

Single-Handed Helical Wrapping of Single-Walled Carbon Nanotubes by Chiral, Ionic, Semiconducting Polymers

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Materials.

All manipulations were carried out under argon previously passed through an O₂ scrubbing tower (Schweitzerhall R3-11 catalyst) and a drying tower (Linde 3-Å molecular sieves) unless otherwise stated. Air sensitive solids were handled in a Braun 150-M glove box. Standard Schlenk techniques were employed to manipulate air-sensitive solutions. Tetrahydrofuran (THF), CH₂Cl₂, N,N-dimethylformamide (DMF), methanol, and diethylether were collected from PURE SOLV (innovative technology) solvent purification system. Dioxane and triethylamine were distilled from Na/4-benzoylbiphenyl and NaOH pellets, respectively, under argon; re-distilled diisopropylamine was purchased from Aldrich. All NMR solvents were used as received. The catalysts PdCl₂(PPh₃)₂, Pd(PPh₃)₄ and tris(dibenzylideneacetone)dipalladium(0) (Pd₂dba₃), as well as P(*o*-tol)₃, triphenylarsine (AsPh₃) were purchased from Strem Chemicals and used as received. 1,3-Propane sultone,

phenylacetylene, 4-iodophenol, (triisopropylsilyl)acetylene, (trimethylsilyl)acetylene, 1,4-dimethoxybenzene, 1,4-dibromo-2,5-dimethylbenzene, 1,3-bis(bromomethyl)benzene, triethylene glycol monomethyl ether, and enantiopure (ee 99%) (*R*)-(+)-1,1'-bi(2-naphthol) and (*S*)-(-)-1,1'-bi(2-naphthol) were purchased from Aldrich and used without further purification. Neat bromine, BuLi (2.5 M solution in hexane), tetraoctylammoniumbromide (TOAB) and tetrabutylammoniumfluoride (TBAF; 1M in THF) were purchased from Aldrich and used as received, where the N-bromosuccinimide (NBS) was recrystallized from water and dried under vacuum at 70 °C overnight prior to use.

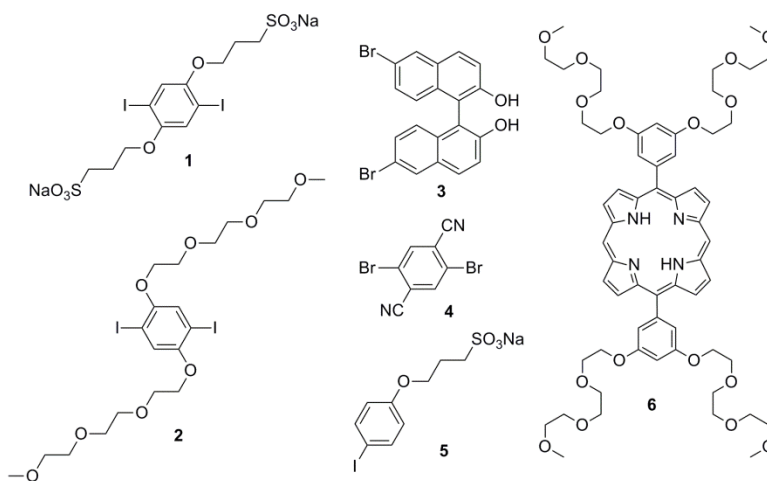


Chart S1: Precursor molecules and key building blocks used for the chiral polymers; these compounds were synthesized following established literature procedure (see SI-text)

Various starting materials (**Chart S1**), such as {[2,5-diiodo-1,4-bis(3-propoxy-sulfonic acid)benzene] sodium salt} (**1**),¹ 1,4-bis(9-methoxy-1,4,7-trioxanonyl)-2,5-diiodobenzene (**2**),² (*R*)- and (*S*)-6,6'-dibromo-2,2'-dihydroxy-1,1'-binaphthyl (**R-3**, **S-3**),³ 1,4-dicyano-2,5-dibromobenzene (**4**),⁴ {[1-iodo-4-(3-propoxy-sulfonic acid)benzene] sodium salt} (**5**),^{1a,5} and 5,15-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphyrin (**6**)⁶ were prepared according to the published procedures. CoMoCat SWNTs were obtained from Sigma Aldrich as freeze dried powder and used as starting material for density gradient (DG) purification to obtain samples enriched with (6,5) chirality tubes. Raw SWNTs prepared via pulsed laser vaporization (PLV-SWNTs) were obtained from NREL, Denver, Colorado, and

raw few-walled carbon nanotubes (FWNTs) were prepared via chemical vapor deposition were obtained from Prof. J. Liu (Duke University); these materials were used without further purification. Flash and size exclusion column chromatography were performed on the bench top, using respectively silica gel (EM Science, 230–400 mesh) and Bio-Rad Bio-Beads SX-1 as media.

Instrumentation.

Free, unbound polymer in each polymer/CNT sample was removed by GE/ÅKTApurifier HPLC system (GE Healthcare Bio-Science AB, Björkgatan, Uppsala, Sweden) equipped with two preparative columns (160x16 mm each; stationary phase: sephacryl S-500 and S-200) connected in a series in the order S-500 and S-200. The HPLC system uses a three-wavelength detection unit (each ranging from 200-700 nm; *vide infra*), which was used to distinguish fractions with and without SWNTs. Electronic spectra were recorded on a Varian 5000 UV/vis/NIR spectrophotometry system. All spectroscopic measurements were carried out at 23 ± 1 °C. CD spectra of the polymer-CNT samples were recorded on an AVIV/Model 202 /UV/Vis CD instrument that uses a PMT detector and a Xe Lamp light source (bandwidth 1 nm). All the CD spectra were acquired as a single scan over 200-700 nm range with 3s averaging at each 2 nm steps. Transmission electron microscopy images (JEOL TEM-2010; accelerate voltage, 200 kV) were obtained from samples prepared via drop casting on lacy Formvar copper grids stabilized with carbon followed by drying in a desiccators overnight. Atomic force microscopy (AFM; Digital Instruments Dimension 3100) images were obtained via intermittent contact mode (scan rate = 0.6 Hz, ambient temperature) using super-sharp Si-tips (FORTA-SS-10 from AppNano; tip radius < 5 nm, cantilever resonant frequency ~70 kHz). AFM samples were prepared by drop-casting SWNT suspensions on Si wafer surfaces (cleaned with acetone and 2-propanol); such samples were then desiccator-dried for overnight. AFM data are presented with a 1st order plane fit. X-ray photoelectron spectroscopic (XPS) data were obtained at CHANL/UNC Chapel Hill. All XPS data were taken with a Kratos Axis Ultra DLD system with a monochromatic Al K α radiation source. Survey spectra and high resolution scans were acquired at pass energies of 80 and 20 eV, respectively. All peaks were calibrated to the C-1s peak at 284.6 eV. NMR

spectra were recorded on a 400 and 500 MHz AC-Bruker spectrometer. Chemical shifts for ^1H NMR spectra are relative to residual protium in the deuterated solvents ($\text{CDCl}_3 = 7.24$ ppm, $\text{D}_2\text{O} = 4.75$ ppm). ^{13}C NMR spectra are also referenced to deuterated solvents ($\text{CDCl}_3 = 77.23$ ppm, $\text{DMSO-}d_6$ as 39.35 ppm). All J values are reported in Hertz. MALDI-TOF mass spectroscopic data were obtained with a Perspective Voyager DE instrument (Department of Chemistry, Duke University). Microwave assisted reactions were performed with Emrys Personal Chemistry System (Biotage).

Molecular Models

The molecular potential parameters for chiral polymer repeat units were developed using quantum mechanical calculations and parameters reported in previous work.⁷ The restrained electrostatic potential method was used to obtain effective atomic charges subject to overall neutrality of each aromatic unit. The effective charges were fit using electrostatic energies computed using the HF/6-311G** basis set in Gaussian09.⁸ All parameter information appears in Appendix S1. The polymer structure was prepared with a total of 35 aryl subunits and terminal p -{4-(3-propoxysulfonicacidsodiumsalt)}phenylene]ethylene units; **S-PBN(b)-Ph₅** contained 5 repeat segments with an additional **Ph₅** segment (Figure S30). For the helical initial configurations of the polymer, all phenyl rings were positioned in the same manner on each monomer; there were no "ring flips," and the aryl subunits were translationally invariant along the contour of the polymer. The naphthalene-naphthalene dihedral potential of the binaphthyl unit was parameterized to be consistent with known potentials of methoxy-binaphthyl units.⁹ For helical initial conditions of the polymer, binaphthyl interplanar torsional angle (ϕ , Scheme 1) was set to 90° and all side chains were positioned in the same manner (all trans) on each aromatic unit. The initial helical structure was generated by aligning the polymer to an ideal helix having radius r and pitch p , as described previously.¹⁰ In building the helix, rigid body motions were used to position each monomer by equivalent ethynyl carbon positions that span each binaphthyl and phenyl subunit.

Similar to our previous work on conjugated polymer-wrapped SWNT, an achiral [(10,0) SWNT] was selected.^{7a,10} Coordinates for the tube were generated using the VMD Nanotube Builder¹¹ and was

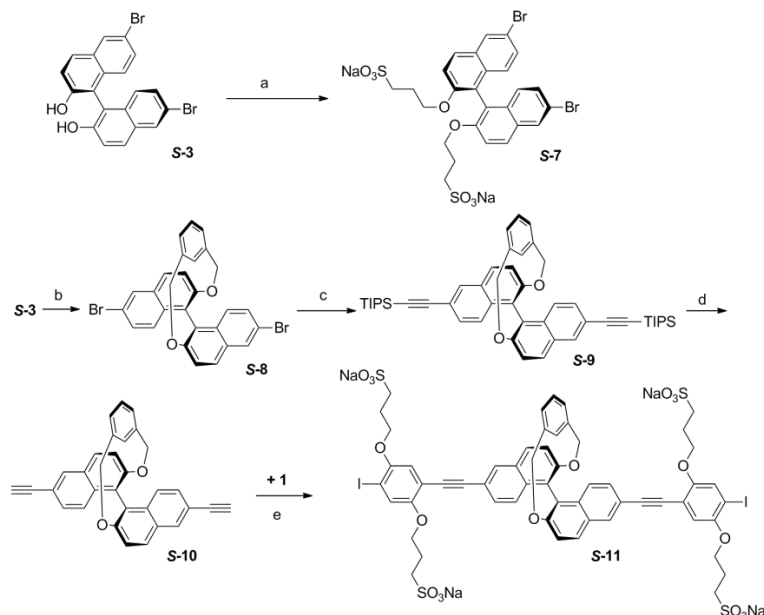
used for simulations as generated nanotube without any relaxation of nuclear coordinates of the tube was performed. Each atom of the SWNT was parameterized as sp^2 carbon atoms of the CHARMM force field¹² with zero net atomic charge. The nanotube length in each simulation was 29.6 nm with an internuclear diameter of 0.793 nm. The nanotube length was more than twice that of the extended polymer, and at no point during the simulation did the polymer approach nanotube ends. The coordinates of all atoms within each nanotube were fixed in all simulations with C-C bonds constrained to their equilibrium lengths of 1.42 Å.

Molecular Dynamics Simulations

All simulations were performed using the molecular dynamics program NAMD2.7.¹³ Orthorhombic periodic boundary conditions were applied in all three Cartesian dimensions, and the average dimensions were 60 Å x 60 Å x 330 Å. The equations of motion were integrated with a time step of 2 fs. Covalent bonds involving hydrogen atoms were constrained to their equilibrium length by means of the SHAKE/RATTLE algorithms.¹⁴ Long-range electrostatic forces were evaluated by means of the particle-mesh Ewald (PME) approach¹⁵ with a 1 Å mesh, and van der Waals interactions were truncated smoothly with a spherical cutoff of 12 Å. For solvated simulations, the TIP3P¹⁶ water model was used. The aqueous system was ensured to be electrostatically neutral via the addition of sodium and chloride ions using the VMD module AUTOIONIZE,¹⁷ consistent with a salt concentration (ionic strength) of 0.2 mol/L. The simulations in the aqueous phase included ~ 35,960 TIP3P waters placed using the VMD module SOLVATE,¹⁷ yielding a total of 111,902 atoms including the polymer, counter ions and the (10,0) nanotube. Aqueous simulations were carried out in the isothermal-isobaric ensemble; pressure and temperature were maintained at 1 bar and 300K by employing Langevin dynamics with damping coefficient of 5 ps⁻¹ and the Langevin piston pressure control with an oscillation period of 100 fs and decay time of 50 fs.¹⁸ Preparation, visualization, and analysis of structures and trajectories utilized the VMD package.¹⁷ The length of the trajectory was 80 ns, and configurations were sampled every 20 ps for a total of 4,000 configurations.

Simulations of the isolated binaphthyl units, unbridged **S-BN** and bridged **S-BN(b)**, in TIP3P aqueous solvent (300 K, 1 atm) were performed in an analogous manner. The number of water molecules and atoms were: 6,871 atoms (2,267 water molecules) for **S-BN**, and 5,390 atoms (1,768 water molecules) for **S-BN(b)**. The length of each trajectory was 40 ns, and configurations were sampled every 20 ps for a total of 2,000 configurations. The data were consistent with the expected properties of unbridged and bridged moieties;¹⁹ for **S-PBN**, the average dihedral angle was $\varphi=87 \pm 17^\circ$, while for the bridged **S-PBN(b)**, $\varphi=107 \pm 10^\circ$.

Synthesis, Sample Preparation, and Characterization



Scheme S1: Synthesis of 1,1'-binaphthalene based dihalo units used for chiral polymer syntheses: (a) 1 M aqueous NaOH, 1,3-propane sultone in dioxane; (b) K_2CO_3 , 1,3-bis(bromomethyl)benzene, DMF, 80°C ; (c) Triisopropylsilylacetylene, $\text{PdCl}_2(\text{PPh}_3)_2$, CuI, Et_3N , THF; (d) TBAF, THF; (e) {[2,5-diiodo-1,4-bis(3-propoxy-sulfonic acid) benzene] sodium salt} (**1**), $\text{Pd}(\text{PPh}_3)_4$, CuI, $i\text{-Pr}_2\text{NH}$, DMF, 80°C .

***R*- and *S*- {[6,6'-dibromo-2,2'-bis(3-propoxysulfonic acid)-1,1'-binaphthalene] sodiumsalt}** (**R-7** and **S-7**). **R-7** and **S-7** compounds were prepared separately. Enantiopure *S*- or *R*- 6,6'-dibromo-1,1'-binaphthalene-2,2'-diol (19 g, 43 mmol) was dissolved in a degassed aqueous solution of sodium hydroxide (4.3 g, 107.5 mmol, 0.4 M) in a round bottomed flask equipped with an addition funnel under argon. The addition funnel was then charged with a degassed (argon purged for 30 min) solution of 1,3-propanesultone (13.2 g, 108.0 mmol) in dioxane (70 ml) and added dropwise to the aqueous reaction

mixture. The resulting mixture was then stirred at room temperature overnight; during this time thick silky slurry formed. The reaction mixture was then stirred at 80° C for 30 min followed by cooling in a water/ice bath. The solid was filtered through a glass frit and washed with ice cold water. The off-white solid was crystallized from water. Yield = 25 g (80%, based on 19 g *S*- or *R*- 6,6'-dibromo-1,1'-binaphthalene-2,2'-diol). ¹H NMR (500 MHz, D₂O as 4.75 ppm, **Figure S1A**): δ 7.923 (d, 2 H, *J* = 1.5 Hz), 7.889 (d, 2H, *J* = 9.0 Hz), 7.467 (d, 2H, *J* = 9.5 Hz), 6.821 (dd, 2H, *J* = 9.0, 1.5 Hz), 6.455 (d, 2H, *J* = 9.0 Hz), 4.095-4.055 (m, 2H), 3.918-3.875 (m, 2H), 2.171-2.111 (m, 2H), 2.043-1.985 (m, 2H), 1.740-1.684 (m, 4H). ¹³C NMR (125 MHz, DMSO-*d*₆ as 39.52 ppm): δ 154.352, 131.924, 129.806, 129.760, 129.275, 128.799, 126.685, 118.464, 116.382, 116.276, 67.888, 47.589, 25.248. MP: 310 °C.

(*S*)-3,17-Dibromo-8,12-dihydrobenzo[*hi*]-dinaphtho[2,1-*b* : 1,2-*d'*][1,6]dioxacycloundecine, (*S*-8). Enantiopure *S*-6,6'-dibromo-1,1'-binaphthalene-2,2'-diol, **S-3**, (13.3 g, 30 mmol), K₂CO₃ (66.5 g, 480 mmol) and 500 ml of dry, degassed DMF were taken in a two-neck 1 L round bottomed flask and the mixture was stirred for 15 min at 80 °C under argon. A solution of 1,3-bis(bromomethyl)benzene (10.16 g, 38.5 mmol) in 40 ml anhydrous DMF was added to the reaction mixture *via* syringe pump over 16 h, following which it was cooled, diluted with 100 ml H₂O, and extracted several times with CH₂Cl₂. The combined organic layers were washed with water, saturated aq. NaCl, and dried over Na₂SO₄. After the solvent was evaporated, the residue was chromatographed on silica gel using 3:7 CH₂Cl₂:hexanes as the eluent (*R*_f ~ 0.5). Yield = 9 g (55%, based on 13.3 g of *S*-6,6'-dibromo-1,1'-binaphthalene-2,2'-diol). ¹H NMR (500 MHz, CDCl₃, **Figure S1B**): δ 7.930 (d, 2H, *J* = 2.0 Hz), 7.757 (d, 2H, *J* = 9.0 Hz), 7.403 (s, 1H), 7.390 (d, 2H, *J* = 9.0 Hz), 7.306 (dd, 2H, *J* = 9.0, 2.0 Hz), 7.053 (d, 2H, *J* = 9.0 Hz), 6.951-6.922 (m, 1H), 6.873 (d, 2H, *J* = 7.0 Hz), 5.214 (d, 2H, *J* = 12.5 Hz), 5.044 (d, 2H, *J* = 12.5 Hz). ¹³C NMR (500 MHz, CDCl₃): δ 154.067, 138.186, 132.697, 131.305, 130.030, 130.013, 129.548, 129.374, 127.951, 127.819, 127.722, 125.743, 121.819, 118.994, 75.515. EI MS *m/z* : 546 [(M)+] (calcd 546).

(*S*)-3,17-Bis((triisopropylsilyl)ethynyl)-8,12-dihydrobenzo[*hi*]-dinaphtho[2,1-*b* : 1,2-*d'*][1,6]dioxacycloundecine, (*S*-9). Compound **S-8** (2.92 g, 5.35 mmol), PdCl₂(PPh₃)₂ (0.225 g, 0.321

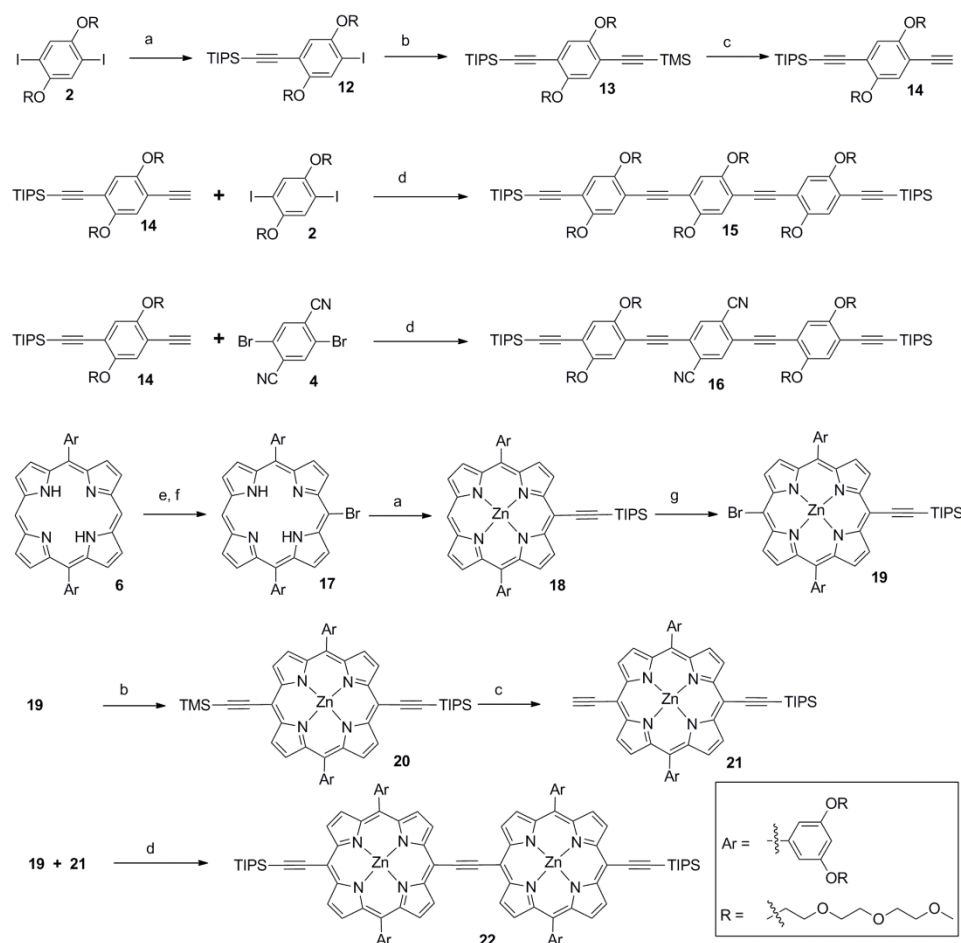
mmol), CuI (0.061 g, 0.321 mmol) were transferred to a 100 ml Schlenk tube in dry box. A solvent mixture of anhydrous THF (40 ml), triethylamine (8 ml) and (triisopropylsilyl)acetylene (5.94 ml, 26.75 mmol) was degassed by three successive freeze-pump-thaw cycles and transferred to the reaction tube via a cannula. The reaction mixture was stirred at 55 °C overnight; following which it was cooled, poured into 150 ml H₂O, and extracted several times with CH₂Cl₂. The combined organic layers were washed with water, saturated aq. NaCl, and dried over Na₂SO₄. After the solvent was evaporated, the residue was chromatographed on silica gel using 3:7 CH₂Cl₂:hexanes as the eluent (*R_f* ~ 0.77). The 1st column band was collected as the desired bis- TIPS-ethyne (*S*)-3,17-bis((triisopropylsilyl)ethynyl)-8,12-dihydrobenzo[*hi*]-dinaphtho[2,1-*b* : 1,2-*d*][1,6]dioxacycloundecine product; the mono- TIPS-ethyne product and unreacted compound **S-8** were recovered from the 2nd and 3rd column bands respectively. Yield = 1.71 g (43%, based on 2.9 g of compound **S-8**). ¹H NMR (500 MHz, CDCl₃): δ 7.940 (d, 2H, *J* = 1.5 Hz), 7.800 (d, 2H, *J* = 9.0 Hz), 7.402 (s, 1H), 7.381 (d, 2H, *J* = 9.0 Hz), 7.301 (dd, 2H, *J* = 9.0, 1.5 Hz), 7.144 (d, 2H, *J* = 9.0 Hz), 6.935-6.906 (m, 1H), 6.856 (d, 2H, *J* = 7.0 Hz), 5.212 (d, 2H, *J* = 12.5 Hz), 5.024 (d, 2H, *J* = 12.5 Hz), 1.120-1.086 (m, 6H). ¹³C NMR (500 MHz, CDCl₃): δ 154.537, 138.243, 133.684, 131.918, 129.981, 129.691, 129.635, 129.564, 127.709, 127.673, 126.132, 125.805, 121.331, 119.932, 107.696, 90.864, 75.484, 18.679, 11.557. MS (MALDI-TOF): 727.01 [(M+Na)⁺] (calcd 726.19).

(S)-3,17-Bis(ethynyl)-8,12-dihydrobenzo[*hi*]-dinaphtho[2,1-*b* : 1,2-*d*][1,6]dioxacycloundecine, (S-10**).** Tetrabutylammonium fluoride (1 M in THF, 10.00 ml, 10.00 mmol) was added to a ice cold solution of **S-9** (3.285 g, 4.40 mmol) in 30 ml of THF under argon and stirred at 0 °C for 20 min. The solution was extracted with CH₂Cl₂, dried over CaCl₂, and evaporated. The residue was chromatographed on silica gel using 3:7 CH₂Cl₂:hexanes as the eluent (*R_f* ~ 0.50). Evaporation of the organic solvent provided a white solid which was immediately used to synthesize compound **S-11**. Yield = 1.88 g (98%, based on 3.285 g of the **S-9** compound). ¹H NMR (500 MHz, CDCl₃, **Figure S1C**): δ 7.953 (d, 2H, *J* = 1.5 Hz), 7.807 (d, 2H, *J* = 11.0 Hz), 7.434 (s, 1H), 7.398 (d, 2H, *J* = 11.0 Hz), 7.293

(dd, 2H, $J = 11.0, 2.0$ Hz), 7.136 (d, 2H, $J = 11.0$ Hz), 6.954-6.916 (m, 1H), 6.873 (d, 2H, $J = 10.0$ Hz), 5.227 (d, 2H, $J = 15.5$ Hz), 5.046 (d, 2H, $J = 15.5$ Hz), 3.059 (s, 2 H).

