Efficient Ion Fragmentation in Structures for Lossless Ion Manipulations

Pacific Northwest National Laboratory, Richland, WA

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 quantification 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 nanoelectrospray ionization at 300 nL/min at +3000 V.
- DC bias was applied to the RF of the top SLIM surface via a 40 kΩ coupling resistor to fragment ions.
- 30 V, 200 m/s traveling wave with 1 MHz, 250 Vpp 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

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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References


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CONTACT: Ian K. Webb, Ph.D.
Biological Sciences Division
Pacific Northwest National Laboratory
E-mail: ian.webb@pnnl.gov