Helical Conjugated Ladder Polymers: Synthesis, Characterization and Carbon Nanotubes Wrapping

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TABLE OF CONTENT

GENERAL METHODS

Chemical reagents were supplied by Sigma-Aldrich Co. Canada, Alfa Aesar Co., TCI America Co. or Oakwood Products Inc. and were used as received. Toluene (Tol), tetrahydrofuran (THF) and dichloromethane (DCM) used for organic synthesis were purchased from Fisher Chemical Co., EMD Millipore Co. and CFS Chemical Co. as HPLC grade. These solvents were degassed, dried and purified with a Solvent Purifier System (SPS) (Vacuum Atmosphere Co., Hawthorne, USA) prior to their use. Anhydrous decahydronaphtalene (decalin, mixture of cis/trans) was used as received for photochemical reactions and other anhydrous solvents were bought from Sigma-Aldrich Co. Canada. Anhydrous and air sensitive reactions were launched in oven-dried pressure vessels purchased from Synthware™. These reactions were performed under positive nitrogen stream. Analytical thin-layer chromatographies were performed with silica gel 60 F254, 0.25 mm pre-coated TLC (Silicycle, Québec, Canada). Compounds were revealed by a 254 nm and/or 365 nm UV wavelength and/or aqueous K_2CO_3 and NaOH solution of potassium permanganate. Purification steps were performed through flash column chromatography with 230-400 mesh silica gel R10030B (Silicycle, Québec, Canada). 2,3-dichloro-1,4-iodobenzene was synthesized according to literature procedures and further purified by recrystallization in *i*PrOH.[1]

APPARATUS

Photochemical reactions were performed in a CCP-ICH2 Luzchem® photochemical reactor equipped with a thermostat and a heating mantle. Photochemical reactions were conducted in a 50 mL quartz round-bottom flask bought from Chemglass®. Nuclear magnetic resonance (NMR) spectra were recorded on a Varian Inova AS400 spectrometer (Varian, Palo Alto, USA) at 400 MHz (^{1}H) and 100 MHz (^{13}C) and an Agilent DD2 spectrometer at 500 MHz (^{1}H), 126 MHz (^{13}C). Chemical shifts were reported as values (ppm) relative to residual solvent peak. High-resolution mass spectra (HRMS) were recorded with an Agilent 6210 Time-of-Flight (TOF) LC-MS apparatus equipped with an APPI ion source (Agilent Technologies, Toronto, Canada). Number-average (M_n) and weight-average (M_w) molecular weights were obtained by size exclusion chromatography (SEC) using a high temperature Varian Polymer Laboratories GPC220 equipped with an RI detector. The column set consists of 2 PL gel Mixed C (300 x 7.5 mm) columns and a PL gel Mixed C guard column. The flow rate was mixed at 1 mL min^{-1} using 1,2,4-trichlorobenzene (TCB) (with 0.0125% BHT w/v) as the eluent. The temperature of the system was set to 110 $^{\circ}$C. All the samples were prepared at a nominal concentration of 1.0 mg mL^{-1} in TCB. Dissolution was performed using a Varian Polymer Laboratories PL-SP 260VC sample preparation system. The sample vials were held at 110 ºC with shaking for 1 h for complete dissolution. The solutions were filtered through a 2 mm porous stainless steel filter used with a 0.40 mm glass filter into a 2 mL chromatography vial. The calibration method used to generate the reported data was the classical polystyrene method using polystyrene narrow standards Easi-Vials PS-M from Varian Polymer Laboratories which were dissolved in TCB. FT-IR spectra were recorded in ATR mode on Infrared spectrometer (Thermo-Nicolet Magne 850) equipped with Golden Gate. UV-visible absorption and photoluminescence spectra were recorded on a Varian diode-array spectrophotometer (model Cary 500) and Varian Cary Eclipse Fluorescence Spectrofluorimeter respectively, using 10-mm path length quartz cells.

EXPERIMENTAL SECTION

Prepapration of the borylated monomers (SCHEME 1)

4',6'-Dibromo-4,4''-didodecyl-1,1':3',1''-terphenyl (1)

To a pressure vessel charged with 1,5-dibromo-2,4-diiodobenzene (1.50 g, 2.55 mmol), 4-dodecylphenyl-1-boronic ester (2.52 g, 6.77 mmol.) and K_2CO_3 (1.87 g, 13.5 mmol) was added DME (9.3 mL) and H_2O (1.2 mL). The mixture was degassed for 10 minutes with a nitrogen stream. $PdCl_2(PPh_3)_2$ (32.4 mg, 46.1 μmol) was added and the reaction mixture was further degassed for 10 minutes. The flask was stirred at 100 °C for 24 hours. Once cooled to room temperature, the reaction mixture was dissolved with EtOAc (20 mL) and a saturated solution of NH_4Cl (20 mL) was added. The aqueous phase was extracted three times with EtOAc, the organic layers were combined, washed with brine and dried over Na_2SO_4. The solvent was evaporated and the crude material was purified by silica gel chromatography (hexanes) to afford the expected product (1.00 g, 45%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (s, 1H), 7.34 (d, 4H, *J* = 8.1 Hz), 7.31 (s, 1H), 7.23 (d, 4H, *J* = 8.2 Hz), 2.65 (t, 4H, *J* = 7.7 Hz), 1.65 (q, 4H, *J* = 8.3 Hz), 1.40-1.23 (bm, 36H), 0.89 (t, 6H, *J* = 7.0 Hz). ^{13}C NMR (126 MHz, $CDCl_3$): δ 139.63, 134.62, 108.75, 34.42, 31.93, 31.42, 31.20, 29.66, 29.36, 29.08, 22.69, 14012, 13.88.

4',6'-Bis-(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)-4,4''-didodecyl-1,1':3',1''-terphenyl (2)

A dry flask under nitrogen was charged with compound **1** (800 mg, 1.10 mmol), $PdCl_2$DtBPF (28.7 mg, 44.2 μmol) and flushed 3 times with a vacuum/nitrogen cycle. Anhydrous dioxane (5.5 mL) and triethylamine (1.23 mL, 8.83 mmol) were separately degassed using a continuous flow of nitrogen for 10 min and transferred via syringe to the

reaction flask. 4,4,5,5-Tetramethyl-1,2,3-dioxaborolane (0.640 mL, 4.42 mmol) was added, and the reaction mixture was sealed and heated at 85 °C for 24 h. Once cooled to room temperature, a saturated NH_4Cl solution was added and the aqueous layer was extracted 3 times with EtOAc (20 mL). The organic layer was dried over Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was purified by silica gel chromatography (Et_2O/hexanes 4:96) to afford compound **3** as a white solid (0.561 g, 62%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.42 (s, 1H), 7.33 (d, 4H, *J* = 8.2 Hz), 7.16 (d, 4H, *J* = 7.9 Hz), 2.64 (t, 4H, *J* = 7.6 Hz), 1.63 (q, 4H, *J* = 6.8 Hz), 1.37-1.24 (bm, 36H), 1.23 (s, 24H), 0.88 (t, 6H, *J* = 6.6 Hz). ^{13}C NMR (126 MHz, $CDCl_3$): δ 149.29, 141.82, 140.72, 140.58, 129.55, 129.12, 128.03, 83.76, 35.78, 32.08, 31.76, 29.85, 29.81, 29.74, 29.52, 29.37, 24.86, 22.85, 14.29. HRMS (APPI+): calcd for $C_{54}H_{84}B_2O_4$ $(M)^+$ 816.66284, found 816.64826.

5,5'-(4,6-dibromo-1,3-phenylene)bis(2-dodecylthiophene) (3)

To a pressure vessel charged with 1,5-dibromo-2,4-diiodobenzene (2.00 g, 4.10 mmol), 5-dodecylthiophene-2-boronic ester (3.57 g, 9.43 mmol.) and Cs_2CO_3 (12.3 g, 37.7 mmol) was added THF (41 mL) and H_2O (10 mL). The mixture was degassed for 10 minutes with a nitrogen stream. $PdCl_2(PPh_3)_2$ (32.4 mg, 46.1 μmol eq.) was added and the reaction mixture was further degassed for 10 minutes. The flask was stirred at 80 °C for 24 hours. Once cooled to room temperature, the reaction mixture was dissolved with EtOAc (20 mL) and a saturated solution of NH_4Cl (20 mL) was added. The aqueous phase was extracted three times with EtOAc, the organic layers were combined, washed with brine and dried over Na_2SO_4. The solvent was evaporated and the crude material

was purified by silica gel chromatography (hexanes) to afford the expected product (1.96 g, 65 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.56 (s, 1H), 7.15 (d, 2H, *J* = 3.7 Hz), 7.16 (d, 4H, *J* = 3.9 Hz), 2.82 (t, 2H, *J* = 7.6 Hz), 1.71 (q, 4H, *J* = 7.6 Hz), 1.45-1.20 (bm, 36H), 0.88 (t, 6H, *J* = 6.8 Hz). ^{13}C NMR (126 MHz, $CDCl_3$): δ 147.78, 137.87, 137.56, 135.06, 133.79, 127.98, 124.30, 121.34, 32.07, 31.77, 30.30, 29.86, 29.82, 29.80, 29.70, 29.51, 29.33, 22.85, 14.29.

