Abstract Submitted
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Spectral Signatures of 3_{10}- and α-Helices Revealed by Two-Dimensional Infrared Spectroscopy[1] NIEN-HUI GE, HIROAKI MAEKAWA, Department of Chemistry, University of California at Irvine, CLAUDIO TONIOLO, Department of Chemistry, University of Padova, Italy, QUIRINUS BROXTERMAN, DSM Research, Life Sciences, Advanced Synthesis and Catalysis, The Netherlands — Femtosecond two-dimensional infrared (2D IR) spectroscopy is applied to the amide I modes of the homo-octapeptide Z-[L-(αMe)Val]$_8$-OtBu in $CDCl_3$, TFE and HFIP solutions to acquire 2D spectral signatures that distinguish between 3_{10}- and α-helix structures. Suppression of diagonal peaks by controlling polarizations of IR pulses clearly reveals cross-peak patterns that are crucial for structural determination. A doublet feature is observed when the peptide forms a 3_{10}-helix in $CDCl_3$ and TFE, and when it is at the initial stage of 3_{10}- to α-helix transition in HFIP. In contrast, the 2D IR spectrum shows a multiple peak pattern after the peptide has become an α-helix in HFIP. This is the first report on the experimental 2D IR signature of a 3_{10}-helical peptide. These results for a model octapeptide demonstrate the powerful capability of 2D IR spectroscopy to discriminate between different helical structures.

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