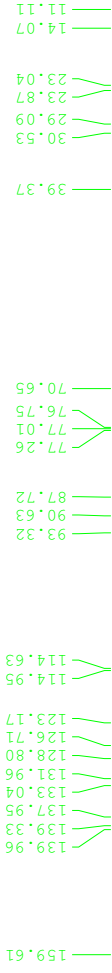


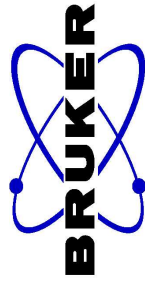


NAME ek-2-006
EXNO 2
PROCNO 1
Date_ 20130815
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 810
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.5 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

===== 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



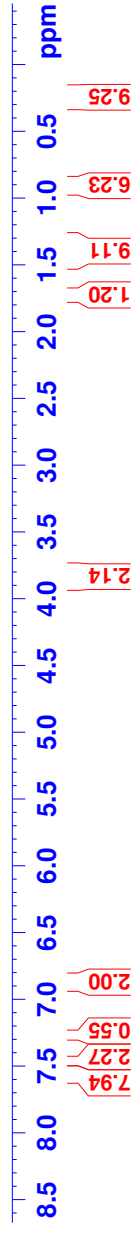
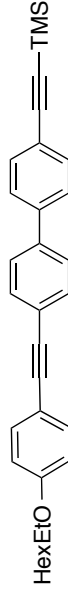
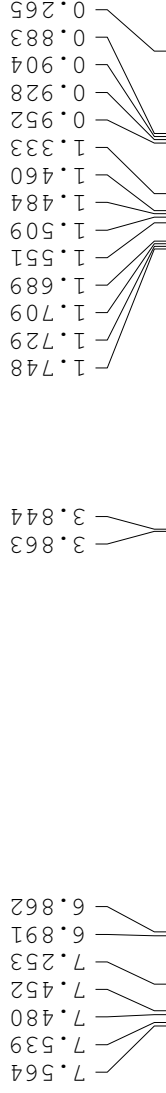


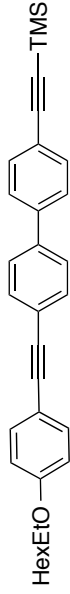
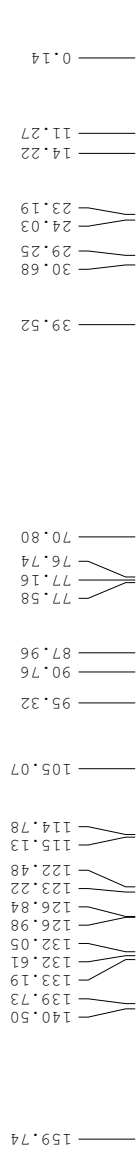
Current Data Parameters
NAME ek-2-008
EXPNO 1
PROCNO 1

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
D11 1
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

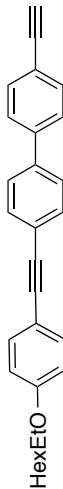




16a

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
PULPROG zgpg30
TD 65536
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
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

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



16

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 CDC13
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 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 20.00 usec
PL1 1.00 dB
PL1W 17.75783539 W
SF01 500.1318364 MHz
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ppm

6.23

8.96

1.02

0.92

2.02

2.00

0.44

2.04

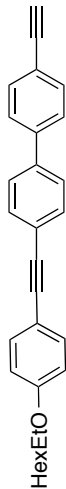
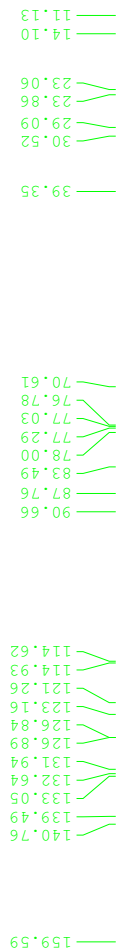
7.95



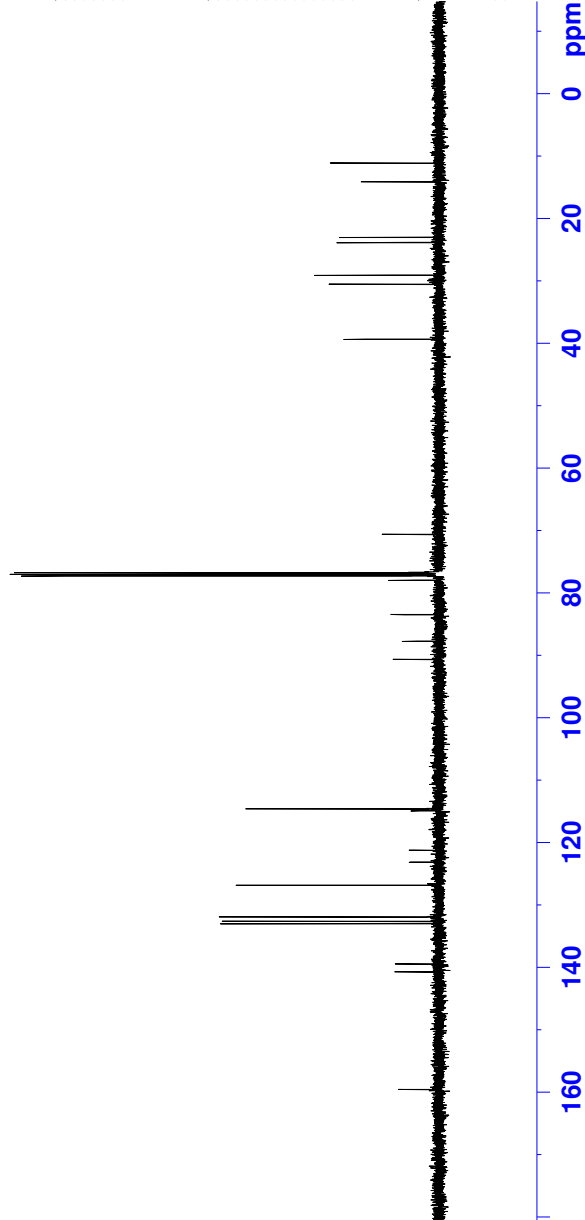
NAME ek-2-010
EXNO 2
PROCNO 1
Date_ 20130820
Time 13.35
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 175
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.3 K
D1 0.5000000 sec
D11 0.0300000 sec
TD0 1

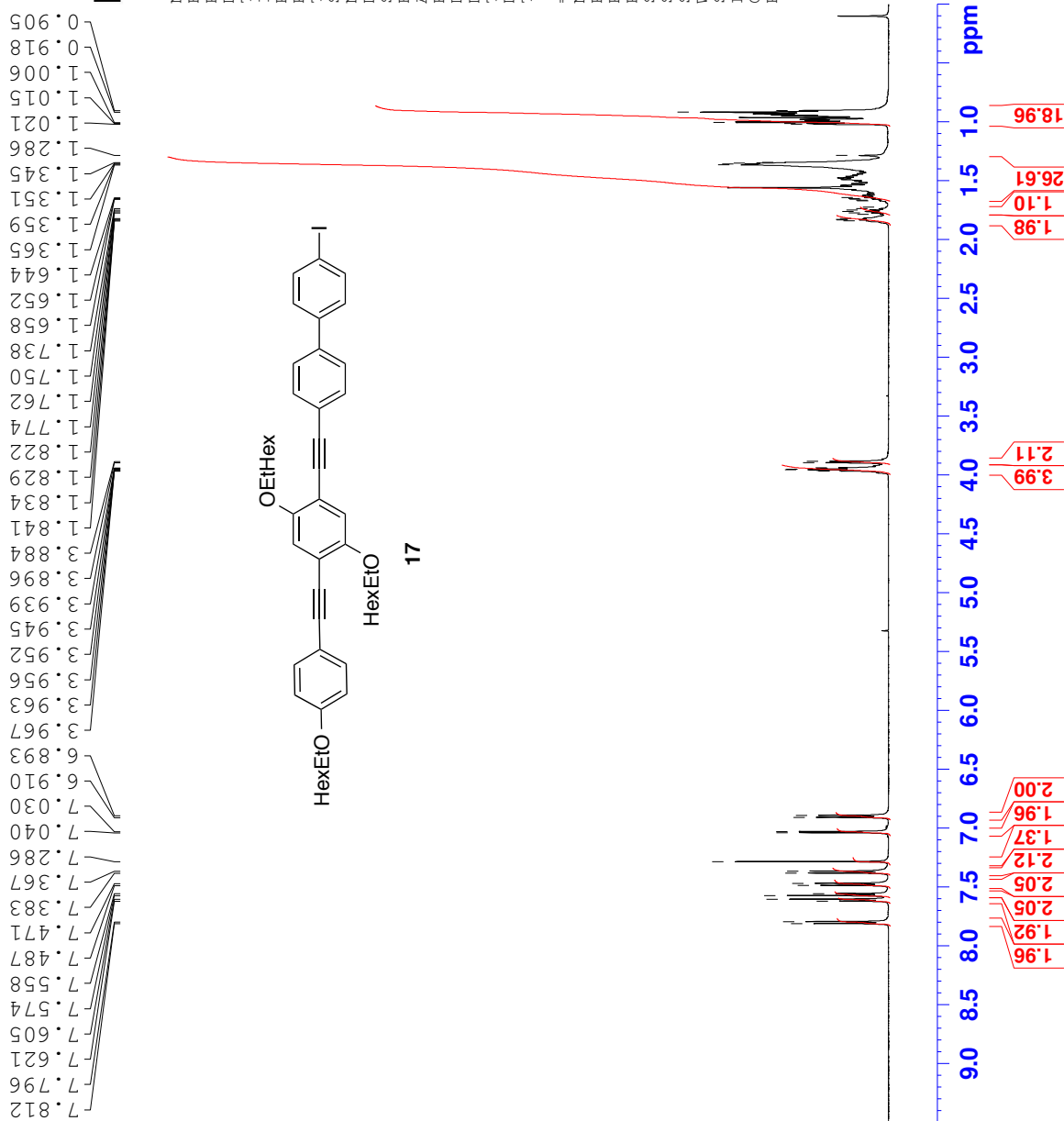
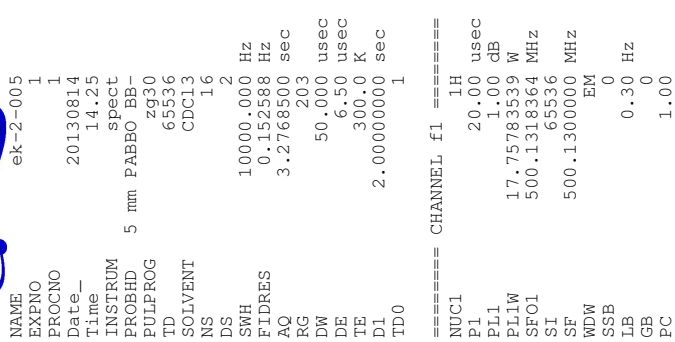
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 0.00 dB
PL1W 89.92553711 W
SFO1 125.7703643 MHz

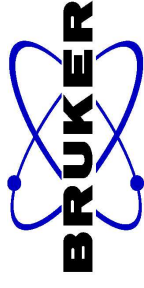
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL12W 17.75783539 W
PL12W 1.11017132 W
PL13W 0.46707872 W
SFO2 500.1320005 MHz
SI 65536
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



16







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

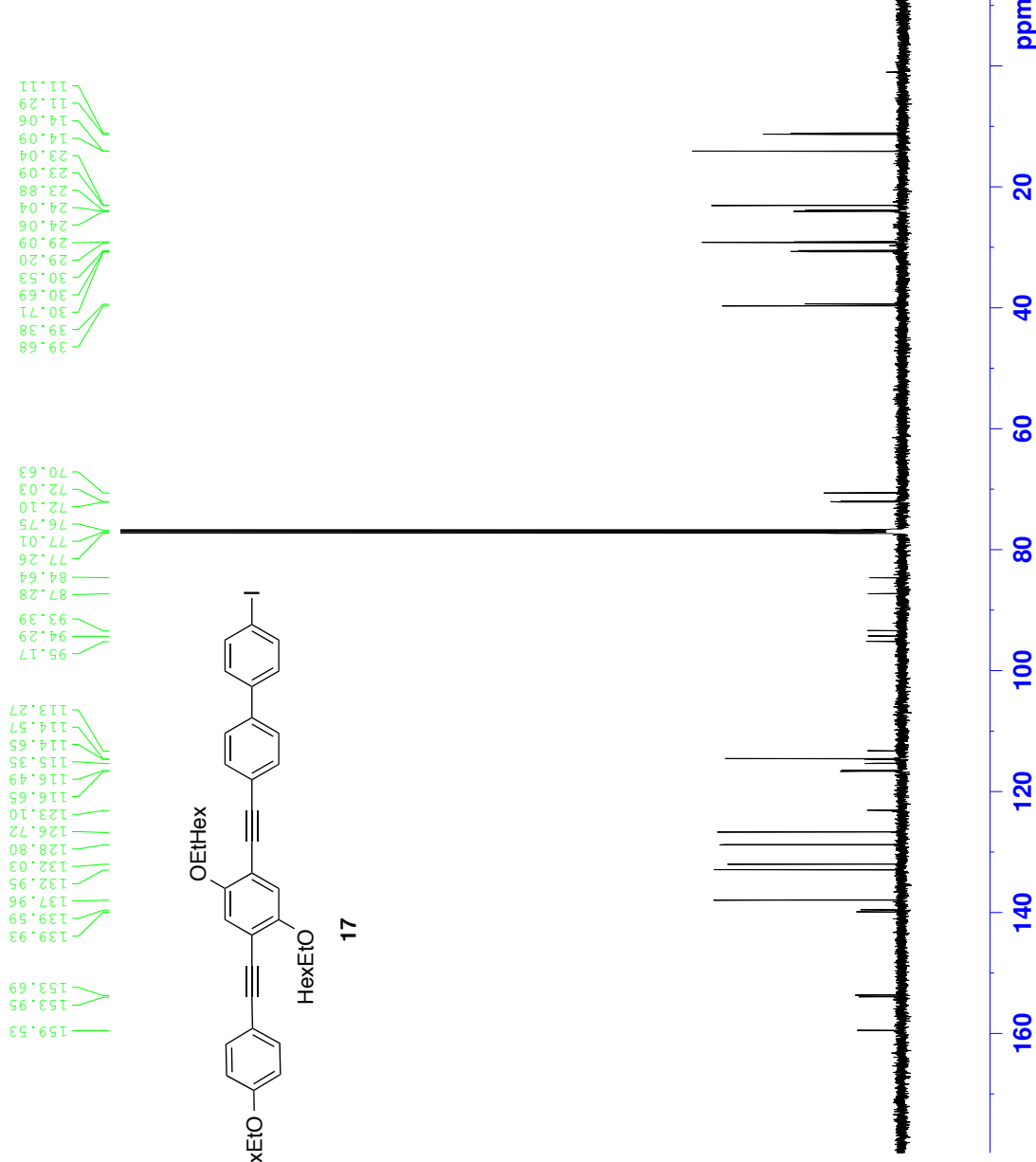
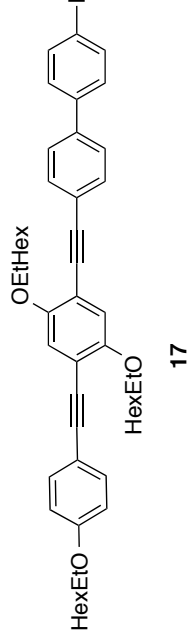
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 0.00 dB
PL1W 89.92553711 W
SFO1 125.7703643 MHz

