Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Influence of Regiochemistry in the Selective Dispersion of Metallic Carbon Nanotubes Using Electron Poor Conjugated Polymers

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General

Raw HiPCO SWNTs were purchased from NanoIntegris (batch #R10-02) and used without further purification. All reagents were purchased from commercial chemical suppliers and used as received, with the exception of 1,4-benzenediboronic acid bis(pinacol) ester which was recrystallized in a 9:1 (v/v) mixture of acetone:ethanol. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on Bruker Avance 600 MHz and 700 MHz spectrometers. High-resolution electron ionization mass spectrometry (HR-EIMS) measurements were carried out on a Micromass Ultima Global instrument (quadrupole time-of-flight). Polymer molecular weights and polydispersity indices (PDI) were assessed by gel permeation chromatography (GPC) using a Waters 2695 separation module, equipped with a Waters 2414 refractive-index detector and a Jordi Fluorinated DVB mixed-bed column. The instrument was calibrated using polystyrene standards, with THF as the solvent at a flow rate of 3.0 mL/min. Sonication was performed in a Branson Ultrasonic B2800 bath sonicator. Centrifugation of the polymer samples was performed using a Beckman Coulter Allegra X-22 centrifuge. All filtrations were done through Teflon membranes (Sartorius), with 200 nm pore diameter. UV-Vis-NIR absorption spectra were recorded on a Cary 5000 spectrometer in dual beam mode, using matching 10 mm quartz cuvettes. Fluorescence spectra were measured on a Jobin-Yvon SPEX Fluorolog 3.22 equipped with a 450 W Xe arc lamp, digital photon counting photomultiplier, and an InGaAs detector, also using a 10 mm quartz cuvette. Slit widths for both excitation and emission were set to 10 nm band-pass, and correction factor files were applied to account for instrument variations. Photoluminescence (PL) maps were obtained at 25 °C with 5 nm intervals for both the excitation and emission. Raman

spectra were collected with a Renishaw InVia Laser Raman spectrometer, using three different lasers: a 25 mW argon ion laser (514 nm, 1800L/mm grating); a 500 mW HeNe Renishaw laser (633 nm, 1800 L/mm grating); and a 300 mW Renishaw laser (785 nm, 1200 L/mm grating). Laser intensity for both 514 and 633 nm excitations was set to 5% for all SWNT dispersions. For spectra obtained at 785 nm, laser intensity was set to 0.1% for all samples.

Synthesis

2,7-dibromofluorene (1)[1]

A 250 mL round bottom flask equipped with a stir bar was charged with fluorene (8.3 g, 50 mmol), NBS (17.4 g, 100 mmol) and acetic acid (100 mL). The mixture was stirred at room temperature and 48% HBr (2.5 mL) was slowly added. The reaction mixture was stirred at room temperature for 3 h. Water (50 mL) was then added and the resulting suspension was filtered to obtain an orange-white solid. The solid was recrystallized from a 2.5:1 mixture of EtOH:acetone (~ 425 mL total volume), the mother liquor was recrystallized again from the same solvent mixture (~300 mL total volume) and the crops were combined to afford a white solid (8.78 g, 54%). ^{1}H NMR (600 MHz; $CDCl_3$): δ = 7.67 (d, J = 0.9 Hz, 2H), 7.61 (d, J = 8.1 Hz, 2H), 7.52-7.50 (m, 2H), 3.88 (s, 2H).

Bis(hexadecyl)-2,7-dibromofluorene (2)[2]

A 300 mL round-bottom flask equipped with a stir bar was charged with bromohexadecane (12.7 g, 41.6 mmol). 30 mL of toluene and 60 mL of saturated KOH was added and the mixture was sparged with nitrogen for 1 hour, followed by the addition of **1** (5 g, 15.43 mmol). The mixture was stirred at 60 °C under N_2 for 6 h. It was then cooled to room temperature, and the toluene layer was separated and evaporated to

dryness, leaving a light brown oil that crystallized overnight. The solid was taken up in a minimum amount of hexanes, and purified by a silica plug using 100% hexanes. The product was evaporated to dryness and transferred to a 50 mL round-bottom flask fitted with a condenser, where the excess alkyl bromide was removed by distillation at 0.2 mbar, heating to 140 °C. The residue was then recrystallized in hexanes to yield a white crystalline solid. Yield: 7.0 g (59%). ^{1}H NMR (700 MHz; $CDCl_3$): δ = 7.51 (dd, *J* = 8.0, 0.4 Hz, 2H), 7.45-7.43 (m, 4H), 1.91-1.89 (m, 4H), 1.24-1.04 (m, 52H), 0.88 (t, *J* = 7.1 Hz, 6H), 0.59-0.57 (m, 4H). ^{13}C NMR (700 MHz; $CDCl_3$): δ = 152.7, 139.2, 130.3, 126.3, 121.6, 121.3, 55.8, 40.3, 32.1, 29.7, 23.8, 22.9, 14.3. HRMS(EI): *m/z* calculated for $C_{45}H_{68}Br_2$ $[M]^+$: 770.4001; found: 770.3997.

Bis(hexadecyl)-4-nitro- 2,7-dibromofluorene (3)[3]

A 100 mL round-bottom flask equipped with a stir bar was charged with **2** (1.20 g, 1.56 mmol). 20.8 mL of glacial acetic acid was added, followed by 20 mL of CH_2Cl_2. The mixture was stirred until homogeneous, and 4.2 mL of fuming nitric acid was added. The mixture was stirred at room temperature for 6 h, and 20 mL of 0.5 M sodium bicarbonate solution was slowly added. It was then extracted with CH_2Cl_2, dried over magnesium sulphate, and evaporated to dryness leaving a yellow solid. The solid was taken up in a minimal amount of warm hexanes and CH_2Cl_2 (10:1) and purified by column chromatography (silica gel) using 93:7 hexanes:CH_2Cl_2 to elute the product that, after drying, was a yellow crystalline solid. Yield: 0.96 g (75%). ^{1}H NMR (600 MHz; $CDCl_3$): δ = 8.00 (d, *J* = 1.7 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.66 (d, *J* = 1.8 Hz, 1H), 7.50-7.48 (m, 2H), 1.95 (m, *J* = 8.6 Hz, 4H), 1.16 (m, *J* = 115.3 Hz, 52H), 0.87 (t, *J* = 7.1 Hz, 6H), 0.52 (m, *J* = 0.4 Hz, 4H). ^{13}C NMR (176 MHz; $CDCl_3$): δ = 156.0, 153.7, 145.2, 135.0,

132.4, 131.0, 130.4, 126.4, 126.1, 124.3, 120.8, 55.5, 40.5, 32.1, 29.6, 23.6, 22.8, 14.3. HRMS(EI): *m/z* calculated for $C_{45}H_{69}Br_2N_1O_2$ $[M]^+$: 815.3852; found: 815.3861.

Bis(hexadecyl)-4,6-dinitro-2,7-dibromofluorene (4)[3]

A 100 mL round-bottom flask equipped with a stir bar was charged with **2** (1.20 g, 1.56 mmol). 20.8 mL of glacial acetic acid was added, followed by 15 mL of chloroform. The mixture was stirred until homogeneous, and 6.8 mL of anhydrous nitric acid was added. The mixture was stirred at reflux for 3 hours, and 20 mL of 0.5 M sodium bicarbonate solution was slowly added. It was then extracted with CH_2Cl_2, dried over magnesium sulphate, and evaporated to dryness, leaving a red oil. The oil was taken up in a minimum of warm hexanes and CH_2Cl_2 (10:1) and purified by column chromatography (silica gel) using 95:5 hexanes:CH_2Cl_2 to elute the product that, after drying, was a white solid. Yield: 0.651 g (48%). ^{1}H NMR (600 MHz; $CDCl_3$): δ = 8.58 (s, 1H), 8.15 (d, *J* = 1.8 Hz, 1H), 7.73 (d, *J* = 1.8 Hz, 1H), 7.68 (s, 1H), 2.01 (m, *J* = 10.3, 6.6 Hz, 4H), 1.29-1.06 (m, 52H), 0.87 (t, *J* = 7.1 Hz, 6H), 0.53-0.50 (m, 4H). ^{13}C NMR (700 MHz; $CDCl_3$): δ = 156.6, 156.0, 149.8, 145.2, 136.4, 131.0, 130.7, 128.8, 127.4, 122.7, 122.5, 115.7, 55.9, 40.4, 32.1, 29.5, 23.7, 22.8, 14.3. HRMS(EI): *m/z* calculated for $C_{45}H_{70}Br_2N_2O_4$ $[M]^+$: 860.3702; found: 860.3629.

