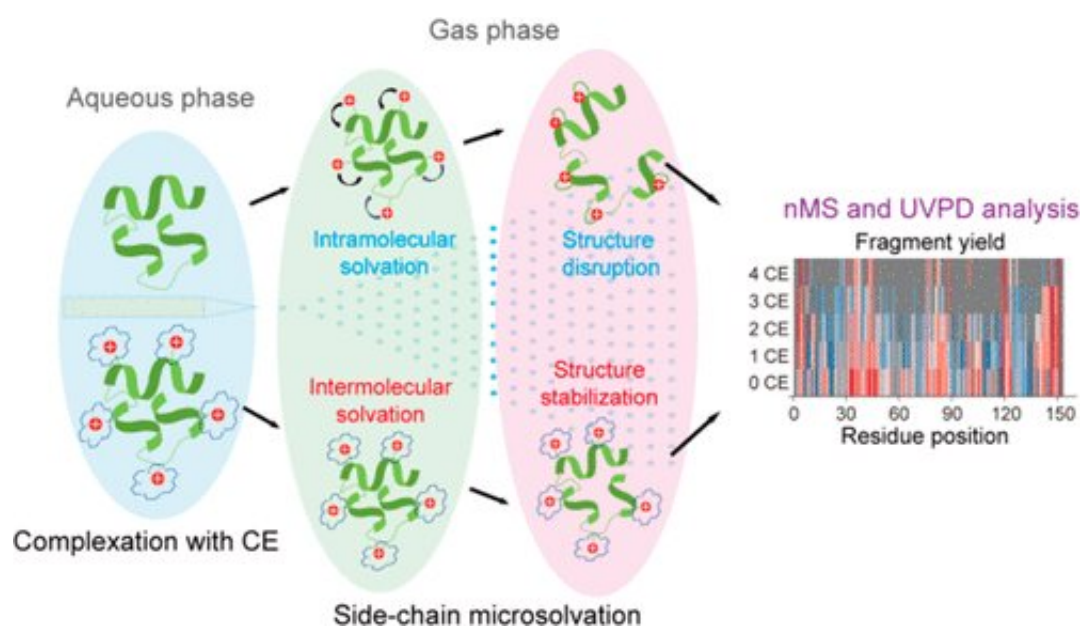


Researchers reveal molecular mechanism of crown ether microsolvation effect on gas-phase native-like protein structure

February 21 2023, by Li Yuan



Graphical abstract. Credit: *Journal of the American Chemical Society* (2022). DOI: 10.1021/jacs.2c11210

A research group led by Prof. Wang Fangjun from the Dalian Institute of Chemical Physics (DICP) of the Chinese Academy of Sciences (CAS), in collaboration with Prof. Shun Feng from Southwest Jiaotong University, has revealed the molecular mechanism of the crown ether microsolvation effect on the gas-phase native-like protein structure by integrating native mass spectrometry (nMS) with 193 nm ultraviolet

photodissociation (UVPD).

This study was published in the *Journal of the American Chemical Society* on Dec. 30, 2022.

The nMS is a cutting-edge technique for studying the composition and structure of proteins and their complexes. Non-denaturing electrospray ionization uses biocompatible solutions to transfer proteins from liquid to gas phase while maintaining higher order structure and interactions.

However, positive charged residues in [protein](#) will form [hydrogen bonds](#) with protein backbone carbonyls to stabilize the positive charges of the side chains through intramolecular solvation.

Although the change of protein collision cross-sectional area caused by intramolecular solvation has been detected by ion mobility-mass spectrometry, there is still a lack of effective analytical means to accurately characterize the specific site where it occurs and the region that causes structural changes.

In this work, the researchers applied the self-built nMS-UVPD platform and home-developed MS data process software to monitor [conformational changes](#) induced by intramolecular solvation. Based on the UVPD fragmentation pattern of myoglobin-heme complex, they determined detailed microsolvation sites and regions with conformational changes.

Then, they systematically characterized the protein structure alternations between protein ions with different charge states. They found that the gas phase [structure of proteins](#) in the high charge state was easily affected by the intramolecular solvation effect and deviated from the solution state structure, and the gas phase structure of low charge protein ions was closer to solution state.

"The complexation of the crown ether 18C6 with protein mainly occurred in solution, and then played an important role in stabilizing the [protein structure](#) during the electrospray ionization process," said Prof. Wang.

UVPD-nMS analysis revealed that the crown ether was mainly bound to protein region with high charge density, and the gas phase structure of the protein was closer to the solution state by blocking the intramolecular solvation of the charged side chain.

"This work demonstrates the significant advantages of UVPD-nMS in simultaneously obtaining [protein sequence](#) and dynamic structure information and provides theoretical and technical insights for the maintenance and efficient characterization of protein [solution](#) structures in nMS," said Prof. Wang.

More information: Lingqiang Zhou et al, Ultraviolet Photodissociation Reveals the Molecular Mechanism of Crown Ether Microsolvation Effect on the Gas-Phase Native-like Protein Structure, *Journal of the American Chemical Society* (2022). [DOI: 10.1021/jacs.2c11210](#)

Provided by Chinese Academy of Sciences

Citation: Researchers reveal molecular mechanism of crown ether microsolvation effect on gas-phase native-like protein structure (2023, February 21) retrieved 29 April 2024 from <https://phys.org/news/2023-02-reveal-molecular-mechanism-crown-ether.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.