

Aggregation of the amphipathic peptides (AAKA)_n into antiparallel β -sheets

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Supporting Information

Materials H-(AAKA)₂-OH, Ac-(AAKA)₃-NH₂ and Ac(AAKA)₃-NH₂ were custom synthesized by Celtek Peptides (Nashville, TN). For the IR, VCD, and Raman measurements of Ac-(AAKA)₄-NH₂, the peptide was dissolved in acidic D₂O (pD = 1.4), and a concentration of ~15 mg/mL (~0.01 M), where the D₂O was made acidic by the addition of DCl (Sigma-Aldrich). The peptide formed a hydrogel shortly after dissolution in D₂O, and the measurements were acquired on the hydrogel. The measurements for the gelled state of the 12-mer, Ac-(AAKA)₃-NH₂ (shown below), were carried out similarly, at a concentration of ~27 mg/mL in D₂O (pD = 1.4). The x-polarized Raman solution spectrum of H-(AAKA)₂-OH was obtained at a concentration of ~37 mg/mL (0.05 M). For the ECD measurements, Ac-(AAKA)₃-NH₂ and H-(AAKA)₄-OH were dissolved in acidic D₂O at concentrations of 2.4 mg/mL and 1 mg/mL, respectively, and the samples were measured at room temperature.

Instrumentation. The IR and VCD spectra were recorded with a Chiral IRTM Fourier Transform VCD spectrometer from Bio Tools. The sample was placed into a cell with a pathlength of 42.5 μ m. The spectral resolution was 4 cm⁻¹. The absorptivity values of these spectra were converted to molar extinction (M⁻¹ cm⁻¹ residue⁻¹) by using Beer-Lambert's law. The Raman spectra were obtained with the 442 nm (40 mW) excitation from a HeCd laser (Model IK 4601R-E, Kommon Electrics, USA) and recorded with a RM 100 Remishaw confocal microscope. The UV ECD spectra in the wavelength range of 180 – 250 nm of all dipeptides listed above were measured with a JASCO J-810 spectropolarimeter in a 0.1 mm quartz cell with 0.05 nm resolution, at the Drexel University Medical School. The samples were placed in a nitrogen purged JASCO CD

module. The temperature at the cuvette was controlled by means of a Peltier-type heating system (accuracy $\pm 1^\circ\text{C}$) set to 20°C . The spectra were obtained by averaging ten scans and were collected as ellipticity as a function of wavelength, and converted to units of molar absorptivities via the equation:

$$\Delta\epsilon = \frac{\theta}{32980 \cdot l \cdot c}$$

where θ is the ellipticity in [mdeg], l is the pathlength of the cuvette in [cm] and c is the concentration in [M].

The IR and Raman spectra were treated with the program MULTIFIT which we also used for determining the wavenumber of band peaks. All spectra were finally produced with the SIGMA Plot 6.0 software.

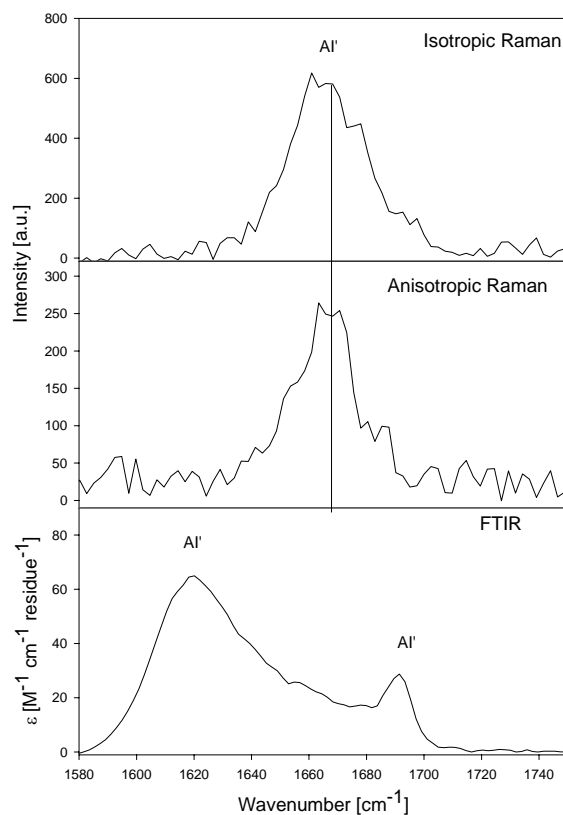


Figure S1. Isotropic and Anisotropic Visible Raman, and FTIR amide I' band spectra of the aggregated state of Ac-(AKA)₃-NH₂.

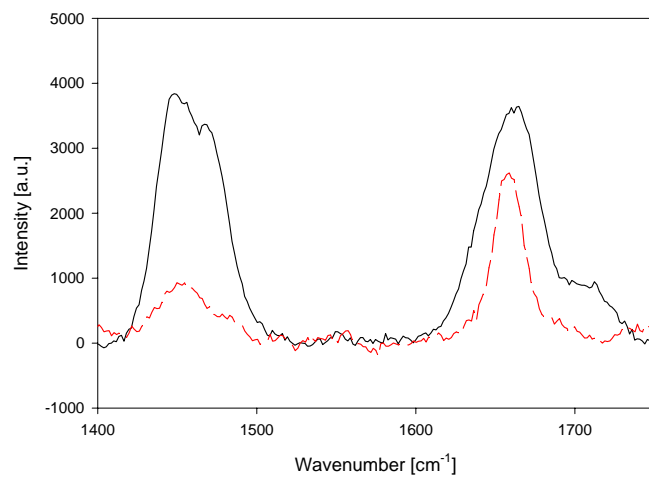


Figure S2: Comparison of x-polarized Raman spectra in the amide I' and II' of unaggregated (AAKA)₂ (solid black line) and the aggregated hydrogel of Ac-(AAKA)₄-NH₂ (dashed red line)