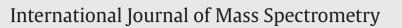
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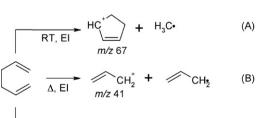
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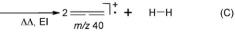
#### 8–15

Radical cation/radical reactions: A Fourier transform ion cyclotron resonance study of allyl radical reacting with aromatic radical cations

Amber L. Russell, Henry W. Rohrs, David Read, Daryl E. Giblin, Peter P. Gaspar, Michael L. Gross

A method for the study of reactions of open-shell neutrals (radicals) and radical cations is described. Pyrolysis (25–1500 °C) of thermally labile compounds, such as, 1,5-hexadiene via a Chen nozzle yields a seeded beam of reactive species in helium. The pyrolysis products are then analyzed by electron ionization (EI) or reacted with stored ions.





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#### **16–20**

### The reactivity of metallated nitrenium ions studied by FT-ICR

Michael J. Yurkovich, Penggao Duan, Ryan C. Shea, Michael A. Watkins, Sarah M. Mandell, Eric M. Tippmann, Sen Jason Li, Matthew S. Platz, Hilkka I. Kenttämaa

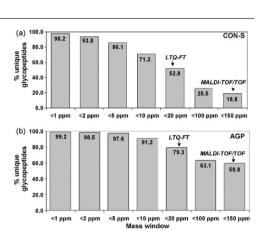
Two metallated nitrenium ions show drastically different reactivity. While the Mg-nitrenium ion reacts by radical mechanisms, the Cu-nitrenium ion follows non-radical pathways.

#### 21–26

# When can glycopeptides be assigned based solely on high-resolution mass spectrometry data?

#### Heather Desaire, David Hua

This work outlines guidelines for when it is (and is not) appropriate to rely heavily on high-resolution mass measurements to assign glycopeptide compositions; such guidelines are potentially useful for anyone conducting glycopeptide analysis by mass spectrometry.



Mg<sup>+</sup> (Nel3s

[Ar]3d<sup>2</sup>4s

Fe

Cu<sup>+</sup> Arl3d<sup>10</sup>

[Ar]3d<sup>6</sup>4

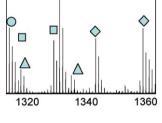
No Reaction

# 27–31

# Rapid and automated processing of MALDI–FTICR/MS data for <sup>15</sup>N-metabolic labeling in a shotgun proteomics analysis

#### Li Jing, I. Jonathan Amster

An automated procedure is presented for matching <sup>15</sup>N-metabolically labeled peptides with their unlabeled counterparts in MALDI-FTICR mass spectra of a batch digested proteome.



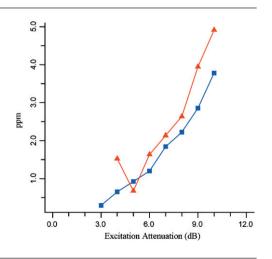
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### 32-38

#### FT-ICR MS optimization for the analysis of intact proteins

Aleksey V. Tolmachev, Errol W. Robinson, Si Wu, Ljiljana Paša-Tolić, Richard D. Smith

Fourier-transform ion cyclotron resonance (FT-ICR) mass spectrometry (MS) remains the technique of choice for the analysis of intact proteins from complex biological systems, i.e., top-down proteomics. Recently, we have implemented a compensated open cylindrical ion trapping cell into a 12 T FT-ICR mass spectrometer.



#### 39-45

# A dual time-of-flight apparatus for an ion mobility-surface-induced dissociation-mass spectrometer for high-throughput peptide sequencing

#### Wenjian Sun, Jody C. May, Kent J. Gillig, David H. Russell

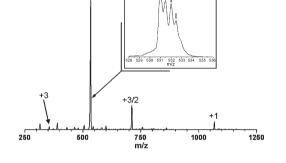
A novel ion mobility (IM)-surface-induced dissociation (SID)-mass spectrometer consisting of two independent time-of-flight (TOF) mass analyzers is described.

#### 46-57

#### A new, higher resolution, ion mobility mass spectrometer

#### Paul R. Kemper, Nicholas F. Dupuis, Michael T. Bowers

We present here a combined IMS–MS instrument able to resolve structures with cross sections differing by less than 1%.



#### 58-69

#### Profiling of phospholipids and related lipid structures using multidimensional ion mobility spectrometry-mass spectrometry

Sarah Trimpin, Bo Tan, Brian C. Bohrer, David K. O'Dell, Samuel I. Merenbloom, Mauricio X. Pazos, David E. Clemmer, J. Michael Walker

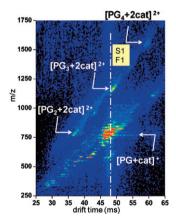
Increasingly comprehensive questions related to the biosynthesis of lipids relevant to understanding new signaling pathways have created daunting tasks for their chemical analysis. Here, ion mobility spectrometry (IMS) and mass spectrometry (MS) techniques combined with electrospray ionization have been used to examine mixtures of closely related lipid structures.

