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α-Synuclein Conformations Followed by Vibrational Optical Activity. Simulation and Understanding of the Spectra

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Supplementary Information

Contents

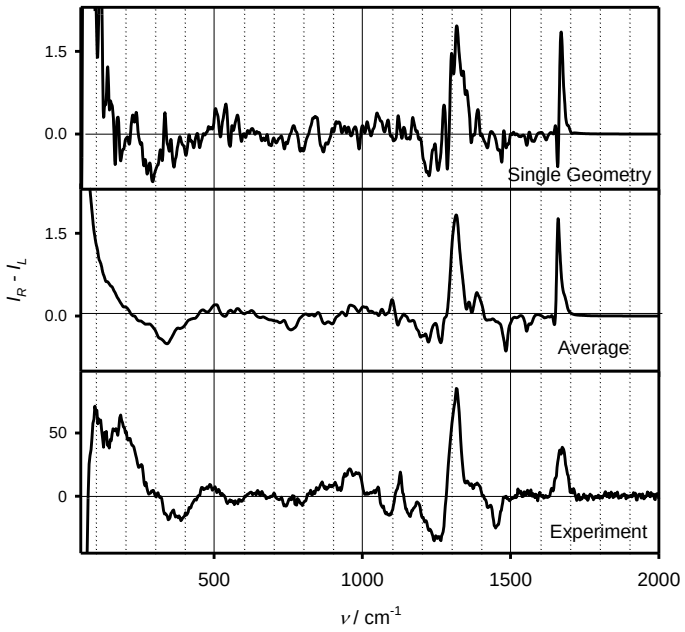


Figure S1. The effect of the averaging: ROA spectrum of disordered αSyn calculated for one MD snapshot geometry, average of 1000 snapshots, and the experiment. (A different water model than in Figure 2 was used in the simulations).

