Supporting Information

Materials

The peptides were designed and synthesized as reported in peptide synthesis part. Fmoc-protected amino acids, MBHA Rink Amide resin, and HBTU were purchased from NovaBiochem and ABCR. All other chemicals were purchased from Fisher, Merck, Alfa Aesar or Aldrich and used as received.

Peptide synthesis and characterization

The peptides were synthesized by solid phase peptide synthesis method. Peptide sequences were constructed on Rink Amide MBHA resin (0.59 mmole/g). 0.25 mmole peptide synthesis was carried out; 2 equivalents (with respect to resin) of amino acids, lauric acid or pyrenebutyric acid were used in each coupling. Amino acids, lauric acid or pyrenebutyric acid (2 eq.) were activated with DIPEA (3 eq.) and HBTU (1.98 eq) prior to coupling. All couplings were carried in dimethylformamide (DMF). At the end of the coupling cycles resin was cleaved from the resin by concentrated trifluoroacetic acid (TFA). For this purpose, a 10 mL cleavage cocktail (TFA:TIS:H_2O = 9.5:0.25:0.25) was prepared; distilled water (H_2O) and triisopropylsilane (TIS) were used as scavengers. Cleaved peptide was collected by dichloromethane (DCM), which was later removed alongside with TFA by rotary evaporation. Residual material was triturated by cold diethyl ether. White (lauryl tale) or yellowish (pyrenebutyryl tale) peptide precipitate was completely separated from ether by centrifugation; the centrifugate was dissolved in water, deep freezed at -80 °C and finally lyophilized. Lyophilized peptide was characterized by high resolution time-of-flight mass spectrometer coupled to liquid chromatography system (Agilent 1200/6210). Purity of the peptide was c.a. 98%.

Pyrene encapsulation

The **2** and **2′** are amphiphilic molecules, which help to solubilize pyrene molecules in water. Encapsulation is driven mainly by the solvophobic effect. 0.1 mL of 3.33 mM solution of pyrene in THF was mixed with 1 mL of 3.33 mM solution of peptide in water. In order to achieve effective encapsulation, pyrene to PA ratio was kept at 1:10. Mixture was homogenized by vigorous vortexing, then sonicated for 40 min at room temperature in sealed vial and for 40 min at 50°C in open vial.

Transmission electron microscopy (TEM) imaging

TEM imaging was performed with a FEI Tecnai G2 F30. Diluted samples were used to collect nanofibers on a Lacey carbon coated 300 mesh copper grid. A 2 wt% aqueous uranyl acetate solution was used for staining organic nanostructures. 20 mL of diluted sample solution was dropped on a parafilm sheet; grid was placed on the top of the droplet and kept there for 1 min.

Then, 20 mL of 2 wt% uranyl acetate solution was dropped on a parafilm sheet, and the grid was transferred to the new droplet and kept there for 2 min. Excess liquid was removed by barely touching the grid with a cleaning tissue. Grids with stained peptide nanofibers were dried prior to imaging.

Fluorescence measurements

Fluorescence measurements were performed on a Varian Cary Eclipse fluorescence spectrophotometer. 3.33 mM solutions of L and D peptides were prepared in water and trifluoroethanol (TFE). 3.33 mM solution of pyrene was prepared in tetrahydrofurane (THF). All solutions were diluted 10 times prior to measurement. Excitation wavelength was 350 nm.

Circular dichroism (CD) and UV-Vis spectroscopy

Jasco J-815 CD spectrophotometer was used for collection of CD and UV-Vis absorption spectra. Solution preparation was identical with fluorescence measurements. CD spectra (Figure 4b) of the samples with encapsulated pyrene were recorded without dilution in pyrene absorption region (230-400 nm); β-sheet region (195-230 nm) of the same samples still required 10 fold dilution.

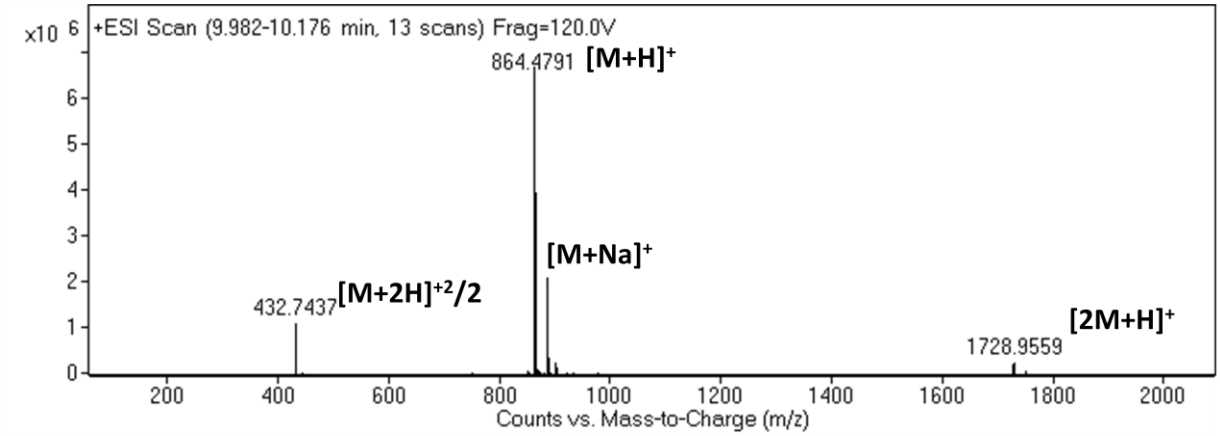

Figure S1. Mass spectrum of pyrenebutyryl-ε-Ahx-VVAGH-Am.

