Supporting Information: Determination of Absolute Orientation of Protein α-helices at Interfaces using Phase Resolved SFG Spectroscopy

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Definition of the transition diploe moments and molecular hyperpolarizability

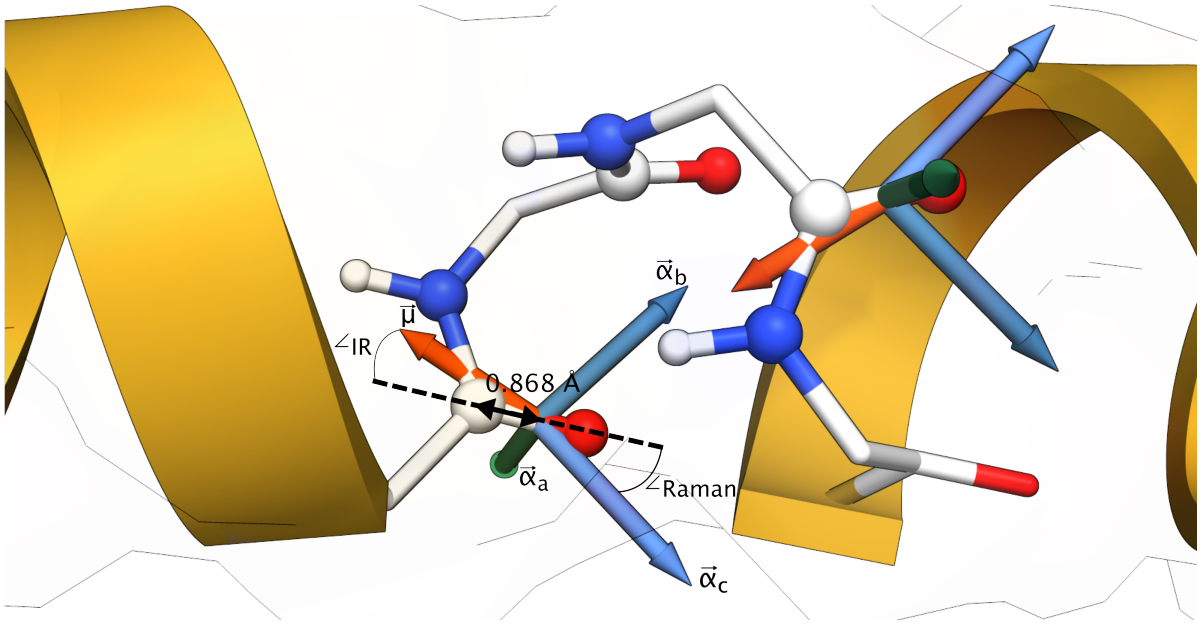

Figure S1. Orientation of the amide-I IR transition dipole moment $\vec{\mu}$ or TDM (orange) and Raman polarizability tensor axes $\vec{\alpha}_a$, $\vec{\alpha}_b$, $\vec{\alpha}_c$, in green, light blue and dark blue, respectively. The backbone C, O, N, H atoms that contribute to the amide-I modes of the three residues are depicted as balls. The TDM is positioned at 0.868 Å from the C atom at the C=O bond (Sandeman, I. Amide Bands in Infra-Red Spectra: the Direction of the Transition Moments of Bands in N, N′-Diacetylhexamethylenediamine. Proc. R. Soc. London, A 1955, 232, 105–113; Moore, W. H.; Krimm, S. Transition Dipole Coupling in Amide I Modes of β-Polypeptides. Proc. Natl. Acad. Sci. U.S.A. 1975, 72, 4933.). The value indicated for the angle between the transition-dipole moment and the C=O bond axis is the average angle calculated using the transition charges, for a typical protein.

Calculation of the peptide orientations

The vectors A and B were constructed between carbon alpha atoms 4 and 5 (A) and 5 and 6 (B). The vectors A and B are summed and normalized to the length of A. The resulting vector is termed V1. The procedure was repeated for carbon alpha atoms 9, 10 and 11, resulting in the normalized Vector V2. For an ideal helix the cross product of V1 and V2 lies in the direction of the helix because V1 and V2 are perpendicular to the helix axis. The angle between the cross product P and the z-axis (surface normal) is determined by trigonometry. The orientation of alpha helices was calculated for frames of the last 50 ns of the 100 ns long simulation (100 frames).