Compound S-11. A 500 ml Schlenk flask was charged with {[2,5-Diiodo-1,4-bis(3-propoxy-sulfonic acid)benzene] sodium salt} (**1**) (6.50g, 10.0 mmol), Pd(PPh₃)₄ (0.175 g, 0.150 mmol), CuI (0.030 g, 0.150 mmol) under argon. A solvent mixture of DMF (150 ml), H₂O (100 ml) and diisopropylamine (50 ml) was degassed by argon purging for 3 h and cannula-transferred to the reaction flask. The resulting slurry was stirred for 5 min at 80 °C under argon. A solution of compound **S-10** (1.352 g, 3.1 mmol) in 40 ml of degassed DMF was added to the reaction mixture *via* syringe pump over 3 h, and the reaction mixture was continued stirring at 60 °C overnight. The reaction was cooled, poured into 1L 5:4:1 Et₂O:Me₂CO:MeOH solvent mixture, and the precipitate was collected by filtration on a glass frit. The solid was washed with 1:1 mixture of Et₂O:Me₂CO and dried. The unreacted diiodo compound (**1**) was separated as white solid *via* crystallization from hot water. The aqueous filtrate was concentrated to ~100 ml, and transferred in a 500 ml round bottomed flask containing 200 ml of DMF. A solution of tetraoctylammonium bromide (NOct₄Br, 30 mmol) in DMF (75 ml) was added to it slowly, following which the mixture was heated to 80 °C, cooled to room temperature and extracted with diethylether. After the solvent was evaporated, the residue was chromatographed on SX-1 using THF as the eluent. The 1st blue-fluorescent column band containing [**S-11-4(NOct₄)**] complex was collected and mixed with a saturated NaCl solution in 1:1 MeOH:H₂O (200 ml) with stirring, **S-11** was collected as yellow precipitate. The solid was filtered, washed with ice-cold water and dried. Yield = 2.42 g (53%, based on 1.352 g of compound **S-10**). ¹H NMR ([**S-11-4(NOct₄)**]; 500 MHz, CDCl₃): δ 8.028 (s, 2H), 7.905 (d, 2H, $J = 9.0$ Hz), 7.462 (s, 1H), 7.369 (dd, 2H, $J = 9.0, 2.5$ Hz), 7.299 (dd, 2H, $J = 9.0, 2.0$ Hz), 7.257 (s, 1H), 7.132 (s, 1H), 7.122 (d, 2H, $J = 9.0$ Hz), 6.961 (s, 1H), 6.935-6.908 (m, 1H), 6.864 (s, 1H), 6.858 (d, 2H, $J = 6.0$ Hz), 5.210 (d, 2H, $J = 12.5$ Hz), 5.020 (d, 2H, $J = 12.5$ Hz), 4.131 (td, 4H, $J = 19.0, 6.5$ Hz), 4.060 (td, 4H, $J = 19.0, 6.5$ Hz), 3.014-2.973 (m, 8H), 2.358-2.282 (m, 8H). ¹H NMR (**S-11**; 500 MHz, 1:1 D₂O:DMSO, δ DMSO = 2.54 ppm; **Figure S2A**): δ 8.183 (d, 2H, $J = 7.0$ Hz), 8.142-8.114 (m, 2H),

7.676 (d, 2H, $J = 8.0$ Hz), 7.442 (d, 2H, $J = 8.0$ Hz), 7.395-7.365 (m, 2H), 7.319 (s, 1H), 7.162 (s, 1H), 7.066-7.016 (m, 6H), 5.389 (d, 2H, $J = 11.5$ Hz), 5.051 (d, 2H, $J = 10.5$ Hz), 4.124-4.046 (m, 4H), 4.030-3.952 (m, 4H), 2.863-2.812 (m, 4H), 2.753-2.705 (m, 4H), 2.114-2.085 (m, 4H), 2.063-2.032 (m, 4H). FTIR (solid, ATR): 3522, 3470 (hydrated sulfonate); 2920 (C_{Ph} -H, str.); 2874 (C_{alk} -H, str.); 1626, 1597, 1490 ($C=C$ ring str.); 1470 (CH_2 scissoring); 1350 (S-O, assym. str.); 1240 (C_{Ph} -O-C, assym. str.); 1203 ($C-SO_3^-$, str.) 1198 (C_{alk} -O-C, assym. str.); 1128 (S-O, sym. str.); 1089 (C_{Ph} -O- C_{alk} , sym. str.); 1029 (C_{alk} -O- C_{alk} , sym. str.); 953, 880, 740, 615, 527 cm^{-1} (various C-H bending, C-S str.). MS (MALDI-TOF) m/z : 1457.32 $[(M - Na)^-]$ (calcd. 1456.93), 1436.6 $[(M - 2Na + H^+)^-]$ (calcd. 1436.01), 1414.52 $[(M - 3Na + 2H^+)^-]$ (calcd. 1414.03), 1392.89 $[(M - 4Na + 3H^+)^-]$ (calcd. 1492.05).



Scheme S2: Synthesis of amphiphilic bis-triisopropylsilylethyne units. (a) (Triisopropylsilyl)acetylene, $PdCl_2(PPh_3)_2$, CuI, Et_3N , THF, 60 $^{\circ}C$; (b) (Trimethylsilyl)acetylene, $PdCl_2(PPh_3)_2$, CuI, Et_3N , THF, 60

⁰C; (c) 1 M NaOH, THF, MeOH; (d) Pd₂(dba)₃, AsPh₃, Et₃N, THF, 60 ⁰C; (e) NBS, 1:9 MeOH:CHCl₃, 0 ⁰C; (f) Zn(OAc)₂, CHCl₃, MeOH, TEA, overnight; (g) NBS, 5:95 pyridine:CHCl₃.

1,4-Bis(9-methoxy-1,4,7-trioxanoyl)-2-((triisopropylsilyl)ethynyl)-5-iodobenzene (12): 1,4-Bis(9-methoxy-1,4,7-trioxanoyl)-2,5-diiodobenzene (**2**) (4.905 g, 7.50 mmol), PdCl₂(PPh₃)₂ (0.350 g, 0.5 mmol) and CuI (0.075 g, 0.4 mmol) were brought together in a 100 ml Schlenk tube. A solvent mixture of THF (50 ml), triethyleamine (10 ml), and (triisopropylsilyl)acetylene (1.70 ml, 7.6 mmol) was degassed via three freeze-pump-thaw cycles, transferred to the reaction flask, and stirred at 60 ⁰C for 4 h. The reaction mixture was poured into water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 4:6 THF:hexanes as the eluent. Compound **12** was collected as the 2nd band. Yield = 2.22 g (42%, based on 4.905 g of the diiodobenzene starting material). ¹H NMR (500 MHz, CDCl₃): δ 7.262 (s, 1 H), 6.848 (s, 1 H), 4.088 (t, 4H, *J* = 5.0 Hz), 3.862 (t, 2H, *J* = 5.0 Hz), 3.798 (t, 2H, *J* = 5.0 Hz), 3.781-3.754 (m, 2H), 3.702-3.675 (m, 2H), 3.674-3.598 (m, 8H), 3.543-3.516 (m, 4H), 3.362 (s, 6H), 1.101 (s, 21H). ¹³C NMR (100 MHz, CDCl₃): 152.98, 124.03, 86.02, 71.98, 71.23, 70.84, 70.62, 70.40, 69.20, 59.04, -0.09; MS (MALDI-TOF) *m/z*: 732.41 [(M+Na)⁺, calcd 731.73].

1,4-Bis(9-methoxy-1,4,7-trioxanoyl)-2-((triisopropylsilyl)ethynyl)-5-((trimethylsilyl)ethynyl)benzene (13): Compound **12** (2.220 g, 3.132 mmol), PdCl₂(PPh₃)₂ (0.110 g, 0.157 mmol) and CuI (0.030 g, 0.157 mmol) were brought together in a 100 ml Schlenk tube. A solvent mixture of THF (50 ml), triethyleamine (10 ml), and (trimethylsilyl)acetylene (0.92 ml, 6.50 mmol) was degassed via three freeze-pump-thaw cycles, transferred to the reaction flask, and stirred at 60 ⁰C for 4 h. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 3:7 THF:hexanes as the eluent. Compound **13** was collected as the 1st band. Yield = 1.44 g (68%, based on 2.22 g of the compound **12**). ¹H NMR (400 MHz, CDCl₃): δ 6.877 (s, 2 H), 4.118-4.074 (m, 4H), 3.850 (t, 2H, *J* = 5.2 Hz), 3.805 (t, 2H, *J* = 5.2 Hz), 3.783-3.759 (m, 2H), 3.710-3.688 (m, 2H), 3.663-

3.610 (m, 8H), 3.547-3.511 (m, 4H), 3.354 (s, 3H), 3.350 (s, 3H), 1.103 (s, 21H). ^{13}C NMR (100 MHz, CDCl_3): 153.41, 118.70, 116.14, 103.12, 100.41, 71.88, 71.11, 70.74, 70.50, 69.63, 69.46, 58.99, 18.62, 11.41, -0.09; FTIR (solid, ATR): 2942, 2865 ($(\text{CH}_3)_2\text{C-H}$, $\text{CH}_3\text{-C}$, str.); 2920 ($\text{C}_{\text{Ph}}\text{-H}$, str.); 2139 ($\text{C}\equiv\text{C}$, str.); 1500, 1414 ($\text{C}=\text{C}$ ring str.); 1460 (CH_2 scissoring); 1273 ($\text{C}_{\text{Ph}}\text{-O-C}$, assym. str.); 1250 (Si-CH_3); 1200 ($\text{C}_{\text{alk}}\text{-O-C}$, assym. str.); 1108 ($\text{C}_{\text{Ph}}\text{-O-C}_{\text{alk}}$, sym. str.); 1028 ($\text{C}_{\text{alk}}\text{-O-C}_{\text{alk}}$, sym. str.); 862, 841, 762 ($\text{Si-}[\text{CH}(\text{CH}_3)_2]_3$, 950, 857, 744, 619 (various C-H bending); MS (MALDI-TOF) m/z : 701.24 [$(\text{M}+\text{Na}^+)$, calcd 701.40].

1,4-Bis(9-methoxy-1,4,7-trioxanoyl)-2-((triisopropylsilyl)ethynyl)-5-(ethynyl)benzene (14):

Compound **13** (1.436 g, 2.115 mmol) was dissolved in THF (60 ml) and MeOH (40 ml). An aqueous solution of NaOH (1 M, 10 ml) was added dropwise to the reaction flask and stirred at room temperature for 20 min. After the reaction endpoint was confirmed by TLC, the reaction mixture was diluted with water, extracted with CH_2Cl_2 , dried over Na_2SO_4 , and evaporated. The residue was chromatographed on silica gel using 3:7 THF:hexanes as the eluent. Yield = 1.22 g (95%, based on 1.436 g of the compound **13**). ^1H NMR (400 MHz, CDCl_3 ; **Figure S3A**): δ 6.925 (s, 1H), 6.917 (s, 1H), 4.132 (t, 2H, $J = 5.2$ Hz), 4.090 (t, 2H, $J = 5.2$ Hz), 3.847 (t, 2H, $J = 5.2$ Hz), 3.807 (t, 2H, $J = 5.2$ Hz), 3.764-3.741 (m, 2H), 3.710-3.688 (m, 2H), 3.660-3.610 (m, 8H), 3.534-3.510 (m, 4H), 3.352 (s, 6H), 3.300 (s, 1H), 1.105 (s, 21H).

2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-((triisopropylsilyl)ethynyl)phenyl]-ethynyl]-1,4-bis(9-methoxy-1,4,7-trioxanoyl)benzene (15): Compound **14** (2.119 g, 3.50 mmol), $\text{Pd}_2(\text{dba})_3$ (0.148, 0.16 mmol), AsPh_3 (0.390 g, 1.28 mmol), CuI (0.950 g, 0.5 mmol) and compound **2** (1.034, 1.58 mmol) were brought together in a 250 ml Schlenk tube and charged with argon. A solvent mixture of THF (100 ml) and triethylamine (20 ml) was degassed via three freeze-pump-thaw cycles, transferred to the reaction tube and stirred at 60°C overnight. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water and extracted with CH_2Cl_2 , dried over Na_2SO_4 , and evaporated. The residue was chromatographed on silica gel using 10:90 THF: CHCl_3 mixture as eluent to isolate the desired product as a yellow fraction. Yield = 3.267 g (41%, based on 2.119 g of the

ethynylbenzene starting material). ^1H NMR (400 MHz, CDCl_3 as 7.24 ppm, **Figure S3B**): δ 6.994 (s, 2 H), 6.955 (s, 2 H), 6.922 (s, 2 H), 4.174 (t, 8H, $J = 4.80$ Hz), 4.106 (t, 4H, $J = 4.80$ Hz), 3.868-3.806 (m, 12H), 3.741-3.691 (m, 12H), 3.635-3.546 (m, 24H), 3.521-3.430 (m, 12H), 3.336 (s, 6 H), 3.312 (s, 6 H), 3.297 (s, 6 H). ^{13}C NMR (125 MHz, $\text{CDCl}_3 = 77.23$ ppm) δ 154.40, 153.74, 153.48, 119.07, 118.04, 117.20, 114.68, 114.67, 114.63, 102.89, 97.18, 91.70, 91.41, 72.12, 72.08, 71.24, 71.18, 71.10 70.85, 70.74, 70.71, 70.68, 69.88, 69.84, 69.81, 69.23, 68.16, 59.22, 59.18, 59.16, 18.91, 11.53. Vis (THF): 394 nm. MS (MALDI-TOF) m/z : 1610.63 ($(\text{M}+\text{H})^+$; calcd 1611.91).

2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-((triisopropylsilyl)ethynyl)phenyl]-ethynyl]-1,4-dicyanobenzene (16): Compound **14** (0.903 g, 1.48 mmol), $\text{Pd}_2(\text{dba})_3$ (0.065, 0.07 mmol), AsPh_3 (0.183 g, 0.60 mmol) and 1,4-dicyano-2,5-dibromobenzene (**4**) (0.197, 0.688 mmol) were brought together in a 250 ml Schlenk tube and charged with argon. A solvent mixture of THF (40 ml) and triethyleamine (10 ml) was degassed via three freeze-pump-thaw cycles, transferred to the reaction tube and stirred at 60°C overnight. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water and extracted with CH_2Cl_2 , dried over Na_2SO_4 , and evaporated. The residue was chromatographed on silica gel using 4:6 THF:hexanes mixture as eluent to isolate the desired product as a orange-yellow fraction. Yield = 0.577 g (62%, based on 0.688 g of the 1,4-dicyano-2,5-dibromobenzene (**4**) compound). ^1H NMR (500 MHz, CDCl_3 as 7.24 ppm, **Figure S3C**): δ 7.867 (s, 2 H), 6.998 (s, 2 H), 6.978 (s, 2 H), 4.188 (t, 4H, $J = 5.00$ Hz), 4.131 (t, 4H, $J = 5.00$ Hz), 3.911 (t, 4H, $J = 5.00$ Hz), 3.830 (t, 4H, $J = 5.00$ Hz), 3.763-3.744 (m, 4H), 3.717-3.698 (m, 4H), 3.659-3.607 (m, 16H), 3.534-3.492 (m, 8H), 3.350 (s, 6 H), 3.328 (s, 6 H), 1.117 (s, 42H). ^{13}C NMR (125 MHz, $\text{CDCl}_3 = 77.23$ ppm) δ 154.28, 154.20, 136.17, 126.69, 118.53, 118.09, 117.44, 117.37, 116.77, 115.79, 111.85, 102.57, 98.55, 97.08, 89.41, 72.08, 71.077, 70.84, 70.70, 69.78, 69.50, 69.29, 59.17, 18.88, 11.49; FTIR (solid, ATR): 2949, 2864 ($(\text{CH}_3)_2\text{C-H}$, $\text{CH}_3\text{-C}$, str.); 2203 ($\text{C}\equiv\text{N}$ str.); 2139 ($\text{C}\equiv\text{C}$); 1608, 1594, 1561, 1500, 1414 ($\text{C}=\text{C}$ ring str.); 1470 (CH_2 scissoring); 1240 ($\text{C}_{\text{Ph}}\text{-O-C}$, assym. str.); 1194 ($\text{C}_{\text{alk}}\text{-O-C}$, assym. str.); 1092 ($\text{C}_{\text{Ph}}\text{-O- C}_{\text{alk}}$,

sym. str.); 1018 (C_{alk}-O- C_{alk}, sym. str.); 855, 790 (Si-[CH(CH₃)₂]₃, 948, 853, 741, 615, 524 cm⁻¹ (various C-H bending); Vis (THF): 334 nm, 433 nm. MS (MALDI-TOF) m/z: 1361.54 [(M+Na⁺), calcd 1360.81].

(5-Bromo-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphyrinato)zinc(II) (17).

Compound **6** (1.863 g, 1.676 mmol) was dissolved in a mixture of 180 ml of chloroform and 20 ml of MeOH. The reaction mixture was cooled to -5 °C and a solution of N-bromosuccinimide (0.290 g, 1.63 mmol) in chloroform (60 ml) was added dropwise to the reaction mixture over 15 min. After the reaction endpoint was confirmed by TLC (30:1 CHCl₃:MeOH), the reaction mixture was poured into water; the organic layer was separated, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 30:1 CHCl₃:MeOH as the eluant, evaporated and dissolved in a mixture of 200 ml chloroform and 15 ml triethylamine. A solution of Zinc acetate dihydrate (1.23 g, 5.60 mmol) in methanol (50 ml) was added, and the reaction mixture was stirred overnight at room temperature. After the completion of the reaction, the solvent was evaporated, and the residue was chromatographed on silica gel using 30:1 CHCl₃:MeOH as the eluent. The mono-bromo porphyrinatozinc compound (**17**) was collected as a mixture along with di-bromo and unreacted porphyrinatozinc compounds and was used for next step without further purification. ¹H NMR (400 MHz, CDCl₃): δ 10.107 (s, 1H), 9.721 (d, 2H, *J* = 4.8 Hz), 9.269 (d, 2H, *J* = 4.8 Hz), 9.051 (d, 2H, *J* = 3.2 Hz), 9.039 (d, 2H, *J* = 3.2 Hz), 7.414 (d, 4H, *J* = 2.4 Hz), 6.942 (t, 2H, *J* = 2.4 Hz), 4.296 (t, 8H, *J* = 4.6 Hz), 3.889 (t, 8H, *J* = 4.6 Hz), 3.708-3.684 (m, 8H), 3.583-3.559 (m, 8H), 3.359-3.329 (m, 8H), 3.171-3.140 (m, 8H), 2.972 (s, 12H).

(5-((Triisopropylsilyl)ethynyl)-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]-porphyrinato)zinc(II) (18). The mono-bromo compound **17**, mixed with dibromo and un-brominated (total of ~1.56 mmol) porphyrinatozinc compounds, was taken in a 100 ml Schlenk tube and charged with argon. The catalysts PdCl₂(PPh₃)₂ (0.070 g, 0.100 mmol) and CuI (0.019 g, 0.100 mmol) were added to the reaction tube in dry box. A solvent mixture of THF (50 ml), triethylamine (10 ml), and (triisopropylsilyl)acetylene (0.90 ml, 4.00 mmol) was degassed via three freeze-pump-thaw cycles,

transferred to the reaction flask, and stirred at 60 °C for 4 h. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 1:50 MeOH: CHCl₃ as the eluent. Compound **18** was collected as the 2nd band. Yield = 1.44 g (62% overall yield based on 1.863g of the compound **17**). ¹H NMR (400 MHz, CDCl₃; **Figure S4A**): δ 10.120 (s, 1H), 9.781 (d, 2H, *J* = 4.4 Hz), 9.266 (d, 2H, *J* = 4.8 Hz), 9.063 (d, 2H, *J* = 4.4 Hz), 9.039 (d, 2H, *J* = 4.4 Hz), 7.438 (d, 4H, *J* = 2.0 Hz), 6.877 (t, 2H, *J* = 2.0 Hz), 4.264 (t, 8H, *J* = 4.4 Hz), 3.831 (t, 8H, *J* = 4.8 Hz), 3.624-3.601 (m, 8H), 3.426-3.438 (m, 8H), 3.099-3.073 (m, 8H), 2.850 (t, 8H, *J* = 4.8 Hz), 2.680 (s, 12H), 1.506-1.422 (m, 21H).

(5-Bromo-15-((triisopropylsilyl)ethynyl)-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphyrinato)zinc(II) (19). Compound **18** (2.30 g, 1.697 mmol) was dissolved in 200 ml of chloroform and 10 ml of pyridine. The reaction mixture was cooled to -5 °C and a solution of N-bromosuccinimide (0.400 g, 2.247 mmol) in chloroform (60 ml) was added dropwise to the reaction mixture over 15 min. After the reaction endpoint was confirmed by TLC (30:1 CHCl₃:MeOH), the reaction mixture was poured into water; the organic layer was separated, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 30:1 CHCl₃:MeOH as the eluant. Yield = 2.11 g (87%, based on 2.30g of the compound **18**). ¹H NMR (400 MHz, CDCl₃): δ 9.671 (d, 2H, *J* = 4.4 Hz), 9.609 (d, 2H, *J* = 4.8 Hz), 8.948 (d, 2H, *J* = 4.8 Hz), 8.911 (d, 2H, *J* = 4.8 Hz), 7.353 (d, 4H, *J* = 2.0 Hz), 6.833 (t, 2H, *J* = 2.0 Hz), 4.238-4.214 (m, 8H), 3.811 (t, 8H, *J* = 4.8 Hz), 3.629-3.606 (m, 8H), 3.486-3.472 (m, 8H), 3.229-3.204 (m, 8H), 3.040-3.015 (m, 8H), 2.858 (s, 12H), 1.484-1.395 (m, 21H).

(5-((Triisopropylsilyl)ethynyl)-15-((trimethylsilyl)ethynyl)-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphyrinato)zinc(II) (20). Compound **19** (1.180 g, 0.823 mmol), PdCl₂(PPh₃)₂ (0.034 g, 0.050 mmol) and CuI (0.009 g, 0.050 mmol) were brought together in a 100 ml Schlenk tube and charged with argon. A solvent mixture of THF (50 ml), triethylamine (10 ml), and (trimethylsilyl)acetylene (0.80 ml, 5.76 mmol) was degassed via three freeze-pump-thaw cycles,

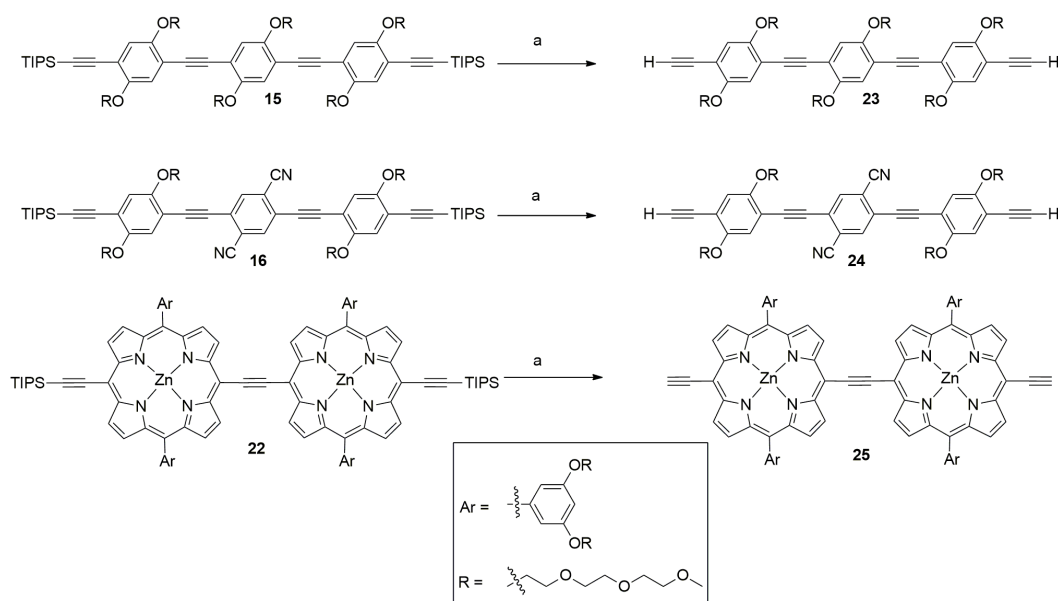
transferred to the reaction flask, and stirred at 60 °C for 4 h. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 1:50 MeOH: CHCl₃ as the eluent.

Yield = 1.101 g (92%, based on 1.18 g of the compound **19**). ¹H NMR (400 MHz, CDCl₃): δ 9.672 (d, 2H, *J* = 4.6 Hz), 9.620 (d, 2H, *J* = 4.6 Hz), 8.948-8.928 (m, 2H), 7.420 (d, 4H, *J* = 2.4 Hz), 6.882 (t, 2H, *J* = 2.2 Hz), 4.298-4.275 (m, 8H), 3.861-3.838 (m, 8H), 3.626-3.614 (m, 8H), 3.466-3.451 (m, 8H), 3.042-3.018 (m, 8H), 2.783-2.758 (m, 8H), 2.596 (s, 12H), 1.506-1.422 (m, 21H), 0.587 (s, 9H).

(5-((Triisopropylsilyl)ethynyl)-15-(ethynyl)-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphyrinato)zinc(II) (21). Compound **20** (1.101 g, 0.759 mmol) was dissolved in THF (30 ml), MeOH (20 ml). An aqueous solution of NaOH (1 M, 4 ml) was added dropwise to the reaction flask and stirred at room temperature for 20 min. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 3:7 THF:hexanes as the eluent. Yield = 1.00 g (96%, based on 1.101 g of the compound **20**). ¹H NMR (400 MHz, CDCl₃; **Figure S4B**): δ 9.685 (d, 2H, *J* = 4.4 Hz), 9.630 (d, 2H, *J* = 4.8 Hz), 8.948-8.932 (m, 4H), 7.375 (d, 4H, *J* = 2.0 Hz), 6.805 (t, 2H, *J* = 2.0 Hz), 4.203 (t, 8H, *J* = 4.4 Hz), 4.125 (s, 1H), 3.761 (t, 8H, *J* = 4.8 Hz), 3.547 (t, 8H, *J* = 4.8 Hz), 3.375 (t, 8H, *J* = 4.4 Hz), 3.035-3.007 (m, 8H), 2.798 (t, 8H, *J* = 4.8 Hz), 2.636 (s, 12H), 1.420-1.405 (m, 21H).

Bis[(5,5'-15-triisopropylsilylethynyl-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphyrinato)zinc(II)]ethyne (22). Compound **21** (1.00 g, 0.729 mmol), Pd₂(dba)₃ (0.065, 0.07 mmol), AsPh₃ (0.183 g, 0.60 mmol) and compound **19** (0.930, 0.648 mmol) were brought together in a 250 ml Schlenk tube and charged with argon. A solvent mixture of THF (40 ml) and triethylamine (10 ml) was degassed via three freeze-pump-thaw cycles, transferred to the reaction tube and stirred at 60 °C overnight. After the reaction endpoint was confirmed by TLC, the reaction mixture was poured into water and extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was

chromatographed on silica gel using 1:49 MeOH: CHCl₃ mixture as eluent to isolate the desired product, which was then further purified via passing through SX-1 SEC using THF as eluent. Yield = 1.40 g (79%, based on 0.93 g of the compound **19**). ¹H NMR (400 MHz, CDCl₃ as 7.24 ppm, **Figure S4C**): δ 10.432 (d, 4H, *J* = 4.4 Hz), 9.659 (dd, 4H, *J* = 4.8, 0.8 Hz), 9.202 (d, 2H, *J* = 4.4 Hz), 8.938 (d, 2H, *J* = 4.4 Hz), 7.429 (d, 4H, *J* = 2.0 Hz), 6.703 (s, br, 2H), 4.130-4.038 (m, 16H), 3.597 (t, 16H, *J* = 4.4 Hz), 3.405 (t, 16H, *J* = 4.4 Hz), 3.264 (t, 16H, *J* = 4.4 Hz), 2.982 (t, 16H, *J* = 4.8 Hz), 2.787 (t, 16H, *J* = 4.8 Hz), 2.645 (s, 24H), 1.454-1.395 (m, 42H). Vis (THF): 423 (5.22), 437 (5.20), 487 (5.47), 573 (4.25), 738 (4.91). MS (MALDI-TOF) *m/z*: 2732 ((M+H)⁺; calcd. 2732).



Scheme S3: Synthesis of amphiphilic bis-ethyne units. (a) TBAF, THF, 0 °C.

