Supporting Information

Toxic amyloid tape: A novel mixed antiparallel/parallel β-sheet structure formed by Aβ on GM1 clusters

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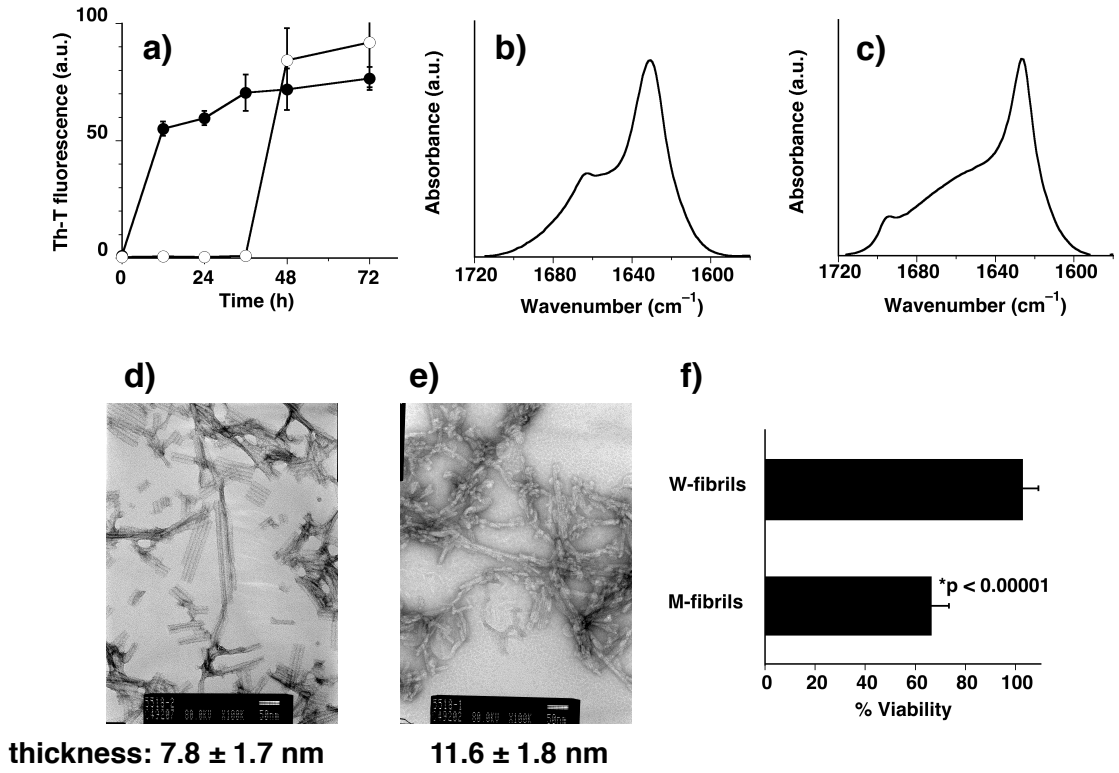

Figure S1. Characterization of W- and M-fibrils. a) Kinetics of fibril formation by Aβ-(1–40) (50 μM) with (closed circles) or without (open circles) GM1-containing liposomes (GM1:sphingomyelin:cholesterol=1:1:1) at an Aβ-to-GM1 ratio of 1 at 37 °C, as determined by the Th-T assay (mean ± S.D., n = 6). FTIR spectra of b) W- and c) M-fibrils. TEM images of d) W- and e) M-fibrils. Bars represent 50 nm. f) Cytotoxicity of W- and M-fibrils against SH-SY5Y human neuroblastoma cells at 25 μM after a 24-h incubation at 37 °C (mean ± S.D., n = 6).

* Two sample t-test.