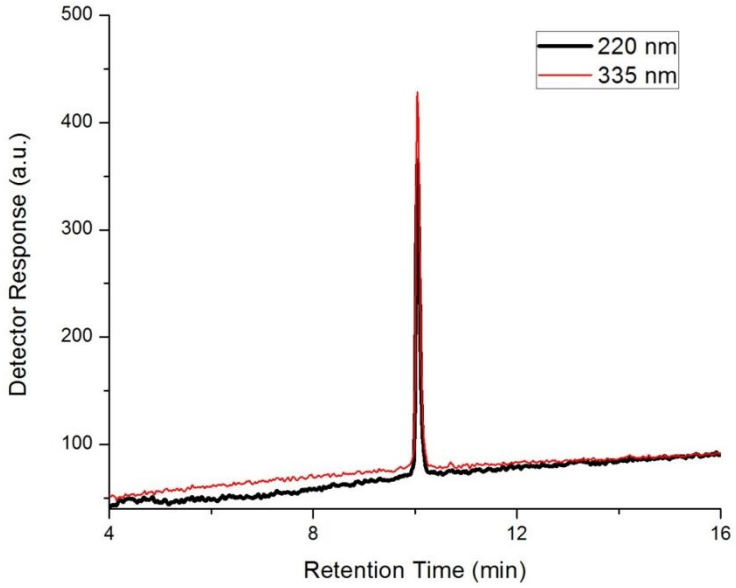

Figure S2. Liquid chromatogram of pyrenebutyryl-ε-Ahx-VVAGH-Am.

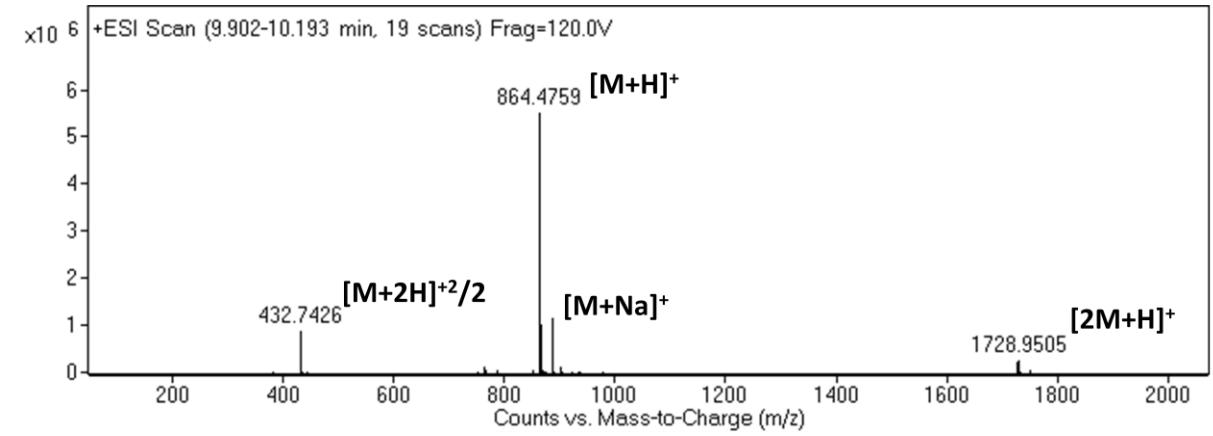

Figure S3. Mass spectrum of pyrenebutyryl-ε-Ahx-vvaGh-Am.

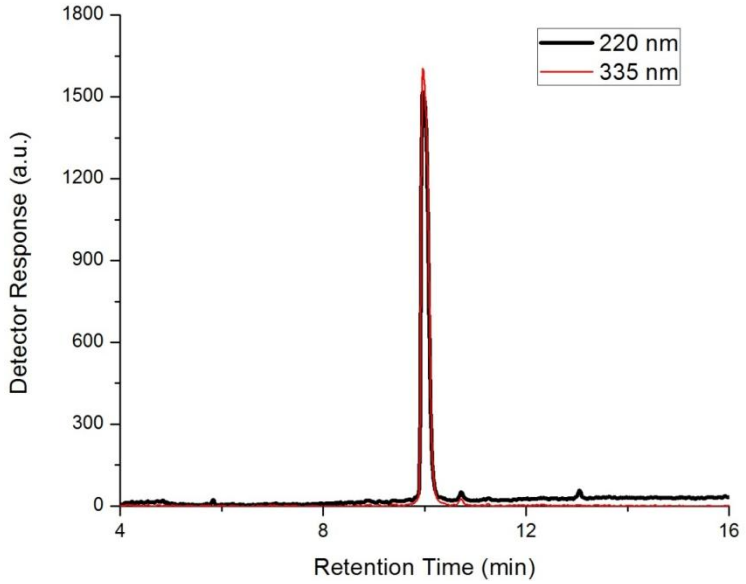

Figure S4. Liquid chromatogram of pyrenebutyryl-ε-Ahx-vvaGh-Am.

