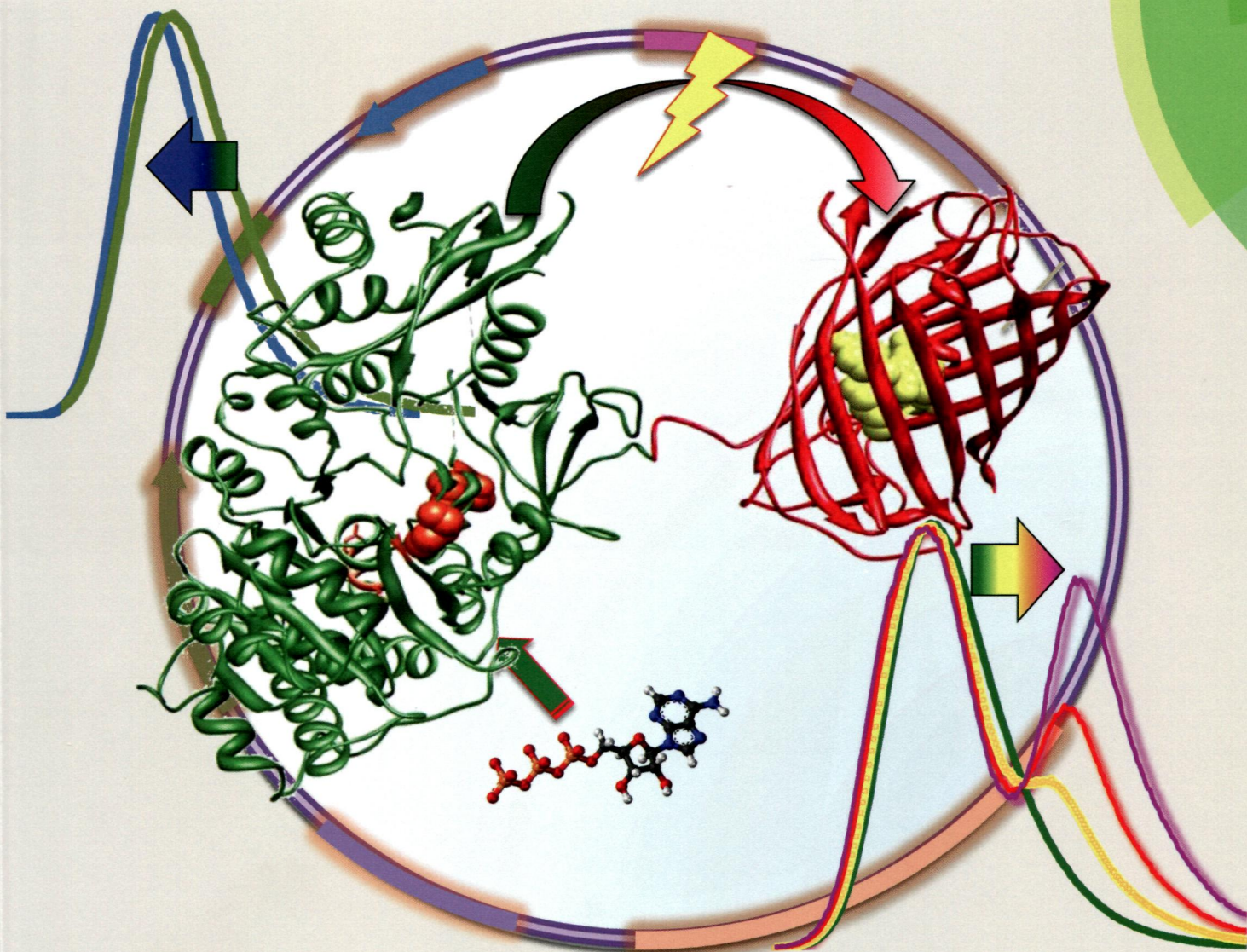
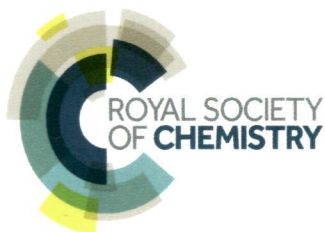