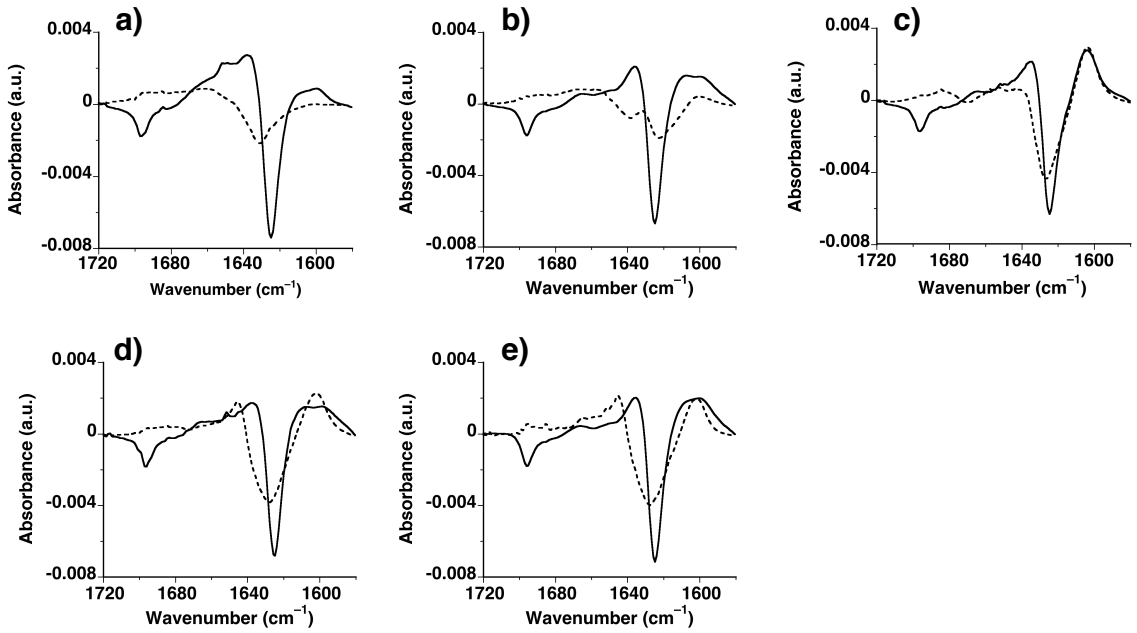

Figure S2. FTIR difference spectra (1-^{13}C-labeled Aβ-(1–40) – unlabeled Aβ-(1–40)) of W-fibrils (dotted line) and M-fibrils (solid line). Labeled residue: a, F4; b, V12; c, F19; d, V24; e, V36.

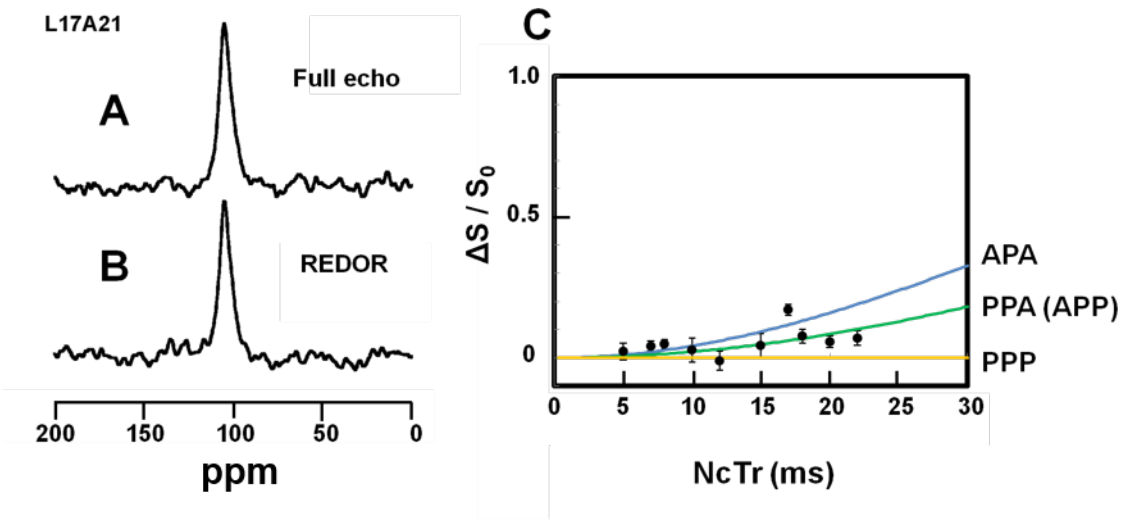

Figure S3. (A) Full echo and (B) REDOR ^{15}N NMR spectra of [^{15}N]L17, [1-^{13}C]A21-Aβ(1-40) M-fibrils at NcTr=20 ms. (C) The plots of $\Delta S/S_0$ against NcTr values. Three calculated REDOR curves were obtained for PPP, PPA (APP) and PAP β-sheet units by considering the shortest interatomic distances for the PPP unit and the two shortest interatomic distances for PPA (APP) and APA units as shown in the solid arrows in Figure 7.

