Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information

Isotope-edited FTIR reveals distinct aggregation and structural behaviors of unmodified and pyroglutamylated amyloid β peptides

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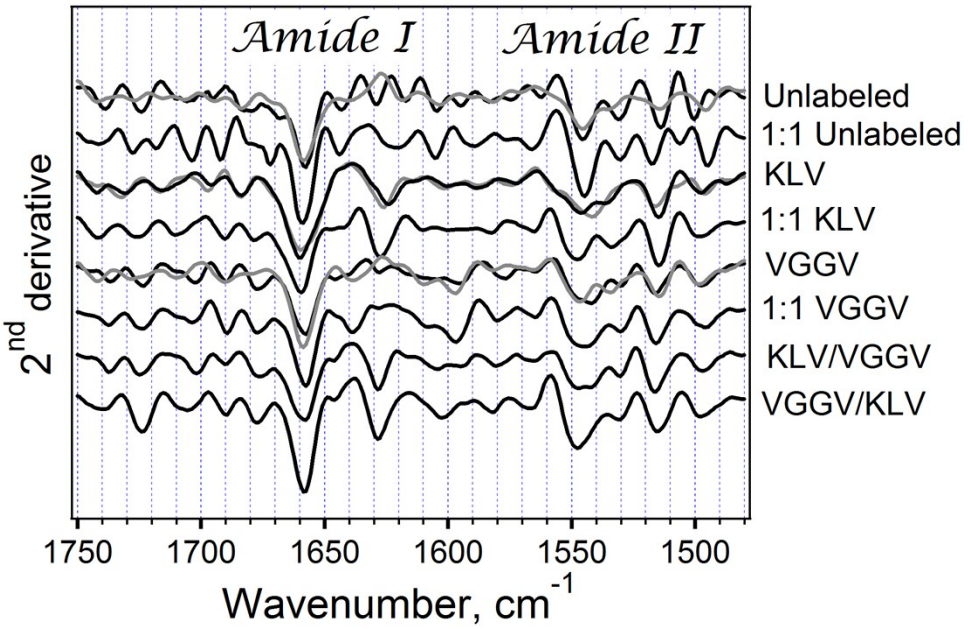

Figure S1. Second derivatives of the FTIR spectra of dry peptides in amide I and amide II regions, shown in Figure 2 of main text. Spectra for unlabeled and isotopically labeled $A\beta_{1\text{-}42}$ and $A\beta pE_{3\text{-}42}$ peptides and their 1:1 combinations are presented. Gray lines correspond to $A\beta pE_{3\text{-}42}$, and solid lines correspond either to $A\beta_{1\text{-}42}$ or to combined samples, as indicated. KLV or VGGV imply the peptides have been labeled at $K^{16}L^{17}V^{18}$ or $V^{36}G^{37}G^{38}V^{39}$, respectively. In KLV/VGGV or VGGV/KLV samples, the first stretch applies to $A\beta_{1\text{-}42}$ and the second to $A\beta pE_{3\text{-}42}$.