Poly(bis(hexadecyl)fluorene-*co*-phenylene) (PF-P_{25})

A 25 mL schlenk flask was equipped with a stir bar and charged with **2** (77.29 mg, 0.10 mmol), and 1,4-benzenediboronic acid bis(pinacol) ester (33.04 mg, 0.10 mmol). 0.6 mL of toluene and 0.8 mL of 3 M K_3PO_4 were added and the vessel was degassed via three freeze-pump-thaw cycles. Bis(tris(2-methylphenyl)phosphine)palladium (3.58 mg, 0.005 mmol) was added and the vessel was sealed under vacuum, charged with nitrogen, and stirred at 85 °C for 24 hours. After it was cooled to room temperature, the reaction mixture was extracted in toluene and purified through an alumina plug, followed by a celite plug, and evaporated to dryness. The product was taken up in a minimum of toluene and precipitated into 100 mL of methanol. The precipitate was filtered through a membrane filter, yielding a white solid. Yield: 45 mg (73 %). ^{1}H NMR (600 MHz; $CDCl_3$): δ = 7.82 (m), 7.66 (m), 2.10-2.08 (m), 1.29-1.11 (m), 0.88 (t), 0.81 (m). GPC results: M_n = 25,396 Da, M_w = 53,761 Da, PDI = 2.12, DP = 37.

Poly(bis(hexadecyl)-4-nitrofluorene-*co*-phenylene) (PMNF-P_{25})

A 25 mL schlenk flask was equipped with a stir bar and charged with **3** (81.8 mg, 0.10 mmol), and 1,4-benzenediboronic acid bis(pinacol) ester (33.0 mg, 0.10 mmol). 0.8 mL of toluene and 0.8 mL of 3 M K_3PO_4 were added and the vessel was degassed via three freeze-pump-thaw cycles, after which bis(tris(2-methylphenyl)phosphine)palladium (3.58 mg, 0.005 mmol) was added. The vessel was then sealed under vacuum, charged with nitrogen, and stirred at 85 °C for 24 h. After cooling to room temperature, the reaction mixture was extracted in toluene and purified through an alumina plug, followed by a celite plug, and evaporated to dryness. The product was taken up in a minimum of

toluene and precipitated into 100 mL of methanol. The precipitate was filtered through a membrane filter, yielding a yellow solid. Yield: 62 mg (84 %). ^{1}H NMR (600 MHz; $CDCl_3$): δ = 8.21 (m), 7.87-7.83 (m), 7.73-7.68 (m), 2.17-2.11 (m), 1.22-1.10 (m), 0.88-0.81 (m), 0.71 (m). GPC results: M_n = 25,356 Da, M_w = 53,498 Da, PDI = 2.11 DP = 35.

Poly(bis(hexadecyl)-4,6-dinitrofluorene-*co*-phenylene) (PDNF-P_{23})

A 25 mL schlenk flask was equipped with a stir bar and charged with **4** (86.2 mg, 0.1 mmol) and 1,4-benzenediboronic acid bis(pinacol) ester (33.0 mg, 0.1 mmol). 0.8 mL of toluene and 0.8 mL of 3 M K_3PO_4 was added and the vessel was degassed via three freeze-pump-thaw cycles, and bis(tris(2-methylphenyl)phosphine)palladium (3.58 mg, 0.005 mmol) was added; the vessel was sealed under vacuum, charged with nitrogen, and stirred at 85 °C for 24 h. After cooling to room temperature, the reaction mixture was extracted with toluene and purified through an alumina plug, followed by a celite plug, and evaporated to dryness. The product was taken up in a minimum of toluene and precipitated into 100 mL of methanol. The precipitate was filtered through a membrane filter, yielding a yellow-green solid. Yield: 70 mg (78 %). ^{1}H NMR (600 MHz; $CDCl_3$): δ = 8.75 (m), 8.34 (m), 7.89 (m), 7.61-7.50 (m), 3.65-3.64 (m), 2.24 (m), 1.44-1.04 (m), 0.89-0.79 (m), 0.70-0.68 (m). GPC results: M_n = 23,323 Da, M_w = 48,903 Da, PDI = 2.09, DP = 30.

NMR Spectra

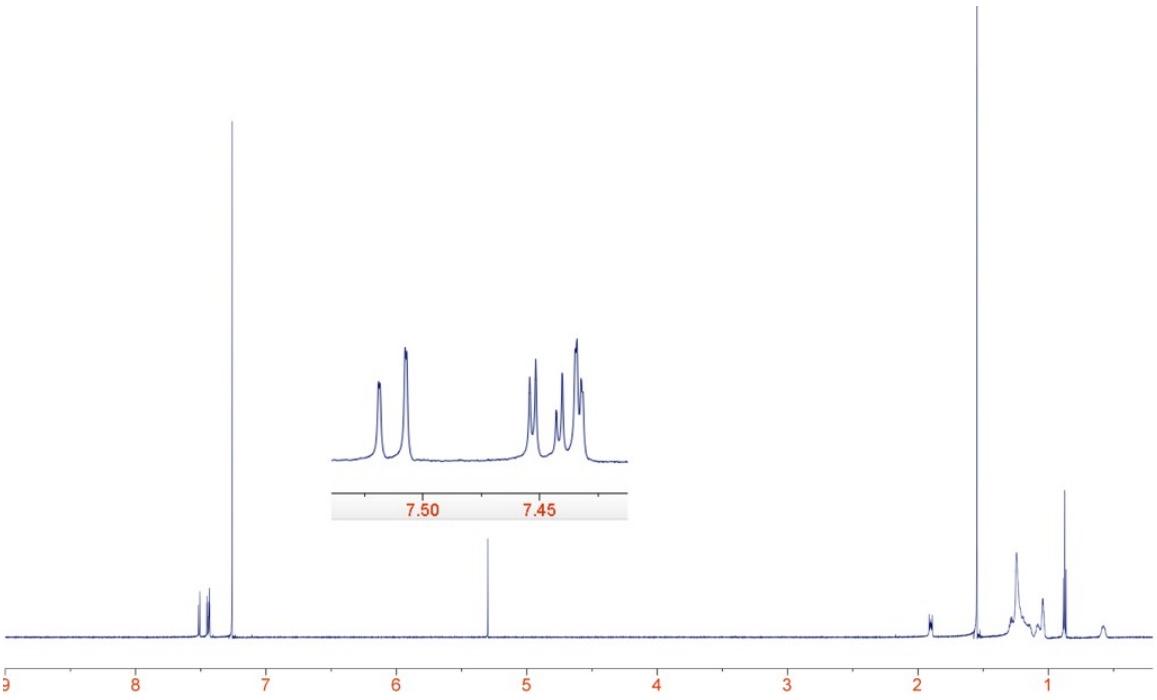

Figure S1. ^{1}H NMR of bis(hexadecyl)-2,7-dibromofluorene in $CDCl_3$.