5,5'-(4,6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolane)-1,3-phenylene)bis(2-dodecylthiophene) (4)

A dry flask under nitrogen was charged with compound **3** (1.00 g, 1.36 mmol), $PdCl_2$DtBPF (35.4 mg, 54.2 μmol) and flushed 3 times with a vacuum/nitrogen cycle. Anhydrous dioxane (6.8 mL) and triethylamine (1.51 mL, 10.8 mmol) were separately degassed using a continuous flow of nitrogen for 10 min and transferred via syringe to the reaction flask. 4,4,5,5-Tetramethyl-1,2,3-dioxaborolane (0.788 mL, 5.43 mmol) was added, the reaction mixture was sealed and heated at 85 °C for 24h. Once cooled to room temperature, a saturated NH_4Cl solution was added and the aqueous layer was extracted 3 times with EtOAc (20 mL). The organic layer was dried over Na_2SO_4 and the solvent was evaporated under reduced pressure. The crude product was purified by silica gel chromatography (Et_2O/hexanes 4:96) to afford compound **3** as a white solid (0.710 g, 63%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.51 (s, 1H), 6.94 (d, 2H, *J* = 3.5 Hz), 6.70 (d, 2H, *J* = 3.5 Hz), 2.81 (t, 4H, *J* = 7.4 Hz), 1.68 (q, 4H, *J* = 7.2 Hz), 1.43-1.28 (bm, 36H), 1.27 (s, 24H), 0.88 (t, 6H, *J* = 6.8 Hz). ^{13}C NMR (126 MHz, $CDCl_3$): δ 146.55, 142.11, 141.54, 140.73, 129.74, 126.12, 124.31, 83.92, 32.08, 31.98, 30.40, 29.82, 29.79,

29.74, 29.56, 29.51, 29.27, 24.92, 22.85, 14.28. HRMS (APPI+): calcd for $C_{50}H_{80}B_2O_4S_2$ $(M)^+$ 828.57568, found 828.56556.

Polymerization procedure for P1, P2 (SCHEME 2)

A flask charged with the bisborylated compound (1.00 equiv.), 2,3-dichloro-1,4-diiodobenzene (1.00 equiv.), LiOH•H_2O (8 equiv.), THF (0.2 M) and water (1.0 M). The solution was degassed using a continuous flow of nitrogen for 10 minutes. $Pd_2(dba)_3$•$CHCl_3$ (0.05 equiv.) and SPhos (0.20 equiv.) were added and the flask was flushed 3 times using a vacuum/nitrogen cycle. The reaction mixture was heated at 60 °C for 48 hours. Once cooled to room temperature, the polymer was precipitated in cold MeOH and directly filtered in an extraction thimble. The residue was purified by Soxhlet extraction in acetone for 16 hours and recovered with hexanes through the extraction thimble. The solvent was evaporated with the exclusion of light, dissolved in a minimum amount of hexanes, precipitated in MeOH, filtered and dried under vacuum for 24 h.

Polymer P1 (SCHEME S2)

Compound **2** (0.450 g, 0.550 mmol) and 1,2-dichloro-3,6-diiodobenzene (0.219 g, 0.550 mmol) were copolymerized according to the procedure described above. Polymer **P1** is isolated as a white powder (0.352 g, 90 %).

Polymer P2 (SCHEME S2)

Compound **4** (0.250 g, 0.301 mmol) and 1,2-dichloro-3,6-diiodobenzene (0.120 g, 0.301 mmol) were copolymerized according to the procedure described above. Polymer **P2** is isolated as a white powder (0.188 g, 87 %).

Photochemical cyclodehydrochlorination procedure for the synthesis of *m*-HGNR, *m*-TGNR (SCHEME 2)

Precursor polymer (P1, P2) was dissolved in anhydrous decahydronaphtalene (0.002 M) in a 50 mL quartz round-bottom flask. The solution was degassed with a continuous flow of argon for 10 min. The solution was heated to 125 °C and irradiated with 16 x 7.2 W low pressure Hg lamp at 254 nm or 300 nm for 48 hours while maintaining a continuous flow of argon. Once cooled down to room temperature, the solvent was distillated off and the residue was precipitated from a concentrated hexanes solution in MeOH. The residue was filtered and purified by Soxhlet extraction in acetone. Hexanes was used to recover the expected polymer and concentrated to a minimum amount of solvent. The polymer was precipitated in MeOH, filtered and dried under vacuum for 24 h.

L-P1

This reaction has been carried out in duplicate. Polymer **P1** (0.064 g) was photochemically cyclodehydrochlorinated at 254 nm according to the procedure described above. **L-P1** is isolated as a light orange solid (109.5 mg, 96 %).

L-P2

Polymer **P2** (0.060 g) was photochemically cyclodehydrochlorinated at 300 nm according to the procedure described above. **L-P2** is isolated as a dark orange powder (52.4 mg, 97 %).

NMR SPECTRA

Compound 1

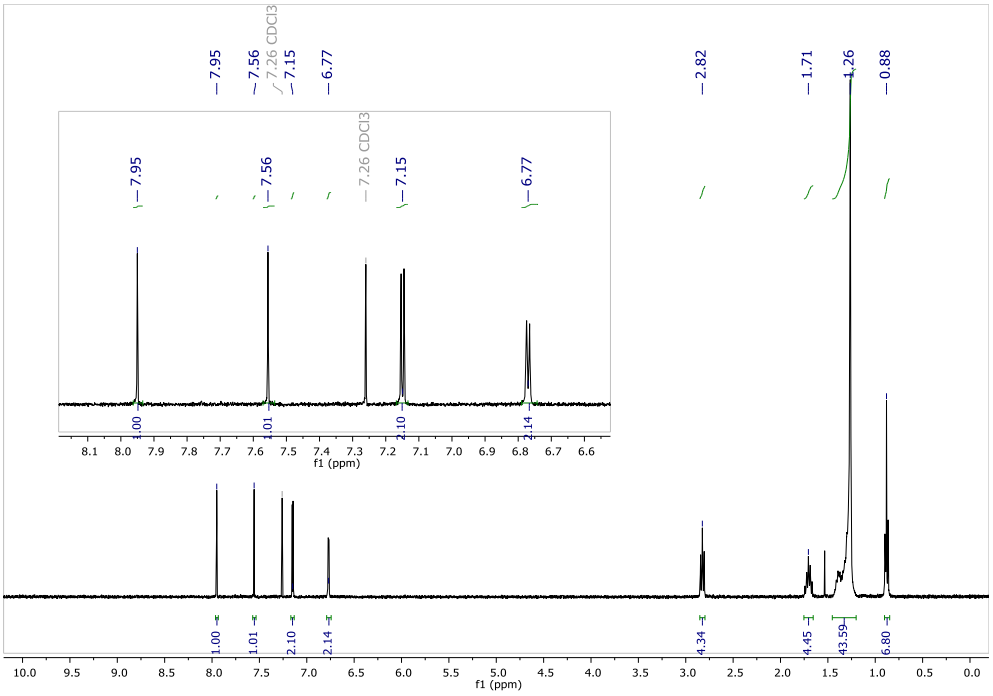

Figure S1: ^{1}H NMR spectrum of compound **1** in $CDCl_3$.

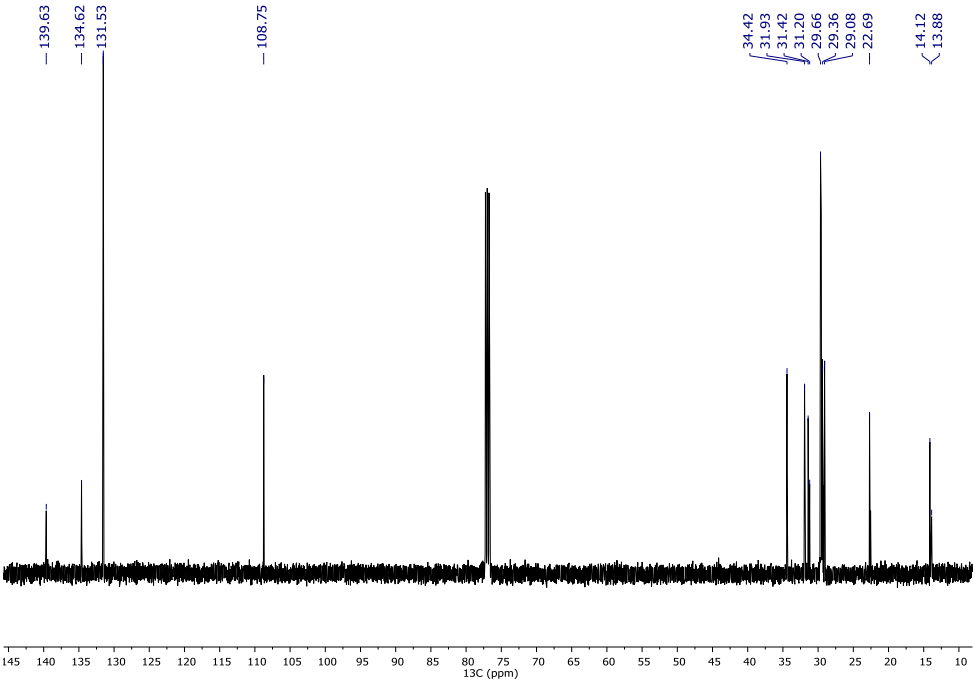

Figure S2 : ^{13}C NMR spectrum of compound **1** in $CDCl_3$.

