An Examination of SID for Different Protonation States and Conformations of GGKG-H$^+$

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Abstract: Collisions between protonated peptide ions and organic surfaces frequently result in peptide fragmentation. The fragmentation patterns generated are quite characteristic and form a "fingerprint" of the peptide, hence making surface-induced dissociation (SID) a well-used analytic technique. Here, we present results from molecular dynamics simulations performed on three different conformations of the GGKG-H$^+$ straight-chain peptide colliding with a perfluorinated self-assembled monolayer (FSAM). Two of the GGKG-H$^+$ conformations have the excess proton located on the lysine side-chain, while the third places it on the N-terminus. The simulations show a slower rate of fragmentation for the lysine protonated conformations, compared to prior simulations of the octaglycine peptide. Examining proton hop patterns occurring prior to fragmentation illustrates that the lysine protonated conformers also exhibit similar proton transfer pathways. These proton hop patterns provide crucial information in understanding how fragmentation events occur. It is also known from experiment, that peptides that contain the lysine side-chain are less prone to fragmentation. Our results, therefore, suggest that the excess proton is located on the lysine side-chain in experiment.