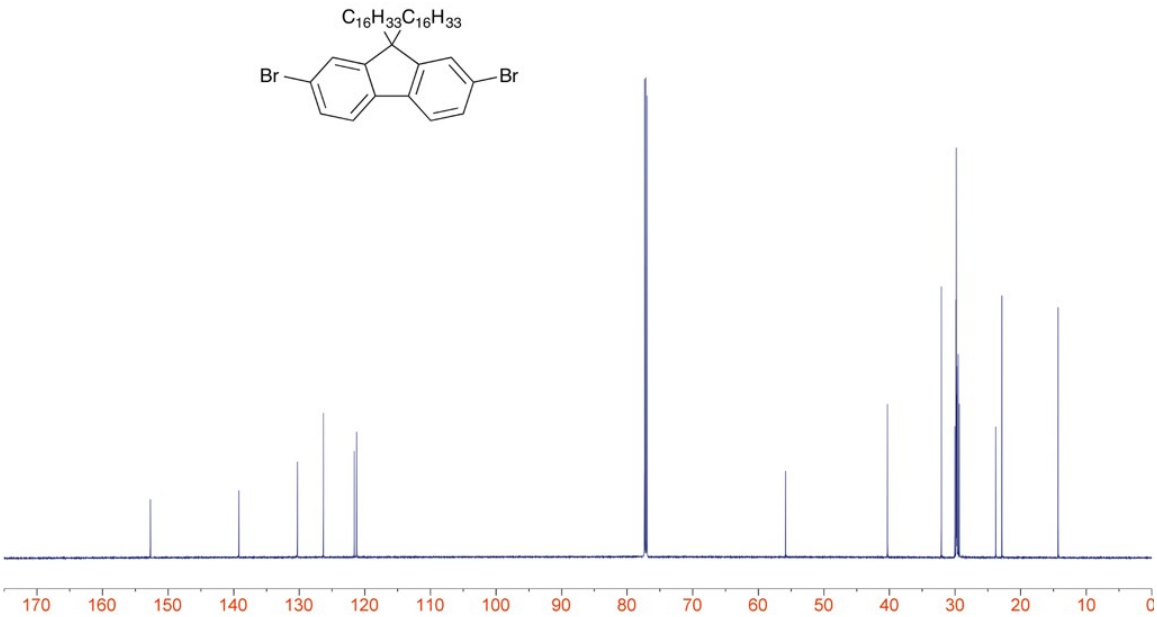

Figure S2. ^{13}C NMR of bis(hexadecyl)-2,7-dibromofluorene in $CDCl_3$.

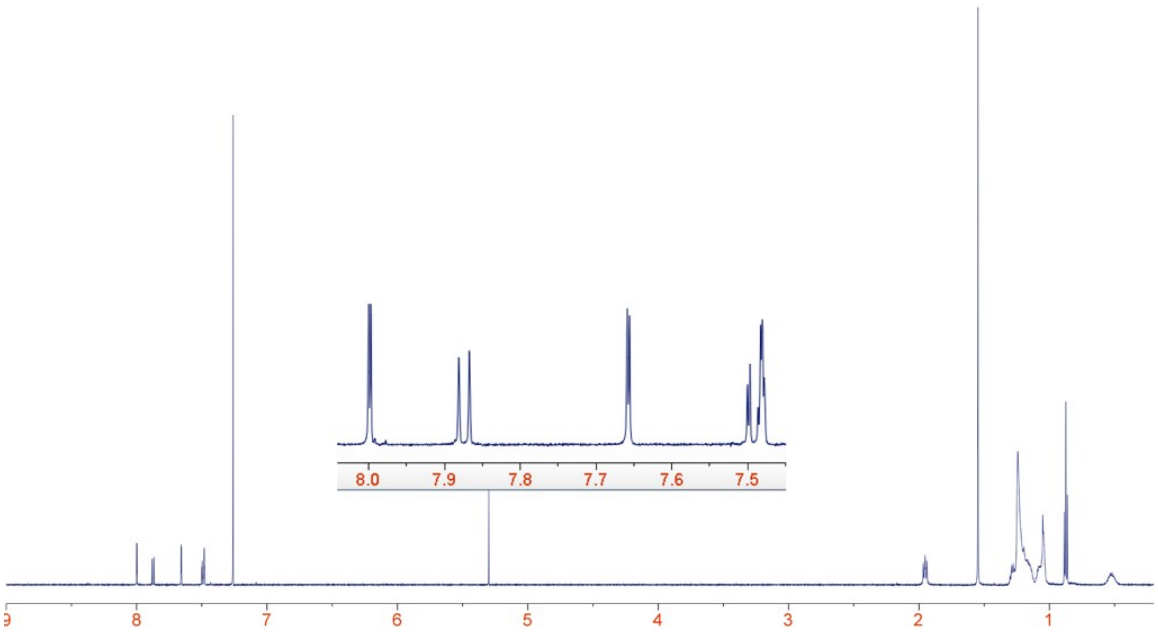

Figure S3. ^{1}H NMR of bis(hexadecyl)-4-nitro-2,7-dibromofluorene in $CDCl_3$.

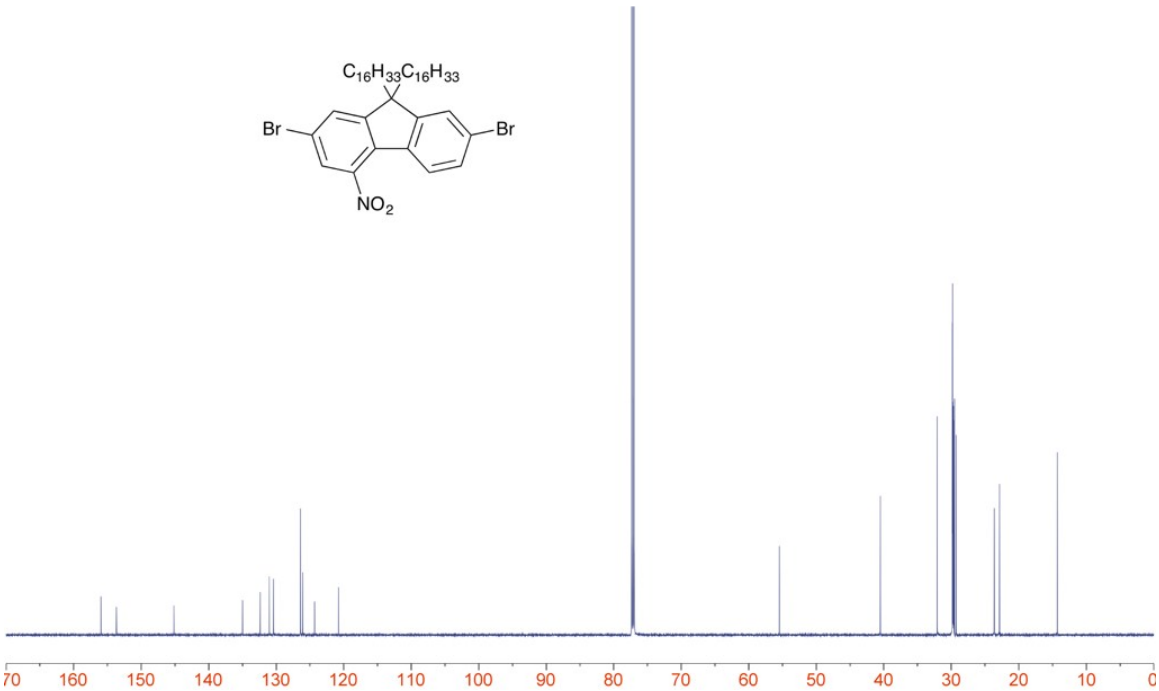

Figure S4. ^{13}C NMR of bis(hexadecyl)-4-nitro-2,7-dibromofluorene in $CDCl_3$.

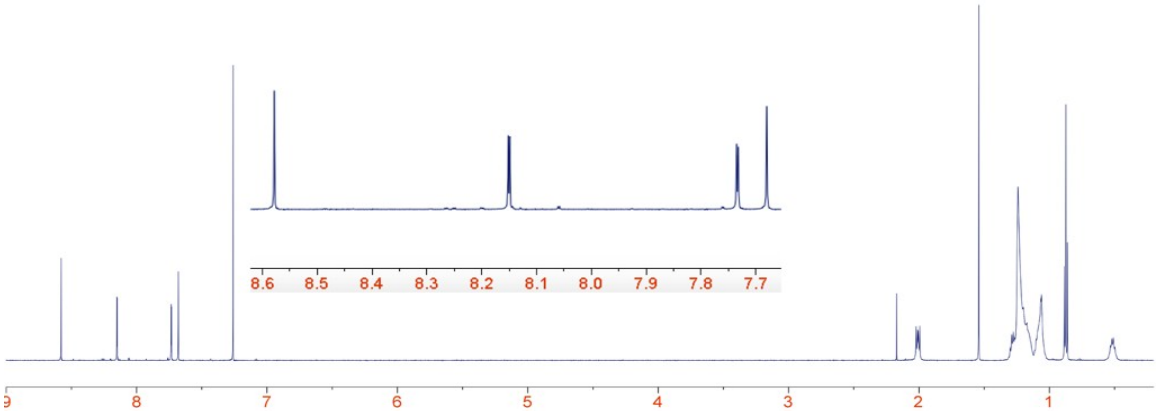

Figure S5. ^{1}H NMR of bis(hexadecyl)-4,6-dinitro-2,7-dibromofluorene in $CDCl_3$.