Compound 2

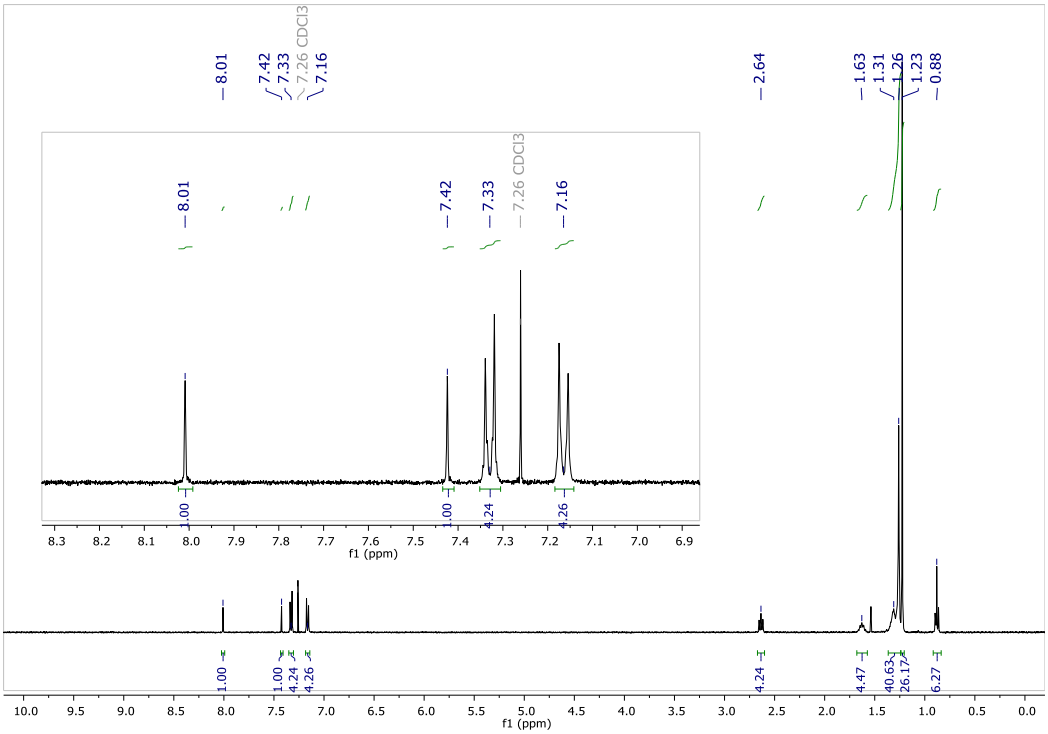

Figure S3: ^{1}H NMR spectrum of compound **2** in $CDCl_3$.

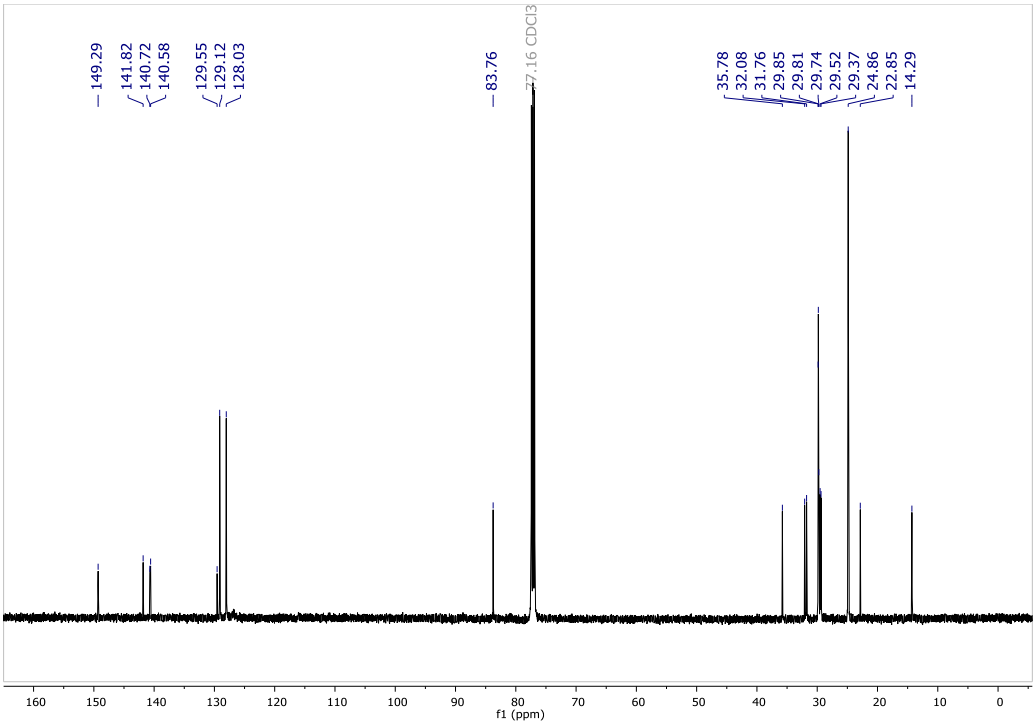

Figure S4 : ^{13}C NMR spectrum of compound **2** in $CDCl_3$.

Compound 3

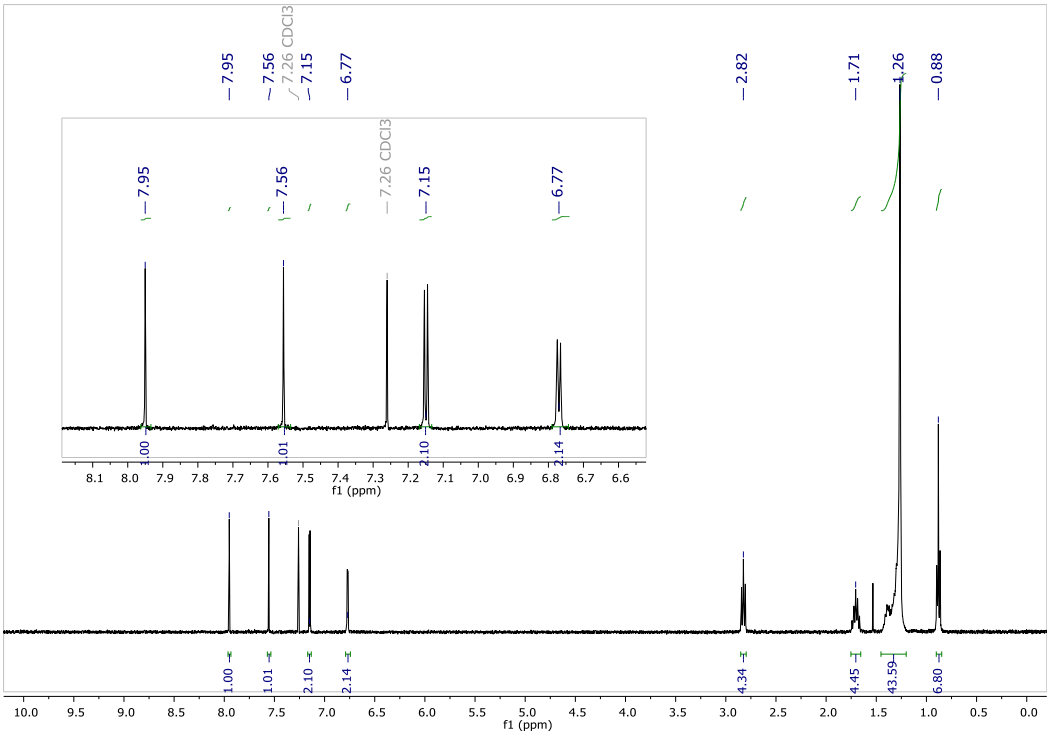

Figure S5 : ^{1}H NMR spectrum of compound **3** in $CDCl_3$.

