Analysis of Structural Changes with High Resolution Structures for Lossless Ion Manipulations (SLIM) Ion Mobility-Mass Spectrometry

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Introduction

• Ion mobility allows for the study of gas phase biomolecule shape (collision cross section)

• Limited resolution of mobility analyzers makes characterization of some structural changes elusive

• We introduce a Structures for Lossless Ion Manipulations multi-pass module to increase IMS resolution
**IM Separations with SLIM**

**Structures for Lossless Ion Manipulations**
- rf and DC confinement
- Straight, 90° turn, switch, and trap segments
- Effectively lossless design → Long path length IM

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Experimental Arrangement

Ion switch:
- Ions either continue on path or are switched to MS

$\text{N}_2$ drift gas
Experimental Arrangement

IM Path Length = 1.25 m + N(14.65 m),
N is the # of passes

42 cm x 68 cm

Switching electrodes alternate between DC only and travelling wave.
4 Passes through SLIM Module

$m/z$ 622 from Agilent Low Concentration Tuning Mix

Intensity (au)

Arrival Time (ms)
• Ion losses due to deleterious ion/molecule reactions

• Ion current measurements show no losses in the first pass
Resolving Power Increases with $\sqrt{\text{Drift Length}}$
Isomers: Sodiated 3,5-Dicaffeoleoyquinic Acid

3,5-diCQA is a plant natural product. CQAs have antioxidant, anti-HIV, and anti-inflammatory activity.

Molecular Weight 516.45 Da

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0 Hours UV Irradiation

3 Hours UV Irradiation

Agilent 6560 IM/qTOF

Arrival time (ms)
Isomers: Sodiated 3,5-Dicaffeoylquinic Acid

Molecular Weight 516.45 Da

0 Hours UV Irradiation

3 Hours UV Irradiation

16 m SLIM

trans/trans

cis/cis

3cis/5trans

3trans/5cis

trans/trans

Arrival Time (ms)
Isomers: Sodiated Oligosaccharides

Cellopentaose

Maltopentaose

Mannopentaose

Molecular Weight 828.72 Da
Isomers: Sodiated Oligosaccharides

Oligosaccharides are baseline resolved

Drift Tube IMS

31m SLIM

31m SLIM, Mixture

Cellopentaose
Maltopentaose
Mannopentaose
Separation of a Phosphopeptide Mixture

Peptide 1: APLpSFRGSLPKSYVK
Peptide 2: APLSFRGpSLPKSYVK
Peptide 3: APLSFRGSLPKpSYVK

Drift Tube IMS

Separation of a Phosphopeptide Mixture

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Summary and Future Directions

• Initial evaluation of a multi-pass SLIM Module yielded resolving power over 500 (singly charged) after a 60 meter path length

• Elucidation of structural isomers inseparable by drift tube IMS (1 meter)

• Optimization of materials needed to minimize outgassing

• Short term applications: small molecules and small sample sizes
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