Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Insight into Vibrational Circular Dichroism of Proteins by Density Functional Modeling

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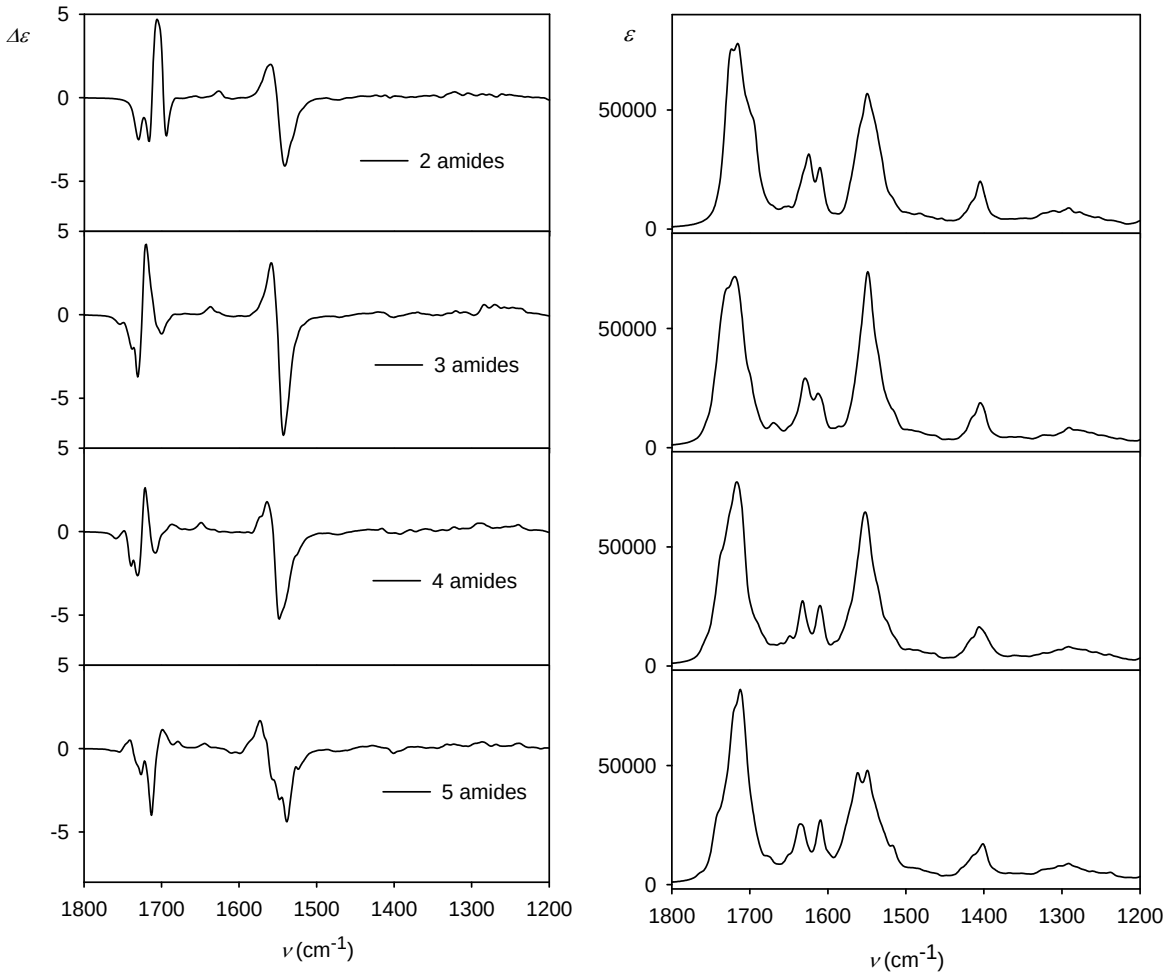


Figure S1. Lactalbumin VCD and IR spectra simulated with fragments of different sizes.