# 70-76

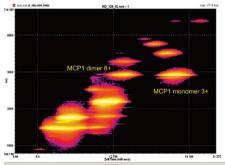
# An ion mobility-mass spectrometry investigation of monocyte chemoattractant protein-1

### Matthew R. Schenauer, Julie A. Leary

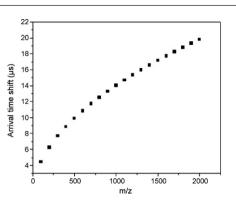
In the present article we describe the gas-phase dissociation behavior of the dimeric form of monocyte chemoattractant protein-1 (MCP-1) using quadrupole-traveling wave ion mobility spectrometry-time of flight mass spectrometry (q-TWIMS-TOF MS) (Waters *Synapt*<sup>TM</sup>).







MCP-1 dimer and monomer, normally overlapping in mass spectrum, are separated by ion mobility



#### 77-86

# MALDI-induced fragmentation of leucine enkephalin, nitro-Tyrleucine enkaphalin, and d<sub>5</sub>-Phe-nitro-Tyr-leucine enkephalin

# Xianquan Zhan, Dominic M. Desiderio

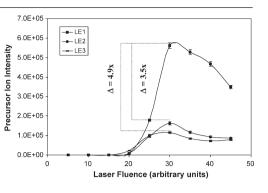
The long-term objective of this study is to use MALDI MS and MS/MS to study the fragmentation pattern of *in vitro* nitrotyrosine-containing peptides in order to assist the interpretation of MS-identification of endogenous nitroproteins in human tissues and fluids. The short-term objective is to study synthetic leucine enkephalin, nitro-Tyr-leucine enkephalin, and d<sub>5</sub>-Phe-nitro-Tyr-leucine enkephalin with a vacuum matrix-assisted laser desorption/ionization linear ion-trap mass spectrometer (vMALDI-LTQ).

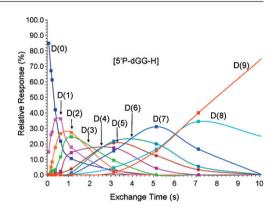
#### 87-95

# Gas-phase hydrogen/deuterium exchange of dinucleotides and 5'-monophosphate dinucleotides in a quadrupole ion trap

# Joseph E. Chipuk, Jennifer S. Brodbelt

Gas-phase hydrogen/deuterium (H/D) exchange reactions of four deprotonated dinucleotides (dAA, dAG, dGA, dGG) and their 5'-monophosphate analogs (5'-dAA, 5'-dAG, 5'-dGA, 5'-dGG) with  $D_2O$  were performed in a quadrupole ion trap mass spectrometer.



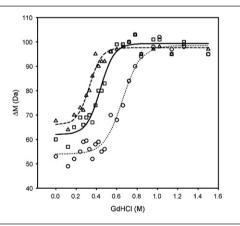


### 96–104

# Comparison of two ESI-MS based H/D exchange methods for extracting protein folding energies

Rohana Liyanage, Nagarjuna Devarapalli, Latisha M. Puckett, N.H. Phan, Jennifer Gidden, Wesley E. Stites, Jackson O. Lay Jr.

In this report, the model proteins staphylococcal nuclease and ubiquitin were used to test the applicability of two new hydrogen/deuterium exchange (HX) electrospray ionization mass spectrometry (ESI-MS) methods for estimating protein folding energies.

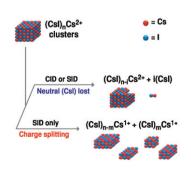


### 105–113

# Influence of cluster size and ion activation method on the dissociation of cesium iodide clusters

### Asiri S. Galhena, Christopher M. Jones, Vicki H. Wysocki

The gas-phase dissociation of cesium iodide clusters was studied by collision-induced dissociation (CID) and surface-induced dissociation (SID) in a quadrupole time-of-flight mass spectrometer. SID was found to deposit more internal energy into these clusters, providing access to alternative, high energy dissociation pathways.



#### 114-118

# The concept of electrostatic non-orbital harmonic ion trapping

#### Claus Köster

A new, more general type of electrostatic ion trap mass analyzer is described. The potential distribution of the electrical field in this trap can be expressed as a combination of a quadrupolar and logarithmic-Cassinian potential.

#### 119-127

#### Wavelength dependence on the level of post-source metastable ion decay observed in infrared matrix-assisted laser desorption ionization

#### Edward E. Durrant, Robert S. Brown

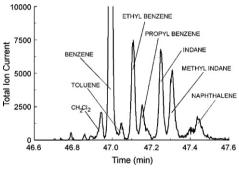
The levels of post-source metastable ion decay (PSD) observed in several peptides and proteins ionized by matrix-assisted laser desorption ionization time-of-flight mass spectrometry (MALDI TOF-MS) are measured utilizing both infrared (IR) and ultraviolet (UV) desorption wavelengths.

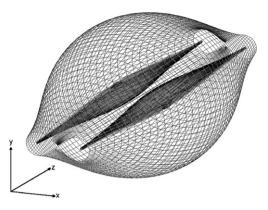
#### 128-133

#### Isoconversion effective activation energies derived from repetitive injection fast gas chromatography/mass spectrometry

#### Robert L. White

Evolved gas analysis by using fast temperature programmed gas chromatography/mass spectrometry is described.





[M+H]

102000

toble [M+H]

104000 106000

104000 106000

100000

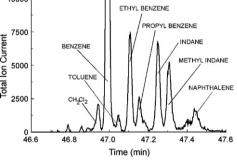
60 (a)

20

30

20

00000



100000 102000

000 Time-of-Flight (nsec)