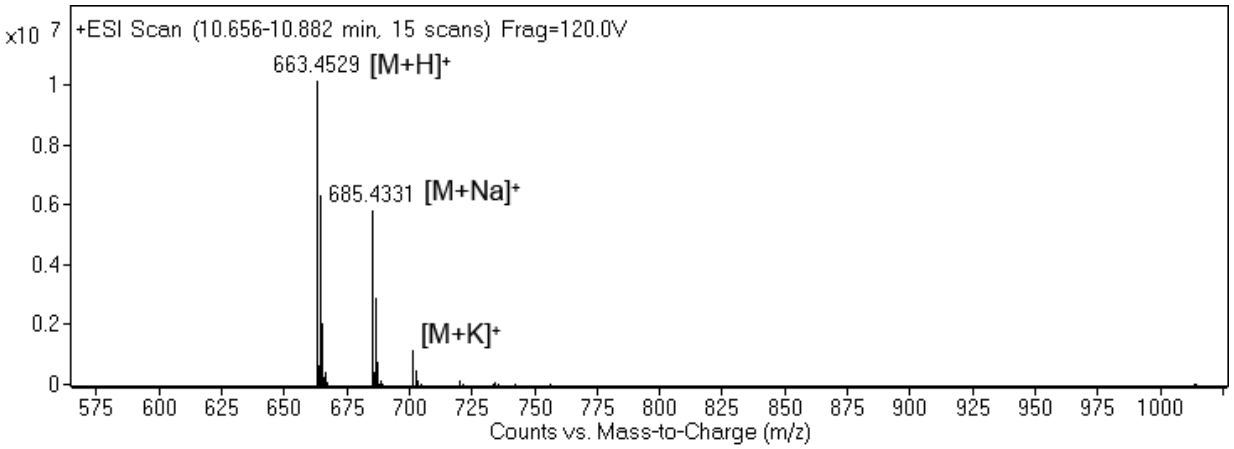

Figure S5. Mass spectrum of lauryl-VVAGH-Am.

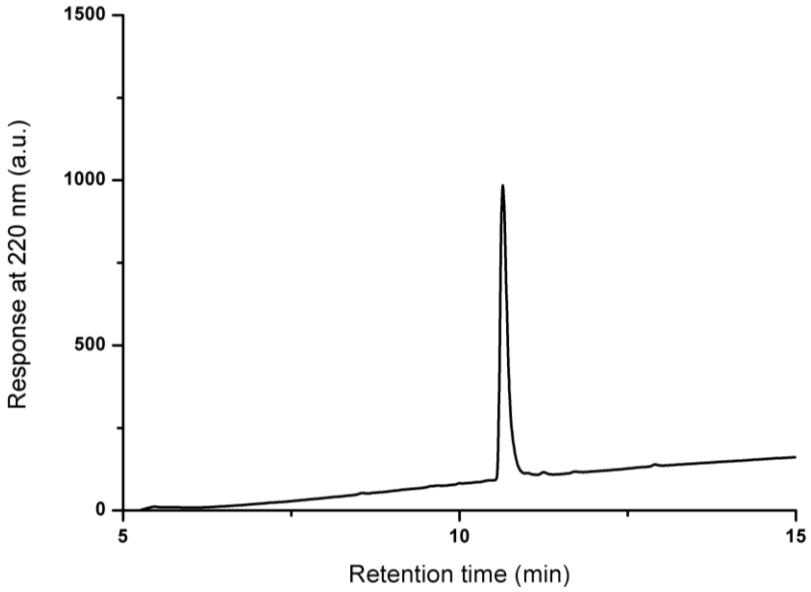

Figure S6. Liquid chromatogram of lauryl-VVAGH-Am.

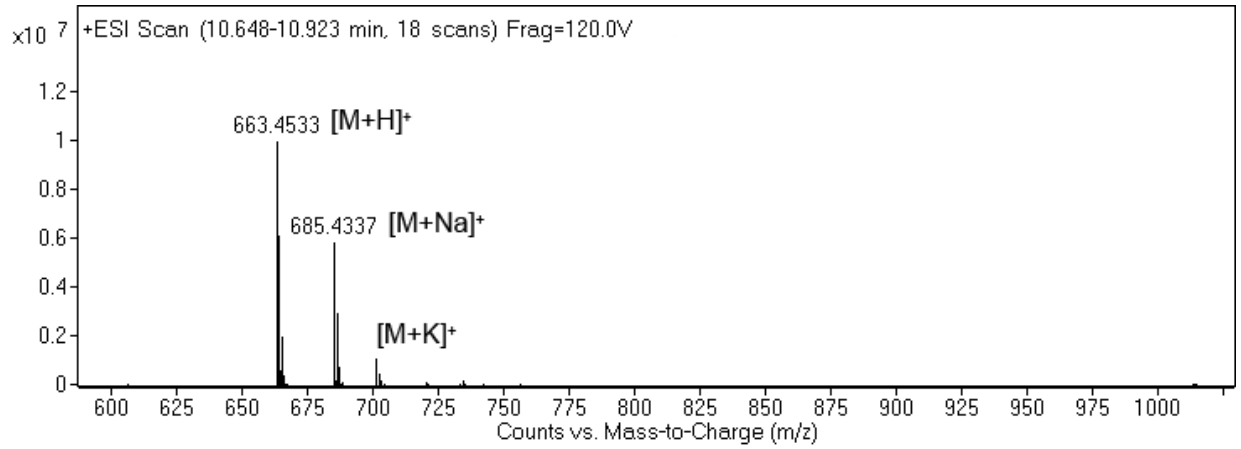

Figure S7. Mass spectrum of lauryl-vvaGh-Am.

