

Rippled β -sheet formation by an amyloid- β fragment suggests the generality of enantiomeric β -sheet peptide coassembly

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SUPPLEMENTARY MATERIAL

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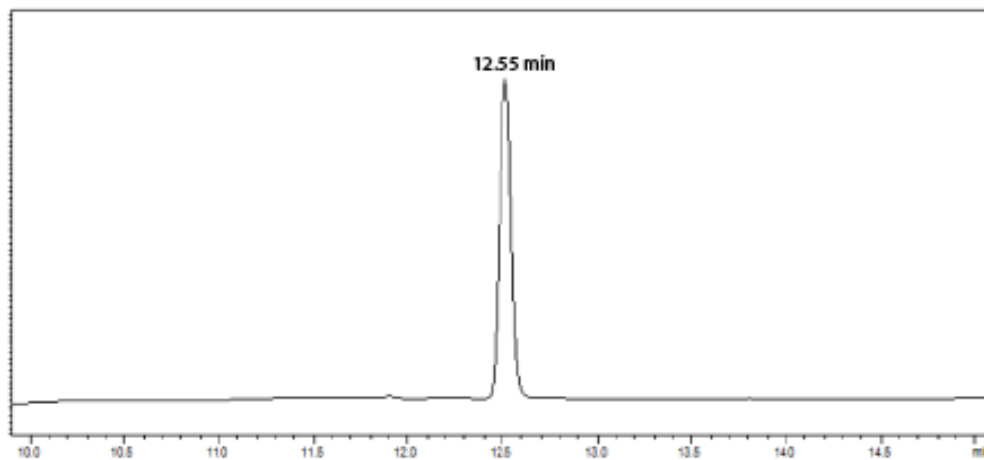
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Table S1. Analytical HPLC gradient conditions

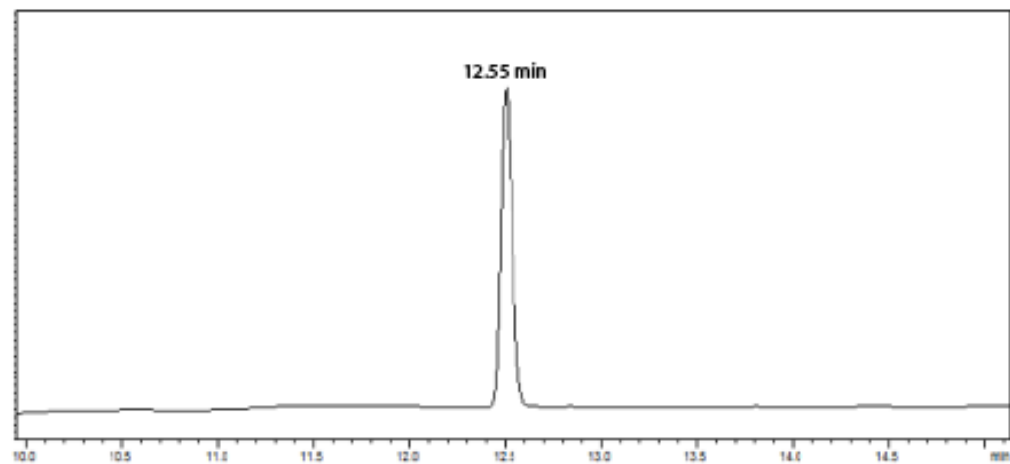
Peptide	Sequence	Retention Time (min)	Gradient (soln A: water/0.5% TFA; soln B: acetonitrile/0.5% TFA)
L-A β (16-22)	Ac-KLVFFAE-NH ₂	12.55	Isocratic 5% B 5 min, 5-95% B over 10 min, 95% B 5 min
D-A β (16-22)	Ac-klvffae-NH ₂	12.55	Isocratic 5% B 5 min, 5-95% B over 10 min, 95% B 5 min
L17/F20 ¹³ C L-A β (16-22)	Ac-K ¹³ LVF ¹³ FAE-NH ₂	12.55	Isocratic 5% B 5 min, 5-95% B over 10 min, 95% B 5 min
F19 ¹³ C L-A β (16-22)	Ac-KLV ¹³ FFAE-NH ₂	12.35	Isocratic 5% B 5 min, 5-95% B over 10 min, 95% B 5 min
F20 4F-Phe L-A β (16-22)	Ac-KLVF(4F-Phe)AE-NH ₂	12.43	Isocratic 5% B 5 min, 5-95% B over 10 min, 95% B 5 min
F20 D-4F-phe D-A β (16-22)	Ac-klvf(4F-phe)AE-NH ₂	12.43	Isocratic 5% B 5 min, 5-95% B over 10 min, 95% B 5 min

Figure S1. Analytical HPLC traces of synthetic peptides at 215 nm.