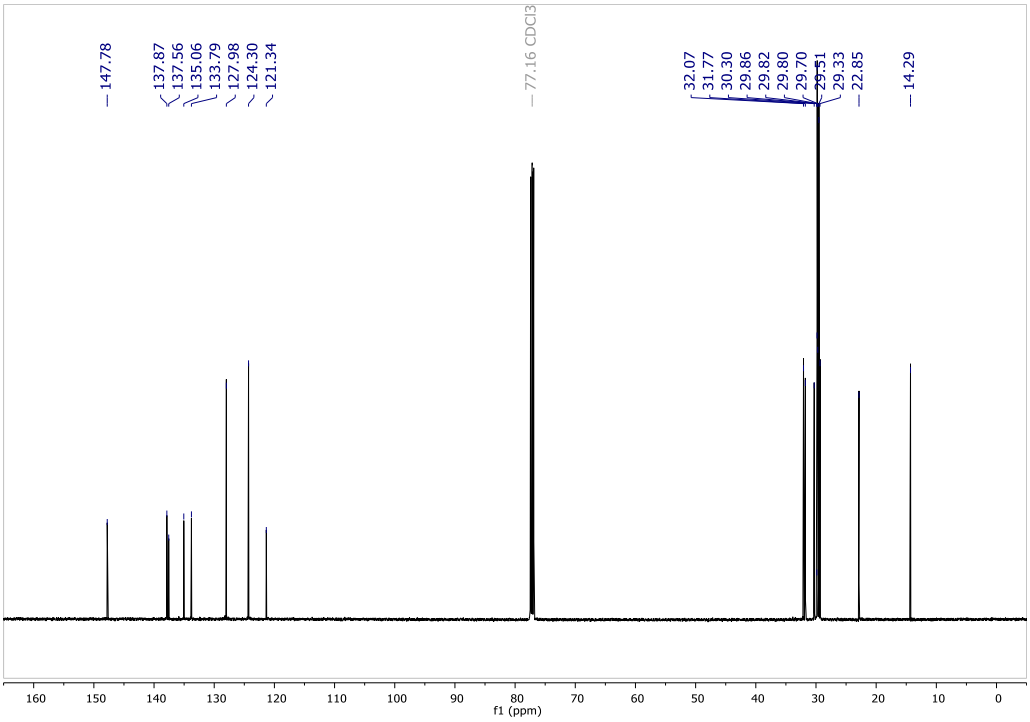

Figure S6 : ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

Compound 4

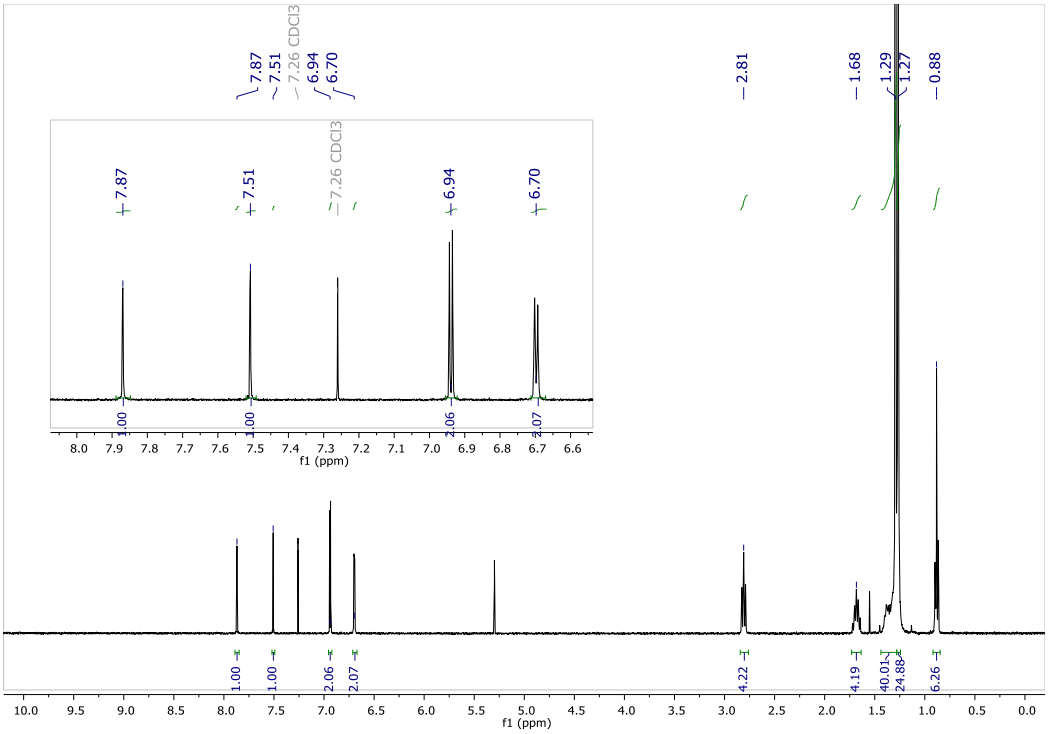

Figure S7 : ^{1}H NMR spectrum of compound **4** in $CDCl_3$.

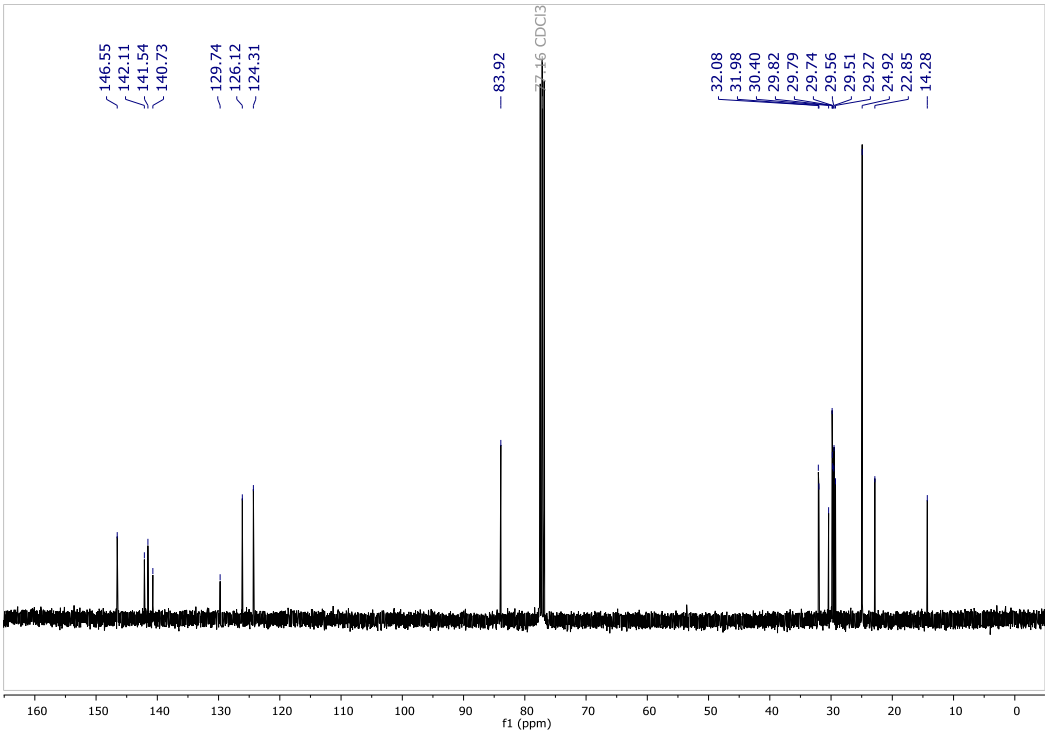

Figure S8: ^{13}C NMR spectrum of compound **4** in $CDCl_3$.

Polymer P1 and L-P1

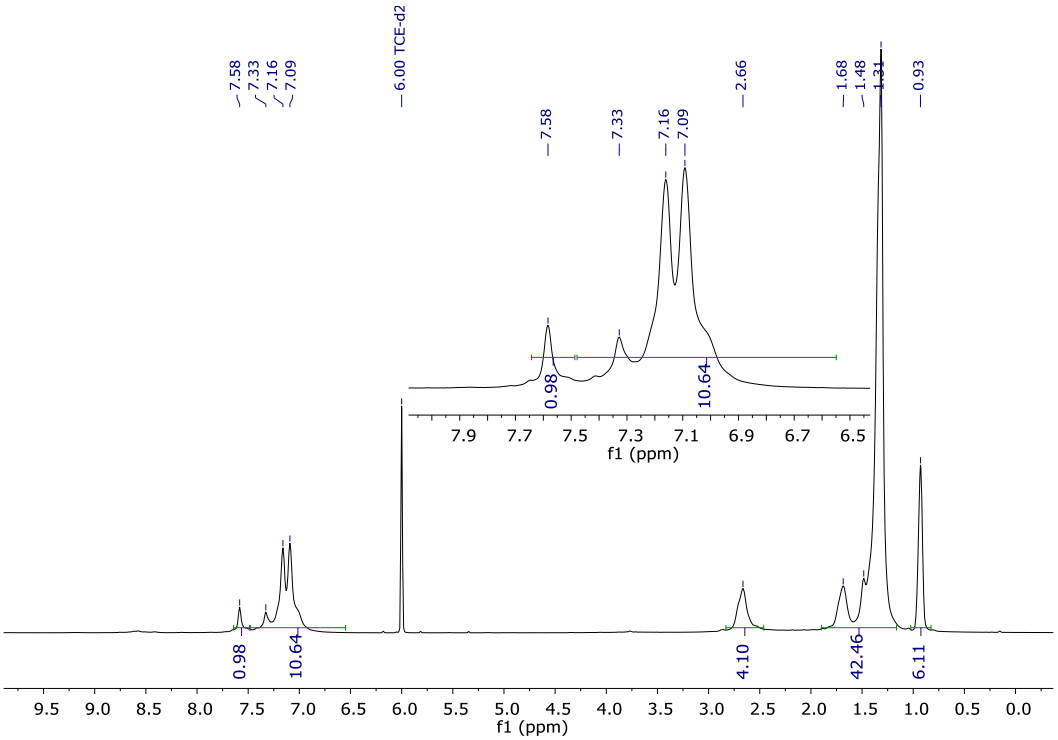

Figure S9 : ^{1}H NMR spectrum of **P1** in TCE-d_2 at 383 K.

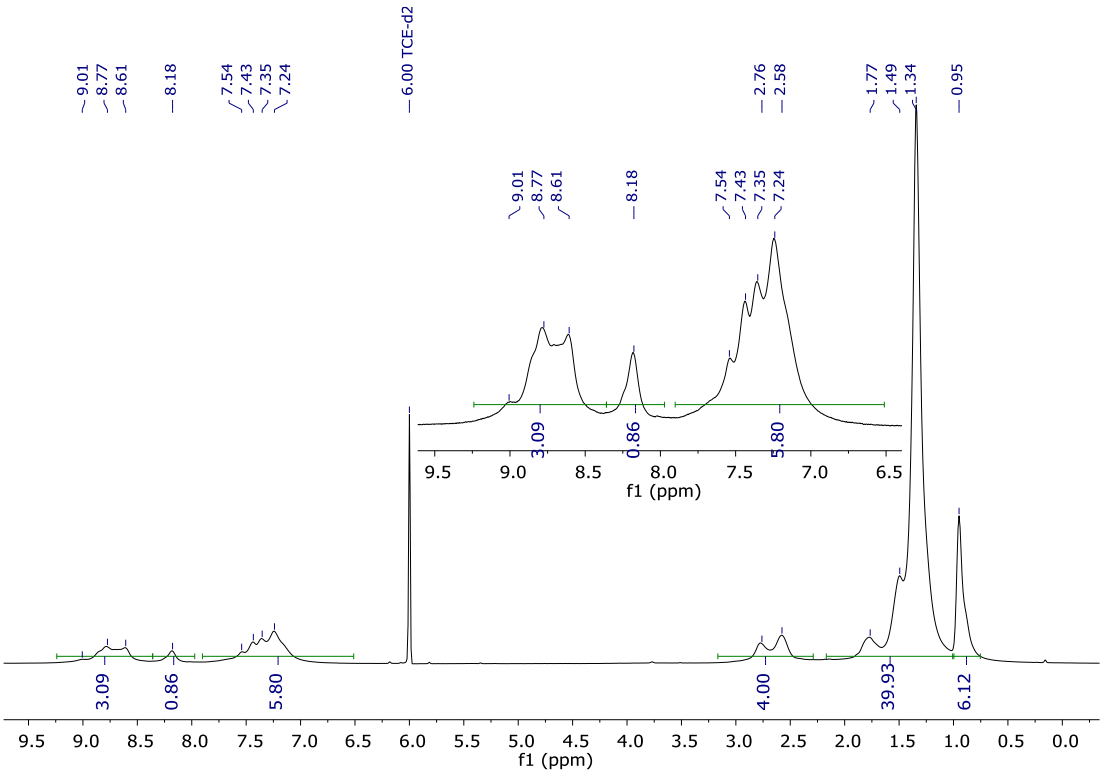

Figure S10: ^{1}H NMR spectrum of **L-P1** in TCE-d_2 at 383 K.