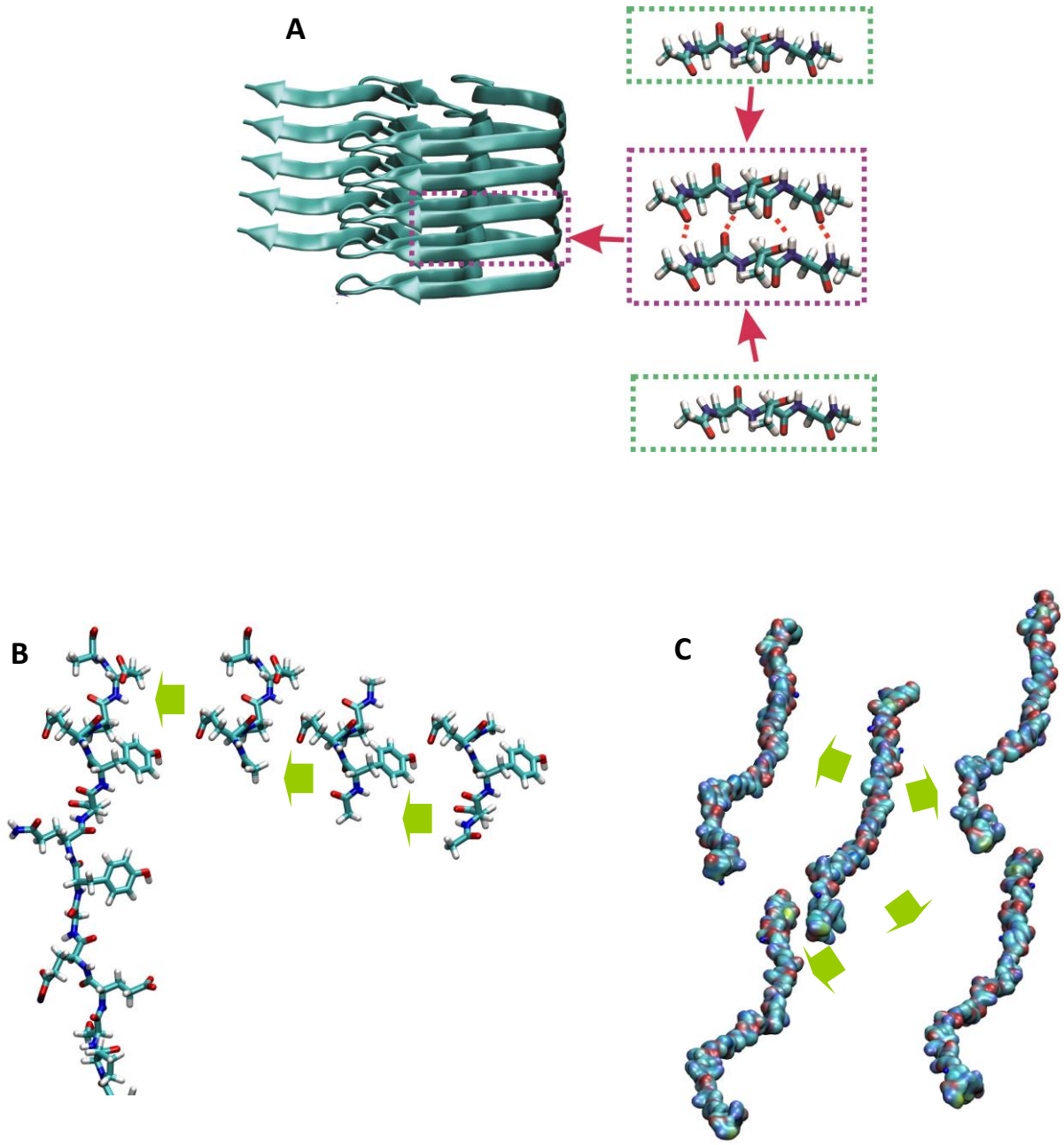


Figure S2. The fragments used to calculate vibrational properties by the CCT method. A) For fibrils, 8-amide fragments (magenta frame) were calculated in a smaller 6-31G** basis, 4-amide fragments (green) were calculated using a bigger 6-31++G** basis set. B) The fragments were partially overlapped, incremented by one amide, illustration for the disordered form. C) Vibrational parameters obtained for one snapshot were distributed to all others (disordered and α-helical forms only).

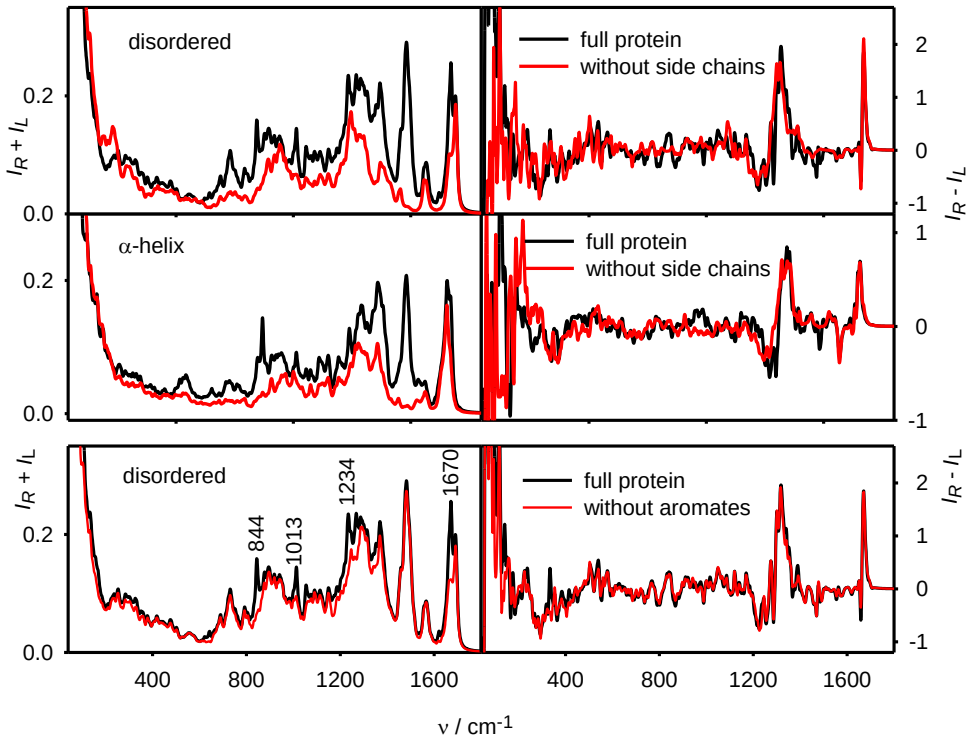


Figure S3. Raman and ROA spectra calculated with and without side chains or aromatic residues.

