Supporting information

for

Fabrication of single-chain nanoparticles through the dimerization of pendant

anthracene groups via photochemical upconversion

Tamuka Chidanguro,^a Danielle R. Blank,^{a b} Alexandra Garrett,^a Cassandra M. Reese,^a Jacob M. Schekman,^a Xinjun Yu,^{c,§} Derek L. Patton,^a Neil Ayres,^c and Yoan C. Simon^a*

^a School of Polymer Science and Engineering, The University of Southern Mississippi, 118

College Dr. #5050 Hattiesburg 39406 MS USA

^b Department of Chemistry, University of Wisconsin-Stevens Point, Stevens Point, WI 55481,

USA

^c Department of Chemistry, University of Cincinnati, Cincinnati, OH 45221, USA

[§]Current address: Applied Biomimetic, 942 Clopper RD, Gaithersburg, MD, 20878

*Author to whom correspondence should be addressed: Email: yoan.simon@usm.edu

Table of Contents

| Instrumentation and Characterization | S-2 |
|--------------------------------------|-----|
| NMR spectra | S-3 |
| UV-vis absorbance data | |
| Size-exclusion chromatography data | S-8 |

Instrumentation and Characterization

¹H NMR spectra were recorded on Varian 300 MHz and 600 MHz Bruker spectrometers and all chemical peaks were referenced to TMS. Atomic force microscopy (AFM) was performed using a Bruker Dimension Icon instrument. AFM height images were collected in tapping mode (in air) to obtain thin film morphology. The samples were scanned using RTESPA-300 probes (from Bruker) with a nominal spring constant of 40 N/m. The AFM height images were analyzed using the SPIP software.

Size-exclusion chromatography (SEC) was done using a Wyatt GPC consisting of a Waters Alliance 2695 separations module and an interferometric refractometer (refractive index detector, Optilab TrEX, Wyatt Technology Inc.) (operating at 35 °C and 685 nm), an on-line multi-angle laser light scattering (MALLS) detector fitted with a gallium arsenide laser (power: 20 mW) operating at 658 nm (miniDAWN TREOS, Wyatt Technology Inc.), and two PLgel (Polymer Laboratories Inc.) mixed 3E columns (3 µm bead size, pore size range 50-103Å,). Freshly distilled THF was used as the mobile phase at a flow rate of 1.0 mL/min and sample volume of 100 uL was injected for each run. All the detector signals were recorded and analyzed using ASTRA 6 software (Wyatt Technology Inc). dn/dc values were calculated from the refractive index detector response assuming 100% mass recovery for use with MALLS to determine the absolute molecular weights. All comparisons of the retention times were done with polymers whose chromatograms were taken during the same run to ensure that the only changes observed would be due to the irradiation. All UV-vis absorbance measurements were taken on a Lambda 35 UV-vis Spectrophotometer (Perkin Elmer).

NMR spectra



Fig. S1. ¹H NMR spectra of the anthracene sample before (top) and after (bottom) irradiation, showing that the dimerization powered by TTA-UC was successful.



Scheme S1. Synthesis of polymer samples via RAFT polymerization.



Fig. S2. ¹HNMR spectra of polymer sample P1.

UV-vis absorbance data



Fig. S3. ¹HNMR spectra of polymer sample P2.



Fig. S4. Uv-vis absorbance data for the reversibility of dimerization in **P1** by using 254 nm light. The initial solution (black) was first irradiated at 366 nm for 20 minutes to dimerize the anthracene pendant groups. The dimerized sample (red) was then irradiated with 254 nm light and the absorbance was measured at the noted intervals to test the reversibility of SCNP formation.



Fig. S5. UV-vis absorbance data for a) P1 and b) P2 at indicated time intervals with 2.7×10^{-5} M and 3.4×10^{-5} M PtOEP concentration in THF.



Fig. S6 UV-vis absorbance data for a solution of PtOEP in THF after irradiation with 532 nm in the absence of polymer sample.



Fig. S7. UV-vis absorbance data for (a) P1 and (b) P2 after irradiation with 532 nm in the absence of PtOEP.

Size-exclusion chromatography data



Fig. S8 Changes in retention times upon TTA-UC irradiation as observed with the dRI detector.