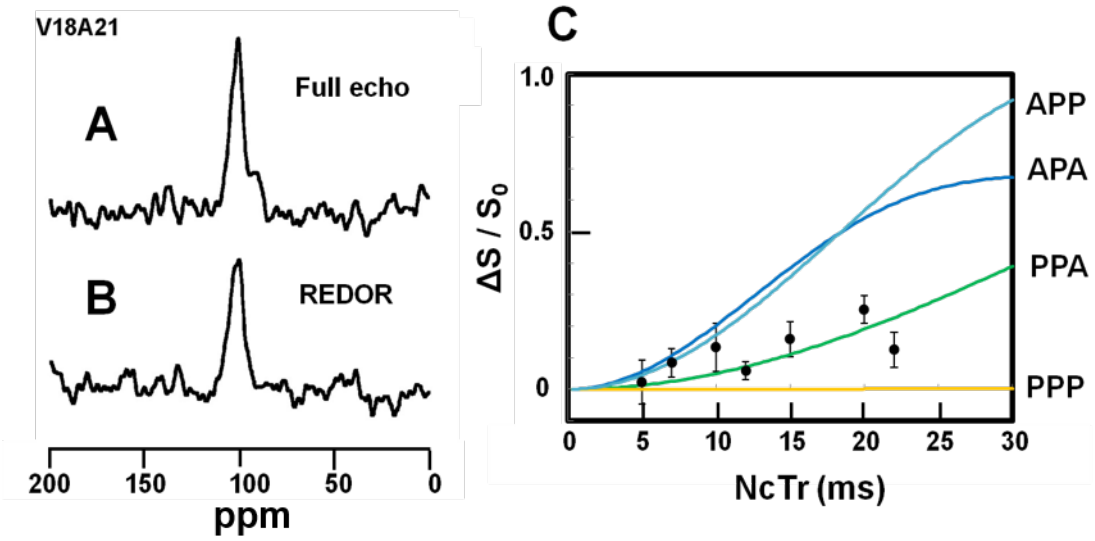

Figure S4. (A) Full echo and (B) REDOR ^{15}N NMR spectra of [^{15}N]V18, [1-^{13}C]A21-Aβ(1-40) M-fibrils at NcTr=20 ms. (C) The plots of $\Delta S/S_0$ against NcTr values. Four calculated REDOR curves were obtained for PPP, PPA, APP and APA β-sheet units by considering the shortest interatomic distances for the PPP unit and the two shortest interatomic distances for PPA, APP and APA units as shown by the solid arrows in Figure 7.

