

Efficient Ion Fragmentation in Structures for Lossless Ion Manipulations



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Overview

- Fragmentation of peptide cations has been achieved in structures for lossless ion manipulations (SLIM).

- A DC offset was applied to RF electrodes on one of two parallel SLIM surfaces.

- b and y-type sequence fragment ions were produced.

Introduction

- SLIM have been used for ultra high resolution ion mobility separations.¹

- Flexibility of design and continuous RF confinement allow complex 3D ion manipulations over extended times.²

- SLIM are being applied to separations and quantitation of complex omics mixtures.

- Identification of unknown compounds without internal standards is difficult.

- Mass spectrometric fragmentation (e.g. collision induced dissociation, CID) allows for identification of unknown compounds.

- Therefore, ion fragmentation in SLIM has been developed.

- Ion trajectories were simulated and electric fields were modeled to assist in the inference of the activation mechanism.

Methods

- Micromolar concentration peptides and proteins were infused by nano electrospray ionization at 300 nl/min at +3000 V.

- DC bias was applied to the RF of the top SLIM surface via a 100 k Ω coupling resistor to fragment ions.

- 30 V, 200 m/s traveling wave with 1 MHz, 250 V_{pp} RF

- SLIM was held at 3 Torr N₂.

- Simulations were performed in Simion 8.1 with the SDS collision model.

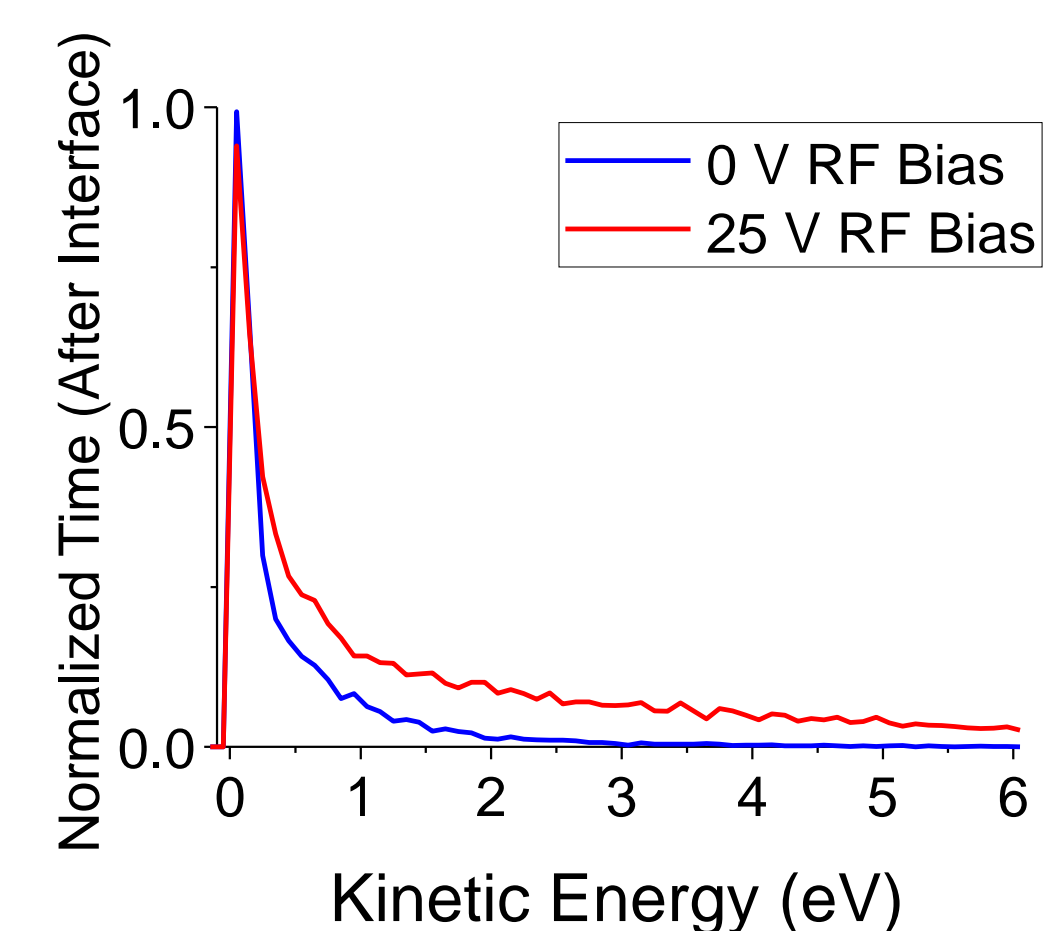
Results

Simulated Ion Trajectories and Kinetic Energies for Triply Protonated Neurotensin

