

Fundamental investigation of peptide fragmentation by collision mass spectrometry: structure/dissociation relationship

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In this project, our aim is to push further the knowledge of the peptide ion decomposition process for the diverse ion activation methods (collision against neutral, electron activation, photoactivation...) to implement new mechanisms, specific to targeted peptide sequences.

In this presentation, I will focus on a mechanistic study on the unexpected c/z decomposition upon CID in different peptide sequences. I will give insights of the interest of combining various approaches such as tailor-made peptide design and synthesis, more fundamental studies to determine the thermodynamics and kinetics of the fragmentation reactions of the decomposing peptide ions, and molecular dynamics, to better understand peptide fragmentation pathways.

