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Highly site-selective fragmentation of peptides induced by swift heavy ions

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The interaction of swift heavy ions (SHI) with organic matter is highly relevant for applications such as cancer therapy and the development of biomaterials based on SHI irradiation. Furthermore, the interaction of SHI with complex molecular systems such as biomolecules is interesting from a fundamental point of view in terms of the excitation mechanisms involved and how the energy deposited in the system is coupled into the molecular degrees of freedom relevant for bond breaking. SHI-induced fragmentation of peptides is an ideal model system for studying these processes due to the variety of functional groups and bonds in peptide molecules.

The study of molecular fragmentation by external stimuli, however, requires an analytical tool that does not introduce fragments itself. Therefore, we make use of Desorption/Ionization induced by Neutral SO2 Clusters (DINeC), an extremely soft desorption method [1], in combination with mass spectrometry (MS). DINeC-MS has proven to be an ideal tool for analyzing fragmentation processes. In particular, DINeC-MS was employed to investigate the fragmentation of peptides by SHI impact [2].

In this study, we examine whether the interaction of SHI with peptides can lead to bond-specific and/or selective fragmentation. We find, in addition to specific fragmentation, i.e, peptide bond cleavages restricted to the peptide backbone [2], a high site-selectivity of SHI-induced fragmentation. This means that only selected peptide bonds within the amino acid sequence are broken efficiently, while others remain intact. Furthermore, experiments with peptides in which single amino acid units were exchanged relative to a reference peptide revealed that this selectivity is independent of the amino acids present in the direct neighborhood of the cleavage site; rather, the overall peptide structure was found to be the determining factor.

[1] Gebhardt, et al., Angw. Chem. Int. Ed. 48, 4162 (2009).
[2] Schneider, et al., Sci. Rep. 12, 17975 (2022).

Author: HERRMANN, Aaron (Justus-Liebig-Universität Gießen(JULGi))

Co-authors: KELLER, Philip (Justus-Liebig-Universität Gießen(JuLGi-2PI)); SCHNEIDER, Pascal (Justus-Liebig-Universität Gießen(JuLGi-2PI)); SCHUBERT, Ina (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI)); KOCH, Frieder (GSI Helmholtzzentrum für Schwerionenforschung); Dr SIMON, Pascal (GSI Helmholtzzentrum für Schwerionenforschung GmbH(GSI)); DÜRR, Michael (Justus-Liebig-Universität Gießen(JULGi))

Presenter: HERRMANN, Aaron (Justus-Liebig-Universität Gießen(JULGi))

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