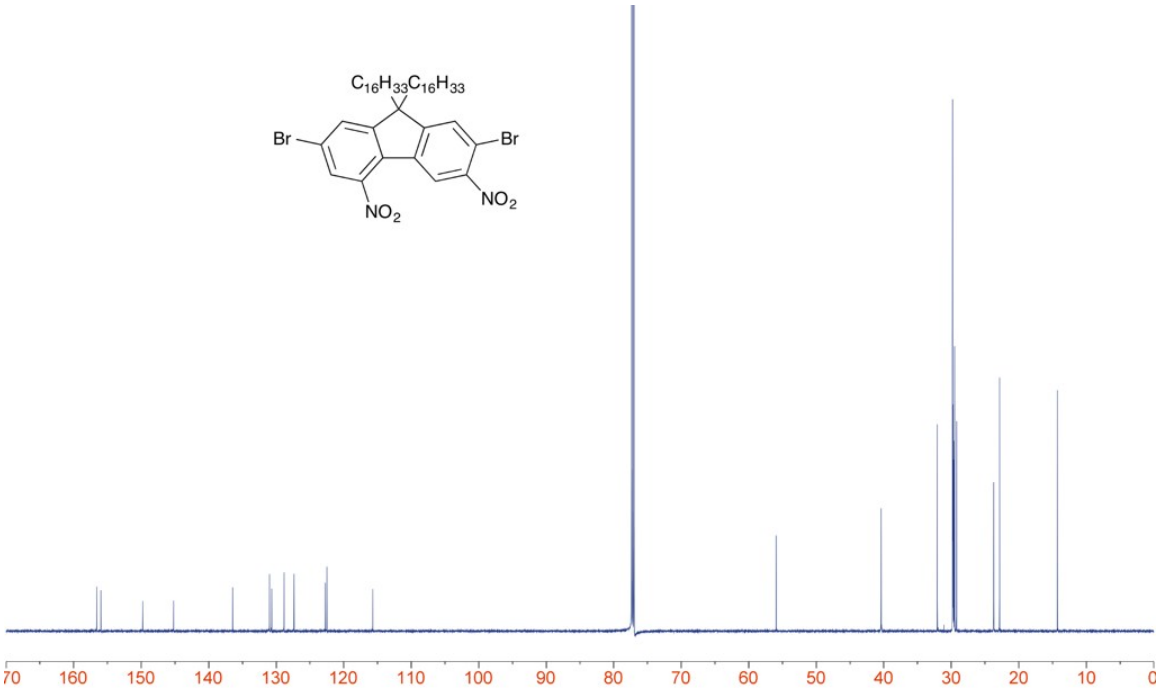

Figure S6. ^{13}C NMR of bis(hexadecyl)-4,6-dinitro-2,7-dibromofluorene in $CDCl_3$.

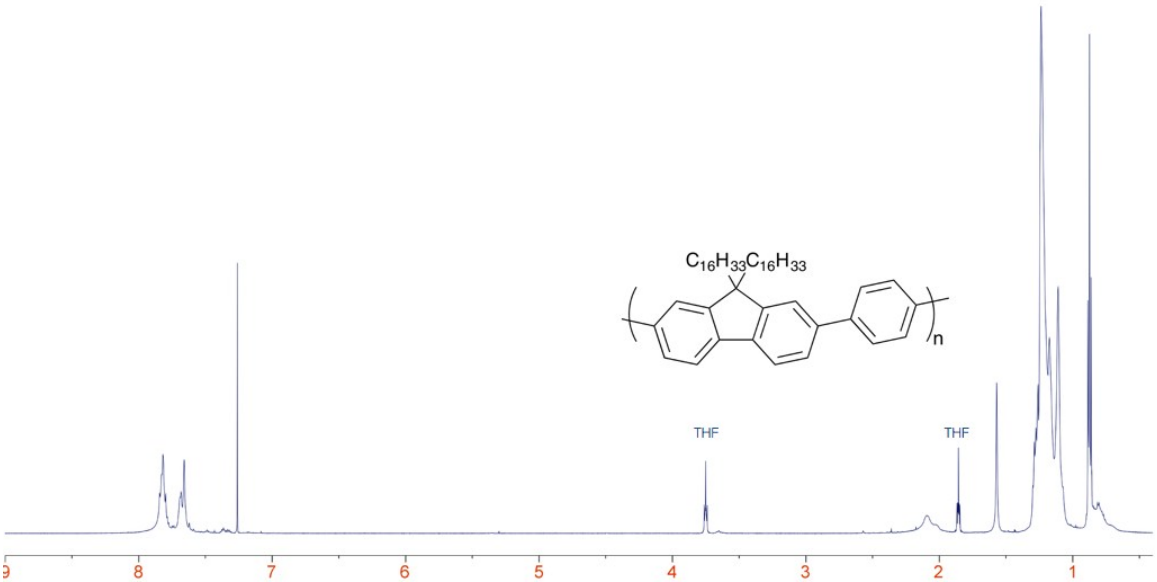

Figure S7. ^{1}H NMR of PF-P_{25} in $CDCl_3$.

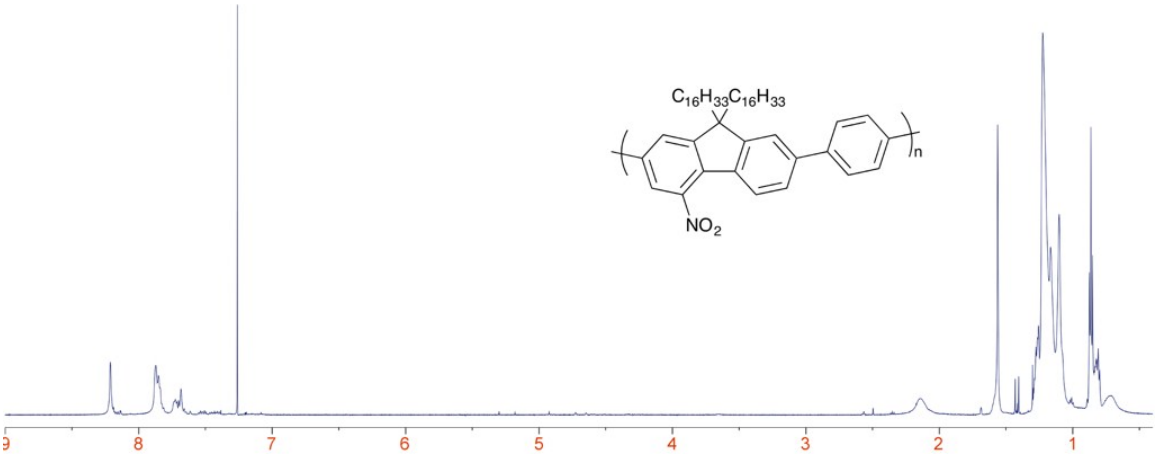

Figure S8. ^{1}H NMR of PMNF-P_{25} in $CDCl_3$.