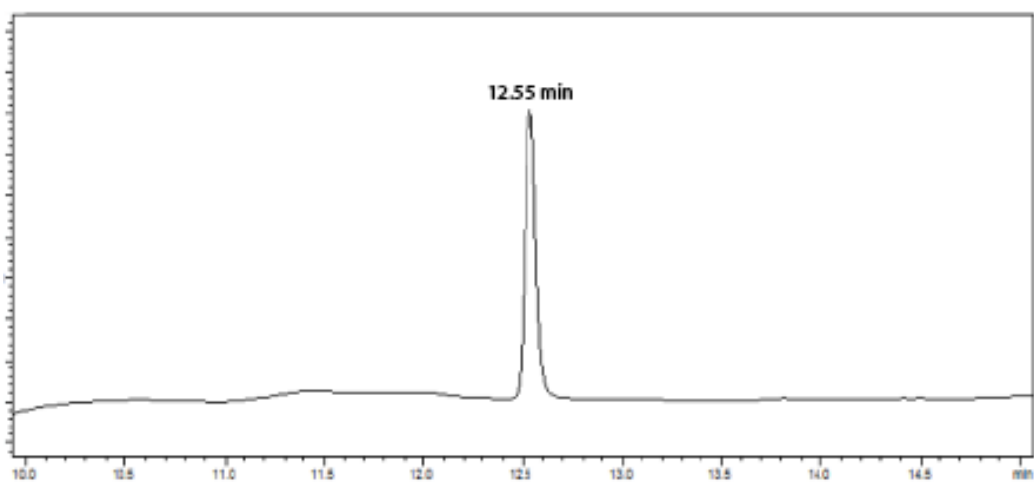
A. L-A β (16-22), Ac-KLVFFAE-NH₂



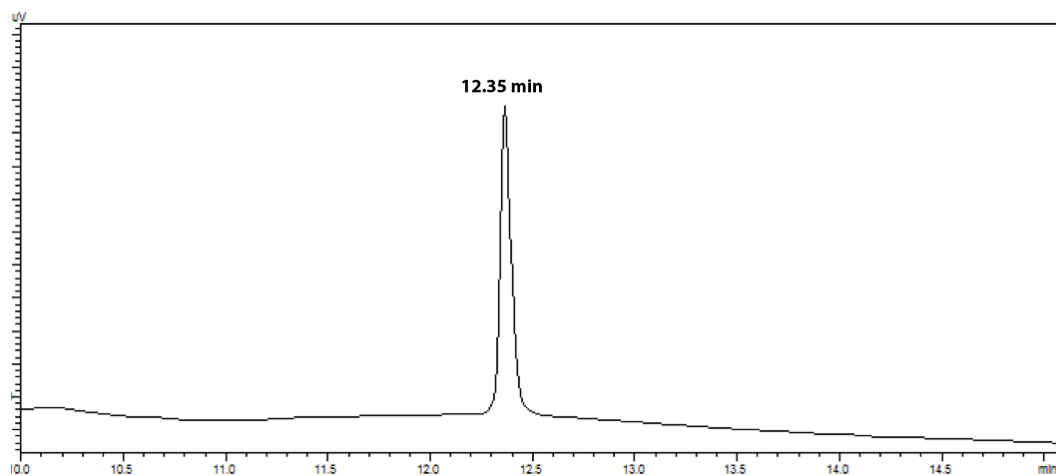
B. D-A β (16-22), Ac-klvffae-NH₂



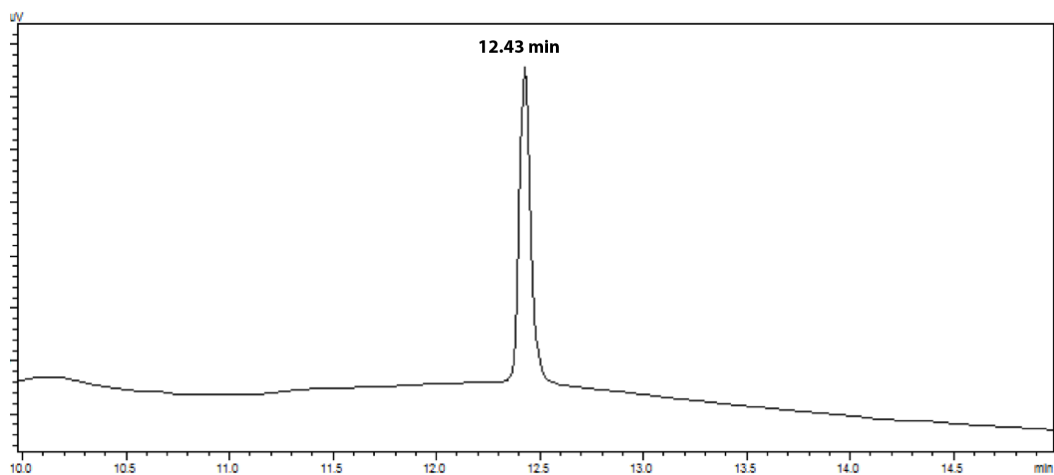
C. L17/F20 ¹³C L-A β (16-22), Ac-K¹³LVF¹³FAE-NH₂



