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## Contents

#### **Regular articles**

#### 1–5

## A theoretical and mass spectrometry study of the novel mechanism of N-glycosidic bond cleavage in nucleoside

Jihong Liu, Shuxia Cao, Bin Jia, Donghui Wei, Xincheng Liao, Jiansha Lu, Yufen Zhao

The fragmentation pathways of ribonucleosides, deoxynucleosides and isopropylidenenucleosides were investigated by electrospray ionization tandem mass spectrometry (ESI-MS/MS) in both positive and negative mode. Novel fragmentation pathways investigated using deuterium-label experiment provided important insight on the nature of N-glucosidic bond cleavage.



#### 6–12

## Comparison between mass spectra of individual organic particles generated by UV laser ablation and in the IR/UV two-step mode

#### Alla Zelenyuk, Juan Yang, Dan Imre

Individual particle mass spectra generated in IR/UV mode exhibit greatly diminished particle-toparticle fluctuations and significantly improved mass spectral quality than those produced by UV laser ablation.



#### 13-20

## Low energy photoelectron resonance capture ionization aerosol mass spectrometry of small peptides with cysteine residues: Cys-Gly, $\gamma$ -Glu-Cys, and glutathione ( $\gamma$ -Glu-Cys-Gly)

#### Scott Geddes, James Zahardis, Jessica Eisenhauer, Giuseppe A. Petrucci

The photoelectron resonance capture ionization (PERCI) of Cysteine (Cys)and small gas-phase neutral peptides that contain the Cys residue (Cys-Gly, \_-Glu-Cys, and glutathione (\_-Glu-Cys-Gly)) is reported.





#### 21–27

# Influence of temperature and crown ether complex formation on the charge partitioning between z and c fragments formed after electron capture by small peptide dications

Anneli Ehlerding, Camilla S. Jensen, Jean A. Wyer, Anne I.S. Holm, Palle Jørgensen, Umesh Kadhane, Mikkel K. Larsen, Subhasis Panja, Jean Christophe Poully, Esben S. Worm, Henning Zettergren, Preben Hvelplund, Steen Brøndsted Nielsen

The effect of crown ether complex formation on the fragmentation of  $[{\rm GHK}+2{\rm H}]^{2_+}$  after electron capture.

#### 28-37

## Proton transfer mass spectrometry at 11hPa with a circular glow discharge: Sensitivities and applications

#### D.R. Hanson, M. Koppes, A. Stoffers, R. Harsdorf, K. Edelen

A circular glow discharge ion source is easy to construct and deploy in proton transfer mass spectrometry studies at ~11 hPa. A high sensitivity for detection of VOCs is maintained for time periods of many days to months.





#### 38-44

#### Modeling and optimization of dual-cylinder image current detector in electrostatic ion beam trap for mass spectrometry

#### Qi Sun, Li Ding, Changxin Gu

This detector acquires the differential current with strengthened intensity, and the configuration is modified further to improve the waveform of the signal.



#### 45–49

## In vivo analysis of palm wine (Elaeis guineensis) volatile organic compounds (VOCs) by proton transfer reaction-mass spectrometry

#### Ola Lasekan, Sabine Otto

The in vivo volatile organic compounds (VOCs) release patterns in palm wine was carried out using the PRT-MS. In order to analyze the complex mixtures of VOCs in palm wine, the fragmentation patterns of 14 known aroma compounds of palm wine were also investigated.



#### **50–55**

## MALDI, AP/MALDI and ESI techniques for the MS detection of amyloid $\beta\text{-peptides}$

#### Giuseppe Grasso, Placido Mineo, Enrico Rizzarelli, Giuseppe Spoto

We analyzed A s solutions by MALDI-TOF, AP MALDI and ESI. Cleavage sites produced by interaction of A s with IDE have also been identified.

#### 56-63

64-69

conditions

protonated, cationized, and negative ions

#### Density functional theory study of $C_nF_3$ - (*n* = 1-9) clusters

J.Y. Qi, H. Liang, M.D. Chen, W. Wu, Q.E. Zhang, C.T. Au

We provide explanations on the ground-state  $C_nF_3-(n = 1-9)$  of even/odd alternation based on the geometrical structure, bonding character, *VDE*, and incremental binding energy.

Mass spectral study of hybrid peptides derived from (R)-aminoxy

ester and  $\beta$ -amino acids: The influence of aminoxy peptide bond (CO-NH-O) on peptide fragmentation under electrospray ionization

Influence of aminoxy peptide bond (CO-NH-O) on fragmentation of some Boc-protected aminoxy hybrid peptides have been studied by electrospray ionization tandem mass spectrometry of their

V. Ramesh, M. Ramesh, R. Srinivas, G.V.M. Sharma, V. Manohar



Long-path detector

 $D_{5}^{+}(1)$ 

8 9 10 11 12 13

D<sub>e</sub><sup>+</sup>(1)

16 17 18

#### 70-76

#### High-energy Coulomb explosions in ultra-dense deuterium: Timeof-flight-mass spectrometry with variable energy and flight length

#### Shahriar Badiei, Patrik U. Andersson, Leif Holmlid

Laser fragmentation of ultra-dense deuterium named D(-1) is studied by TOF-MS with two detectors at different distances. The measurements prove that the distance D–D is 2.3 pm.



H<sup>+</sup>(1)

D<sup>+</sup>/1

200

100 D

2 3

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