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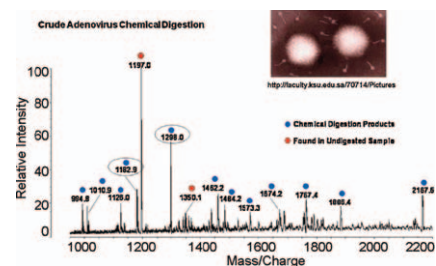
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Regular articles

7–11

Microwave assisted acid cleavage for denaturation and proteolysis of intact human adenovirus

Catherine Fenselau, Olli Laine, Stephen Swatkoski

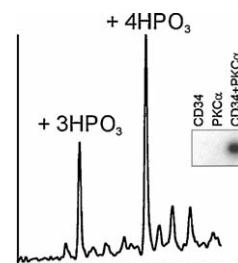


12–21

CD34 antigen: Determination of specific sites of phosphorylation *in vitro* and *in vivo*

Leesa J. Deterding, Jason G. Williams, Margaret M. Humble, Robert M. Petrovich, Sung-Jen Wei, Carol S. Trempus, Matthew B. Gates, Feng Zhu, Robert C. Smart, Raymond W. Tennant, Kenneth B. Tomer

The sites of phosphorylation on the CD34 antigen were determined both *in vitro* from PKC and AKT2 kinase assays as well as *in vivo*.

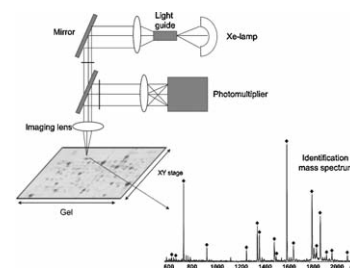


22–28

Mass spectrometric protein identification from two-dimensional gel separation with stain-free detection and visualization using native fluorescence

Iuliana Susnea, Bogdan Bernevic, Eliska Svobodova, Diliana Dancheva Simeonova, Michael Wicke, Carsten Werner, Bernhard Schink, Michael Przybylski

We describe here an approach for the mass spectrometric identification of proteins from gel electrophoretic separation using stain-free detection and visualization based on native fluorescence.

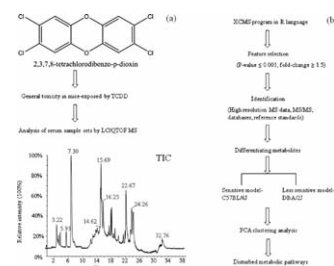


29–36

LC/MS-based non-targeted metabolomics for the investigation of general toxicity of 2,3,7,8-tetrachlorodibenzo-*p*-dioxin in C57BL/6J and DBA/2J mice

Shuhai Lin, Zhu Yang, Yang Shen, Zongwei Cai

Non-targeted metabolomics was applied for investigating different metabolic patterns associated with TCDD exposure in aryl hydrocarbon receptor sensitive C57BL/6J and less sensitive DBA/2J mouse strains.

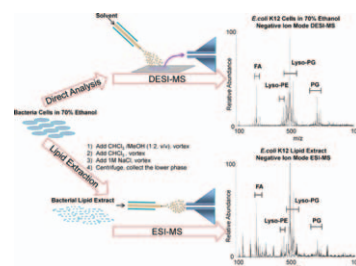


37–44

Rapid direct lipid profiling of bacteria using desorption electrospray ionization mass spectrometry

J. Isabella Zhang, Nari Talaty, Anthony B. Costa, Yu Xia, W. Andy Tao, Rebecca Bell, John H. Callahan, R. Graham Cooks

Synopsis: Polar lipids from intact bacterial samples directly detected by DESI-MS give highly similar spectra to those of lipid extracts examined by ESI-MS.



45–54

Relative and absolute bond dissociation energies of sodium cation–alcohol complexes determined using competitive collision-induced dissociation experiments

Jay C. Amicangelo, P.B. Armentrout

Absolute $(R_1OH)Na^+-(R_2OH)$ and relative and absolute $Na^+-(ROH)$ bond dissociation energies are determined experimentally by competitive collision-induced dissociation of $(R_1OH)Na^+(R_2OH)$ complexes with xenon in a guided ion beam mass spectrometer.