D. F19 ¹³C L-A β (16-22), Ac-KLV¹³FFAE-NH₂



E. F20 4F-Phe L-A β (16-22), Ac-KLVF(4F-Phe)AE-NH₂



F. F20 D-4F-phe D-A β (16-22), Ac-klvf(4F-phe)AE-NH₂

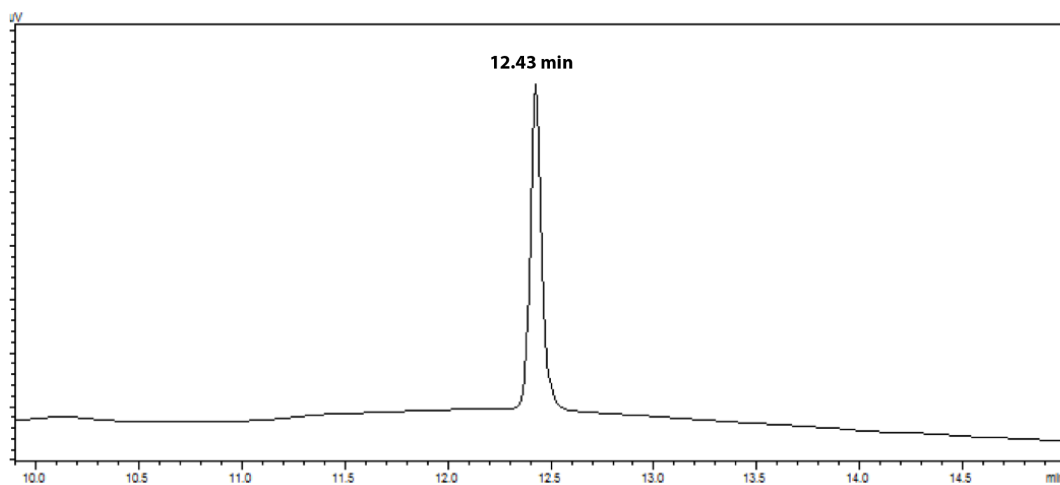


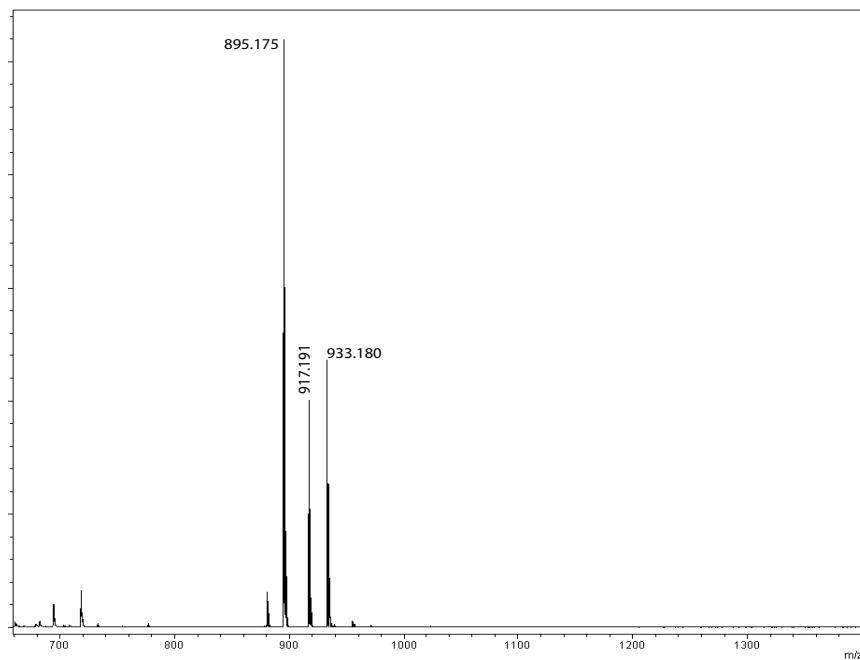
Table S2. Calculated and observed m/z for all peptides by MALDI-TOF-MS.