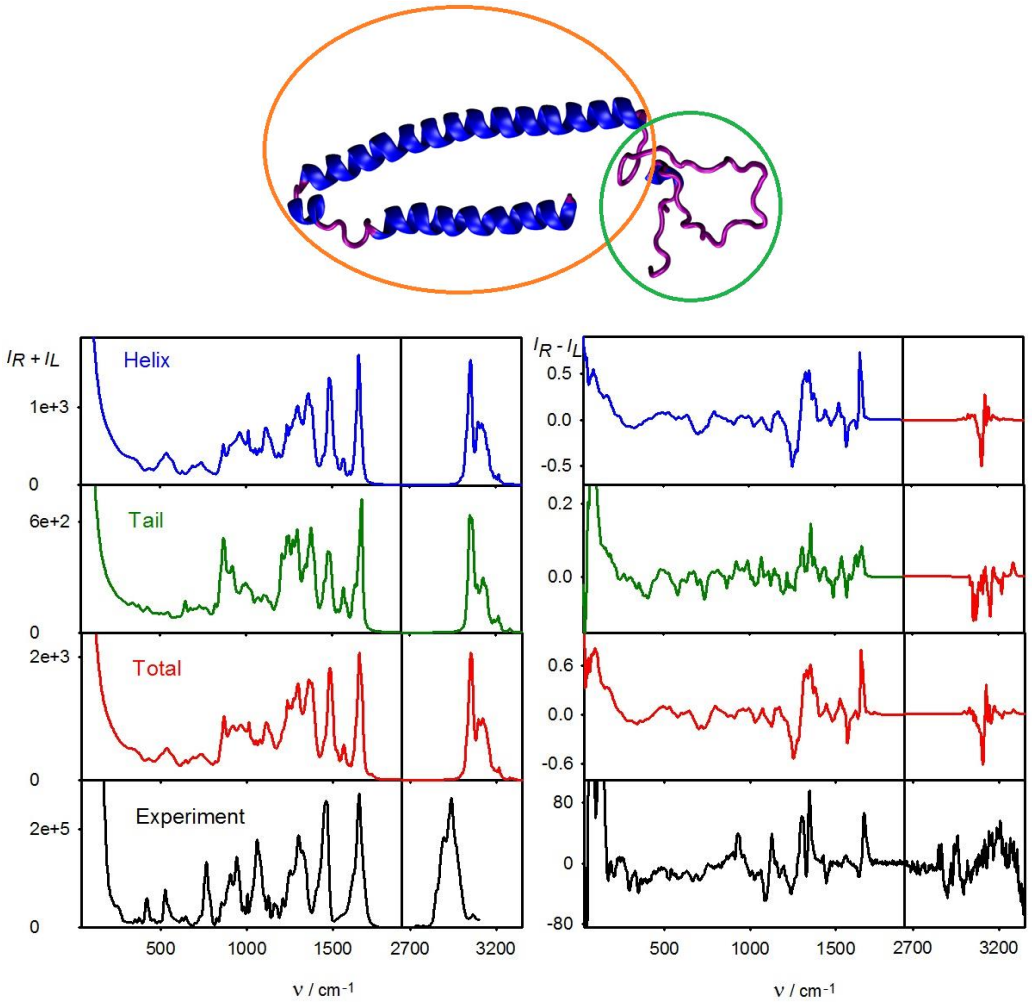


Figure S4. Contribution of the disordered and α-helical parts to α-helical αSyn Raman and ROA spectra.

