

# **Investigating the Formation of a Repulsive Hydrogel of a Cationic 16mer Peptide at Low Ionic Strength in Water by Vibrational Spectroscopy and Rheology**

*David DiGuseppi<sup>1</sup>, Jodi Kraus<sup>1</sup>, Siobhan E. Toal<sup>2</sup>, Nicolas Alvarez<sup>3</sup>,  
and Reinhard Schweitzer-Stenner<sup>1\*</sup>*

<sup>1</sup>Department of Chemistry and <sup>3</sup>Department of Chemical and Biological Engineering, Drexel University and <sup>2</sup>Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104, USA

## *Supporting Information*

\*Corresponding author: Reinhard Schweitzer-Stenner, Phone: 215-895-2268, Email: [rschweitzer-stenner@drexel.edu](mailto:rschweitzer-stenner@drexel.edu)



Wavenumber [ $\text{cm}^{-1}$ ]	Half-width [ $\text{cm}^{-1}$ ]
1431.80	14.69
1445.52	15.43
1455.60	16.43
1522.79	35.23
1557.04	21.16
1620.18	28.82
1648.60	24.62
1674.70	25.43
1695.26	15.30

**Table S1a:** Wavenumbers and halfwidths of spectral bands obtained from the decomposition of the FTIR spectrum of solid AK-16 shown in Figure 1. The values in parenthesis are referring to the Lorentzian contribution to a Voigtian profile, the remaining halfwidth values reflect Gaussian band profiles or Gaussian contributions to Voigtian profiles.

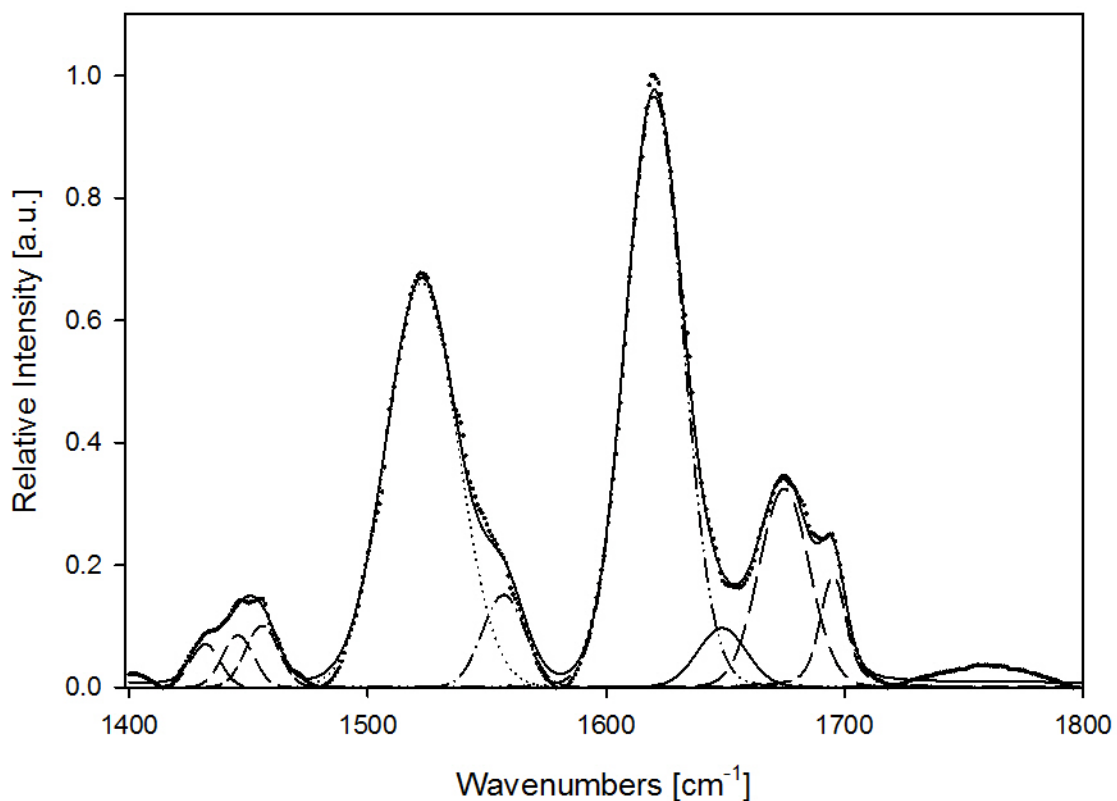
Wavenumber [ $\text{cm}^{-1}$ ]	Half-width [ $\text{cm}^{-1}$ ]
1453.91	43.63
1469.60	23.84
1530.19	22.82
1555.05	20.05
1616.10	16.43
1632.00	40.00
1646.12	40.00
1672.13	19.16
1693.31	19.16