Peptide	calc [MH ⁺]	obs [MH ⁺]	calc [MNa ⁺]	obs [MNa ⁺]	calc [MK ⁺]	obs [MK ⁺]
L-A β (16-22)	895.07	895.175	917.07	917.191	933.17	933.180
D-A β (16-22)	895.07	894.693	917.07	916.685	933.17	932.671
L17/F20 ¹³ C L-A β (16-22)	897.05	896.834	919.05	918.835	935.15	934.821
F19 ¹³ C L-A β (16-22)	896.06	896.311	918.06	918.340	934.16	934.335
F20 4F-Phe L-A β (16-22)	913.06	913.494	935.06	935.522	951.16	951.523

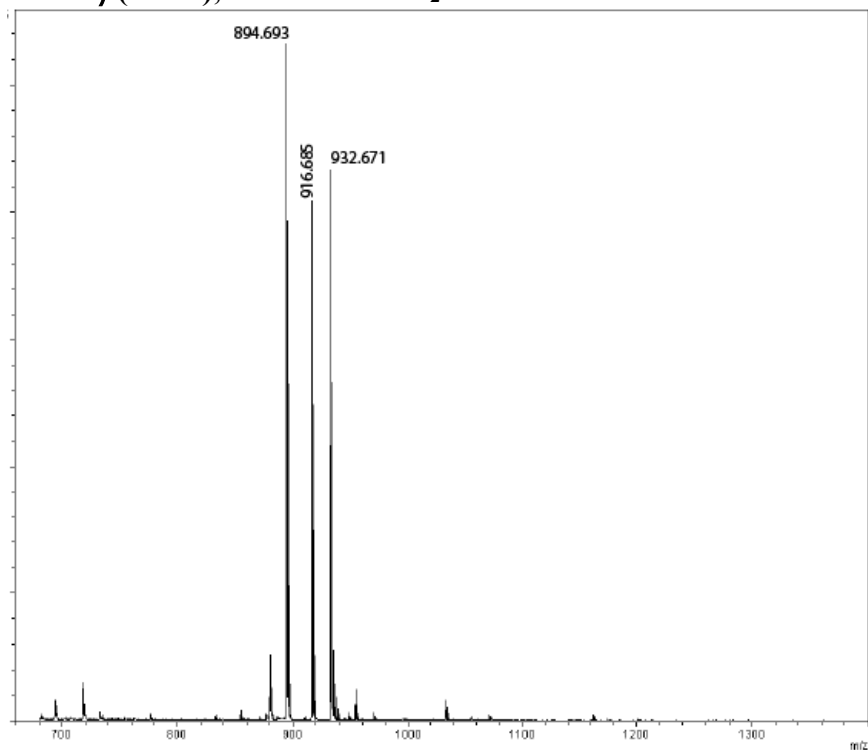
F20 D-4F-phe D-A β (16-22)	913.06	913.497	935.06	935.532	951.16	951.530
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Figure S2. MALDI-TOF spectra for all peptides.