# Analyst

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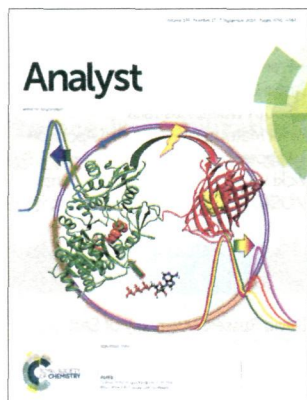
ISSN 0003-2654



PAPER  
Golnaz Borghei and Elizabeth A. H. Hall  
BRET-linked ATP assay with luciferase

## IN THIS ISSUE

ISSN 0003-2654 CODEN ANALAO 139(17) 4091–4384 (2014)



### Cover

See Golnaz Borghei and Elizabeth A. H. Hall, pp. 4185–4192. Image reproduced by permission of Elizabeth Hall from *Analyst*, 2014, **139**, 4185.



### Inside cover

See Royston Goodacre *et al.*, pp. 4193–4199. Image reproduced by permission of Royston Goodacre from *Analyst*, 2014, **139**, 4193.

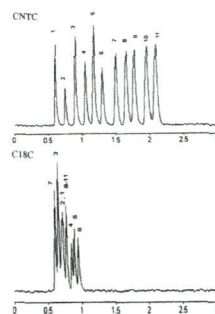
## MINIREVIEWS

4103

### Nanoparticle-based monoliths for chromatographic separations

Sheng Tang, Yong Guo, Chunming Xiong, Shujuan Liu,\* Xia Liu and Shengxiang Jiang\*

As an intriguing member of the monolith family, nanoparticle-based monoliths have recently emerged as a new class of promising substrates in analytical sample preparation and separation science because of their many distinct characteristics such as high permeability and readily available tailored surface chemistries.

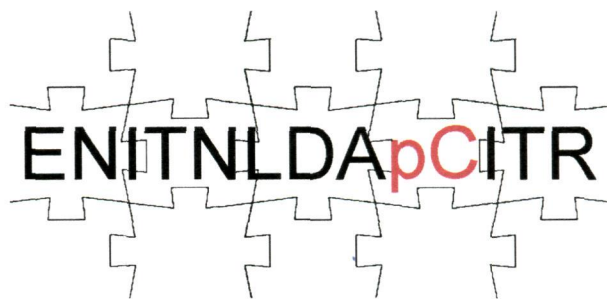


4118

### Puzzling over protein cysteine phosphorylation – assessment of proteomic tools for S-phosphorylation profiling

A. K. Buchowiecka\*

The article provides useful information necessary for designing experiments in the emerging cysteine phosphoproteomics.

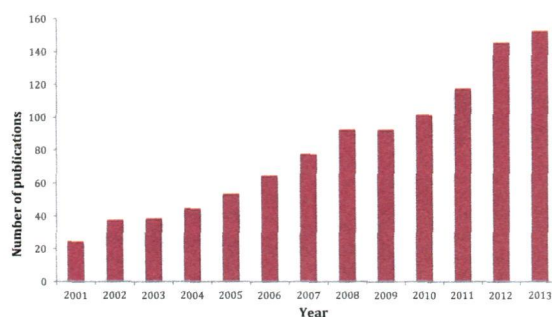


4124

### Detection of proteins by hyphenated techniques with endogenous metal tags and metal chemical labelling

Beatrice Campanella and Emilia Bramanti\*

The absolute and relative quantitation of proteins plays a fundamental role in modern proteomics, as it is the key to understand still unresolved biological questions in medical and pharmaceutical applications.

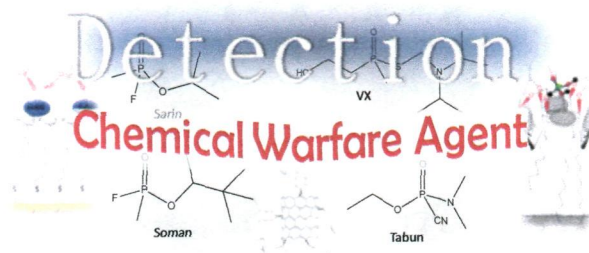


4154

### Surface-immobilization of molecules for detection of chemical warfare agents

Indrani Bhowmick\* and Neelam

Surface-based detection of chemical warfare agents through immobilization of inorganic-organic molecular entities.