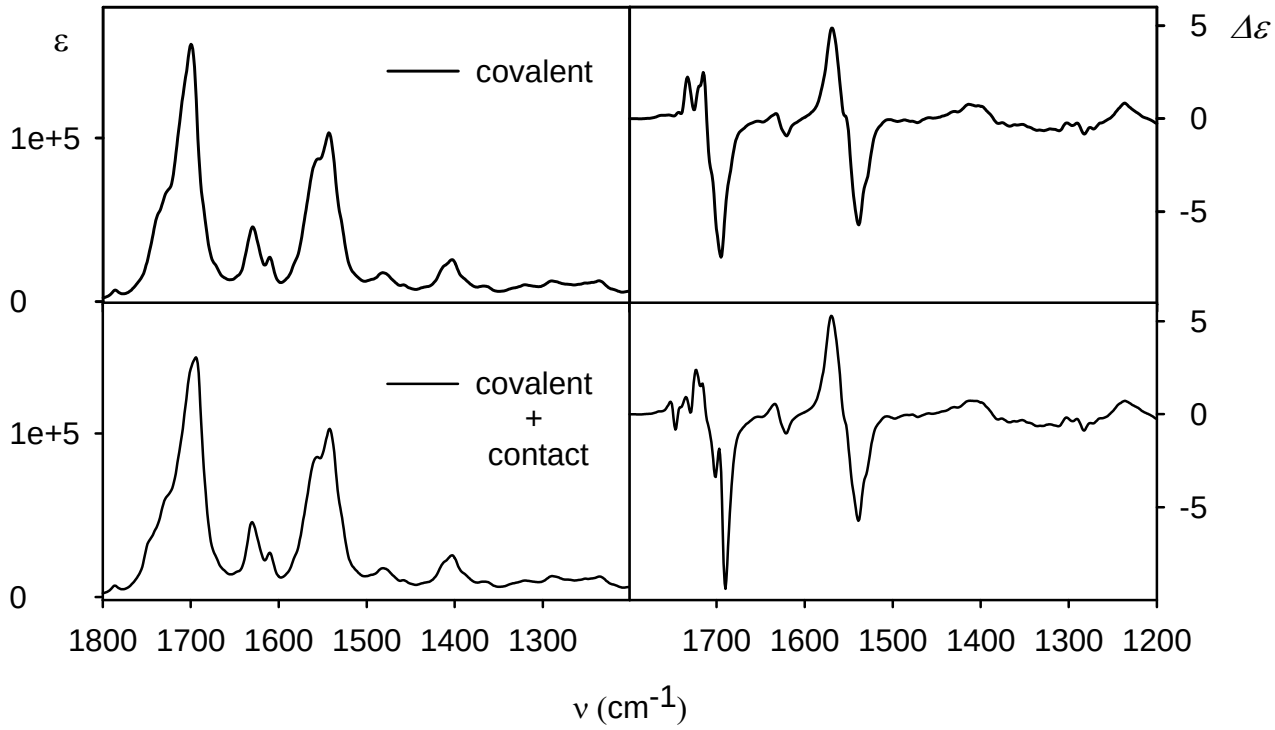


Figure S2. Concanavalin A IR and VCD spectra simulated with covalent fragments and when "contact" fragments across peptide chains were added.