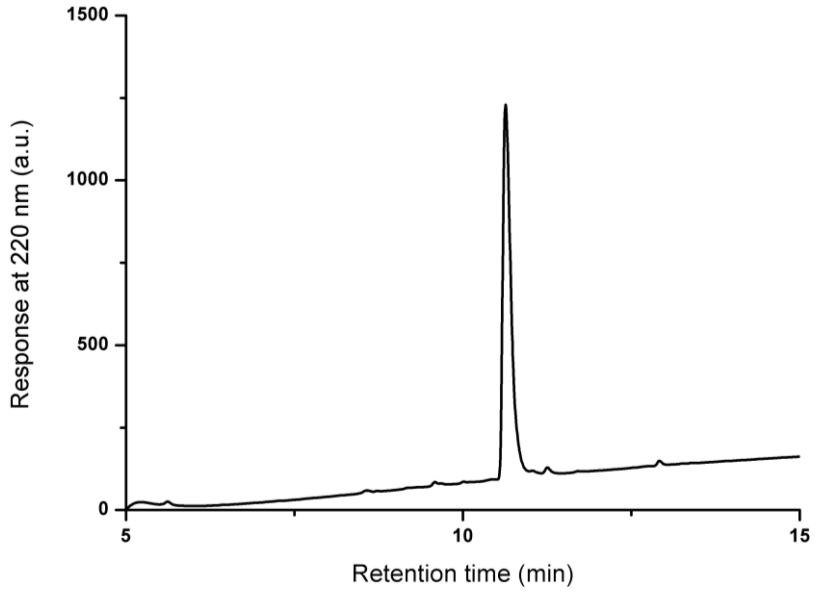

Figure S8. Liquid chromatogram of lauryl-vvaGh-Am.

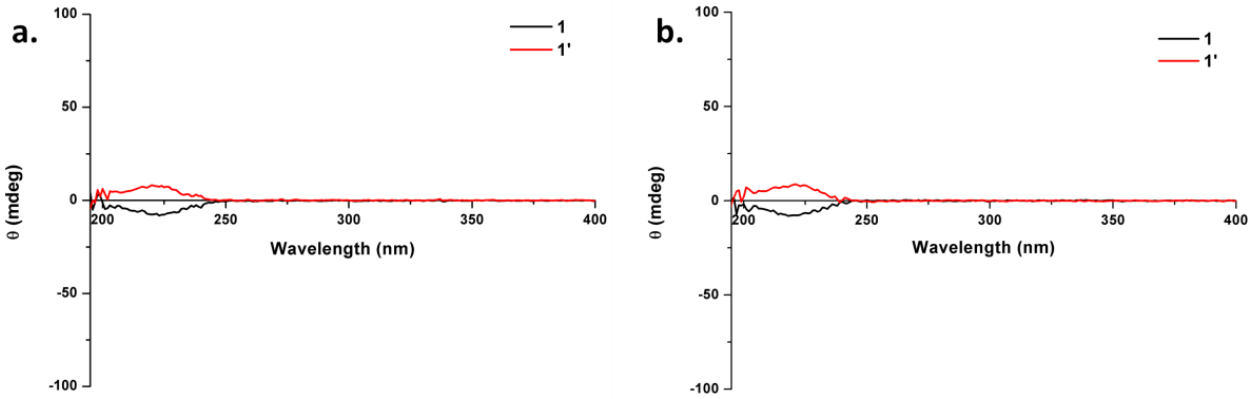

Figure S9. CD spectra of **a) 1** and **1′** directly in TFE (0.333 mM) and **b)** pre-assembled **1** and **1′** in TFE (0.333 mM).

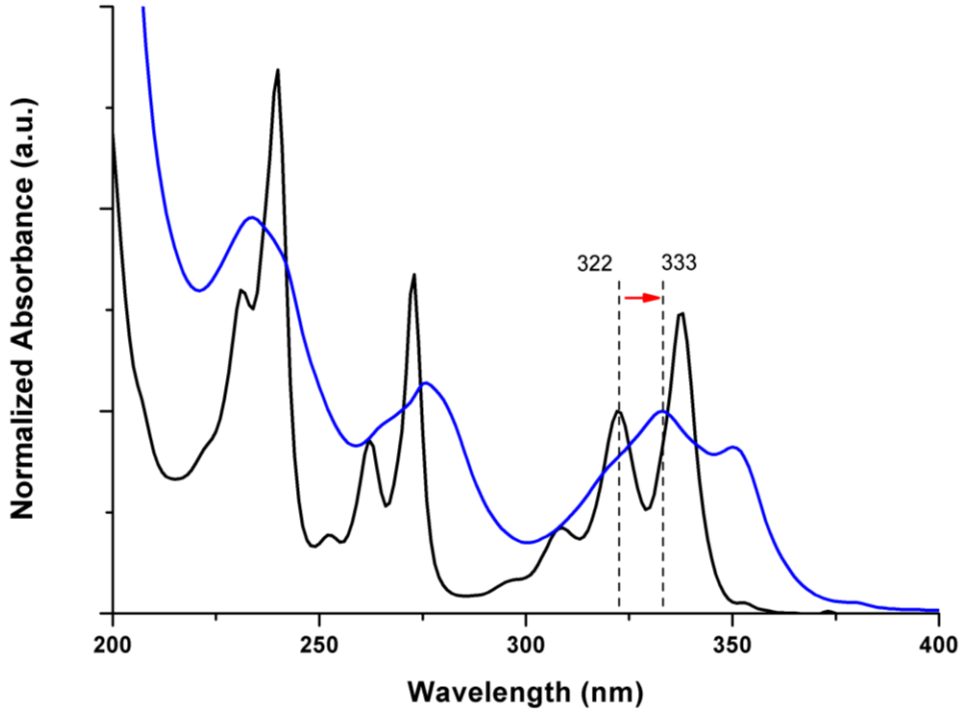

Figure S10. Absorption spectra of nanofibers of **1** in H_2O (blue) and **1** dissolved in TFE (black). The same holds for **1′** as well (see Figure S11).