2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-ethynylphenyl]-ethynyl]-1,4-bis(9-methoxy-1,4,7-trioxanoyl)benzene (23**):** Tetrabutylammonium fluoride (1M in THF, 0.90 ml, 0.90 mmol) was added to a solution of **15** (0.590 g, 0.366 mmol) in THF (50 ml) under argon at 0 °C. The reaction mixture was stirred for 15 minutes at 0 °C, quenched with water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 4:20:76 MeOH:THF:CHCl₃ as the eluent. Yield = 0.426 g (89%, based on 0.590 g of compound **15**). ¹H NMR

(500 MHz, CDCl₃ as 7.24 ppm): δ 7.013 (s, 2H), 7.005 (s, 2H), 6.980 (s, 2H), 4.193-4.169 (m, 8H), 4.145 (t, 4H, J = 4.75 Hz), 3.874-3.840 (m, 12H), 3.776-3.703 (m, 12H), 3.664-3.624 (m, 8H), 3.610-3.560 (m, 12H), 3.530-3.511 (m, 4H), 3.495-3.446 (m, 8H), 3.345 (s, 6H), 3.324 (s, 6H), 3.32 (s, 2H), 3.307 (s, 6H). ¹³C NMR (125 MHz, CDCl₃ = 77.23 ppm) δ 154.446, 153.771, 153.583, 119.164, 118.120, 117.580, 115.237, 114.690, 113.281, 91.582, 91.427, 82.981, 79.950, 72.146, 72.098, 72.074, 71.268, 71.227, 70.910, 70.893, 70.875, 70.755, 70.736, 70.710, 69.903, 69.859, 69.820, 69.759, 69.674, 68.170, 59.228, 59.202, 59.179, 25.807. Vis (λ_{max} (THF): 396 nm. MS (MALDI-TOF) m/z : 1299.10 ((M+H)⁺; calcd. 1298.64).

2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-ethynylphenyl]-ethynyl]-1,4-dicyanobenzene (24): Tetrabutylammonium fluoride (1M in THF, 0.70 ml. 0.700 mmol) was added to a solution of **16** (0.406 g, 0.303 mmol) in THF (50 ml) under argon at 0 °C. The reaction mixture was stirred for 15 minutes at 0 °C, quenched with water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 4:20:76 MeOH:THF:CHCl₃ as the eluent. Yield = 0.252 g (81%, based on 0.406 g of compound **16**). ¹H NMR (400 MHz, CDCl₃ as 7.24 ppm): δ 7.864 (s, 2H), 7.035 (s, 2H), 7.014 (s, 2H), 4.177-4.134 (m, 8H), 3.927-3.844 (m, 8H), 3.763-3.725 (m, 8H), 3.648-3.595 (m, 16H), 3.525-3.481 (m, 8H), 3.374 (s, 2H), 3.337 (s, 6H), 3.316 (s, 6H). Vis (THF): 334 nm, 433 nm. MS (MALDI-TOF) m/z : 1052.95 [(M+H)⁺, calcd 1053.49].

Bis[(5,5'-15-ethynyl-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphinato)zinc(II)]-ethyne (25). Tetrabutylammonium fluoride (1M in THF, 0.40 ml. 0.400 mmol) was added to a solution of **22** (0.470 g, 0.172 mmol) in THF (50 ml) under argon at 0 °C. The reaction mixture was stirred for 15 minutes at 0 °C, quenched with water, extracted with CH₂Cl₂, dried over Na₂SO₄, and evaporated. The residue was chromatographed on silica gel using 4:20:76 MeOH:THF:CHCl₃ as the eluent. Yield = 0.384 g (91%, based on 0.406 g of compound **22**). ¹H NMR (300 MHz, CDCl₃ as 7.24 ppm): δ 10.448 (d, 2H, J = 4.8 Hz), 9.612 (d, 2H, J = 4.8 Hz), 9.190 (d, 2H, J =

4.8 Hz), 8.925 (d, 2H, $J = 4.8$ Hz), 7.393 (d, 4H, $J = 2.1$ Hz), 6.641 (t, 2H, $J = 2.1$ Hz), 4.133 (s, 2H), 4.086-3.957 (m, 16H), 3.543 (t, 16H, $J = 4.2$ Hz), 3.391-3.361 (m, 16H), 3.263-3.233 (m, 16H), 3.091-3.060 (m, 16H), 2.955-2.924 (m, 16H), 2.796 (s, 24H). Vis (THF): 421 (5.22), 433 (5.20), 485 (5.47), 563 (4.25), 720 (4.91). MS (MALDI-TOF) m/z : 2419 ((M+H)⁺; calcd. 2420).

General polymer synthesis: Binaphthalene-based ionic conjugated polymers were synthesized via Sonogashira polycondensation reaction following a modified literature² procedure. A bis-ethynyl compound (1 equiv), a **S-7** or **R-7** or **S-11** (~1 equiv), Pd(PPh₃)₄ (~0.05 equiv) and CuI (~0.05 equiv) were brought together in a 25 ml microwave tube, sealed and charged with argon. These reagents were dissolved in an aqueous solvent mixture and diisopropyl amine that were previously degassed via argon purging for 3 h; the reaction mixture was stirred at 160 °C for 1 h in a microwave irradiation cavity. The reaction mixture was then stirred in oil bath at 70 °C for an additional 18 h under argon. Degassed DMSO solutions (1 ml) of {[4-iodo-1-(3-propoxy-sulfonicacid)benzene]sodium salt} (**5**, ~0.25 equiv) and phenylacetylene (~0.5 equiv) were sequentially added to the reaction mixture, and the reaction mixture was stirred for 2 h at 70 °C following each addition. The reaction mixture was cooled to room temperature and the crude product was precipitated by pouring the viscous reaction mixture into 500 ml of 5:4:1 acetone, diethyl ether, and MeOH mixture. The precipitate was collected, dissolved in aqueous solvent mixture and filtered through a 0.20 micron hydrophilic PTFE membrane (Millipore) to remove black metallic and organic impurities. The filtrate was collected, concentrated to ~20 ml in volume and was again precipitated by pouring it into 500 ml of 5:4:1 acetone, diethyl ether and methanol mixture. The precipitate was collected, dissolved in ~30 ml of 5 mM carbonate/15 mM NaCl buffer (pH ~9) aqueous buffer and was then passed through a size exclusion column (3.6 × 60 cm) packed with sephacryl-based separatory medium S-100 (Sigma Aldrich, MW fractionation range globular proteins 1 × 10³ – 1 × 10⁵) using 5 mM carbonate/15 mM NaCl buffer (pH ~9) aqueous buffer as eluent. The size exclusion chromatography enabled separation of the polymeric products from the starting materials; the front running polymeric band was collected as 10 fractions of 50 ml each. Among these fractions only the 1st

two fractions that contain the longest polymeric stands ($M_n = 14\text{--}21$ kDa) were collected together and desalted and concentrated via centrifuging through Microcon centrifugal filter YM-100 (Millipore, Bedford, MA) while washing ($\sim 7 \times 5$ ml) with aqueous solvent mixture containing no salt. The concentrated polymer solution was collected, diluted to ~ 20 ml and pH was adjusted to 7.5 by adding 2–5 μl of 0.2 M NaOH solution. The neutralized solution was then poured into 300 ml 5:4:1 acetone: diethyl ether: methanol and filtered. The solid product was collected and dried to get the desired polymeric product as solid glassy film.

General polymer characterizations: These polymers were characterized via UV-Vis-NIR absorption, XPS, and FTIR spectroscopy (**Figures S6-9**) (^1H NMR spectra of these polymers were inconclusive due to broad spectral evolution as a result of aggregated nature of these amphiphilic polymers in NMR solution). Degree of polymerization (DP) of these polymeric samples were estimated via GPC technique: a diluted (OD @ 400 nm ~ 1 in 1 cm pathlength cell) solution of each polymer was run through a GE/ÄKTA purifier HPLC system (GE Healthcare Bio-Science AB, Björkgatan, Uppsala, Sweden) equipped with GPC column (160x16 mm each; stationary phase: sephacryl S-200; Sigma Aldrich; MW fractionation range 1–80 kDa (dextran)) using 5 mM carbonate/15 mM NaCl buffer (pH ~ 9) aqueous buffer as eluent. The GPC profile of each polymer was compared against a MW profile that was generated from the GPC traces of various poly(sodium 4-styrenesulfonate) standards (Sigma-Aldrich) and the estimated MW of each polymeric compound was corrected for their structural rigidity according to literature description.²⁰ Previously reported related ionic conjugated polymer poly[2,6-{1,5-bis(3-propoxysulfonic acid sodium salt)} naphthylene]ethynylene (PNES; DP measured via ion exchange chromatography = 40²¹) was measured via GPC technique described above as a control experiment; estimated DP measured via GPC was found to be 41.

R/S-PBN-Ph₃. Reagents: **R-7** or **S-7** (257 mg, 0.350 mmol), 2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-ethynylphenyl]-ethynyl]-1,4-bis(9-methoxy-1,4,7-trioxanoyl)benzene (**23**) (445 mg, 0.342 mmol), Pd(PPh₃)₄ (20 mg, 0.0175 mmol), CuI (3.5 mg, 0.0180 mmol). Reaction solvent: DMF (9 ml),

H₂O (6 ml), and diisopropylamine (3 ml). Reaction quenchers: {[4-iodo-1-(3-propoxy-sulfonicacid)benzene]sodium salt} (**5**, 30 mg, 0.087 mmol) and phenylacetylene (18 mg, 0.174 mmol). Purification and HPLC solvents: 3:7 MeOH:H₂O. Isolated yield = 0.120 g (from the 1st two fractions of size exclusion chromatographic separation). GPC (5 mM carbonate/15 mM NaCl buffer in 3:7 MeOH:H₂O, 25 °C, **Fig. S5**): M_p = 21.3 kD, and 14.0 kD (as 4:6 mixture; DP = 11 and 8; correspond to 44 and 32 total aromatic units, respectively). Vis (3:7 MeOH:H₂O, log ϵ , **Fig. S6**): 406 nm (4.8) (extinction coefficient is reported with respect to concentration of the repeating unit). XPS (neat, **Fig. S7A**) obtained atomic con%: O:C:S:Na = 23.7:72.46:1.25:0.99 (expected: 32:94:2:2); High resolution XPS: C1s BE of 286.11 eV (54%, expected 55%, for C bound to O), and 284.61 eV (46% expected 45%, for C bound to C and S). FTIR (solid, ATR; **Fig. S9A**): 3425 (hydrated sulfonate); 2925 (C_{Ph}-H, str.); 2872 (C_{alk}-H, str.); 1610, 1589, 1490, 1415 (C=C ring str.); 1465 (CH₂ scissoring); 1350 (S-O, assym. str.); 1240 (C_{Ph}-O-C, assym. str.); 1197 (C_{alk}-O-C_{alk}, assym. str.); 1128 (S-O, sym. str.); 1097 (C_{Ph}-O-C_{alk}, sym. str.); 1033 (C_{alk}-O-C_{alk}, sym. str.); 947, 846, 732, 688, 597, 522 cm⁻¹ (various C-H bending, C-S str.). Note that the peak for the C≡C stretching was extremely weak in the IR spectrum owing to its symmetric nature in the polymeric backbone but was observed at 2195 cm⁻¹ as an intense peak in the Raman spectrum of the related PNES polymer (458 nm laser excitation).²²

S-PBN(b)-Ph₅. Reagents: **S-11** (483 mg, 0.327 mmol), 2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-ethynylphenyl]-ethynyl]-1,4-bis(9-methoxy-1,4,7-trioxanoyl)benzene (**23**) (426 mg, 0.327 mmol), Pd(PPh₃)₄ (20 mg, 0.0175 mmol), CuI (3.5 mg, 0.0180 mmol). Reaction solvent: DMF (9 ml), H₂O (6 ml), and diisopropylamine (3 ml). Reaction quenchers: {[4-iodo-1-(3-propoxy-sulfonicacid)benzene]sodium salt} (**5**, 30 mg, 0.087 mmol) and phenylacetylene (18 mg, 0.174 mmol). Purification and HPLC solvents: 3:7 MeOH:H₂O. Isolated yield = 0.080 g (from the 1st two fractions of size exclusion chromatographic separation). GPC (5 mM carbonate/15 mM NaCl buffer in 3:7 MeOH:H₂O, 25 °C, **Fig. S5**): M_p = 20.8 kD (DP = 8; correspond to 48 total aromatic units). Vis (3:7

MeOH:H₂O, log ϵ , **Fig. S6**): 406 nm (4.9) (extinction coefficient is reported with respect to concentration of the repeating unit). XPS (neat, **Fig. S7B**) obtained atomic con%: O:C:S:Na = 32.50:65.34:1.11:0.92 (expected: 42:124:4:4); High resolution XPS: C1s BE of 284.6 eV (52.5%, expected 51.6%, for C bound to O and S), 286 eV (39%, expected 38.7%, for C bound the sp³ and sp² C), and 288.7 eV (8.5% expected 9.7%, for C bound to Sp C). FTIR (solid, ATR; **Fig S9B**): 3425 (hydrated sulfonate); 2922 (C_{ph}-H, str.); 2872 (C_{alk}-H, str.); 1598, 1552, 1504, 1419 (C=C ring str.); 1454 (CH₂ scissoring); 1352 (S-O, assym. str.); 1240 (C_{ph}-O-C, assym. str.); 1199 (C_{alk}-O-C, assym. str.); 1128 (S-O, sym. str.); 1095 (C_{ph}-O- C_{alk}, sym. str.); 1029 (C_{alk}-O- C_{alk}, sym. str.); 947, 850, 733, 609, 522 cm⁻¹ (various C-H bending, C-S str.). Note that the peak for the C≡C stretching was extremely weak in the IR spectrum owing to its symmetric nature in the polymeric backbone but it was observed at 2195 cm⁻¹ as an intense peak in the Raman spectrum of the related PNES polymer (458 nm laser excitation).²²

S-PBN(b)-Ph₄PhCN. Reagents: **S-11** (370 mg, 0.25 mmol), 2,5-Bis[2'-[1',4'-bis(9-methoxy-1,4,7-trioxanoyl)-5'-ethynylphenyl]-ethynyl]-1,4-dicyanobenzene (**24**) (260 mg, 0.25 mmol), Pd(PPh₃)₄ (17 mg, 0.0150 mmol), CuI (3.0 mg, 0.0150 mmol). Reaction solvent: DMF (9 ml), H₂O (6 ml), and diisopropylamine (3 ml). Reaction quenchers: {[4-iodo-1-(3-propoxy-sulfonicacid)benzene]sodium salt} (**5**, 30 mg, 0.087 mmol) and phenylacetylene (18 mg, 0.174 mmol). Purification and HPLC solvents: 3:7 MeOH:H₂O. Isolated yield = 0.120 g (from the 1st two fractions of size exclusion chromatographic separation). GPC (5 mM carbonate/15 mM NaCl buffer in 3:7 MeOH:H₂O, 25 °C, **Fig. S5**): M_p = 14.5 kD (DP = 6.5; correspond 38 total aromatic units). Vis (3:7 MeOH:H₂O, log ϵ , **Fig. S6**): 393 nm (4.8), 438 nm (4.6) (extinction coefficient is reported with respect to concentration of the repeating unit). XPS (neat, **Fig. S7A**) obtained atomic con%: O:C:S:N:Na = 24.4:70.26:1.36:2.09:1.90 (expected: 34:112:4:2:4); High resolution XPS: C1s BE of 284.6 eV (38%, expected 39%, for C bound to sp² and sp³ C), 286.1 eV (41%, expected 43%, for C bound to O), and 286.9 eV (21%, expected 17%, for Sp C and phenyl ring carbon of Ph(CN)₂ ring); N1s BE 399.45. FTIR (solid, ATR; **Fig. S9C**): 3408 (hydrated

sulfonate); 2920 (C_{Ph} -H, str.); 2874 (C_{alk} -H, str.); 2229 (weak, $C\equiv N$ str.); 1612, 1591, 1552, 1502, 1415 ($C=C$ ring str.); 1470 (CH_2 scissoring); 1350 (S-O, assym. str.); 1240 (C_{Ph} -O-C, assym. str.); 1198 (C_{alk} -O-C, assym. str.); 1128 (S-O, sym. str.); 1089 (C_{Ph} -O- C_{alk} , sym. str.); 1029 (C_{alk} -O- C_{alk} , sym. str.); 947, 850, 733, 609, 522 cm^{-1} (various C-H bending, C-S str.). Note that the peak for the $C\equiv C$ stretching was extremely weak in the IR spectrum owing to its symmetric nature in polymeric backbone but it was observed at 2195 cm^{-1} as an intense peak in the Raman spectrum of the related PNES polymer (458 nm laser excitation);²² similarly the $C\equiv N$ stretching peak at 2229 cm^{-1} in the IR spectra is very weak due the symmetric nature of the 1,4 dicyanophenyl moiety.

R-PBN-PZn₂. Reagents: **R-7** (130 mg, 0.18 mmol), bis[(5,5'-15-ethynyl-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphinato)zinc(II)]-ethyne (**25**) (412 mg, 0.17 mmol), $Pd(PPh_3)_4$ (12 mg, 0.010 mmol), CuI (2.0 mg, 0.010 mmol). Reaction solvent: DMF (6 ml), H_2O (4 ml), diisopropylamine (3 ml), and THF (5 ml). Reaction quenchers: {[4-iodo-1-(3-propoxy-sulfonic acid)benzene]sodium salt} (**5**, 20 mg, 0.058 mmol) and phenylacetylene (13 mg, 0.124 mmol). Purification and HPLC solvents: 5:4:2 H_2O :MeOH:THF. Isolated yield = 0.120 g (from the 1st two fractions of size exclusion chromatographic separation). GPC (5 mM carbonate/15 mM NaCl buffer in 5:4:2 H_2O :MeOH:THF, 25 °C, **Fig. S5**): M_p = 21.6 kD (DP = 7; correspond to 21 total aromatic units). Vis (5:4:2 H_2O :MeOH:THF, log ϵ , **Fig. S6**): 445 nm (5.18), 494 nm (5.24), 580 nm (4.2), 753 nm (4.85) (extinction coefficient is reported with respect to concentration of the repeating unit). XPS (on indium paste, **Fig. S8A**) obtained atomic con%: O:C:S:N:Zn = 22.5:72.70:0.53:2.36:0.52 (expected: 40:152:2:8:2; note that Na peaks are masked by the In peaks); High resolution XPS: C1s BE of 286.4 eV (53%, expected 51.4%, for C bound to O, S, and Sp C), and 284.6 eV (47%, expected 48.6%, for C bound to sp^2 and sp^3 C); N1s 398 eV; Zn 2P_{3/2} 1020.6 (for TPPZn, reported BE of N1S is 397.9 eV and Zn 2P_{3/2} is 1021.5 eV).²³ FTIR (solid, ATR, **Fig. S9D**): 3388 (hydrated sulfonate); 2916 (C_{Ph} -H, str.); 2872 (C_{alk} -H, str.); 1585, 1493, 1431 ($C=C$ ring str.); 1450 (CH_2 scissoring); 1344 (S-O, assym. str. + CH_2 bending); 1244 (C_{Ph} -O- C_{alk} , sym. str.); 1201 (C_{alk} -O- C_{alk} ,

assym. str.); 1164 (C_{α} -N str. C_{β} -H bend); 1120 (S-O, sym. str.); 1101 (C_{Ph} -O- C_{alk} , sym. str.); 1066, 1029 (C_{alk} -O- C_{alk} , sym. str.); 947, 848, 823, 792, 713, 696, 599, 522 cm^{-1} (various C-H bending, C-S str.).

Note that the peak for the $C\equiv C$ stretching was extremely weak in the IR spectrum owing to its symmetric nature in the polymeric backbone but was observed at 2195 cm^{-1} as an intense peak in the Raman spectrum of the related PNES polymer (458 nm laser excitation).²²

S-PBN(b)-Ph₂PZn₂. Reagents: **S-11** (235 mg, 0.16 mmol), bis[(5,5'-15-ethynyl-10,20-bis[3,5-bis(9-methoxy-1,4,7-trioxanonyl)phenyl]porphinato)zinc(II)]-ethyne (**25**) (384 mg, 0.16 mmol (12 mg, 0.010 mmol), CuI (2.0 mg, 0.010 mmol). Reaction solvent: DMF (5ml), H₂O (5 ml), THF (5 ml) and diisopropylamine (3 ml). Reaction quenchers: {[4-iodo-1-(3-propoxy-sulfonic acid)benzene]sodium salt} (**5**, 20 mg, 0.058 mmol) and phenylacetylene (13 mg, 0.124 mmol). Purification and HPLC solvents: 5:4:2 H₂O:MeOH:THF. Isolated yield = 0.070g (from the 1st two fractions of size exclusion chromatographic separation). GPC (5 mM carbonate/15 mM NaCl buffer in 5:4:2 H₂O:MeOH:THF, 25 °C, **Fig. S5**): M_p = 20.05 kD (DP = 5.5; correspond to 28 total aromatic units). Vis (5:4:2 H₂O:MeOH:THF, log ϵ , **Fig. S6**): 430 nm (5.23), 490 nm (5.34), 562 nm (4.5), 733 nm (4.84) (extinction coefficient is reported with respect to concentration of the repeating unit). XPS (solid, **Fig. S7A**) obtained atomic con%: O:C:S:N:Zn:Na = 16.7:78.67:0.38:2.36:1.55:0.31 (expected: 50:182:4:8:2:4); High resolution XPS: C1s BE of 286.1 eV (51%, expected 51%, for C bound to O, S, and Sp C), and 284.6 eV (49%, expected 49%, for C bound to sp² and sp³ C); N1s 398 eV; Zn 2P_{3/2} 1021.9 (for TPPZn, reported BE of N1S is 397.9 eV and Zn 2P_{3/2} is 1021.5 eV).²³ FTIR (solid, ATR, **Fig. S9E**): 3400 (hydrated sulfonate); 2918 (C_{Ph} -H, str.); 2871 (C_{alk} -H, str.); 1585, 1494, 1431 ($C=C$ ring str.); 1452 (CH_2 scissoring); 1344 (S-O, assym. str. + CH_2 bending); 1242 (C_{Ph} -O- C_{alk} , sym. str.); 1199 (C_{alk} -O- C_{alk} , assym. str.); 1166 (C_{α} -N str. C_{β} -H bend); 1120 (S-O, sym. str.); 1099 (C_{Ph} -O- C_{alk} , sym. str.); 1066, 1031 (C_{alk} -O- C_{alk} , sym. str.); 947, 848, 823, 790, 713, 696, 603, 520 cm^{-1} (various C-H bending, C-S str.).

Note that the peak for the $C\equiv C$ stretching was extremely weak in the IR spectrum owing to its symmetric

nature in the polymeric backbone. but was observed at 2195 cm^{-1} as an intense peak in the Raman spectrum of the related PNES polymer (458 nm laser excitation).²²

Sample preparation: Sodium cholate dispersions of carbon nanotubes (SC–CNTs), SC–CoMoCat, SC–PLVs and SC–FWNTs, were prepared using the standard ultrasonication centrifugation technique;^{7a,24} a 20 ml aqueous solution of SC (2 wt%) was sonicated with 8 mg of CoMoCat SWNTs or PLV SWNTs or FWNTs in direct contact with a tip horn sonicator (20 kHz; 12 W total power; @ 0 °C), and centrifuged (90000 g; 0.5 h, 2x). The upper 60% of the suspension volume was collected and used as the starting material to prepare polymer CNT samples.

Surfactant solubilized (6,5) chirality enriched tubes suspensions SC–[(6,5) SWNTs]/H₂O and SC–[(6,5) SWNTs]/D₂O were prepared from an aqueous SC–CoMoCat dispersion using an established method²⁵ of a two-cycle, density gradient ultracentrifuge (DGU) separation technique that utilizes a step-gradient, composed of 30% (3 ml) and 12% (1.5 ml) iodixanol density gradient layers, and a mixed surfactant system (0.4 and 1.6 wt% SDS and SC, respectively).

General procedure for chiral polymer-wrapped carbon nanotube (polymer–CNT) suspensions

(choose a more descriptive and consistent abbreviation): 10 ml aqueous suspension of SC–CNT (SC–CNT (either SC–[(6,5) SWNTs] or SC–PLVs or SC–FWNTs; with CNT concentration of ~0.1 mg/ml) was added over a course of 3 h to a 5 ml polymer solution (1.6 mg/ml).²⁵ The mixture was stirred overnight and was exchanged into a 5 mM carbonate/15 mM NaCl buffer (pH ~9) using either a Microcon centrifugal filter YM-100 (Millipore, Bedford, MA) or filtering and washing through a 200 nm PTFE membrane (Millipore) with the appropriate buffer solution. Free, unbound polymers in each polymer–CNT sample were removed via gel permeation chromatography: a 2 ml of polymer–CNT solution (CNT concentration of ~0.5 mg/ml) was injected into a series of two preparative columns (160x16 mm each) consist of sephacryl-based separatory medium connected in the order of S-500 (Sigma

Aldrich; MW fractionation range 40-20000 kDa (dextran)) and S-200 (Sigma Aldrich; MW fractionation range 1-80 kDa (dextran)), mounted on a GE/ÄKTApurifier HPLC system (GE Healthcare Bio-Science AB, Björkgatan, Uppasala, Sweden), and eluted with 5 mM carbonate/15 mM NaCl buffer (pH ~9) at a flow rate of 1 ml/min; with three-wavelength detection (for all samples, carbon nanotubes were detected at 580 nm; phenyleneethynylene polymers were detected at 315 and 440 nm, where as porphyrin-based polymers were detected at 400 and 700 nm) was used to identify fractions that did not contain CNTs. For **S/R-PBN-Ph₃**, **S-PBN(b)-Ph₅** and **S-PBN(b)-Ph₄PhCN** wrapped CNT samples, a 5 mM carbonate/15 mM NaCl buffer in 3:7 MeOH:H₂O solvent mixture was used as eluent, while a 5 mM carbonate/15 mM NaCl buffer in 2:4:5 THF:MeOH:H₂O solvent mixture was used for **R-PBN-PZn₂-** and **S-PBN(b)-Ph₂PZn₂-** based samples. The fractions were collected as 1 ml aliquots; the polymer–CNT fractions eluted at an earlier time (eluted at 20-27 min range) followed by the free, unbound polymers (eluted at 28-48 min range; see **Figures S10-11**). Polymer–CNT-containing fractions (eluted at 20-27 min range) were collected together and exchanged into corresponding D₂O-based solvents via filtering, washing, and resuspending to provide final sample that correspond to a SWNT concentrations of ~1 mg/ml. The pH of these samples was adjusted to ~8 by adding appropriate amount of 0.1 mM NaOD in D₂O and stored in a clean, sealed vial. Samples utilized for spectroscopic studies were diluted with the appropriate solvent such to provide a CNT concentration of ~0.06 mg/ml. To test the stability of these polymer–CNT samples in absence of free polymers in the suspension, polymer–CNT fractions collected from the 1st GPC run were left for one week, concentrated in the appropriate eluting buffer and subjected to a 2nd GPC run; no de-wrapped polymeric strand from the collected polymer–CNT suspension was detected during the 2nd GPC run (**Figure S10-B**).

