Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Terahertz Spectroscopy Technology for Interpreting the Formation and Hierarchical Structures of Silk Fibroin Oligopeptides

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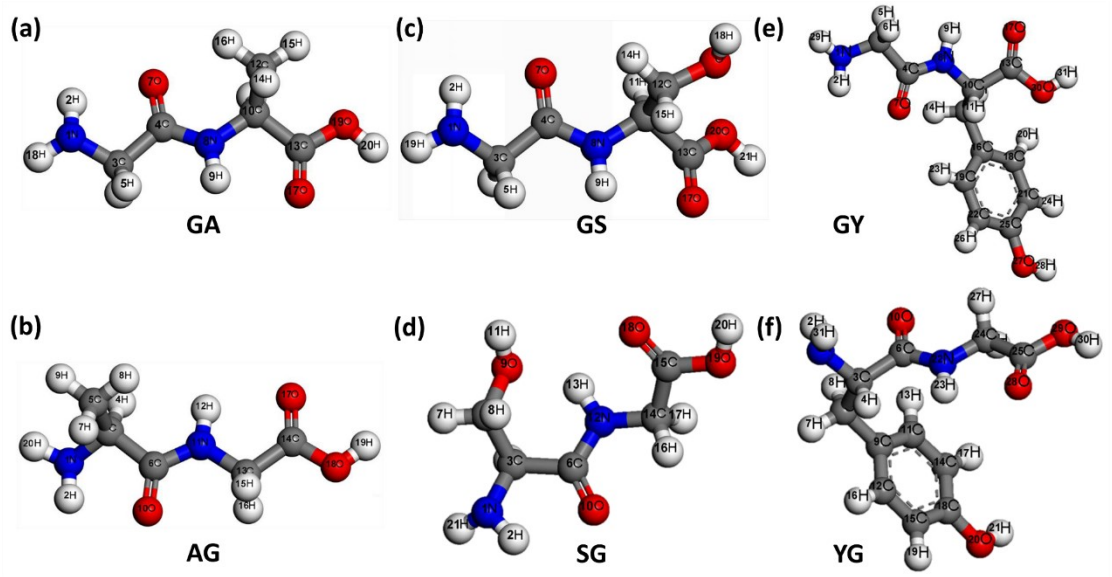

Figure S1 The molecular structures of six dipeptides after optimization: (a) GA, (b) AG, (c) GS, (d) SG, (e) GY, (f) YG.

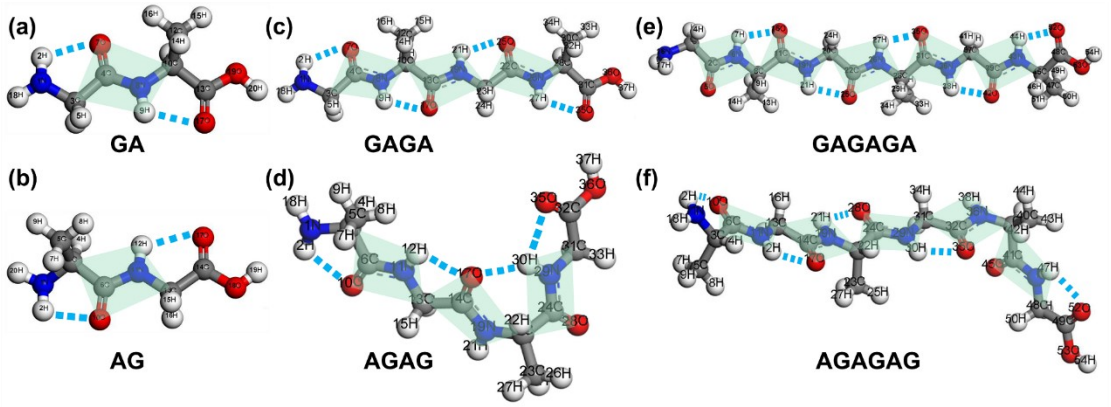

Figure S2 DFT simulated molecular structures of six oligopeptides: (a) GA, (b) AG, (c) GAGA, (d) AGAG, (e) GAGAGA, and (f) AGAGAG.