**Table S1b:** Wavenumbers and halfwidths of Gaussian spectral bands obtained from the decomposition of the FTIR spectrum of 15 mg/mL AK-16 in  $\text{D}_2\text{O}$  right after incubation, as shown in Figure 2.

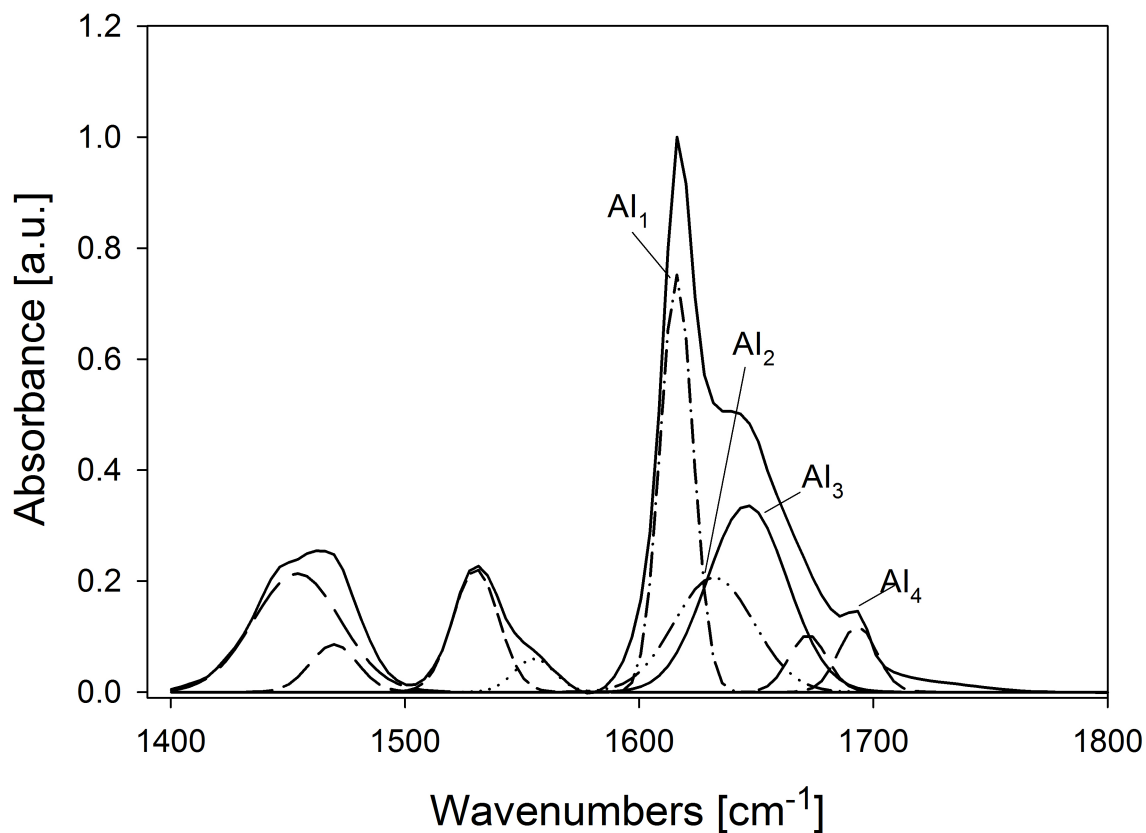
**Table S2:** Spectroscopic parameters obtained from the decomposition of the IR-spectrum of solid AK16 obtained from batch 2.