$(R_1OH)Na^+(R_2OH) + Xe$ CID
(Energies in kJ/mol)

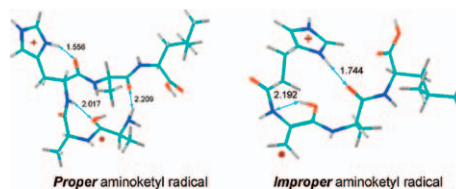
t-BuOH (121.0)				
s-BuOH (120.2)				
2-ProH (115.5)			3.47	4.61
i-BuOH (115.4)			0.27	0.14
n-BuOH (115.3)				
1-ProH (113.5)			2.77	2.86
EtOH (110.0)	10.91	10.70	6.50	6.47
			6.44	3.44

55–61

Proper and improper aminoketyl radicals in electron-based peptide dissociations

Thomas W. Chung, František Tureček

Proper and improper aminoketyl radicals and cation-radicals are two types of intermediates that are distinguished by structure and reactivity.

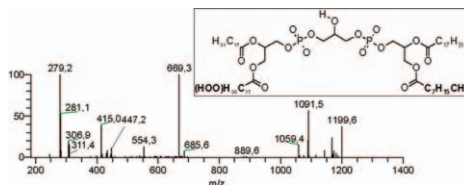


62–73

Cardiolipin and oxidative stress: Identification of new short chain oxidation products of cardiolipin in *in vitro* analysis and in nephrotoxic drug-induced disturbances in rat kidney tissue

Elisabete Maciel, Pedro Domingues, Diane Marques, Cláudia Simões, Ana Reis, Maria Manuel Oliveira, Romeu A. Videira, Francisco Peixoto, M. Rosário M. Domingues

This work describes the identification of new short chain products (with fatty acyl shortened) formed during CL oxidation and their characterization by LC-ESI-MS/MS. The short chain products identified resulted from β -cleavage of alkoxyl radicals at C9 and C13.

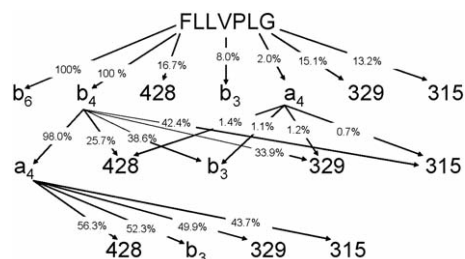


74–83

The effect of ion trap temperature on the dissociation of peptide ions in a quadrupole ion trap

April L. Jue, Alawee H. Racine, Gary L. Glish

Product ion formation pathway tree for FLLVPLG obtained by double resonance/CID at a bath gas temperature of 100 °C.

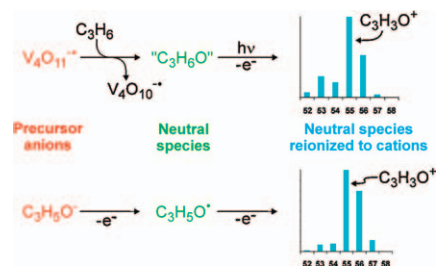


84–89

Neutralization–reionization study of the allyloxide anion

Detlef Schröder, Helmut Schwarz, Jana Roithová

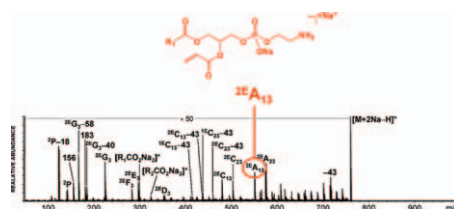
The pattern of $C_3H_nO^+$ ions formed upon neutralization–reionization of $CH_2CHCH_2O^-$ show similarities to the photoionized oxygenates formed from $V_4O_{11}^{4-}$ and propene, suggesting occurrence of initial allylic C–H bond activation followed by oxygenation.