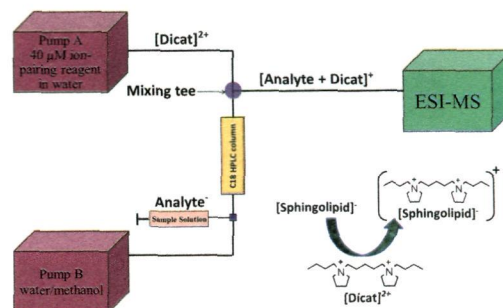
## COMMUNICATIONS

4169

### Separation and sensitive determination of sphingolipids at low femtomole level by using HPLC-PIESI-MS/MS

Chengdong Xu, Eduardo Costa Pinto and Daniel W. Armstrong\*

A highly sensitive paired ion electrospray ionization mass spectrometry (PIESI-MS) approach was developed for the trace determination of sphingolipids.

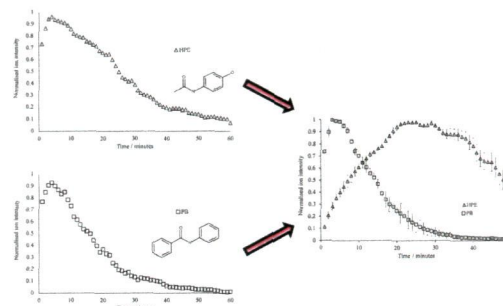


4176

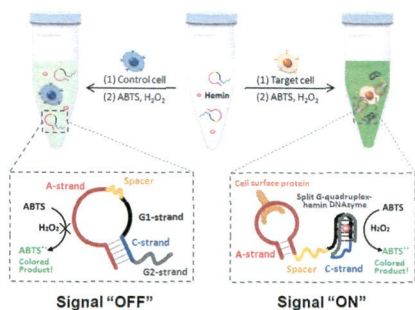
### Parameters affecting ion intensities in transmission-mode direct analysis in real-time mass spectrometry

Lindsay P. Harding,\* Gareth M. B. Parkes\* and James D. Townsend

The first systematic study of thermal parameters affecting ion intensities in transmission mode DARTMS is presented.



4181



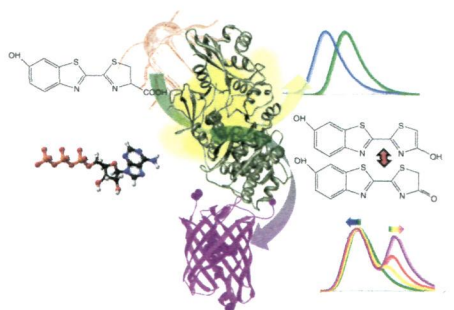
### A label-free activatable aptamer probe for colorimetric detection of cancer cells based on binding-triggered *in situ* catalysis of split DNAzyme

Hui Shi, Duo Li, Fengzhou Xu, Xiaoxiao He,<sup>\*</sup> Kemin Wang,<sup>\*</sup> Xiaosheng Ye, Jinlu Tang and Chunmei He

A label-free activatable aptamer probe was developed for cancer cell detection through recognition-switched split DNAzyme activity on a living cell surface.

## PAPERS

4185

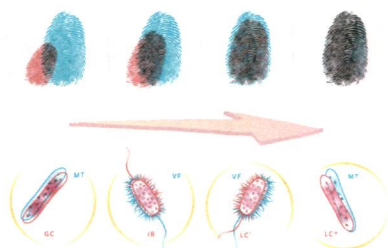


### BRET-linked ATP assay with luciferase

Golnaz Borghei and Elizabeth A. H. Hall<sup>\*</sup>

A Bioluminescence Resonance Energy transfer (BRET) pair with firefly luciferase and mCherry provides a new method for ATP measurement via the shift in the mCherry emission wavelength.

4193

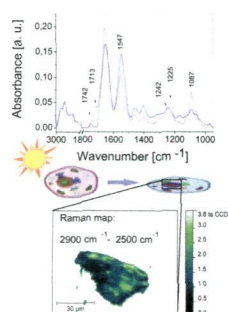


### Multiple metabolomics of uropathogenic *E. coli* reveal different information content in terms of metabolic potential compared to virulence factors

Haitham AlRabiah, Yun Xu, Nicholas J. W. Rattray, Andrew A. Vaughan, Tarek Gibreel, Ali Sayqal, Mathew Upton, J. William Allwood and Royston Goodacre<sup>\*</sup>

No single analytical method can cover the whole metabolome and the choice of which platform to use may inadvertently introduce chemical selectivity.

