



Contents

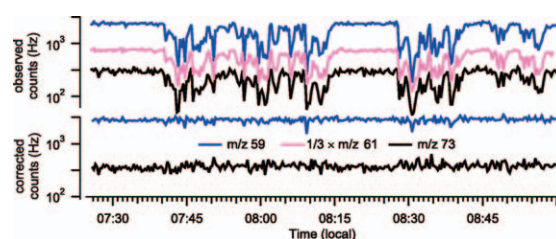
Regular Articles

1–9

On quantitative measurements of peroxydicarboxylic nitric anhydride mixing ratios by thermal dissociation chemical ionization mass spectrometry

Levi H. Mielke, Hans D. Osthoff

► Iodide ion CIMS is applied to measure peroxydicarboxylic nitric anhydrides. ► Matrix effects arising from NO, NO₂, and organic acids were characterized. ► Minor PANs may not be accurately measured in polluted environments.

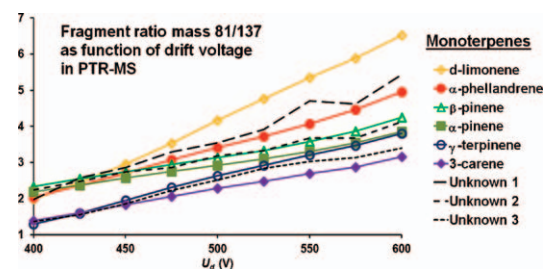


10–19

Development of PTR-MS selectivity for structural isomers: Monoterpenes as a case study

P.K. Misztal, M.R. Heal, E. Nemitz, J.N. Cape

► An alternating drift voltage (AD) mode expands the analytical capabilities of PTR-MS. ► Discrimination of structural isomers is possible with a PTR-MS running in AD mode. ► Different drift energies yield variation in isomer fragmentation/clustering. ► Ratios of m/z 81–137 in the AD mode characterise monoterpenes in the ppb range. ► The method is likely to be effective for other structural isomeric species.

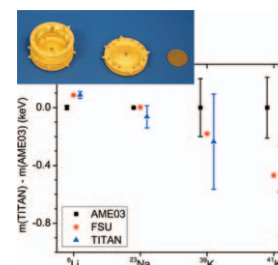


20–31

Verifying the accuracy of the TITAN Penning-trap mass spectrometer

M. Brodeur, V.L. Ryjkov, T. Brunner, S. Ettenauer, A.T. Gallant, V.V. Simon, M.J. Smith, A. Lapierre, R. Ringle, P. Delheij, M. Good, D. Lunney, J. Dilling

► Detailed systematic studies of the TITAN Penning trap mass spectrometer. ► New electrical potential compensation method is derived and demonstrated. ► Mass measurements on stable nuclei shows sub-part-per-billion accuracy.

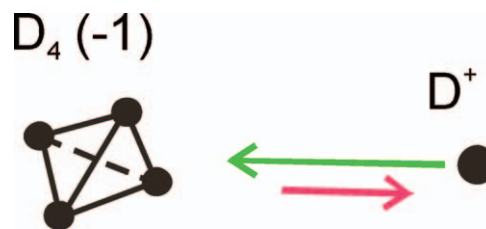


32–43

Cluster ions D_N^+ ejected from dense and ultra-dense deuterium by Coulomb explosions: Fragment rotation and D^+ backscattering from ultra-dense clusters in the surface phase

Patrik U. Andersson, Leif Holmlid

► Cluster ions D_N^+ from D(1) are observed with $N = 3, 4, 12$ and 17 , not in close-packed forms. ► Clusters $D_N(1)$ from D(1) are mainly in the form of chains of D_2 and D_3 groups. ► Only atomic ions D^+ with initial kinetic energy of hundreds of eV are observed from D(-1). ► Half of the D^+ ions are ejected from the emitter surface, half of them penetrate into the ultra-dense D(-1) layer on the emitter surface. This second half of the ions is reflected completely from the surface layer formed by clusters $D_3(-1)$ and $D_4(-1)$.

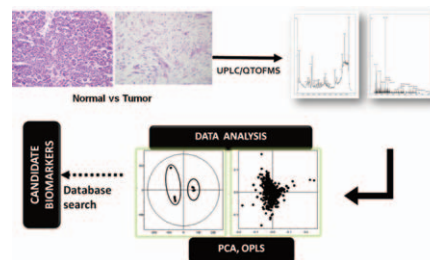


44–51

Metabolomic profiling for biomarker discovery in pancreatic cancer

Prabhjit Kaur, Kathryn Sheikh, Alexander Kirilyuk, Ksenia Kirilyuk, Rajbir Singh, Habtom W. Resson, Amrita K. Cheema

► One of the first reports that tests the feasibility of discerning novel biomarkers from pancreas tumor and normal tissue. ► Use of state of art technology. ► Use of two independent data analysis tools to cross-validate findings. ► Functional pathway analysis using the ingenuity pathway analysis which can lead to potential mechanistic insights. ► In future the markers could be evaluated in bio-fluids for developing minimally invasive assays.