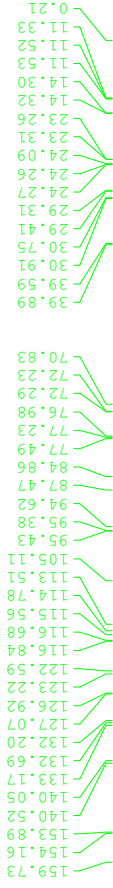
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL2W 17.75783539 W
PL12W 1.11017132 W
PL13W 0.46707872 W
SFO2 500.1320005 MHz
SI 65536
SF 125.7577890 MHz
WDM EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

39.68
39.71
30.69
30.71
30.53
29.20
29.09
24.06
24.04
23.88
23.09
23.04
14.06
14.04
11.29
11.11

95.17
94.29
93.39
87.28
84.64
77.26
77.01
76.75
72.10
72.03
70.63

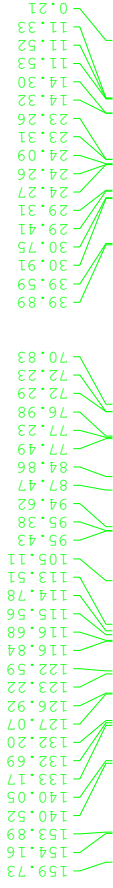
159.53
153.95
153.69
139.93
139.59
137.96
132.95
132.03
128.80
126.72
123.10
116.65
116.49
115.35
114.65
114.57
113.27





```
===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1        0.00 dB
PL1W       89.92553711
SF01       125.7703643 MHz
```

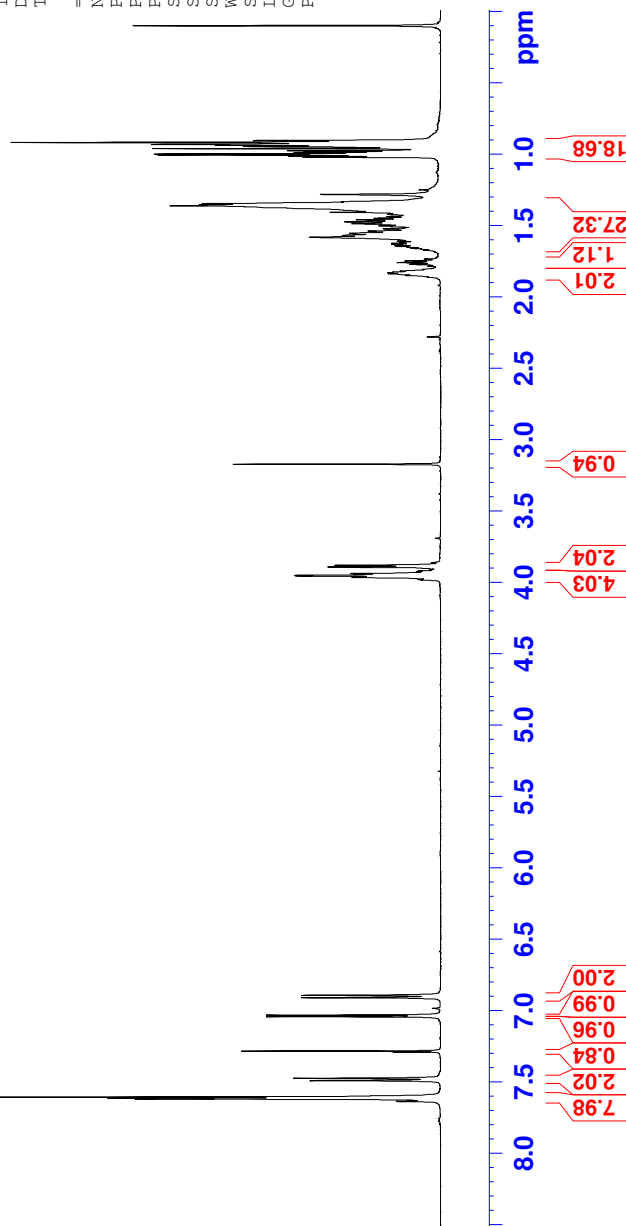
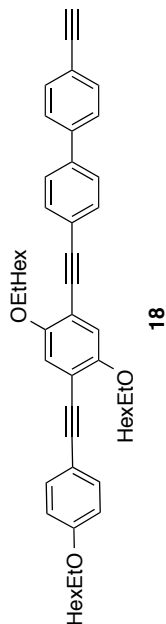
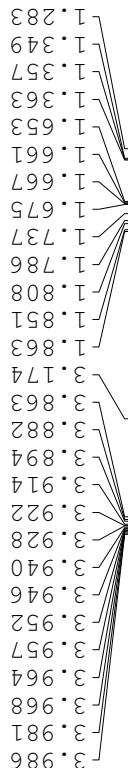
200 180 160 140 120 100 80 60 40 20 0 ppm

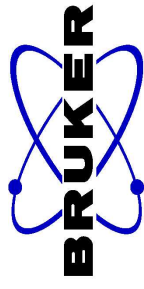




ek-2-009

CHANNEL f1 =====



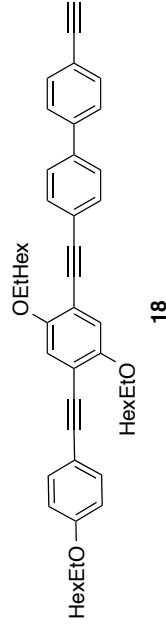


NAME ek-2-009
EXPNO 2
PROCNO 1
Date_ 20130820
Time 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 871
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

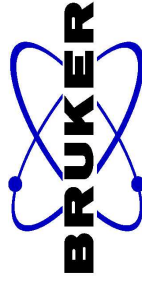
===== CHANNEL f1 =====
NUC1 13C
P1 9.50 usec
PL1 0.00 dB
PL1W 89.92553711 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 13.04 dB
PL13 16.80 dB
PL12W 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

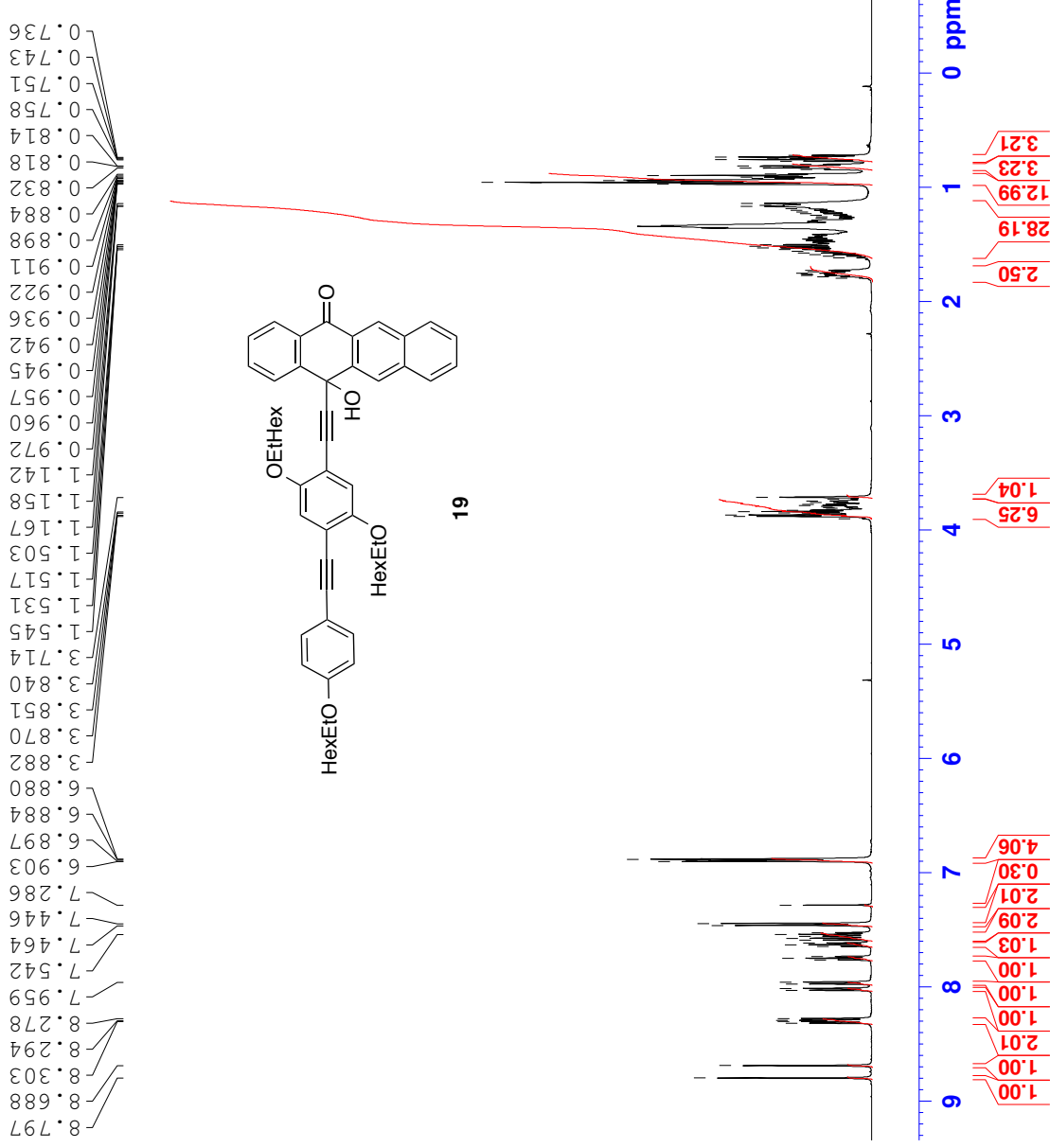
159.73
154.16
153.89
140.94
139.97
133.17
132.86
132.22
127.10
127.06
123.32
121.54
116.84
116.68
115.55
114.83
114.78
113.48
95.39
94.56
87.52
84.85
83.69
78.23
77.48
77.23
76.98
72.29
72.23
70.82



200 180 160 140 120 100 80 60 40 20 0 ppm



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 5.0000000 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



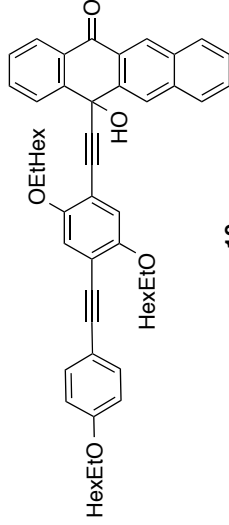


NAME ek-2-021
EXPNO 6
PROCNO 1
Date_ 20130916
Time 9.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1338
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.2 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1

===== 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

183.45
159.56
154.12
153.40
144.24
139.51
135.89
134.19
132.96
132.73
130.03
129.83
129.34
129.01
128.79
128.127
128.15
127.42
127.30
127.22
116.86
116.00
115.21
115.16
114.56
111.69
96.10
95.31
84.47
83.35
77.30
77.05
76.79
72.10
71.29
70.61
67.23
39.63
39.36
39.33
39.31
30.64
30.52
30.21
30.19
29.16
28.92
28.88
23.98
23.87
23.69
23.64
23.07
23.04
22.95
22.93
14.09