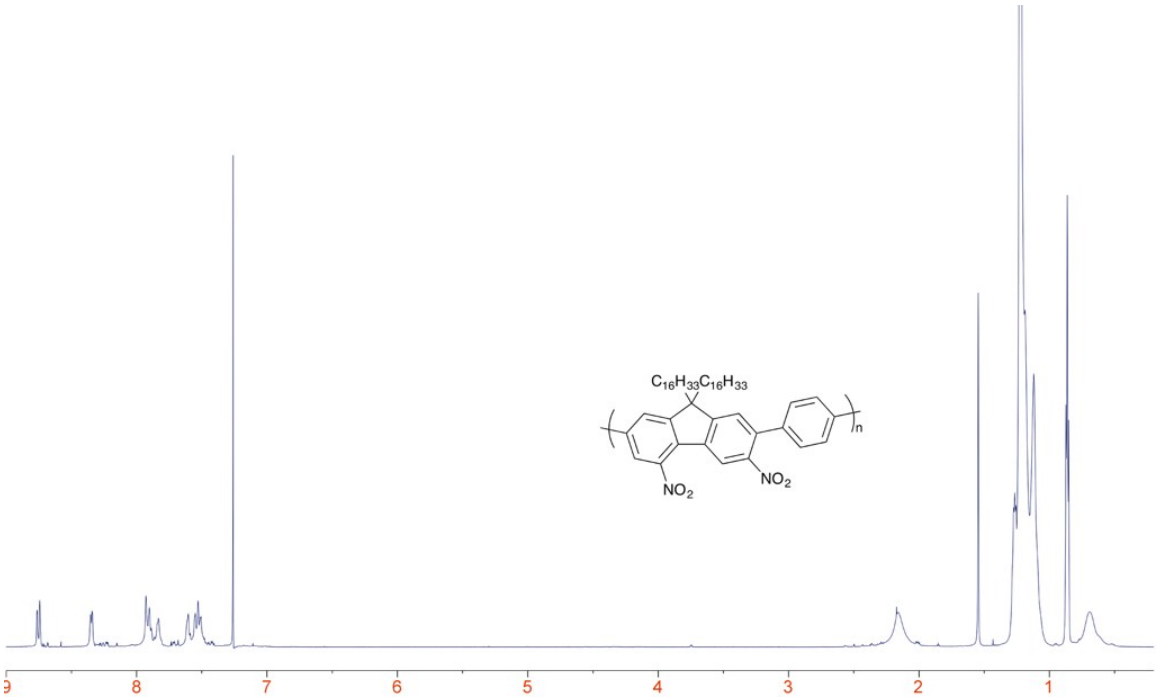

Figure S9. ^{1}H NMR of PDNF-P_{23} in $CDCl_3$.

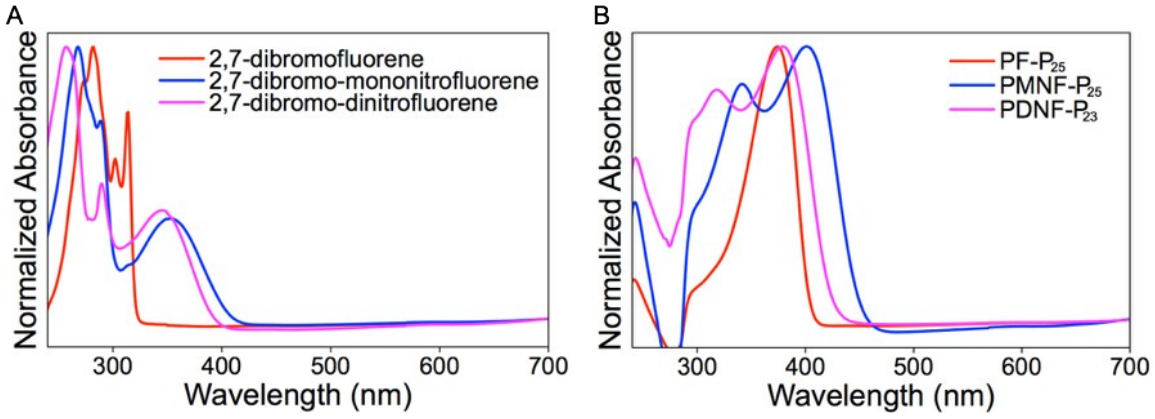

Figure S10: UV-vis absorption spectra of (A) fluorene monomers and (B) three polymers before addition of SWNTs. All spectra have been normalized to the maximum absorbance value.

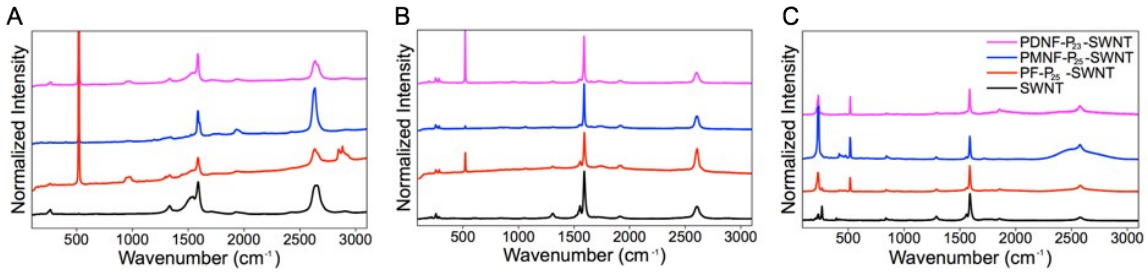

Figure S11. Full Raman spectra of PDNF-P_{23}-SWNT (magenta), PMNF-P_{25}-SWNT (blue), PF-P_{25}-SWNT (red), and raw HiPCO SWNT material (black) obtained at (A) 514 nm, (B) 633 nm, and (C) 785 nm excitation wavelengths.

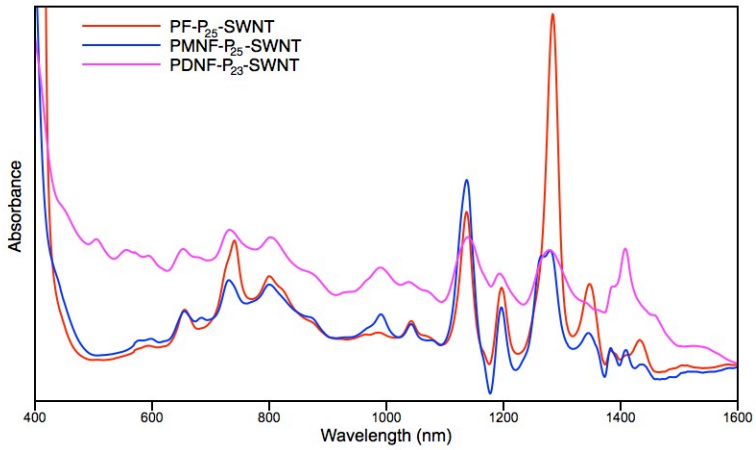

Figure S12. UV-Vis-NIR absorbance spectrum of PF-P_{25}-SWNT, PMNF-P_{25}-SWNT, and PDNF-P_{23}-SWNT with no vertical offset.

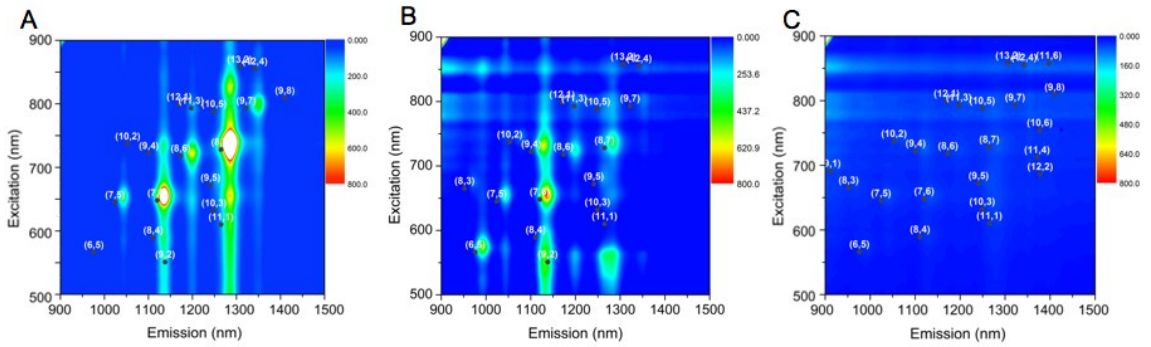

Figure S13. PL maps for (A) PF-P_{25}-SWNT, (B) PMNF-P_{25}-SWNT, and (C) PDNF-P_{23}-SWNT on the same scale.

Computational Methods.

All calculations were run in Mac OS X 10.9.3 on a desktop computer equipped with an Intel i5-3570k processor, using GAMESS.[4] The 6-31G(d) basis set with the M06 density functional was used for all computational calculations. The DFT calculations were used to verify the similar geometries of the oligomers, and to assess the electron density of the polymer backbones. The initial coordinates for the M06 calculations were determined by a molecular mechanics geometry optimization using Avogadro.[5] To minimize computational load, the alkyl chains were replaced by methyl functionalities.

Coordinates of M06/6-31G(d).

