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Supplemental Information

Effect of a Paramagnetic Spin Label on the Intrinsically Disordered Peptide Ensemble of Amyloid-β

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FIGURE CAPTIONS

Figure S1. *Percentages of MTSL-Cys-Aβ42 sub-ensembles containing turn 32-33 for REMD simulations.*

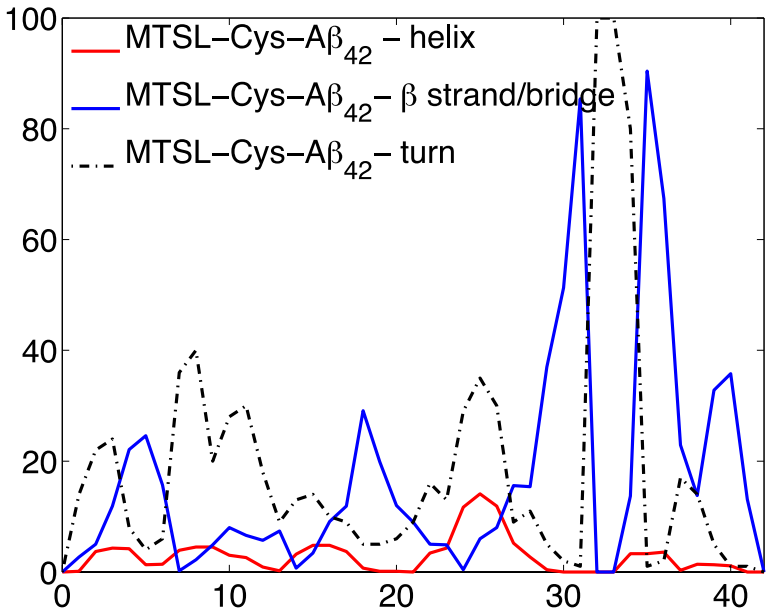
Figure S2. *Plot of the probability of a heavy atom contact between the MTSL-Cys residue and other residues in the Aβ42 sequence for REMD simulations.*

Figure S3: *Calculated SHIFTX2*[2] *proton and carbon secondary chemical shifts by residue for Aβ42 (blue) and MTSL-Cys-Aβ42 (red) REMD simulations.* (a) H_α chemical shifts, (b) H_N chemical shifts, (c) C_α chemical shifts, (d) C_β chemical shifts, and (e) N chemical shifts. Random coil residue specific values taken from are subtracted from both experimental and simulation values.

Figure S4: *J-coupling constants for backbone amides for Aβ42 (blue) and MTSL-Cys-Aβ42 (red) for REMD simulations.* Simulation uncertainty bars represent rms difference between two independent simulations and the average.

Figure S5: *Calculated RDCs for (a) Aβ42 and (b) MTSL-Cys-Aβ42 structural ensembles generated using REMD simulations.* RDCs based on global alignments calculated from PALES.

Figure S6: *Contact map of strong simulated* ^1H-^1H *NOE intensities for MTSL-Cys-Aβ42 from REMD simulations that are dominated by a single contact*. Strong experimental intensities that define β-strands 4-7 and 10-12 (orange), β-strands 3-6 and 31-41 (pink), β-strands 16-21 and 29-36 (cyan), β-strands 27-31 and 33-38 (grey), β-strands 34-36 and 39-40 (yellow) and hydrophobic contacts (outlined black) indicated in the map. The color-coding for helices and turns are shown in the figure.



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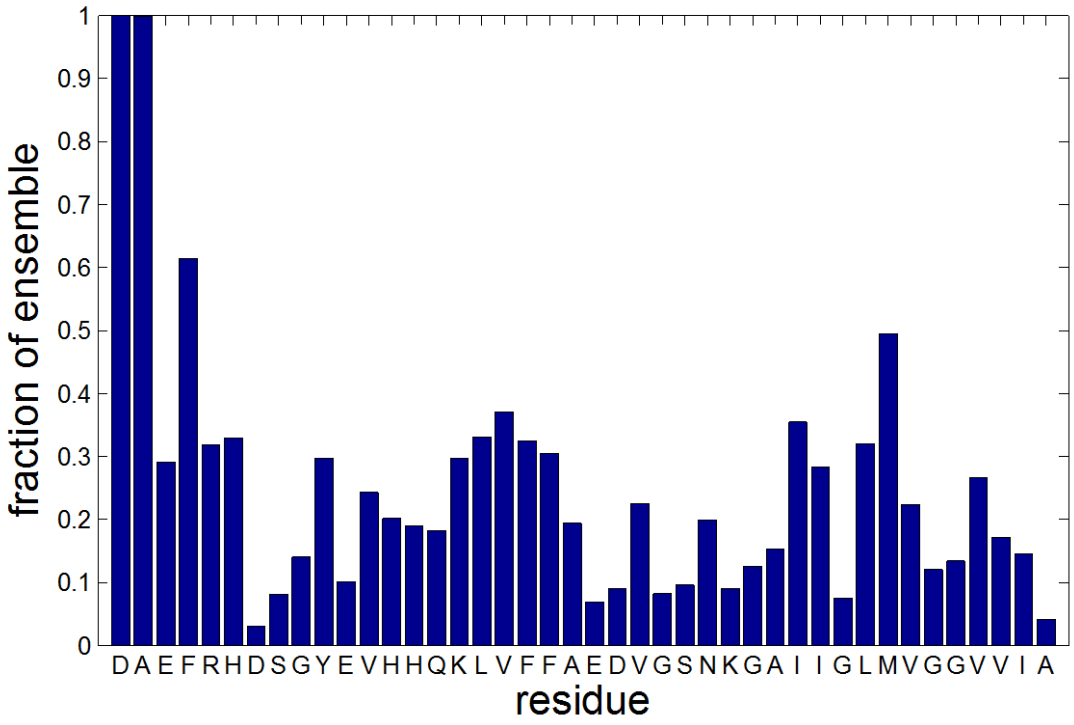