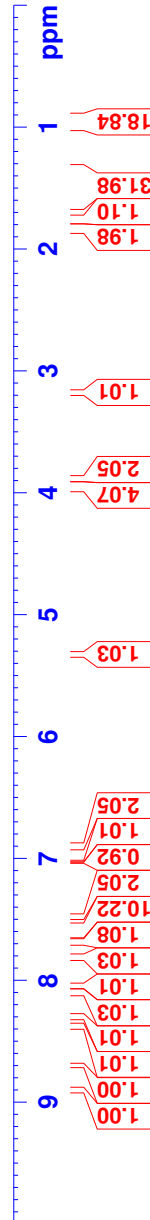


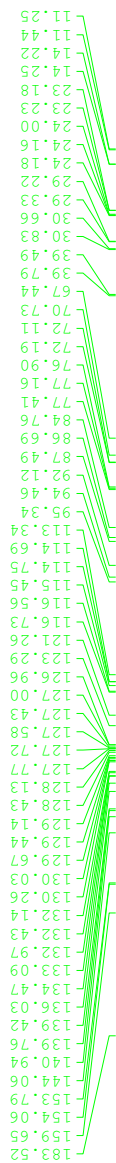
19

200 180 160 140 120 100 80 60 40 20 0 ppm

CCOC1=CC=C(C#CC2=CC=C(C#CC3=CC=C(C#CC4=CC(=C5C(=O)C6=CC=CC=C6C(O)C5=C4)C3)C2)C(=C1)OCC

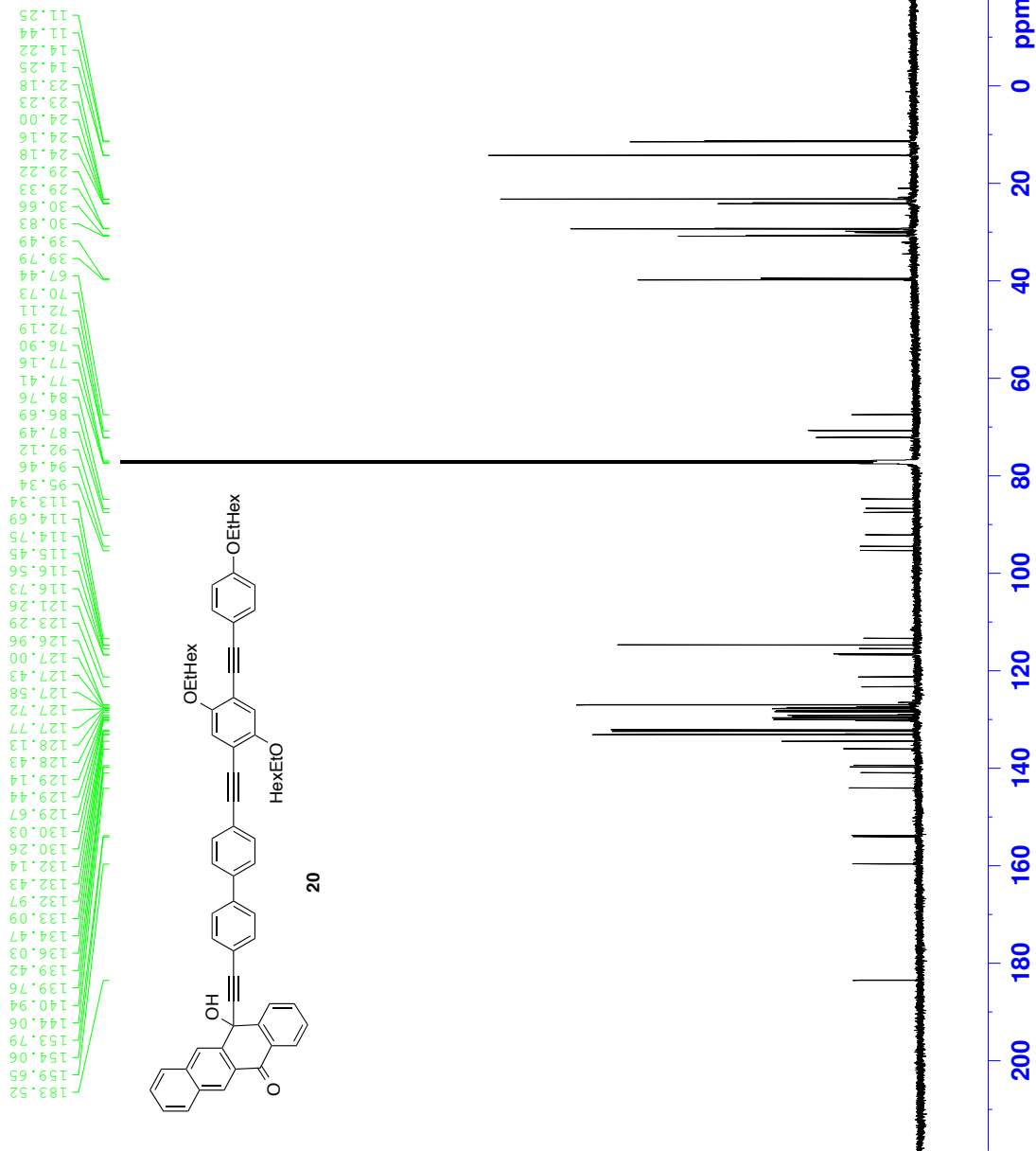
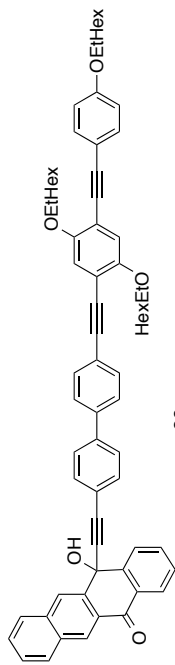
20





EXPNO	1
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
FIDRES	0.454131
AQ	1.1010548
RG	203
DW	16.800
DE	6.50
TE	290.4
D1	0.50000000
D11	0.03000000
TD0	1

=====	CHANNEL f1	=====
NUC1	13C	
P1	9.50 usec	
PL1	0.00 dB	
PL1W	89.92553711 W	
SF01	125.7703643 MHz	
=====	CHANNEL f2	=====
CPDPRG2	waltz16	
NUC2	1H	
PCPD2	80.00 usec	
PL2	1.00 dB	
PL12	13.04 dB	
PL2W	16.80 dB	
PL12W	17.75783539 W	
PL13W	1.11017132 W	
SF02	0.46707872 W	
SI	500.1320005 MHz	
SF1	65536	
WDW	125.7577718 MHz	
SSB	EM	
LB	0	
GB	1.00 Hz	
PC	0	
	1.40	





NAME
EXPNO
PROCNO
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
DS
NS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
TD0

ek-2-016

3

1

20130904

15.49

spect

5 mm PABBO BB-

zg30

65536

CDC13

24

2

10000.000 Hz

0.152588 Hz

3.2768500 sec

114

50.000 usec

6.50 usec

295.2 K

5.0000000 sec

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

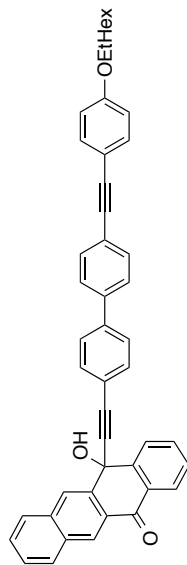
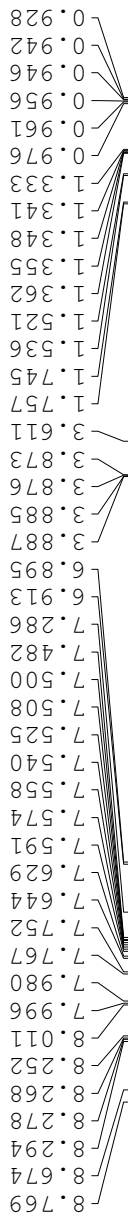
WDW EM

SSB 0

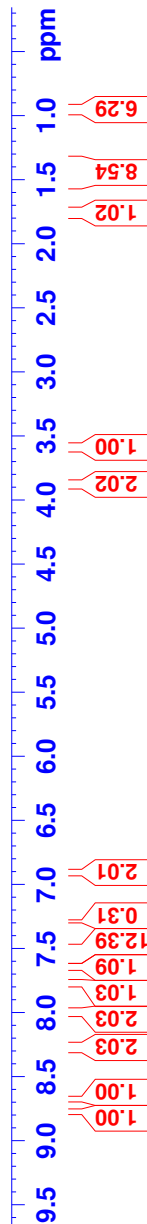
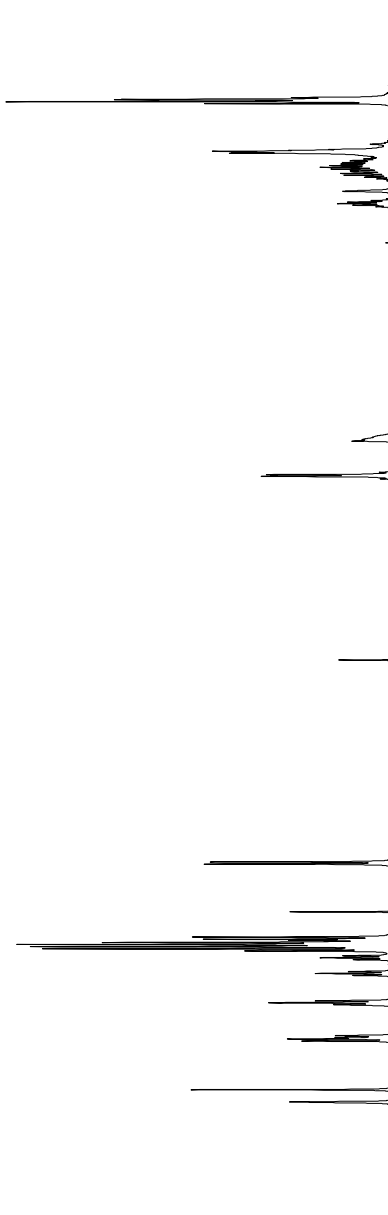
LB 0.30 Hz

GB 0

PC 1.00

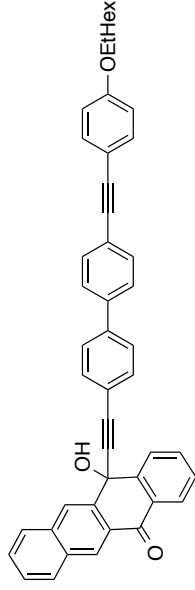
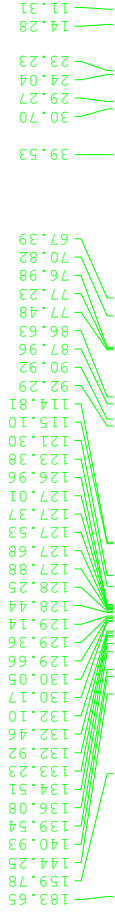