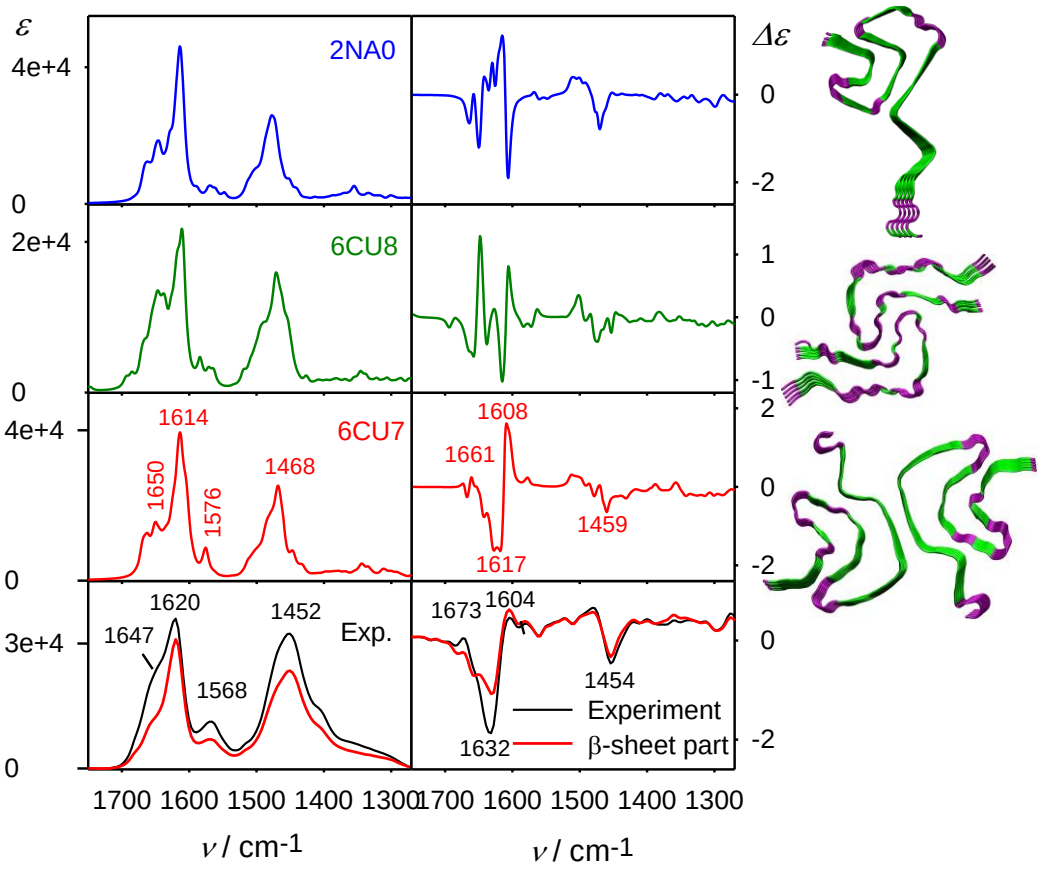


Figure S5. IR and VCD spectra for three PDB αSyn fibril structures calculated for zero twist, and the experiment. In the calculation, 180 monomers were propagated in the periodic model. Pure β-sheet contribution plotted by the red line was obtained by a partial (40%) subtraction of experimental spectra of the disordered form.

