Soft-landing of fragment ions to determine structure

The technique of soft-landing involves using a mass spectrometer to select a molecule of a specific mass and collecting that molecule on a surface for further experimentation. In the Wysocki lab we are using the experimental setup shown below to soft-land fragment ions in hopes to learn more about their structure using infrared spectroscopy and ultimately gain information that will lead to an understanding of the mechanisms by which peptides and proteins fragment.

Currently we are working with several model systems to see if our methods of soft-landing ions will lead to a direct determination of fragment structure. Below is a comparison of a calculated IR spectrum of Val-Pro diketopiperizine and an IR spectrum of soft-landed cyclo-Val-Pro (which has a diketopiperizine structure) on an H-SAM surface in our instrument.

The computational work for this experiment is being performed by JC Poutsma’s group at the College of William and Mary (http://people.wm.edu/~jcpout/faculty.html#R1).