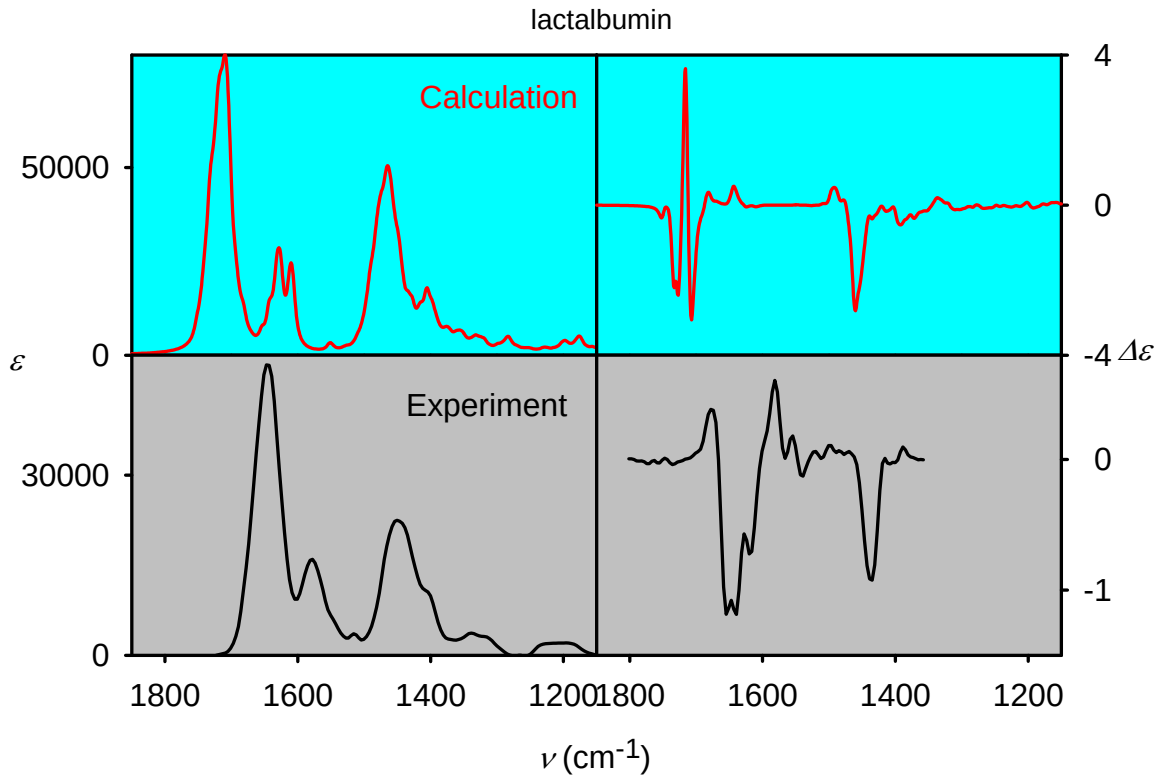


Figure S3. Simulated and experimental α-lactalbumin spectra, measurement in D_2O.