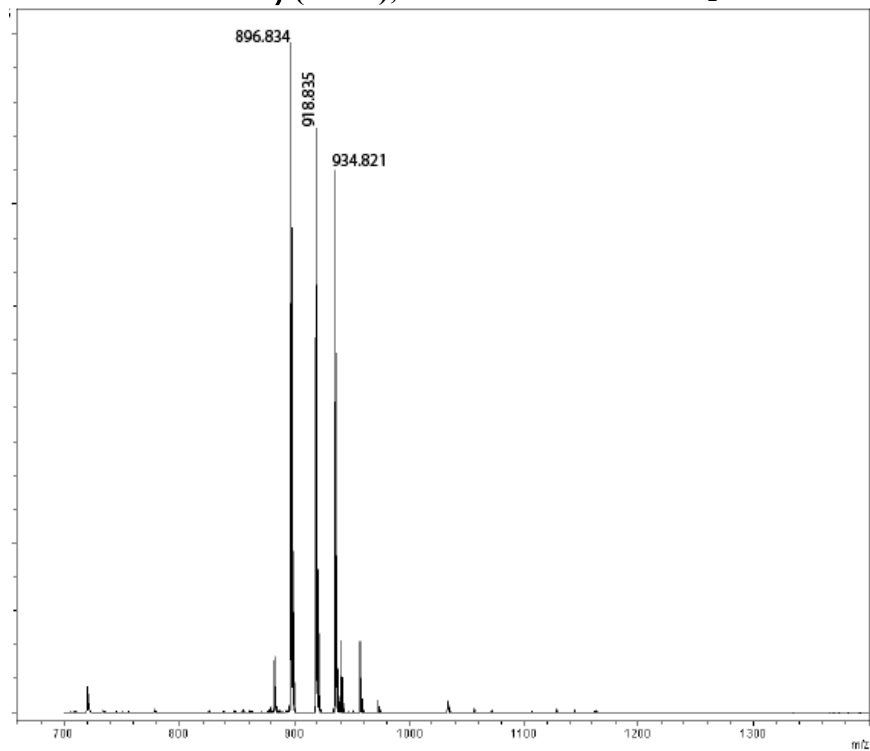
A. L-A β (16-22), Ac-FKLVFFAE-NH₂



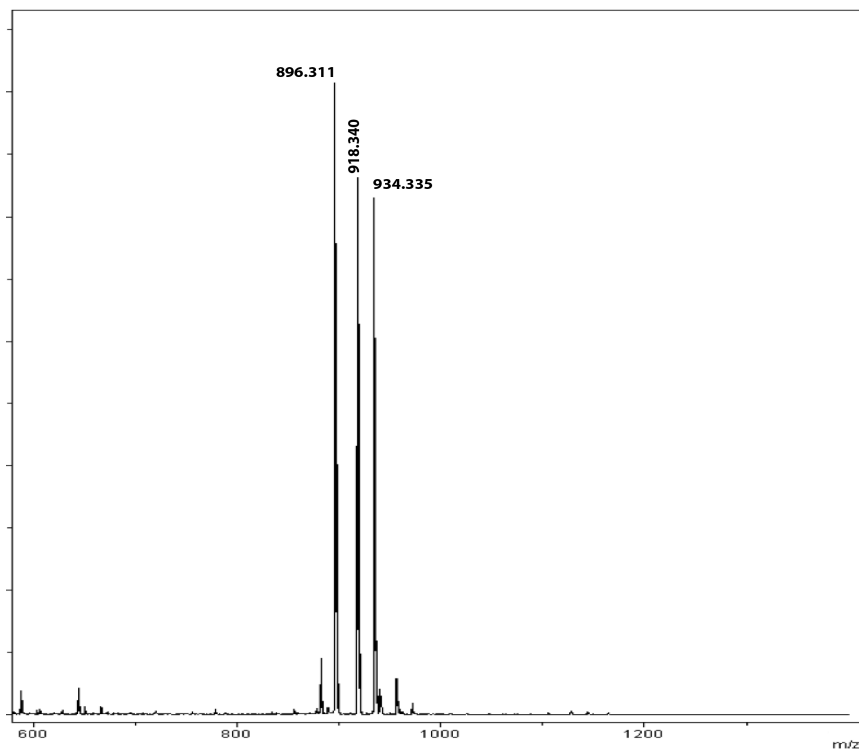
B. D-A β (16-22), Ac-klvffae-NH₂



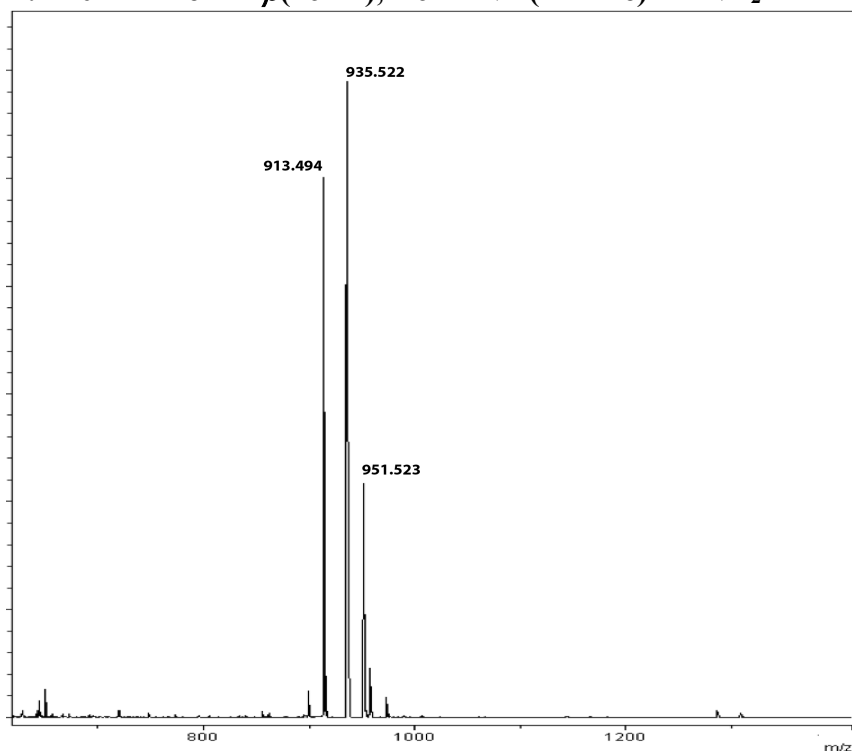
C. L17/F20 ^{13}C L-A β (16-22), Ac-K $^{13}\text{LVF}^{13}\text{FAE-NH}_2$