Data summarized in **Table S1** describe the surface coverage metrics of polymer-wrapped [(6,5) SWNTs]. The average number (tabulated in the right most column) of polymeric repeating unit (1.2-1.5) found to be wrapped on a given length of [(6,5) SWNTs] surface (e.g. 3.5 nm) indicate the these polymer-

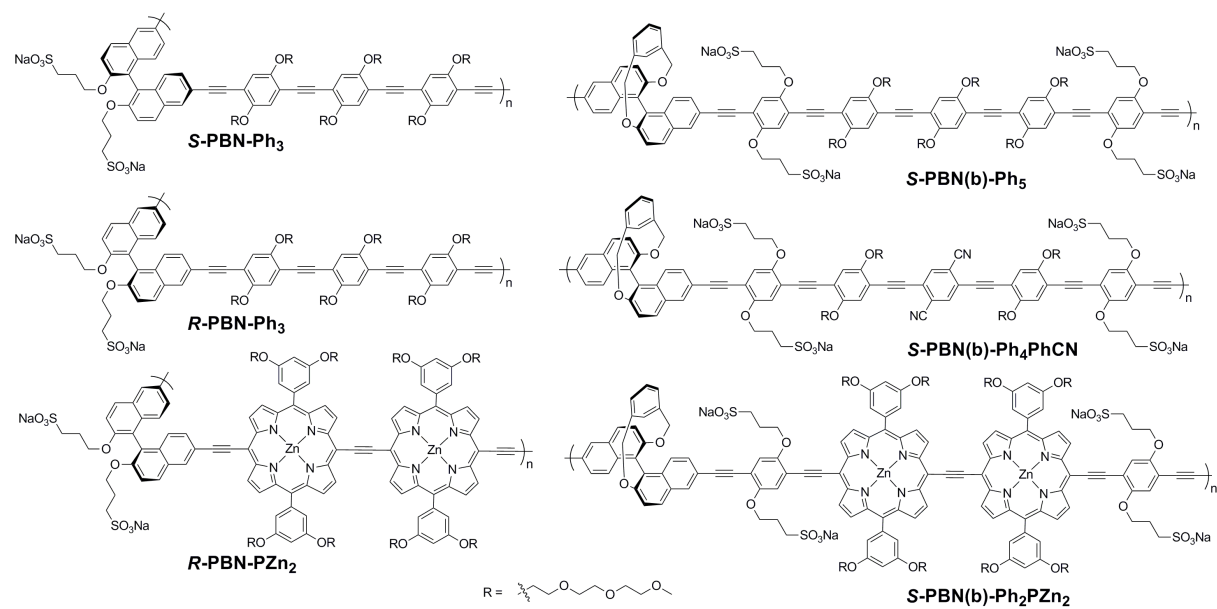
wrapped [(6,5) SWNTs] samples consist of tubes that are ~100% covered via single-chain helical wrapping of each polymer.

Enantio-enriched [-(6,5)] chirality tubes dispersions:

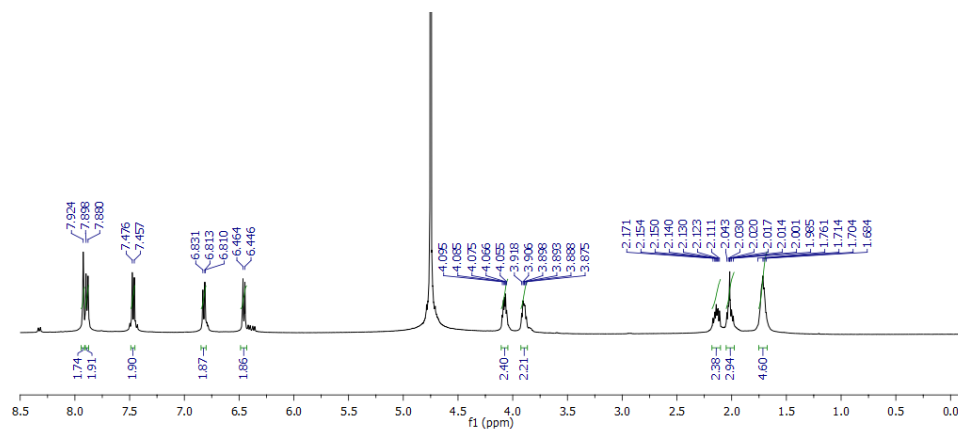
SC-[-(6,5) SWNTs]/D₂O: Surfactant solubilized [-(6,5)] chirality enantio-enriched tube dispersion was prepared using an one-cycle density gradient ultracentrifuge (DGU) separation technique that utilizes a step-gradient, composed of 30% (3 ml) and 15% (1.5 ml) iodixanol density gradient layers, and a mixed surfactant system (0.15 and 0.4 wt% **S-7** and SC, respectively). First, a **S-7** dispersion of carbon nanotube (**S-7**)–CoMoCat was prepared using the standard ultrasonication centrifugation technique;^{7a,24} a 10 ml aqueous solution of **S-7** (0.2 wt%) was sonicated with 6 mg of CoMoCat SWNTs in direct contact with a tip horn sonicator (20 kHz; 8 W total power; @ 0 °C), and centrifuged (90000 g; 0.5 h, 2x). The upper 60% of the suspension volume was carefully collected and was mixed with iodixanol, **S-7** and SC such that the final **S-7**, SC and iodixanol concentrations were 0.15 wt%, 0.4 wt% and 15%, respectively. This suspension (1.5 ml) was deposited on top of a 30% iodixanol layer (3 ml; 0.15 wt% **S-7** and 0.4 wt% SC) to form the step gradient; and these step-gradient layers were centrifuged at an average centrifugal force of ~120,000 g for 12 hrs in a fixed angle TLA-110 (Beckman-Coulter) rotor. The purple colored, one-cycle-DGU separated [-(6,5)] chirality enriched tube suspension was collected in a clean vial. This sample (5 ml) was passed through a short desalting column (ZebaTM, MWCO = 3000; pre-saturated with 0.7% SC in D₂O) using 0.7% SC in D₂O as eluent. The purple colored SC-[-(6,5) SWNTs]/D₂O suspension, void of **S-7** and iodixanol, was collected in a clean vial and used without any further treatment save for dilution to the desired concentration with D₂O prior to spectroscopic studies. The absorption spectrum (**Figure S12 A**) of this SC-[-(6,5) SWNTs]/D₂O sample highlights that the purified suspension is ~85% enriched in (6,5) tubes by mass (as described in the previous section), where as the CD spectrum (**Figure S12 B**) clearly shows intense peaks corresponding to the E₂₂ and E₃₃ parallel-polarized optical transitions of (6,5) SWNTs at 574 and 348 nm, respectively.²⁶

Given the CD signal corresponding to the E_{22} transitions has (-) sign, we assigned the sample to be a [- (6,5) SWNT] enriched sample.²⁶ The cross-polarized peaks corresponding to the E_{12} and E_{13} transition appears at 646 and 444 nm as described in the literature.²⁶⁻²⁷ Though the molar ellipticity (θ) or the CD signal strength (mdegree) of known concentration SWNT sample with 100% ee has not been clearly established, a 27-30% ee of the **SC-[-(6,5) SWNTs]/D₂O** sample (a CD signal of 2.35 mdegree with a SC dispersed [- (6,5) SWNT] sample having OD of 0.35 at E_{22} transition in a 1 cm path length cell) was established relative to the CD signal strength corresponding to the E_{22} transition with the spectra reported by Weisman *et al* (assuming a CD signal intensity of ~20 mdegree with a SDS/SC dispersed [- (6,5) SWNT] sample having OD of ~0.8 at E_{22} transition in a 1 cm path length cell correspond to a 100% ee).²⁶

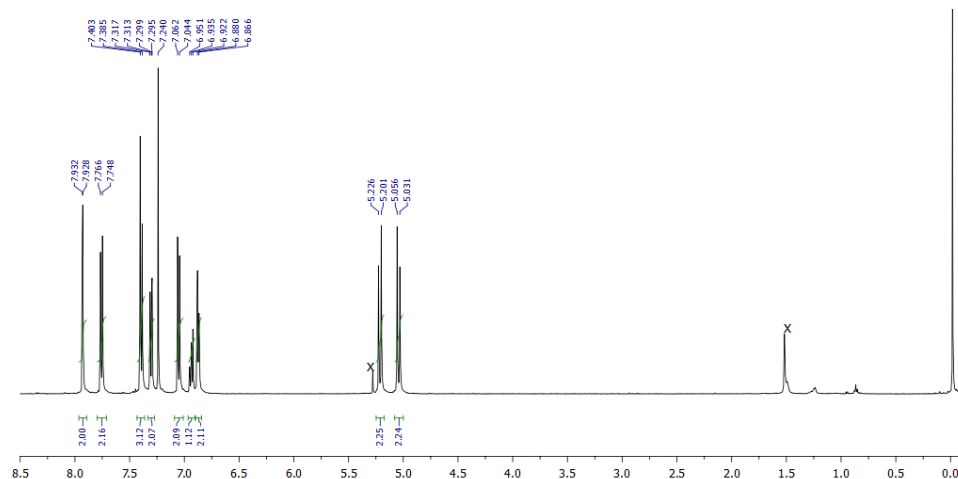
***R/S*-PBN-Ph₃-[-(6,5) SWNT]**: The **SC-[-(6,5) SWNTs]** sample was used to prepare ***R*-PBN-Ph₃-[-(6,5) SWNTs]** and ***S*-PBN-Ph₃-[-(6,5) SWNTs]** according to method discussed in the previous section. The absorption spectra of ***R*-PBN-Ph₃-[-(6,5) SWNTs]** and ***S*-PBN-Ph₃-[-(6,5) SWNTs]** samples (**Figure S13 A**) clearly show that an equal amount of both the *R*- and *S*- chirality polymers bind to a given mass of [- (6,5) SWNTs] indicating no possible preferential binding stemming from the matched helical handedness of the chiral polymers relative to graphene-helicity of the [- (6,5) SWNTs]. Similarly the CD spectra of ***R*-PBN-Ph₃-[-(6,5) SWNTs]** and ***S*-PBN-Ph₃-[-(6,5) SWNTs]** samples (**Figure S13 B**) clearly show that CD signal strength associated with the E_{22} transition of the [- (6,5) SWNT] does not get altered upon chiral polymer wrapping compared to the surfactant-dispersed sample. Likewise, the polymer CD signal does not get changed by the chiral [- (6,5) SWNTs] binding. These data highlight that these enantiopure chiral polymers and enantio enriched SWNTs do not produce induce CD (ICD) signals (as seen for the DNA wrapped racemic SWNTs samples)²⁸ upon binding.

**Chart S2:** Ionic aryleneethynylene polymers based on 1,1'-bi-2-naphthol derivatives.

A.



B.



C.

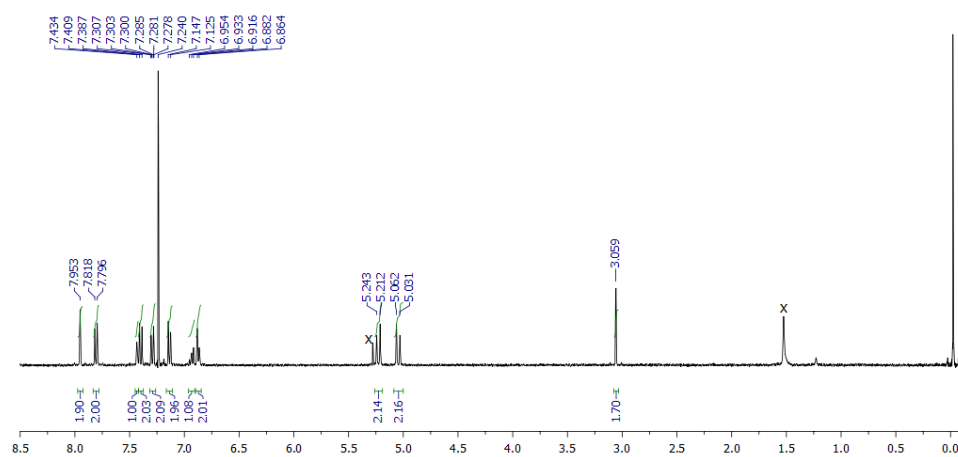
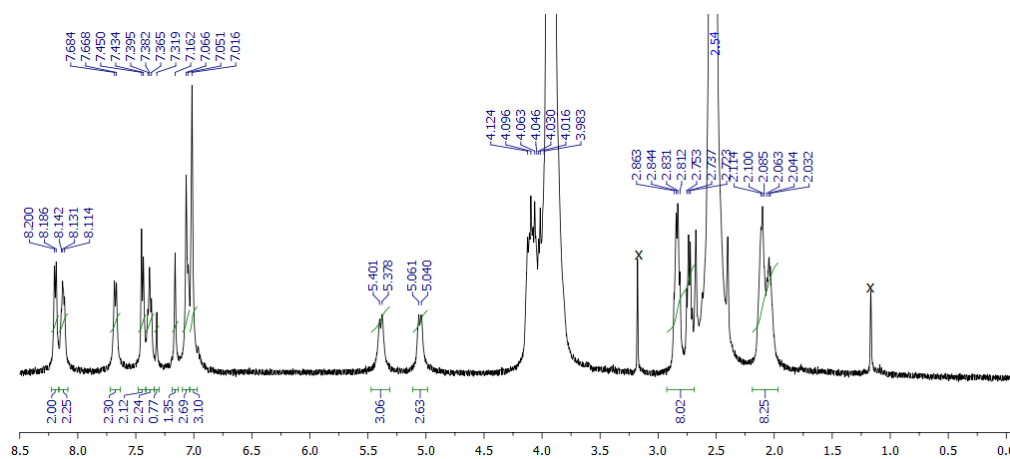


Figure S1. ¹H NMR spectra of (A) **S-7** in D₂O solvent, (B) **S-8**, and (C) **S-10** in CDCl₃ solvent; residual solvent peaks (CH₂Cl₂, H₂O and hexanes) are marked with "X".

A.



C.

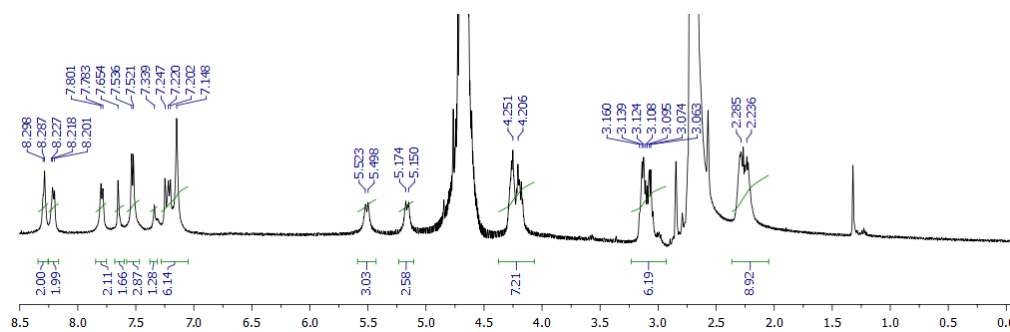
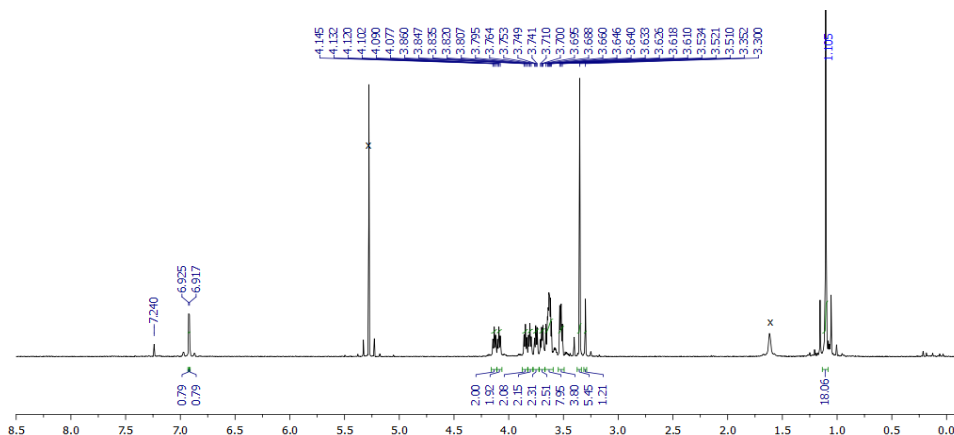
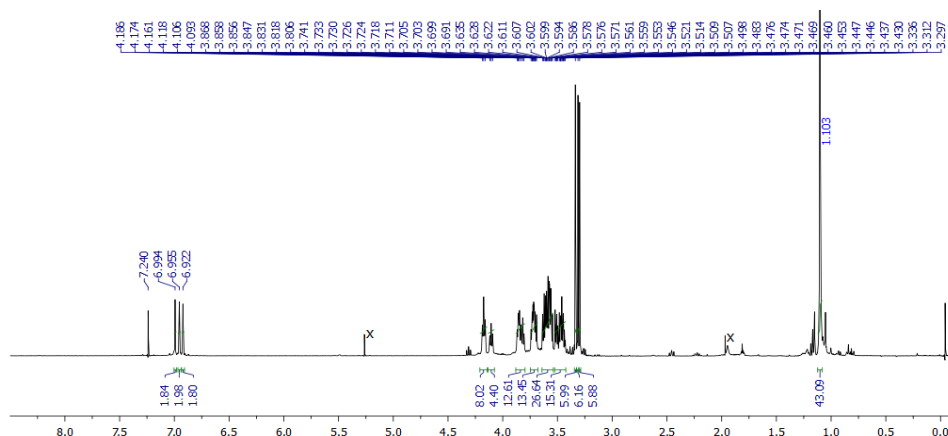


Figure S2. ¹H NMR spectra of **S-11** in (A) 1:1 D₂O:DMSO and (B) 7:3 D₂O:DMSO solvent respectively; residual solvent peaks (MeOH) are marked with "x".

A.



B.



C.

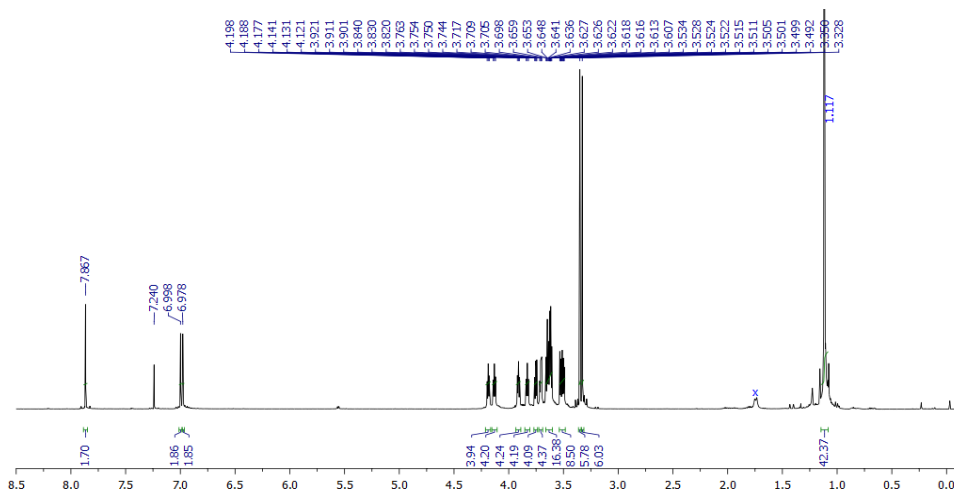
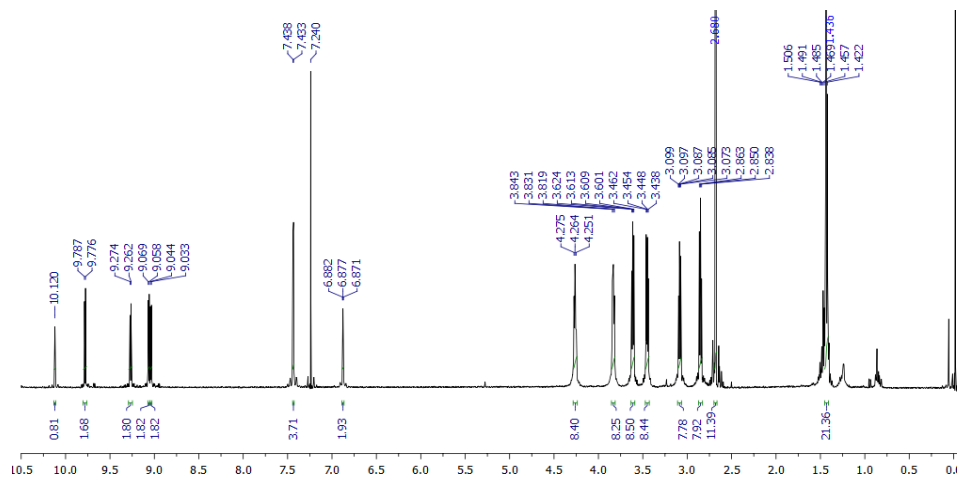
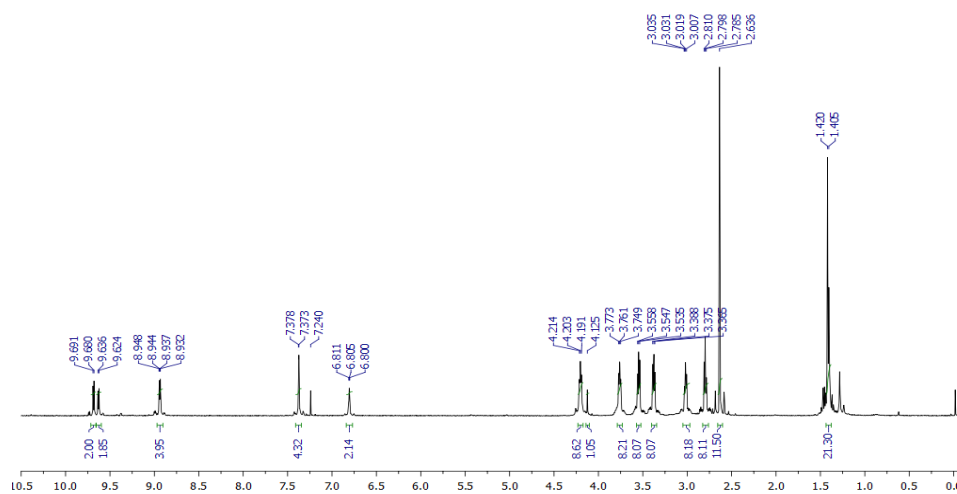


Figure S3. ^1H NMR spectra of (A) **14**, (B) **15**, and (C) **16** in CDCl_3 solvent; residual solvent peaks (CH_2Cl_2 , THF, H_2O and hexanes) are marked with “x”.

A.



B.



C.

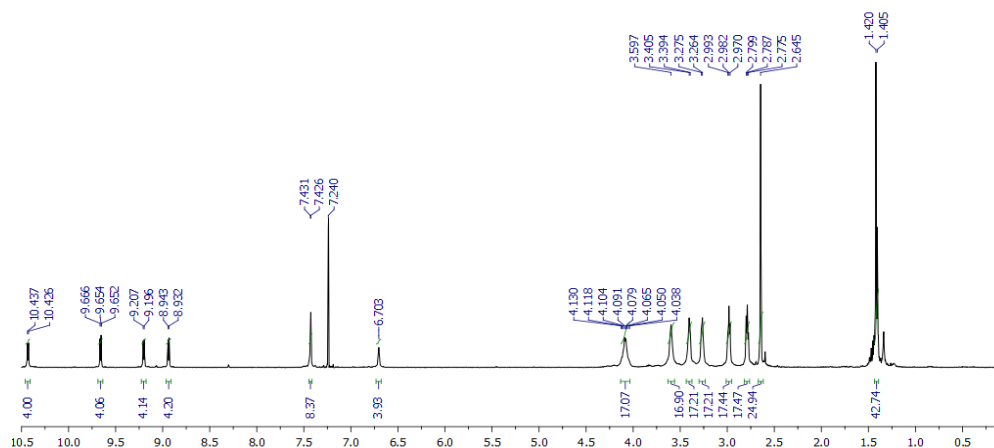


Figure S4. ^1H NMR spectra of (A) **18**, (B) **21** and (C) **22** in CDCl_3 solvent; residual solvent peaks (CH_2Cl_2 , THF, H_2O and hexanes) are marked with “x”.

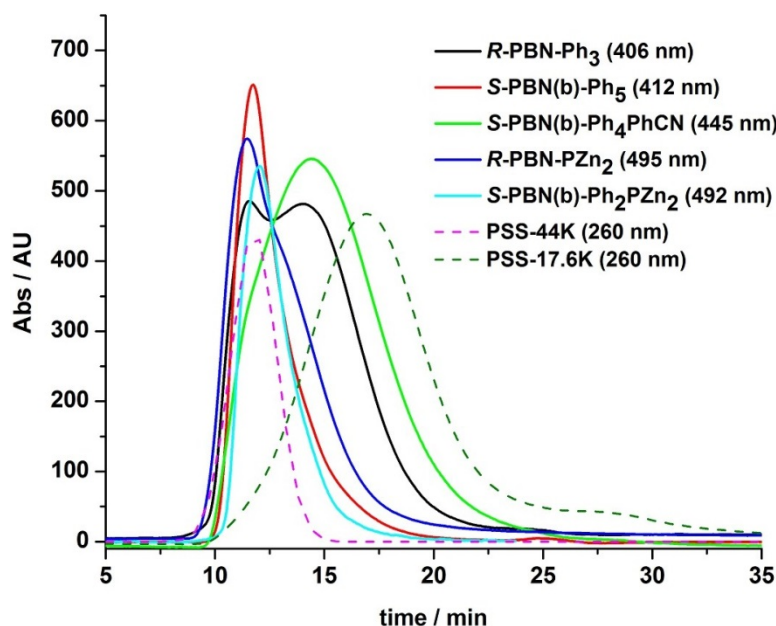


Figure S5. GPC profile of (A) *R*-PBN-Ph₃ (black), (B) *S*-PBN(b)-Ph₅ (red), (C) *S*-PBN(b)-Ph₄PhCN (green) and (D) *R*-PBN-PZn₂ (blue) and (E) *S*-PBN(b)-Ph₂PZn₂ (cyan); GPC profiles of polystyrene sulfonate (PSS) standards ($M_n = 44$ kD (dotted pink) and 17.6 kD (dotted dark green) are plotted for comparison. Eluent: 5 mM carbonate/15 mM NaCl buffer (in 30% MeOH:H₂O mixture); flow rate of 1 ml/min. The polymer detection wavelengths are given in the parenthesis.