Wavenumber [ $\text{cm}^{-1}$ ]	Half-width [ $\text{cm}^{-1}$ ]
1429.30	31.98
1445.33	15.95
1456.56	15.26
1522.79	37.74
1547.04	21.56
1557.04	21.88
1597.28	20.97
1621.51	28.80
1656.39	35.80
1688.30	29.74 (5.59) <sup>a</sup>
1696.29	23.28 (22.28) <sup>a</sup>

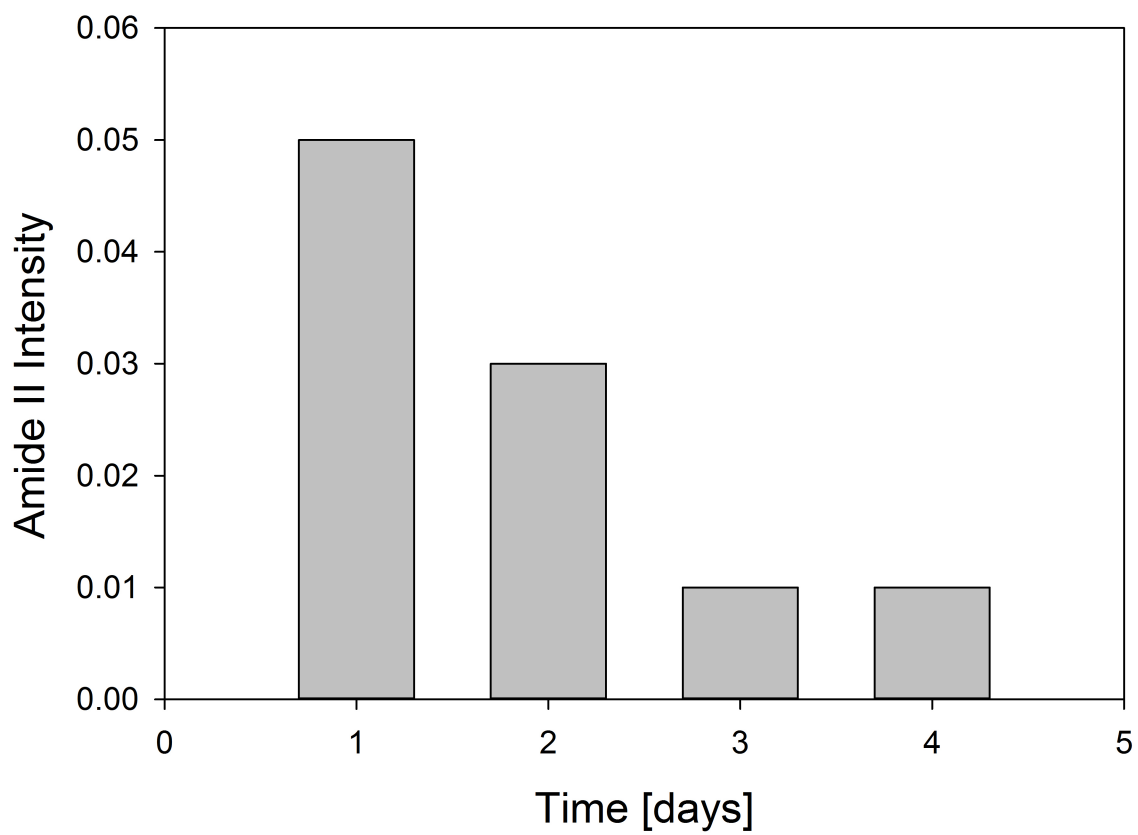
<sup>a</sup>The values in parenthesis are the Lorentzian contributions to the Voigtian sub-bands.



