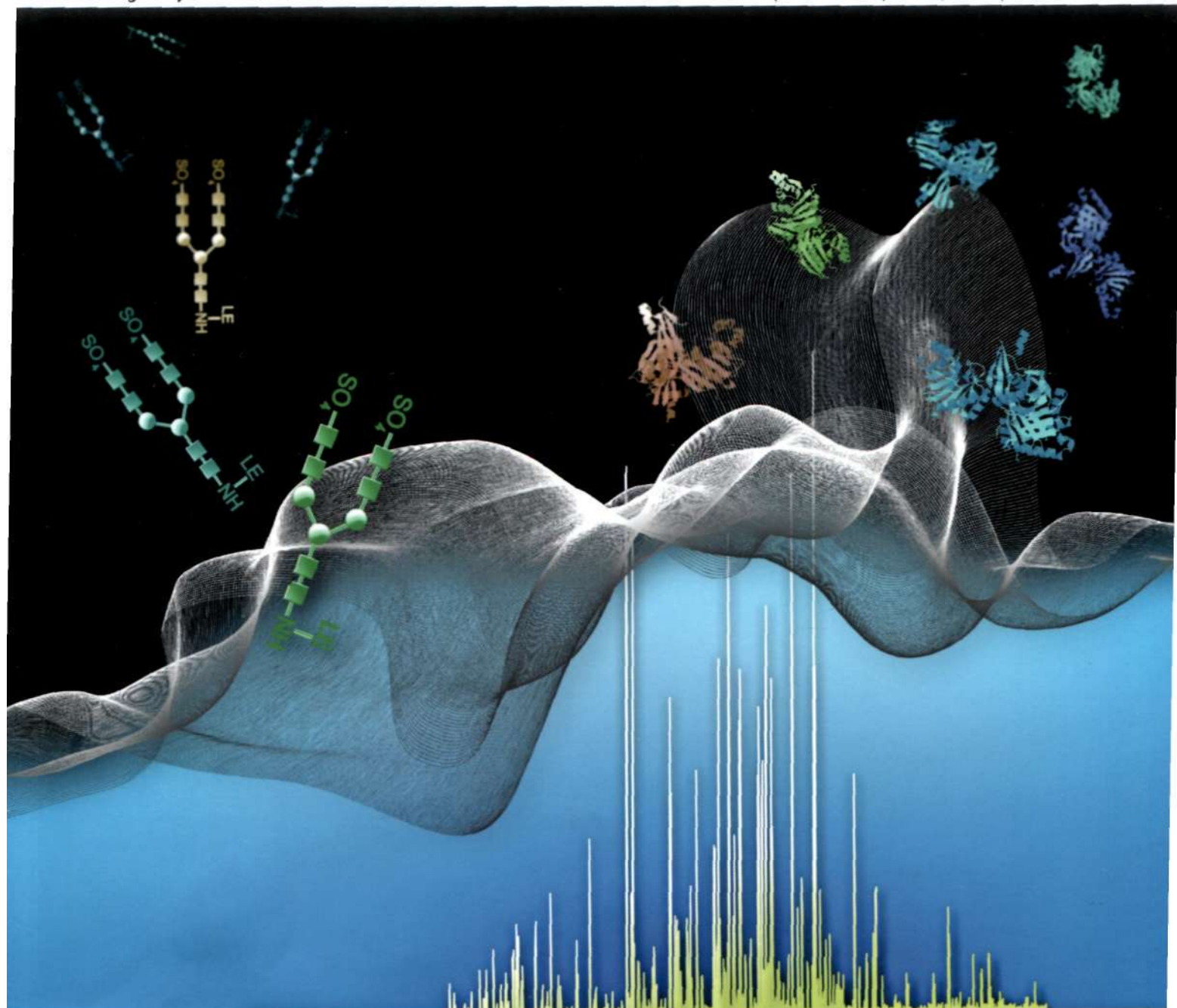


# Analyst

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Volume 138 | Number 10 | 21 May 2013 | Pages 2779–3084