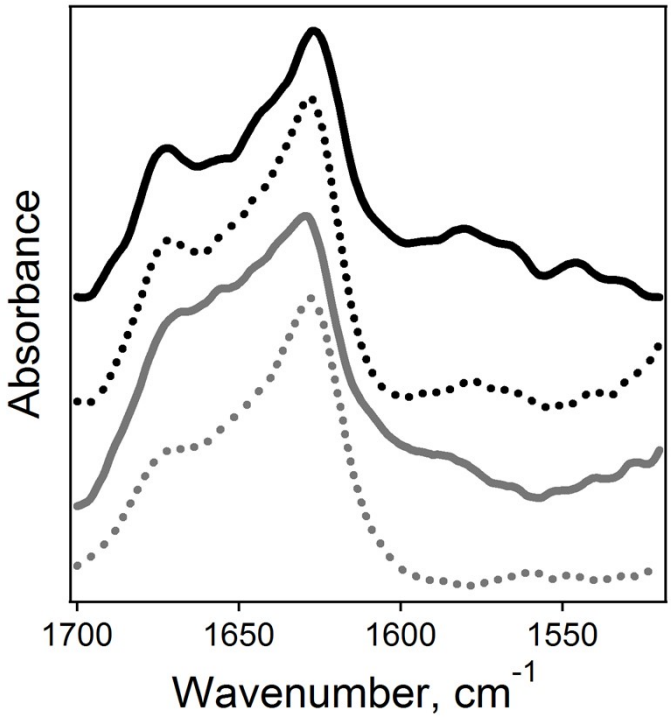

Figure S2. FTIR spectra of $A\beta_{1\text{-}42}$ (solid) and $A\beta pE_{3\text{-}42}$ (dotted) incubated in D_2O-based 50 mM NaCl + 50 mM Na,K-phosphate, pD 7.2 (black lines) or 10 mM Na,K-phosphate, pD 7.2 (gray lines) for 2 hours. Total peptide concentration is 50 μM. Comparison with the spectra of dry samples (Figure 2 of main text) indicates nearly complete loss of amide II bands, implying amide H/D exchange is close to completion.

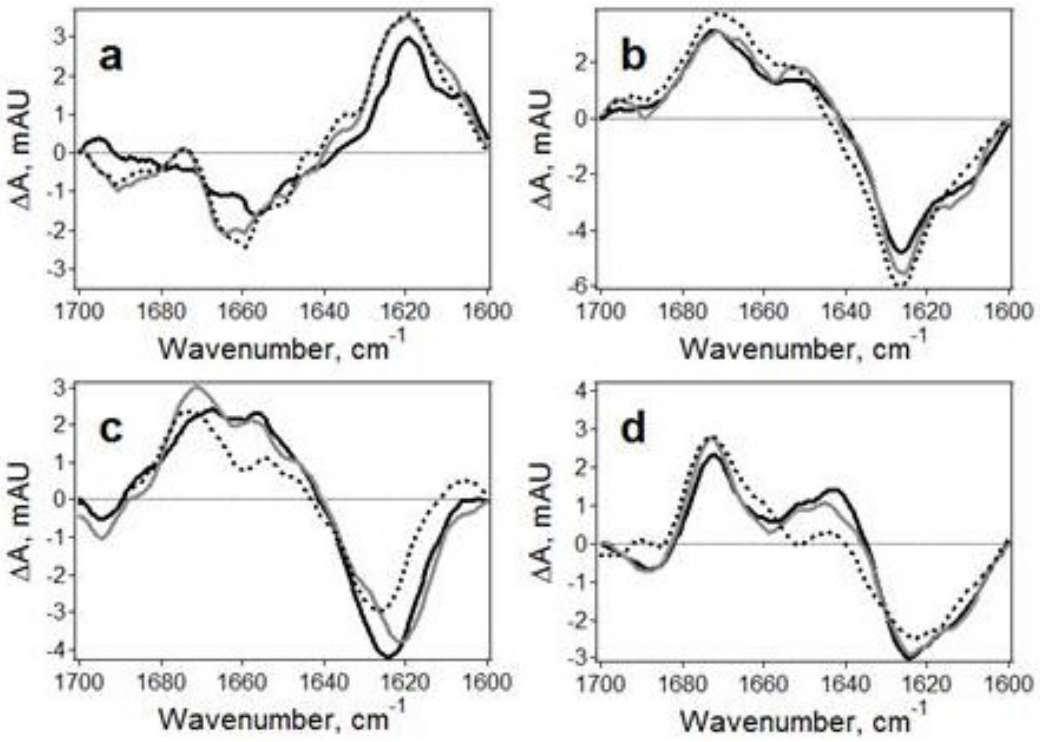

Figure S3. Difference FTIR spectra of $A\beta_{1\text{-}42}$ and $A\beta pE_{3\text{-}42}$ peptides and their equimolar combinations in 50 mM NaCl + 50 mM Na,K-phosphate buffer (a, b) and 10 mM Na,K-phosphate buffer (c, d), pD 7.2 (buffers were made using D_2O). Spectra in a) and c) show the difference $A\beta_{1\text{-}42}$ - $A\beta pE_{3\text{-}42}$, and those in b) and d) show the difference between 1:1 combination and the normalized sum of the spectra of the two peptides. Black, gray, and dashed lines correspond to the peptide samples incubated in a D_2O-based buffer for 10, 60 and 120 min, respectively. Total peptide concentration is 50 μM.