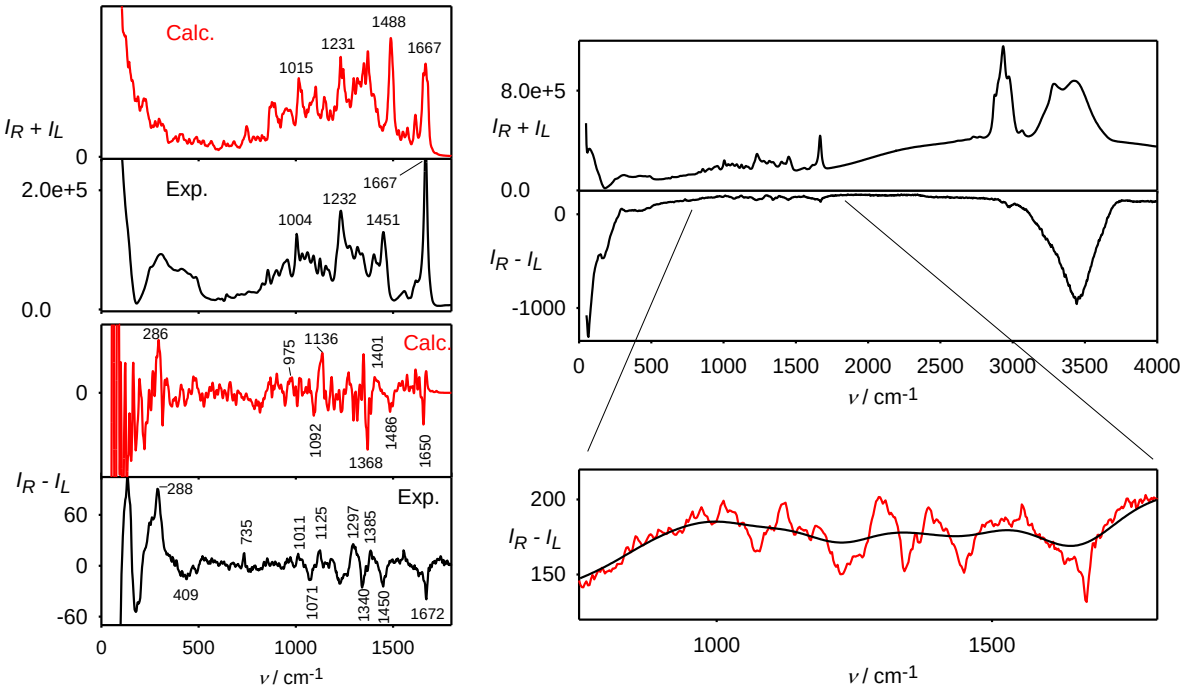
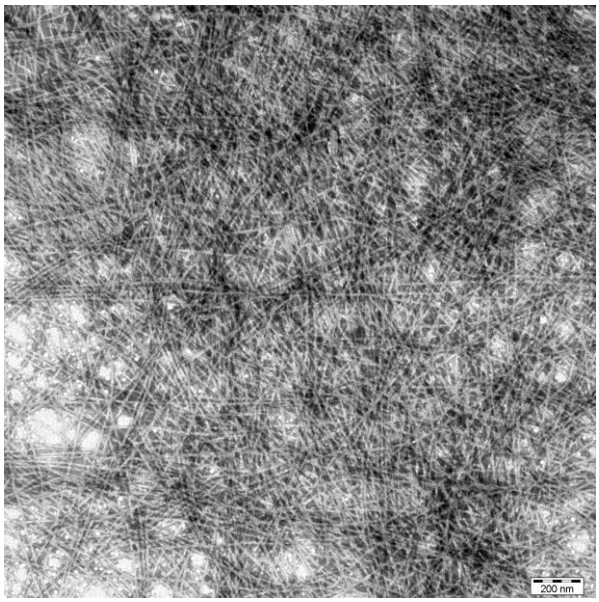


Figure S6. Raman and ROA spectra of αSyn fibrils. Left: simulation (6CU7, 180 molecules, -1° twist) and experimental spectra with subtracted background. Right: raw experimental spectra in the full range, and example of subtraction of the baseline (black) to get the vibrational contributions for ROA.



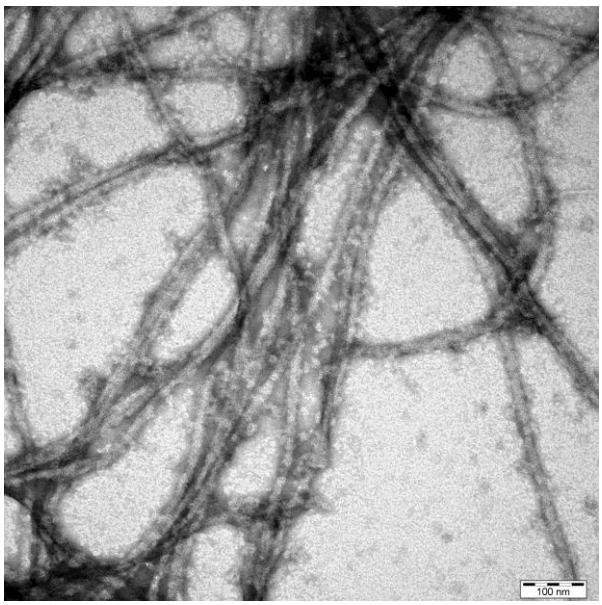


Figure S7. TEM images of αSyn fibrils.