4200



### Monitoring UVR induced damage in single cells and isolated nuclei using SR-FTIR microspectroscopy and 3D confocal Raman imaging

Ewelina Lipiec, Keith R. Bambery, Philip Heraud, Wojciech M. Kwiatek, Don McNaughton, Mark J. Tobin, Christian Vogel and Bayden R. Wood<sup>\*</sup>

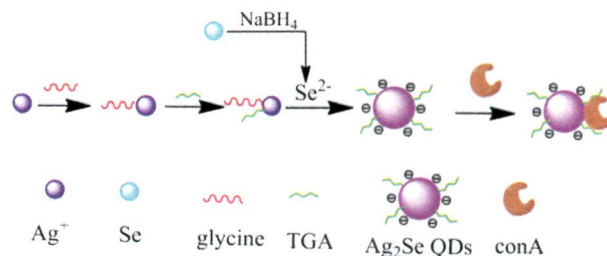
Melanocytes exposed to artificial sunlight and analysed with FTIR and Raman spectroscopy show changes in DNA bands and evidence of lipid accumulation.

4210

### Synthesis of water-soluble Ag<sub>2</sub>Se QDs as a novel resonance Rayleigh scattering sensor for highly sensitive and selective ConA detection

Shuguang Yan, Lichun Zhang, Yurong Tang and Yi Lv\*

Schematic illustration for fabricating TGA and glycine modified Ag<sub>2</sub>Se QDs for RRS detection of ConA.

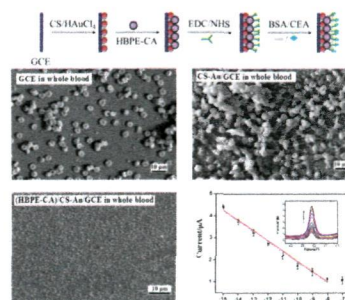


4216

### A chitosan-Au-hyperbranched polyester nanoparticles-based antifouling immunosensor for sensitive detection of carcinoembryonic antigen

Chong Sun, Lie Ma, Qiu-hui Qian, Soniya Parmar, Wenbo Zhao,\* Bo Zhao and Jian Shen\*

An electrochemical immunosensor was developed for the detection of carcinoembryonic antigen in whole blood, based on the antibiofouling properties of carboxylic acid group functionalized hyperbranched polyester nanoparticles.

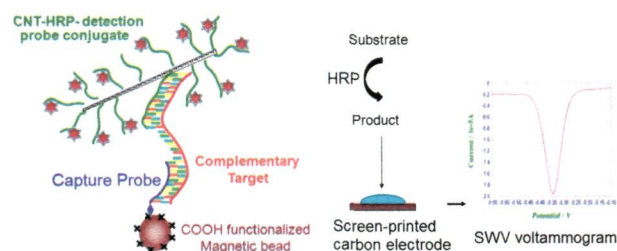


4223

### Electrochemical detection of leukemia oncogenes using enzyme-loaded carbon nanotube labels

Ai-Cheng Lee, Dan Du, Baowei Chen, Chew-Kiat Heng, Tit-Meng Lim\* and Yuehe Lin\*

An ultrasensitive electrochemical nucleic acid assay amplified by carbon nanotubes (CNTs)-based labels for the detection of leukemia oncogenes.

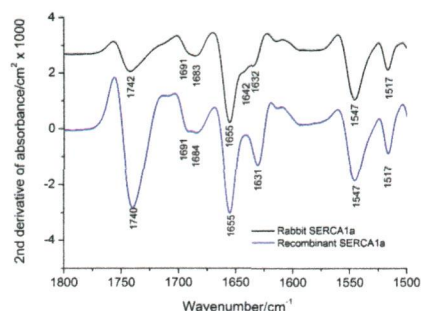


4231

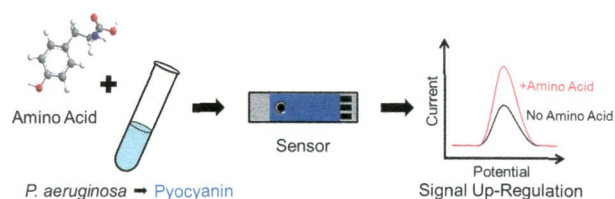
### Quality assessment of recombinant proteins by infrared spectroscopy. Characterisation of a protein aggregation related band of the Ca<sup>2+</sup>-ATPase

Chenge Li, Saroj Kumar, Cédric Montigny, Marc le Maire and Andreas Barth\*

FTIR spectroscopy detects aggregates of recombinantly produced protein and can therefore be used for quality control.



