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### Editorial

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#### Nucleic acids

Patrick A. Limbach, Michael T. Bowers

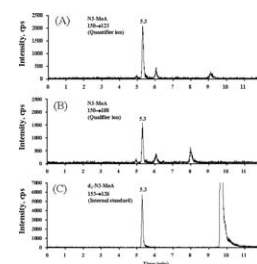
### Regular articles

68–73

#### Quantitative determination of urinary N3-methyladenine by isotope-dilution LC–MS/MS with automated solid-phase extraction

Chiung-Wen Hu, Bo-Huei Lin, Mu-Rong Chao

A highly specific and sensitive isotope-dilution liquid chromatographic–tandem mass spectrometric (LC–MS/MS) method was developed for a direct measurement of urinary N3-methyladenine.

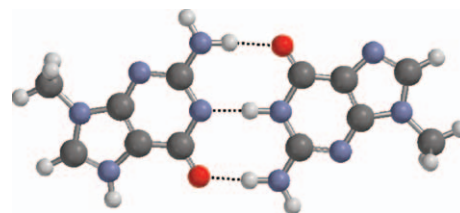


74–82

#### Gas-phase formation and reactions of radical cations of guanosine, deoxyguanosine and their homodimers and heterodimers

Linda Feketeová, Elizabeth Yuriev, John D. Orbell,  
George N. Khairallah, Richard A.J. O'Hair

Investigation of the gas-phase formation and reactions of radical cations of guanosine, deoxyguanosine and their homodimers and heterodimers has revealed a novel tautomeric structure, illustrated above, that may have important biological implications.

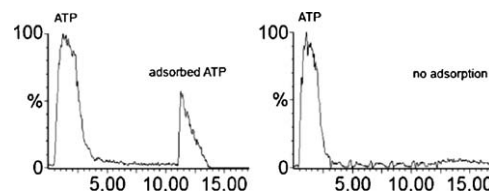


## 83–90

### Study on the loss of nucleoside mono-, di- and triphosphates and phosphorylated peptides to a metal-free LC-MS hardware

Thomas De Vijlder, Jasper Boschmans, Erwin Witters, Filip Lemière

Nucleotides and phosphopeptides strongly interact with metal-free LC-ESI hardware. The main site of adsorption is traced back to the fused silica tubing. A solution is suggested.

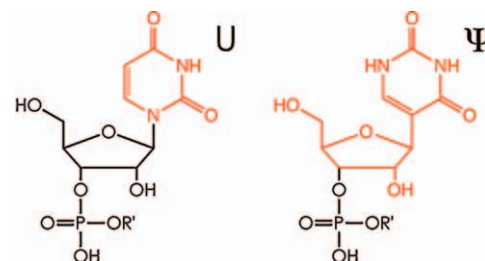


## 91–97

### Identification, localization, and relative quantitation of pseudouridine in RNA by tandem mass spectrometry of hydrolysis products

Monika Taucher, Barbara Ganisl, Kathrin Breuker

Collisionally activated dissociation of RNA gives base loss diagnostic for uridine, and nucleoside loss diagnostic for pseudouridine residues.

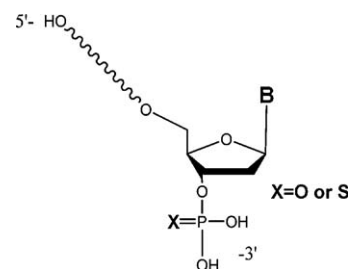


## 98–104

### Detecting low-level synthesis impurities in modified phosphorothioate oligonucleotides using liquid chromatography–high resolution mass spectrometry

Irena Nikcevic, Tadeusz K. Wyrzykiewicz, Patrick A. Limbach

An LC-MS method based on the use of high resolution Fourier transform ion cyclotron resonance mass spectrometry (FTIRCMS) for profiling oligonucleotides synthesis impurities is described.

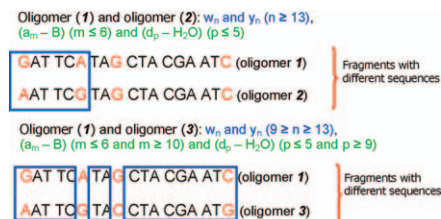


## 105–114

### Differentiation and sequencing of three constitutional isobaric 18-mer DNA oligomers using low-energy collision tandem mass spectrometry

Farid Jahouh, Mina Nashed, Nicolas Joly, Patrick Martin, Joseph Banoub

Differentiation and sequencing of three constitutional isobaric 18-mer DNA oligomers, namely: GATTCATAGCTACGAATC **1**, AATTCGTAGCTACGAATC **2**, and AATTCGTACTACGAATG **3** using electrospray ionization tandem mass spectrometry with a hybrid QqToF-MS/MS instrument.