21

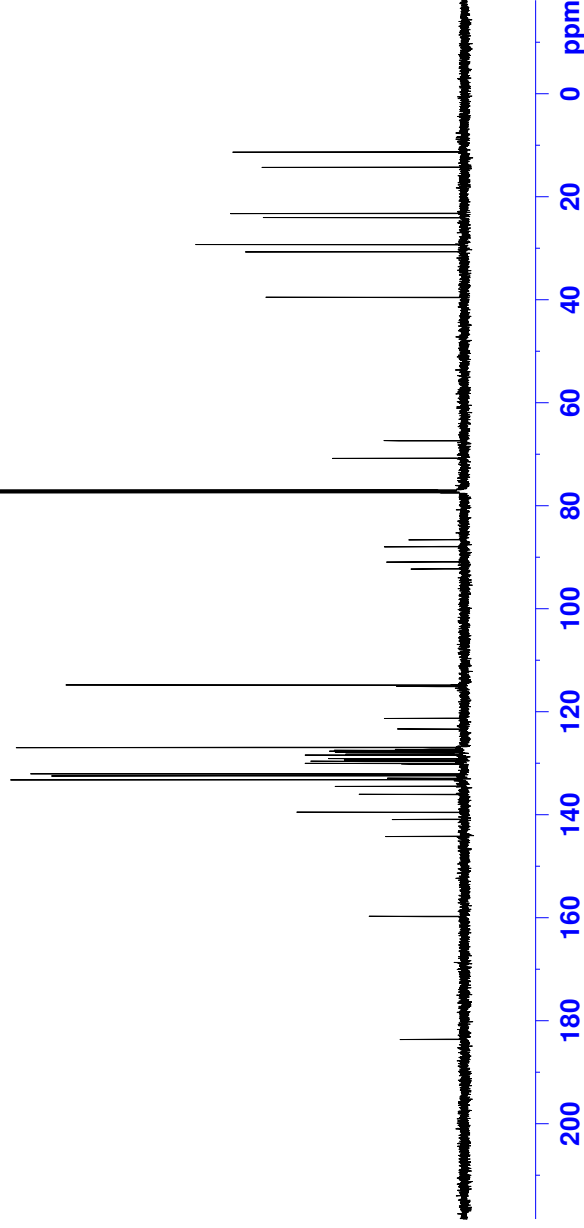


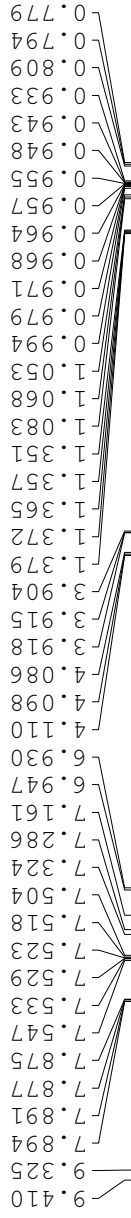
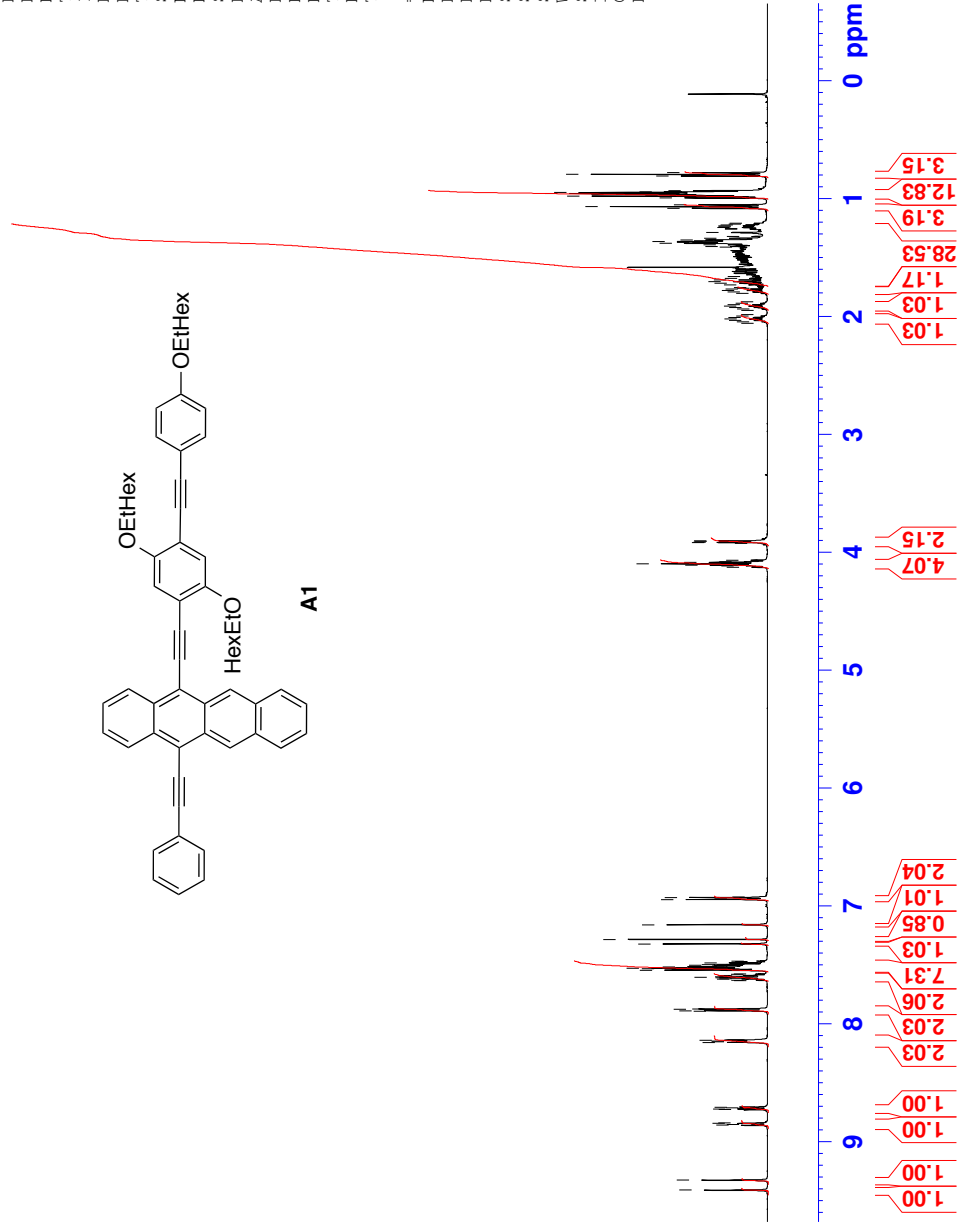


NAME ek-2-016
EXPNO 4
PROCNO 1
Date_ 20130904
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 560
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.4 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL f1 =====
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



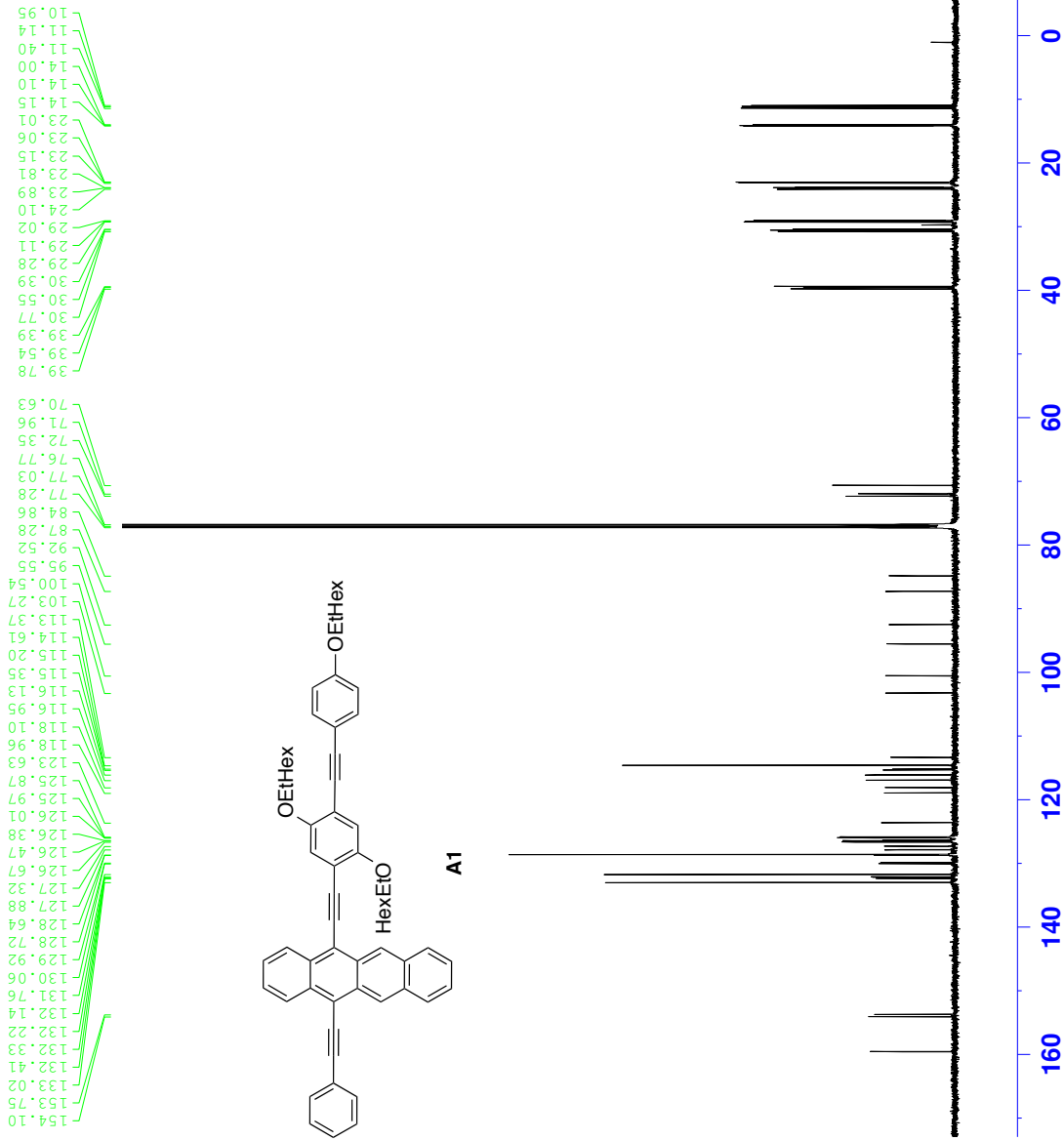
21

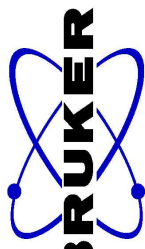


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8=CC=CC=C348C349=CC=CC=C349C350=CC=CC=C350C351=CC=CC=C351C352=CC=CC=C352C353=CC=CC=C353C354=CC=CC=C354C355=CC=CC=C355C356=CC=CC=C356C357=CC=CC=C357C358=CC=CC=C358C359=CC=CC=C

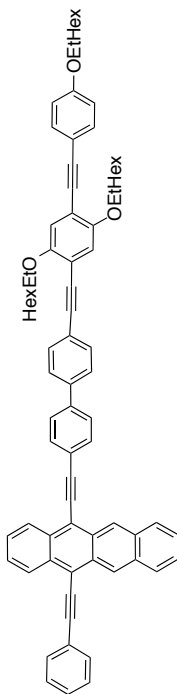


NAME ek-2-023
EXENO 8
PROCNO 1
Date_ 20130924
Time 10.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 4475
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 295.0 K
D1 0.50000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL f1 =====
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

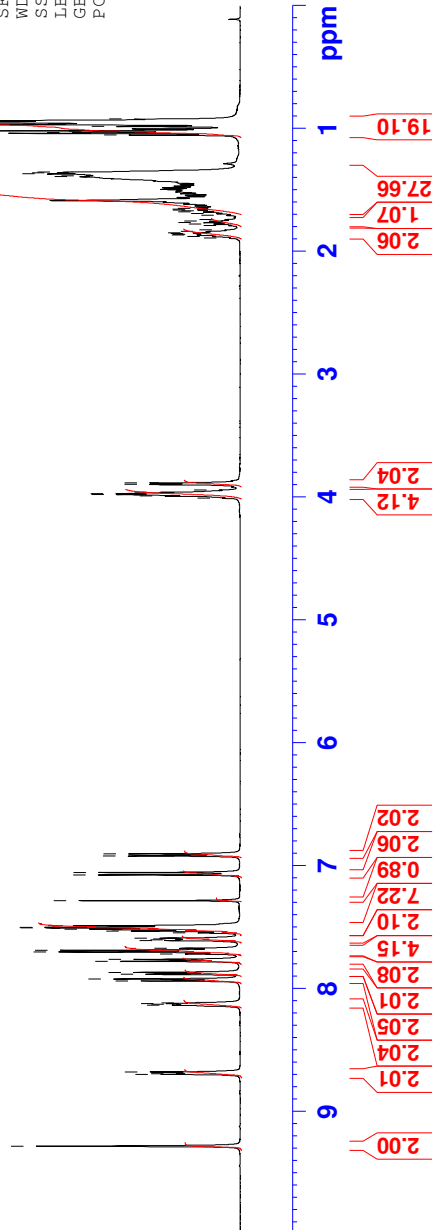




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8.681
7.940
7.924
7.885
7.871
7.780
7.764
7.704
7.690
7.611
7.591
7.534
7.518
7.507
7.504
7.490
7.286
7.077
7.057
6.923
6.905
3.992
3.981
3.974
3.962
3.898
3.886
1.393
1.387
1.370
1.363
1.356
1.054
1.040
1.034
1.024
0.985
0.970
0.965
0.951
0.938
0.924



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-2-018

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

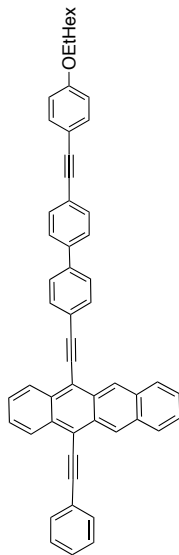
SSB 0

LB 0.30 Hz

GB 0

PC 1.00

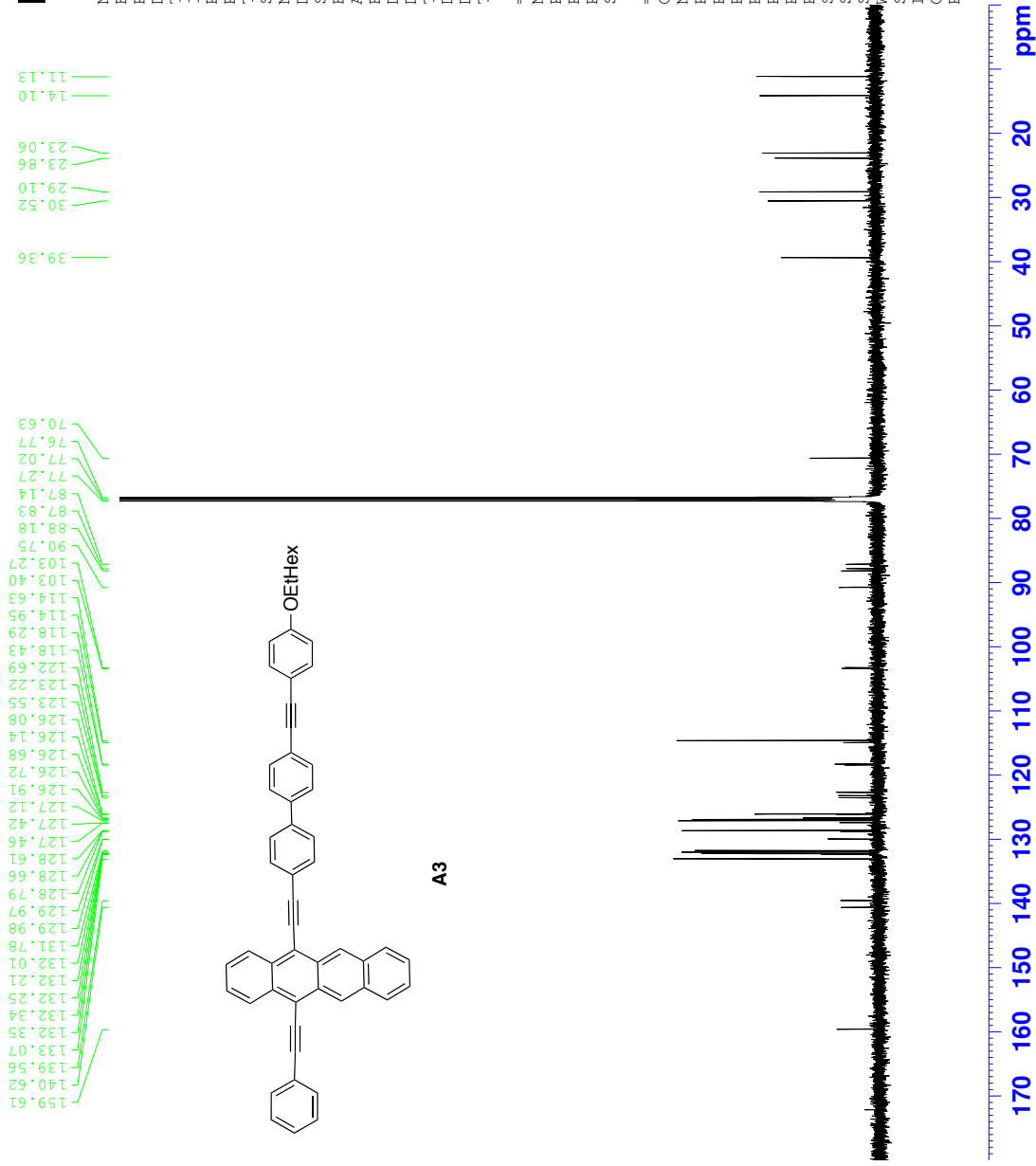
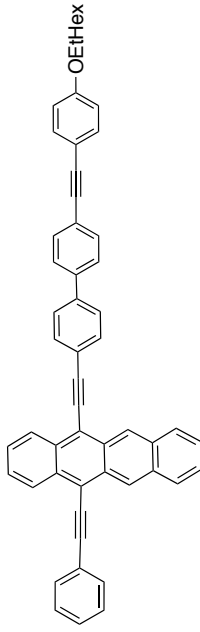
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9.342
8.748
8.744
8.720
8.177
8.147
7.960
7.943
7.894
7.880
7.788
7.771
7.711
7.652
7.636
7.627
7.619
7.608
7.553
7.476
7.286
6.935
6.917
3.906
3.904
3.895
3.892
1.794
1.782
1.745
1.561
1.354
1.278
1.278
0.984
0.930