PF-P Oligomer:

E = -2429.0220330713

		COORDINATES (BOHR)		
ATOM	*CHARGE*	*X*	*Y*	*Z*
C	*6.0*	*-6.3499139557*	*-5.0401637709*	*1.3784039300*
C	*6.0*	*-4.9524804851*	*-6.6700146408*	*-0.1978732082*
C	*6.0*	*-2.5174173718*	*-5.9877290729*	*-1.0014035954*
C	*6.0*	*-1.5348732417*	*-3.6753469708*	*-0.2016715574*
C	*6.0*	*-2.8907138434*	*-2.0696467990*	*1.3411007390*

C	6.0	-5.3180668746	-2.7210164497	2.1578592081
C	6.0	0.8725242831	-2.5319682619	-0.7379946900
C	6.0	0.9945816846	-0.2376897347	0.4700882367
C	6.0	-1.4125323813	0.3164157194	1.9409375620
C	6.0	2.8590420359	-3.4253929144	-2.1957860087
C	6.0	5.0391433189	-1.9370447265	-2.4334757434
C	6.0	5.2398133215	0.4622269766	-1.2047948035
C	6.0	3.1411781258	1.2863553771	0.2707599395
H	1.0	-6.3859510303	-1.4652935309	3.3679452444
H	1.0	-8.2257504574	-5.5768837459	1.9911853760
H	1.0	-5.7587698722	-8.4533679527	-0.7911337848
H	1.0	-1.4358704973	-7.2311876701	-2.2116597070
H	1.0	2.7365122028	-5.2383204380	-3.1343373178
H	1.0	6.5381117668	-2.7024971350	-3.5696923908
C	6.0	7.6052400321	2.0783017440	-1.4617597433
H	1.0	3.1164416127	3.0646442233	1.2506962477
C	6.0	-2.7574314695	2.6786487931	0.9250964600
C	6.0	-0.8879633444	0.5500614405	4.7853909132
H	1.0	-4.5925443762	2.9566085886	1.9061666038
H	1.0	-1.5753511724	4.3861107093	1.2320257550
H	1.0	-3.1269106946	2.4878431601	-1.1340245652
H	1.0	0.0850187722	-1.1695892083	5.4988569599
H	1.0	0.3335366368	2.2128691316	5.1728414325
H	1.0	-2.6846959162	0.7847087164	5.8456216786
C	6.0	7.9022104711	4.3416643541	-0.0789338545
C	6.0	10.0737135008	5.8252315352	-0.3133732605
C	6.0	12.0660705069	5.1297178855	-1.9470602742
C	6.0	11.7683063831	2.8672623439	-3.3312467657
C	6.0	9.5987686683	1.3813896970	-3.0934058529
H	1.0	9.5283763753	-0.3043592676	-4.2240478086
H	1.0	13.1931597778	2.1898900636	-4.6105345676
H	1.0	6.4848214940	5.0101360249	1.2132607759
H	1.0	10.1361311502	7.5203157462	0.8036248735
C	6.0	14.4302311011	6.7473422282	-2.2062172961
C	6.0	14.8241444833	8.9175980388	-0.6437162605
C	6.0	17.0029040608	10.4075524938	-0.8843917623
C	6.0	18.7942698109	9.7450145625	-2.6796881424
C	6.0	18.4826350983	7.6764827018	-4.2133330622
C	6.0	16.3343756982	6.1542706242	-4.0181243677
C	6.0	21.1558414805	10.9423638456	-3.2986489924
C	6.0	22.2901117101	9.6068377983	-5.2112217673
C	6.0	20.6965246819	7.3559851743	-6.0159426819
C	6.0	22.2699294365	13.0781321569	-2.2649499798
C	6.0	24.6126983326	13.8807176812	-3.2095106175
C	6.0	25.8550986832	12.5399759901	-5.2007526853
C	6.0	24.6241311748	10.3571723990	-6.1907801303
H	1.0	16.1966146736	4.5694519246	-5.2800833823
H	1.0	13.4892609428	9.4888811021	0.7759403878
H	1.0	17.2754592400	12.0425812129	0.3134488496
H	1.0	21.3543949900	14.1107729229	-0.7557014225
H	1.0	25.4164365897	15.5359097766	-2.3502144164
C	6.0	28.3968368285	13.4099491431	-6.2276297871
H	1.0	25.4074792885	9.2397207307	-7.6944917905
C	6.0	22.0879110294	4.8518903707	-5.5511834725
C	6.0	19.8530643845	7.5891962585	-8.7830684457
H	1.0	20.8372525762	3.2241559940	-5.9910360934

H	*1.0*	*23.7950516922*	*4.7237669488*	*-6.7662205908*
H	*1.0*	*22.6887116127*	*4.7046051273*	*-3.5436519667*
H	*1.0*	*18.8490529673*	*9.4076228847*	*-9.0962905282*
H	*1.0*	*21.5134910209*	*7.5180669723*	*-10.0656065763*
H	*1.0*	*18.5558808775*	*6.0185882983*	*-9.2904598734*
C	*6.0*	*29.7360667387*	*11.9700157350*	*-8.0321291327*
C	*6.0*	*32.0697460527*	*12.7676879717*	*-8.9749890170*
C	*6.0*	*33.1904480497*	*15.0515919032*	*-8.1689641915*
C	*6.0*	*31.8504055573*	*16.4923567907*	*-6.3657498595*
C	*6.0*	*29.5189750172*	*15.6923601911*	*-5.4193561876*
H	*1.0*	*28.6280825976*	*16.9103452819*	*-4.0599251065*
H	*1.0*	*32.5672164190*	*18.2489893771*	*-5.6402462583*
H	*1.0*	*29.0275895686*	*10.2046526145*	*-8.7444802411*
H	*1.0*	*32.9517945547*	*11.5590570244*	*-10.3484796594*
C	*6.0*	*35.7303720580*	*15.9234736794*	*-9.1986569850*
C	*6.0*	*37.1895995685*	*14.3551144931*	*-10.8470082723*
C	*6.0*	*39.5300252043*	*15.1602511475*	*-11.7952160811*
C	*6.0*	*40.4243569253*	*17.5267927964*	*-11.1089809859*
C	*6.0*	*39.0778893645*	*19.0850797431*	*-9.5319668547*
C	*6.0*	*36.7422447354*	*18.3363514095*	*-8.5550541081*
C	*6.0*	*42.7324115549*	*18.7805504002*	*-11.8123936904*
C	*6.0*	*42.7978527658*	*21.1074644952*	*-10.6682401938*
C	*6.0*	*40.4535720890*	*21.5648159787*	*-9.0717429876*
C	*6.0*	*44.6786970414*	*17.9557794929*	*-13.3624414318*
C	*6.0*	*46.7582082101*	*19.5504436649*	*-13.7596807317*
C	*6.0*	*46.8963471798*	*21.9889082849*	*-12.6018456190*
C	*6.0*	*44.8421205448*	*22.7390350157*	*-11.0279117411*
H	*1.0*	*35.7758010708*	*19.6460071081*	*-7.3408484692*
H	*1.0*	*36.5702985678*	*12.5062443813*	*-11.4146252672*
H	*1.0*	*40.6139531336*	*13.9508832071*	*-13.0381455550*
H	*1.0*	*44.6001600294*	*16.1168304424*	*-14.2537873857*
H	*1.0*	*48.2202892068*	*18.8440640907*	*-14.9786862746*
H	*1.0*	*44.7842193406*	*24.5304574576*	*-10.0742048296*
C	*6.0*	*38.9237066211*	*23.8250416436*	*-10.0584445148*
C	*6.0*	*41.1279397050*	*21.8983337183*	*-6.2687880191*
H	*1.0*	*37.1359124532*	*24.0301525023*	*-8.9773889691*
H	*1.0*	*40.0258515090*	*25.6007037707*	*-9.8600043889*
H	*1.0*	*38.4468342681*	*23.5623319368*	*-12.0873488216*
H	*1.0*	*42.2342797845*	*20.2522878967*	*-5.5764491089*
H	*1.0*	*42.2756836809*	*23.6339714490*	*-5.9908849153*
H	*1.0*	*39.3859335977*	*22.0626642902*	*-5.1088364133*
C	*6.0*	*49.1514138927*	*23.7209177417*	*-13.0327220414*
C	*6.0*	*49.2223920008*	*26.2019578882*	*-12.0117030903*
C	*6.0*	*51.3002213133*	*27.7820144784*	*-12.4164634996*
C	*6.0*	*53.3501582703*	*26.9479650164*	*-13.8343816000*
C	*6.0*	*53.3354939966*	*24.5271315398*	*-14.8580650648*
C	*6.0*	*51.2716675537*	*22.9240391899*	*-14.4720507373*
H	*1.0*	*51.3869408389*	*21.0774178520*	*-15.3085568430*
H	*1.0*	*54.9341832850*	*23.8816011424*	*-15.9593973704*
H	*1.0*	*54.9537041544*	*28.1803498193*	*-14.1405927990*
H	*1.0*	*51.3152257377*	*29.6677720415*	*-11.6232510162*
H	*1.0*	*47.7004444848*	*26.9675047831*	*-10.9065724354*