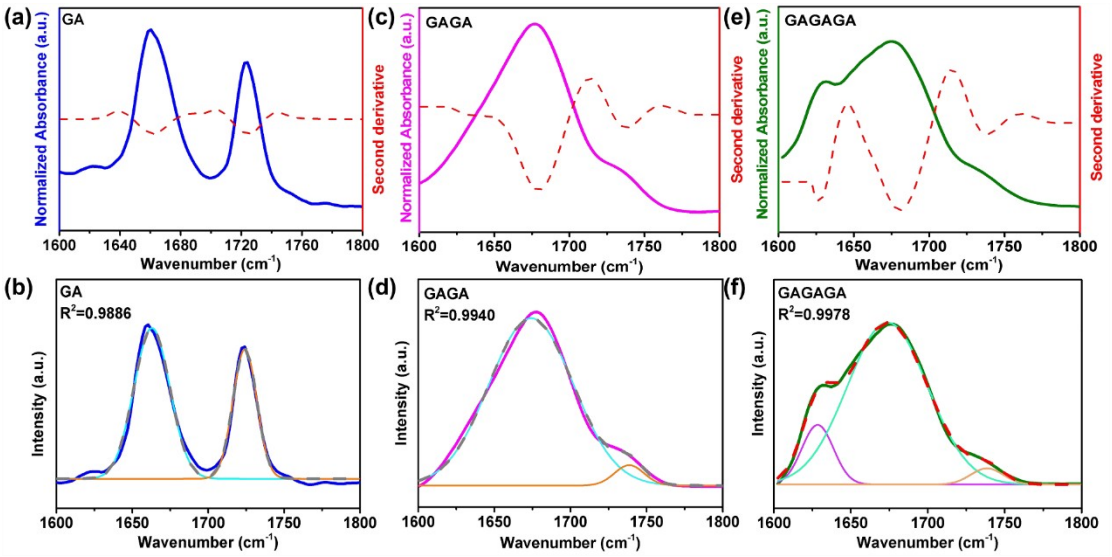

Figure S3 Second derivative absorbance spectra in the Amide I region (1600–1800) cm^{-1} for samples (GA, GAGA, and GAGAGA) indicating various secondary structures like α-helix (the orange solid line), random coils (light blue solid line), and β-sheet (purple solid line). The red dotted line represents the second derivative of the infrared spectrum of the three samples, respectively. The gray dotted line shows the fitting curve.

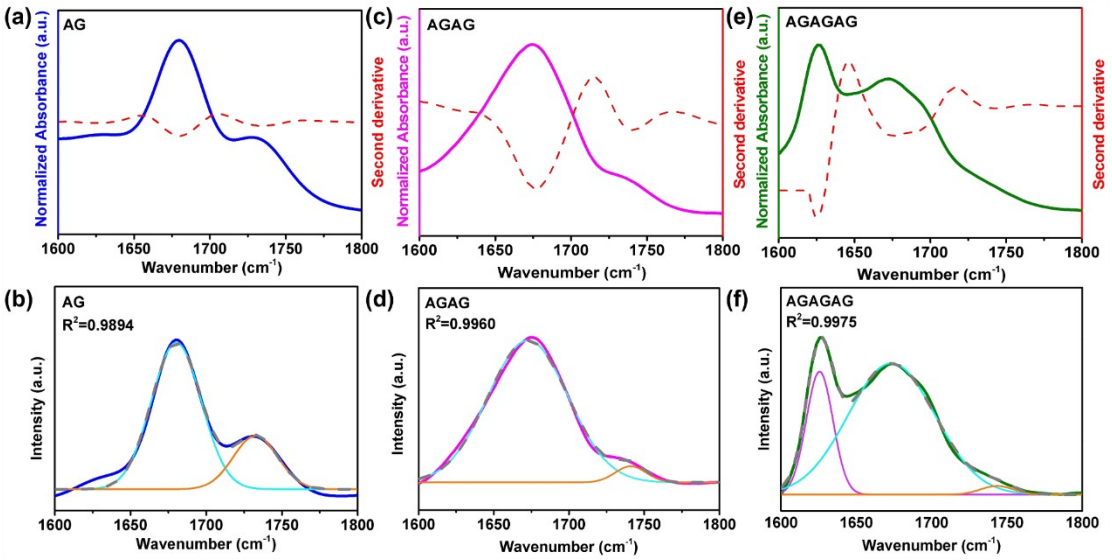

Figure S4 Second derivative absorbance spectra in the Amide I region (1600–1800) cm^{-1} for samples (AG, AGAG, and AGAGAG) indicating various secondary structures like α-helix (the orange solid line), random coils (light blue solid line), and β-sheet (purple solid line). The red dotted line represents the second derivative of the infrared spectrum of the three samples, respectively. The gray dotted line shows the fitting curve.

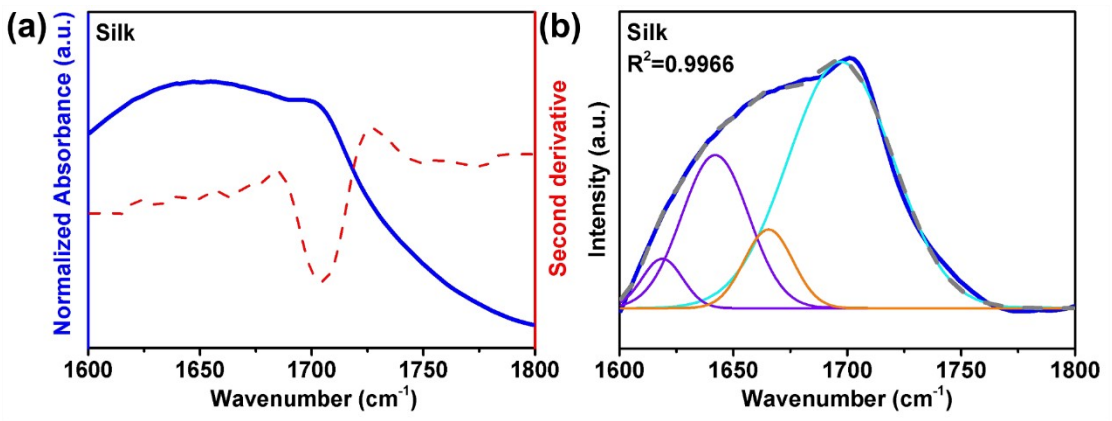

Figure S5 Second derivative absorbance spectra in the Amide I region (1600–1800) cm^{-1} for silk indicating various secondary structures like α-helix (the orange solid line), random coils (light blue solid line), and β-sheet (purple solid line). The red dotted line represents the second derivative of the infrared spectrum of the three samples, respectively. The gray dotted line shows the fitting curve.