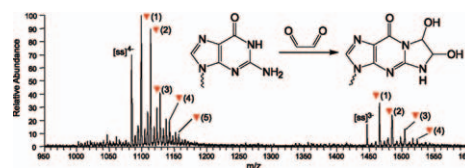


## 115–123

### Investigation of the reactivity of oligodeoxynucleotides with glyoxal and $\text{KMnO}_4$ chemical probes by electrospray ionization mass spectrometry

Carol Parr, Sarah E. Pierce, Suncerae I. Smith, Jennifer S. Brodbelt

The reactions of glyoxal and potassium permanganate with oligodeoxynucleotides are monitored by electrospray ionization mass spectrometry to evaluate the influence of the sequence of DNA.

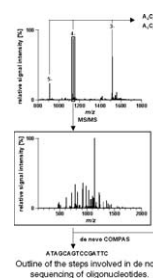


## 124–129

### Tandem mass spectrometric de novo sequencing of oligonucleotides using simulated annealing for stochastic optimization

Herbert Oberacher, Florian Pitterl

A global strategy for tandem mass spectrometric de novo sequencing of oligonucleotides is presented which is based on finding among all possible sequences the sequence, whose simulated tandem mass spectrum shows the highest degree of similarity to the measured spectrum.

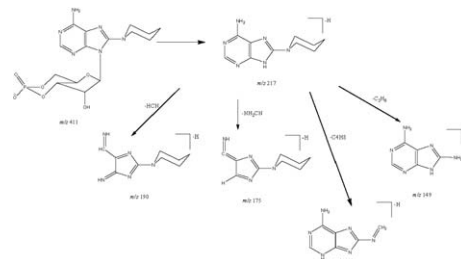


## 130–139

### Mass spectrometric fragmentation behaviour of cAMP analogues

A.E. Bond, S. Ding, C.M. Williams, R.P. Newton, E. Dudley

The mass spectrometric fragmentation of analogues of the biological second messenger, adenosine 3',5'-cyclic monophosphate was undertaken to study the effect of modifications on the tandem mass spectrometry data obtained.

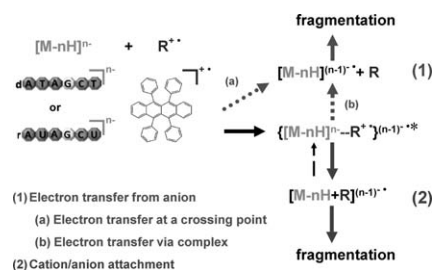


## 140–147

### Gas-phase ion/ion reactions of rubrene cations and multiply charged DNA and RNA anions

Teng-yi Huang, Scott A. McLuckey

The major processes relevant to the reaction of multiply charged DNA or RNA anions ( $[\text{M-nH}]^{n-}$ ) with ionized rubrene ( $\text{R}^{+}$ ).

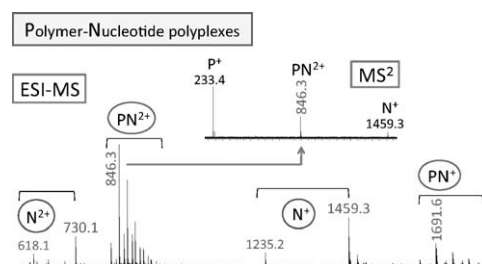


## 148–153

### Non-covalent complexes between single-stranded oligodeoxynucleotides and poly(ethylene imine)

Danijela Smiljanic, Chrys Wesdemiotis

The dominant polyplexes formed by pentadeoxynucleotides with poly(ethylene imine) 400 or 800 have 1:1 stoichiometry. Solution and intrinsic stabilities of these non-covalent complexes follow the same order, with thymine-rich nucleotides showing the highest binding affinities.

