Conformational dynamics in peptides: Ultrafast triggering and transient two-dimensional infrared spectroscopy

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Picosecond conformational transition and equilibration of a cyclic peptide

Ultrafast IR spectroscopy is a useful tool to study the conformational dynamics of a cyclic peptide. We investigated the conformational transition of a cyclic peptide at two separated wavelengths. A conformational change is induced by light, allowing the probing of the peptide backbone. The results show the importance of the peptide backbone in controlling the conformational transition.

Photo-control of an α-helix

The linear peptide was designed to show a strong propensity to form an α-helix. Upon excitation, a strong change in helix content is observed. In contrast to the original peptide, the helix content is reduced, indicating that the peptide backbone plays a crucial role in controlling the conformation.

How small can a photoswitch be?

Replacing D by S is one of the simplest and most widely used methods to create a photoswitch. However, this approach has limitations. For example, a single atom compared to the original peptide molecule differs. To characterize this type of photoswitch, we investigated N-methylthioacetamide (NMTAA).

Towards measuring transient structures

2D-IR spectroscopy is a powerful tool to study transient structures. We extend the application of 2D-IR spectroscopy to the measurement of non-equilibrium states. Here, we investigate the conformational transition of the cyclic peptide. The time dependence of the 2D-IR spectra shows a significant time dependence, where the 1D spectrum changes only slightly. We use 2D-IR spectroscopy to extract structural parameters and understand the transient structure.