Polymer P2 and L-P2

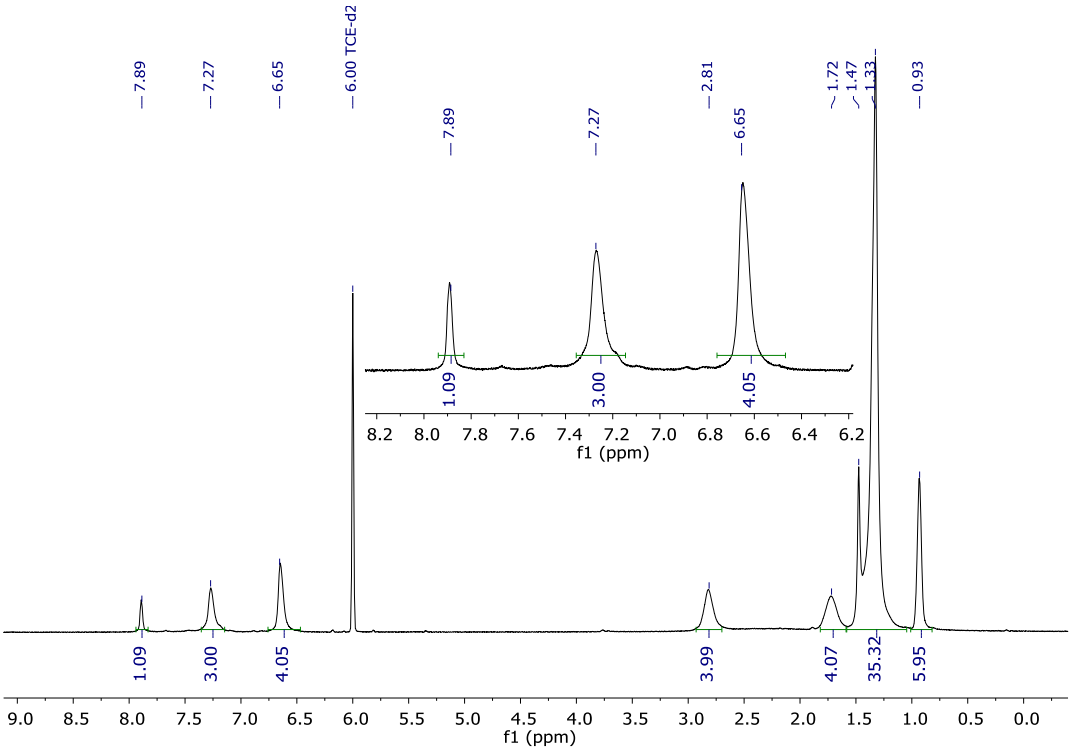

Figure S11 : ^{1}H NMR spectrum of **P2** in TCE-d_2 at 383 K.

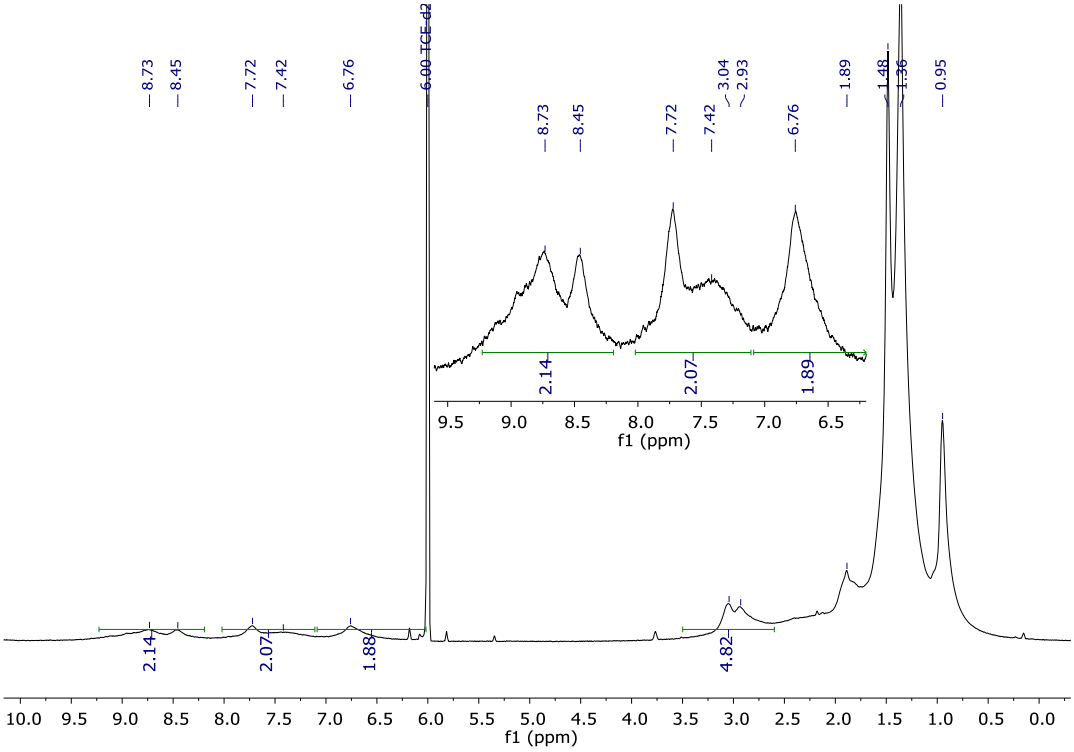

Figure S12: ^{1}H NMR spectrum of **L-P2** in TCE-d_2 at 383 K.

SIZE EXCLUSION CHROMATOGRAPHY:

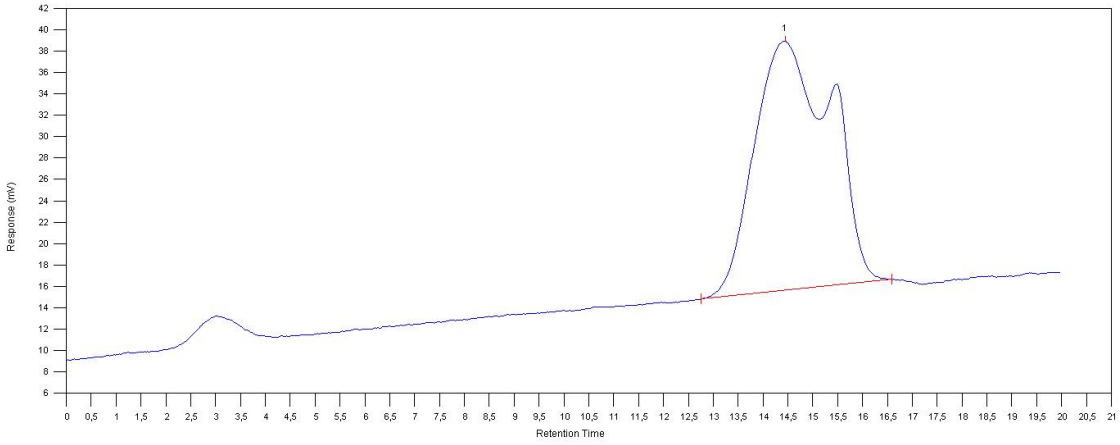

Figure S13 : Size exclusion chromatography trace for **P1** (M_n : 9 800, M_w : 16 900, I_p : 1.7).

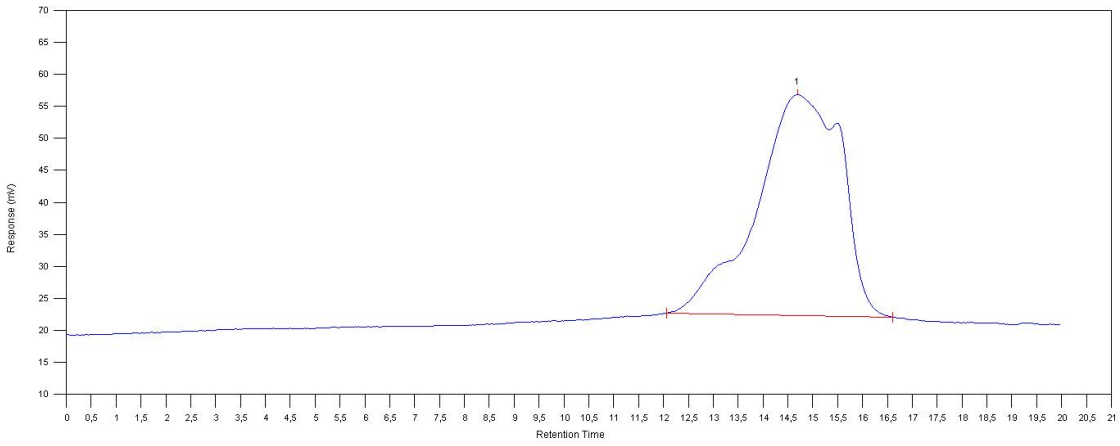

Figure S14 Size exclusion chromatography traces for **L-P1** (M_n : 9 400, M_w : 21 000, I_p : 2.2).