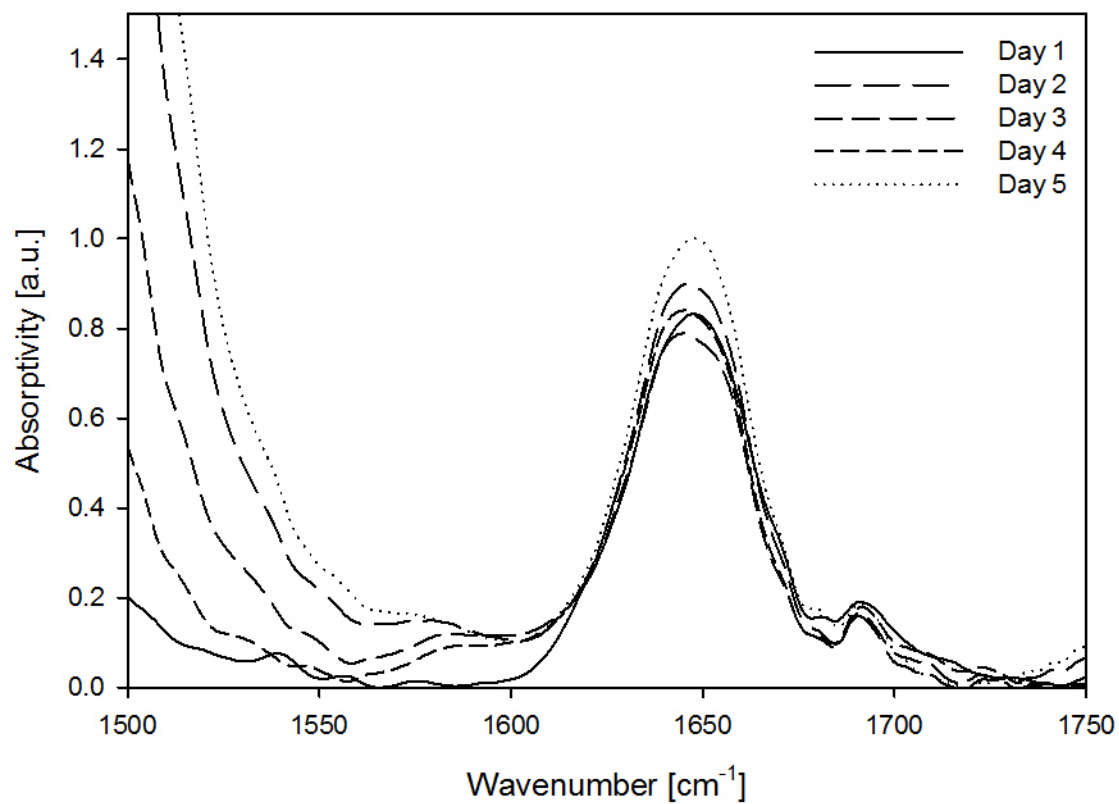
**Figure S1:** FTIR spectra of solid AK-16 (batch 1) in the region between 1400 and 1800  $\text{cm}^{-1}$ . The spectrum was decomposed into Gaussian subbands in the region between 1400 and 1600  $\text{cm}^{-1}$  and Voigtian subbands in the amide I region between 1600 and 1700  $\text{cm}^{-1}$ . The FTIR data is plotted as a scatter plot ( $\bullet$ ), while the overall fit of the decomposition is a solid line. The spectrum was normalized to the 1620  $\text{cm}^{-1}$  band.



**Figure S2:** Decomposition of the amide I' band profile (solid line) of 15 mg/mL AK-16 in D<sub>2</sub>O recorded between 1400 and 1800 cm<sup>-1</sup> into Gaussian bands (solid, dashed, dashed-dot). The spectrum was measured right after the incubation of the peptide and normalized to the 1616cm<sup>-1</sup> band. The FTIR spectrum is plotted as a scatter plot (•) while the overall fit with our spectral model is presented by a solid line. The amide I' sub-band utilized in the main paper are indicated.