ISSN 0003-2654

**CRITICAL REVIEW**

Heather Desaire *et al.*

Software for automated interpretation of mass spectrometry data from glycans and glycopeptides

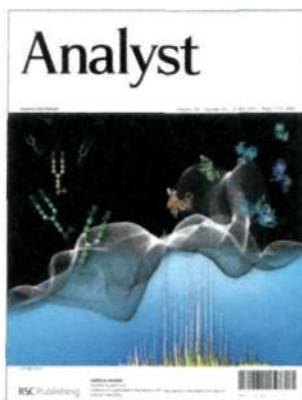


0003-2654 (2013)138:10;1-0

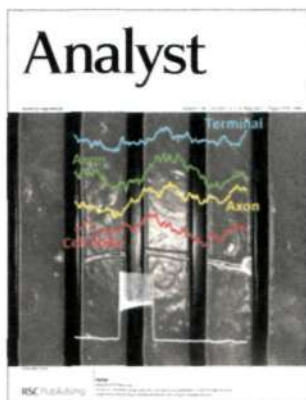
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## IN THIS ISSUE

ISSN 0003-2654 CODEN ANALAO 138(10) 2779–3084 (2013)



**Cover**  
See Heather Desaire *et al.*,  
pp. 2793–2803.  
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2013, **138**, 2793.



**Inside cover**  
See Bhavik Anil Patel *et al.*,  
pp. 2833–2839.  
Image reproduced by permission  
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2013, **138**, 2833.

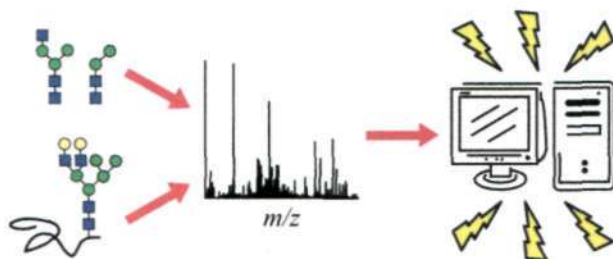
## CRITICAL REVIEW

2793

### Software for automated interpretation of mass spectrometry data from glycans and glycopeptides

Carrie L. Woodin, Morgan Maxon and Heather Desaire\*

This review focuses on recent advances in software development for assigning MS data of glycans and glycopeptides.



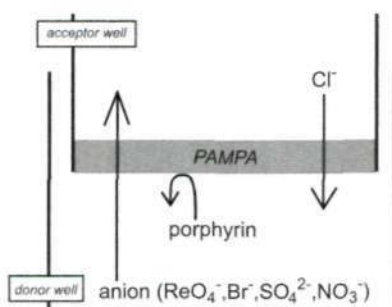
## COMMUNICATIONS

2804

### Study of receptor mediated selective anion transmembrane transport using parallel artificial membrane permeability assay

Lenka Veverková, Kamil Záruba and Vladimír Král\*

Separation of inorganic anions  $\text{ReO}_4^-$ ,  $\text{Br}^-$ ,  $\text{SO}_4^{2-}$ , and  $\text{NO}_3^-$  using porphyrin–alkaloid quaternary salt transporters is examined using a parallel artificial membrane permeability assay.



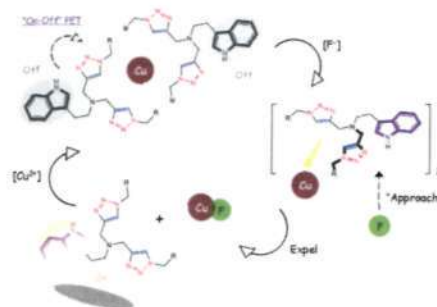


2808

### Bis-triazolyl indoleamines as unique "off-approach-on" chemosensors for copper and fluorine

De-Tai Shi, Bin Zhang, Ya-Xi Yang, Chu-Chu Guan, Xiao-Peng He,\* Yuan-Chao Li,\* Guo-Rong Chen\* and Kaixian Chen

Unique fluorescence "off-approach-on" chemosensors for detection of copper and fluorine based on "clicked" indoleamines are reported.