4241

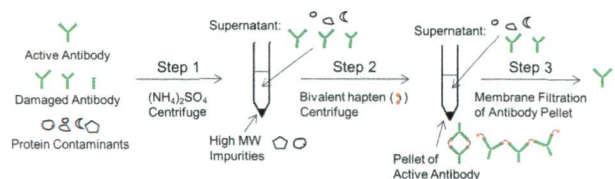


### Up-regulating pyocyanin production by amino acid addition for early electrochemical identification of *Pseudomonas aeruginosa*

Hunter J. Sismaet, Thaddaeus A. Webster and Edgar D. Goluch\*

A simple and rapid electrochemical detection method for *Pseudomonas aeruginosa* is demonstrated using amino acids as up-regulatory molecules for pyocyanin production.

4247

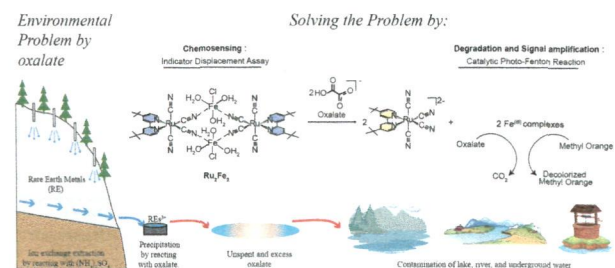


### Affinity-based precipitation via a bivalent peptidic hapten for the purification of monoclonal antibodies

Michael W. Handlogten, Jared F. Stefanick, Peter E. Deak and Basar Bilgicer\*

An affinity-based precipitation method was developed for the rapid and facile purification of bivalently active antibodies from complex biological solutions.

4256

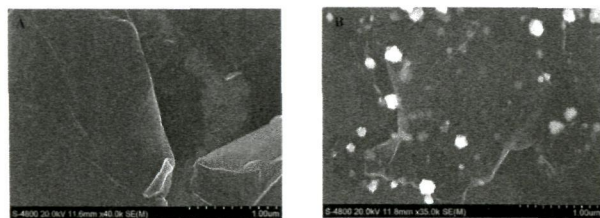


### An Ru(II)–Fe(III) bimetallic complex as a multifunctional device for detecting, signal amplifying, and degrading oxalate

Cheuk-Fai Chow,\* Pui-Yu Ho and Cheng-Bin Gong

A multifunctional device that can monitor the level of pollutants, magnify weak signals, and subsequently degrade pollutants is highly desirable. A new Ru(II)–Fe(III) complex— $[\text{Ru}^{\text{II}}(\text{Bubpy})(\text{CN})_4]_2\text{—}[\text{Fe}^{\text{III}}(\text{H}_2\text{O})_3\text{Cl}]_2 \cdot 8\text{H}_2\text{O}$  (1, 'Bubpy' = 4,4'-di-*tert*-butyl-2,2'-bipyridine)—was synthesized and characterized.

4264



### Cleavage-based hybridization chain reaction for electrochemical detection of thrombin

Yuanyuan Chang, Yaqin Chai,\* Shunbi Xie, Yali Yuan, Juan Zhang and Ruo Yuan\*

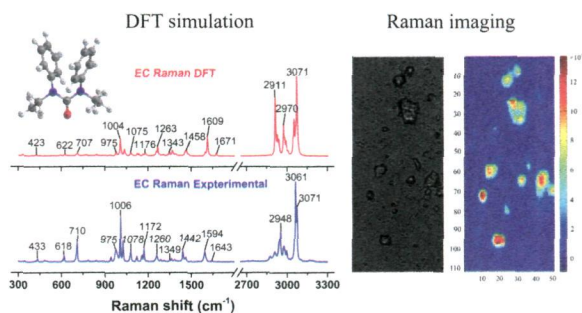
In the present work, we constructed a new label-free "inter-sandwich" electrochemical aptasensor for thrombin (TB) detection by employing a cleavage-based hybridization chain reaction (HCR).