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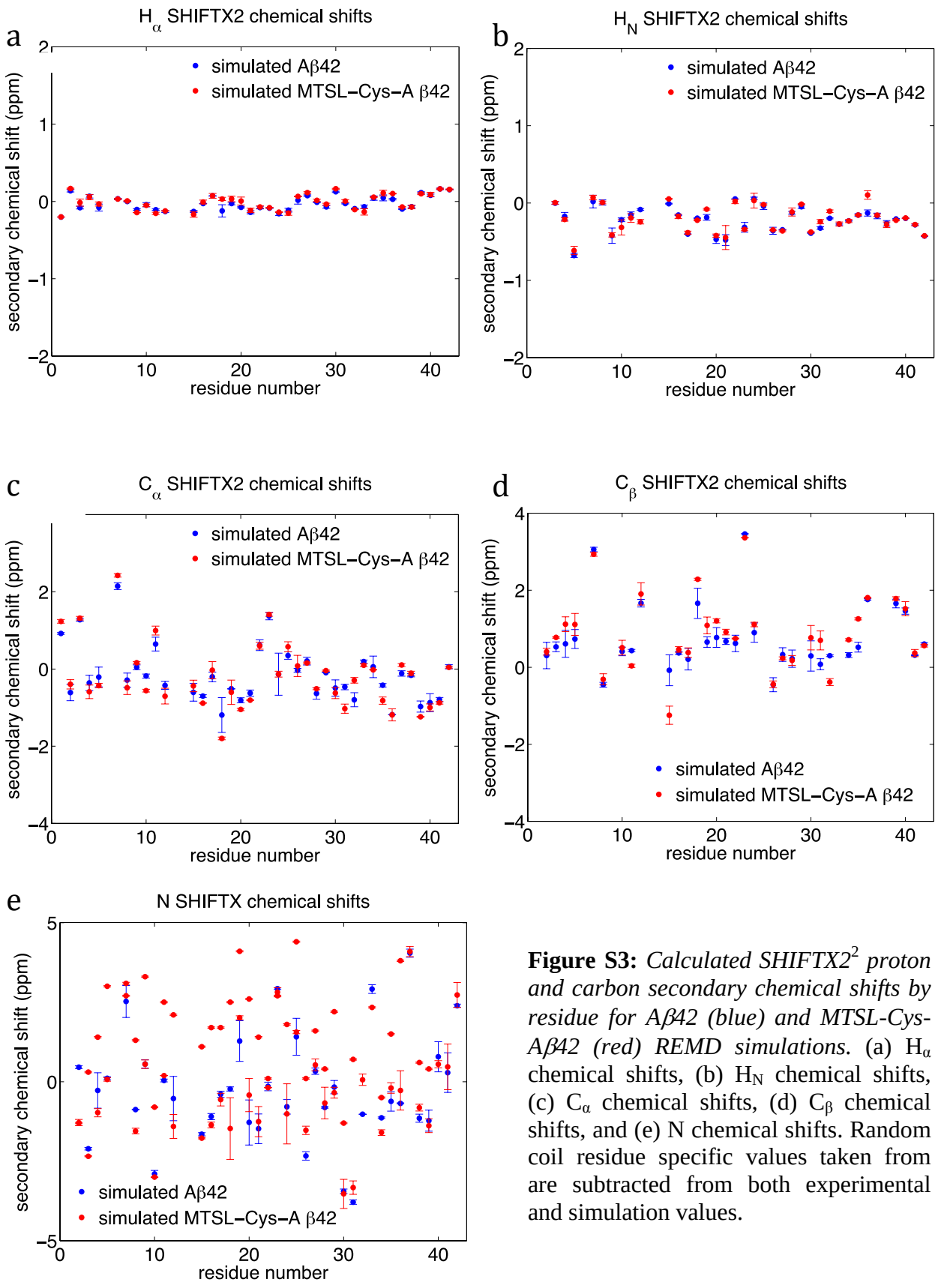