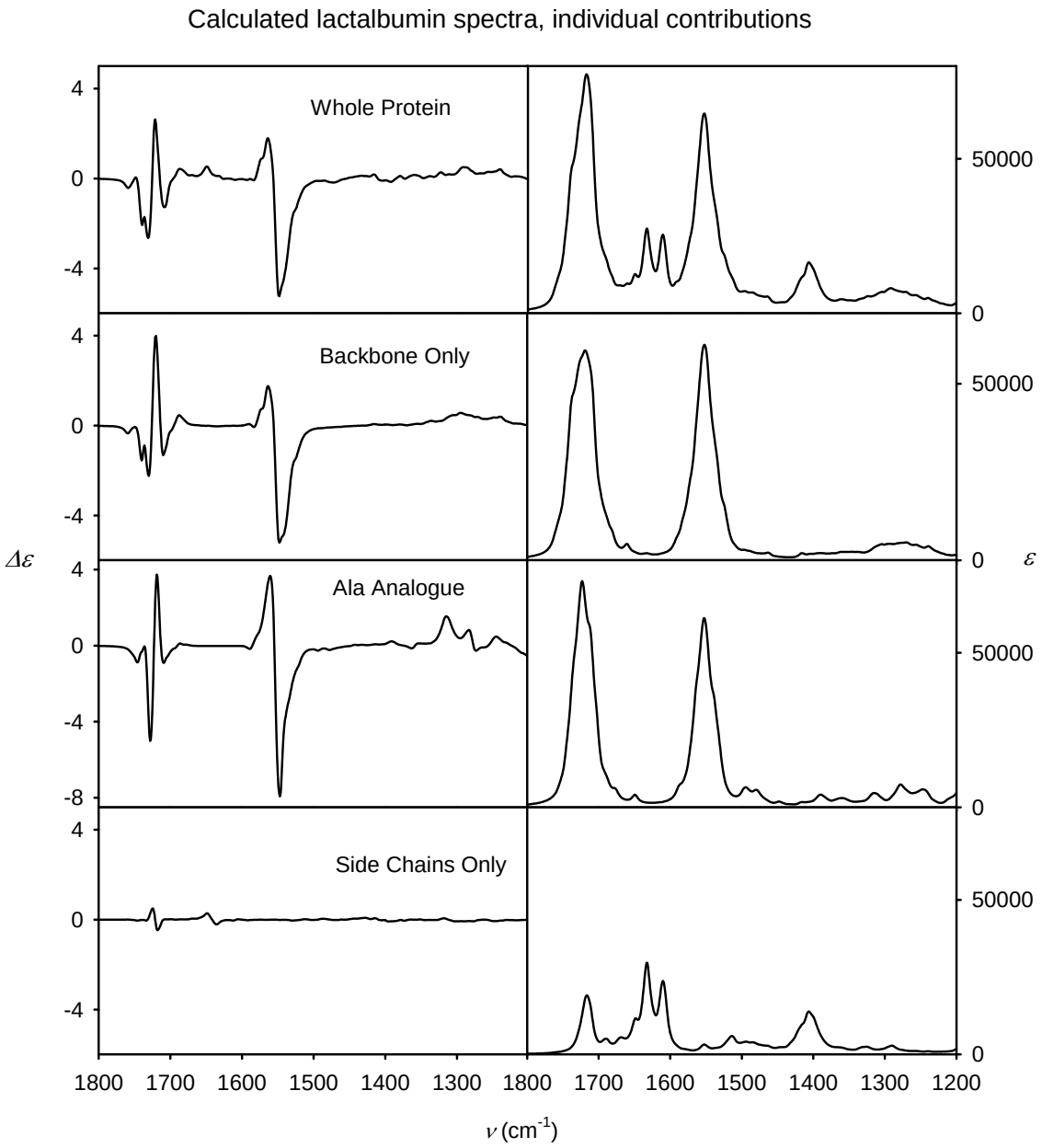
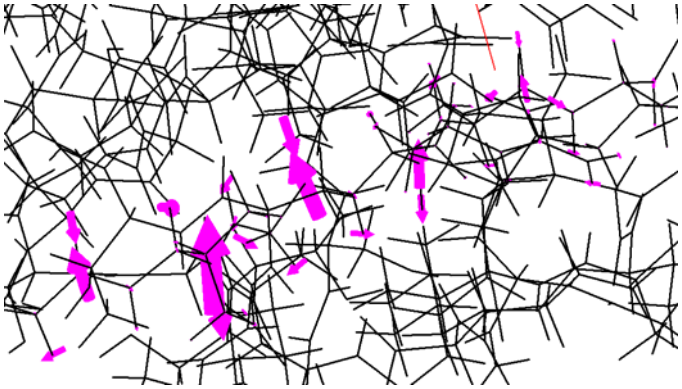
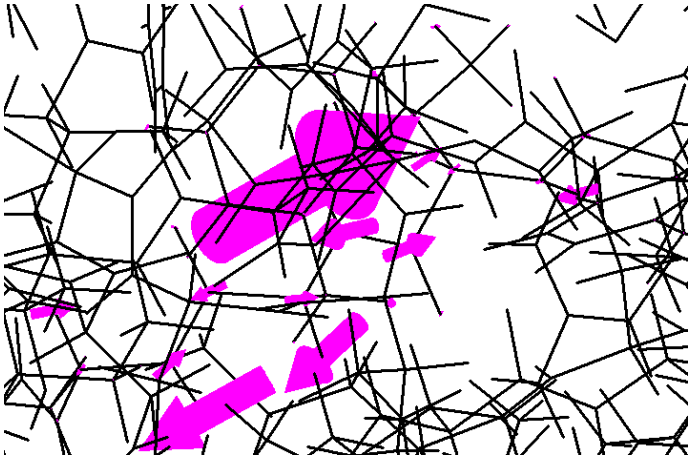


Figure S4. α-lactalbumin spectra simulated for the whole protein, signal from the backbone only, the all-Ala analogue, and signal from the side chains.