4278

### Analysis of ethyl and methyl centralite vibrational spectra for mapping organic gunshot residues

Jianbo Zeng, Ji Qi, Fuquan Bai, Jorn Chi Chung Yu and Wei-Chuan Shih\*

Detection of ethyl and methyl centralites in gunshot residues is important in forensic science due to their limited contamination from environmental sources compared to other organic residues.

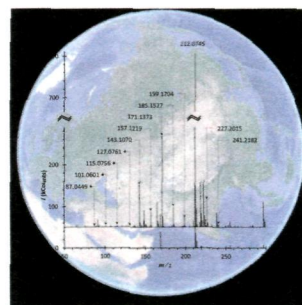


4279

### High throughput volatile fatty acid skin metabolite profiling by thermal desorption secondary electrospray ionisation mass spectrometry

Helen J. Martin, James C. Reynolds, Svetlana Riazanskaia and C. L. Paul Thomas\*

Global VOC skin metabolite profiling. Thermal desorption secondary electrospray ionisation time-of-flight mass spectrometry classifies skin odour phenotypes by targeted volatile fatty analysis. Examination of the mass spectra reveals the potential for global metabolic studies.

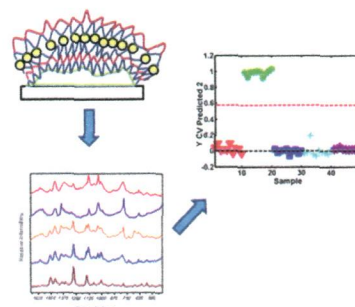


4287

### Layer-by-layer polyelectrolyte encapsulation of *Mycoplasma pneumoniae* for enhanced Raman detection

Omar E. Rivera-Betancourt, Edward S. Sheppard, Duncan C. Krause and Richard A. Dluhy\*

*Mycoplasma pneumoniae* is a major cause of respiratory disease in humans and accounts for as much as 20% of all community-acquired pneumonia.

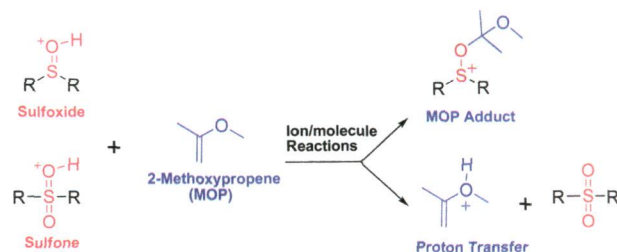


4296

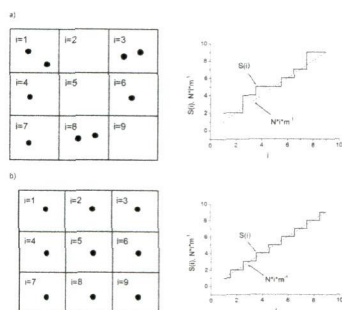
### Identification of the sulfoxide functionality in protonated analytes via ion/molecule reactions in linear quadrupole ion trap mass spectrometry

Huaming Sheng, Peggy E. Williams, Weijuan Tang, Minli Zhang and Hilkka I. Kenttämäa\*

A mass spectrometric method utilizing gas-phase ion/molecule reactions of 2-methoxypropene (MOP) has been developed for the identification of the sulfoxide functionality in protonated analytes in a LQIT mass spectrometer.



4303

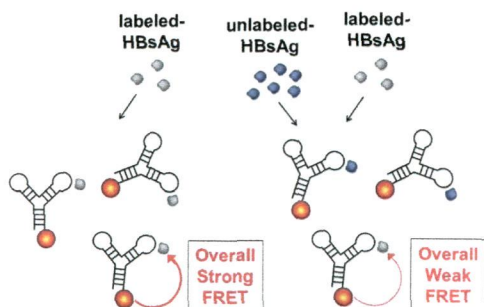


### A sample-effective calibration design for multiple components

Dmitry Kirsanov,\* Vitaly Panchuk, Marina Agafonova-Moroz, Maria Khaydukova, Alexander Lumpov, Valentin Semenov and Andrey Legin

The experimental design of mixtures for multivariate calibration is introduced. The idea of this design is based on uniform distribution of experimental points in a concentration hypercube and does not employ the concept of fixed concentration levels.

