Fragmentation and Ring-Opening during Collisions between Cyclic GGKG-H^+ and a Perfluorinated Self-Assembled Monolayer

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Abstract: We present the results from direct dynamic simulations involving the collision between a cyclic protonated peptide (c(-GGKG-)-H^+) and perfluorinated self-assembled monolayer (FSAM) surface with a focus on post-collision fragmentation and ring-opening events. In comparison to prior work on the octaglycine peptide, significantly fewer fragmentation events occur as a result of proton motion within the peptide. Although it is common for ring-opening to occur prior to fragmentation, it is not required. The most common site for ring-opening to occur is at the C5-C6 bond, which is adjacent to the lysine side-chain. Within the timeframe of our simulations, fragmentation is less common for this cyclic peptide than observed in N-protonated octaglycine. There are several possible explanations for the reduction in fragmentation efficiency including the relative isolation of the excess proton from the backbone, the basic nature of the lysine side-chain, and the slowed dynamics due to ring-openings. Future studies will investigate these possibilities.