1696 cm^{-1}:



1570 cm^{-1}:



1526 cm^{-1}:

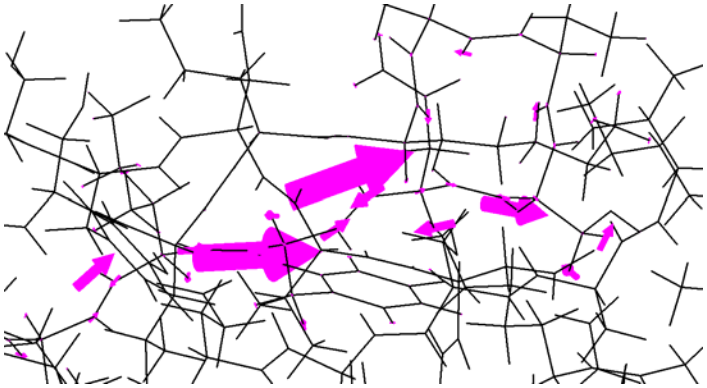


Figure S5. Examples of concanavalin β-strand vibrational modes, 1696 cm^{-1} (amide I, out of phase "+-" C=O stretching), 1570 and 1526 cm^{-1} (amide II, most visible is the in-phase NH bending).

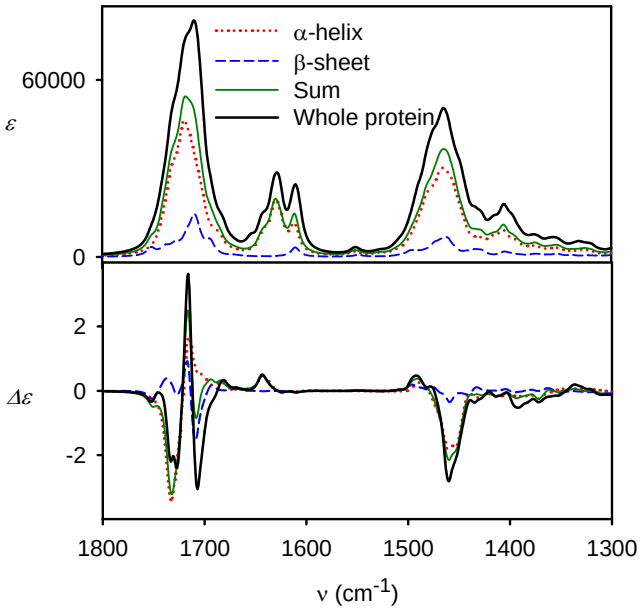


Figure S6. Absorption and VCD spectra of deuterated α-lactalbumin, simulated separately for the whole protein, and α-helical and β-sheet parts.

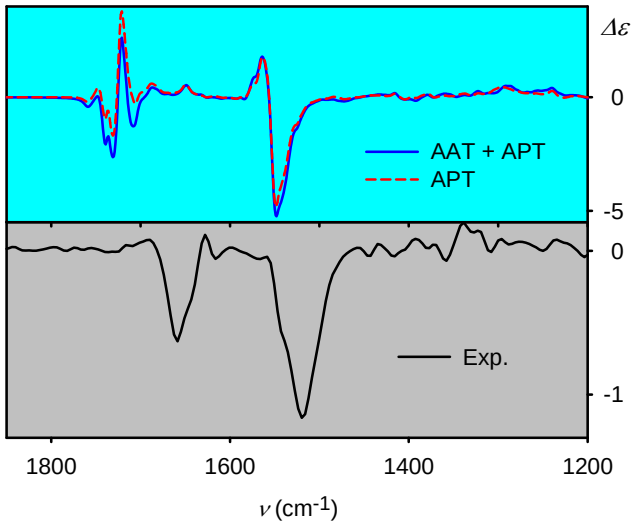


Figure S7. VCD α-lactalbumin spectra simulated with both the AAT and APT contributions, with the APT part only, and experiment.