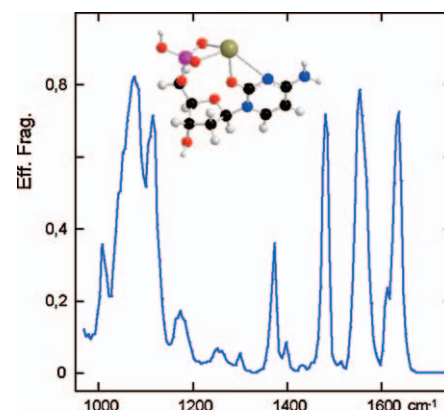


## 154–164

### Structure of $Pb^{2+}$ /dCMP and $Pb^{2+}$ /CMP complexes as characterized by tandem mass spectrometry and IRMPD spectroscopy

Jean-Yves Salpin, L titia Gamiette, Jeanine Tortajada, Thierry Besson, Philippe Ma tre

Formation of macrochelate forms for  $Pb^{2+}$ /deoxycytidine-5'-monophosphate and  $Pb^{2+}$ /cytidine-5'-monophosphate complexes is demonstrated by tandem mass spectrometry and mid-infrared multiple-photon dissociation (IRMPD) spectroscopy.

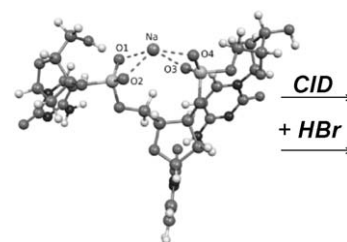


## 165–171

### Alkali cation regulation of the dissociation and hydrobromination of a deprotonated trideoxynucleotide

Janna Anichina, Andreas Krapp, Einar Uggerud, Diethard K. Bohme

► Alkali cation regulation of the gas-phase dissociation of the deprotonated trideoxycytoside dianion  $(CCC-2H)^{2-}$  is measured by CID using ESI mass spectrometry. ► Sodium cation regulation of the gas-phase chemical reactivity of  $[Na(CCC-2H)]^-$  anion with HBr is measured using ESI/SIFT/QqQ tandem mass spectrometry. ► Quantum chemical calculations (RI-MP2) provide structural and energetic results for the alkaliation and hydrobromination of  $(CCC-2H)^{2-}$  and  $[M(CCC-2H)]^-$  anions.

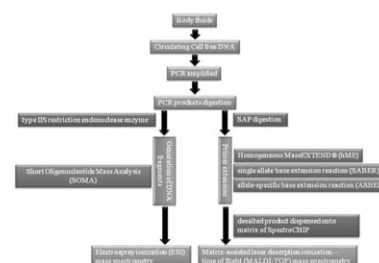


## 172–183

### Mass spectrometric based analysis, characterization and applications of circulating cell free DNA isolated from human body fluids

Vaneet K. Sharma, Paul Vouros, James Glick

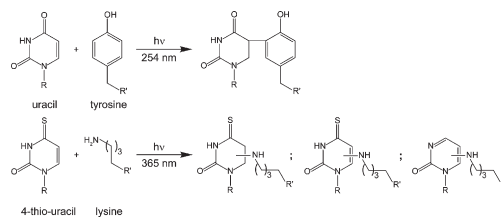
► The use of circulating cell free DNA in clinical diagnostics. ► Application of mass spectrometry to circulating cell free DNA. ► The use of PCR and mass spectrometry for fetal disease diagnosis. ► New developments of mass spectrometry for circulating cell free DNA in biofluids.



**184–194****Mass-spectrometric analysis of proteins cross-linked to 4-thio-uracil- and 5-bromo-uracil-substituted RNA**

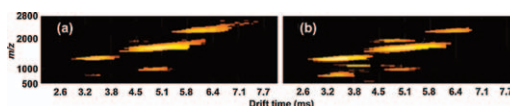
Katharina Kramer, Petra Hummel, He-Hsuan Hsiao, Xiao Luo, Markus Wahl, Henning Urlaub

- MS analysis of protein-RNA cross-links derived from 4-thio-uracil substituted RNA.
- Implementation of novel, automated data analysis approach. ► MASCOT identification of cross-linked peptides enabled by novel procedure.

**195–203****Assessment of the gas phase stability of quadruplex DNA using travelling wave ion mobility mass spectrometry**

Karina C. Porter, Jennifer L. Beck

- ESI-TWIMS enabled distinction of ions of the same  $m/z$  that corresponded to folded and unfolded qDNA. ► ESI-TWIMS supported that ions carrying 4 and 5 negative charges arose from folded intra molecular qDNA. ► This work shows the utility of ESI-TWIMS in distinguishing among different conformations and structures of qDNA.

**204–208****Analysis of nucleosides using the atmospheric-pressure solids analysis probe for ionization**

Jef Rozenski

- ASAP is an ionization technique suitable for non-polar compounds. ► Nucleosides are considered to be non-volatile compounds. ► This work shows that nucleosides are ionizable with ASAP. ► The method works also for naturally occurring and synthetically modified nucleosides. ► Presence of cations is not as critical as with electrospray ionization.