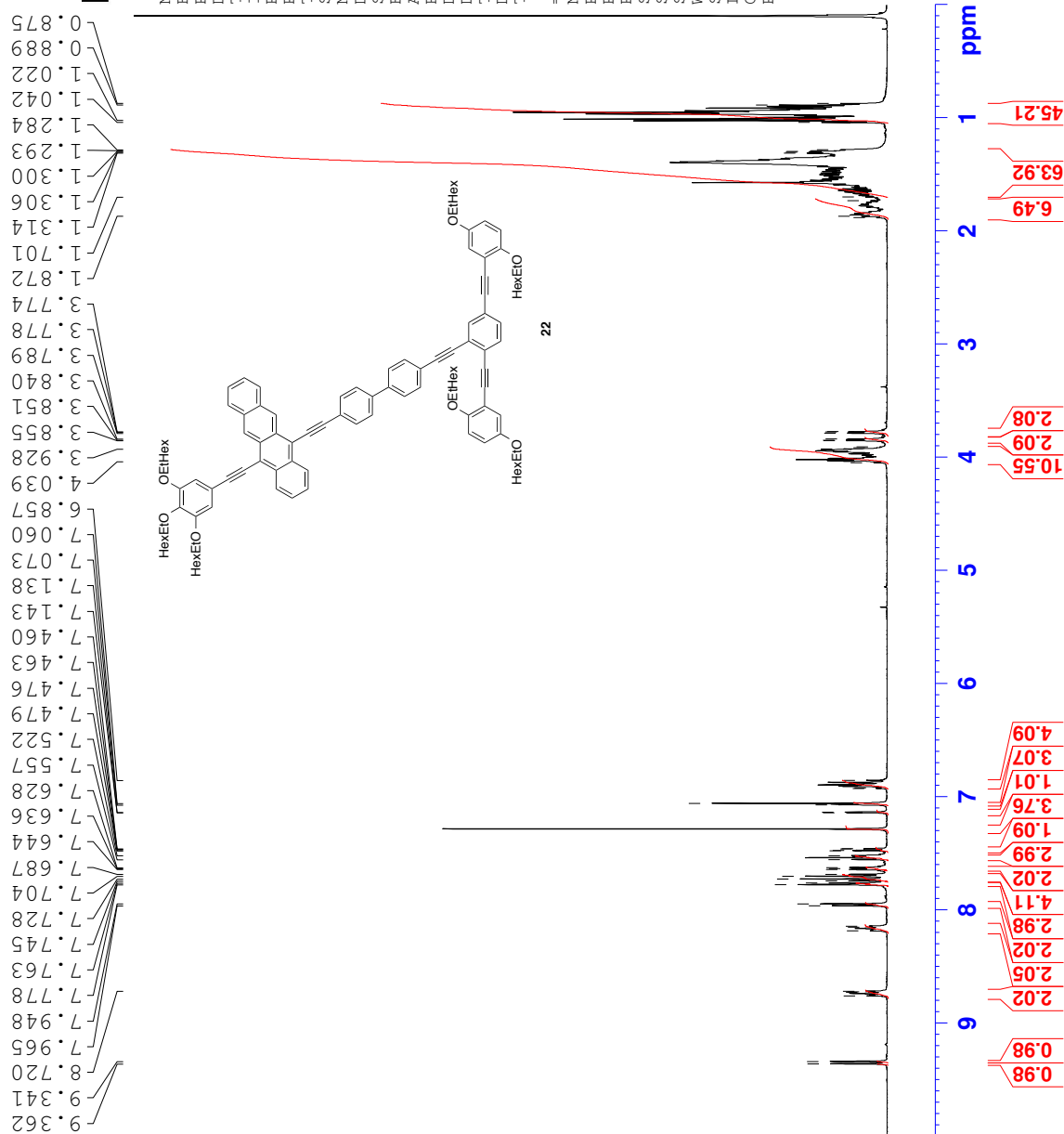
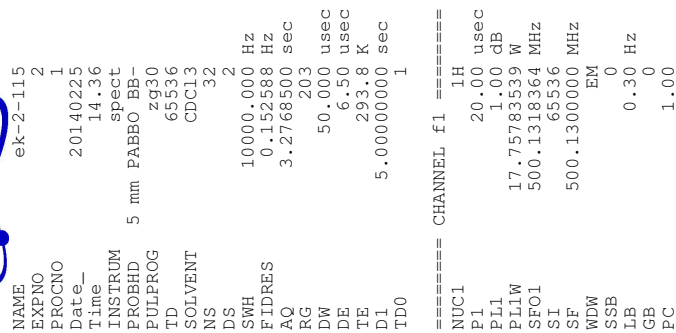
A3

10 9 8 7 6 5 4 3 2 1 ppm

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1.97
1.98
2.01
1.99
2.19
4.36
2.11
7.21
6.41
2.07
2.12
1.11
10.27
6.57



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	500.13200005 MHz
SI	65536
SF	125.7577890 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	0.10

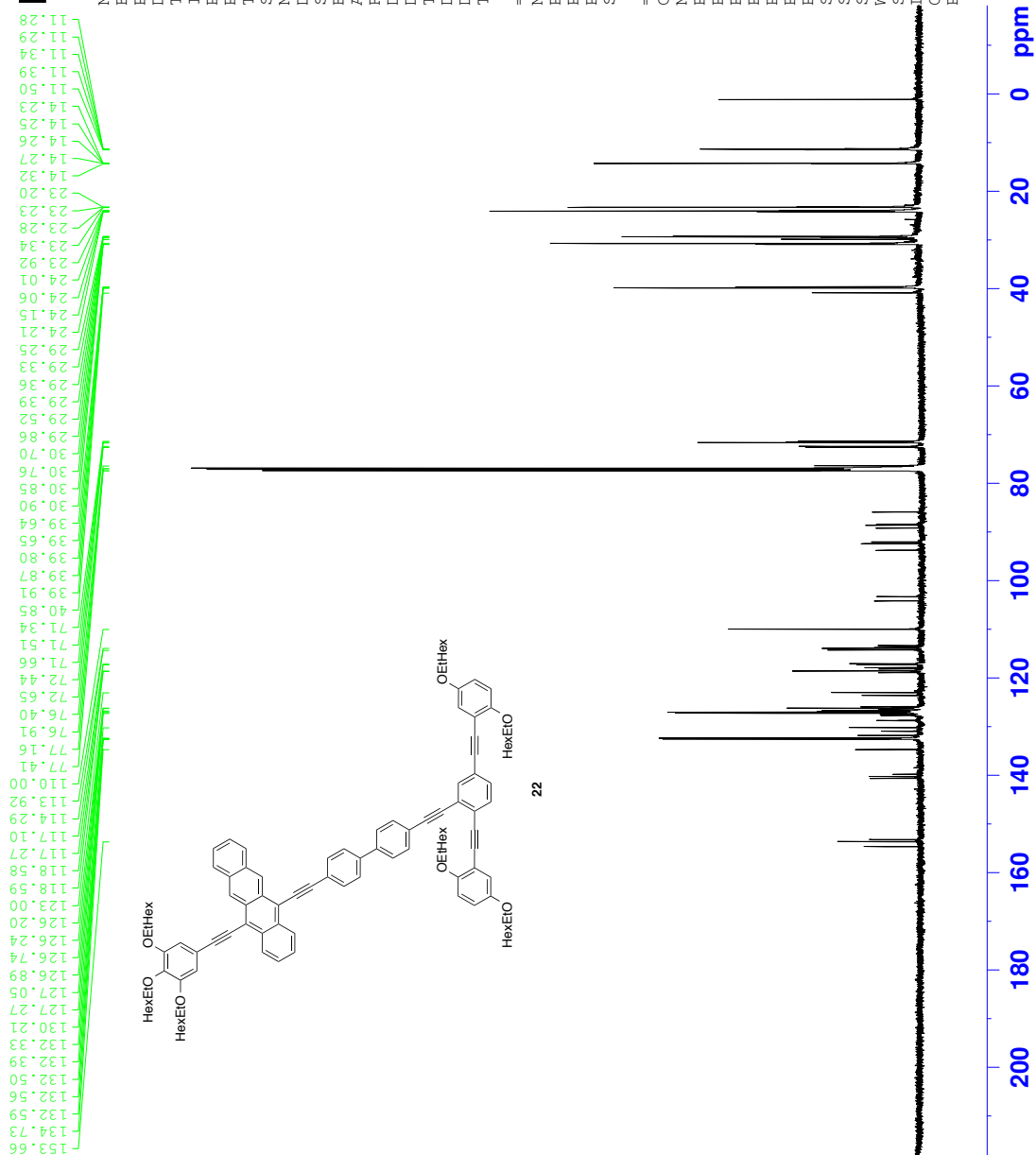




NAME	ek-2-115
EXPNO	7
PROCNO	1
Date_	20140415
Time	17:42
INSTRUM	spect
5 mm PABBO BS-	
PROBHD	zpg9
PULPROG	65536
TD	CDCL3
NS	33378
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.0110548 sec
RG	203
DE	16.800 usec
DE	6.50 usec
TE	300.3 K
DD1	0.50000000 sec
DD11	0.03000000 sec
TD0	40

```
===== CHANNEL f1 =====
NUC1      13C
P1        9.50 usec
PL1       0.00 dB
PL1W      89.92553711 W
SF01     125.7703643 MHz
```

=====	CHANNEL f2	=====
CDPRG2	waltz16	
NUC2	IH	
PCFD2	80.00 usec	
Pf2	1.00 dB	
PL12	13.04 dB	
PL13	16.80 dB	
PL11	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 0.5000000 sec
TD0 1

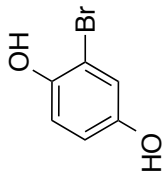
===== CHANNEL f1 =====
NUC1 1H
P1 20.00 usec
PL1 1.00 dB
PL1W 17.75783539 W
SF01 500.1318364 MHz
SI 65536
SF 500.1300185 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1.727

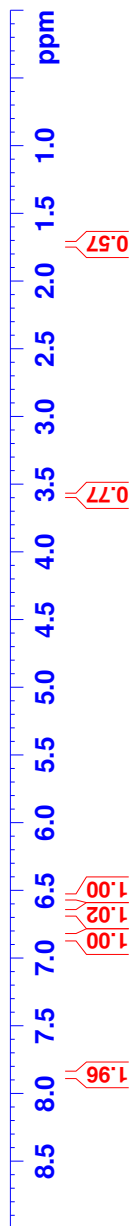
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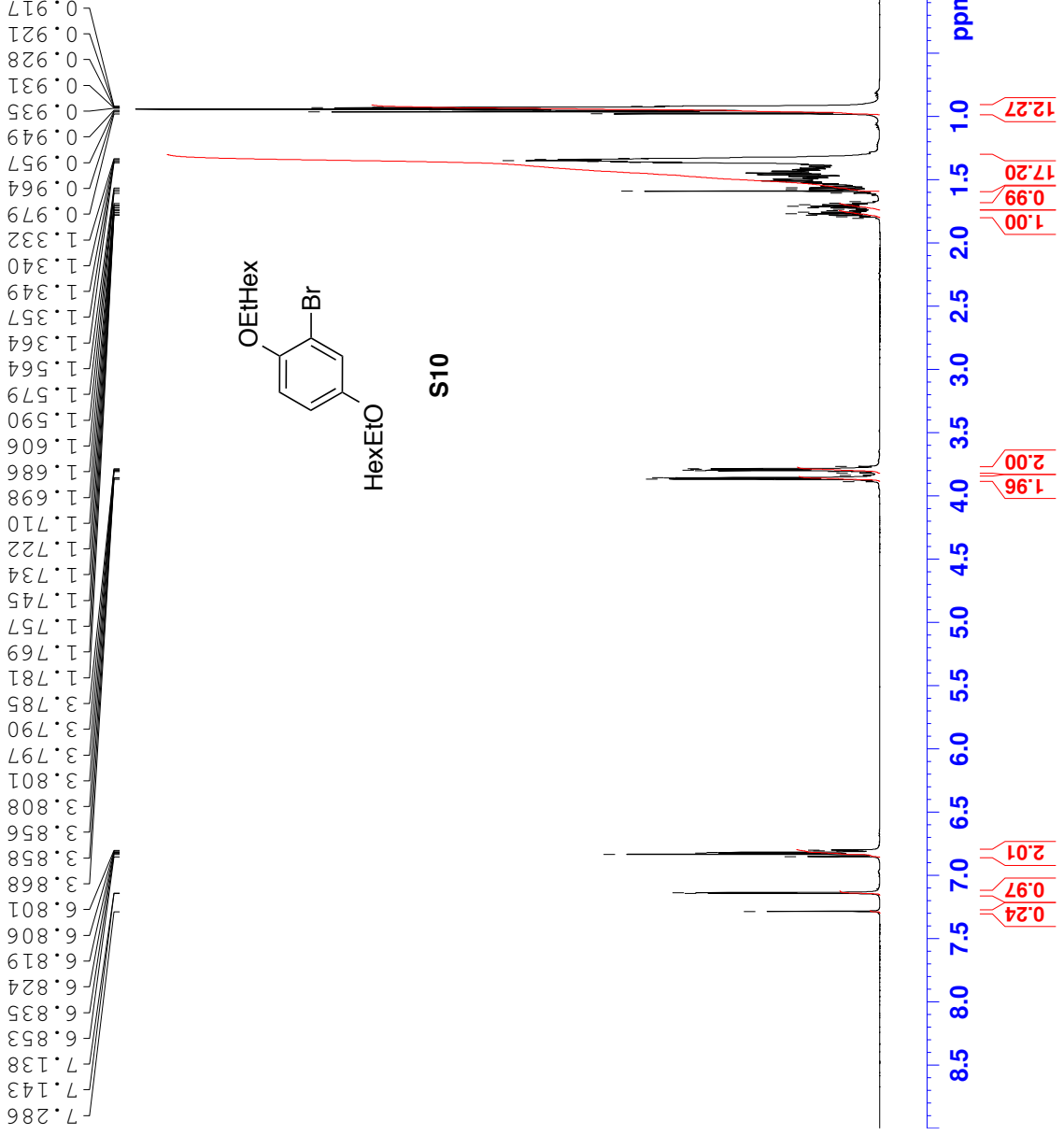
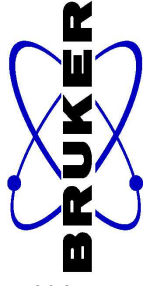
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6.874
6.657
6.559
6.553
6.541
6.536

