# The Amide I Spectrum of Proteins – Optimization of Transition Dipole Coupling Parameters using Density Functional Theory Calculations

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The two spreadsheets contain a comparison of the reconstructed DFT F matrices and theTDC F matrices with optimized TDM parameters. Each file shows the coupling constants grouped by the type of arrangement between the interacting amide groups as well as the deviations between TDC and DFT coupling constants. Each individual interaction is indicated by the numbers of the interacting amide groups. For example, in the “Intrachain parallel” section, “1-3” indicates the parallel arrangement between the C=O bonds of amide groups 1 and 3. Additional listed information is: the distance between the TDMs of the amide groups (in Å) calculated with our optimized position (see Tab. 1 of the main text); the angle between the TDMs of the amide groups (in degrees); the angle between the TDM of the first amide group and the connecting vector between the amide groups (in degrees); the angle between the TDM of the second amide group and the connecting vector between the amide groups (in degrees).
Each file contains also the DFT F matrix and the TDC F matrix, then the absolute and squared differences for each element.

“SI - f matrix analysis all” → Optimization using the six structural models together. The F matrices from Matlab are obtained using the optimized parameters for our optimized position for the TDM (see Tab. 1 of the main text).

“SI - f matrix analysis secondary structure” → Optimization for each secondary structure separately. The F matrices from Matlab are obtained using our optimized position for the TDM (see Tab. 1 of the main text) and the best value for A for each secondary structure (see Tab. 2 of the main text).

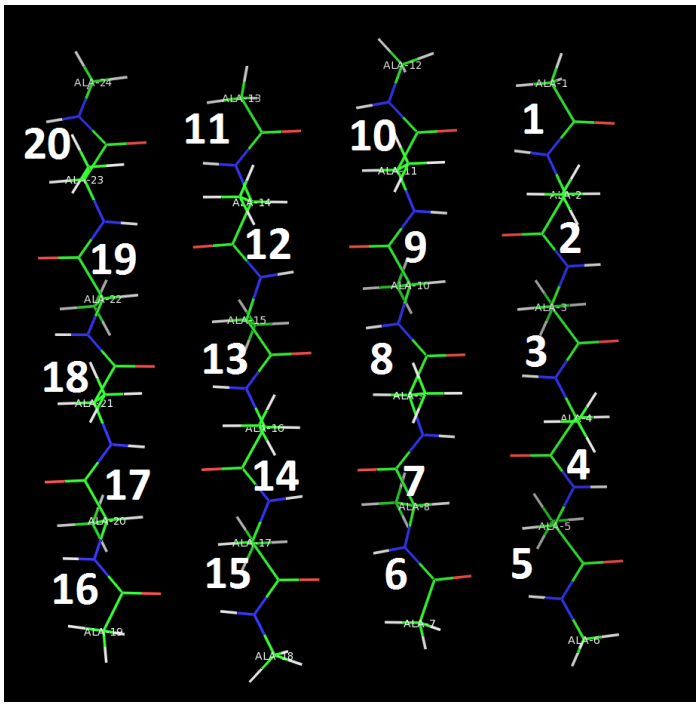


*Figure S1. Antiparallel β-sheet model structure, with 4 strands and 5 amide groups per strand. The number of the amide groups is indicated.*

