

**Automated Transition State Search Applied to Protonated Diglycine:
Moving Towards a Simulated CID Mass Spectra**

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Abstract:

Gaining an understanding of the fragmentation patterns that occur for protonated peptides within tandem mass spectrometry is a computationally challenging task. During tandem mass spectrometry, the ion undergoes collisions which results in a highly energized species that is expected to fragment. The fragmentation pattern serves as a “finger print” for the peptide. However, it is not uncommon for unexpected fragmentation products to be observed. Computer simulations can be used to improve our understanding of these high-energy systems. We have implemented the Transition State Search Using Chemical Dynamics Simulation (TSSCDS) technique to explore the important reaction pathways for diglycine. Specifically, we have performed 68,200 500 fs trajectories, for a total simulation time of 34.1 nanoseconds. These trajectories were analyzed and resulted in 1625 transition states. Using Kinetic Monte Carlo (KMC) calculations the most important reaction pathways were determined and final product branching ratios obtained.