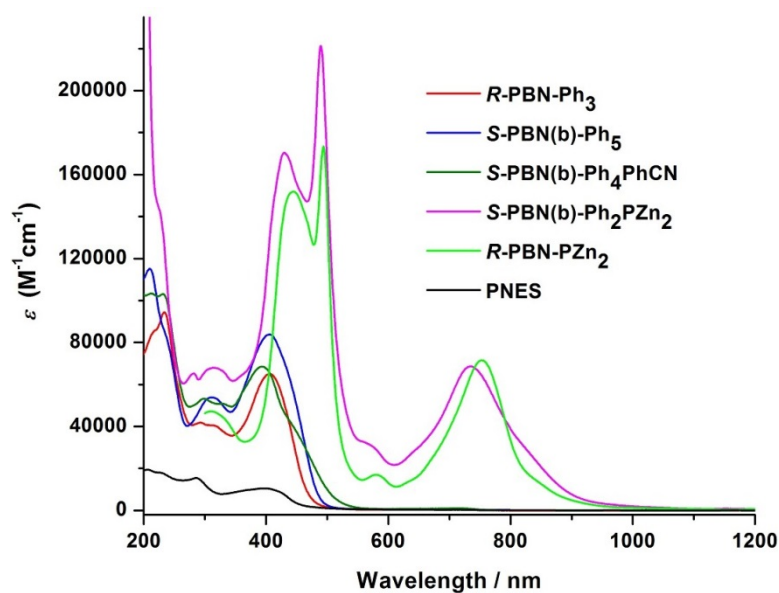
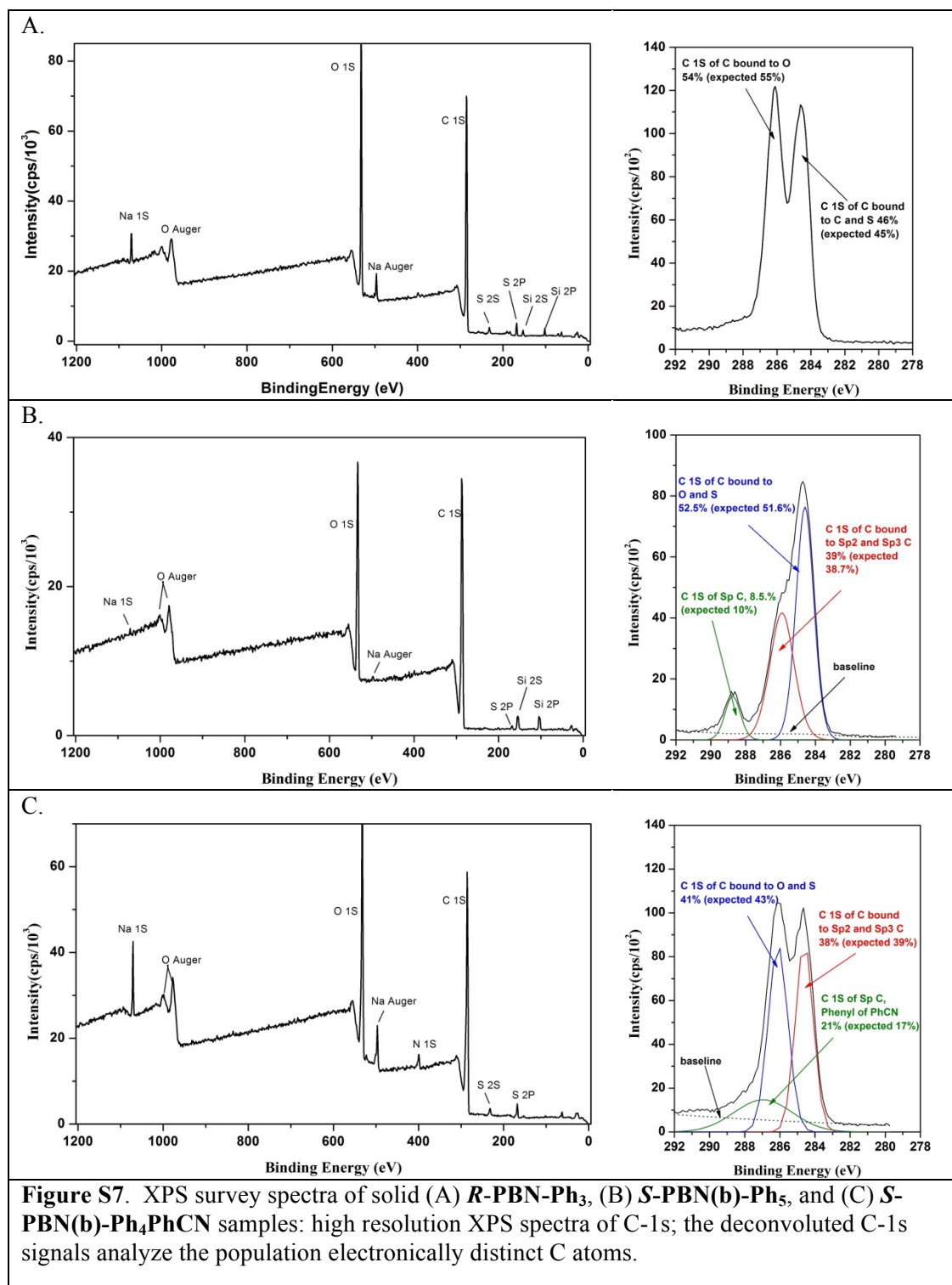
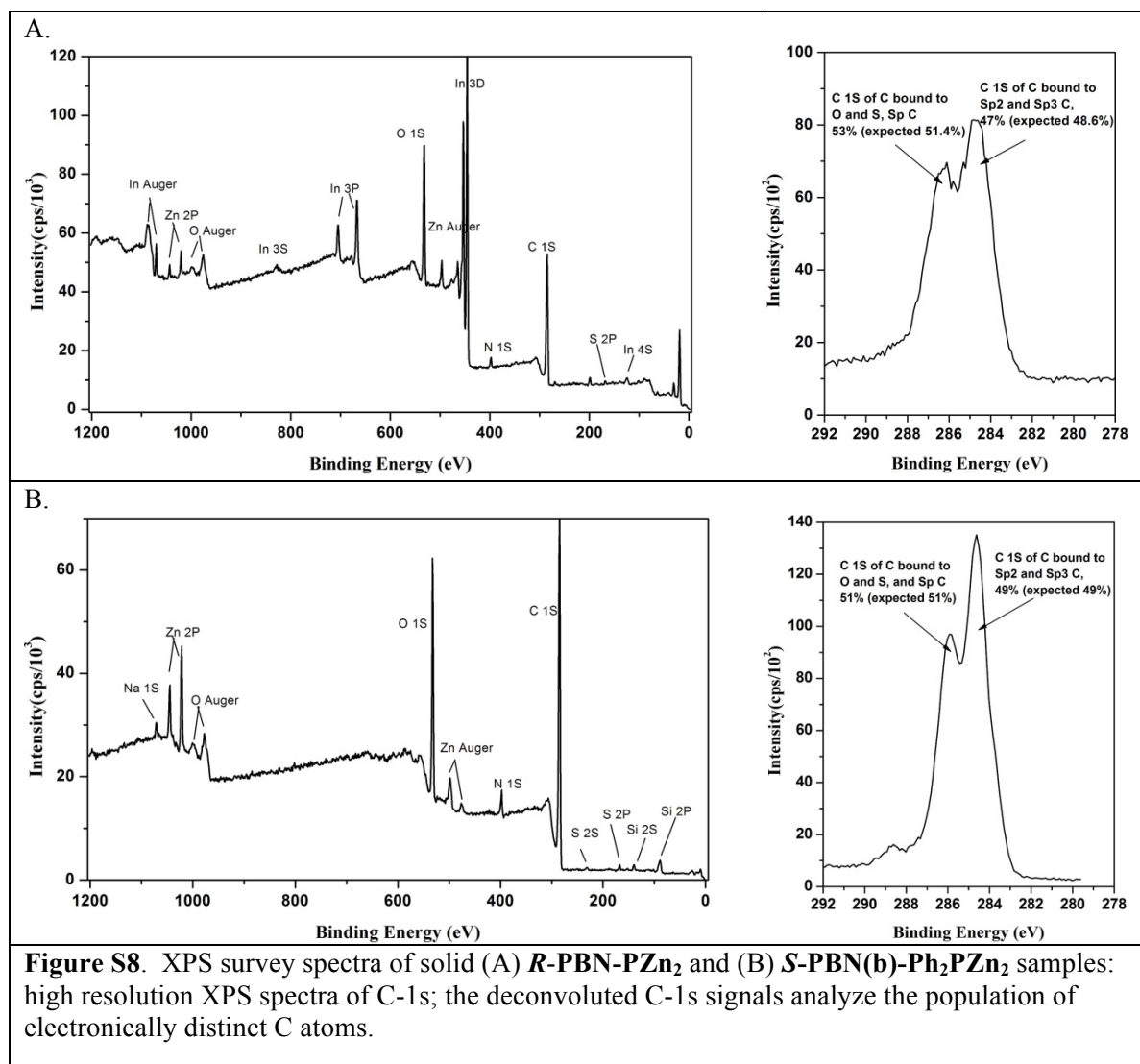


Figure S6. Absorption spectra of (A) *R*-PBN-Ph₃ (red), (B) *S*-PBN(b)-Ph₅ (blue), (C) *S*-PBN(b)-Ph₄PhCN (deep green) in a 3:7 MeOH:H₂O mixed solvent system and (D) *R*-PBN-PZn₂ (green) and (E) *S*-PBN(b)-Ph₂PZn₂ (magenta) in 5:4:2 D₂O:MeOH:THF mixed solvent system; the black spectrum corresponding to PNES²¹ benchmark in 3:7 MeOH:H₂O solvent. The extinction coefficient is shown relative to the number of moles of the repeating unit of each polymer.





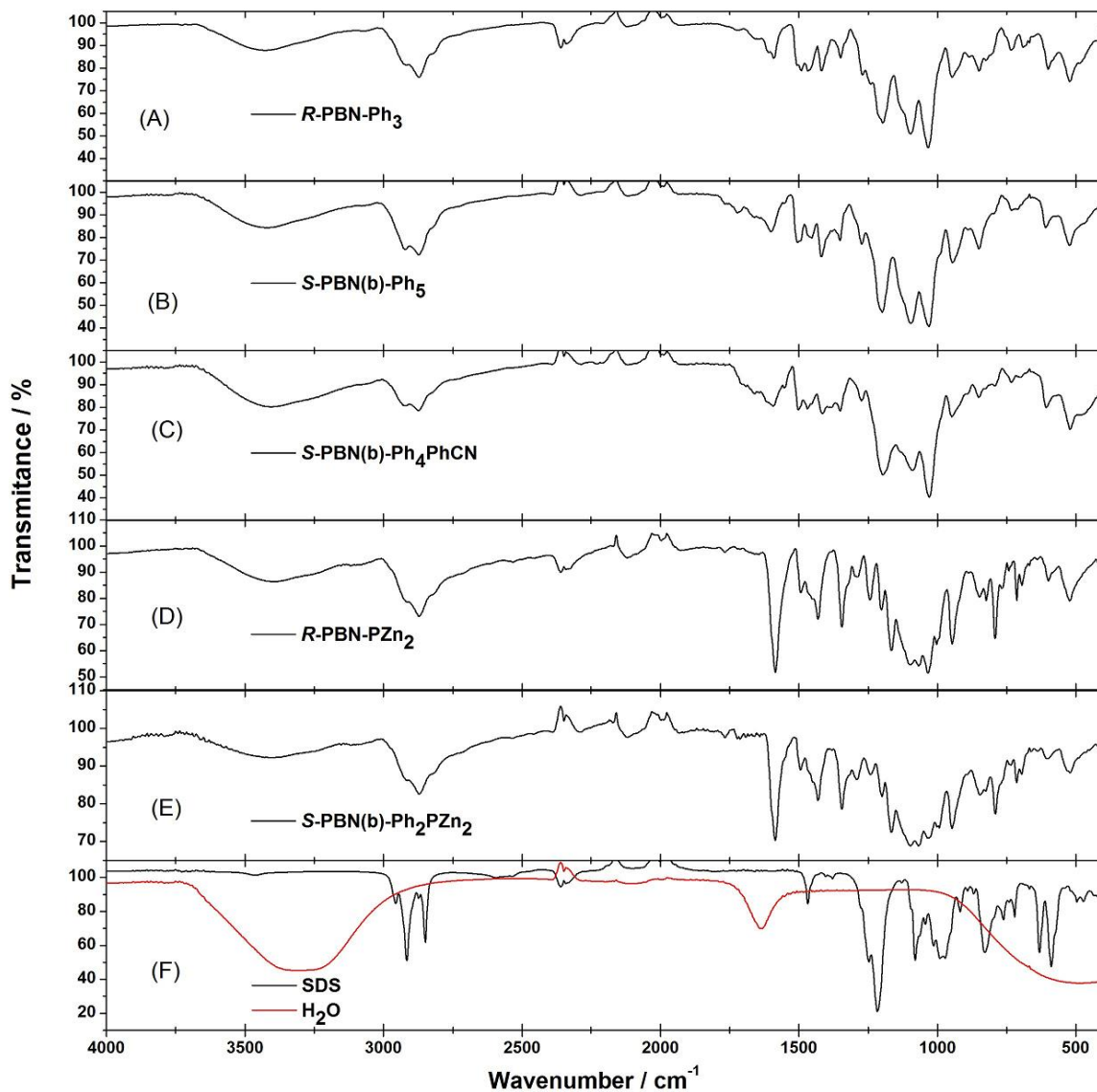


Figure S9. FTIR (ATR) spectra of solid (A) $R\text{-PBN-Ph}_3$, (B) $S\text{-BN(b)-Ph}_5$, (C) $S\text{-PBN(b)-Ph}_4\text{PhCN}$ (D) $R\text{-PBN-PZn}_2$ (E) $S\text{-PBN(b)-Ph}_2\text{PZn}_2$ polymer samples. Panel (F) show the FTIR (ATR) spectra of solid SDS (black) and neat water (red) for comparison purpose.

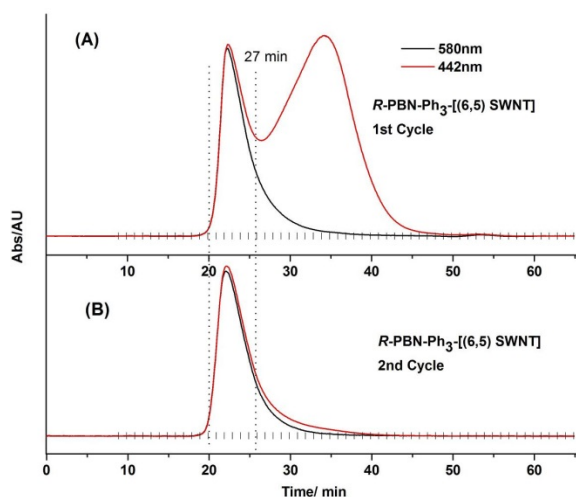


Figure S10. Exemplary GPC profile highlighting the purification process of the polymer–CNT suspension. (A) 1st cycle GPC of ***R*-PBN-Ph₃-[(6,5) SWNT]** suspension; the red trace shows the detection of polymer absorption at 442 nm whereas the black trace detects the E₂₂ of [(6,5) SWNT] at 580 nm. The collected fractions of polymer–wrapped CNT correspond to retention times that range from 20–27 min (denoted by dotted lines). (B) 2nd cycle GPC of the ***R*-PBN-Ph₃-[(6,5) SWNT]** suspension using the fractions collected at 20–27 min of the 1st GPC run (note that the ***R*-PBN-Ph₃-[(6,5) SWNT]** suspension collected after the 1st GPC was equilibrated at ambient condition for 1 week before running the 2nd GPC). These samples were eluted using a 5 mM carbonate/15 mM NaCl buffer (in 30% MeOH:H₂O mixture) over a 65 minute duration at a flow rate of 1 ml/min.

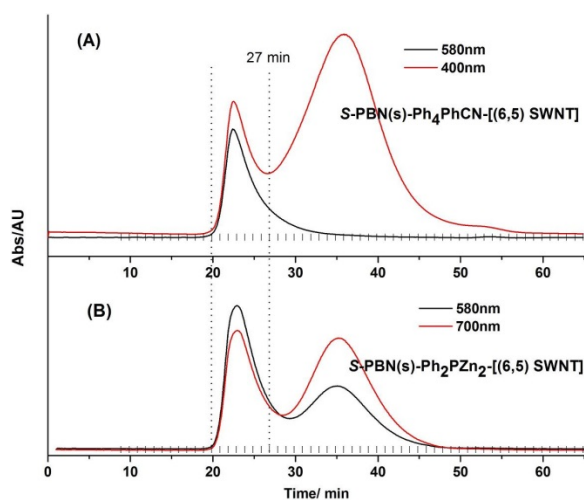


Figure S11. GPC profile of (A) ***S*-PBN(b)-Ph₄PhCN-[(6,5) SWNT]** suspension, and (B) ***S*-PBN(b)-Ph₂PZn₂-[(6,5) SWNT]** suspension; the red trace show the detection of polymer absorption at 400 and 700 nm, respectively, whereas the black trace detect the E₂₂ of [(6,5) SWNT] at 580 nm. The polymer–CNT suspensions eluted at 20–27 min (denoted by dotted lines) were collected. These samples were eluted using a 5 mM carbonate/15 mM NaCl buffer (in 30% MeOH:H₂O mixture for ***S*-PBN(b)-Ph₄PhCN-[(6,5) SWNT]** and in 5:4:2 D₂O:MeOH:THF mixture for ***S*-PBN(b)-Ph₂PZn₂-[(6,5) SWNT]** suspensions) over a 65 minute duration at a flow rate of 1 ml/min.

Description/ system	Polymer concentration ^a	SWNT concentration ^b	# of polymeric repeat units per 700 nm SWNT ^c	# of repeat units per 3.5 nm SWNT
<i>R</i>-BN-Ph₃/[(6,5) SWNT]	2.4297x10 ⁻⁵ M	~9.00x10 ⁻⁸ M	275	1.4
<i>S</i>-BN(b)-Ph₅/[(6,5) SWNT]	2.741x10 ⁻⁵ M	~9.00x10 ⁻⁸ M	304	1.5
<i>S</i>-BN(b)-Ph₄PhCN/[(6,5) SWNT]	2.06x10 ⁻⁵ M	~9.00x10 ⁻⁸ M	233	1.2
<i>S</i>-BN(b)-Ph₂PZn₂/[(6,5) SWNT]	3.05x10 ⁻⁵ M	~9.00x10 ⁻⁸ M	260	1.3
SC/[(6,5) SWNT]		~9.00x10 ⁻⁸ M		

Table S1. Surface coverage metrics of polymer-wrapped [(6,5) SWNTs]. ^aConcentration of the bound polymer in each sample was calculated as a concentration of its repeating units from the absorption spectra shown in **Figures 1,10** and **S6**. ^bConcentration of the bound SWNT was calculated from absorption spectra (Figure 1 and 10 in the main text and Figure S6); estimated mass/vol (E_{11} OD = 1 in 2 mm path length cell) was converted into concentration by dividing with MW of a 700 nm [(6,5) SWNTs]. ^cThe experimentally measured (AFM) average length of [(6,5) SWNTs] samples is 700 nm. The average numbers (summarized in the right most column) of polymeric repeating units found to be wrapped on a given length of a [(6,5) SWNTs] surface (e.g. 3.5 nm) indicate that the these polymer-wrapped [(6,5) SWNTs] samples consist of tubes that are ~100% covered via single-chain helical wrapping of each corresponding polymer.

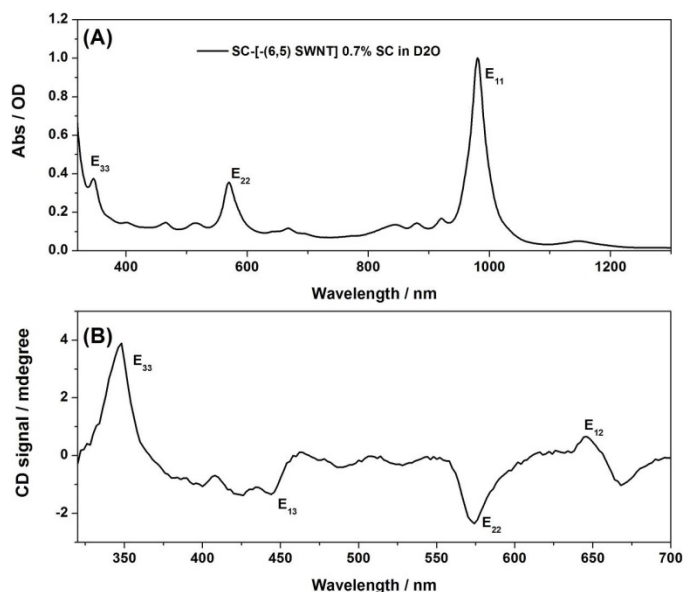


Figure S12. (A) Absorption and (B) CD spectra of SC-[-(6,5) SWNT] sample in D₂O solvent. Experimental condition: optical path length 1 cm, 23 °C, 3 second exposure time at each wavelength.

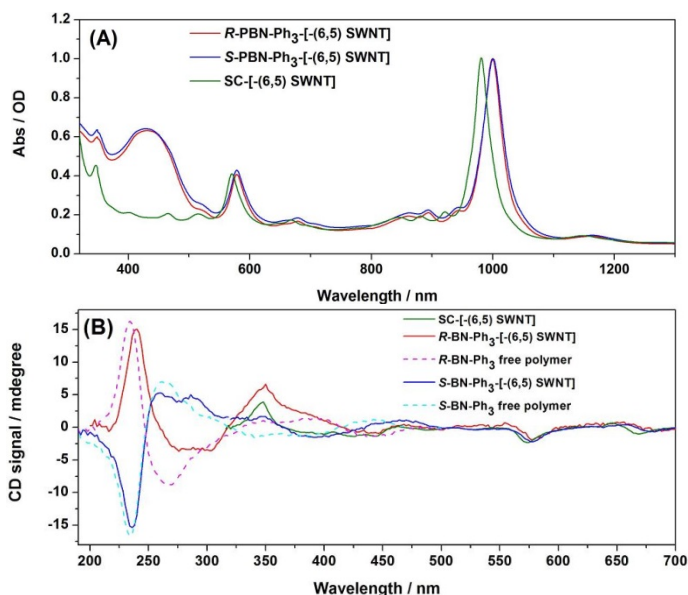


Figure S13. (A) Absorption and (B) CD spectra of **R-PBN-Ph₃-[-(6,5) SWNT]** (red), **S-PBN-Ph₃-[-(6,5) SWNT]** (blue), and **SC-[-(6,5) SWNT]** (green) samples. CD spectra of free **R-PBN-Ph₃** (dashed, cyan) and **S-PBN-Ph₃** (dashed, magenta) samples of identical polymer concentration relative to the corresponding polymer-[-(6,5) SWNT] samples are plotted for comparison purpose. Data presented in panel (B) also establish that the CD signal strength of neither the [-(6,5) SWNTs] (at 580 nm for E₂₂ transition) nor the polymers (at 233 nm) change upon polymer wrapping of SWNTs. Experimental condition: optical path length 1 cm; 23 °C; solvent: polymer-based samples 3:7 MeOH:D₂O solvent, SC-SWNT D₂O solvent; 3 second exposure time at each wavelength.

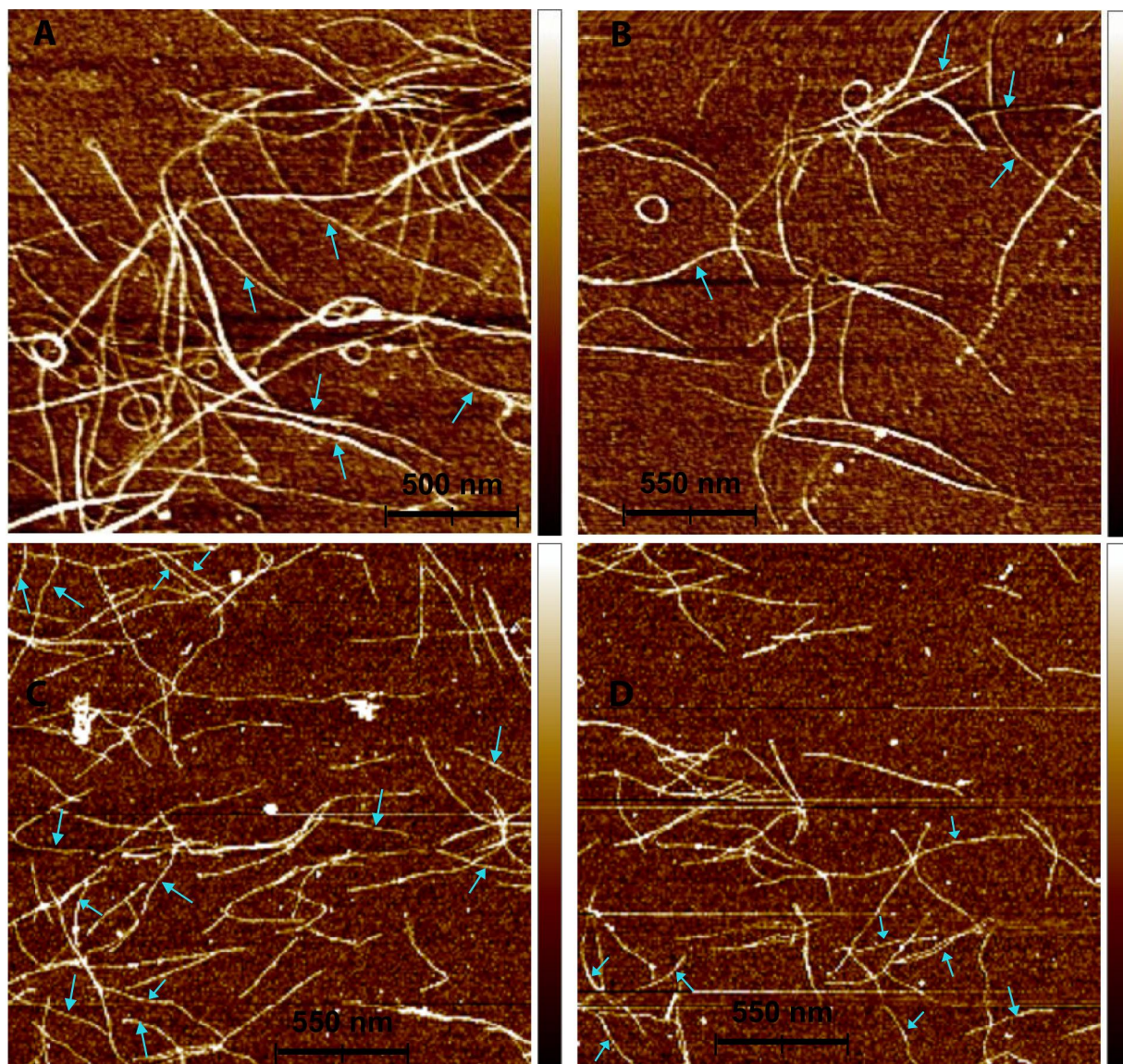


Figure S14. Topographic intermittent contact AFM image of: (A) *R*-PBN-Ph₃-[(6,5) SWNTs], (B) *S*-PBN-Ph₃-[(6,5) SWNTs], (C) *R*-PBN-Ph₃-[(6,5) SWNTs], and (D) *S*-PBN-Ph₃-[(6,5) SWNTs] deposited on Si surface from their corresponding aqueous suspensions. The height color code on the right side of each panel indicates range of -1.5 (dark) to +1.5 nm (white). Polymer-wrapped SWNT structures that evince the unexpected polymer helical wrapping chirality are marked with cyan arrows.