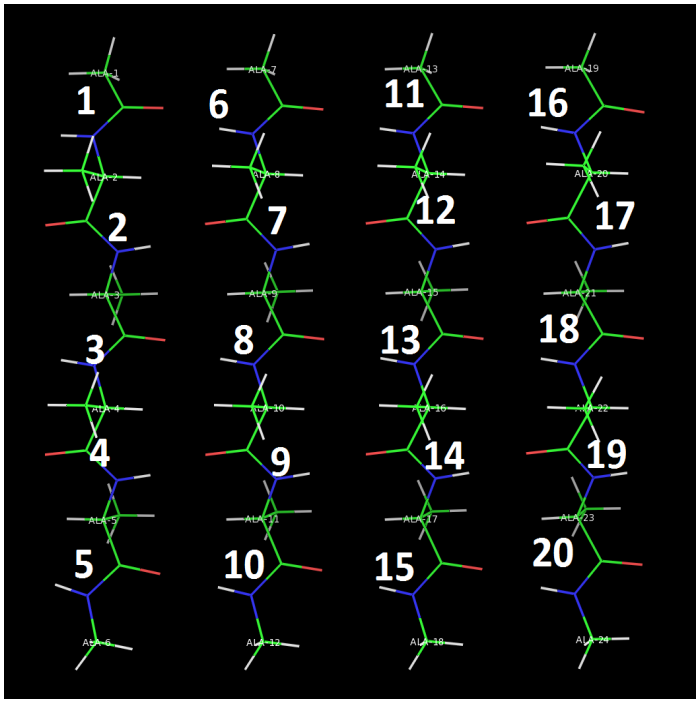


*Figure S2. Parallel β-sheet model structure, with 4 strands and 5 amide groups per strand. The number of the amide groups is indicated.*

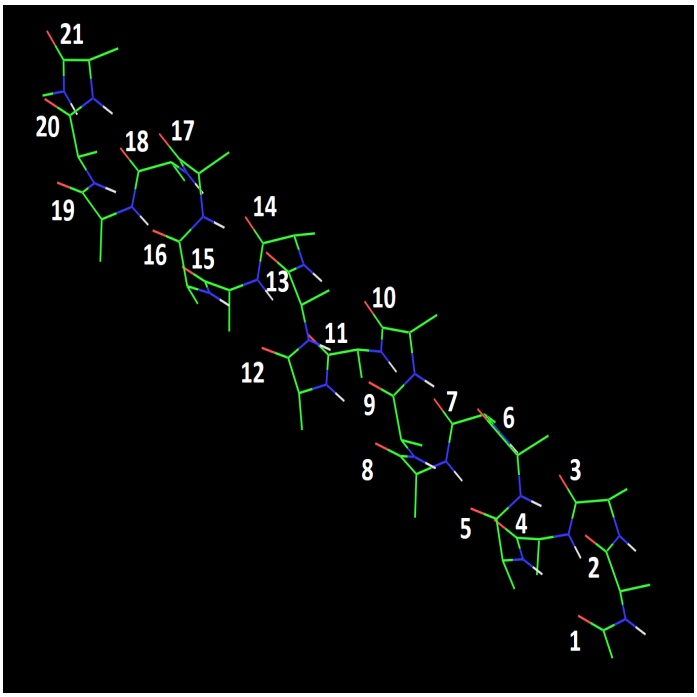


*Figure S3. α-helix with 21 amide groups and indicated number of the amide groups.*