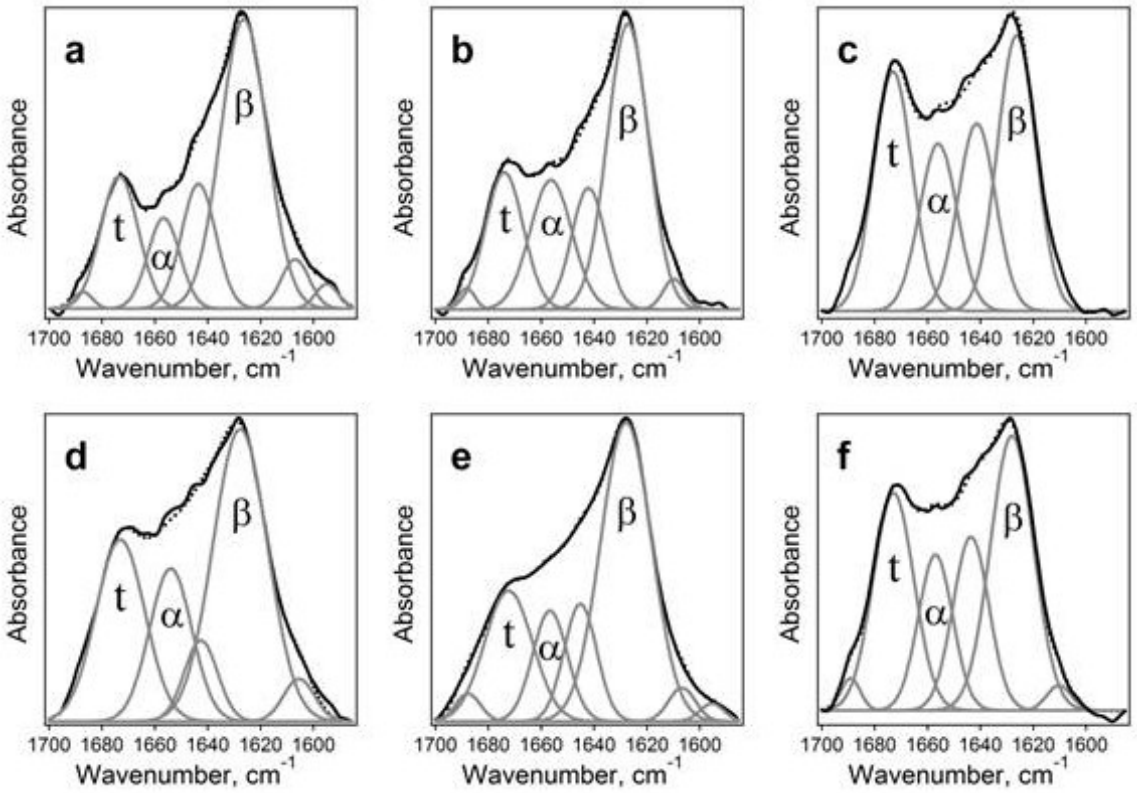

Figure S4. Curve-fitted FTIR spectra of unlabeled $A\beta_{1\text{-}42}$ (a, d), $A\beta pE_{3\text{-}42}$ (b, e), and their 1:1 combination (c, f) incubated in 50 mM NaCl + 50 mM Na,K-phosphate buffer (a, b, c) or 10 mM Na,K-phosphate buffer (d, e, f), pD 7.2, for 2 hours. Total peptide concentration is 50 μM. The measured spectra are shown in black solid lines, the amide I components in gray lines, and the curvefit, i.e. the sum of all components, in dotted lines. Components marked t, α, and β are assigned to turn, α-helix, and β-sheet structures, respectively.