4310

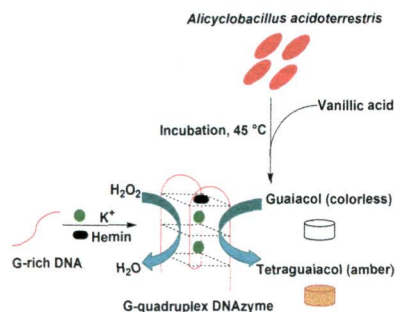


### Aptamer-based competitive binding assay for one-step quantitation of hepatitis B surface antigen

Sung-Kwan Suh, Seongeun Song, Heung-Bum Oh, Sang-Hyun Hwang\* and Sang Soo Hah\*

A robust aptamer- and FRET-based competitive binding assay is reported for the one-step quantitation of hepatitis B surface antigen.

4315

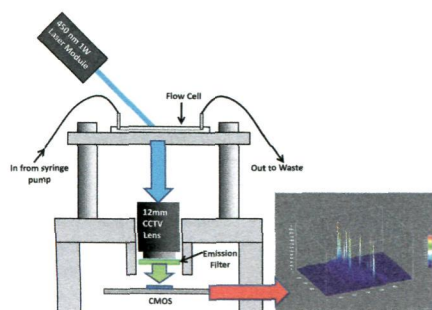


### A G-quadruplex DNAzyme-based colorimetric method for facile detection of *Alicyclobacillus acidoterrestris*

Tao Liu, Xiao Zhang, Wenxin Zhu, Wei Liu, Daohong Zhang\* and Jianlong Wang\*

A novel G-quadruplex DNAzyme-based colorimetric method was developed for the first time for a rapid detection of *Alicyclobacillus acidoterrestris*.

4322



### Webcam-based flow cytometer using wide-field imaging for low cell number detection at high throughput

Joshua Balsam, Hugh Alan Bruck and Avraham Rasooly\*

Here we describe a novel low-cost high throughput flow cytometer based on a webcam capable of low cell number detection in a large volume which may overcome the limitations of current flow cytometry.

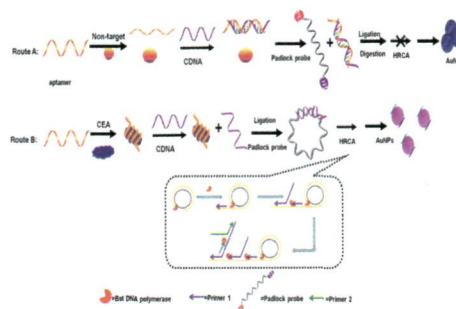


4330

### Ultrasensitive colorimetric carcinoembryonic antigen biosensor based on hyperbranched rolling circle amplification

Kai Liang, Shuiting Zhai, Zhidong Zhang, Xiaoyang Fu, Jingwei Shao,\* Zhenyu Lin, Bin Qiu\* and Guo-nan Chen

A hyperbranched rolling circle amplification (HRCA)-based colorimetric biosensor for carcinoembryonic antigen (CEA) with high sensitivity and specificity has been developed.

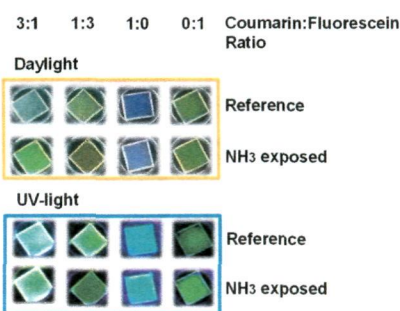


4335

### Coumarin meets fluorescein: a Förster resonance energy transfer enhanced optical ammonia gas sensor

Susanne Widmer, Marko Dorrestijn, Agathe Camerlo, Špela Korent Urek, Aleksandra Lobnik, Catherine E. Housecroft, Edwin C. Constable and Lukas J. Scherer\*

The incorporation of a FRET-based sensing system into an organic modified silica matrix resulted in a quantitative and reversible optical ammonia gas sensor with a linear response.