D. F19 ^{13}C L-A β (16-22), Ac-KLV $^{13}\text{FFAE-NH}_2$



E. F20 4F-Phe L-A β (16-22), Ac-KLVF(4F-Phe)AE-NH₂



F. F20 D-4F-phe D-A β (16-22), Ac-klvf(4F-phe)AE-NH₂

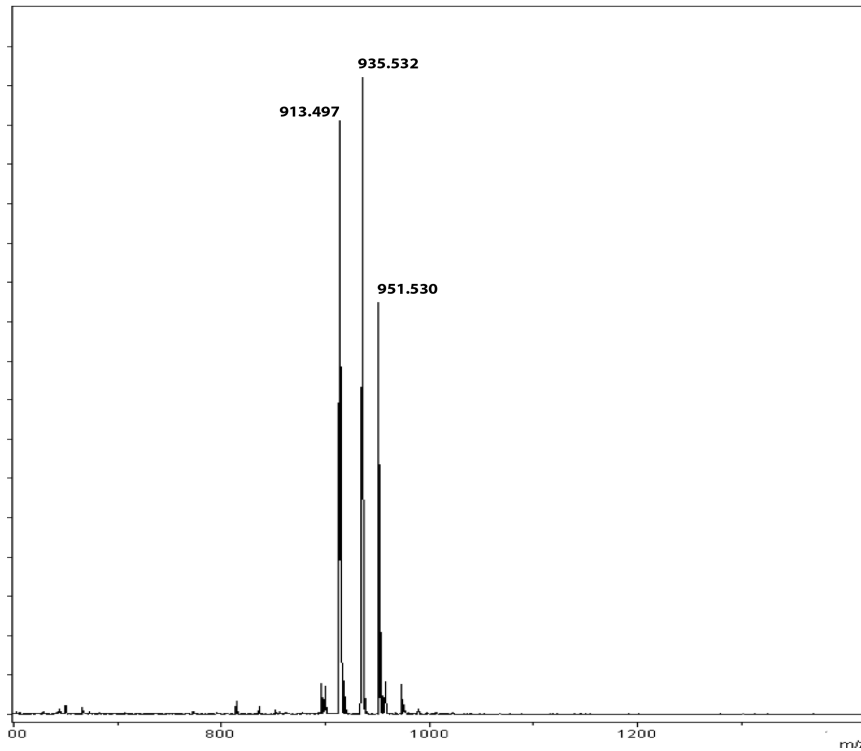
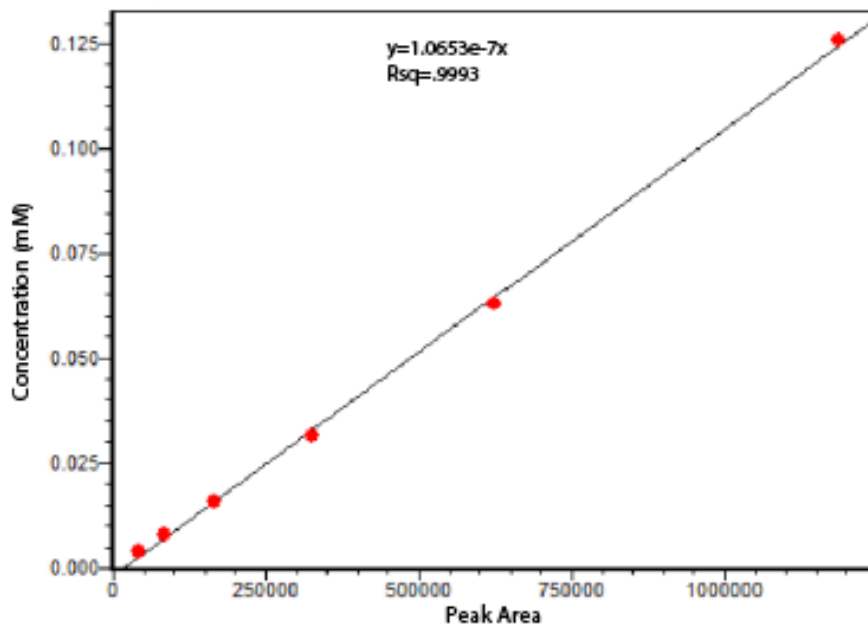


Figure S3. Peptide concentration curves used to determine concentrations of all peptides used in this study.