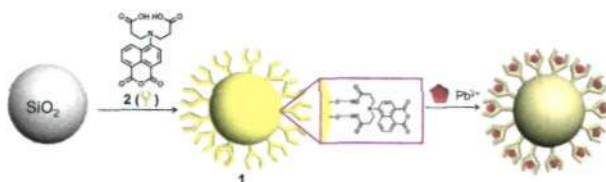


2812

### A thin-layered chromatography plate prepared from naphthalimide-based receptor immobilized SiO<sub>2</sub> nanoparticles as a portable chemosensor and adsorbent for Pb<sup>2+</sup>

Sunhong Park, Jin Hyeok Lee and Jong Hwa Jung\*

We have prepared naphthalimide-functionalized SiO<sub>2</sub> nanoparticles **1** that act as a new type of fluorogenic chemosensor. **1** exhibits high affinity and high selectivity for Pb<sup>2+</sup> over a number of other metal ions tested and successfully detects and separates Pb<sup>2+</sup> at pH 7.

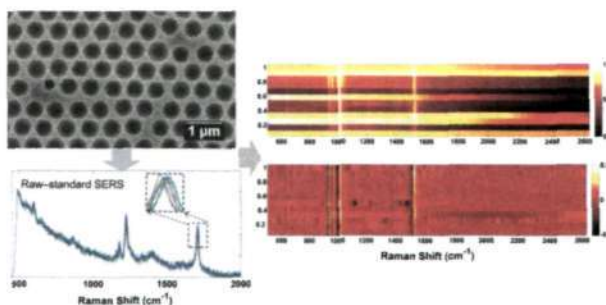


2816

### Wavelength modulated surface enhanced (resonance) Raman scattering for background-free detection

Bavishna B. Praveen, Christian Steuwe, Michael Mazilu, Kishan Dholakia\* and Sumeet Mahajan\*

The 'background' in surface enhanced (resonance) Raman scattering is eliminated and the signal to noise ratio is enhanced using wavelength modulation.

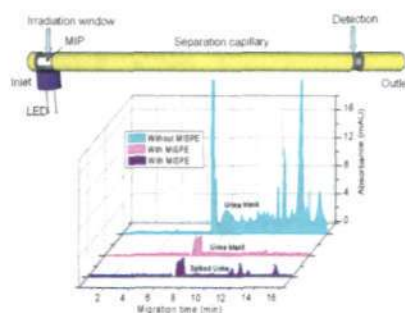


2821

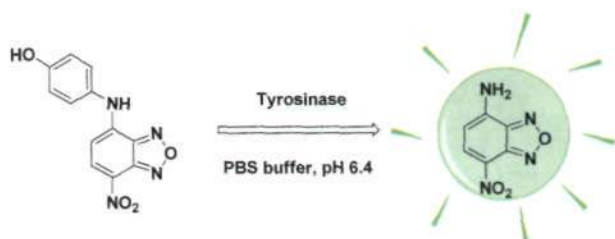
### LED-induced in-column molecular imprinting for solid phase extraction/capillary electrophoresis

Xinfeng Zhang, Shuxia Xu, Yong-Ill Lee\* and Steven A. Soper

A novel light-emitting diode-induced polymerization technology was demonstrated, which could be applied for the on-line construction of an in-column molecularly imprinted solid phase extraction concentrator for capillary electrophoresis. Such a strategy exhibited the advantages of simplicity, zero dead volume, and ease of renewing the concentrator.



2825

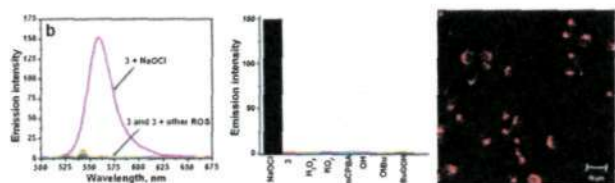


### A turn-on fluorescent probe for detection of tyrosinase activity

Changcheng Wang, Shengyong Yan, Rong Huang, Shuo Feng, Boshi Fu, Xiaocheng Weng\* and Xiang Zhou\*

A new fluorescent probe was developed for tyrosinase activity detection through the enzyme-catalyzed formation of NBD-NH<sub>2</sub>.