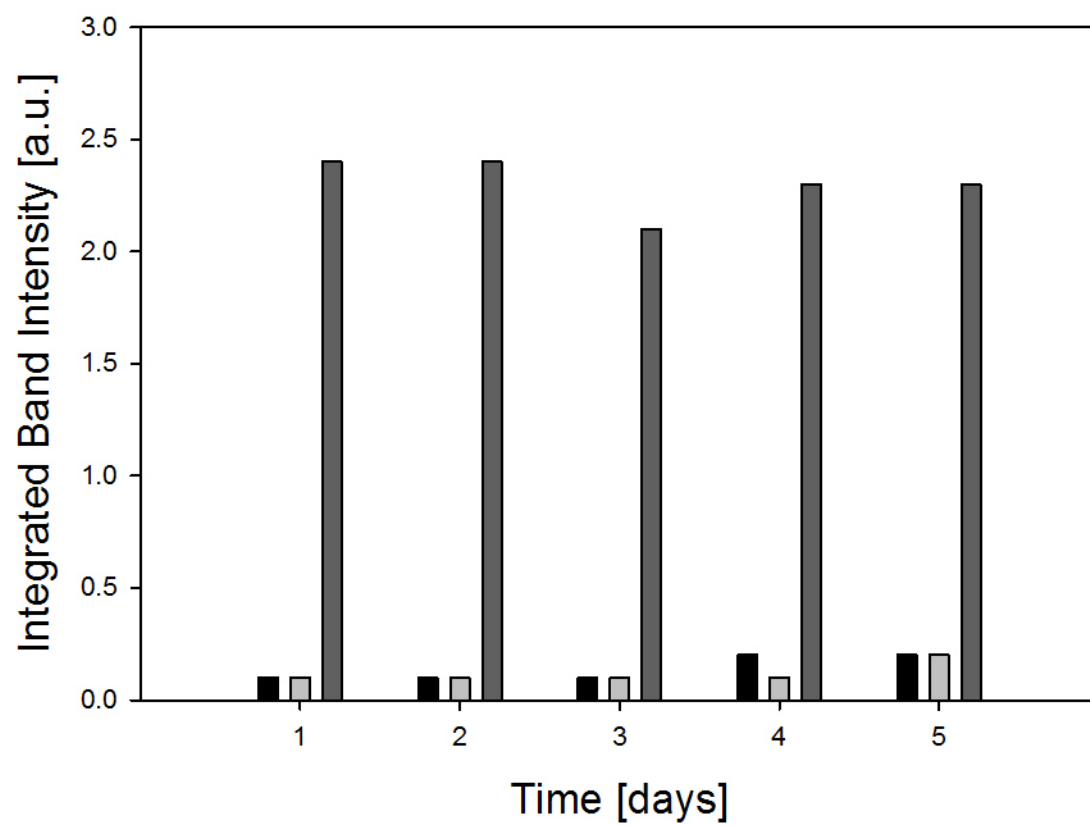


**Figure S3:** Integrated IR intensity of amide II of AK16 at the indicated time after incubation.

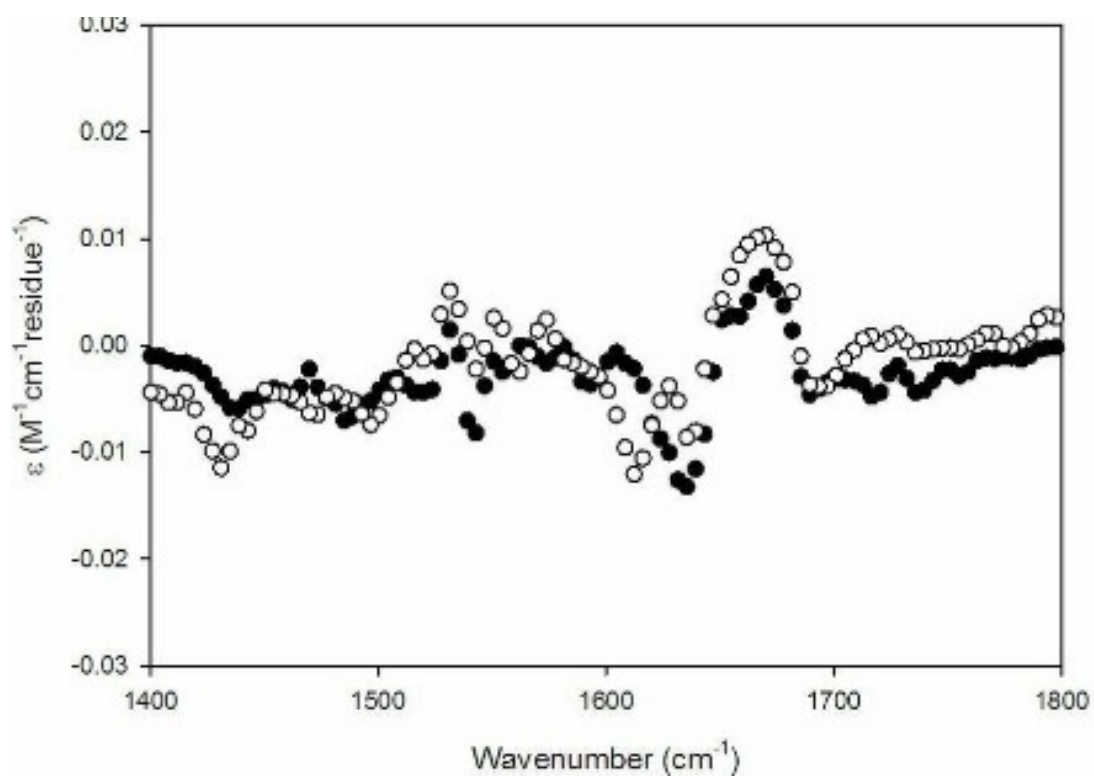


**Figure S4.** IR spectrum of 10mg/mL AK-16 measured between 1500 and 1750 cm<sup>-1</sup> immediately after preparation (Day 1) and measured over time on a daily basis. The spectra are normalized to the 1648cm<sup>-1</sup> peak of Day 5.