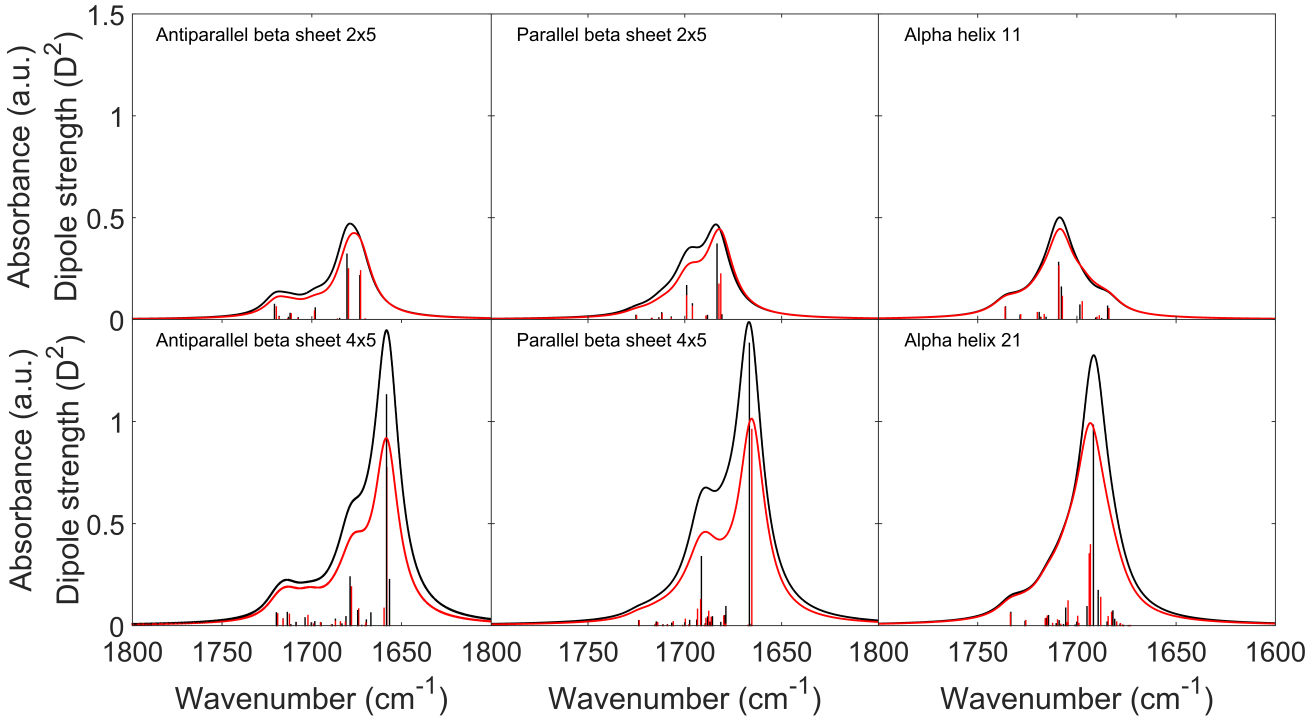


*Figure S4. Comparison between IR spectra from DFT calculations (black) and TDC calculations (red), using optimized TDM parameters and TDC F matrices after applying the cutoff on the coupling constants (between -0.002 and 0.001 mdyn Å$^{-1}$ u$^{-1}$). The dipole strengths of the normal modes are shown as bars.*