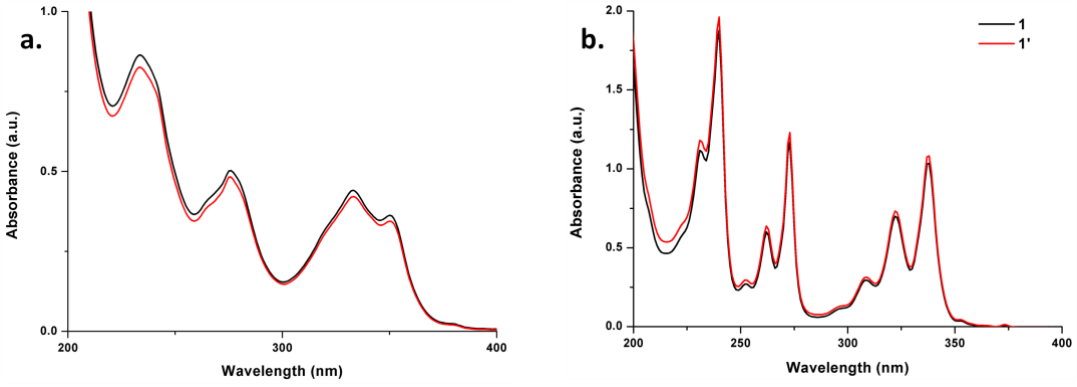

Figure S11. Absorption spectra of **a)** nanofibers of **1** and **1′** in H_2O, and **b)** of **1** and **1′** dissolved in TFE (pyrene moiety absorption region).

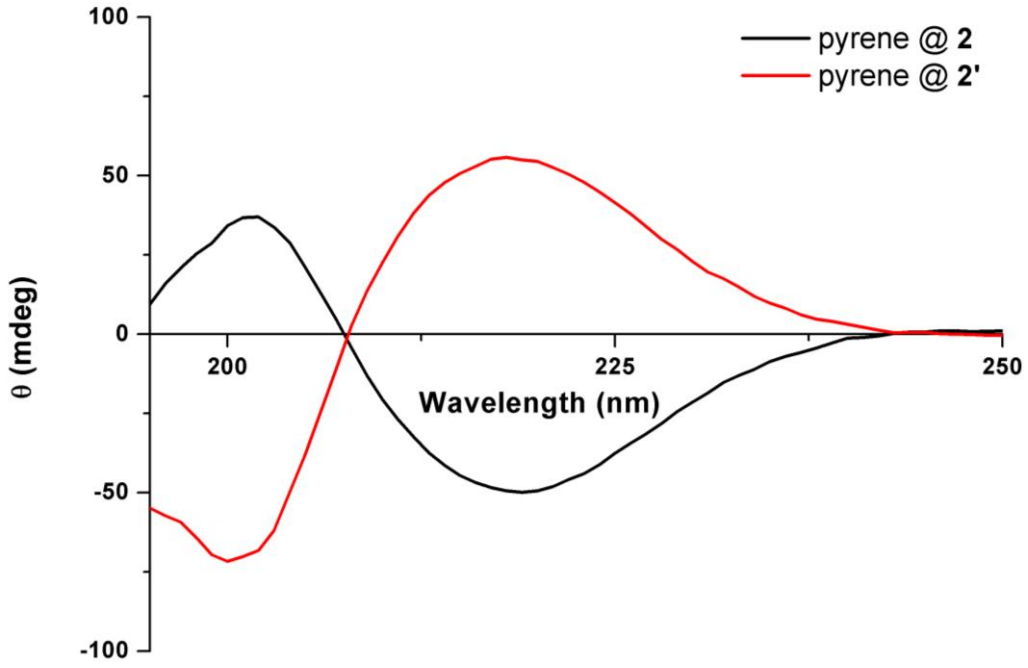

Figure S12. CD spectra of **2** and **2′** nanofibers with encapsulated pyrene (β-sheet region).

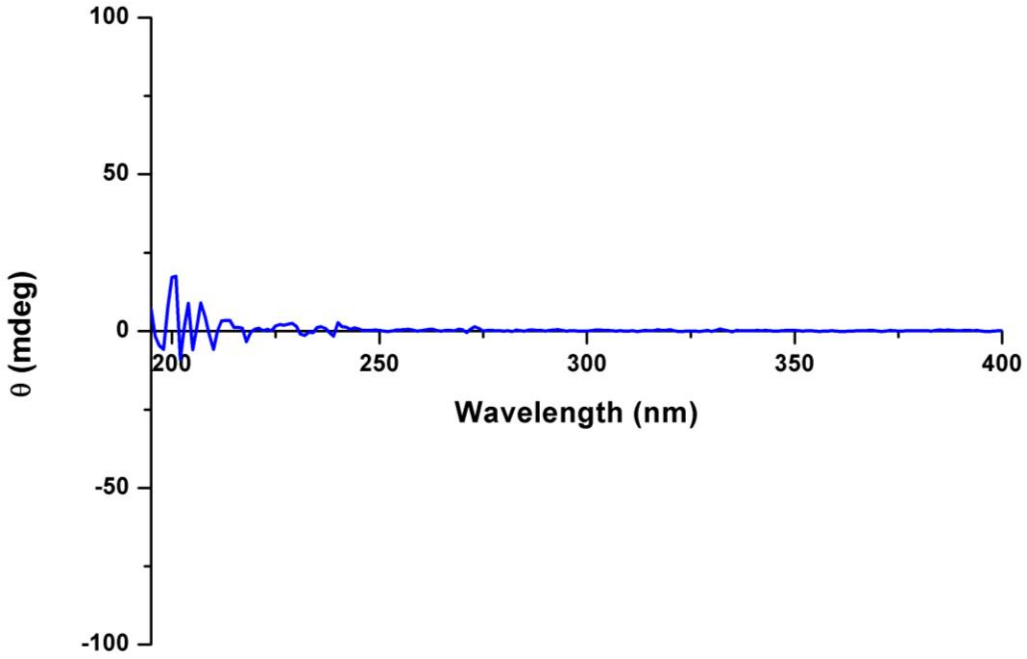

Figure S13. CD spectrum of pyrene in THF (0.333 mM).