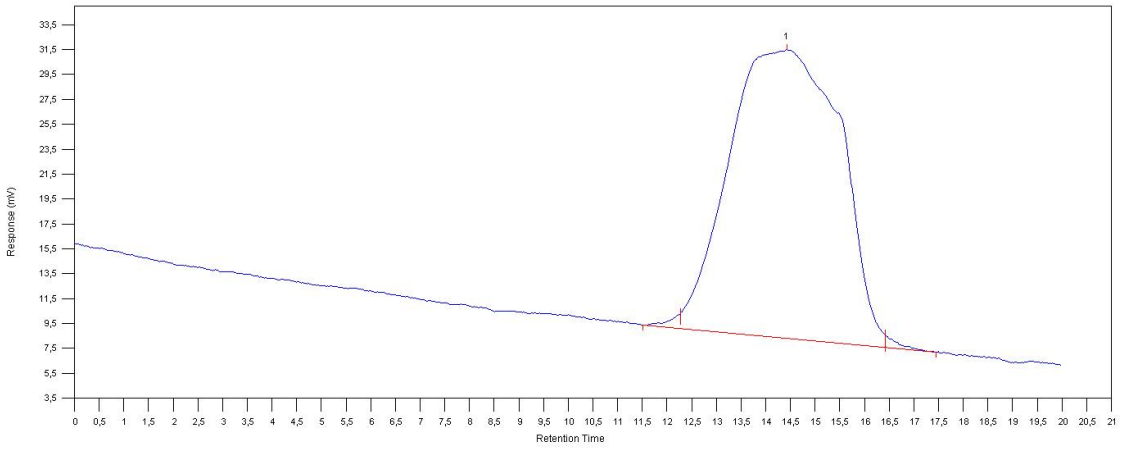

Figure S15 Size exclusion chromatography traces for **P2** (M_n : 11 100, M_w : 28 700, I_p : 2.6).

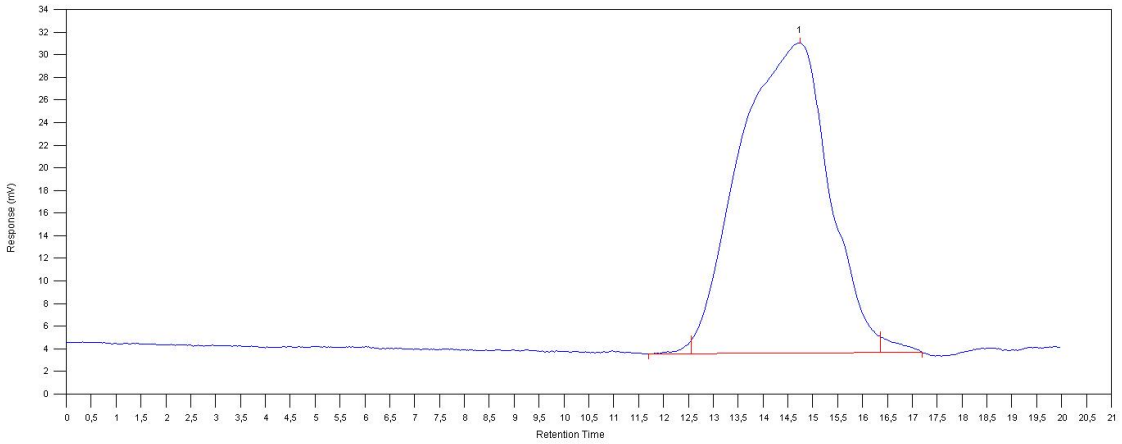

Figure S16 Size exclusion chromatography traces for **L-P2** (M_n : 12 200, M_w : 25 600, I_p : 2.1).

INFRARED SPECTROSCOPY:

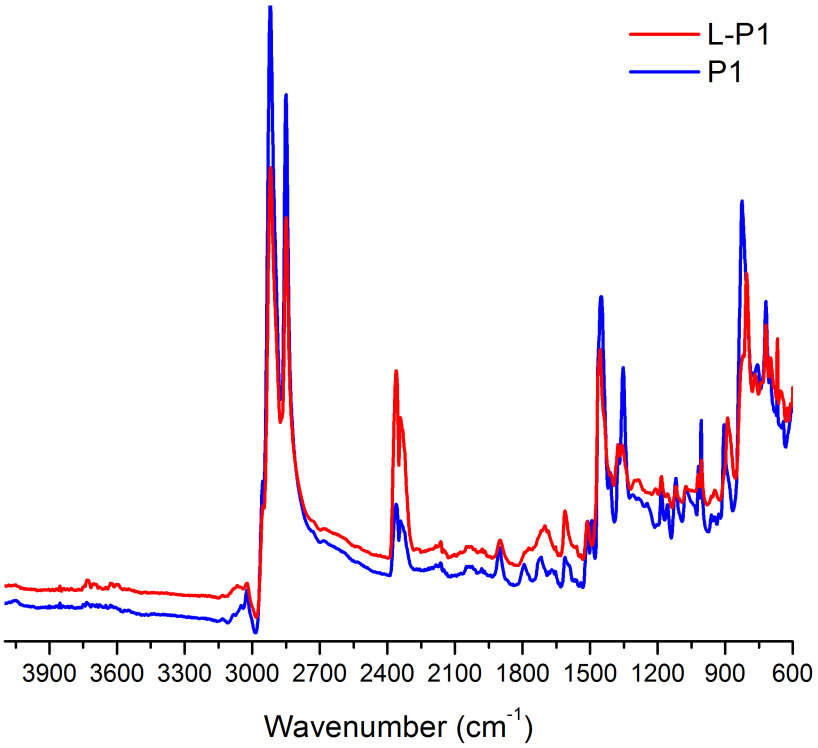

Figure S17: Infrared spectrum of **P1** and **L-P1**.

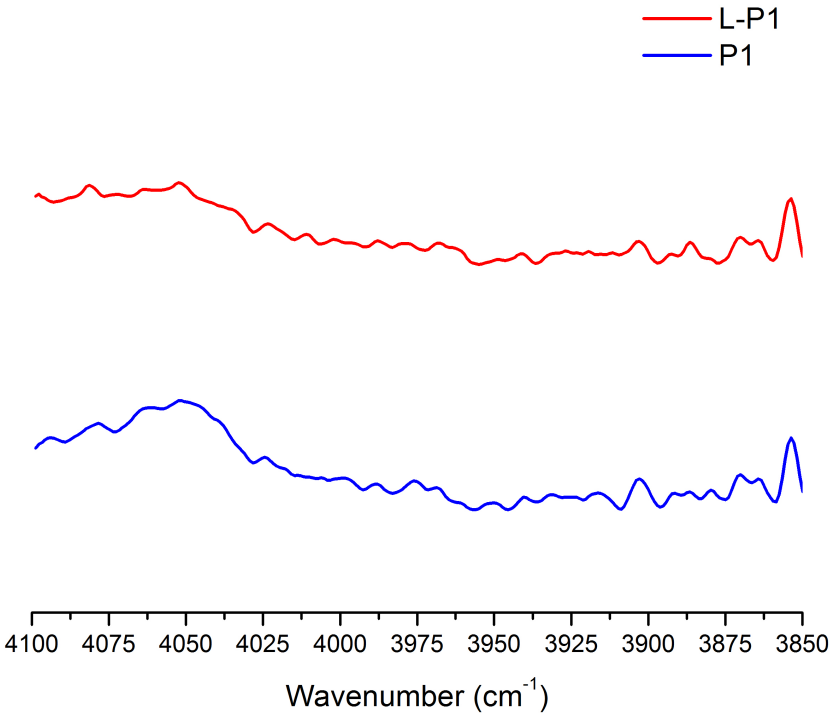

Figure S18: Infrared spectrum of **P1** and **L-P1** zoomed.

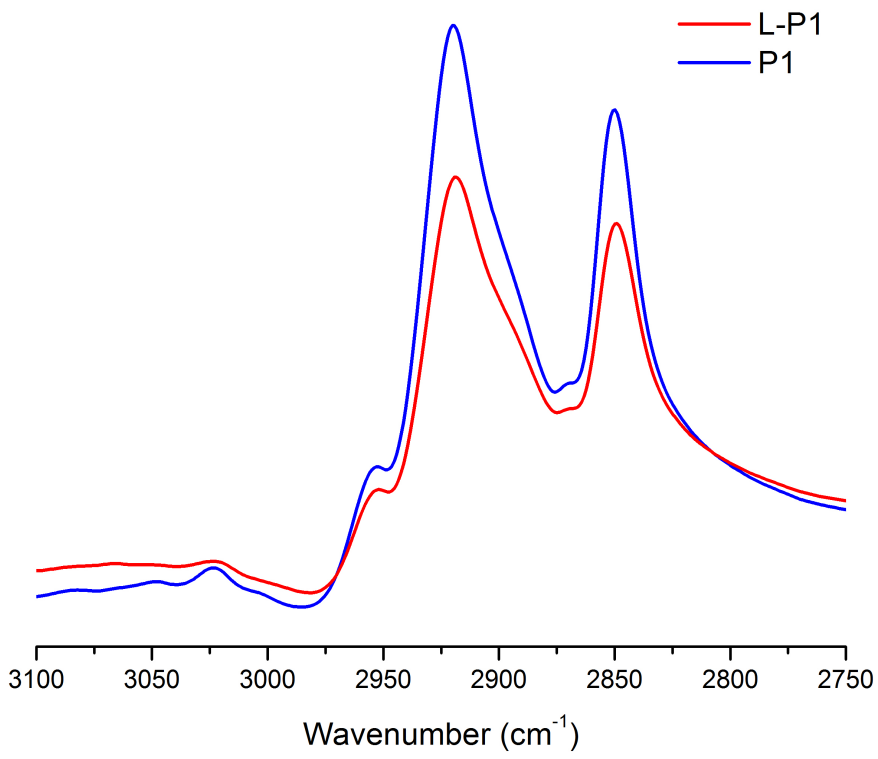

Figure S19: Infrared spectrum of **P1** and **L-P1** zoomed.

