

Solvent-Enhanced Conformational Flexibility of Cyclic Tetrapeptides



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The front cover artwork is provided by the groups of Prof. Wolfram Sander (Ruhr-Universität Bochum) and Prof. Elsa Sanchez-Garcia (University of Duisburg-Essen). The image shows the structure of a cyclic tetrapeptide in solution. The dynamics of the peptide in explicit solvent was investigated using several computational and experimental techniques at different temperatures. Read the full text of the Article at 10.1002/cphc.201900345.

What is the most significant result of this study?

We propose a mechanism behind the temperature-dependent solvent-controlled conformational flexibility of cyclopeptides. Rather than by strong and specific solvent-peptide interactions, this regulation is achieved by changes in the intramolecular interaction pattern of the peptide due to the combined contribution of several weak intermolecular interactions. This mechanism of solvent regulation of protein structural properties can find applications in the development of peptide ligands that regulate protein-protein interactions.

What inspired you for the cover image?

The interdisciplinary character of our research, within the framework of the Excellence Initiative RESOLV (EXC-2033). The interplay between computations and experiments allowed us to address the complexities of peptides' dynamics and interactions with the solvent.

Who designed the cover?

The cover was designed by Dr. Joel Mieres-Perez.

What other topics are you working on at the moment?

The group of Prof. Wolfram Sander specializes in physical organic chemistry, with focus on the chemistry of highly reactive intermediates such as carbenes, nitrenes and polyradicals. The group of Prof. Elsa Sanchez-Garcia focuses on theoretical approaches to investigate the structural properties and reactivity

of complex chemical and biological systems, with emphasis on multiscale approaches.

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