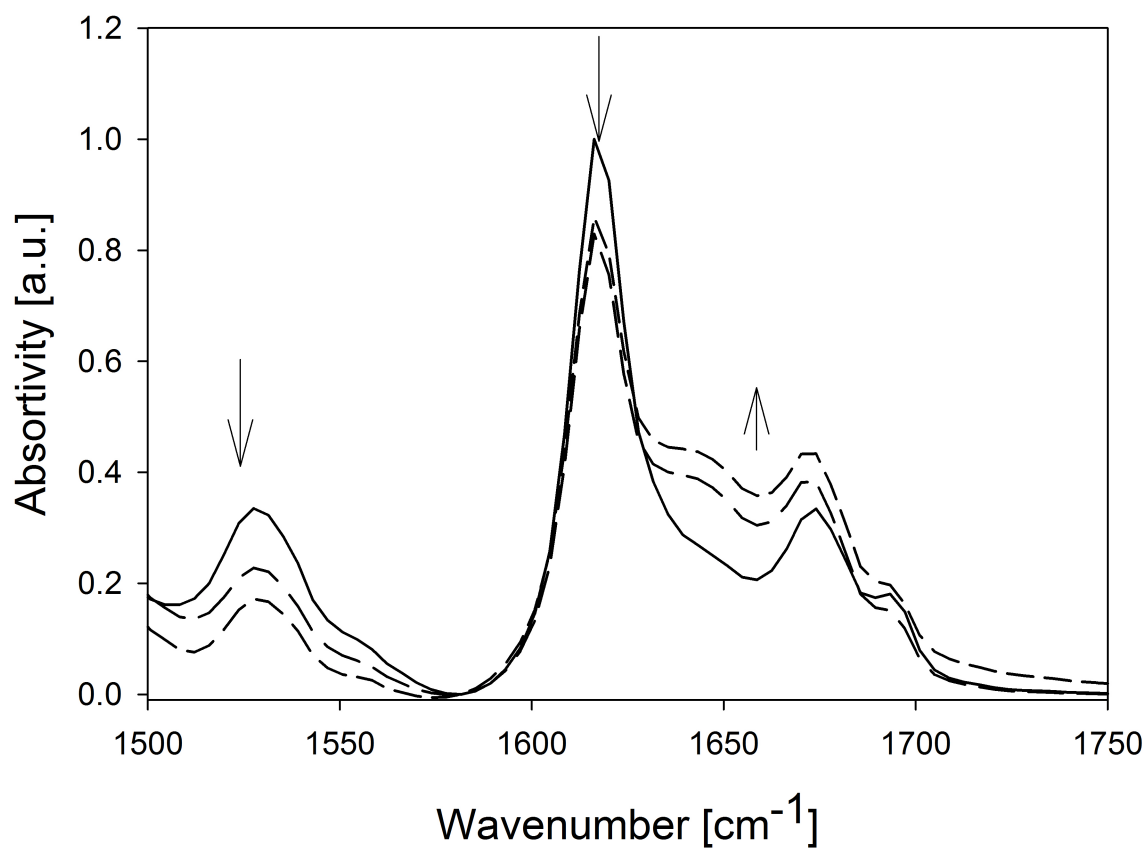




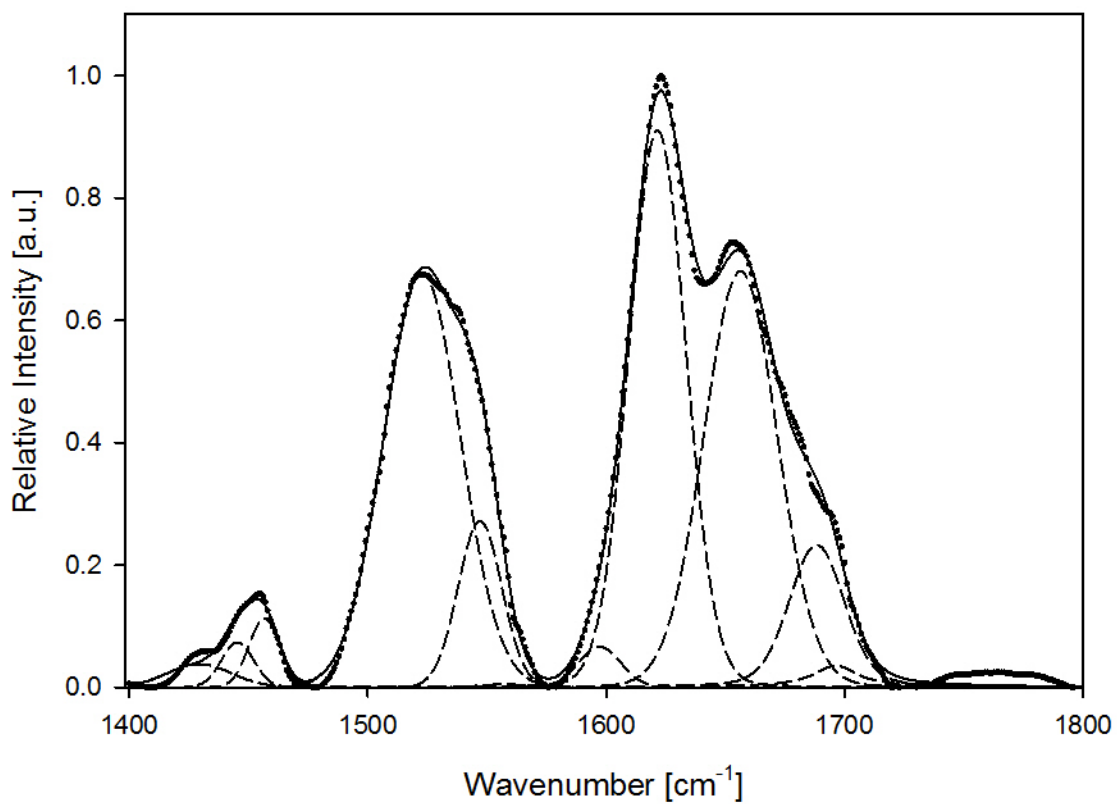
**Figure S5.** Integrated intensities of the AI<sub>1</sub> (left), AI<sub>2</sub> (middle), and AI<sub>3</sub> (right) obtained from the spectral decomposition of the amide I' band profiles in Figure S4.



**Figure S6:** VCD spectra of 20 mg/mL AK-16 recorded between 1580 and 1800 cm<sup>-1</sup> at the beginning (filled symbols) and the end (open symbols) of the investigated incubation time period of 5 days.



**Figure S7:** IR spectrum of the amide II and amide I' region of 17.5 mg/mL AK16 measured 1 day, 30 days and 60 days after incubation. The time course of spectral changes is indicated by arrows.



**Figure S8:** IR spectrum of solid AK16 obtained from the second batch investigated. The dashed lines represent the band profiles obtained from the spectral decomposition described in the paper.