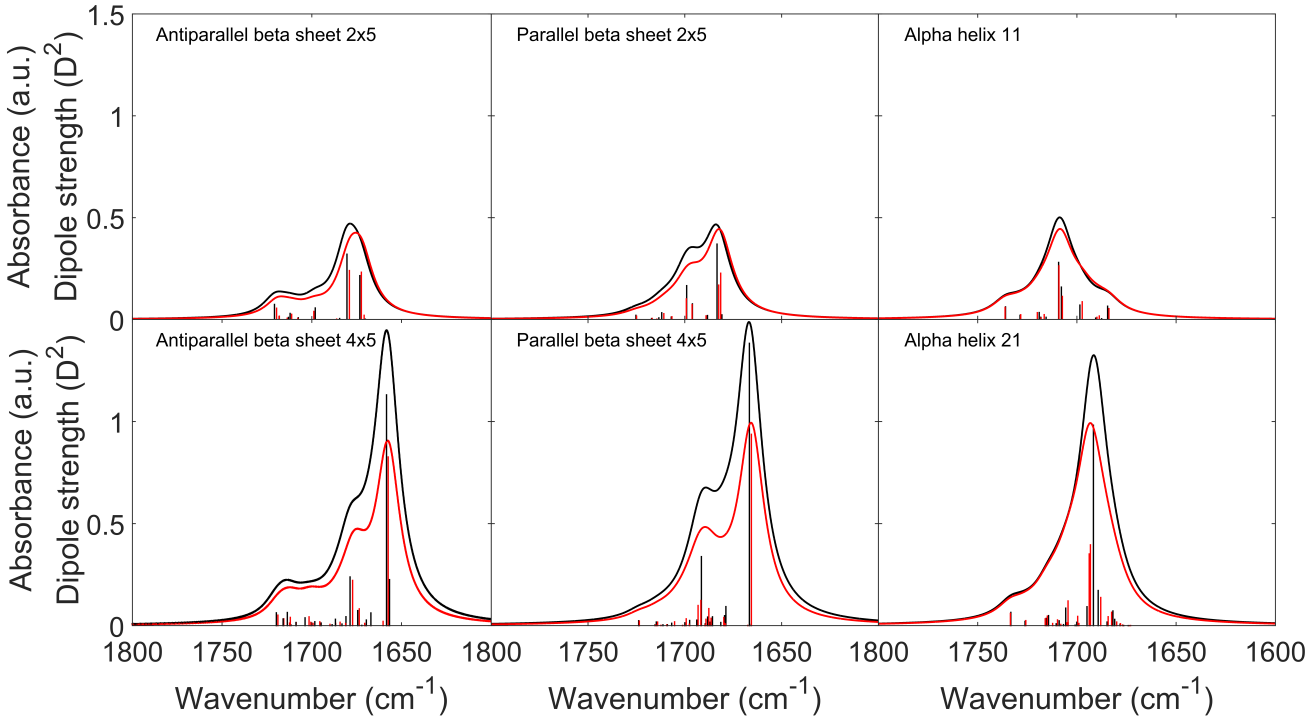


*Figure S5. Comparison between IR spectra from DFT calculations (black) and TDC calculations (red), using optimized TDM parameters and TDC F matrices after applying the cutoff on the coupling constants (between -0.002 and 0.002 mdyn Å$^{-1}$ u$^{-1}$). The dipole strengths of the normal modes are shown as bars.*

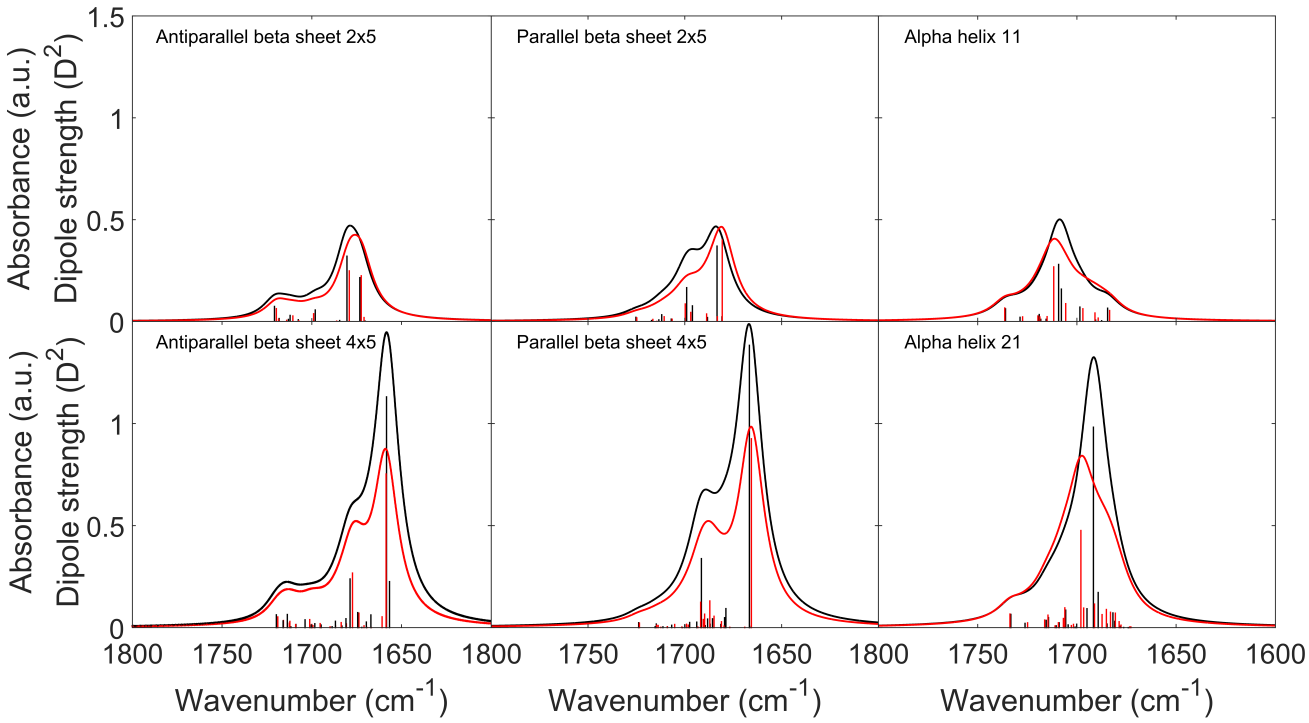


*Figure S6. Comparison between IR spectra from DFT calculations (black) and TDC calculations (red), using optimized TDM parameters and TDC F matrices after applying the cutoff on the coupling constants (between -0.005 and 0.005 mdyn Å$^{-1}$ u$^{-1}$). The dipole strengths of the normal modes are shown as bars.*