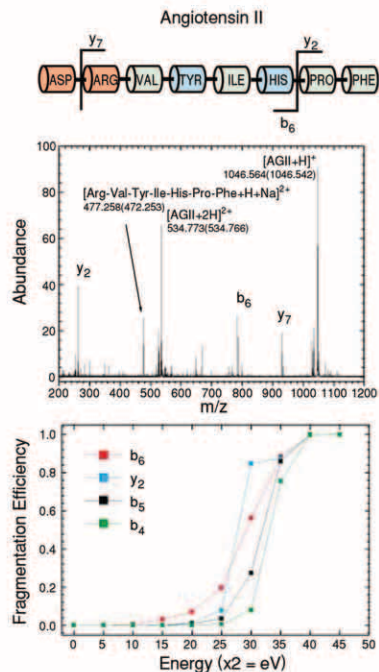


# Fragmentation Studies for Peptides Using Mass Spectrometry: Experiment and Simulation

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In recent years there has been significant interest in fragmentation analysis of peptides and proteins using mass spectrometry (MS) combined with infrared multiphoton dissociation (IRMPD) and collision induced dissociation (CID) technique. We investigate the cleavage of polypeptides induced at the backbone amine bonds by using the CO<sub>2</sub> laser peptide cleavage IRMPD technique. MS experiments are performed in electrospray ionization fourier-transform ion cyclotron resonance (FTICR) MS, and the results are compared with those of CID experiment. In addition, we theoretically model the fragmentation of the peptides under vacuum conditions using molecular dynamics. The dissociation energy and proton affinity for the peptide bonds (C'-N bond) are also obtained using *ab initio* calculations.



ESI-FTICR Spectrum and product efficiency curves obtained from CID experiment