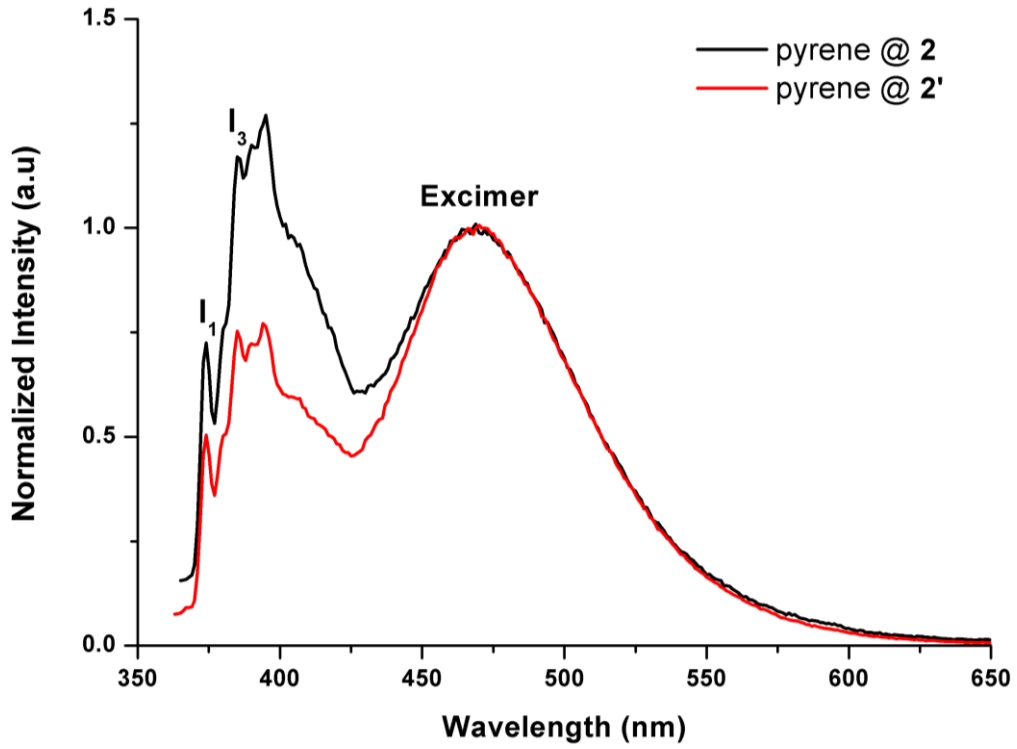

Figure S14. Emmision spectra of pyrene in nanofibers of **2** and **2′** in H_2O (0.333 mM pyrene).

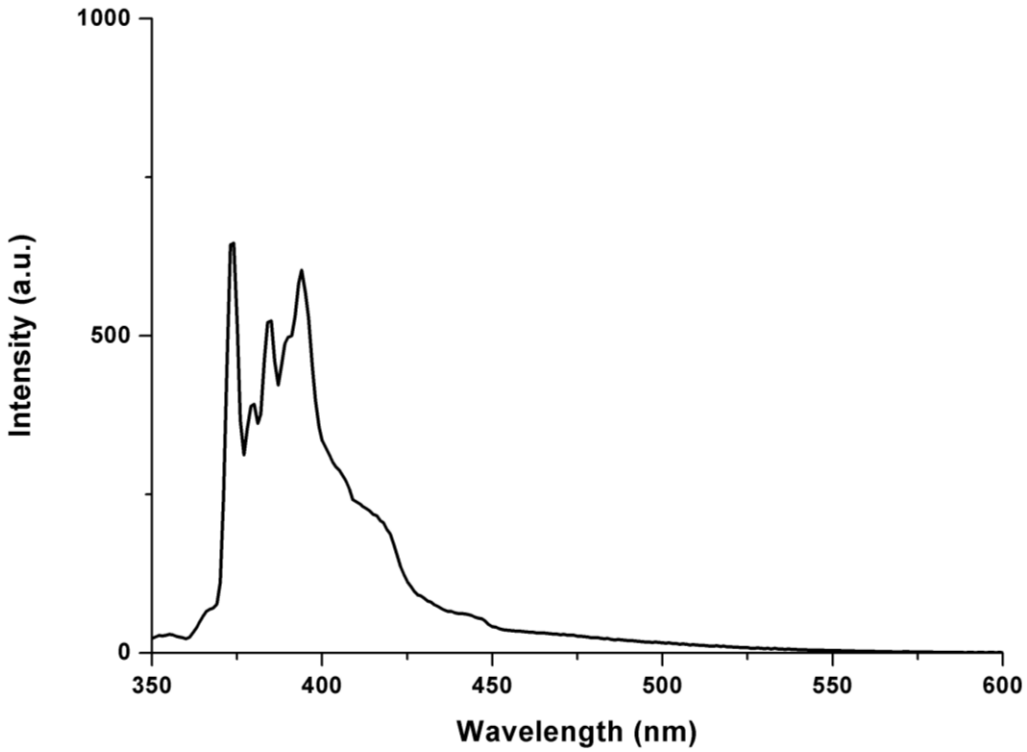

Figure S15. Emission spectrum of pyrene in THF (0.333 mM).