PMNF-P Oligomer:

E = -3042.212754368

		COORDINATES (BOHR)		
ATOM	*CHARGE*	*X*	*Y*	*Z*
C	*6.0*	*-5.2648899854*	*-6.7548066459*	*2.4831944342*
C	*6.0*	*-3.5198792138*	*-8.6845948245*	*2.0269011972*
C	*6.0*	*-1.0121939308*	*-8.1492921440*	*1.2561008640*
C	*6.0*	*-0.2910178021*	*-5.5405065207*	*1.0360611700*
C	*6.0*	*-2.0973123875*	*-3.6659550326*	*1.4667864144*
C	*6.0*	*-4.5684503698*	*-4.2403372466*	*2.1801768720*
C	*6.0*	*2.0991265244*	*-4.2115189253*	*0.4349582306*
C	*6.0*	*1.6228210892*	*-1.6395451642*	*0.4219947103*
C	*6.0*	*-1.0817736417*	*-1.0278030675*	*1.0730620049*
C	*6.0*	*4.5733069656*	*-5.0616877499*	*0.0058581506*
C	*6.0*	*6.4966133841*	*-3.3159399852*	*-0.5202604617*
C	*6.0*	*6.0145442847*	*-0.6745943831*	*-0.6032383298*
C	*6.0*	*3.5119045701*	*0.1334713465*	*-0.0969429432*
C	*6.0*	*8.1073780216*	*1.2116923033*	*-1.1762410438*
C	*6.0*	*7.7125764682*	*3.8407357892*	*-0.9476597883*
C	*6.0*	*9.6321601265*	*5.5736901090*	*-1.4782192566*
C	*6.0*	*12.0538250825*	*4.7724462902*	*-2.2673121373*
C	*6.0*	*12.4473794167*	*2.1417398454*	*-2.4960823654*
C	*6.0*	*10.5267564091*	*0.4092201626*	*-1.9651827464*
C	*6.0*	*-2.4321718325*	*0.3147527605*	*-1.1203807436*
C	*6.0*	*-1.2425137342*	*0.5388931599*	*3.5162509399*
C	*6.0*	*14.1495312029*	*6.6570322232*	*-2.8534484469*
C	*6.0*	*13.6691628568*	*9.2945416816*	*-2.9660950131*
C	*6.0*	*15.5883874672*	*11.0879294384*	*-3.4886609405*
C	*6.0*	*18.0752290726*	*10.1680675194*	*-3.9961468545*
C	*6.0*	*18.5449015695*	*7.5906324502*	*-3.8349154332*
C	*6.0*	*16.6543063079*	*5.8440343088*	*-3.2751974929*
C	*6.0*	*20.4873131178*	*11.3757725009*	*-4.7408878662*
C	*6.0*	*22.3204418122*	*9.5194190741*	*-4.8822393701*
C	*6.0*	*21.2828688614*	*6.9276409847*	*-4.3213497997*
C	*6.0*	*21.1298766454*	*13.8685667431*	*-5.3699209557*
C	*6.0*	*23.6256566547*	*14.4605612032*	*-6.0330635994*
C	*6.0*	*25.5438230185*	*12.5801704619*	*-6.1176099401*
C	*6.0*	*24.8219098967*	*10.0656065763*	*-5.5382199522*
C	*6.0*	*28.2506098315*	*13.2332030715*	*-6.8435481782*
C	*6.0*	*30.1067553884*	*11.3402267551*	*-7.1556553224*
C	*6.0*	*32.5889671651*	*11.9406304959*	*-7.8285489521*
C	*6.0*	*33.3535691970*	*14.4684413606*	*-8.2190986220*
C	*6.0*	*31.4983118113*	*16.3607373757*	*-7.9013600944*
C	*6.0*	*29.0160811374*	*15.7599745869*	*-7.2344757933*
C	*6.0*	*22.5311273626*	*5.7626438105*	*-1.9713432531*
C	*6.0*	*21.5503595749*	*5.1751091037*	*-6.6256816691*
C	*6.0*	*36.0558017704*	*15.1320564357*	*-8.9552602777*
C	*6.0*	*37.8291962263*	*13.2364534002*	*-9.6335774210*
C	*6.0*	*40.3589346116*	*13.8047884910*	*-10.3080962151*
C	*6.0*	*41.0986300549*	*16.4012908954*	*-10.3735563233*
C	*6.0*	*39.3686048104*	*18.2423186444*	*-9.6604304273*
C	*6.0*	*36.8981471294*	*17.6617759237*	*-8.9579436886*
C	*6.0*	*43.4447059714*	*17.7472293329*	*-11.0966977670*
C	*6.0*	*43.0803101092*	*20.3012506971*	*-10.6818273237*
C	*6.0*	*40.4611120957*	*20.8823225410*	*-9.7302935971*

C	*6.0*	*45.7411576835*	*16.9292614391*	*-12.1382013479*
C	*6.0*	*47.6578311638*	*18.6862341762*	*-12.6514887207*
C	*6.0*	*47.3294912734*	*21.3084746485*	*-12.1658291418*
C	*6.0*	*44.9656519326*	*22.0857567418*	*-11.1749324229*
C	*6.0*	*49.4132543256*	*23.2104649579*	*-12.7241486849*
C	*6.0*	*49.1555901871*	*25.7983691090*	*-12.0608737605*
C	*6.0*	*51.0779706399*	*27.5344603740*	*-12.5785075030*
C	*6.0*	*53.2921247852*	*26.7549295068*	*-13.7611169234*
C	*6.0*	*53.5993942308*	*24.2322964912*	*-14.4326688477*
C	*6.0*	*51.6959110379*	*22.4718655556*	*-13.9266758172*
C	*6.0*	*39.0188165301*	*22.5715486014*	*-11.6064324549*
C	*6.0*	*40.5276493477*	*22.0785568858*	*-7.0839213239*
H	*1.0*	*-4.4606415022*	*0.6086807406*	*-0.6669598901*
H	*1.0*	*-1.5617073508*	*2.1894554266*	*-1.4865340510*
H	*1.0*	*-2.3036137736*	*-0.8311392839*	*-2.8763897204*
H	*1.0*	*-0.2625774260*	*-0.4468257098*	*5.0916777013*
H	*1.0*	*-0.3454041160*	*2.4178666068*	*3.2499696509*
H	*1.0*	*-3.2446406237*	*0.8433091193*	*4.0682210036*
H	*1.0*	*-5.9329459165*	*-2.7530284080*	*2.5099718514*
H	*1.0*	*-7.1755919315*	*-7.2204351292*	*3.0457469635*
H	*1.0*	*-4.1518035841*	*-10.6186159894*	*2.2324277956*
H	*1.0*	*5.1098379681*	*-7.0028520790*	*0.0981523678*
H	*1.0*	*8.3550833040*	*-4.0791247226*	*-0.8249409827*
H	*1.0*	*2.9804380333*	*2.0932683739*	*-0.0932390802*
H	*1.0*	*10.9825583174*	*-1.5555846386*	*-2.2118675768*
H	*1.0*	*5.9349679233*	*4.6150699100*	*-0.3407364928*
H	*1.0*	*9.1686859308*	*7.5357359103*	*-1.2314588372*
H	*1.0*	*14.2228336740*	*1.3668388069*	*-3.1099976470*
H	*1.0*	*11.8025482180*	*10.0053243173*	*-2.6239412257*
H	*1.0*	*17.1894389131*	*3.8874498156*	*-3.1788781593*
H	*1.0*	*19.7921774132*	*15.3776641223*	*-5.4215482697*
H	*1.0*	*23.9981972359*	*16.4017822241*	*-6.4996369457*
H	*1.0*	*26.1331340678*	*8.5165225952*	*-5.5865591430*
H	*1.0*	*29.6905054451*	*9.3685244540*	*-6.9011092318*
H	*1.0*	*27.7334107259*	*17.3210772254*	*-7.0286468387*
H	*1.0*	*31.9094405972*	*18.3312680466*	*-8.1794332735*
H	*1.0*	*33.8779681586*	*10.3811530218*	*-8.0116067085*
H	*1.0*	*21.6383830114*	*3.9230900478*	*-1.4968330576*
H	*1.0*	*24.5764344909*	*5.4326787558*	*-2.3092073625*
H	*1.0*	*22.3294747024*	*7.0441236946*	*-0.3190235412*
H	*1.0*	*20.6417604228*	*6.0323455035*	*-8.3148699350*
H	*1.0*	*23.5746529502*	*4.8334466451*	*-7.0635122832*
H	*1.0*	*20.6419871899*	*3.3197383344*	*-6.2547851495*
H	*1.0*	*37.0397820922*	*22.8628120679*	*-10.9710498861*
H	*1.0*	*39.9358816547*	*24.4531298702*	*-11.7633930955*
H	*1.0*	*38.9800582501*	*21.6912197501*	*-13.5136006135*
H	*1.0*	*41.5751433600*	*20.8449815555*	*-5.7445024410*
H	*1.0*	*41.4772555538*	*23.9496501753*	*-7.1436933569*
H	*1.0*	*38.5808158407*	*22.3531529690*	*-6.3487234284*
H	*1.0*	*35.6927098191*	*19.2061733844*	*-8.4238504327*
H	*1.0*	*37.2843693268*	*11.2841396877*	*-9.6257728527*
H	*1.0*	*46.1181391208*	*15.0062762740*	*-12.6166421735*
H	*1.0*	*49.3795038194*	*17.9428159726*	*-13.4313219440*
H	*1.0*	*44.5286339007*	*24.0331760639*	*-10.8028075814*
H	*1.0*	*52.0516519551*	*20.5575164383*	*-14.5035713667*
H	*1.0*	*55.3238447837*	*23.6306644285*	*-15.3544771845*