90–101

A universal product ion nomenclature for $[M-H]^-$, $[M+H]^+$ and $[M+nNa-(n-1)H]^+$ ($n = 1-3$) glycerophospholipid precursor ions based on high-energy CID by MALDI-TOF/RTOF mass spectrometry

Ernst Pittenauer, Günter Allmaier

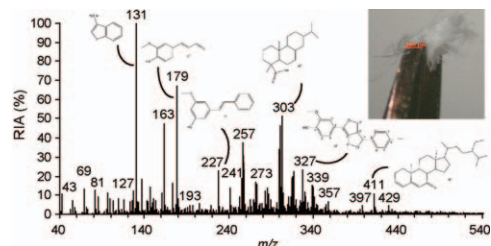


109–126

Analysis of printing and writing papers by using direct analysis in real time mass spectrometry

Jeanette Adams

- DART-MS can differentiate printing and writing papers made from different types of pulps.
- Non-volatile polar organic compounds can be directly determined.
- Analysis is fast and reproducible.
- Microgram samples can be characterized.

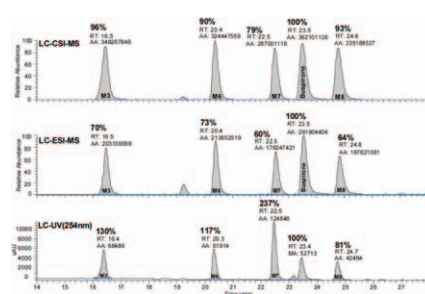


127–135

A low flow ionization technique to integrate quantitative and qualitative small molecule bioanalysis

Ragu Ramanathan, Nirmala Raghavan, S. Nilgun Comezoglu, W. Griffith Humphreys

- LC-Captive Spray Ionization (CSI)-MS allows integration of quantitative and qualitative bioanalysis.
- LC-CSI-MS provides near equimolar response for drugs and metabolites.
- LC-CSI-MS provides opportunities to quantify drugs and metabolites without reference standards.

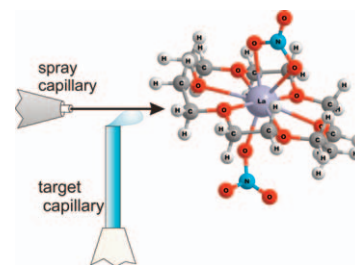


136–142

Characterization of coordination complexes by desorption electrospray mass spectrometry with a capillary target

G.S. Groenewold, A.D. Appelhans, M.E. McIlwain, G.L. Gresham

Desorption electrospray mass spectrometry is used with a capillary target to generate metal coordination complexes directly from sample solutions.

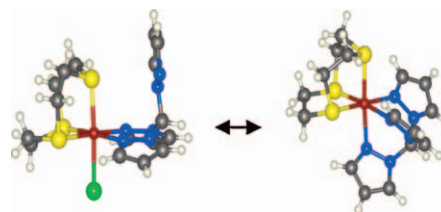


143–150

Investigation of the coordination modes of tris(pyrazolylmethane)/1,4,7-trithiacyclononane ruthenium(II) complex ions by electrospray ionization mass spectrometry

Raul A. Izquierdo, J. Madureira, Catarina I.V. Ramos, M. Graça O. Santana-Marques, Teresa M. Santos

- The denticities of Ru^{II} complexes with [9]aneS₃ and HCpz₃ were investigated by ESIMS.
- The relative abundances of the [Ru([9]aneS₃)(HCpz₃)]²⁺ ions, *m/z* 248, point to rapid Cl losses.
- The ions *m/z* 248 and *m/z* 531, [Ru([9]aneS₃)(HCpz₃)Cl]⁺, coexist in solution up to 16 h.
- A *k*³-HCpz₃ coordination is proposed for the *m/z* 248 ions.
- For the *m/z* 531 ions two isomeric *k*²-HCpz₃ species are proposed: fully coordinated Cl and ion pairs.

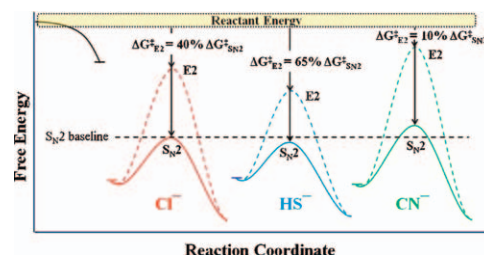


151–158

Mechanistic investigation of S_N2 dominated gas phase alkyl iodide reactions

John M. Garver, Nicole Eyt, Stephanie M. Villano, Zhibo Yang, Veronica M. Bierbaum

► Relative $E2/S_N2$ barriers favor the S_N2 pathway for methyl, ethyl, and isopropyl iodide reactions. ► Reactivity trends can be explained using electronegativity and looseness parameters. ► More normal isotope effects and looser S_N2 transition states occur upon alkyl substitution. ► Results substantiates significantly tighter transition states in the gas phase versus solution.