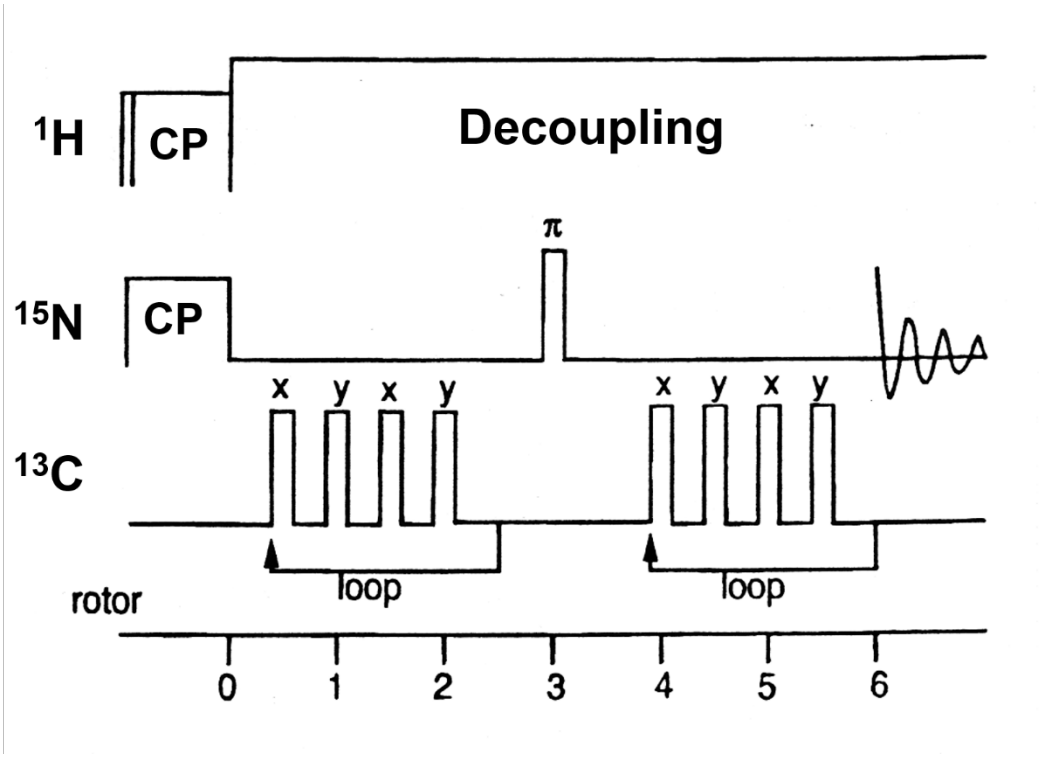

Figure S5. Pulse sequence for rotational echo double resonance (REDOR) experiments. ^{15}N nuclei are excited by CP pulse with duration of 2 ms. After the CP pulse, ^{13}C π-pulses were applied at the center of rotor period (x-pulse) and at the rotor period (y-pulse) to recouple the ^{15}N-^{13}C dipolar interaction, alternately with series of $(xyxy)_n$ phase modulated pulses with each π-pulse duration of 13.4 μs and ^{15}N π-pulse is applied as an Hahn echo pulse with the duration of 11.5 μs. After applying same duration of $(xyxy)_n$ pulses which are called xy four pulses, ^{15}N rotational echo signals were acquired after *NcTr* time, where *Nc* is the number of rotor cycles and *Tr* is the rotor cycle period. In this experiment, *Tr* is 0.25 ms corresponding to 4 kHz rotor spinning frequency. To accumulate the echo signals, repetition time was set to 4 s. REDOR signals were acquired at 20 °C and made Fourier transformation with 100 Hz Lorentzian line broadening. Typically, 2000, 4000, 8000 and 16000 transients were accumulated for *NcTr* values of 5, 10, 15, and 20 ms, respectively. The signal peak heights were evaluated and used as REDOR signal intensity $S_{REDOR}(t)$. On the other hand, ^{15}N Hahn echo signal (full echo signal) intensity $S_{fullecho} = S_0$ were also acquired without applying ^{13}C-$(xyxy)_n$ pulses. Finally $\Delta S/S_0 = (S_{fullecho} - S_{REDOR})/S_{fullecho}$ (REDOR factor) values were plotted against *NcTr* time (REDOR curve) to evaluate ^{15}N-^{13}C dipolar dephasing patterns for each fibril sample.

Table S1: Summary of ^{13}C spectral shifts (cm^{-1})

		W-fibrils			M-fibrils		
labeled	residue	100% ^{13}C (%area)	25% ^{13}C	difference	100% ^{13}C(%area)	25% ^{13}C	difference
F4			not detected		14.9 (6.3)	14.1	0.8
V12			not detected		15.7 (5.6)	14.8	0.9
F19		24.1 (5.7)	18.9	5.2	19.3 (5.9)	17.3	2.0
F20		25.4 (4.4)	19.8	5.6	19.4 (6.4)	18.0	1.4
V24		23.1 (4.6)	17.9	5.2	16.0 (7.1)	14.1	1.9
V36		23.8 (3.2)	15.0	8.8	14.5 (6.2)	14.3	0.2