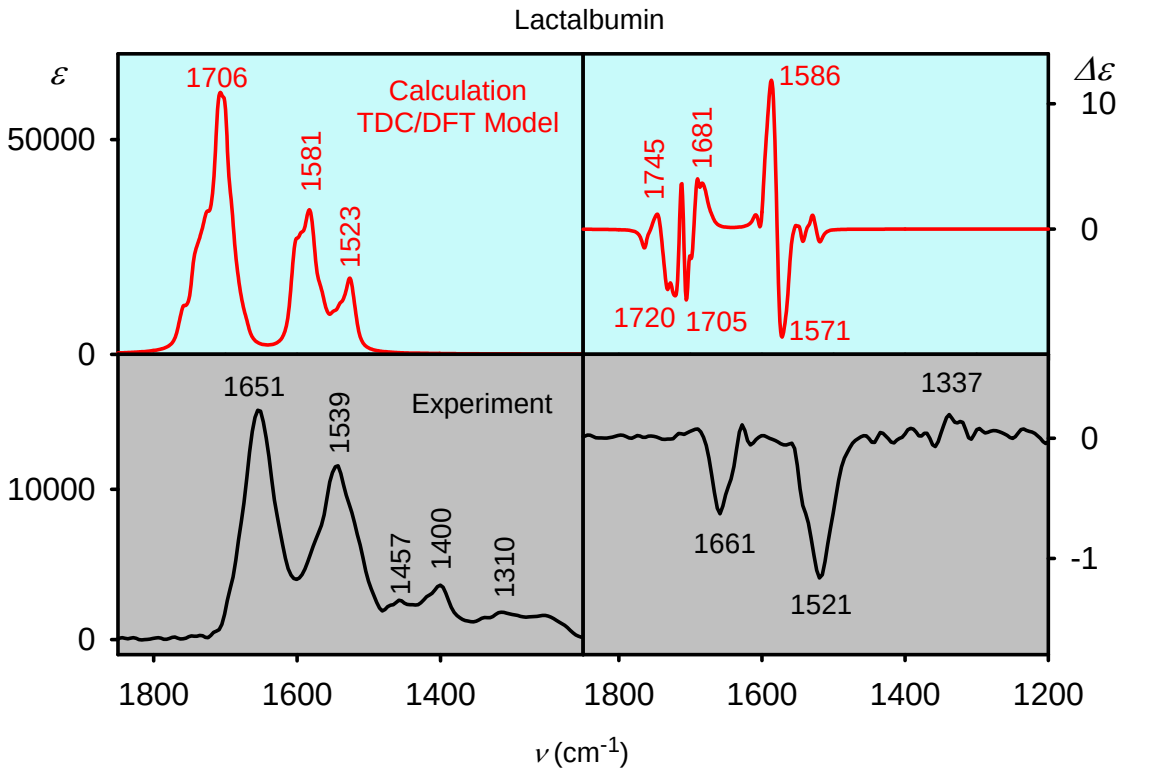


Figure S8. (Top) α-lactalbumin IR and VCD spectra calculated using the TDC model (DFT parameters) and (bottom) the experiment.

