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Department of Chemistry Research Seminar Series



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Combining Spectroscopy with Mass Spectrometry for the Structural Analysis of Biomolecules

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Combining Spectroscopy with Mass Spectrometry for the Structural Analysis of Biomolecules

Mass spectrometry (MS) is a powerful tool for analyzing the sequence of biomolecules. However, MS provides limited information regarding the three-dimensional structure of ionized biomolecular ions. In the last years, more and more mass spectrometry setups have been combined with lasers to perform various forms of spectroscopy, such as infrared, UV-Vis, or fluorescence. Due to the low density of ions in an ion trap, absorption spectroscopy is not feasible. Instead, we monitor the effect of laser radiation on the ions in a wavelength-dependent manner. In this talk, I will discuss infrared and fluorescence spectroscopy of trapped ions.

Reactive intermediates, with short lifetimes in solution, are generated using electrospray ionization followed by in-source fragmentation. In the gas phase, these intermediates survive long enough for their vibrational modes to be examined. The investigated ions are then accumulated in an ion trap and picked up by superfluid helium droplets (0.4 K). The doped droplets are excited by the infrared beam of a free-electron laser, leading to the release of the ions from the droplets, which are detected by a time-of-flight detector. The ion count as a function of the photon wavenumber provides an infrared spectrum. The resulting infrared patterns help determine the ion's structure by comparing them with calculated patterns of candidate structures. This method has been applied to several reactive intermediates, such as glycosyl cations, fluorenyl cations, and intermediates of RNA autohydrolysis.

Protonated polypeptides carrying fluorescent labels are generated by electrospray ionization. To understand how collisional and photon-based activation influences the structure of peptides, we hyphenated MS with time-resolved fluorescence emission spectroscopy, known as Förster resonance energy transfer (FRET). In the presence of a fluorescence quencher, the fluorescence lifetime is reduced in a distance-dependent manner, allowing us to estimate the distance between the quencher and the label. By studying this signal, it is possible to determine to what extent collisional and photon-based activation unfold investigated peptides.