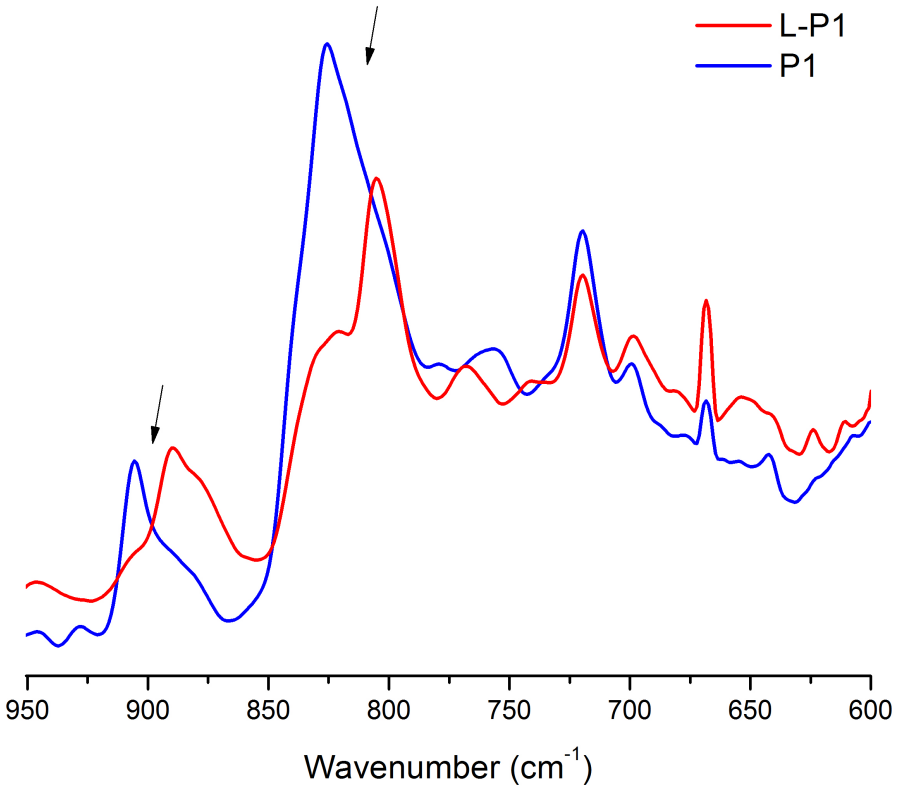

Figure S20: Infrared spectrum of **P1** and **L-P1** zoomed.

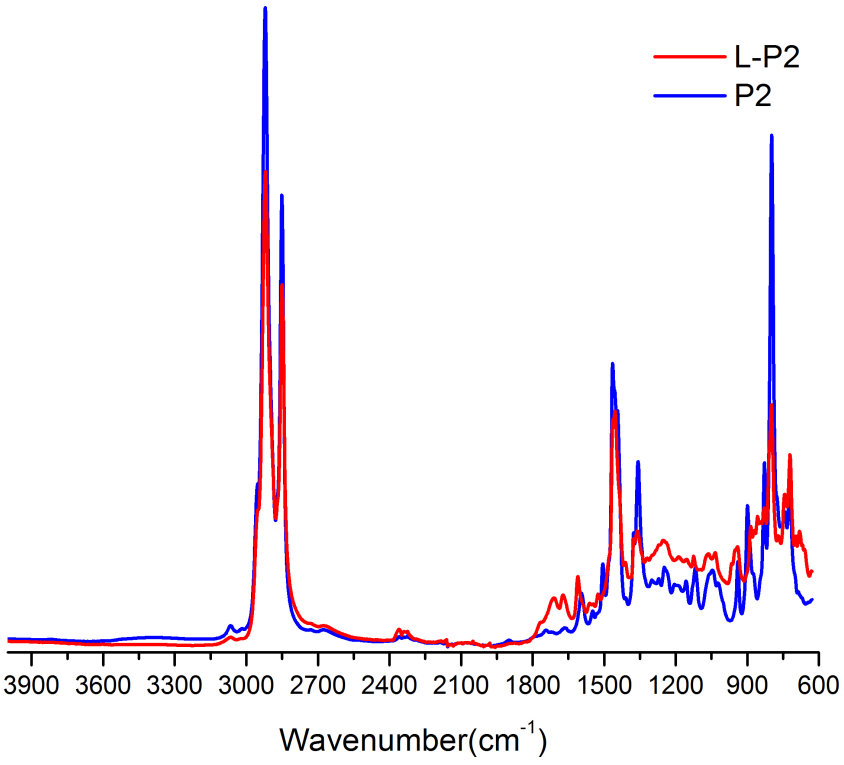

Figure S21: Infrared spectrum of **P2** and **L-P2**.

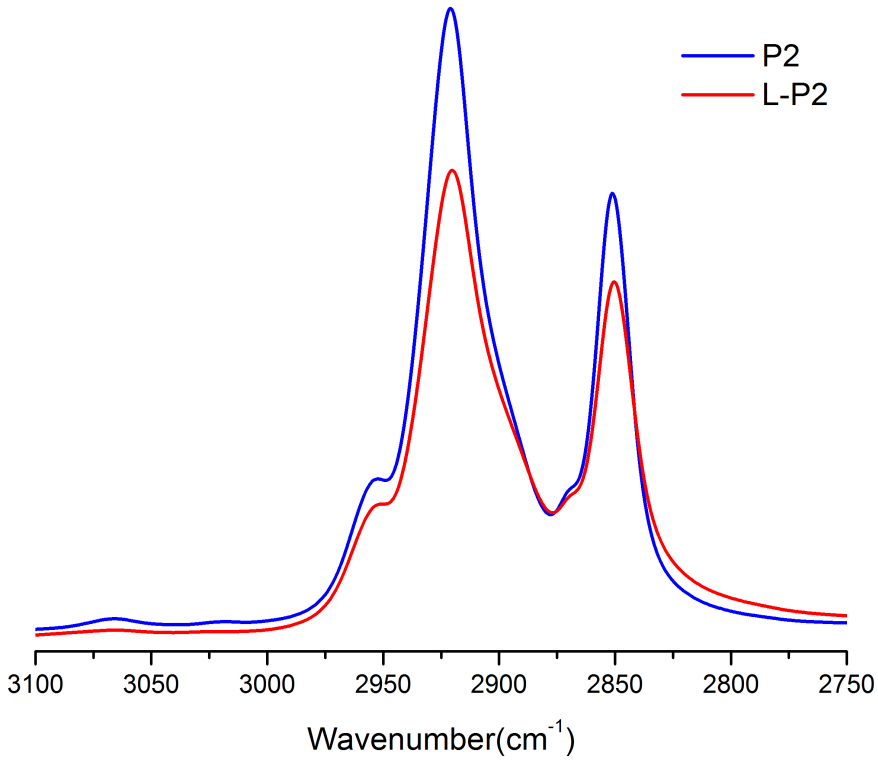

Figure S22: Infrared spectrum of **P2** and **L-P2** zoomed.

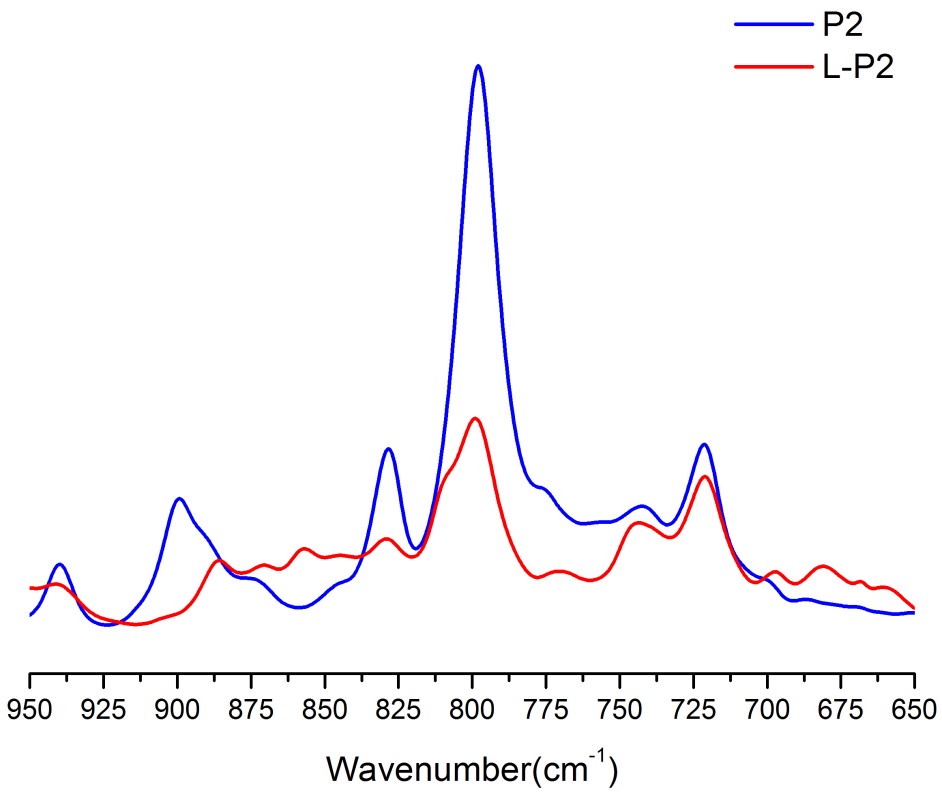

Figure S23: Infrared spectrum of **P2** and **L-P2** zoomed.