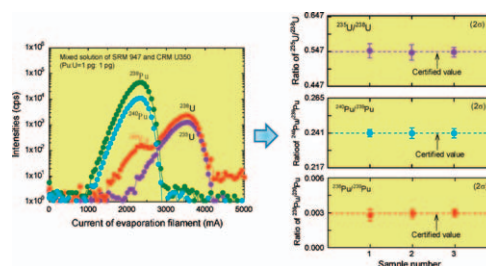


52–56

Application of a continuous heating method using thermal ionization mass spectrometry to measure isotope ratios of plutonium and uranium in trace amounts of uranium–plutonium mixture sample

Yoko Saito-Kokubu, Daisuke Suzuki, Chi-Gyu Lee, Jun Inagawa, Masaaki Magara, Takaumi Kimura

► The continuous heating method by TIMS was confirmed as an effective method for measuring simultaneously isotope ratios of Pu and U in Pu/U mixture samples without chemical separation. ► Particularly, $^{238}\text{Pu}/^{239}\text{Pu}$ ratio was obtained by using a correcting method in which ^{238}Pu intensity was calculated by subtracting the ^{238}U intensity estimated from the ^{235}U intensity and the $^{235}\text{U}/^{238}\text{U}$ ratio.

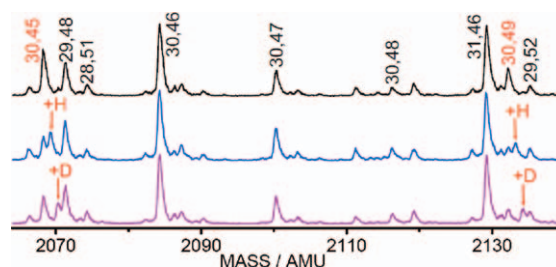


57–64

C–H bond activation by nanosized scandium oxide clusters in gas-phase

Xiao-Nan Wu, Bo Xu, Jing-Heng Meng, Sheng-Gui He

► C–H bond activation of *n*-butane by nanosized scandium oxide cluster cations. ► C–H bond activation is facilitated by bridgingly bonded oxygen-centred radicals. ► Local spin effect on C–H bond activation is demonstrated for small clusters. ► C–H bond activation by a series of oxygen-very-rich clusters $(\text{Sc}_2\text{O}_3)_{4-22}\text{O}_4^+$.

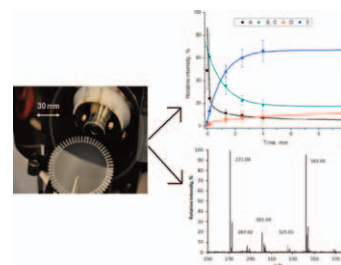


65–71

Rotating multitip micropillar array electrospray ionization-mass spectrometry for rapid analysis and high-throughput screening

Teemu Nissilä, Nina Backman, Marjo Kolmonen, Antti Leinonen, Alexandros Kiriazis, Jari Yli-Kauhaluoma, Lauri Sainiemi, Risto Kostianen, Sami Franssila, Raimo A. Ketola

- ▶ A microfabricated rotating multitip electrospray ionization platform for mass spectrometry.
- ▶ Rapid screening of benzodiazepines from urine with ZipTip extraction and μ PESI/MS.
- ▶ Determination of synthetic reaction products on-line. ▶ Only very small volumes of samples are needed.



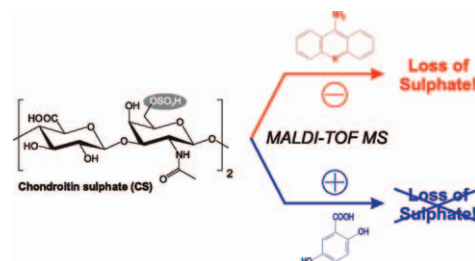
Short Communication

72–76

Positive ion MALDI-TOF mass spectra are more suitable than negative ion spectra to characterize sulphated glycosaminoglycan oligosaccharides

Kathrin Nimptsch, Rosmarie Süß, Matthias Schnabelrauch, Ariane Nimptsch, Jürgen Schiller

- ▶ Glycosaminoglycans (GAGs) are acidic polysaccharides – often sulphated. ▶ Sulphate loss is an important, but unwanted fragmentation in the mass spectra of GAG. ▶ Positive ion MS leads to less pronounced sulphate loss than negative ion MS. ▶ Positive ion MS is only slightly less sensitive. Reduced sulphate loss is a significant advantage for mixture analysis.



77–80

Electrospray tandem mass spectrometric analysis of duboscic acid, exploring the structural features of a new class of triterpenoids, dubosane

Syed Ghulam Musharraf, Madiha Goher, Pascal Wafo, Ramsay S.T. Kamdem

- ▶ First report on CID-MS/MS analysis of dubosane triterpenoid, duboscic acid. ▶ Identification of key fragments and proposal of logical fragmentation pathways. ▶ Characteristic fragments are formed due to the cleavage of seven membered ring C.