7.861



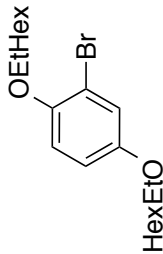
S9







153.75
149.94
119.52
114.34
114.29
112.73
77.28
77.02
76.77
72.45
71.33
39.52
39.41
30.50
29.09
23.89
23.83
23.06
14.10
11.18
11.10



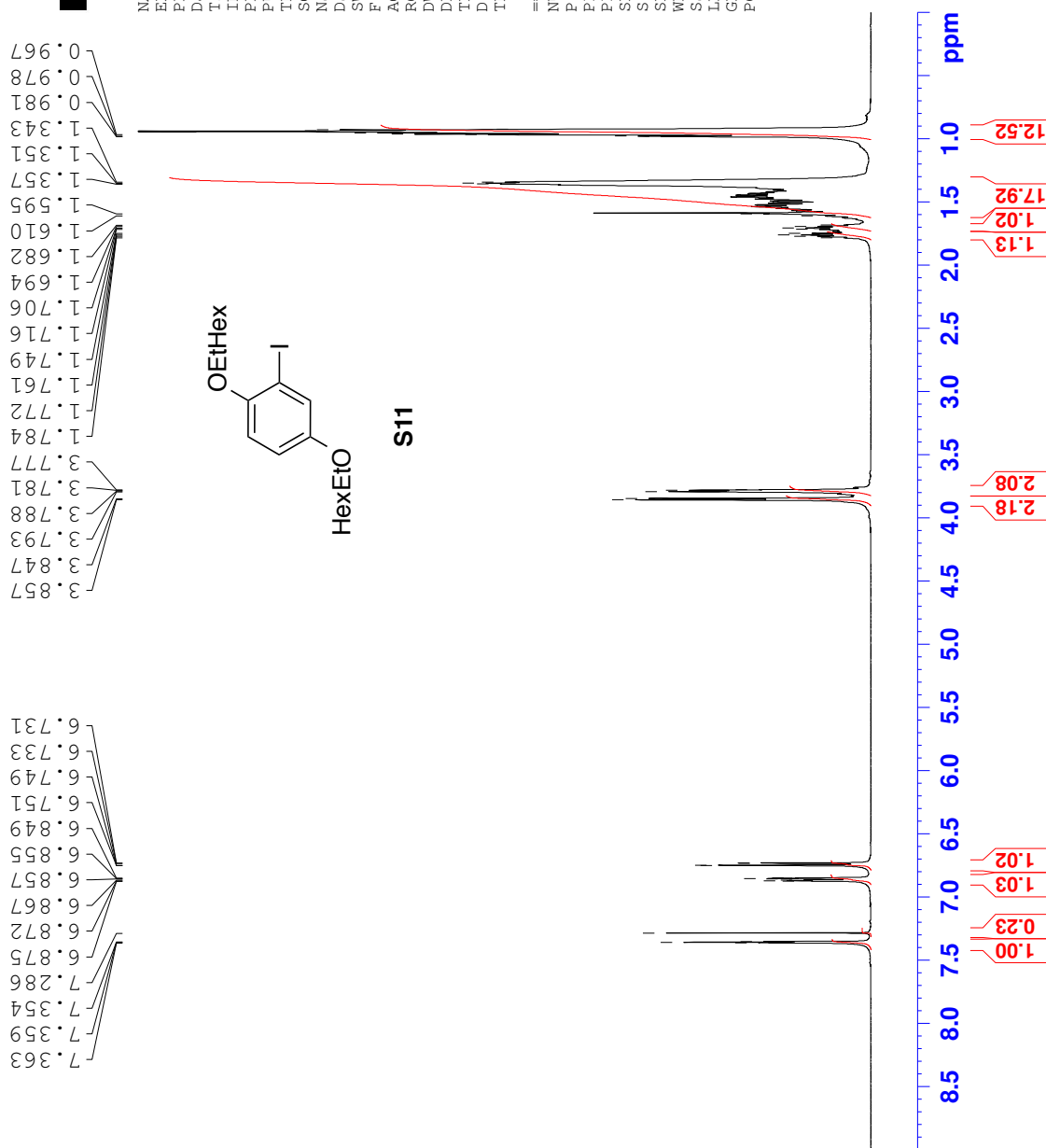
S10

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

ppm



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 CDC13
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 0.5000000 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-2-078

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

SF 65536

SI 125.7577890 MHz

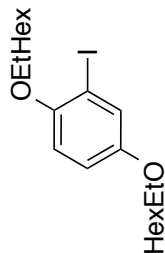
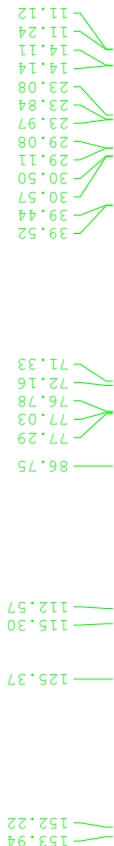
WDW EM