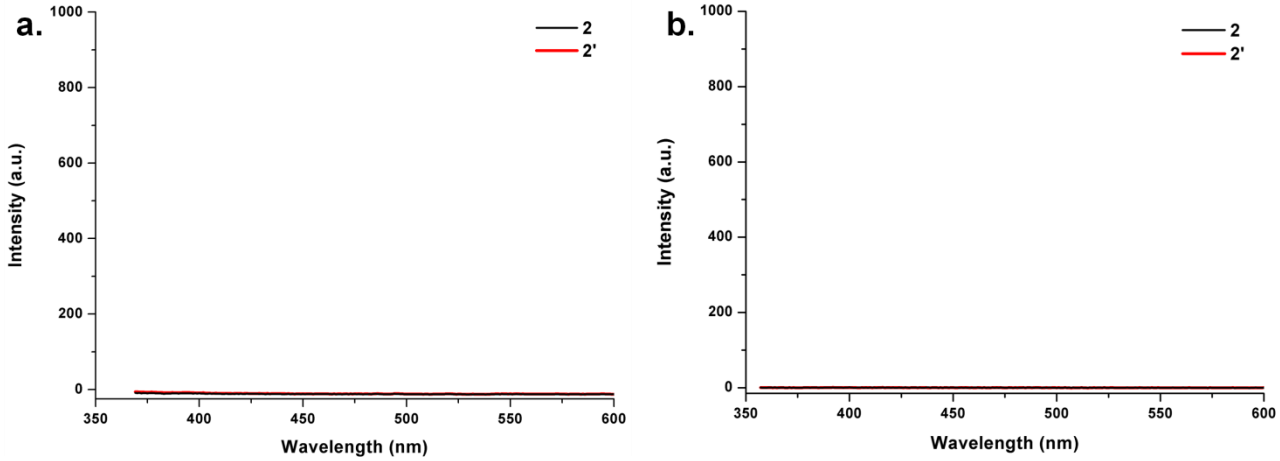

Figure S16. Emisson spectra of **2** and **2′** in **a)** H_2O and **b)** TFE.

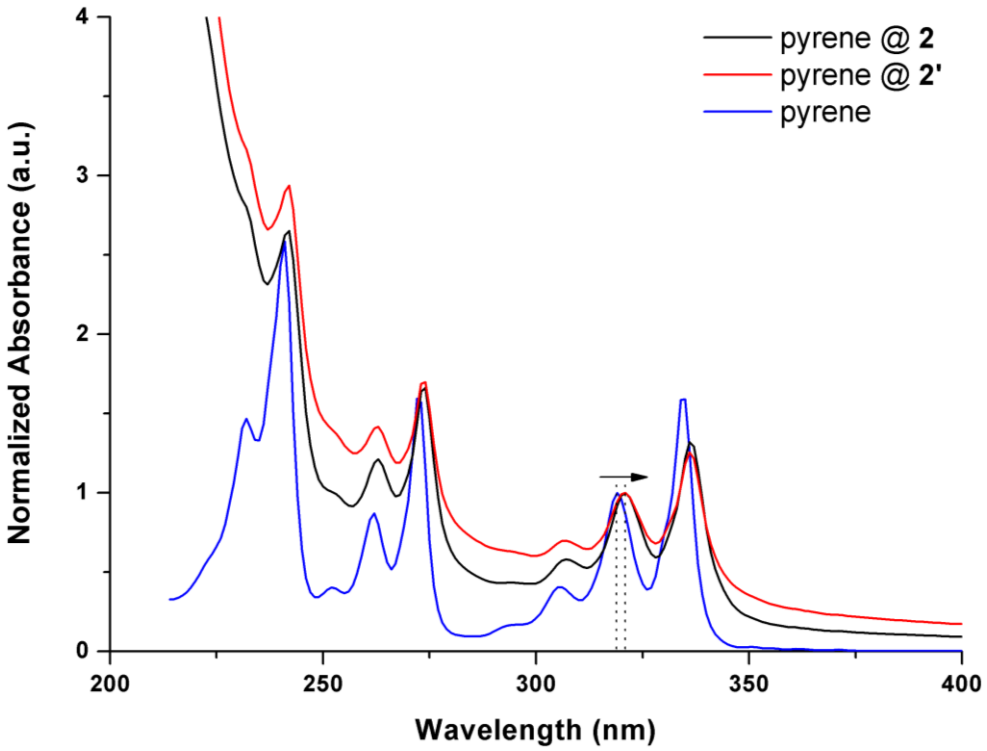

Figure S17. Absorption spectra of pyrene in THF (blue), pyrene encapsulated in **2** (black) and **2′** (red) in H_2O.