CARBON NANOTUBES WRAPPING

HiPCo CNTs were a courtesy of Yuming Zao from Memorial University. Dispersions of CNTs were prepared according to a slightly modified procedure developed by Loo *et al*.[2] A 50 mL Becker was charge with 10 mg of **L-P1/L-P2** , 2.0 mg of CNTs and 40 mL of toluene. The resulting suspensions were pre-sonicated at room temperature for 10 minutes in a standard Branson® 2510 sonicator bath, followed by ultrasonication with a Fisher Scientific Ultrasonic Dismembrator, Model 500 at 70% of its maximum power for 30 minutes in an ice-water bath. The dispersion was then centrifugated at 20 500 *g* for 60 minutes before the supernatant was carefully collected using a pipette. UV-Vis-NIR analysis of the resulting solution was performed on a Agilent Cary 5000 UV-Vis-NIR spectrophotometer. The 2D photoluminescence (PL) spectra were measured with a Horiba Jobin Yvon Nanolog spectrofluorimeter equipped with a 450 W xenon lamp as a source, a double monochromator for excitation, a iHR320 imaging spectrometer and a NIR (950-1700 nm) Hamamatsu photomultiplier tube (PMT) for the detection. Emission wavelength was set from structural analysis of the CNTs dispersions were performed on a thin dried film of the dispersion solution using a micro Raman spectrometer (Renishaw inVia model) coupled with a Leica DM2700 microscope. A back-scattering geometry was used in the frequency range of 130–600 cm^{-1}. The excitation light sources were a 633 nm and a 785 nm laser. The laser beam was focused with a 50 x objective. The wave number uncertainty was estimated to be ±2 cm^{-1}. The collected data were then processed using Wire4 software.

HYPERCHEM^{TM} STRUCTURAL OPTIMIZATION

Structural optimization of molecular oligomers avec L-P1, L-P2 and L-P2/ (3, 3) CNTs have been conducted on HyperChem^{TM} 8.0 using molecular mechanics (MM^{+}) due to high computing time of regular DFT B3LYP 6/31-G (d,p) calculations. (3, 3) CNTs coordinates have been generated by TubeGen Online – Version 3.4, a web-accessible nanotube structure generator, TubeGen 3.4 (web-interface), J. T. Frey and D. J. Doren, University of Delaware, Newark DE, 2011.[3]

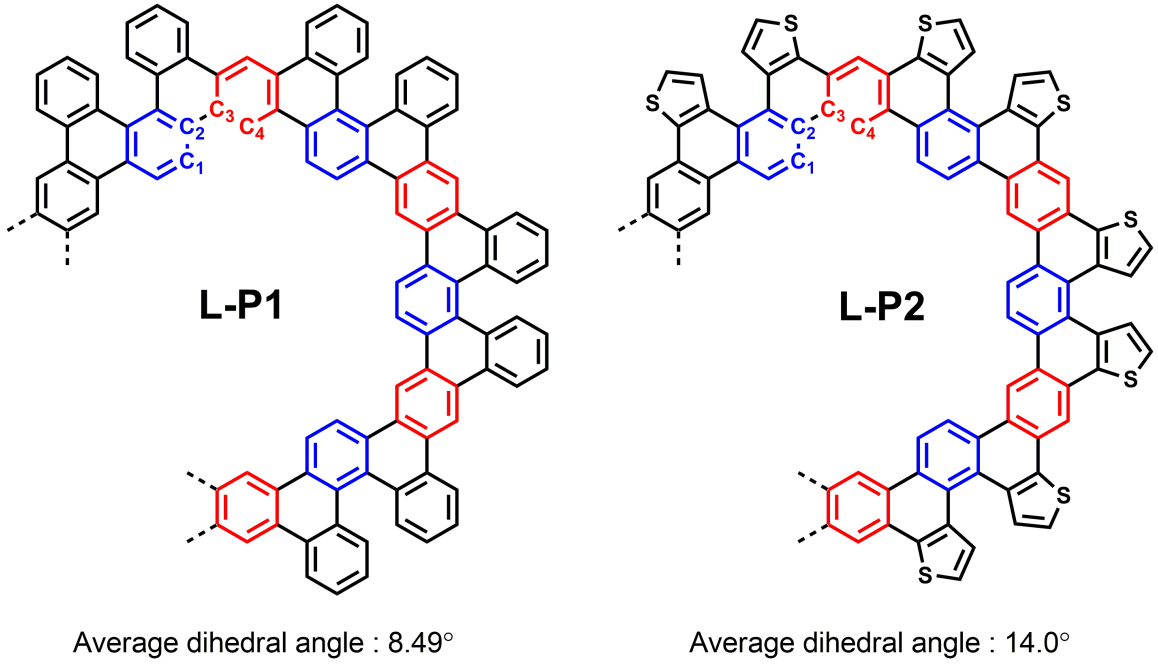

Figure S24 : Schematic representation of the dihedral angle (C_1-C_2-C_3-C_4) located in the bay region on the inner edge of the coils measured after structural optimization.

LP-1 coordinates and connectivity

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C	18.39940000	11.07070000	19.18290000
C	17.40400000	11.19770000	20.10500000
C	17.75930000	11.35320000	21.53160000
C	19.02290000	11.18180000	21.95110000
C	20.04770000	10.77450000	20.99510000
C	19.74080000	10.70050000	19.68990000
H	7.82020000	7.18990000	15.92490000
H	3.40790000	7.87000000	17.79930000
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L-P2 coordinates and connectivity

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L-P2 and (3, 3) CNT coordinates and connectivity

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C	19.98470000	6.54020000	-19.13160000
C	20.58430000	7.14260000	-20.26260000
C	21.59110000	8.11430000	-20.03210000
C	18.03110000	7.79460000	-10.91760000
C	16.91510000	7.21110000	-11.56930000
C	16.85090000	7.32080000	-12.97630000
C	16.76730000	6.11760000	-13.72200000
C	17.10630000	6.17660000	-15.09170000
C	18.13350000	5.31600000	-15.55450000

C	18.73770000	5.62860000	-16.79370000
C	20.14150000	5.82900000	-16.80440000
C	20.69350000	6.52210000	-17.90690000
C	16.62950000	4.83870000	-11.65480000
C	17.06070000	4.93940000	-12.99700000
C	18.29030000	4.32160000	-13.33790000
C	18.91970000	4.72840000	-14.53620000
C	20.24840000	5.21580000	-14.44630000
C	20.73280000	5.98760000	-15.52830000
C	19.09270000	3.94160000	-12.23750000
C	20.28340000	4.69050000	-12.06490000
C	20.68470000	5.52350000	-13.13510000
C	20.53020000	5.11060000	-10.73590000
C	20.03630000	3.82350000	-7.27680000
C	20.24970000	4.72420000	-8.34510000
C	19.77310000	6.04990000	-8.18460000
C	19.60580000	6.82830000	-9.35250000
C	18.31720000	7.36510000	-9.60230000
C	19.76360000	3.43520000	-4.88730000
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C	18.87920000	6.23820000	-7.10410000
C	17.53190000	6.47860000	-7.47570000
C	17.27560000	6.80760000	-8.82520000
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C	18.37200000	4.93290000	-3.65840000
C	18.10390000	5.54810000	-4.90130000
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C	15.92140000	4.71320000	-7.51200000
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C	18.78250000	3.48380000	-1.30030000
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C	17.31050000	4.75180000	-2.74390000
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C	12.94970000	-5.90140000	0.13760000
C	14.01720000	-6.63250000	-0.41720000
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C	18.54000000	-4.55490000	3.13240000
C	17.23140000	-4.99520000	2.88350000
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S	11.41960000	-6.35660000	-2.25680000
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S	16.54760000	-7.92350000	-2.10740000
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C	19.61220000	-2.81040000	-2.59710000
S	20.86220000	-1.92350000	-1.66920000
C	22.71490000	0.34330000	2.76590000
S	23.76200000	1.23020000	1.60690000
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RAMAN SPECTRA AND HYPERCHEM OPTIMIZED STRUCTURE OF AN NONSELECTIVE DISPERSION MECHANISM

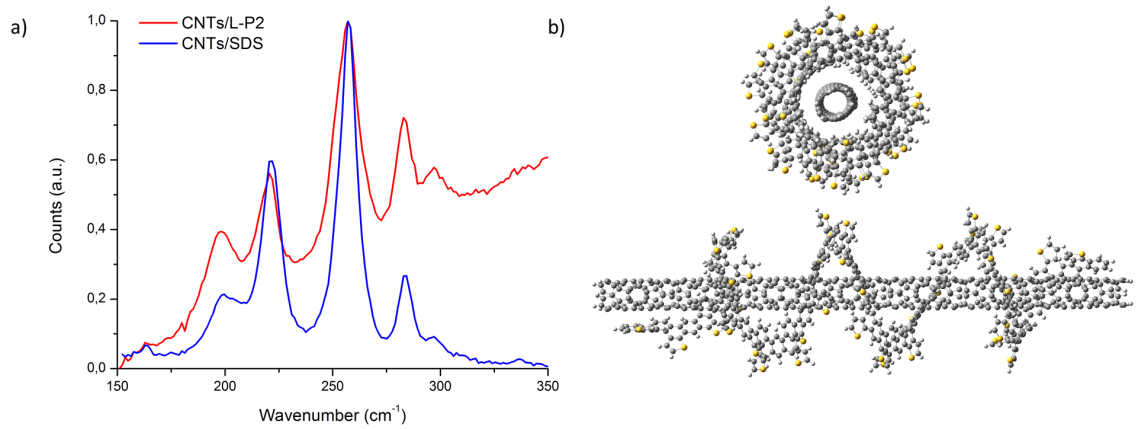

Figure 25 : a) Raman spectra of L-P2/HiPco CNTs and SDS/HiPco blends using a 634 nm laser wavelength. b) Possible nonselective CNTs dispersion mechanism.

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