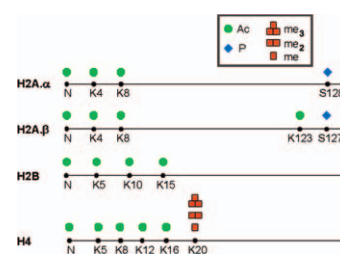


159–165

Mapping post-translational modifications of histones H2A, H2B and H4 in *Schizosaccharomyces pombe*

Lei Xiong, Yinsheng Wang

► PTMs of histones H2A, H2B and H4 from *Schizosaccharomyces pombe* were mapped by LC-nano-ESI-MS/MS. ► Most modification sites were conserved among *Schizosaccharomyces pombe* and other organisms. ► Novel modification sites were found in H2A and H2B.

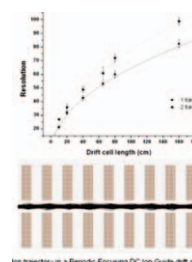


166–173

Increased ion transmission in IMS: A high resolution, periodic-focusing DC ion guide ion mobility spectrometer

Ryan C. Blase, Joshua A. Silveira, Kent J. Gillig, Chaminda M. Gamage, David H. Russell

► Electrode geometry effects on ion transmission and mobility resolution for a periodic-focusing DC ion guide (PDC IG) drift cell. ► Increased ion transmission with a PDC IG drift cell with minimal degradation in mobility resolution. ► Ion mobility resolution increase on increased length PDC IG drift cell agrees with diffusion limited resolving power equation without a decrease in ion transmission.

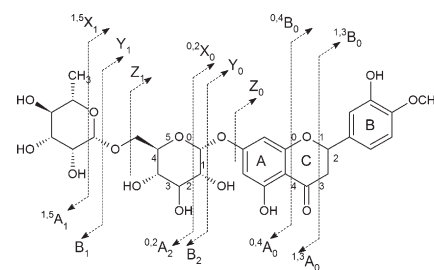


174–183

The formation and fragmentation of flavonoid radical anions

Linda Feketeov, Christopher K. Barlow, Timothy M. Simone J. Rochfort, Richard A.J.

► CID of the $[FeIII(salen)(M-2H)]^-$ complex produces the flavonoid radical anion, $[M-2H]^{\bullet-}$. ► Complexes incorporating a flavonoid containing a disaccharide, dissociation via the elimination of salen or fragmentation of the coordinated flavonoid competes with radical formation. ► Comparison of the CID spectra of the $[M-2H]^{\bullet-}$ radical anions with their corresponding even electron counterparts, $[M-H]^-$, reveals that the radical anion provides a richer CID spectrum. ► CID of the radical anion may provide a means of distinguishing between isomeric flavonoids.

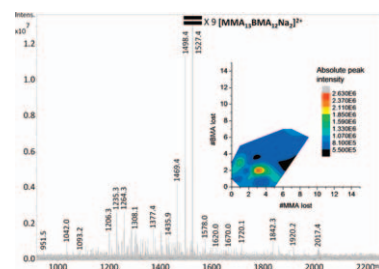


184–194

Tandem Fourier transform mass spectrometry of block and random copolymers

Saša M. Miladinović, Cynthia J. Kaeser, Matthias M. Knust, Charles L. Wilkins

► Random and block copolymers can be differentiated by QCID-FTMS. ► QCID-FTMS and ECD-FTMS result in different fragmentation patterns. ► ECD allows determination of side group losses for polymers.



