Supplmentary Information for Study of the γD-Crystallin Protein Using Two-Dimensional Infrared (2DIR) Spectroscopy : Experiment and Simulation

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The full-width at half-maximum (FWHM) node slopes were determined using the protocol in reference 1. First, the frequencies and FWHM of the diagonal peaks were determined. Next, the points of zero intensity between the positive and negative peaks were located across the FWHM of the diagonal peaks. Finally, we fit these points to a straight line, with the slope yielding the FWHM node slope.

Table S1: Diagonal peak frequencies (ω_{max}) and FWHM node slopes for simulated and experimental *xxxx* 2DIR spectra.

	Simulation		Experiment[1]		
	Node Slope	ω_{max} (cm^{-1})	Node Slope	ω_{max} (cm^{-1})	Assignment
^{12}C-Ntd/^{12}C-Ctd	1.38	1633	1.30	1642	Ntd+Ctd
^{13}C-Ntd/^{13}C-Ctd	1.45	1593	1.25	1598	Ntd+Ctd
^{12}C-Ntd/^{13}C-Ctd	1.43	1594	1.09	1601	Ntd
	1.33	1634	1.32	1640	Ctd
^{13}C-Ntd/^{12}C-Ctd	1.28	1633	1.26	1638	Ctd
	1.35	1595	1.14	1596	Ntd

References

(1) Moran, S., Woys, A., Buchanan, L., Bixby, E., Decatur, S., and Zanni, M. Two-dimensional IR Spectroscopy and Segmental ^{13}C Labeling Reveals the Domain Structure of human γD-Crystallin Amyloid Fibrils. *Proc. Natl. Acad. Sci. USA* 2012, *109(9)*, 3329–3334