SSB 0

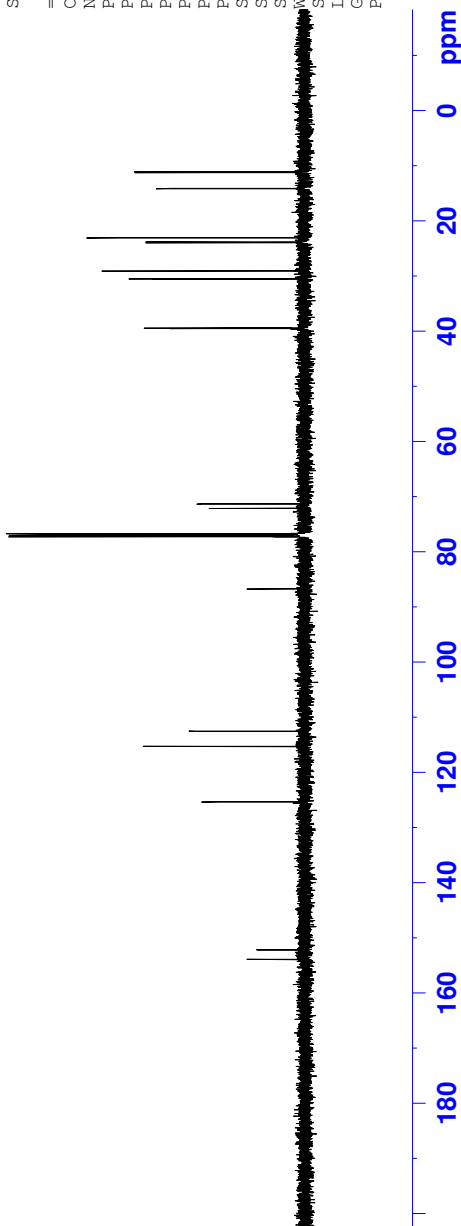
LB 1.00 Hz

GB 0

PC 1.40

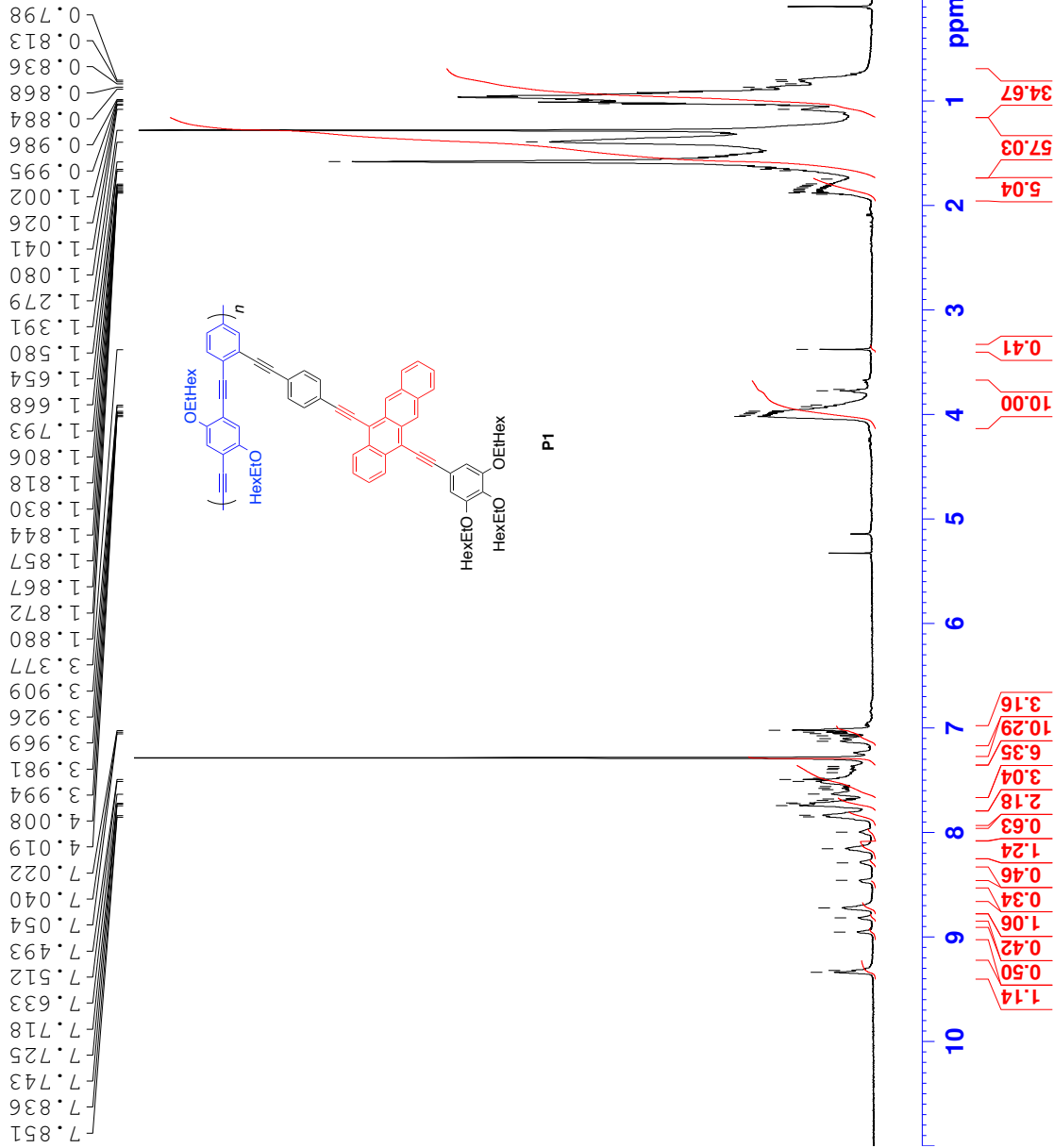


S11





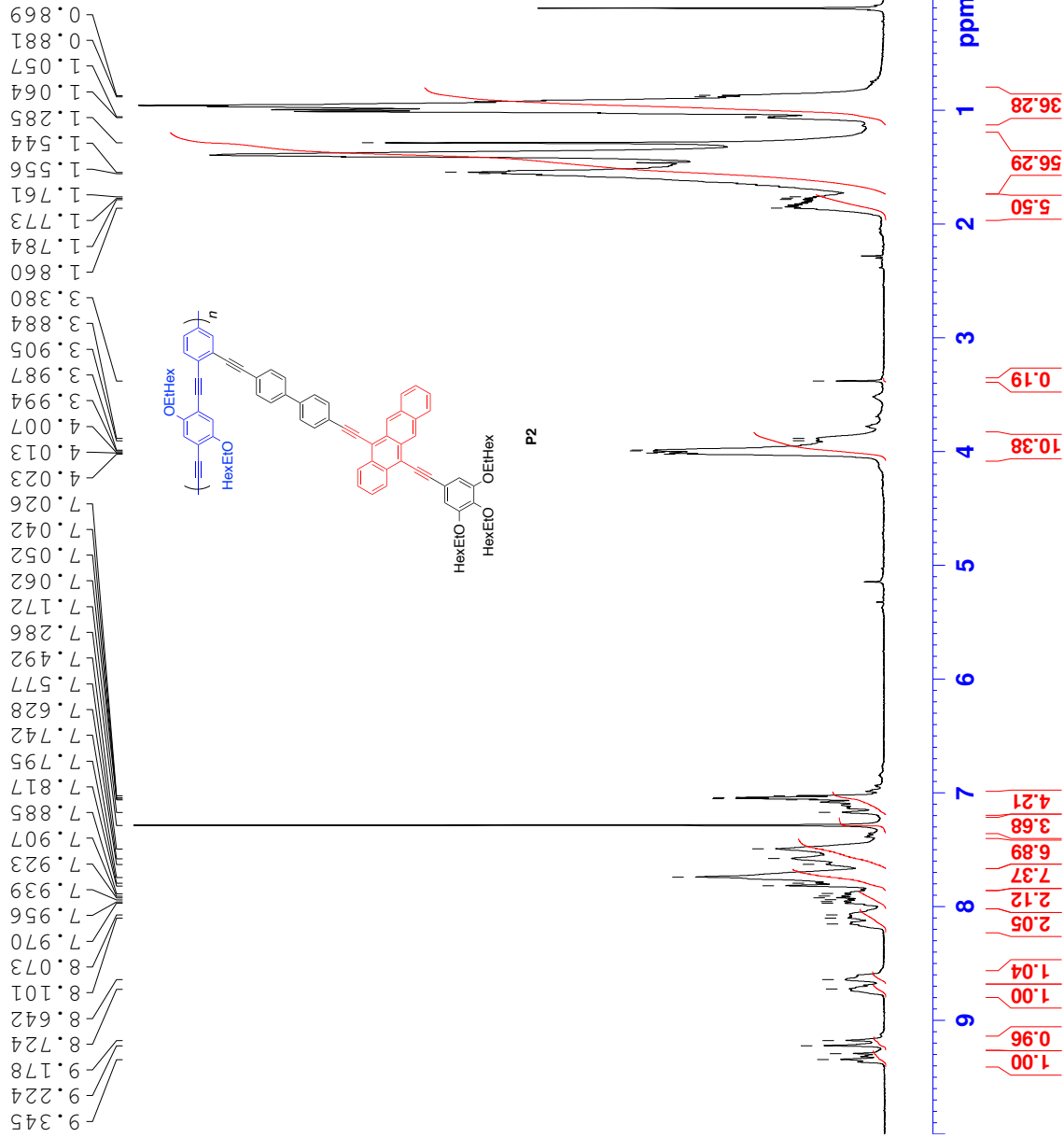
NAME ek-2-129
EXNO 1
PROCNO 1
Date_ 20140403
Time 13.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 254
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 293.6 K
D1 5.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 20.00 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

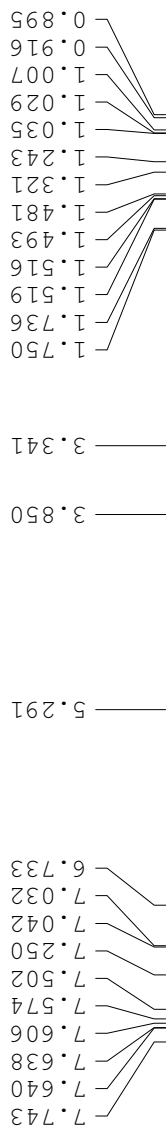




NAME PPE-TET
EXPNO 1
PROCNO 1
Date_ 20131205
Time 15.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 67
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 300.0 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 20.00 usec
PL1 1.00 dB
PL1W 17.75783539 W
SF01 500.1318364 MHz
SI 65536
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