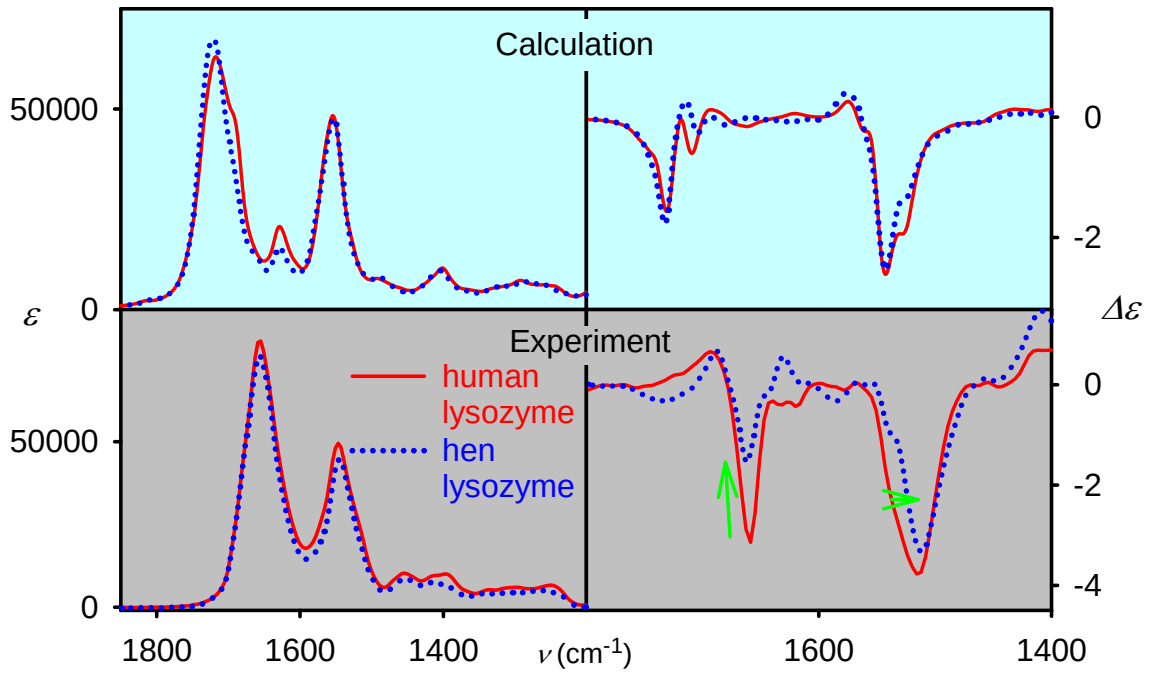


Figure S9. IR and VCD spectra of human and hen egg white lysozyme, simulation (TDC correction not applied) and experiment.

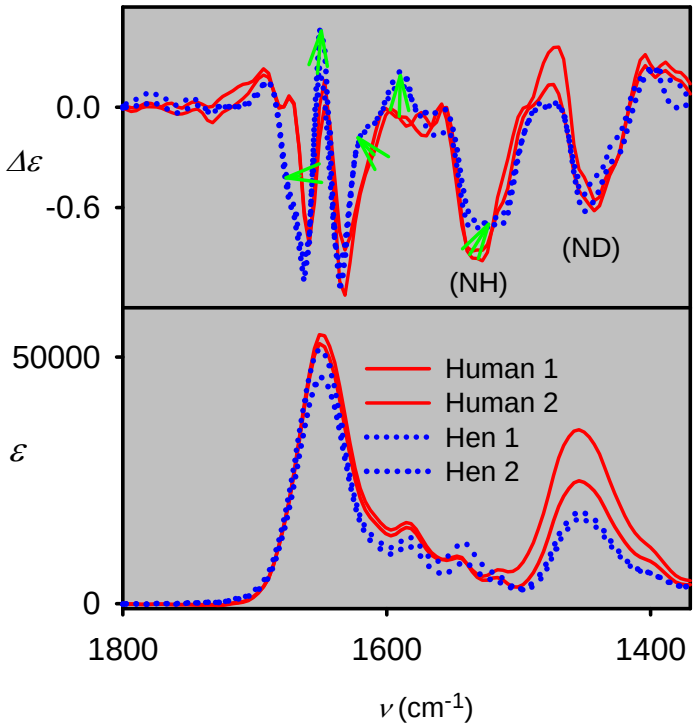


Figure S10. Experimental VCD and IR spectra of human and hen egg white lysozyme in D_2O, two independent measurements for each protein. Because of incomplete H↔D exchange, amide II (NH) is still visible around 1530 cm^{-1}. Around 1460 cm^{-1} the D_2O absorption is difficult to subtract.