H	*1.0*	*54.7734620897*	*28.1086347181*	*-14.1573924630*
H	*1.0*	*50.8447217613*	*29.4982258259*	*-12.0544297949*
H	*1.0*	*47.5007571397*	*26.5237593267*	*-11.1330183005*
N	*7.0*	*42.0351971517*	*11.7411510206*	*-10.8176419304*
O	*8.0*	*44.2474993655*	*11.9735117281*	*-10.5047788959*
O	*8.0*	*41.1186611504*	*9.4442646716*	*-11.0966410752*
N	*7.0*	*0.6102870077*	*-10.2367212645*	*0.6852902322*
O	*8.0*	*2.3501199301*	*-9.9787169754*	*-0.7108771221*
O	*8.0*	*-0.1046152307*	*-12.5481774009*	*1.2677604734*
N	*7.0*	*14.9339753577*	*13.7134769313*	*-3.4099160585*
O	*8.0*	*16.4926213524*	*15.2553799537*	*-2.9200045962*
O	*8.0*	*12.5400893737*	*14.3881658007*	*-3.3227429987*

PDNF-P Oligomer

E = -3655.3831350115

		COORDINATES (BOHR)		
ATOM	*CHARGE*	*X*	*Y*	*Z*
C	*6.0*	*-6.0206669969*	*-5.3838482363*	*0.9510046033*
C	*6.0*	*-4.4116031129*	*-7.4747544527*	*0.8070830721*
C	*6.0*	*-1.7546294769*	*-7.1845870272*	*0.6538073972*
C	*6.0*	*-0.7557959088*	*-4.6629366692*	*0.7409237653*
C	*6.0*	*-2.4205878122*	*-2.6201806710*	*0.8375454550*
C	*6.0*	*-5.0335497299*	*-2.9486906367*	*0.9381544666*
C	*6.0*	*1.8257209685*	*-3.5837708494*	*0.7749955248*
C	*6.0*	*1.6217061509*	*-0.9838480410*	*0.7773954768*
C	*6.0*	*-1.0855341964*	*-0.0979822925*	*0.8113916473*
C	*6.0*	*4.2269201921*	*-4.6964604082*	*0.9174997616*
C	*6.0*	*6.4416223579*	*-3.1833001181*	*0.9538769868*
C	*6.0*	*6.1923108083*	*-0.4743779147*	*0.8144530034*
C	*6.0*	*3.7404669283*	*0.5753270770*	*0.7801355795*
C	*6.0*	*8.3841283925*	*1.3233940065*	*0.6265575485*
C	*6.0*	*8.2939128738*	*3.6938851827*	*1.8184077289*
C	*6.0*	*10.2955673318*	*5.4019518112*	*1.6051710485*
C	*6.0*	*12.4673727177*	*4.8191981111*	*0.1547118666*
C	*6.0*	*12.5178661961*	*2.4436613665*	*-1.0754430596*
C	*6.0*	*10.5133204574*	*0.7414528885*	*-0.8450098727*
C	*6.0*	*-1.7439336278*	*1.4283304906*	*-1.5705323711*
C	*6.0*	*-1.6567227734*	*1.4243620660*	*3.2205277201*
C	*6.0*	*14.6447527953*	*6.6796333461*	*-0.0943162240*
C	*6.0*	*14.8027527851*	*8.8574480606*	*1.4642163871*
C	*6.0*	*16.8192037976*	*10.6103956813*	*1.2849758771*
C	*6.0*	*18.6967410527*	*10.1884198683*	*-0.6063941722*
C	*6.0*	*18.5621169733*	*8.0268756945*	*-2.0876747849*
C	*6.0*	*16.6011105213*	*6.2831121421*	*-1.8624005499*
C	*6.0*	*20.9383529166*	*11.6178275027*	*-1.4754791540*
C	*6.0*	*22.1162947137*	*10.2291434633*	*-3.3385977998*
C	*6.0*	*20.7424450234*	*7.8041903841*	*-3.9218050341*
C	*6.0*	*21.8845576159*	*14.0114489250*	*-0.8452933316*
C	*6.0*	*24.0966897544*	*14.9665542337*	*-2.0238020466*
C	*6.0*	*25.3819490904*	*13.4247834921*	*-3.8664171654*
C	*6.0*	*24.3087737020*	*11.0721313292*	*-4.5233426105*
C	*6.0*	*27.8431660113*	*14.1292544431*	*-5.1001247765*
C	*6.0*	*28.3239689944*	*13.4730470938*	*-7.6276143878*

C	*6.0*	*30.6240300831*	*14.0725248689*	*-8.7766811719*
C	*6.0*	*32.5582402205*	*15.3386223834*	*-7.4292876454*
C	*6.0*	*32.0703696623*	*15.9503833774*	*-4.8709010142*
C	*6.0*	*29.7656220531*	*15.3450852463*	*-3.7350623120*
C	*6.0*	*22.3837098383*	*5.4776164398*	*-3.3469125941*
C	*6.0*	*19.8099597348*	*7.7726886519*	*-6.6751924900*
C	*6.0*	*35.0652074076*	*16.0042594654*	*-8.6683242838*
C	*6.0*	*35.7382522154*	*15.0328080268*	*-11.0765532880*
C	*6.0*	*38.0491036395*	*15.6502759933*	*-12.2816315504*
C	*6.0*	*39.7780895347*	*17.2467920968*	*-10.9594091740*
C	*6.0*	*39.0856939328*	*18.2326054528*	*-8.6280920175*
C	*6.0*	*36.7900925974*	*17.6507399239*	*-7.4762284389*
C	*6.0*	*42.3600977408*	*18.1848142826*	*-11.4906678409*
C	*6.0*	*43.0642663356*	*19.7715605027*	*-9.5475948886*
C	*6.0*	*41.0653708775*	*19.9767280532*	*-7.5306525474*
C	*6.0*	*44.0912568209*	*17.6562957183*	*-13.4266354236*
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C	*6.0*	*-1.3544044099*	*1.0232677251*	*3.4073460312*
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