2829



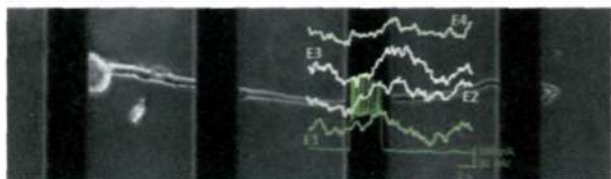
### Extremely selective "turn-on" fluorescence detection of hypochlorite confirmed by proof-of-principle neurological studies via esterase action in living cells

Atul P. Singh, Olga G. Tsay, Dhiraj P. Murale, Taehong Jun, Hyunjeong Liew, Yoo-Hun Suh and David G. Churchill\*

A probe bearing an ancillary 2-sulfide-benzoic acid group allows for selective "turn-on" hypochlorite detection in neuroblastoma media.

## PAPERS

2833

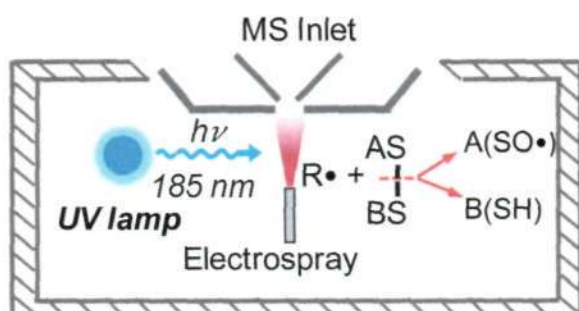


### A planar microelectrode array for simultaneous detection of electrically evoked dopamine release from distinct locations of a single isolated neuron

Bhavik Anil Patel,\* Collin C. Luk, Pei Ling Leow, Arthur J. Lee, Wali Zaidi and Naweed I. Syed

This manuscript shows the first simultaneous electrically evoked recordings of dopamine release from distinct locations of an isolated single neuron.

2840



### Radical induced disulfide bond cleavage within peptides via ultraviolet irradiation of an electro spray plume

Craig A. Stinson and Yu Xia\*

Facile cleavage of disulfide bonds within peptides via UV-induced radical reactions in an ESI plume.

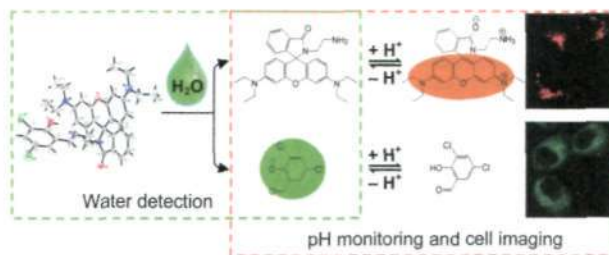


2847

### A dual channel optical detector for trace water chemodosimetry and imaging of live cells

Guangwen Men, Guirong Zhang, Chunshuang Liang, Hailing Liu, Bing Yang, Yuyu Pan, Zhenyu Wang and Shimei Jiang\*

The first dual-channel optical water chemodosimeter and its application in intracellular pH monitoring and cell imaging have been successfully developed.

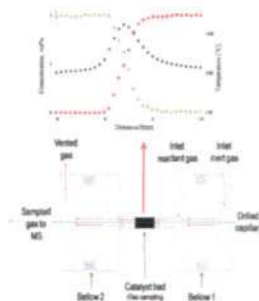


2858

### An *in situ* spatially resolved analytical technique to simultaneously probe gas phase reactions and temperature within the packed bed of a plug flow reactor

Jamal Touitou, Robbie Burch, Christopher Hardacre,\* Colin McManus, Kevin Morgan, Jacinto Sá and Alexandre Goguet\*

An *in situ* spatially resolved analytical technique to probe gas phase reactions and temperature within the packed bed of a plug flow reactor.