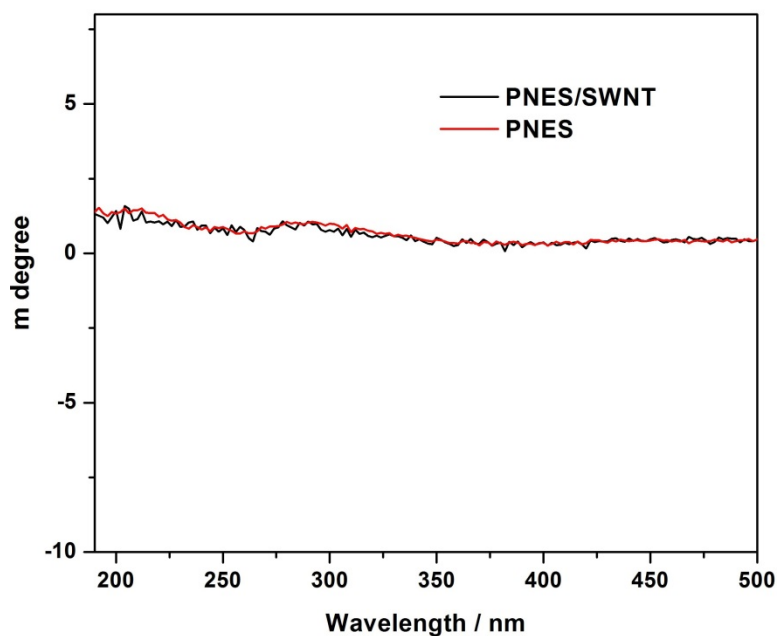


Figure S15. CD spectra of PNES–SWNT (black) and PNES (red) in water.

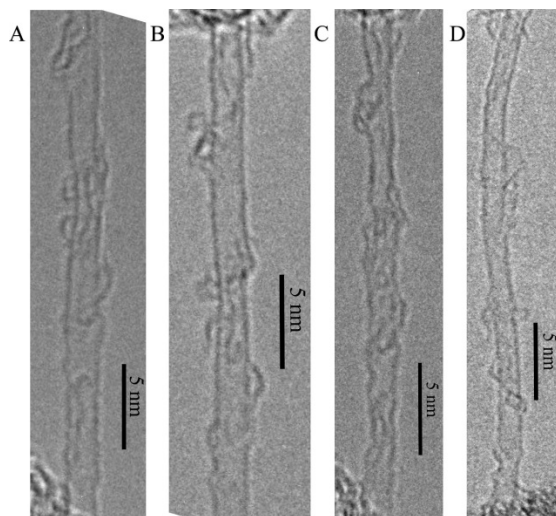


Figure S16. TEM images of *R*-PBN-Ph₃-[PLV SWNTs] obtained from aqueous suspension: individualized tubes wrapped with (A)-(C) expected right-handed helical structures and (D) unexpected left-handed helical wrapping structures.

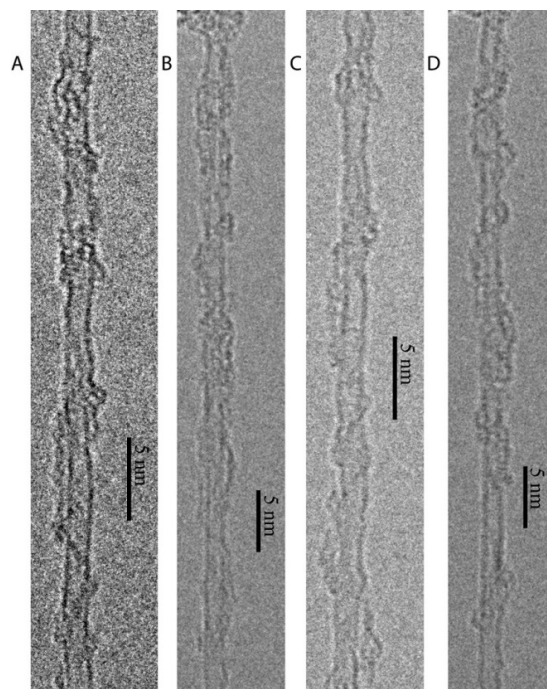


Figure S17. TEM images highlighting expected right-handed helical structures formed by ***R*-PBN-Ph₃**-wrapped individualized [PLV SWNTs] obtained from aqueous suspension.

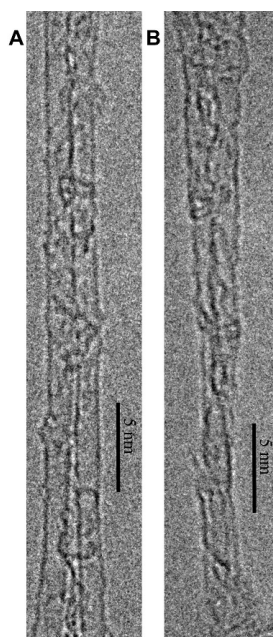


Figure S18. TEM images highlighting expected left-handed helical structures formed by ***S*-PBN-Ph₃**-wrapped two-tube bundle of [PLV SWNTs] obtained from aqueous suspension.

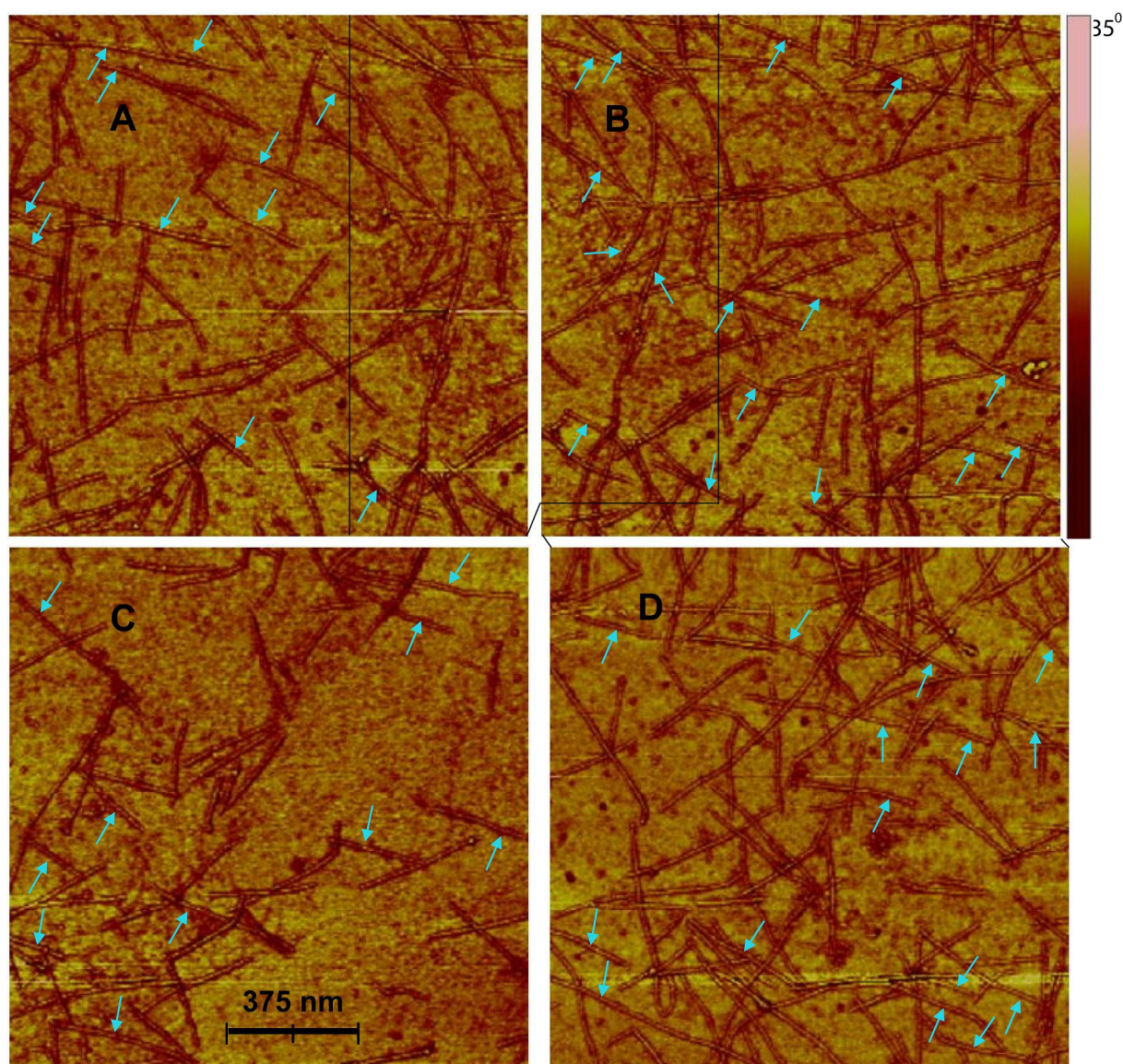


Figure S19. (a)-(d) Phase images derived from intermittent contact mode AFM experiments of ***R*-PBN-Ph₃-[PLV SWNTs]** from an aqueous suspension on a Si surface. Note that a common scanned area in panel A and B is marked with black rectangular box. Polymer-wrapped SWNT structures that evince the unexpected polymer helical wrapping chirality are marked with cyan arrows.

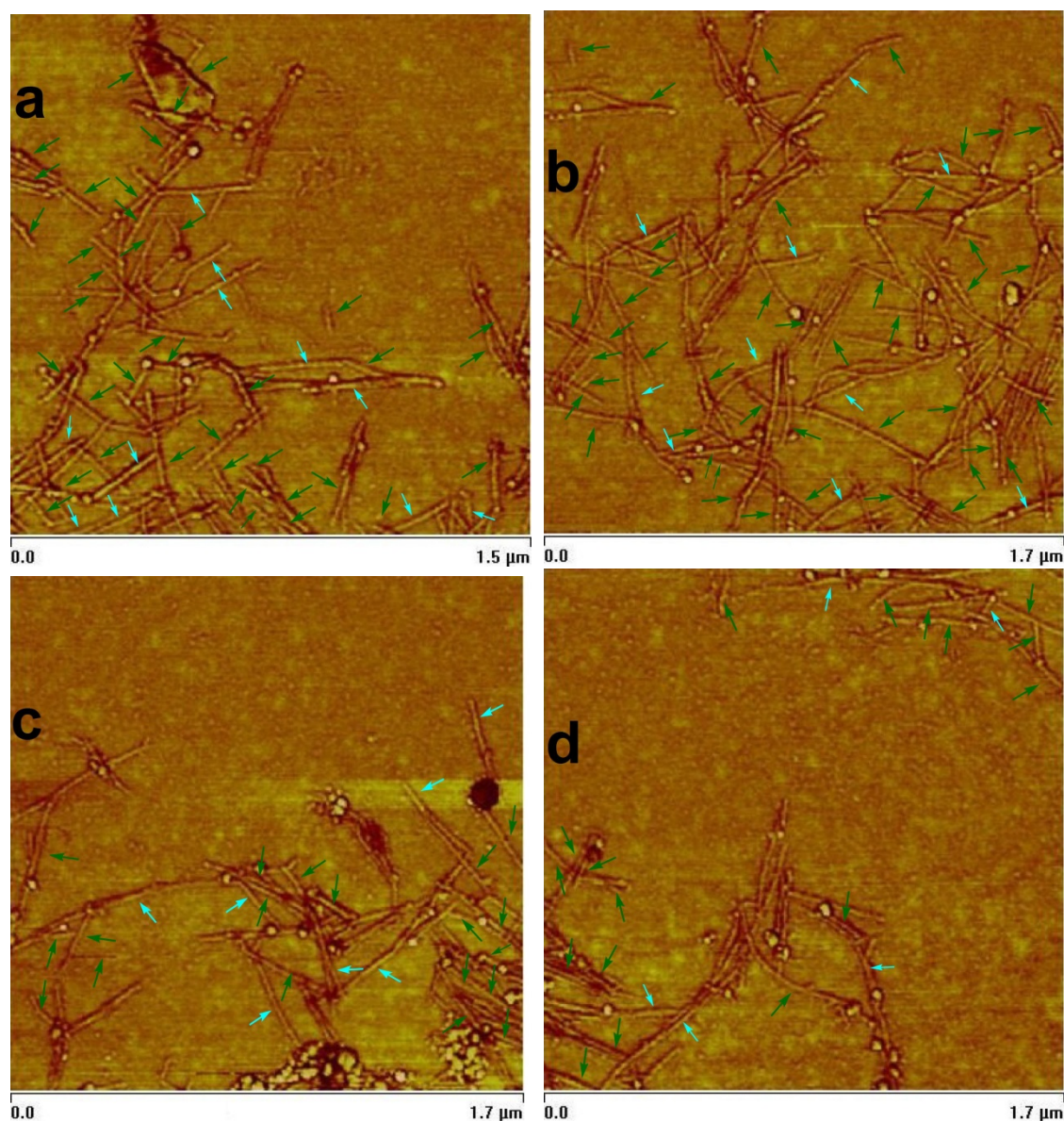


Figure S20. (a)-(d) Phase images derived from intermittent contact mode AFM experiments of ***S*-PBN-Ph₃-[PLV SWNTs]** from an aqueous suspension on a Si surface. Polymer-wrapped SWNT structures that evince the unexpected polymer helical wrapping chirality are marked with cyan arrows.

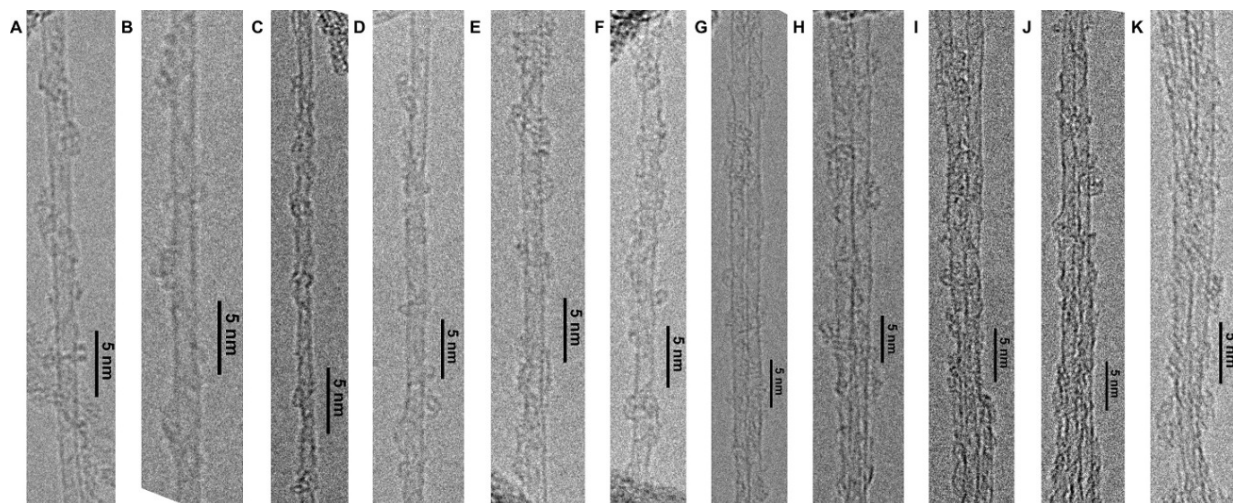


Figure S21. TEM images highlighting expected left-handed helical structures formed by **S-PBN(b)-Ph₅** -wrapped [PLV SWNTs] ($d = 1.4\text{-}2.4$ nm) obtained from aqueous suspension: (A)-(F) individualized tubes and (G) – (K) two-tube bundle. [Panel A and B images were also presented in Figure 6 in the main text]

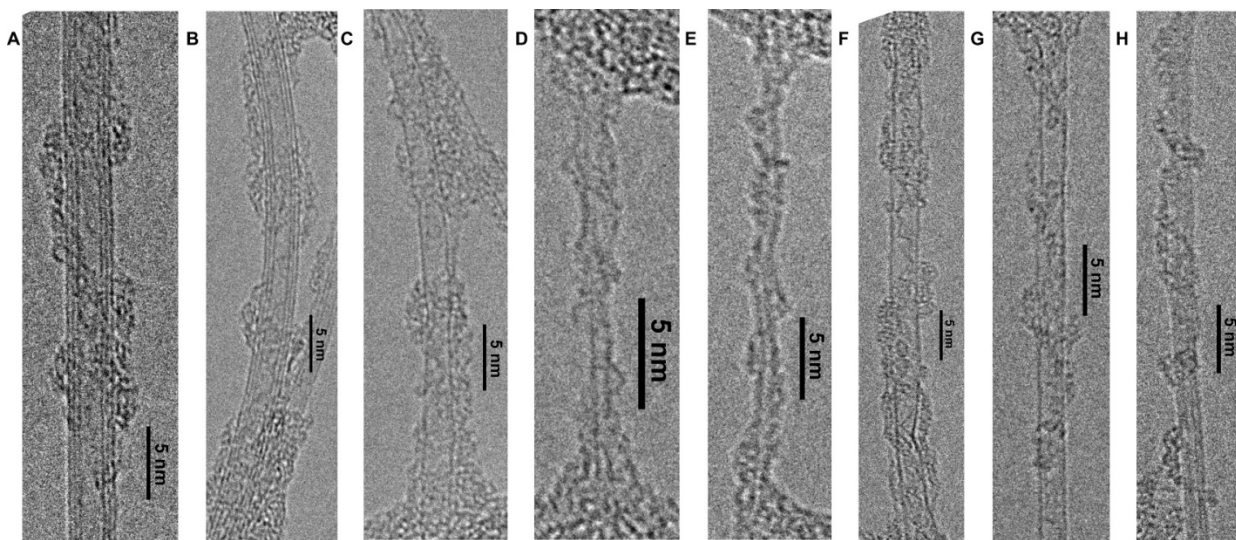


Figure S22. TEM images highlighting expected left-handed helical structures formed by **S-PBN(b)-Ph₅** -wrapped individualized CNTs of various diameter obtained from aqueous suspension: (A)-(D) FWNTs ($d \approx 3.5$ nm), (D)- (E) SWNTs ($d = 1\text{-}1.4$ nm), (F)-(G) large diameter SWNTs ($d \approx 3.5$ nm) and (H) FWNTs ($d = 2.5$ nm). These tubes, with various diameters, present in the unsorted “FWNT” sample.

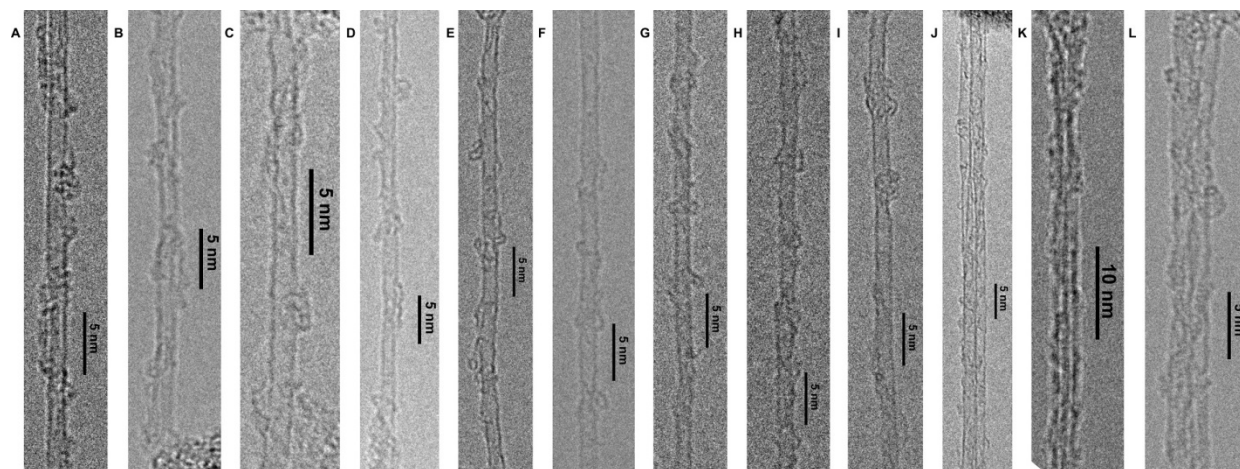


Figure S23. TEM images highlighting expected left-handed helical structures formed by **S-PBN(b)-Ph₄PhCN** -wrapped [PLV SWNTs] ($d = 1.4\text{-}2.4$ nm) obtained from aqueous suspension: (A)-(I) individualized tubes and (J)-(L) two-tube bundle. [Panel G, H and B images were also presented in **Figure 7** in the main text]

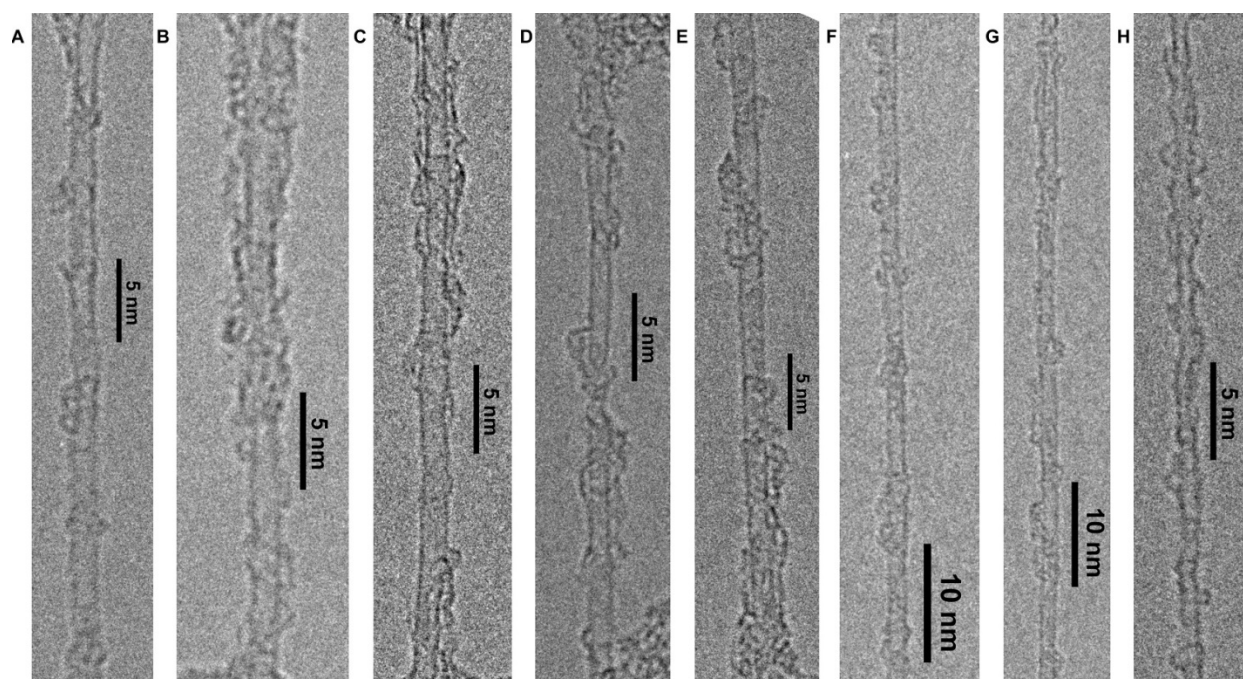


Figure S24. TEM images highlighting expected left-handed helical structures formed by **S-PBN(b)-Ph₂PZn₂**-wrapped individualized [PLV SWNTs] ($d = 1.4\text{-}2.4$ nm) obtained from aqueous suspension. Panel A, C and G images were also presented in **Figure 7** in the main text.