A. Concentration curve used for all peptides *except* those containing 4F-Phe



B. Concentration curve used for peptides containing 4F-Phe

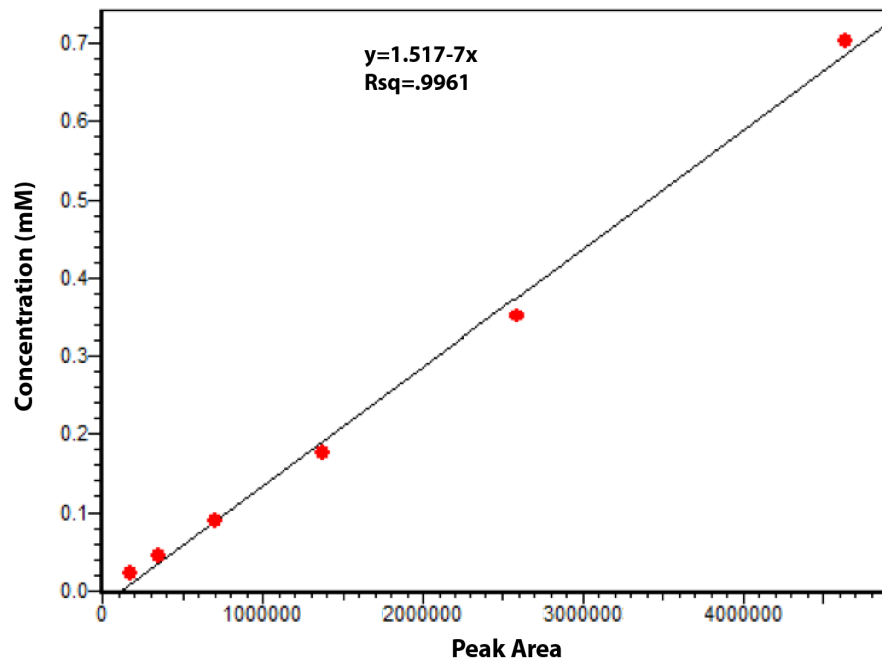
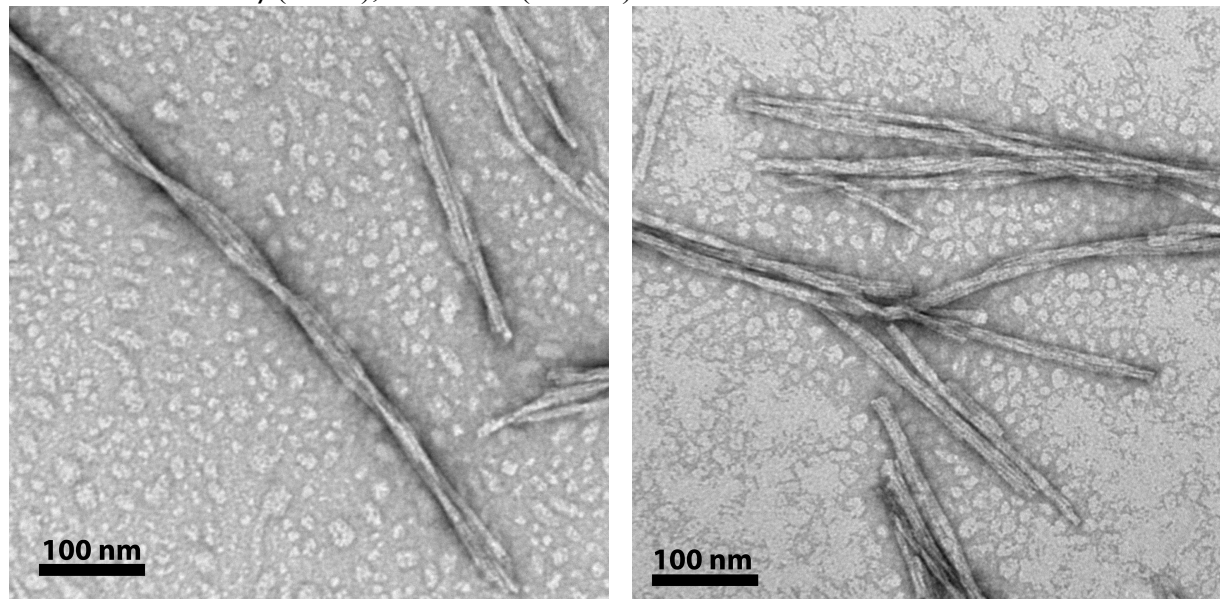
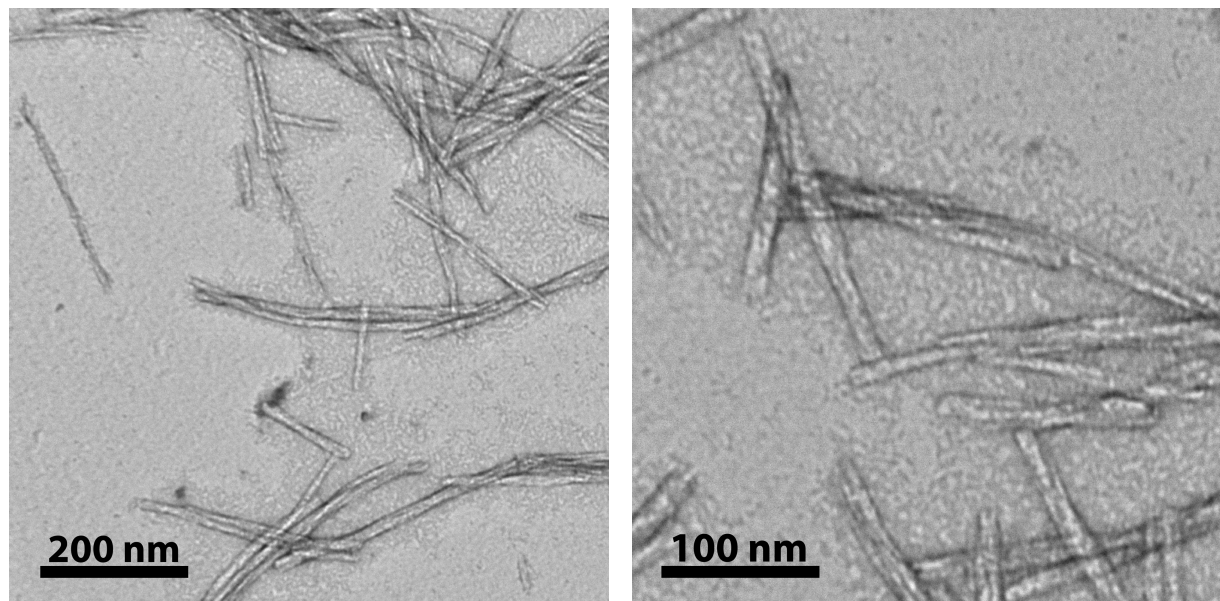