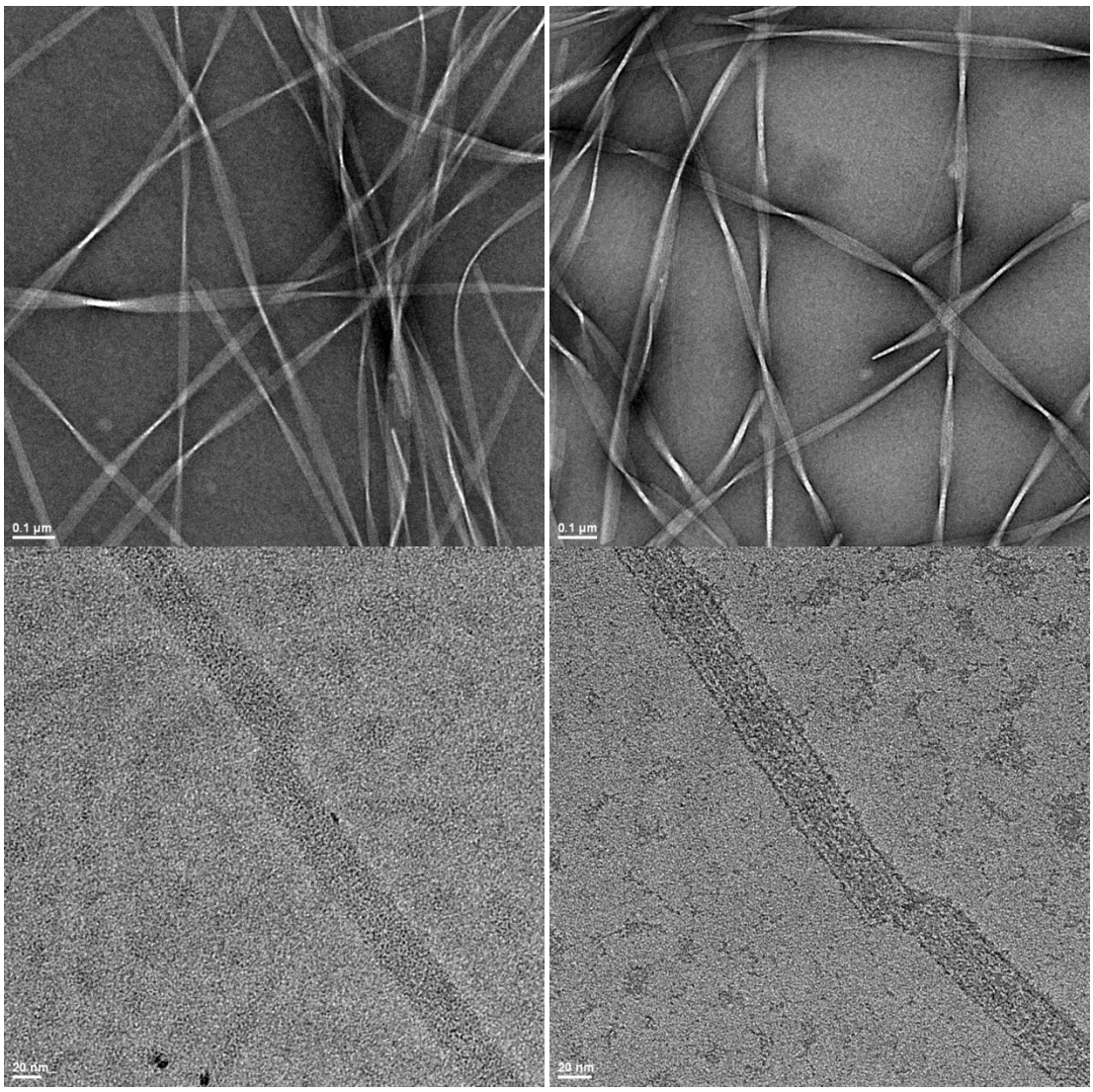

Figure S18. TEM images of nanoribbons of **2** and **2′**.

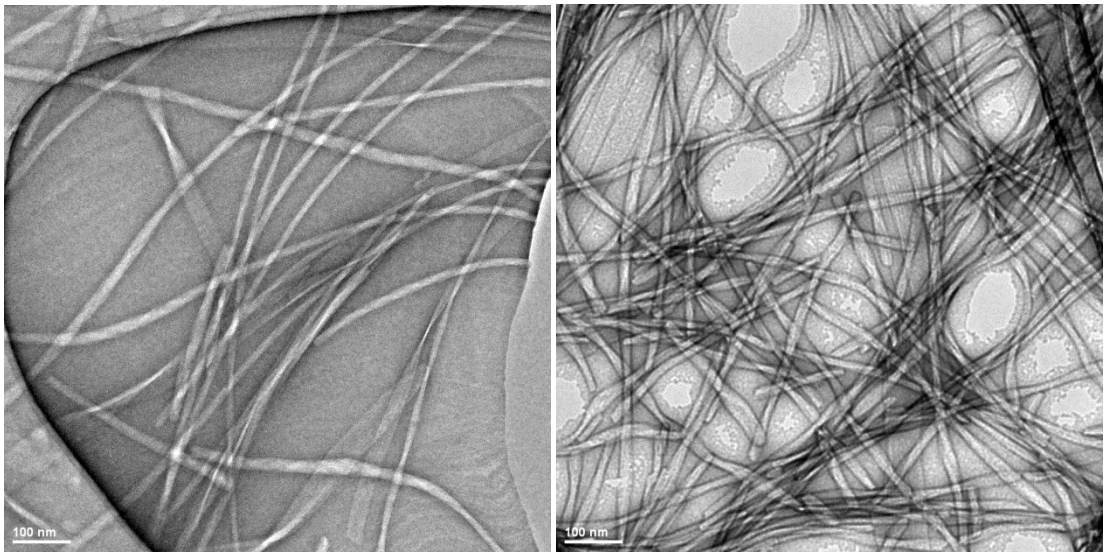

Figure S19. TEM images of nanofibers of **2** (left) and **2′** (right) with encapsulated pyrene.