

Supporting Information

MOMD Analysis of NMR Lineshapes from A β -Amyloid Fibrils: A New Tool for
Characterizing Molecular Environments in Protein Aggregates

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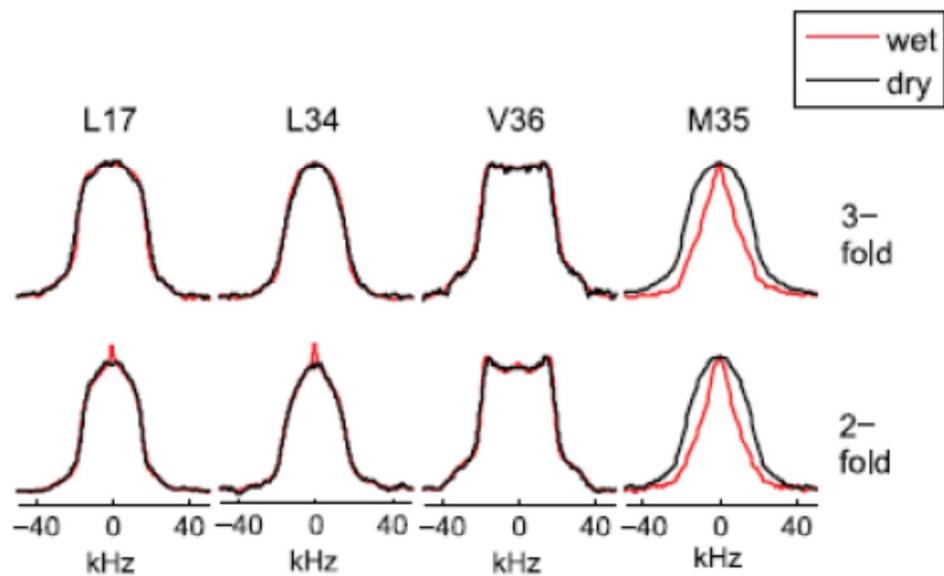


Figure S1. Experimental ^2H lineshapes from the methyl groups of L17, L34 and V36 at 274 K, and the methyl group of M35 at 310 K, in dry (black) and hydrated (red) 3-fold-symmetric $\text{A}\beta_{40}$ fibrils (upper row) and 2-fold-symmetric fibrils (lower row).¹

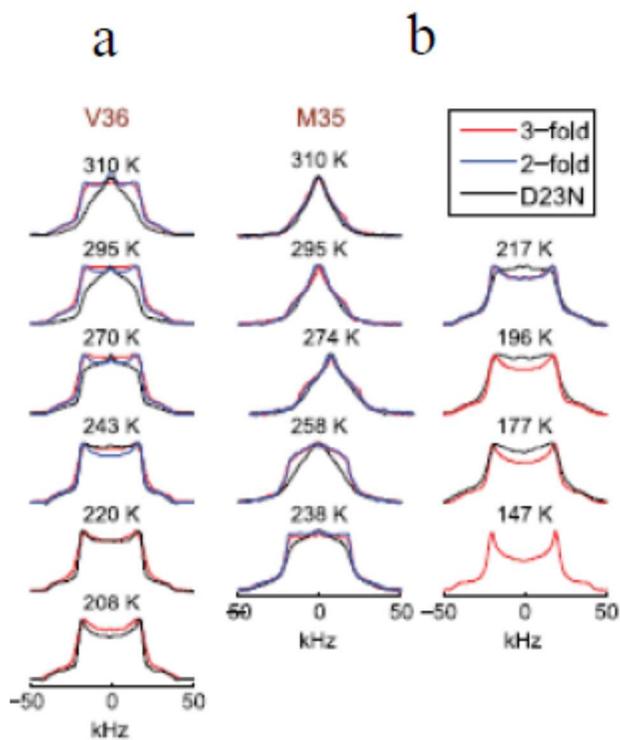


Figure S2. Experimental ^2H lineshapes from the methyl group of V36 (part a) and M35 (part b) in the hydrated 3-fold-symmetric $\text{A}\beta_{40}$ fibrils at the temperatures depicted in the figures. The spectra of the 3-fold-symmetric $\text{A}\beta_{40}$ fibrils, the 2-fold-symmetric $\text{A}\beta_{40}$ fibrils and the protofibrils of the D23N mutant are red, blue and black, respectively.¹

References

1. Vugmeyster, L.; Clark, M. A.; Falconer, I. B.; Ostrovsky, D.; Gantz, D.; Qiang, W. Flexibility and Solvation of Amyloid- β Hydrophobic Cores. *J. Biol. Chem.* **2016**, *291*, 18484-18495.