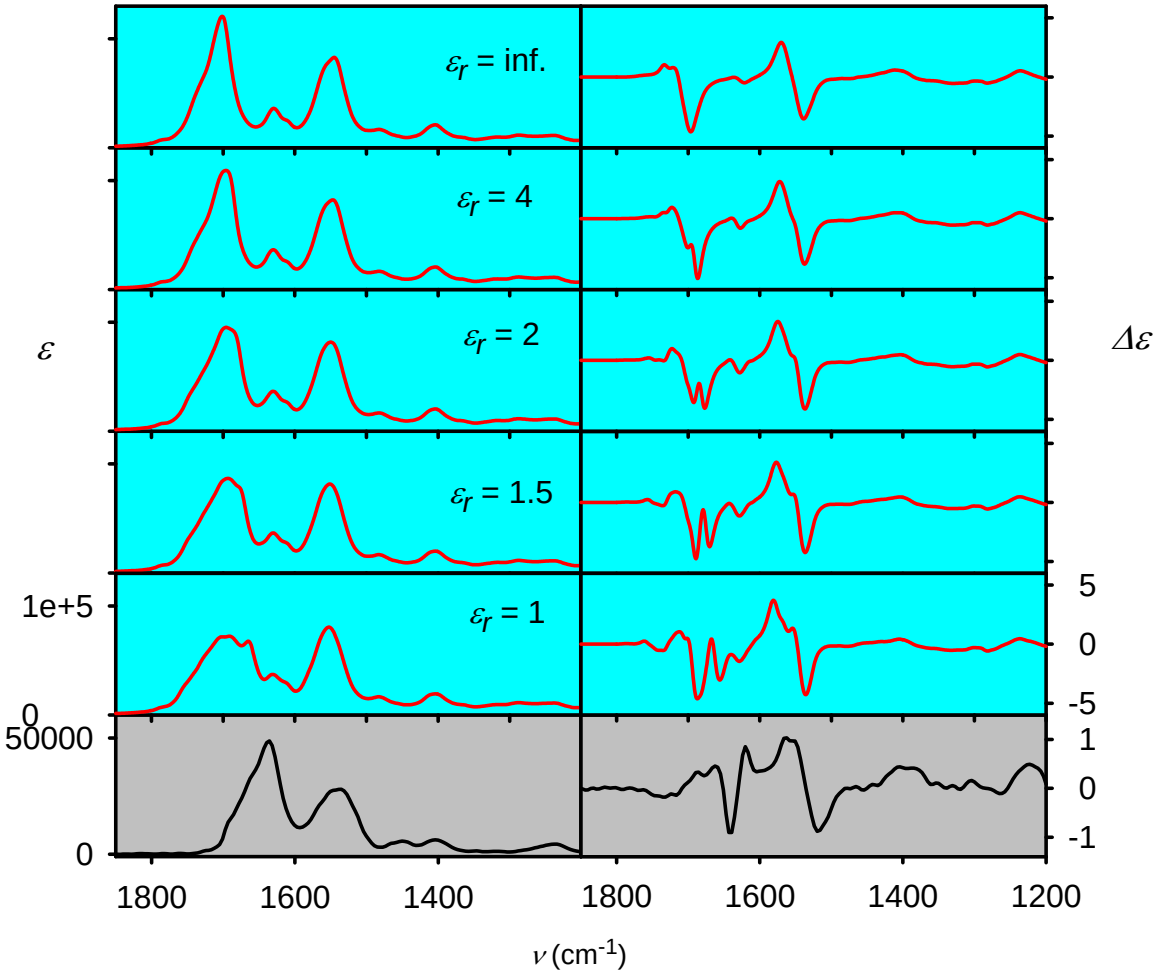


Figure S11. IR and VCD spectra of concanavalin A simulated with the TDC correction, at various values of the dielectric constant; the experiment is at the bottom.