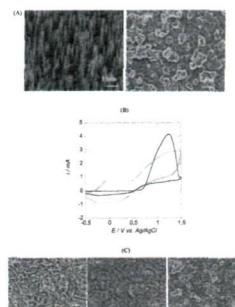


4343

### Diamond nanowires modified with poly[3-(pyrrolyl)carboxylic acid] for the immobilization of histidine-tagged peptides

Palaniappan Subramanian, Ievgen Mazurenko, Vladimir Zaitsev, Yannick Coffinier, Rabah Boukherroub and Sabine Szunerits\*

Coating boron-doped diamond nanowires (BDD NWs) with a conducting polymer, poly[3-(pyrrolyl)carboxylic acid], has been reported.

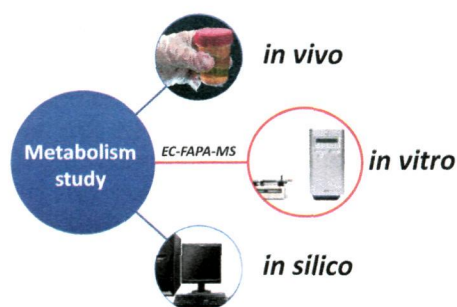


4350

### Determination of psychostimulants and their metabolites by electrochemistry linked on-line to flowing atmospheric pressure afterglow mass spectrometry

Marek Smoluch,\* Przemyslaw Mielczarek, Edward Reszke, Gary M. Hieftje and Jerzy Silberring

A novel EC-FAPA coupling has been shown for analysis of psychostimulants and their metabolites. The capabilities of the FAPA source to accept flowing liquid systems have also been demonstrated.



4356

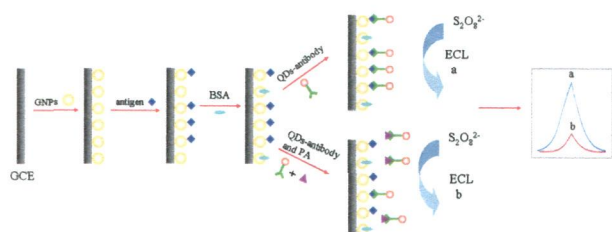


### Synthesis of ZnO nanorods and their application in the construction of a nanostructure-based electrochemical sensor for determination of levodopa in the presence of carbidopa

Elahé Molaakbari, Ali Mostafavi, Hadi Beitollahi\* and Reza Alizadeh

A novel carbon paste electrode modified with ZnO nanorods and 5-(4'-amino-3'-hydroxy-biphenyl-4-yl)-acrylic acid (3,4'-AAZCPE) was fabricated.

4365

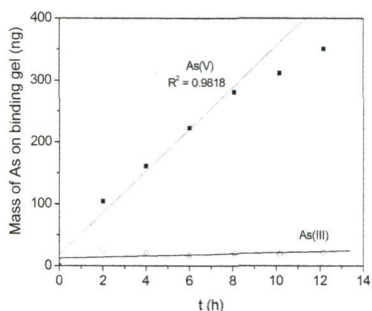


### A quantum dot based electrochemiluminescent immunosensor for the detection of pg level phenylethanolamine A using gold nanoparticles as substrates and electron transfer accelerators

Panpan Yan, Jing Zhang, Qinghui Tang, Anping Deng\* and Jianguo Li\*

This study reports the development of an electrochemiluminescent (ECL) immunosensor for ultrasensitive detection of phenylethanolamine A (PA) based on CdSe quantum dots (QDs) and gold nanoparticles (GNPs).

4373



### Speciation analysis of inorganic arsenic in river water by Amberlite IRA 910 resin immobilized in a polyacrylamide gel as a selective binding agent for As(v) in diffusive gradient thin film technique

Ana M. C. M. Rolisola, Carlos A. Suárez, Amauri A. Menegário,\* Didier Gastmans, Chang H. Kiang, Camila D. Colaço, Daniel L. Garcez and Ricardo E. Santelli

Selective sampling of As(v) by DGT (diffusive gradients in thin films) device containing the Amberlite IRA 910 resin immobilized in polyacrylamide gel.

## ADDITIONS AND CORRECTIONS

4381

Additions and corrections published 31st January to 23rd April 2014