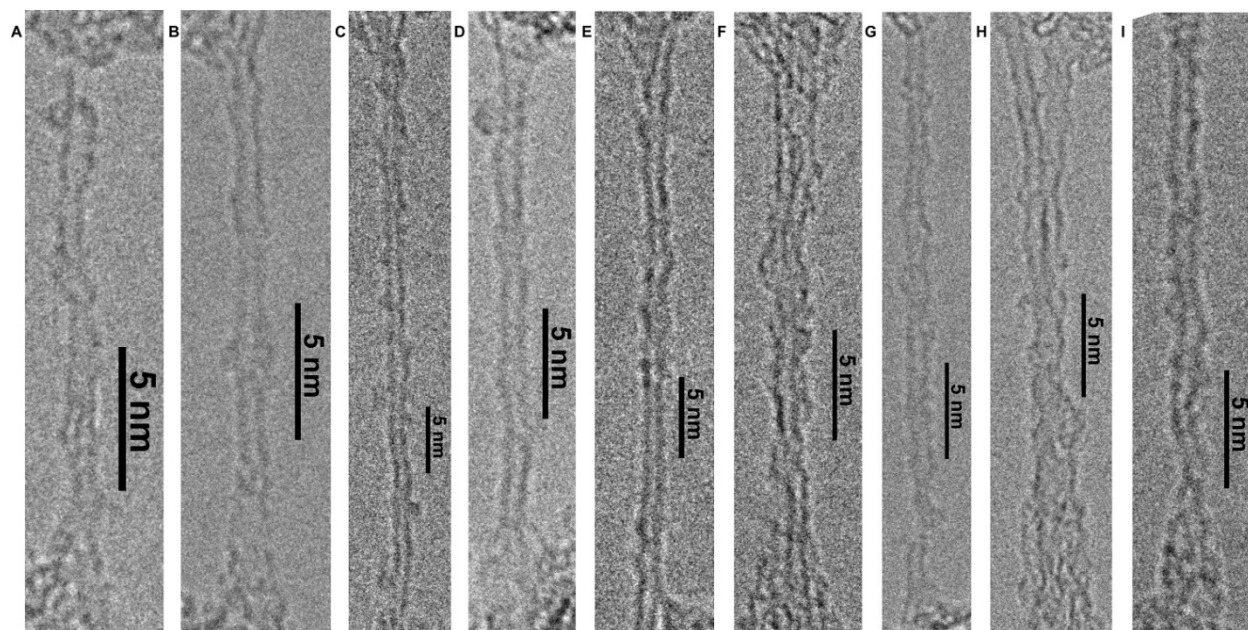
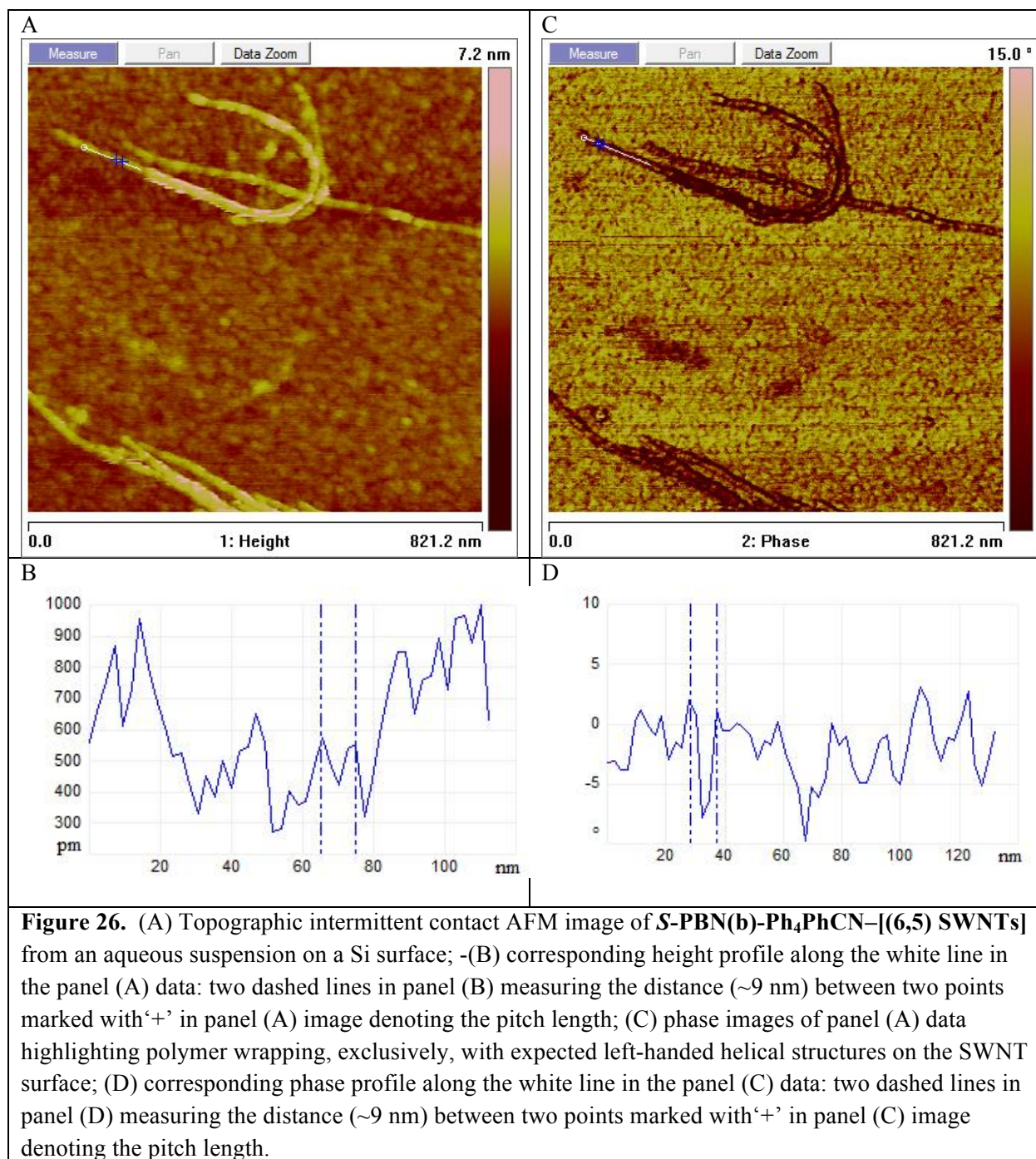
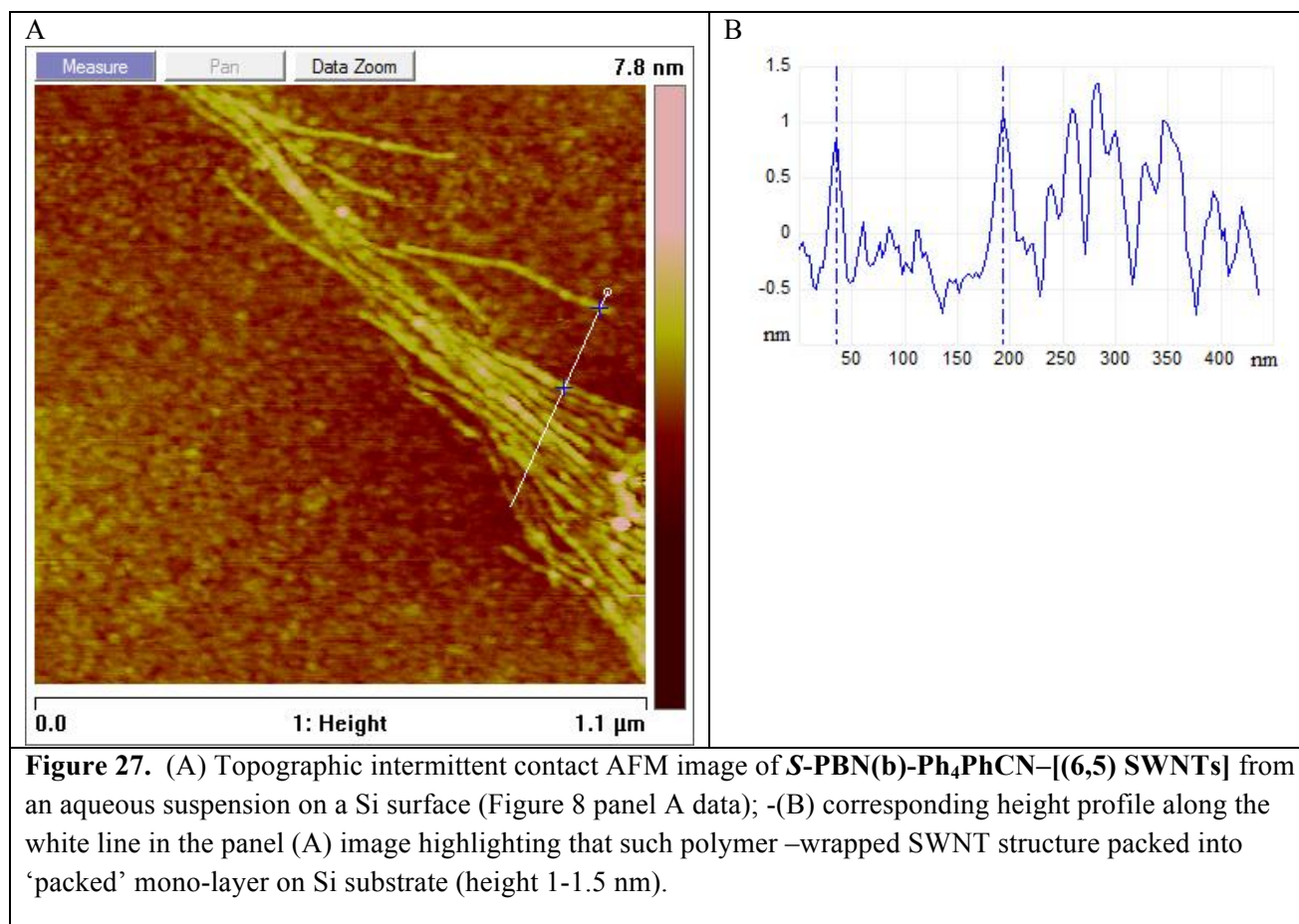


Figure S25. TEM images highlighting expected left-handed helical structures formed by (A)-(C) **S-PBN(b)-Ph₄PhCN**, (D)-(F) **S-PBN(b)-Ph₅** and (G)-(I) **S-PBN(b)-Ph₂PZn₂** –wrapped individualized [(6,5) SWNTs] ($d \approx 0.78$ nm) from aqueous suspensions.





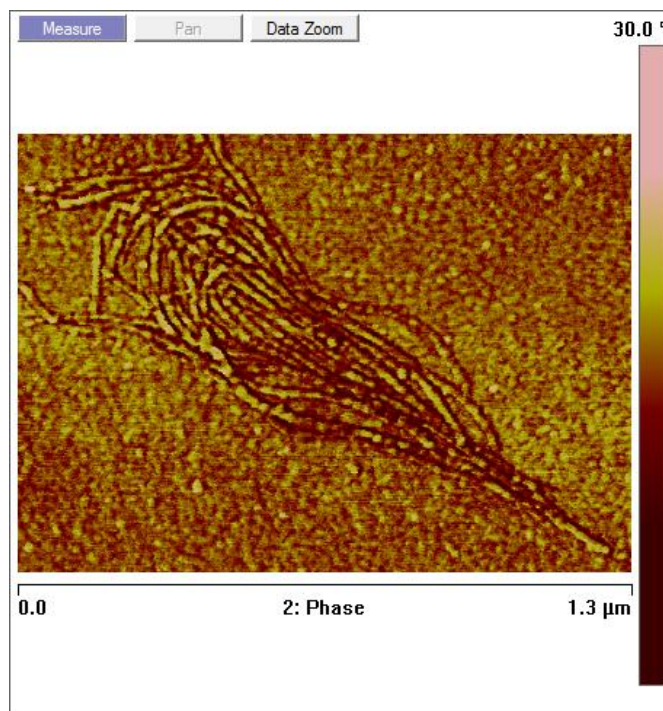


Figure S28. Phase images derived from intermittent contact mode AFM experiments of ***S*-PBN(b)-Ph₄PhCN-[(6,5) SWNTs]** from an aqueous suspension on a Si surface highlighting monolayer formation by these exclusively left-handed helically wrapped polymer/SWNT structures on the Si surface similar to **Figures 8 and S27** data.

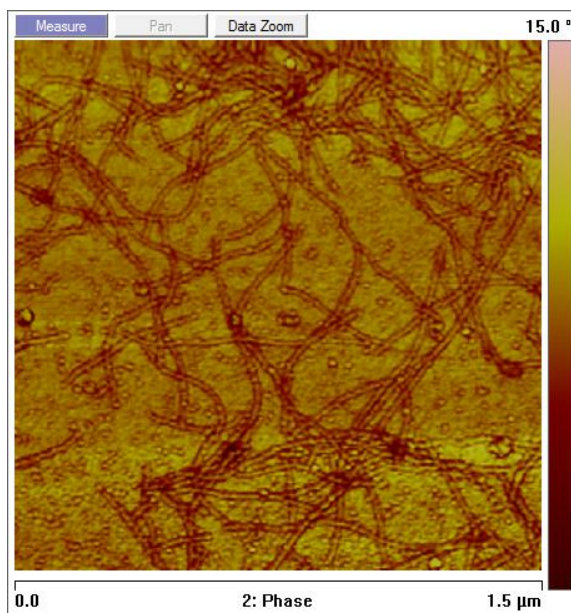


Figure S29. Phase images derived from intermittent contact mode AFM experiments of ***R*-PBN-PZn₂-[(6,5) SWNTs]** from an aqueous suspension on a Si surface highlighting an identical distribution of expected right and unexpected exclusively left-handed helically wrapping structure as that shown in **Figures 4 and S14, S19 and S20** for other *unbridged* polymers.

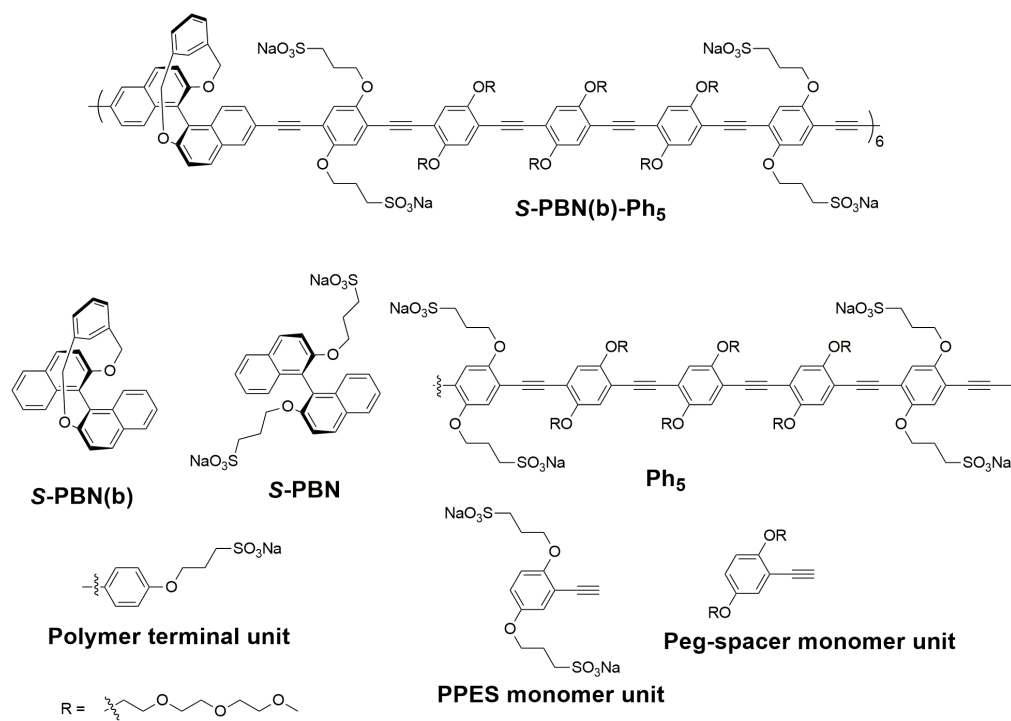
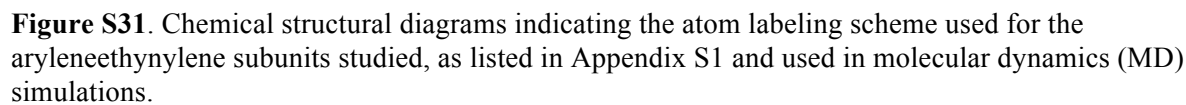


Figure S30. Ionic aryleneethynylene polymer S-PBN(b)-Ph₅ based on 1,1'-bi-2-naphthol derivatives and various monomeric units used in molecular dynamics (MD) simulations.



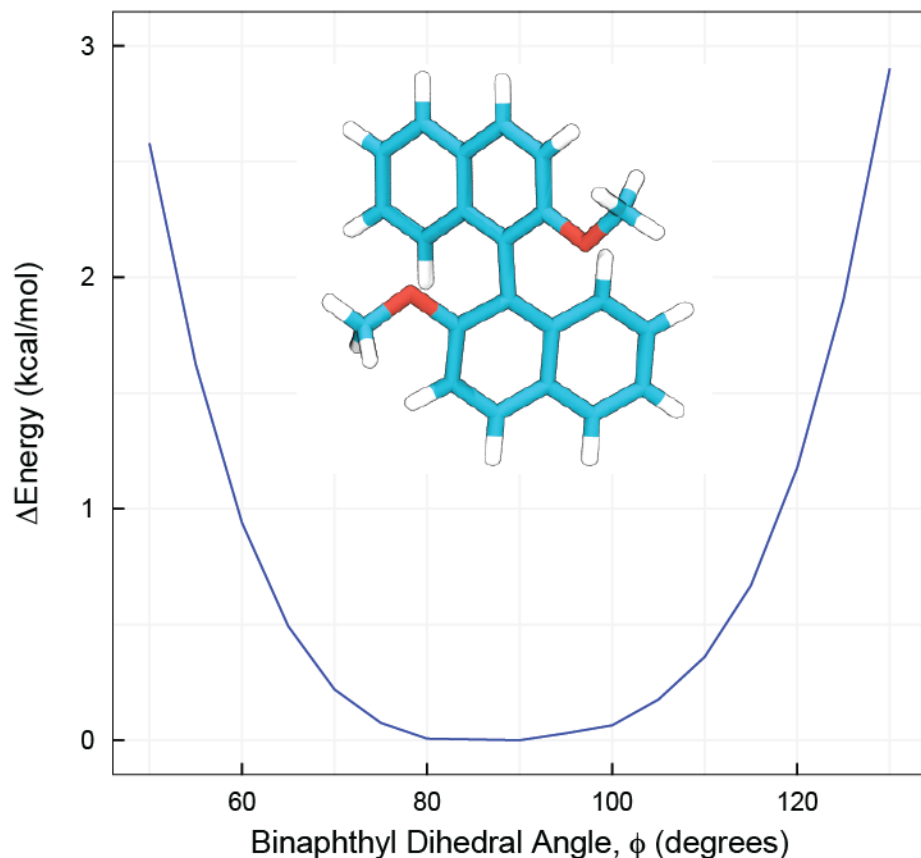


Figure S32. Potential energy curve for dimethoxy-1,1'-binaphthyl as a function of dihedral angle ϕ . Relative energies are based on the sum of the dihedral potential term and nonbonded interactions within the dimethoxy-1,1'-binaphthyl unit in the gas phase (blue line). This potential was estimated from the potential curves for dimethoxy-1,1'-binaphthyl as given by theoretical calculations done at the SCS-MP2/TZVPP and DFT-B97-D/ZTV2P levels. (M. Nishizaka, T. Mori, and Y. Inoue. Experimental and Theoretical Studies on the Chiroptical Properties of Donor-Acceptor Binaphthyls. Effects of Dynamic Conformer Population on Circular Dichroism. *J. Phys. Chem. Lett.* 2010, 1:1809-1812.)