Figure S4. Transmission electron micrographs of peptide fibrils used for solid state NMR.

A. F20 4F-Phe L-A β (16-22), Ac-KLVF(4F-Phe)AE-NH₂



B. TEM images of the L/L-ssNMR sample: F19 ¹³C L-A β (16-22) (Ac-KLV¹³FFAE-NH₂) with F20 4F-Phe L-A β (16-22) (Ac-KLVF(4F-Phe)AE-NH₂).



C. TEM images for the L/D-ssNMR sample: F19 ^{13}C L-A β (16-22) (Ac-KLV ^{13}F FAE-NH $_2$) with F20 D-4F-phe D-A β (16-22) (Ac-klvf(4F-phe)AE-NH $_2$).

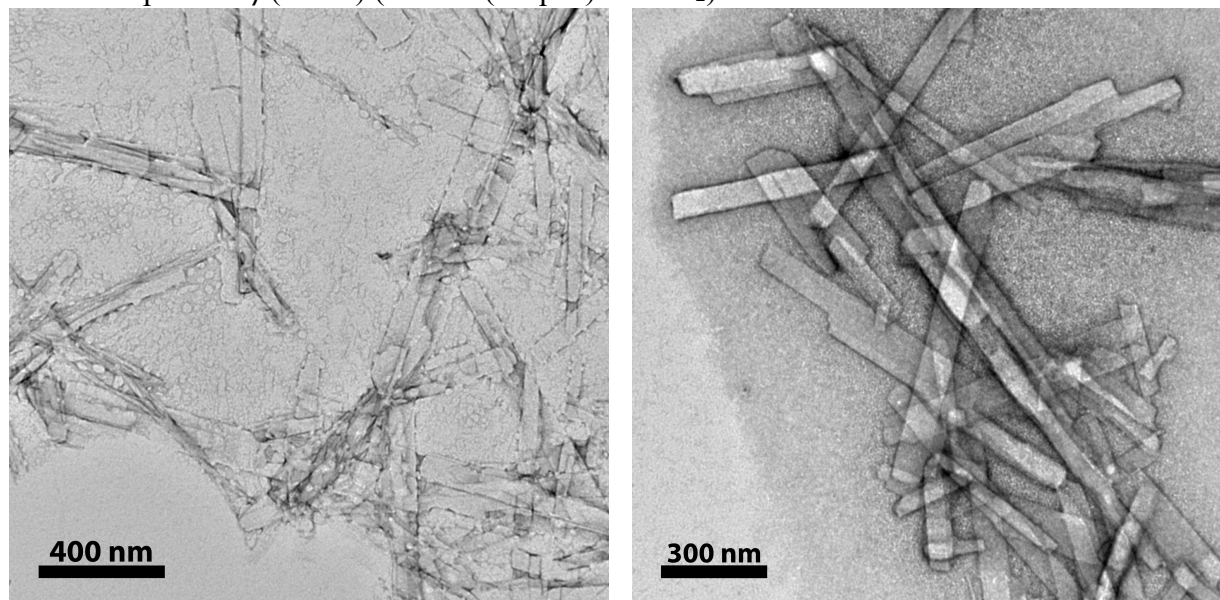


Figure S5. Carbon-13 ssNMR 1D spectra for the L/L- and L/D- A β (16-22) assemblies.

