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EXPLORING BIOMOLECULAR PROPERTIES IN THE GAS PHASE BY USING ADVANCED LIGHT SOURCES

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Biomolecules such as proteins and peptides exhibit complex three-dimensional structures that are crucial for their biological functions. Non-covalent interactions within proteins, particularly those involving sulfur-containing residues like methionine and aromatic amino acids such as tyrosine and tryptophan, significantly contribute to stabilizing their folded structures (Valley et al. 2012). This specific interaction, referred to as S∴π interaction, has been consistently identified in various protein database analyses, underscoring their important role in enhancing the structural stability of proteins (Meyer et al. 2003).

In this work, we study the electronic and structural properties of tailor-made gas-phase peptides that represent a model of the S∴π interaction. By using electrospray ionization (ESI) in combination with synchrotron light sources we perform mass spectrometry-based action spectroscopy. We aim to indicate and characterize the S∴π interaction by measuring the ionization potential (VUV) and investigating the resonant absorption processes occurring at the carbon K-edge (soft X-rays). Additionally, we explore fragmentation channels at specific absorption resonances as distinctive signatures of S∴π interactions. We estimate the preferred orientation of the sulfur atom relative to the aromatic ring using Molecular dynamics (MD) simulations and density functional theory (DFT).

This experimental and computational approach offers a detailed understanding of the S∴π interaction in our tailor-made peptides and contributes to a broader understanding of the structure-function relationship in biomolecules.

References

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