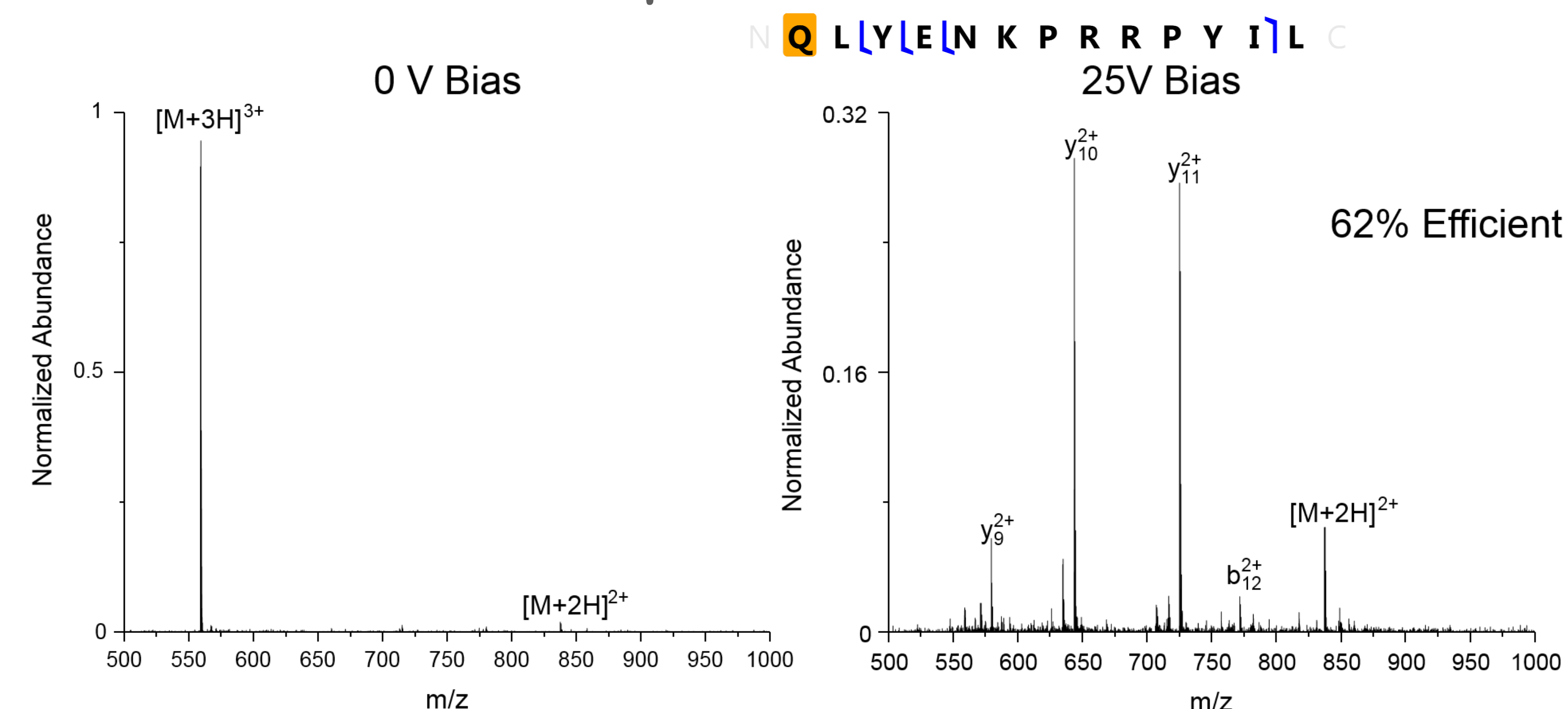


0 V Bias

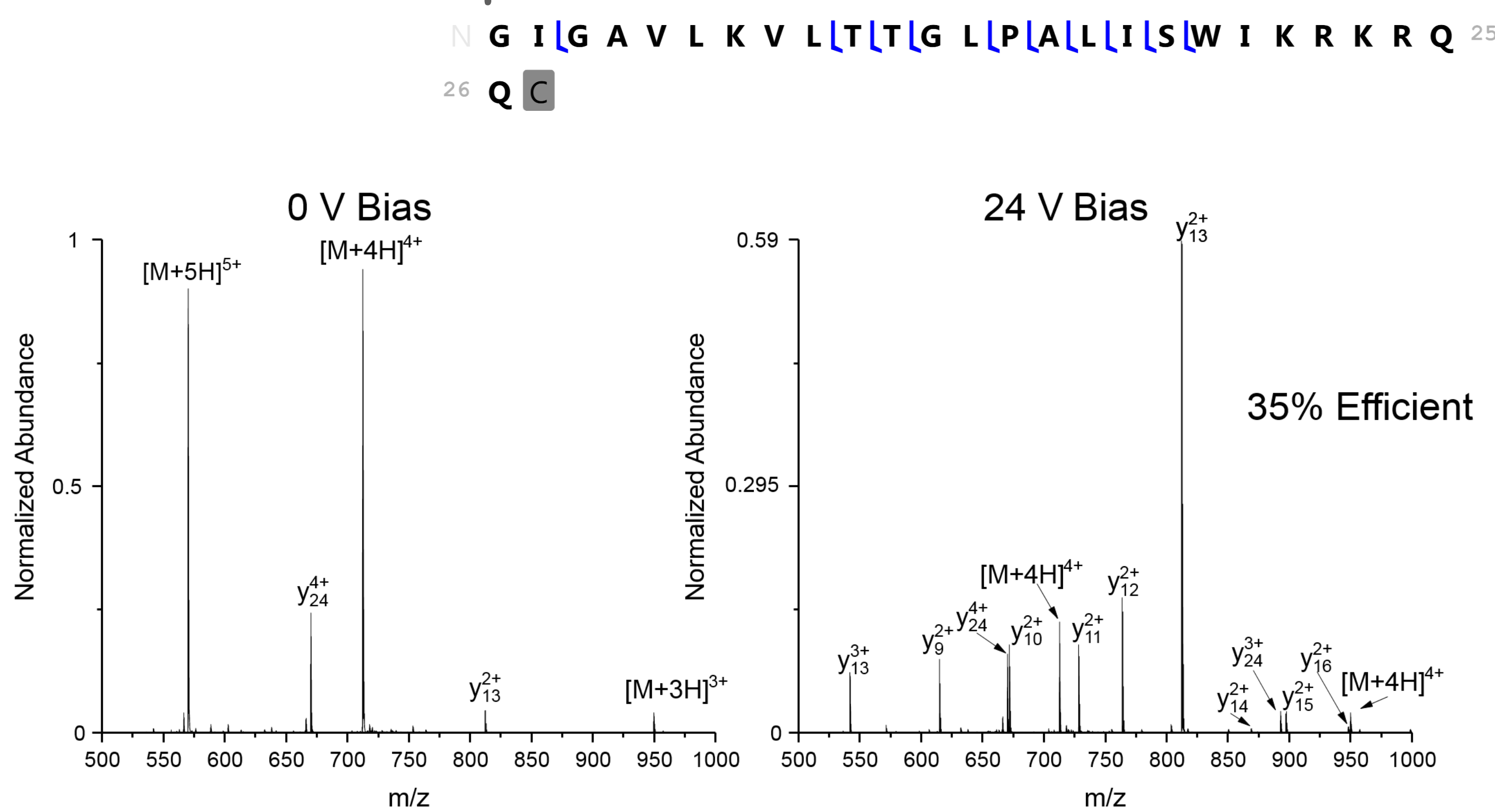
25 V Bias



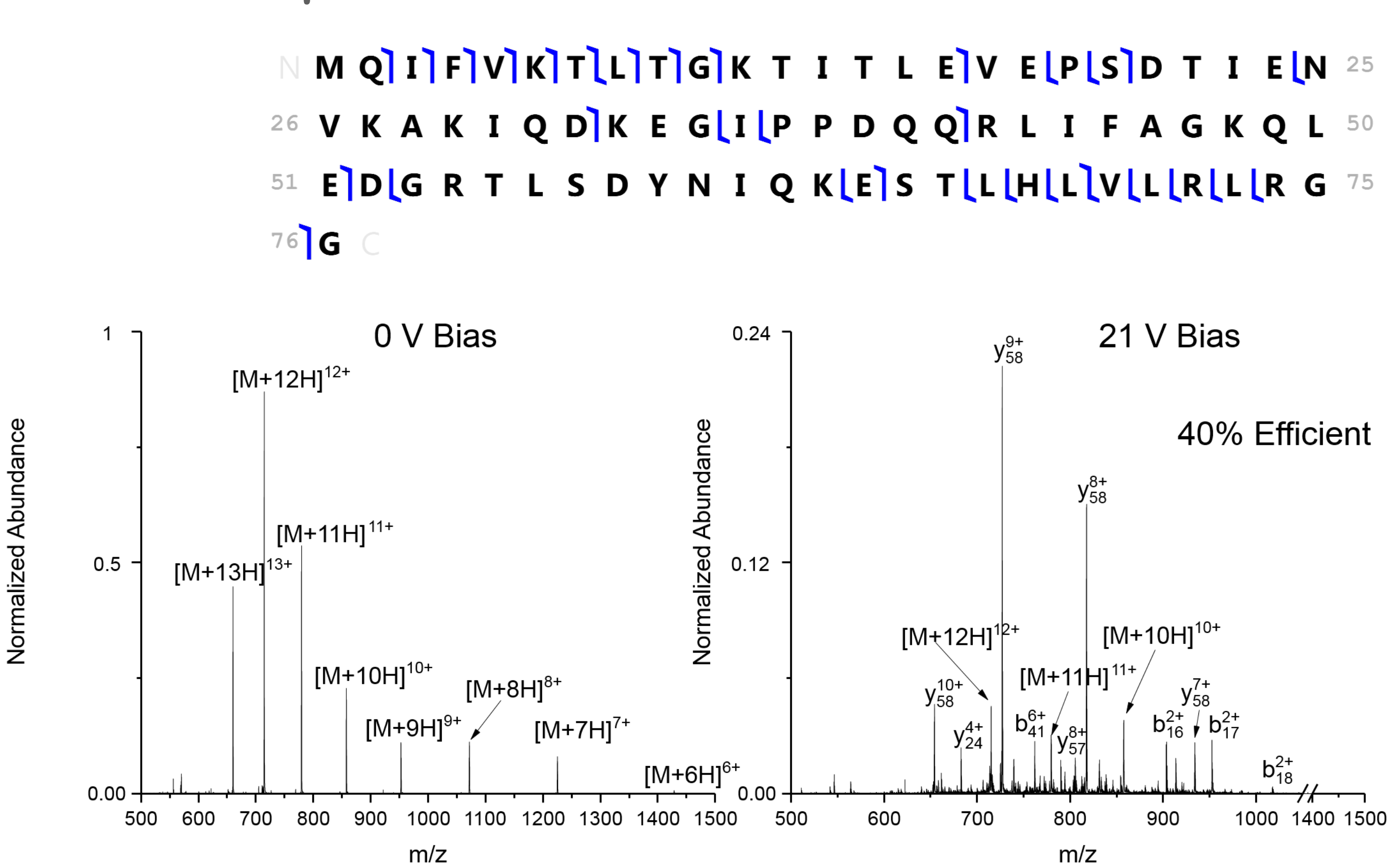
CID of Neurotensin Peptide Cations



CID of Melittin Peptide Cations



CID of Ubiquitin Cations



Conclusions

- A simple method for implementing CID with SLIM has been demonstrated.

- Ion activation was induced by applying a DC bias to the RF on a single SLIM surface..

- Simulations of ion trajectories show ions traveling into regions of higher RF field intensities when bias is applied.

- Resulting ion kinetic energies are higher when bias is applied.

- We plan to implement CID with high resolution ion mobility separations, accumulation of large ion populations, and other manipulations.

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