Appendix S1. Structural parameters for bond distances, bond angles and dihedral angles; atom labels with the respective partial charges used in the simulations are also provided.

```

Parameters

BONDS
!! V(bond) = Kb(b - b0)**2
!!
!! Kb: kcal/mole/A**2
!! b0: A
!! atom_type Kb b0
CT CT 500.000 1.0240 !One-Sun, J. Phys. Chem. B. 106, 11343 (2002)
ON3 S 480.000 1.4500 !from S=O, JACS, vol.113 p4484(1991), macromodel AMBER, One-Sun Lee
OS CT2 340.000 1.4300 !from OS CT3, One-Sun Lee
CPS CT 250.000 1.4900 !pseudo from CA CT
OS CA 340.000 1.4300 !from OS CT3, adm jr., 4/05/91, for PRES CT1 from methylacetate
CPS CA 305.000 1.3750 ! ALLOW ARO, pseudo-bond by One-Sun Lee from CA CA
CPS CPS 0.000 4.0040 !pseudo-bond by One-Sun Lee
CD CD 306.768 1.4986 !CVB, from paratools
CD CA 305.000 1.3750 !from CPS CA
CA CD 305.000 1.3750 !from CA CA
CA CS 305.000 1.3750 ! ALLOW ARO, benzene, JES 8/25/89
CD CS 305.000 1.3750 !from CPS CA
OS CS 340.000 1.4300 !from OS CT3, adm jr., 4/05/91, for PRES CT1 from methylacetate
CA CA 305.000 1.3750 ! ALLOW ARO, benzene, JES 8/25/89
CNT CNT 938.000 1.4000 ! Nature 414, 188 (2001), Carbon Nanotube, One-Sun
CT2 CA 230.000 1.4900 ! ALLOW ALI ARO, phe,tyr, JES 8/25/89
CT2 CT2 222.500 1.5300 ! ALLOW ALI, alkane update, adm jr., 3/2/92
HA CA 340.000 1.0830 ! ALLOW ARO, trp, adm jr., 10/02/89
HA CT2 309.000 1.1110 ! ALLOW ALI, alkane update, adm jr., 3/2/92
HP CA 340.000 1.0800 ! ALLOW ARO, phe,tyr JES 8/25/89
S CT2 198.000 1.8180 ! ALLOW ALI SUL ION, fitted to C-S s 9/26/92 (FL)
! Alkane standard C27 parameters. Not modified from original.
CC32A HCA2 309.00 1.111 ! alkanes, 4/98
CC32A CC32A 222.50 1.530 ! alkanes, 3/92
CC32A OC30A 360.00 1.415 ! DEET, diethylether, alex
OS CC32A 340.000 1.4300 !pseudo-bond by CVB from (OS CT2)
ON3 HA 499.029 0.9607 !CVB, via paratools 9/23/11

ANGLES
!! V(angle) = Ktheta(Theta - Theta0)**2
!! V(Urey-Bradley) = Kub(S - S0)**2
!!
!! Ktheta: kcal/mole/rad**2
!! Theta0: degrees
!! Kub: kcal/mole/A**2 (Urey-Bradley)
!! S0: A
!! atom_types Ktheta Theta0 Kub S0
CPS CPS CT 0.00 180.00 !pseudo
CPS CT CT 44.500 180.00 !pseudo from CA CT CT HF/6-311G** -> 28.81
ON3 S ON3 75.000 118.00 !from macromodel amber*, One-Sun Lee
CT2 S ON3 65.000 109.00 !from macromodel amber*, One-Sun Lee
OS CT2 CT2 55.000 109.00 20.00 2.32600 !from OS CD CT2, One-Sun Lee 55
CPS CA HP 30.000 120.00 22.00 2.15250 ! ALLOW ARO, pseudo from CA CA HP
CA CA OS 75.000 120.00 !pseudo from CA CA CT HF/6-311G**->130.48
CPS CA OS 75.000 120.00 !pseudo from CA CA CT HF/6-311G**->130.48
CPS CA CA 40.000 120.00 35.00 2.41620 ! ALLOW ARO, pseudo from CA CA CA
CA CPS CPS 0.000 120.00 !Pseudo
CA CPS CT 75.000 120.00 !pseudo from CA CA CT HF/6-311G**->130.48
CA CPS CA 40.000 120.00 35.00 2.41620 ! ALLOW ARO, pseudo from CA CA CA
CA OS CT2 40.000 109.60 30.00 2.26510 !from CT3 OS CD, One-Sun Lee
CT2 OS CT2 40.000 109.60 30.00 2.26510
CA CD CD 40.000 120.00 35.00 2.41620
CD CD CA 40.000 120.00 35.00 2.41620
CA CA CD 40.000 120.00 35.00 2.41620
CD CA CA 40.000 120.00 35.00 2.41620
CA CD CA 40.000 120.00 35.00 2.41620
CD CA OS 75.0 120.00
CA CA CS 40.000 120.000 35.00 2.41620 ! ALLOW ARO, JES 8/25/89
CD CS CA 40.000 120.00 35.00 2.41620
CS CD CA 40.000 120.00 35.00 2.41620
CS CD CD 40.000 120.00 35.00 2.41620
CD CS OS 75.0 120.00
CA CS OS 75.000 120.00
CS OS CT2 40.000 109.60 30.00 2.26510 !from CT3 OS CD, One-Sun Lee
HP CA CS 30.000 120.000 22.00 2.15250 ! ALLOW ARO, JES 8/25/89 benzene
CA CT2 OS 40.000 109.60 30.00 2.26510 ! from CS OS CT2 (CVB, need to check this...)
CA CA CA 40.000 120.000 35.00 2.41620 ! ALLOW ARO, JES 8/25/89
CNT CNT CNT 126.000 120.000 35.00 2.41620 !Nature 414, 188 (2001), Carbon Nanotube, One-Sun
CT2 CA CA 45.800 122.300 ! ALLOW ALI ARO, PARALLH19 (JES)
CT2 CT2 CT2 58.350 113.600 11.16 2.56100 ! ALLOW ALI, alkane upd. adm jr 3/2/92,
!Heme vinyl subst. (KK from propene (JCS))
HA CA CA 29.000 120.000 25.00 2.15250 ! ALLOW ARO, trp, adm jr., 10/02/89
HA CT2 CA 49.300 107.500 ! ALLOW ALI ARO, PARALLH19 (JES)
HA CT2 CT2 26.500 110.100 22.53 2.17900 ! ALLOW ALI, alkane update, adm jr., 3/2/92
HA CT2 HA 35.500 109.000 5.40 1.80200 ! ALLOW ALI, alkane update, adm jr., 3/2/92
HP CA CA 30.000 120.000 22.00 2.15250 ! ALLOW ARO, JES 8/25/89 benzene
OS CT2 HA 60.000 109.500 ! ALLOW PEP POL, adm jr. 4/05/91, for PRES CT1 from methyl acetate

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S   CT2 CT2 58.000 114.500 ! ALLOW ALI SUL ION, expt. MeEtS, 3/26/92 (FL)
S   CT2 HA 46.100 111.300 ! ALLOW ALI SUL ION, vib. freq. and HF/6-31G* geo. (DTN) 8/24/90
HT  OT HT 55.000 104.520 ! TIP3P GEOMETRY
! Alkane standard C27 parameters. Not modified from original.
HCA2 CC32A CC32A 26.500 110.10 22.53 2.179 ! alkane, 4/98
CC32A CC32A CC32A 58.350 113.60 11.16 2.561 ! alkane, 3/92
HCA2 CC32A HCA2 35.50 109.00 5.40 1.802 ! alkane, 3/92
CC32A OC30A CC32A 95.00 109.70 ! DEET, diethylether, alex
OC30A CC32A CC32A 45.00 111.50 ! DEET, diethylether, alex
HCA2 CC32A OC30A 60.00 109.50 ! phosphate, alex
CA OS CC32A 40.000 109.60 30.00 2.2651 !pseudo from CA OS CT2, pseudo-bond CVB
HCA2 CC32A OS 60.00 109.50 !pseudo from HCA2 CC32A OC30A, pseudo-bond CVB
OS CC32A CC32A 45.00 111.50 !pseudo from OC30A CC32A CC32A, pseudo-bond CVB
S ON3 HA 40.952 109.51 !CVB, via paratools 9/23/11

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DIHEDRALS

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!! V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!!
!! Kchi: kcal/mole
!! n: multiplicity
!! delta: degrees
!! atom_types Kchi n delta
CA CD CD CS 0.0000 2 0.00 !CVB, from paratools
CA CD CD CA 5.0000 2 180.00 !
CS CD CD CS 0.0000 2 0.00 !
CA CA CA CD 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CA CA CD CD 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CD CD CA CA 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CD CA CA CA 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CD CD CA OS 3.1000 2 180.00 ! from CA CA CA CA
CA CD CA OS 3.1000 2 180.00 ! from CA CA CA CA
CA CA CD CA 3.1000 2 180.00 ! from CA CA CA CA
HP CA CA CD 4.2 2 180.00 ! pseudo from HP CA CA CA
CD CA OS CT2 2.6000 2 180.00 ! from JPC 94 4483 (1990) Kollman
CD CA OS CT2 0.3250 4 180.00 ! from JPC 94 4483 (1990) Kollman
CA CA CA CS 3.1000 2 180.00 ! ALLOW ARO, JES 8/25/89
CA CA CS CD 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CA CS CD CA 3.1000 2 180.00 ! from CA CA CA CA
CA CA CD CS 3.1000 2 180.00 ! from CA CA CA CA
CA CS CD CD 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CD CD CS OS 3.1000 2 180.00 ! from CA CA CA CA
CA CA CS OS 3.1000 2 180.00 ! from CA CA CA CA
CA CD CS OS 3.1000 2 180.00 ! from CA CA CA CA
CD CS OS CT2 2.6000 2 180.00 ! from JPC 94 4483 (1990) Kollman
CD CS OS CT2 0.3250 4 180.00 ! from JPC 94 4483 (1990) Kollman
CA CS OS CT2 2.6000 2 180.00 ! from JPC 94 4483 (1990) Kollman
CA CS OS CT2 0.3250 4 180.00 ! from JPC 94 4483 (1990) Kollman
HP CA CS CD 4.2 2 180.00 ! pseudo from HP CA CA CA
HP CA CA CS 4.2 2 180.00 ! pseudo from HP CA CA CA
HP CA CS OS 4.2000 2 180.00 !pseudo from HP CA CA CT
CA CA CA CPS 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CA CA OS CT2 2.6000 2 180.00 ! from JPC 94 4483 (1990) Kollman
CA CA OS CT2 0.3250 4 180.00 ! from JPC 94 4483 (1990) Kollman
CA CA CA OS 3.1000 2 180.00 ! from CA CA CA CA
CA CA CPS CPS 0.0000 2 180.00 ! ALLOW ARO pseudo
CT CPS CA CA 3.1000 2 180.00 ! pseudo from CT CA CA CA
CA CPS CPS CA 3.1000 2 180.00 ! ALLOW ARO, pseudo from CA CA CA CA
CA CPS CPS CT 0.1150 2 180.00 !PSEUDO J. Phys. Chem 88, 1711 (1984) K. Okuyama 0.29
CA CPS CPS CT 0.0000 2 180.00 ! pseudo
CT CT CPS CA 0.0000 2 180.00 !pseudo
HP CA CPS CA 4.2000 2 180.00 ! ALLOW ARO, pseudo from HP CA CA CA
HP CA CPS CPS 4.2000 2 180.00 ! ALLOW ARO, pseudo from HP CA CA CA
CPS CPS CT CT 0.0000 2 180.00 !pseudo
CPS CPS CA OS 0.0000 2 180.00 !pseudo
CPS CT CT CPS 0.0000 2 180.00 !pseudo
CPS CA CA OS 3.1000 2 180.00 !pseudo from CT CA CA CA
CPS CA OS CT2 2.6000 2 180.00 !from JPC 94 4483 (1990) Kollman
CPS CA OS CT2 0.3250 4 180.00 !from JPC 94 4483 (1990) Kollman
HP CA CA CPS 4.2000 2 180.00 !pseudo from HP CA CA CA
CA CPS CA OS 3.1000 2 180.00 !pseudo from CA CA CA CA
HP CA CA OS 4.2000 2 180.00 !pseudo from HP CA CA CT
CT CPS CPS CT 0.0000 2 180.00 !pseudo
CT CPS CA OS 3.1000 2 180.00 !pseudo
HP CA CPS CT 4.2000 2 180.00 !pseudo from HP CA CA CT
CT2 CT2 S ON3 0.0000 1 180.00 !from macromodel amber*
HA CT2 S ON3 0.3330 3 0.00 !from macromodel amber*
CPS CA CA CPS 3.1000 2 180.00 !from CA CA CA CA
CA CA CA CA 3.1000 2 180.00 ! ALLOW ARO, JES 8/25/89
CNT CNT CNT CNT 3.1000 2 180.00 ! Carbon Nanotube, One-Sun
CT2 CA CA CA 3.1000 2 180.00 ! ALLOW ARO, JES 8/25/89 toluene and ethylbenzene
CT2 CT2 CT2 CT2 0.1500 1 0.00 ! ALLOW ALI, alkane update, adm jr., 3/2/92, butane trans/gauche
HA CA CA CA 3.5000 2 180.00 ! ALLOW ARO, adm jr., 10/02/89
HA CA CA HA 2.5000 2 180.00 ! ALLOW ARO, ADM JR., 10/02/89
HP CA CA CA 4.2000 2 180.00 ! ALLOW ARO, JES 8/25/89 benzene
HP CA CA CT2 4.2000 2 180.00 ! ALLOW ARO, JES 8/25/89 toluene and ethylbenzene

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HP  CA  CA  HP      2.4000  2   180.00  ! ALLOW  ARO, JES 8/25/89 benzene
X   CT2 CA  X      0.0000  6    0.00  ! ALLOW  ALI ARO, toluene, adm jr., 3/7/92
X   CT2 CT2 X      0.1950  3    0.00  ! ALLOW  ALI, alkane update, adm jr., 3/2/92
X   CT2 OS  X      -0.1000  3    0.00  ! ALLOW  PEP POL, adm jr. 3/19/92, from lipid methyl acetate
CT2 CA  CA  CT2     0.0000  1    0.00  ! no explicit dihedral term for the linker... CVB
!! Alkane standard C27 parameters. Not modified from original.
HCA2 CC32A CC32A HCA2    0.19000  3    0.0  ! alkane, 4/98, yin and mackerell
CC32A CC32A CC32A HCA2    0.19000  3    0.0  ! alkane, 4/98, yin and mackerell
CC32A CC32A CC32A CC32A  0.11251  5    0.0  ! alkane, c27r klauda et al 2004
CC32A CC32A CC32A CC32A  0.09458  4    0.0  ! alkane, c27r klauda et al.2004
CC32A CC32A CC32A CC32A  0.14975  3   180.0  ! alkane, c27r klauda et al 2004
CC32A CC32A CC32A CC32A  0.06450  2    0.0  ! alkane, c27r klauda et al 2004
HCA2 CC32A CC32A OC30A  0.19000  3    0.0  ! alkane, 4/98, yin and mackerell
HCA2 CC32A OC30A CC32A  0.28400  3    0.0  ! DEET, diethylether, alex
CC32A CC32A OC30A CC32A  0.57000  1    0.0  ! 1,2 dimethoxyethane, 2/12/05, ATM
CC32A CC32A OC30A CC32A  0.29000  2    0.0  ! 1,2 dimethoxyethane
CC32A CC32A OC30A CC32A  0.43000  3    0.0  ! 1,2 dimethoxyethane
OC30A CC32A CC32A OC30A  0.59000  1   180.0  ! 1,2 dimethoxyethane, Aug 2007, HK Lee
OC30A CC32A CC32A OC30A  1.16000  2    0.0  ! 1,2 dimethoxyethane
OC30A CC32A CC32A CC32A  0.16000  1   180.0  ! methylpropylether, 2/12/05, ATM
OC30A CC32A CC32A CC32A  0.39000  2    0.0  ! methylpropylether
CPS  CA  OS  CC32A  2.6000  2   180.00  !from JPC 94 4483 (1990) Kollman, pseudo-bond CVB
CPS  CA  OS  CC32A  0.3250  4   180.00  !from JPC 94 4483 (1990) Kollman, pseudo-bond CVB
CA   CA  OS  CC32A  2.6000  2   180.00  !from JPC 94 4483 (1990) Kollman, pseudo-bond CVB
CA   CA  OS  CC32A  0.3250  4   180.00  !from JPC 94 4483 (1990) Kollman, pseudo-bond CVB
CC32A CC32A OS  CA  2.6000  2   180.00  !from JPC 94 4483 (1990) Kollman, pseudo-bond CVB
CC32A CC32A OS  CA  0.3250  4   180.00  !from JPC 94 4483 (1990) Kollman, pseudo-bond CVB
HCA2 CC32A OS  CA  0.2840  3    0.00  ! DEET, diethylether, alex, pseudo-bond CVB
OS   CC32A CC32A OC30A  0.5900  1   180.00  ! 1,2 dimethoxyethane, Aug 2007, HK Lee, pseudo-bond
CVB
OS   CC32A CC32A OC30A  1.1600  2    0.00  ! 1,2 dimethoxyethane, pseudo-bond CVB
HCA2 CC32A CC32A OS  0.1900  3    0.00  ! alkane, 4/98, yin and mackerell, pseudo-bond CVB
CT2  S  ON3  HA  0.6286  3    0.00  !CVB, via paratools 9/23/11
ON3  S  ON3  HA  1.4969  3    0.00  !CVB, via paratools 9/23/11

!! V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!!
!! epsilon: kcal/mole, Eps,i,j = sqrt(eps,i * eps,j)
!! Rmin/2: A, Rmin,i,j = Rmin/2,i + Rmin/2,j
!! atom ignored epsilon Rmin/2 ignored eps,1-4 Rmin/2,1-4
HCA2 0.000000 -0.035000 1.340000 ! alkane,propane 11/16/04 viv
HT   0.000000 -0.046000 0.224500 ! TIP3P water
CC32A 0.000000 -0.056000 2.010000 0.000000 -0.010000 1.900000 ! alkane, 4/98, yin, adm jr.
OC30A 0.000000 -0.100000 1.650000 ! THP, tetrahydropyran sng 1/06
OT   0.000000 -0.152100 1.768200 ! TIP3P water
CT   0.000000 -0.020000 2.275000 0.000000 -0.010000 1.900000 !One-Sun Lee test from CT1
CPS  0.000000 -0.070000 1.992400 ! ALLOW ARO lpseudo
C    0.000000 -0.110000 2.000000 ! ALLOW PEP POL ARO ! NMA pure solvent, adm jr., 3/3/93
CA   0.000000 -0.070000 1.992400 ! ALLOW ARO ! benzene (JES)
CS   0.000000 -0.070000 1.992400 ! ALLOW ARO ! benzene (JES)
CD   0.000000 -0.070000 2.000000 ! ALLOW POL ! adm jr. 3/19/92, acetate a.i. and dH of solvation
CNT  0.000000 -0.086000 1.908200 ! Nature 414, 188 (2001) ! Carbon Nanotube, One-Sun Lee
CPA  0.000000 -0.090000 1.800000 ! ALLOW HEM, Heme (6-liganded): porphyrin macrocycle (KK 05/13/91)
CT2  0.000000 -0.055000 2.175000 0.000000 -0.010000 1.900000 ! ALLOW ALI, propane pure solvent
! properties, adm jr, 2/3/92
HA   0.000000 -0.022000 1.320000 ! ALLOW PEP ALI POL SUL ARO PRO ALC,
!methane/ethane a.i. and ethane pure solvent, adm jr, 2/3/92
HP   0.000000 -0.030000 1.358200 0.000000 -0.030000 1.358200 ! ALLOW ARO, JES 8/25/89 values from
! Jorgensen fit to hydration energy
OS   0.000000 -0.152100 1.770000 ! ALLOW ALC ARO, adm jr. 9/17/90, avoid O* wildcard
S    0.000000 -0.450000 2.000000 ! ALLOW SUL ION, adm jr., 3/3/92, methanethiol/ethylmethylsulfide pure
solvent
ON3  0.000000 -0.120000 1.700000

Topologies

!! Beginning Terminal Unit
!!
RESI BEG -1.00
GROUP
ATOM C02 CT -0.116100
ATOM C39 CT -0.116100
GROUP
ATOM C40 CPS 0.010800
ATOM C41 CA -0.1458095
ATOM C42 CA -0.1458095
ATOM C01 CA 0.190206
ATOM C03 CA -0.1458095
ATOM C45 CA -0.1458095
ATOM H33 HP 0.153608
ATOM H34 HP 0.153608
ATOM H35 HP 0.153608
ATOM H36 HP 0.153608
GROUP
ATOM O23 OS -0.410939

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ATOM C46 CT2 0.144746
ATOM C47 CT2 0.048854
ATOM C48 CT2 -0.180965
ATOM S04 S 1.423871
ATOM O24 ON3 -0.768393
ATOM O25 ON3 -0.768393
ATOM O26 ON3 -0.768393
ATOM H37 HA 0.060430
ATOM H38 HA 0.060430
ATOM H39 HA 0.025980
ATOM H40 HA 0.025980
ATOM H41 HA 0.053396
ATOM H42 HA 0.053396

BOND C40 C41 C42 C01 C03 C45 C01 O23
BOND O23 C46 C46 C47 C47 C48 C48 S04 S04 O25
BOND C41 H33 C03 H35 C45 H36 C42 H34 C39 C40
BOND C46 H37 C46 H38 C47 H39 C47 H40 C48 H41 C48 H42
BOND C02 +C01
Double C40 C45 C41 C42 C01 C03 S04 O24 S04 O26
Triple C02 C39

!! PPES Monomer Unit
!!
RESI PPS -2.0
GROUP
ATOM C01 CPS 0.010800
ATOM C07 CA -0.238514
ATOM C06 CA 0.190206
ATOM C04 CPS 0.010800
ATOM C05 CA -0.238514
ATOM C03 CA 0.190206
ATOM C02 CT -0.116100
ATOM C08 CT -0.116100
ATOM H25 HP 0.153608
ATOM H26 HP 0.153608
GROUP
ATOM O09 OS -0.410939
ATOM C10 CT2 0.144746
ATOM C11 CT2 0.048854
ATOM C12 CT2 -0.180965
ATOM S13 S 1.423871
ATOM O14 ON3 -0.768393
ATOM O15 ON3 -0.768393
ATOM O16 ON3 -0.768393
ATOM H27 HA 0.060430
ATOM H28 HA 0.060430
ATOM H29 HA 0.025980
ATOM H30 HA 0.025980
ATOM H31 HA 0.053396
ATOM H32 HA 0.053396
GROUP
ATOM O17 OS -0.410939
ATOM C18 CT2 0.144746
ATOM C19 CT2 0.048854
ATOM C20 CT2 -0.180965
ATOM S21 S 1.423871
ATOM O22 ON3 -0.768393
ATOM O23 ON3 -0.768393
ATOM O24 ON3 -0.768393
ATOM H33 HA 0.060430
ATOM H34 HA 0.060430
ATOM H35 HA 0.025980
ATOM H36 HA 0.025980
ATOM H37 HA 0.053396
ATOM H38 HA 0.053396

BOND C01 C07 C06 C04 C05 C03
BOND C04 C08 C07 H25 C05 H26
BOND C06 O09 O09 C10 C10 C11 C11 C12 C12 S13
BOND S13 O14 S13 O15 S13 O16
BOND C10 H27 C10 H28 C11 H29 C11 H30 C12 H31 C12 H32
BOND C03 O17 O17 C18 C18 C19 C19 C20 C20 S21
BOND S21 O22 S21 O23 S21 O24
BOND C18 H33 C18 H34 C19 H35 C19 H36 C20 H37 C20 H38
BOND C02 +C01
Double C07 C06 C04 C05 C03 C01
Triple C02 C08

!! Unstitched BiNaphthyl Monomer Unit
!!
RESI PBS -2.00
GROUP inapthal group 1
ATOM C06 CD -0.106618
ATOM C28 CS 0.190206

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ATOM C07 CA -0.106618
ATOM C04 CA -0.106618
ATOM C05 CA -0.106618
ATOM C01 CPS 0.010800
ATOM C03 CA -0.106618
ATOM C08 CA -0.106618
ATOM C09 CA -0.106618
ATOM C10 CA -0.106618
ATOM H01 HP 0.153608
ATOM H02 HP 0.153608
ATOM H03 HP 0.153608
ATOM H04 HP 0.153608
ATOM H05 HP 0.153608
GROUP lnapthal group 2
ATOM C11 CD -0.106618
ATOM C12 CS 0.190206
ATOM C13 CA -0.106618
ATOM C14 CA -0.106618
ATOM C15 CA -0.106618
ATOM C16 CPS 0.010800
ATOM C17 CA -0.106618
ATOM C18 CA -0.106618
ATOM C19 CA -0.106618
ATOM C20 CA -0.106618
ATOM H06 HP 0.153608
ATOM H07 HP 0.153608
ATOM H08 HP 0.153608
ATOM H09 HP 0.153608
ATOM H10 HP 0.153608
GROUP ltail on ng1
ATOM O11 OS -0.410939
ATOM C21 CT2 0.144746
ATOM C22 CT2 0.048854
ATOM C23 CT2 -0.180965
ATOM S01 S 1.423871
ATOM O12 ON3 -0.768393
ATOM O13 ON3 -0.768393
ATOM O14 ON3 -0.768393
ATOM H11 HA 0.060430
ATOM H12 HA 0.060430
ATOM H13 HA 0.025980
ATOM H14 HA 0.025980
ATOM H15 HA 0.053396
ATOM H16 HA 0.053396
GROUP ltail on ng2
ATOM O15 OS -0.410939
ATOM C24 CT2 0.144746
ATOM C25 CT2 0.048854
ATOM C26 CT2 -0.180965
ATOM S02 S 1.423871
ATOM O16 ON3 -0.768393
ATOM O17 ON3 -0.768393
ATOM O18 ON3 -0.768393
ATOM H17 HA 0.060430
ATOM H18 HA 0.060430
ATOM H19 HA 0.025980
ATOM H20 HA 0.025980
ATOM H21 HA 0.053396
ATOM H22 HA 0.053396
GROUP ltriple bond
ATOM C27 CT -0.116100
ATOM C02 CT -0.116100

BOND C28 C07 C04 C10 C10 C05
BOND C01 C03 C08 C09 C09 C06
BOND C07 H01 C04 H02 C05 H03 C03 H04 C08 H05
BOND C06 C11 C11 C19 C20 C15 C16 C17 C18 C19
BOND C20 C14 C13 C12
BOND C13 H06 C14 H07 C15 H08 C17 H09 C18 H10
BOND C16 C27
BOND C28 O11 O11 C21 C21 C22 C22 C23 C23 S01 S01 O13
BOND C21 H11 C21 H12 C22 H13 C22 H14 C23 H15 C23 H16
BOND C12 O15 O15 C24 C24 C25 C25 C26 C26 S02 S02 O17
BOND C24 H17 C24 H18 C25 H19 C25 H20 C26 H21 C26 H22
BOND C02 +C01
Double C06 C28 C07 C04 C05 C01 C03 C08 C09 C10
Double C11 C12 C13 C14 C20 C19 C16 C15 C18 C17
Double S01 O12 S01 O14 S02 O16 S02 O18
Triple C27 C02

!! "Stitched" BiNaphthyl Monomer Unit
!!
RESI BNX 0.00
GROUP lnapthal group 1
ATOM C06 CD -0.106618

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ATOM C28 CS      0.190206
ATOM C07 CA     -0.106618
ATOM C04 CA     -0.106618
ATOM C05 CA     -0.106618
ATOM C01 CPS      0.010800
ATOM C03 CA     -0.106618
ATOM C08 CA     -0.106618
ATOM C09 CA     -0.106618
ATOM C10 CA     -0.106618
ATOM H01 HP      0.153608
ATOM H02 HP      0.153608
ATOM H03 HP      0.153608
ATOM H04 HP      0.153608
ATOM H05 HP      0.153608
GROUP          !napthal group 2
ATOM C11 CD     -0.106618
ATOM C12 CS      0.190206
ATOM C13 CA     -0.106618
ATOM C14 CA     -0.106618
ATOM C15 CA     -0.106618
ATOM C16 CPS      0.010800
ATOM C17 CA     -0.106618
ATOM C18 CA     -0.106618
ATOM C19 CA     -0.106618
ATOM C20 CA     -0.106618
ATOM H06 HP      0.153608
ATOM H07 HP      0.153608
ATOM H08 HP      0.153608
ATOM H09 HP      0.153608
ATOM H10 HP      0.153608
GROUP          !linker
ATOM O11 OS     -0.3117998      !-0.410939
ATOM C21 CT2      0.0317127      !0.144746
ATOM H11 HA       0.1064377      !0.060430
ATOM H12 HA       0.1064377      !0.060430
ATOM CX1 CA       -0.0857476      !-0.053961
ATOM CX2 CA       -0.0857476      !-0.053961
ATOM CX3 CA       -0.0857476      !-0.053961
ATOM CX4 CA       -0.0857476      !-0.053961
ATOM CX5 CA       -0.0857476      !-0.053961
ATOM CX6 CA       -0.0857476      !-0.053961
ATOM HX2 HP        0.1622272      !0.153608
ATOM HX3 HP        0.1622272      !0.153608
ATOM HX4 HP        0.1622272      !0.153608
ATOM HX6 HP        0.1622272      !0.153608
ATOM O15 OS       -0.3117998      !-0.410939
ATOM C24 CT2      0.0317127      !0.144746
ATOM H17 HA       0.1064377      !0.060430
ATOM H18 HA       0.1064377      !0.060430
GROUP          !triple bond
ATOM C27 CT       -0.116100
ATOM C02 CT       -0.116100

BOND  C28 C07  C04 C10  C10 C05
BOND  C01 C03  C08 C09  C09 C06
BOND  C07 H01  C04 H02  C05 H03  C03 H04  C08 H05
BOND  C06 C11  C11 C19  C20 C15  C16 C17  C18 C19
BOND  C20 C14  C13 C12
BOND  C13 H06  C14 H07  C15 H08  C17 H09  C18 H10
BOND  C16 C27
BOND  C28 O11  O11 C21  C21 H11  C21 H12
BOND  C12 O15  O15 C24  C24 H17  C24 H18
BOND  C24 CX1  CX1 CX2  CX3 CX4  CX5 CX6  CX5 C21
BOND  CX2 HX2  CX3 HX3  CX4 HX4  CX6 HX6
BOND  C02 +C01
Double C06 C28  C07 C04  C05 C01  C03 C08  C09 C10
Double C11 C12  C13 C14  C20 C19  C16 C15  C18 C17
Double CX2 CX3  CX4 CX5  CX6 CX1
Triple C27 C02

!! PEG Spacer Monomer Unit
!!
RESI PEG  0.0      !taken from top_all135_ethers.rtf
GROUP          !Mackerell.upmaryland.edu
ATOM C01 CPS      0.010800
ATOM C06 CA     -0.238514
ATOM C07 CA      0.190206
ATOM C04 CPS      0.010800
ATOM C05 CA     -0.238514
ATOM C03 CA      0.190206
ATOM C02 CT     -0.116100
ATOM C08 CT     -0.116100
ATOM H31 HP      0.153608
ATOM H32 HP      0.153608
GROUP

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ATOM O09 OS -0.26
ATOM C10 CC32A -0.01
ATOM C11 CC32A -0.01
ATOM O12 OC30A -0.34
ATOM C13 CC32A -0.01
ATOM C14 CC32A -0.01
ATOM O15 OC30A -0.34
ATOM C16 CC32A -0.01
ATOM C17 CC32A -0.01
ATOM O18 OC30A -0.34
ATOM C19 CC32A -0.01
ATOM H33 HCA2 0.09
ATOM H34 HCA2 0.09
ATOM H35 HCA2 0.09
ATOM H36 HCA2 0.09
ATOM H37 HCA2 0.09
ATOM H38 HCA2 0.09
ATOM H39 HCA2 0.09
ATOM H40 HCA2 0.09
ATOM H41 HCA2 0.09
ATOM H42 HCA2 0.09
ATOM H43 HCA2 0.09
ATOM H44 HCA2 0.09
ATOM H45 HCA2 0.09
ATOM H46 HCA2 0.09
ATOM H47 HCA2 0.09
GROUP
ATOM O20 OS -0.26
ATOM C21 CC32A -0.01
ATOM C22 CC32A -0.01
ATOM O23 OC30A -0.34
ATOM C24 CC32A -0.01
ATOM C25 CC32A -0.01
ATOM O26 OC30A -0.34
ATOM C27 CC32A -0.01
ATOM C28 CC32A -0.01
ATOM O29 OC30A -0.34
ATOM C30 CC32A -0.01
ATOM H48 HCA2 0.09
ATOM H49 HCA2 0.09
ATOM H50 HCA2 0.09
ATOM H51 HCA2 0.09
ATOM H52 HCA2 0.09
ATOM H53 HCA2 0.09
ATOM H54 HCA2 0.09
ATOM H55 HCA2 0.09
ATOM H56 HCA2 0.09
ATOM H57 HCA2 0.09
ATOM H58 HCA2 0.09
ATOM H59 HCA2 0.09
ATOM H60 HCA2 0.09
ATOM H61 HCA2 0.09
ATOM H62 HCA2 0.09

BOND C01 C06 C07 C04 C05 C03
BOND C04 C08 C06 H31 C05 H32
BOND C07 O09 O09 C10 C10 C11 C11 O12 O12 C13
BOND C13 C14 C14 O15 O15 C16 C16 C17 C17 O18
BOND O18 C19 C19 H33 C19 H34 C19 H35
BOND C10 H36 C10 H37 C11 H38 C11 H39 C13 H40 C13 H41
BOND C14 H42 C14 H43 C16 H44 C16 H45 C17 H46 C17 H47
BOND C03 O20 O20 C21 C21 C22 C22 O23 O23 C24
BOND C24 C25 C25 O26 O26 C27 C27 C28 C28 O29
BOND O29 C30 C30 H48 C30 H49 C30 H50
BOND C21 H51 C21 H52 C22 H53 C22 H54 C24 H55 C24 H56
BOND C25 H57 C25 H58 C27 H59 C27 H60 C28 H61 C28 H62
BOND C02 +C01
Double C06 C07 C04 C05 C03 C01
Triple C02 C08

!! Ending Terminal Unit
!!
RESI END -1.00
GROUP
ATOM C01 CPS 0.010800
ATOM C30 CA -0.203860
ATOM C03 CA -0.203860
ATOM C02 CA 0.190206
ATOM C33 CA -0.203860
ATOM C34 CA -0.203860
ATOM H23 HP 0.153608
ATOM H24 HP 0.153608
ATOM H25 HP 0.153608
ATOM H26 HP 0.153608
GROUP

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ATOM O19 OS -0.410939
ATOM C35 CT2 0.144746
ATOM C36 CT2 0.048854
ATOM C37 CT2 -0.180965
ATOM S03 S 1.423871
ATOM O20 ON3 -0.768393
ATOM O21 ON3 -0.768393
ATOM O22 ON3 -0.768393
ATOM H27 HA 0.060430
ATOM H28 HA 0.060430
ATOM H29 HA 0.025980
ATOM H30 HA 0.025980
ATOM H31 HA 0.053396
ATOM H32 HA 0.053396

BOND C30 C03 C02 C33 C35 C36 C36 C37 C01 C34
BOND C37 S03 S03 O21 C35 O19 O19 C02
BOND C30 H23 C03 H24 C34 H26 C33 H25
BOND C35 H27 C35 H28 C36 H29 C36 H30 C37 H31 C37 H32
!BOND C02 -C01
Double C01 C30 C03 C02 C33 C34 S03 O20 S03 O22

!! Carbon Nanotube (10,0)
!!
RESI 100 0.0
GROUP
ATOM C1 CNT 0.0
ATOM C2 CNT 0.0
ATOM C3 CNT 0.0
ATOM C4 CNT 0.0
ATOM C5 CNT 0.0
ATOM C6 CNT 0.0
ATOM C7 CNT 0.0
ATOM C8 CNT 0.0
ATOM C9 CNT 0.0
ATOM C10 CNT 0.0
ATOM C11 CNT 0.0
ATOM C12 CNT 0.0
ATOM C13 CNT 0.0
ATOM C14 CNT 0.0
ATOM C15 CNT 0.0
ATOM C16 CNT 0.0
ATOM C17 CNT 0.0
ATOM C18 CNT 0.0
ATOM C19 CNT 0.0
ATOM C20 CNT 0.0
ATOM C21 CNT 0.0
ATOM C22 CNT 0.0
ATOM C23 CNT 0.0
ATOM C24 CNT 0.0
ATOM C25 CNT 0.0
ATOM C26 CNT 0.0
ATOM C27 CNT 0.0
ATOM C28 CNT 0.0
ATOM C29 CNT 0.0
ATOM C30 CNT 0.0
ATOM C31 CNT 0.0
ATOM C32 CNT 0.0
ATOM C33 CNT 0.0
ATOM C34 CNT 0.0
ATOM C35 CNT 0.0
ATOM C36 CNT 0.0
ATOM C37 CNT 0.0
ATOM C38 CNT 0.0
ATOM C39 CNT 0.0
ATOM C40 CNT 0.0

BOND C1 C2 C2 C3 C3 C4 C4 C5 C5 C6 C6 C7 C7 C8 C8 C9 C9 C10
BOND C10 C11 C11 C12 C12 C13 C13 C14 C14 C15 C15 C16 C16 C17 C17 C18 C18 C19 C19 C20 C20 C1
BOND C21 C22 C22 C23 C23 C24 C24 C25 C25 C26 C26 C27 C27 C28 C28 C29 C29 C30
BOND C30 C31 C31 C32 C32 C33 C33 C34 C34 C35 C35 C36 C36 C37 C37 C38 C38 C39 C39 C40 C40 C21
BOND C2 C23 C4 C25 C6 C27 C8 C29 C10 C31 C12 C33 C14 C35 C16 C37 C18 C39 C20 C21
BOND +C24 C3 +C26 C5 +C28 C7 +C30 C9 +C32 C11 +C34 C13 +C36 C15 +C38 C17 +C40 C19 +C22 C1

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