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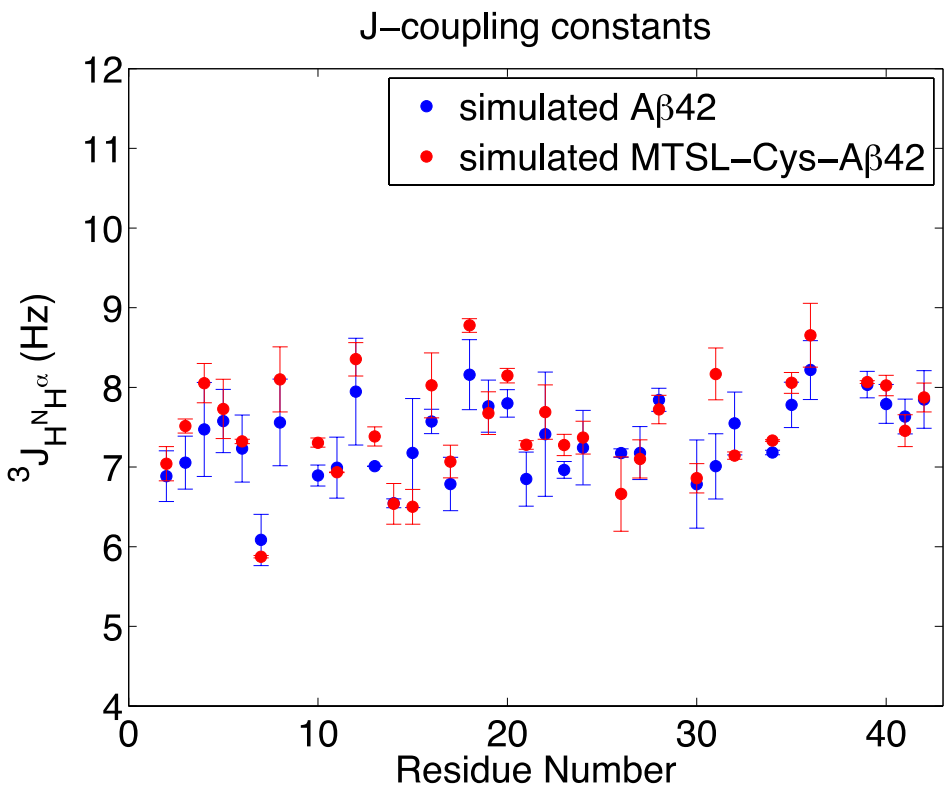

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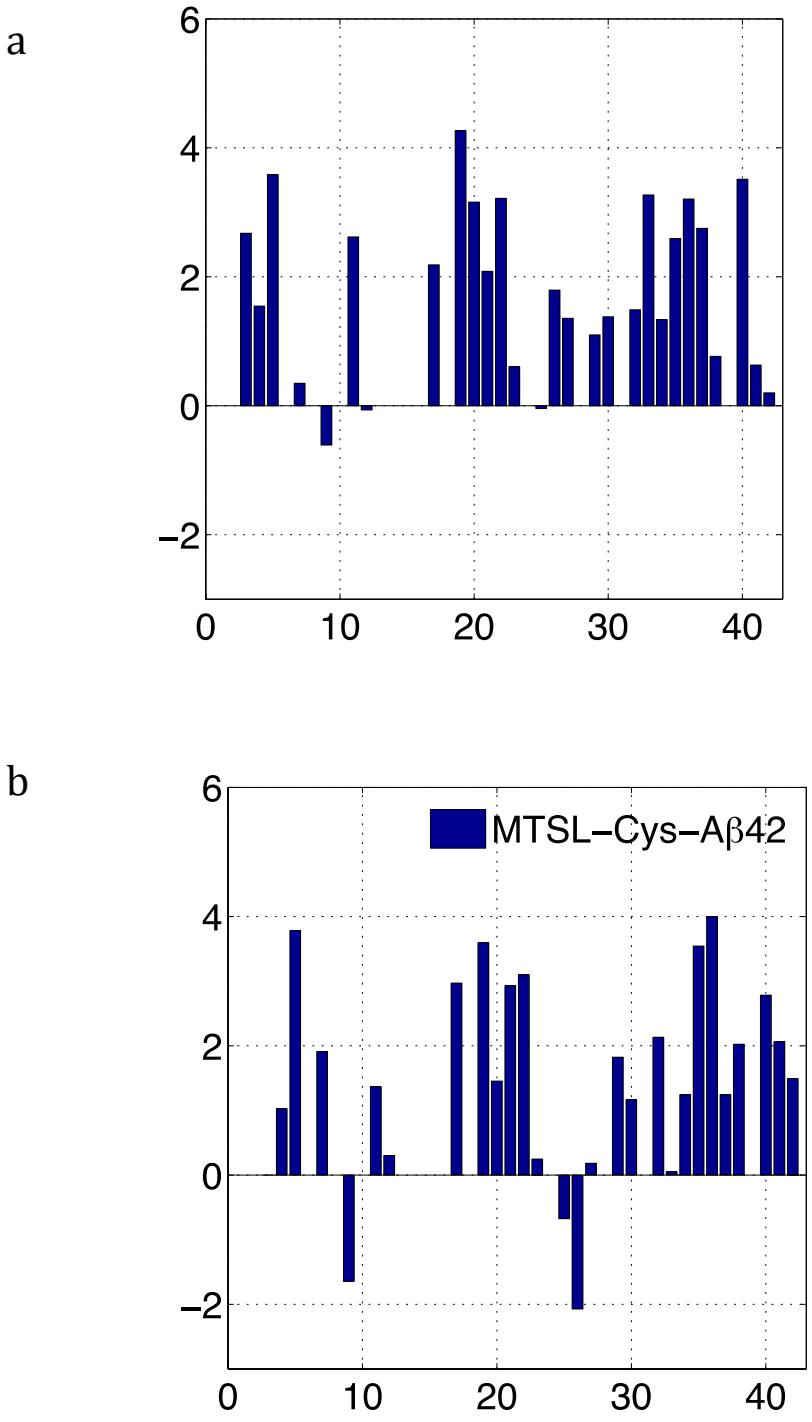