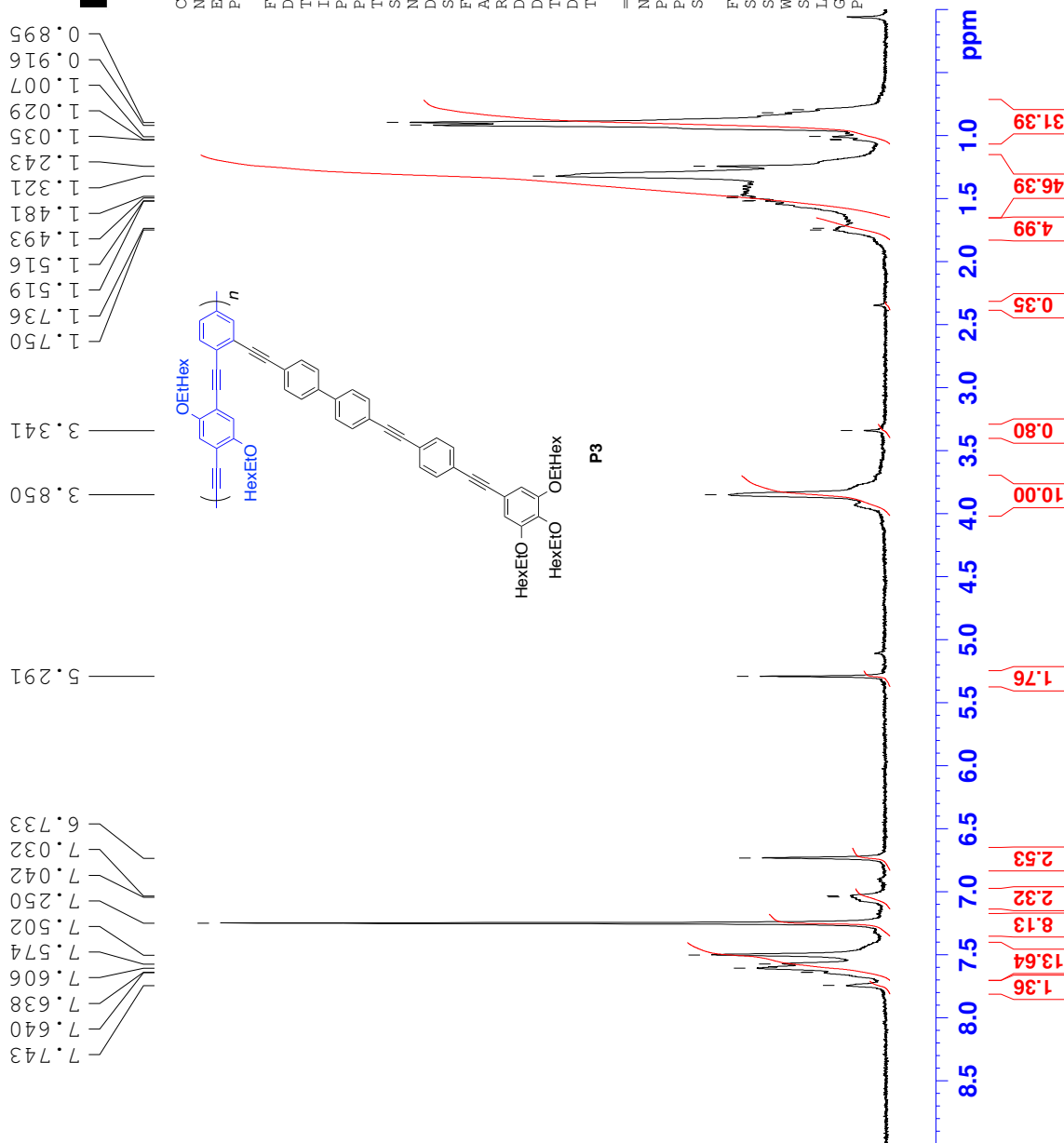


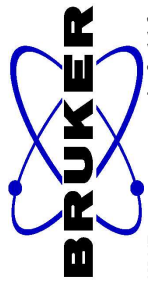


F2 - Acquisition Parameters

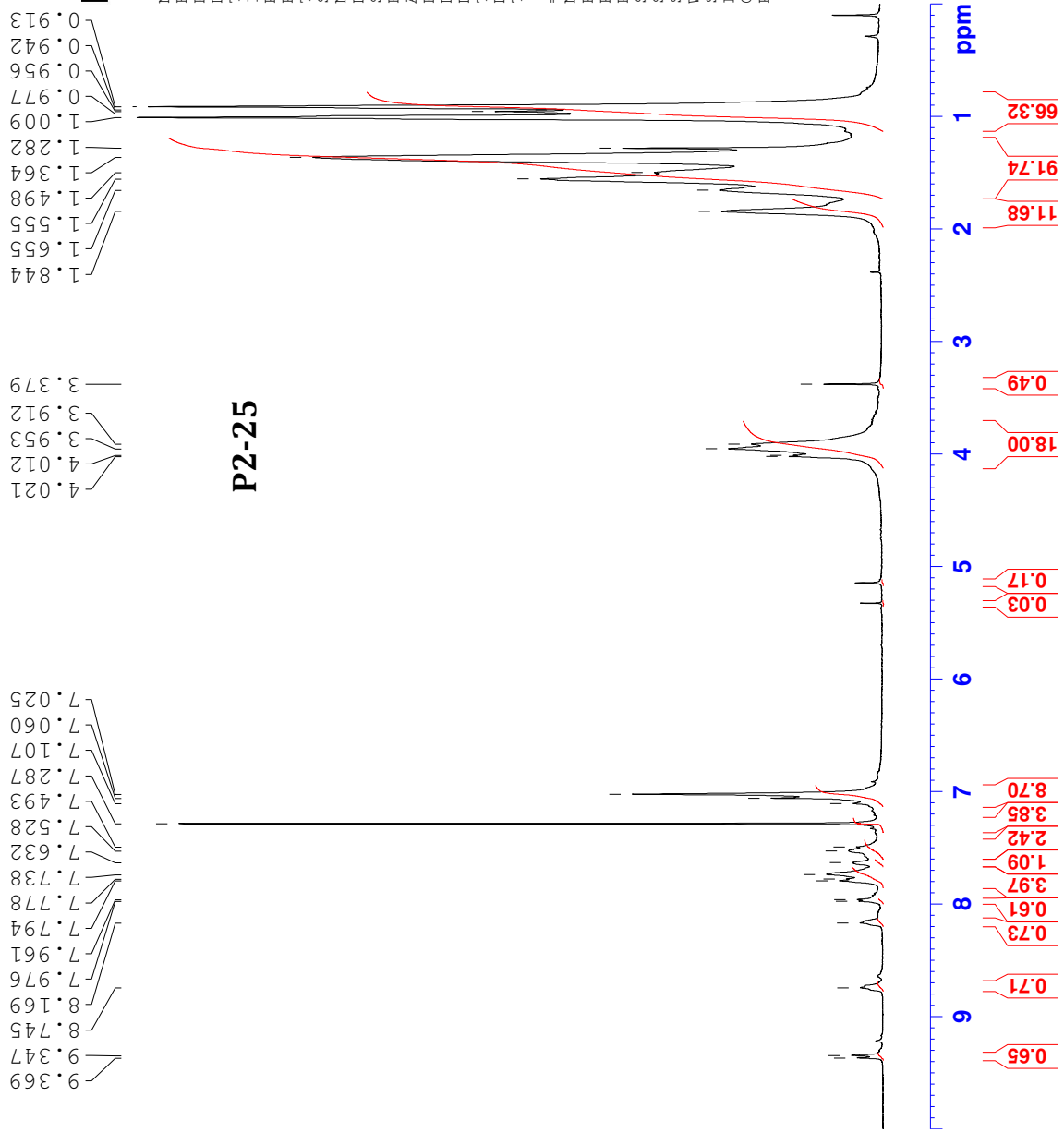
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===== CHANNEL f1 =====
NUC1      1H
P1        12.00 usec
PL1       0.00 dB
SF01      300.3418547 MHz
```

F2 - Processing parameters	
SI	32768
SF	300.340067 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	0.20

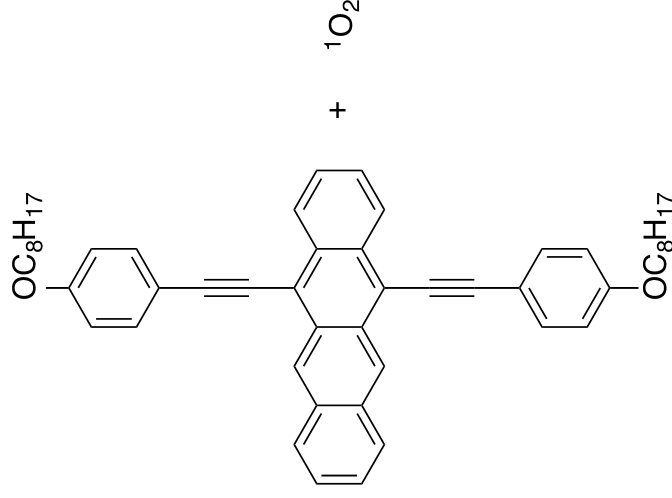




NAME ek-2-116
EXPNO 2
PROCNO 1
Date_ 20140228
Time 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 64
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2768500 sec
RG 203
DW 50.000 usec
DE 6.50 usec
TE 293.6 K
D1 5.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 20.00 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

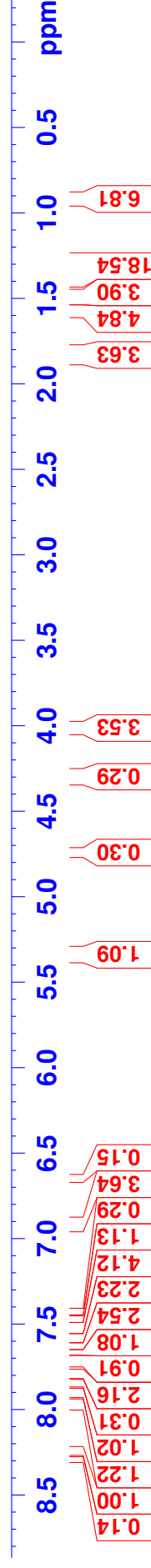
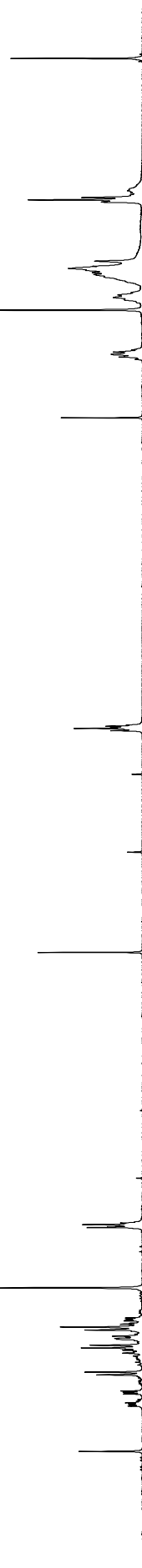


ek-1-296 t=3 h MB removed



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
PC 1.00

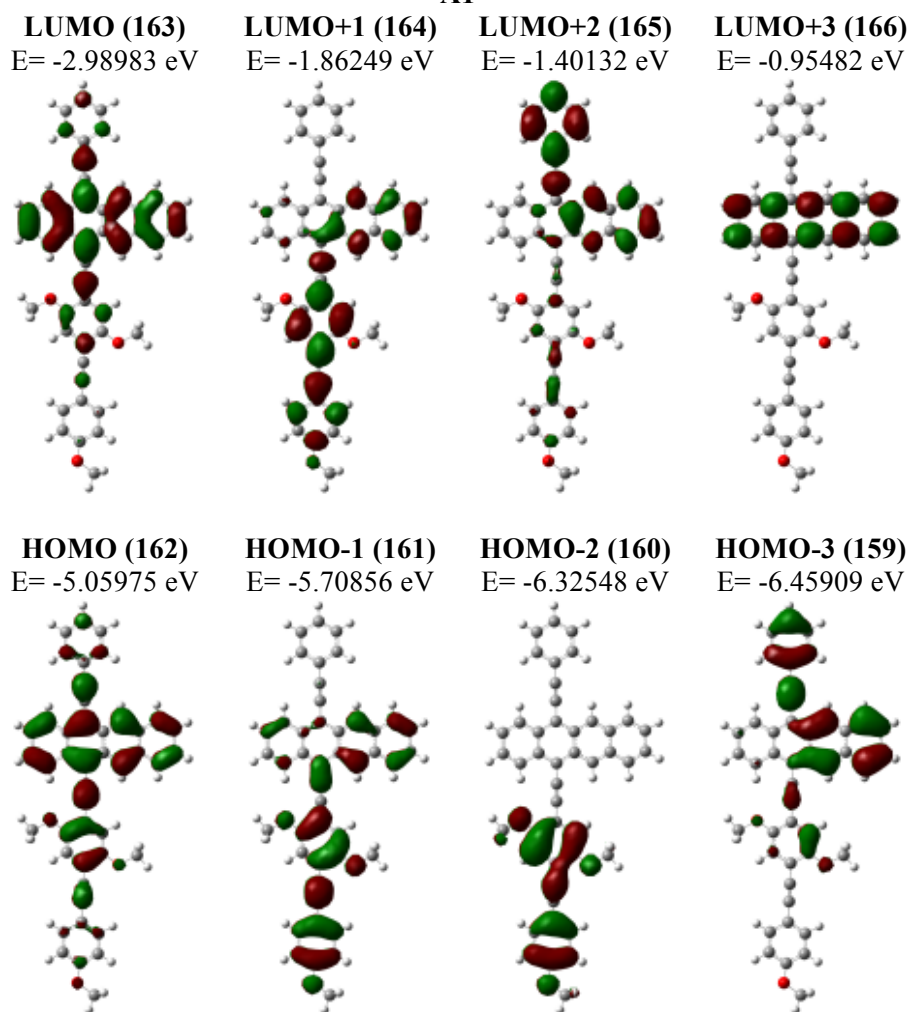


DFT Calculations

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.

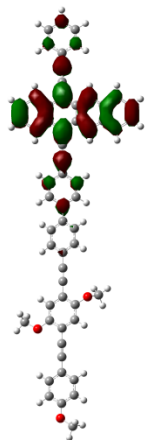
A1



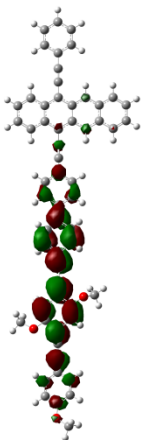
Excited State	Transition	f	λ (nm)	E (eV)
1	162→163 (94 %)	1.5942	624.53	1.9852
3	162→164 (79 %)	0.4557	423.61	2.9269
4	159→163 (54 %), 160→163 (25 %)	0.271	409.33	3.0289
5	160→163 (72 %), 159→163 (23 %)	0.2062	407.37	3.0435
7	162→165 (66 %)	0.3056	365.13	3.3956
9	161→164 (58 %), 156→163 (20 %)	0.3148	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

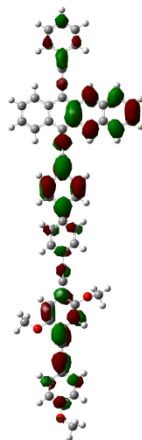
LUMO (209)
E= -3.02202 eV



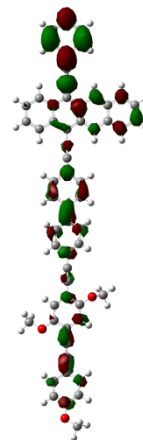
LUMO+1 (210)
E= -2.23998 eV



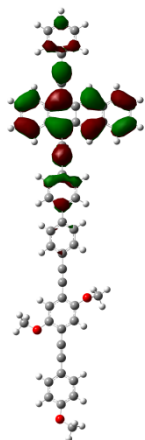
LUMO+2 (211)
E= -1.6287 eV



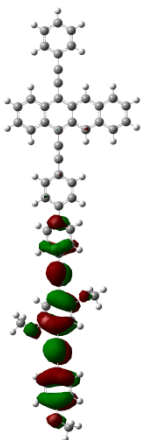
LUMO+3 (212)
E= -1.37803 eV



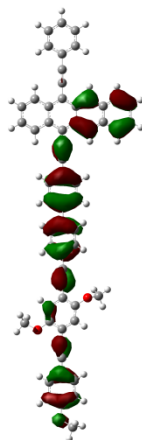
HOMO (208)
E= -5.16429 eV



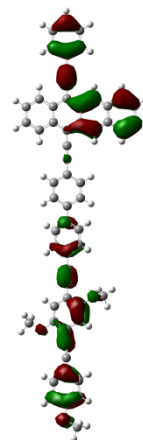
HOMO-1 (207)
E= -5.58023 eV



HOMO-2 (206)
E= -6.26396 eV

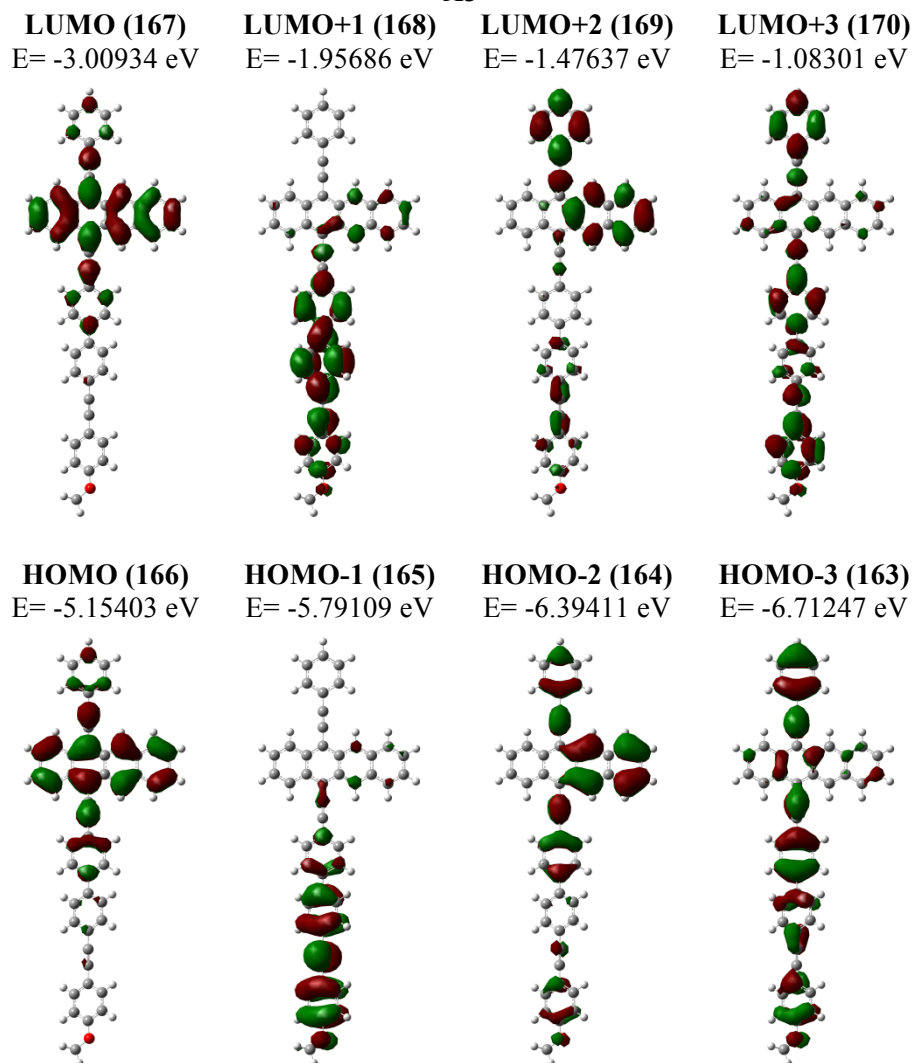


HOMO-3 (205)
E= -6.49949 eV

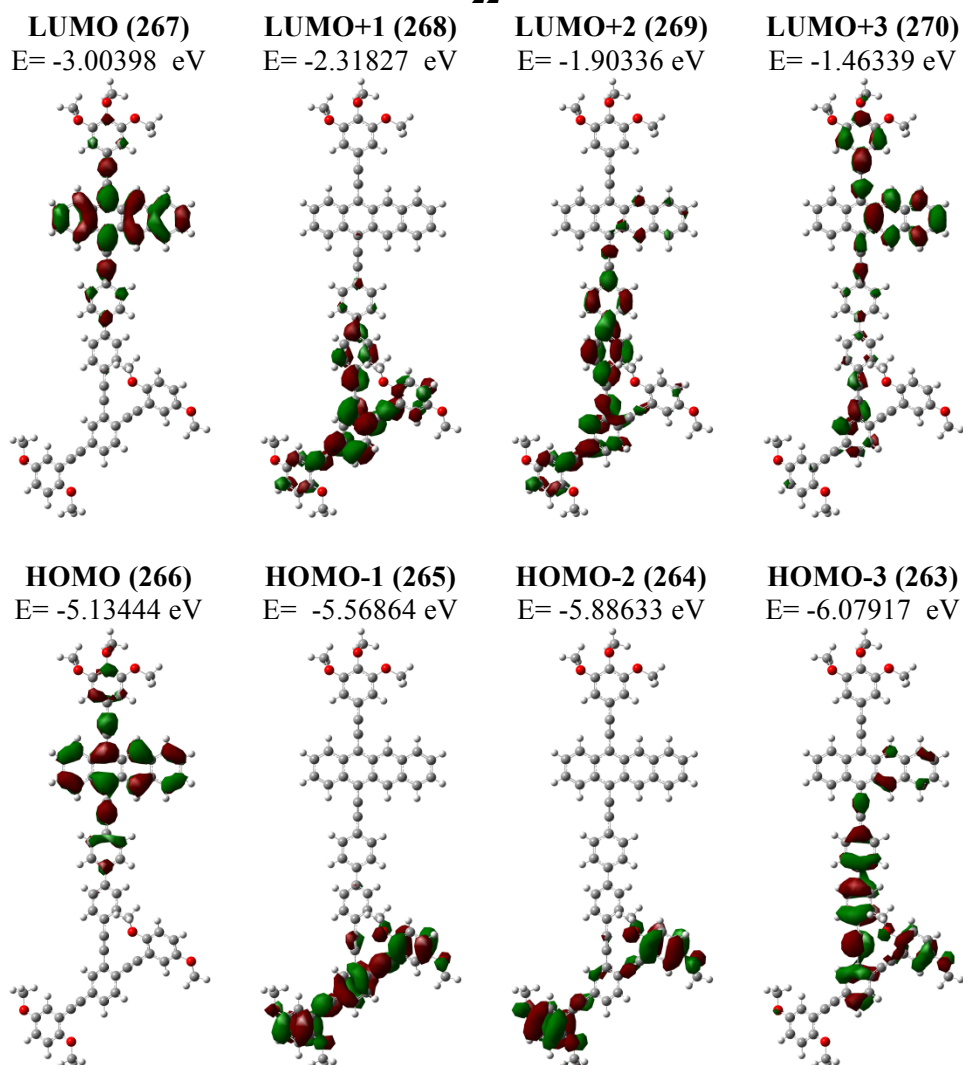


Excited State	Transition	f	λ (nm)	E (eV)
1	208→209 (94 %)	1.602	597.68	2.0744
3	208→210 (91 %)	0.2803	454.81	2.7261
4	206→209 (68 %)	0.7195	431.53	2.8731
5	207→210 (62 %)	1.3442	401.64	3.087
6	205→209 (34 %), 207→210 (27 %)	0.3251	392.68	3.1574
13	207→211 (48 %), 206→210 (42 %)	0.3195	331.95	3.735
26	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



Excited State	Transition	<i>f</i>	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



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