Accurate Determination of Interstrand Distances and Alignment in Amyloid Fibrils by Magic Angle Spinning NMR

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Supporting Information.

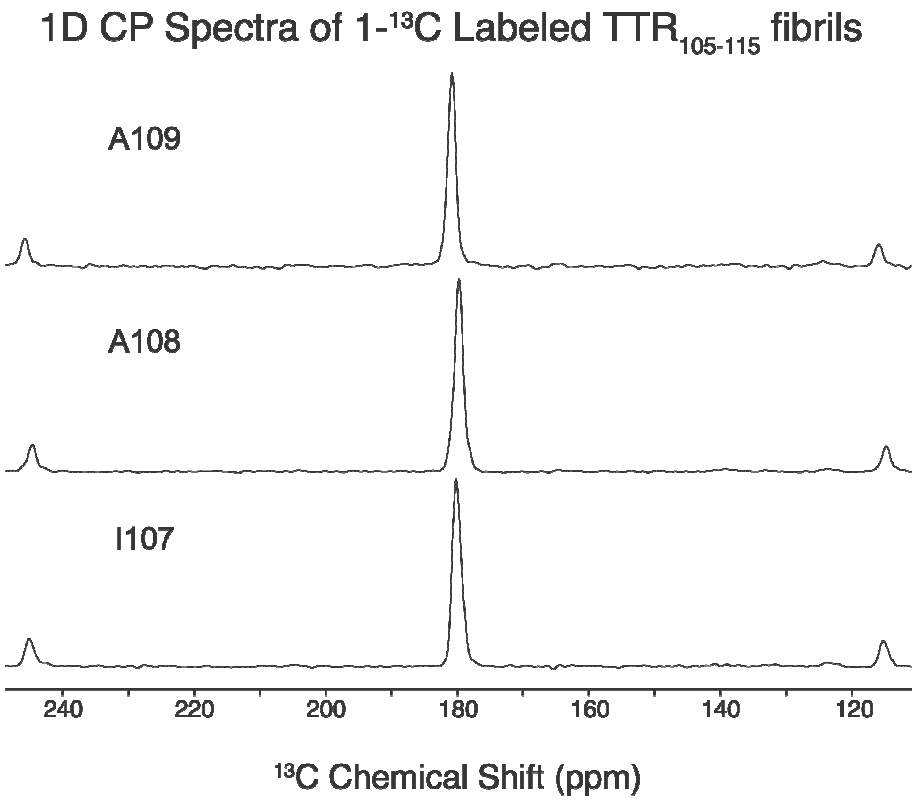

Figure S1. The 1D ^{13}C cross-polarization spectra of three 1-^{13}C labeled $TTR_{105-115}$ peptides are plotted. These were recorded with identical parameters to the DRAWS experiments (5.882 kHz MAS, 83 kHz TPPM proton decoupling, and 256 scans) just before recording and are used to normalize the DRAWS data. The samples exhibit good heterogeneity and ample signal-to-noise.