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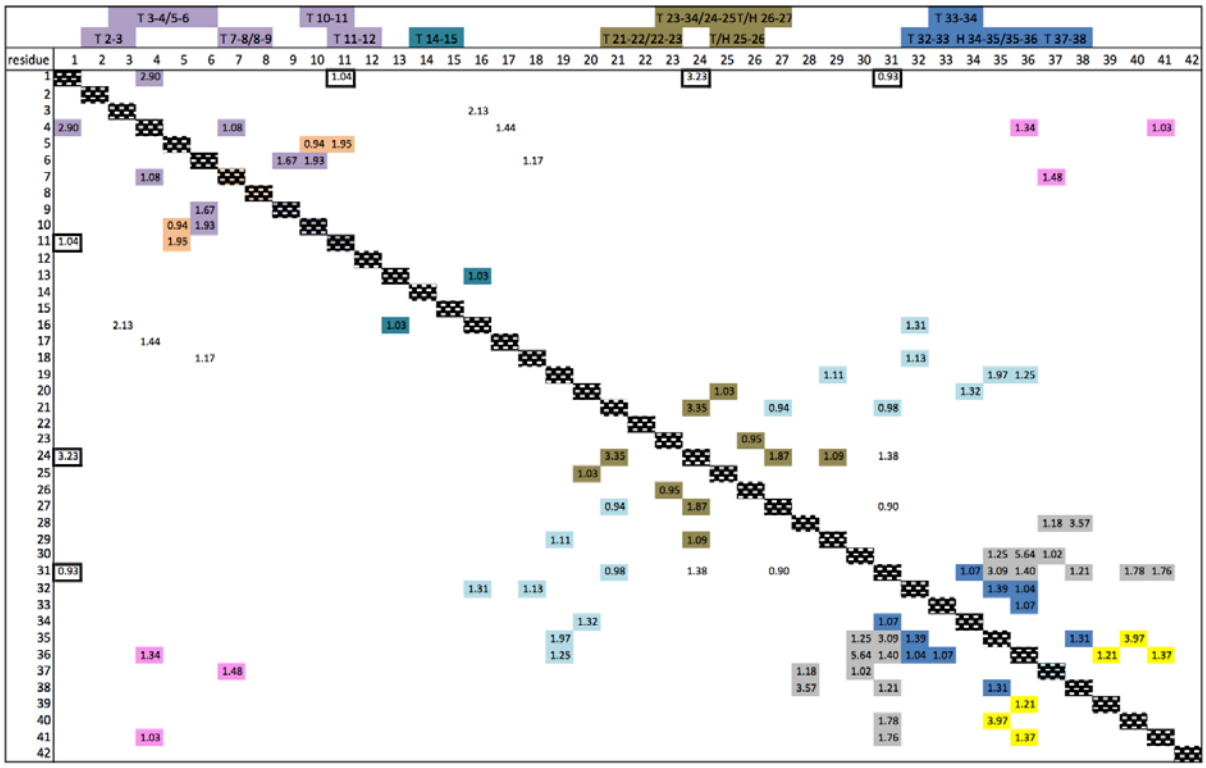

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