195–201

Mass spectrometry analysis of poly(styrene sulfonate sodium salt), a polyanionic electrolyte

Bethany L. Subel, Chrys Wesdemiotis

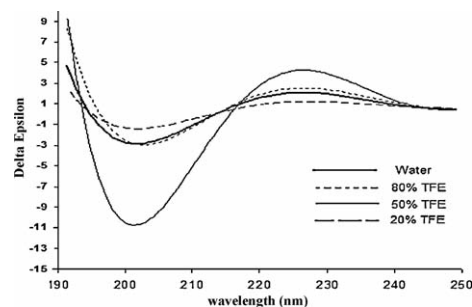
► ESI ionizes efficiently sulfonated styrene poly(electrolytes). ► Such compounds readily undergo sodium/proton exchanges in anionic charge states. ► Polymers with sulfonate salt pendants decompose by charge-remote homolytic chain cleavages via ion/radical complexes. ► Polymers with sulfonic acid pendants degrade by proton-catalyzed sulfur trioxide losses.

202–210

Trifluoroethanol-induced conformational changes in α - and β -neoendorphins monitored using hydrogen/deuterium exchange mass spectrometry and circular dichroism spectroscopy

Hari Kosanam, Chhabil Dass

► H/D exchange, coupled with ESI-MS, can be effectively used to monitor changes in conformational structures of small size peptides. ► In pure water, α -neoendorphin and β -neoendorphin both exist as random coil open structures. ► Both peptides acquire secondary structural elements in the [water + trifluoroethanol] mixed solvent system.

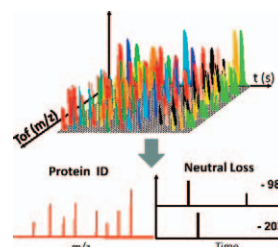


211–219

High-capacity ion trap coupled to a time-of-flight mass spectrometer for comprehensive linked scans with no scanning losses

Sunnie Myung, Herbert Cohen, David Fenyő, Julio C. Padovan, Andrew N. Krutchinsky, Brian T. Chait

► A high-capacity ion trap ($>10^6$ ions) is coupled to a TOF mass spectrometer. ► Comprehensive linked scan analysis of all stored ions in the ion trap is achieved. ► Accurate mass analysis is achieved for both the precursor and fragment ions. ► Comprehensive data set is extracted by a computer algorithm after data acquisition.

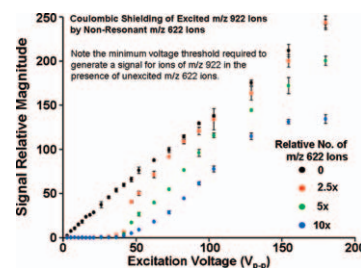


220–223

Coulombic shielding during ion cyclotron excitation in FT-ICR mass spectrometry

Brian M. Ruddy, Steven C. Beu, Nathan K. Kaiser, Christopher L. Hendrickson, Alan G. Marshall

- A trapped ion packet can shield the ions so as to prevent rf resonant excitation in FT-ICR MS.
- In FT-ICR MS, higher resolution ion isolation requires a lower number of trapped ions.

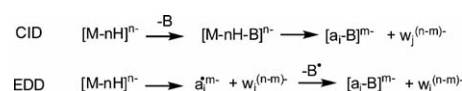


224–233

Concomitant EDD and EID of DNA evidenced by MSⁿ and double resonance experiments

Viet Hung Nguyen, Carlos Afonso, Jean-Claude Tabet

- EID and EDD can be decoupled through double resonance and MS³ experiments.
- EDD is very random along the DNA sequence.
- Sequence dependent cleavages are due to EID processes.
- Mechanism of dissociation processes occurring with EDD of DNA single strands.

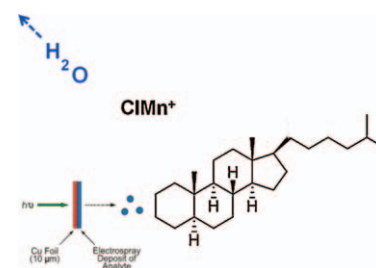


234–239

Characterization of nonpolar lipids and selected steroids by using laser-induced acoustic desorption/chemical ionization, atmospheric pressure chemical ionization, and electrospray ionization mass spectrometry

Zhicheng Jin, Shivani Daiya, Hilkka I. Kenttämä

- Different ionization methods were compared for the mass spectrometric analysis of nonpolar lipids.
- LIAD/CI was found to be superior to ESI and APCI.
- A stable pseudo-molecular ion was formed for all analytes, including saturated hydrocarbons.



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