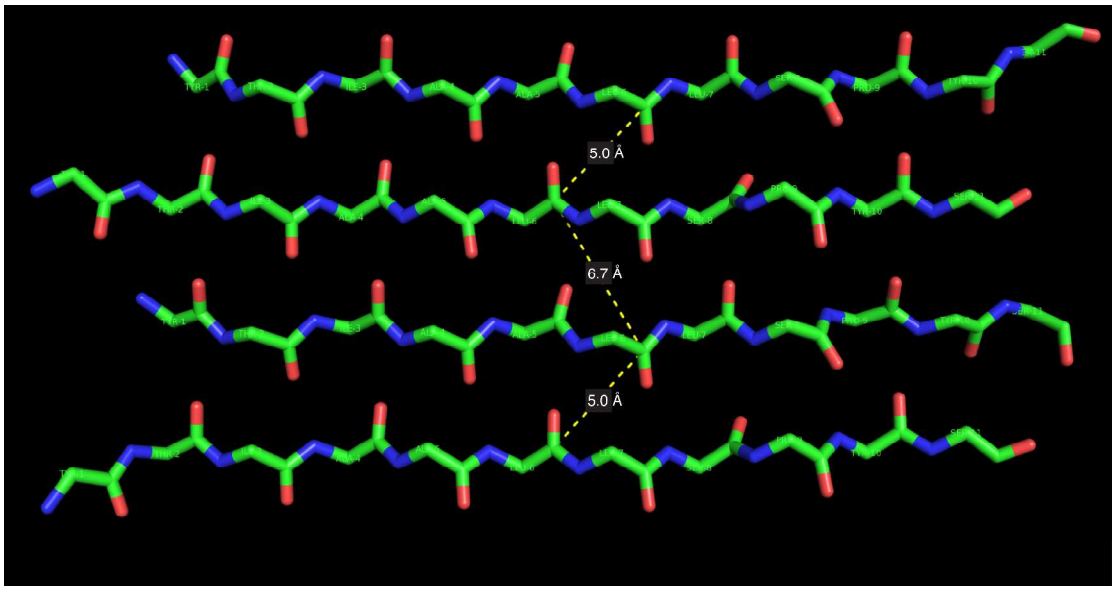

Figure S2: Illustration of expected topology and carbonyl-carbonyl distances for out of register parallel arrangement of β strands. In this geometry, there are multiple distances and all are longer than those seen in the in-register topology. Our measurement of several ^{13}CO-^{13}CO constraints establishes the geometry and registry of the packing.

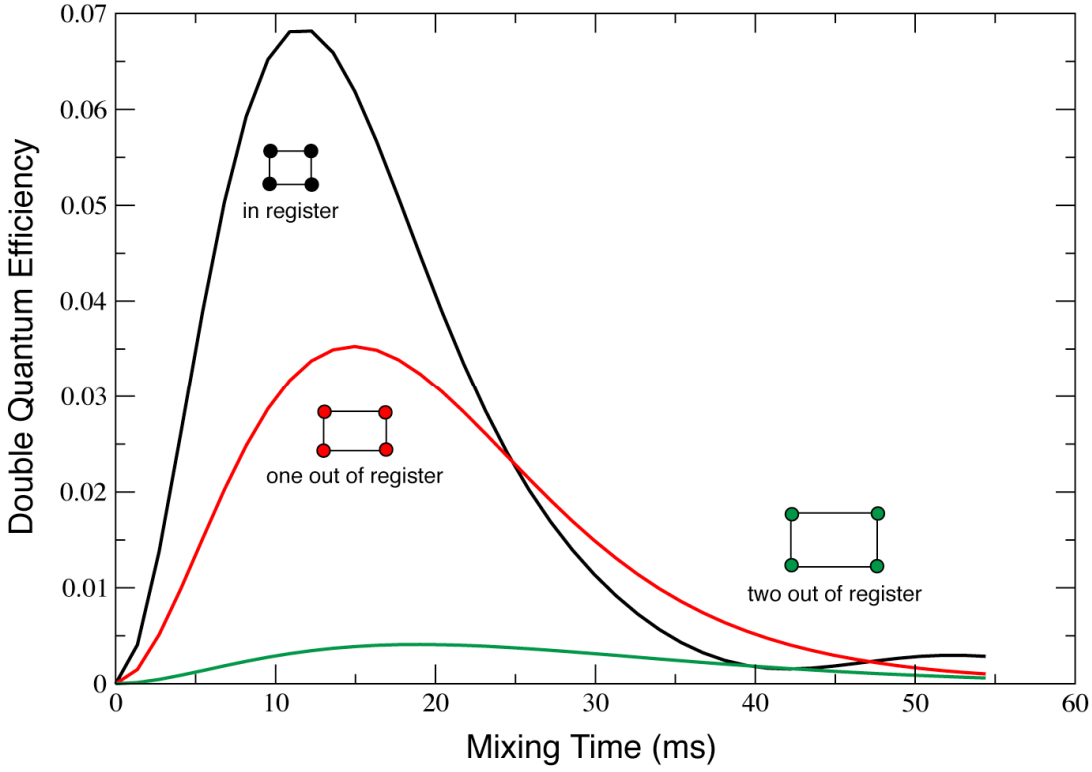

Figure S3: Expected DQ DRAWS build-up trajectory for spin geometries corresponding to parallel, parallel+1, and parallel+2 β-sheets. Note that out of register parallel β-sheets have inequivalent sets of intermolecular couplings which have been included in this simulation. T_2=15ms, 360 MHz ^1H, 5.882 kHz MAS. The maximum filtering efficiency will vary depending on the magnitude of the T_2 relaxation, which is measured to be stronger in the amyloid fibril than in succinate (succinate parameters were used here).