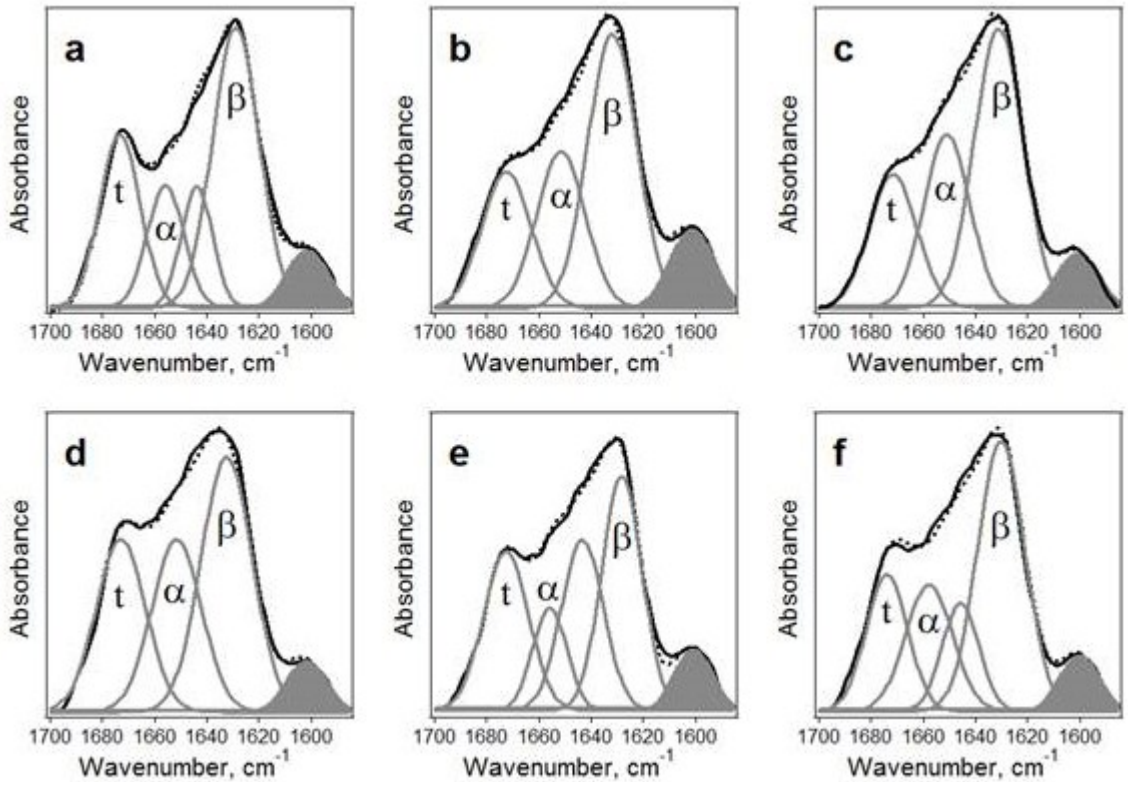

Figure S5. Curve-fitted FTIR spectra of $K^{16}L^{17}V^{18}$-labeled $A\beta_{1\text{-}42}$ (a, d), $A\beta pE_{3\text{-}42}$ (b, e), and their 1:1 combination (c, f) incubated in 50 mM NaCl + 50 mM Na,K-phosphate buffer (a, b, c) or 10 mM Na,K-phosphate buffer (d, e, f), pD 7.2, for 2 hours. Total peptide concentration is 50 μM. The measured spectra are shown in black solid lines, the amide I components in gray lines, and the curvefit, i.e. the sum of all components, in dotted lines. The component generated by the $^{13}C,^{15}N$-labeled segment is shaded. Components marked t, α, and β are assigned to turn, α-helix, and β-sheet structures, respectively.