Freiser Lecture

Structures, Energetics and Mechanisms for Dissociation of Protonated Nucleosides and Protonated Base Pairs

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A major focus of our research has been to provide fundamental information regarding the influence of the local environment and modifications on the structures, stabilities, and reativities of model nucleic acid systems. We utilize several complementary tandem mass spectrometry approaches to examine the energy and wavelength dependences of the dissociation behavior of these systems. To elucidate the influence of the local environment, our investigations include various states of deprotonation, protonation, and metal cationization or complexation of nucleic acid building blocks. The influences of modifications are examined by comparing behavior of the canonical systems to that of naturally occurring and synthetically modified nucleic acid building blocks. Our experimental studies are supported and enhanced by complementary electronic structure calculations. This talk will focus on three sets of recent experiments. In the first, we have studied the wavelength dependence of the fragmentation of protonated DNA, RNA, and modified nucleosides and nucleotides to elucidate structures experimentallly populated and how they are influenced by the nucleobase and sugar moieties and modifications. In the second, we have studied the energy dependence of the fragmentation of protonated DNA, RNA, and modified nucleosides to characterize glycosidic bond stability and how it is influenced by the nucleobase and sugar moieties and modifications. The resulting structural, mechanistic and thermodynamic information is potentially of interest in better understanding and predicting how mass spectrometry can be used to sequence oligonucleotides and nucleic acids. In the third series, we have studied the energy dependence of the fragmentation of protonated DNA, RNA, and modified nucleoside base pairs to characterize the strength of base pairing and how it is influenced by the nucleobase and sugar moieties and modifications. The resulting thermodynamic information is potentially of interest in better understanding nucleic acid i-motif formation and how it is influenced and may be controlled by modifications for applications in medicine and nanotechnology.

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