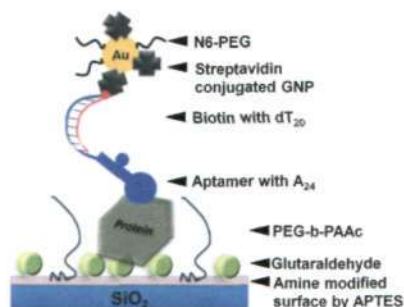


2863

### A high-performance waveguide-mode biosensor for detection of factor IX using PEG-based blocking agents to suppress non-specific binding and improve sensitivity

Thangavel Lakshmi Priya, Makoto Fujimaki, Subash C. B. Gopinath, Koichi Awazu, Yukichi Horiguchi and Yukio Nagasaki\*

PEG-assisted high-performance detection of factor IX with higher sensitivity on the SiO<sub>2</sub> sensing surface.

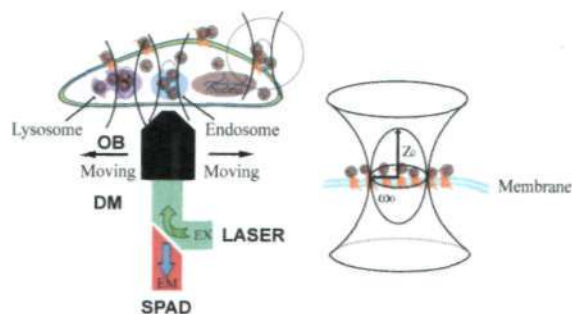


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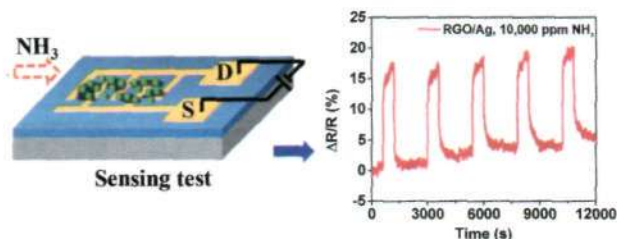
### Probing site-exclusive binding of aqueous QDs and their organelle-dependent dynamics in live cells by single molecule spectroscopy

Chaoqing Dong, Basudev Chowdhury and Joseph Irudayaraj\*

Understanding the biophysical and chemical interactions of nanoprobe and their fate upon entering live cells is critical for developing fundamental insights related to intracellular diagnostics, drug delivery and targeting.



2877

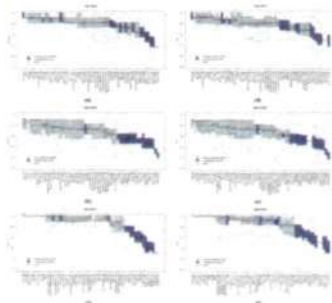


### Controllable synthesis of silver nanoparticle-decorated reduced graphene oxide hybrids for ammonia detection

Shumao Cui, Shun Mao, Zhenhai Wen, Jingbo Chang, Yang Zhang and Junhong Chen\*

A controllable fabrication of Ag nanoparticle-decorated reduced graphene oxide (RGO/Ag) hybrids and their application for fast and selective detection of room-temperature ammonia were demonstrated.

2883

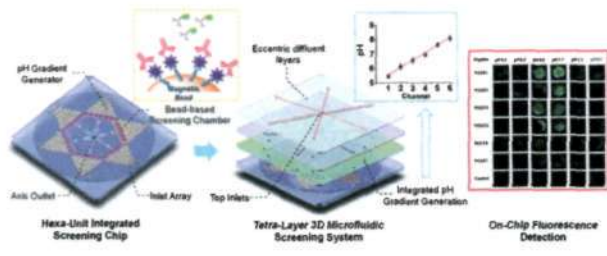


### An automated Pearson's correlation change classification (APC3) approach for GC/MS metabolomic data using total ion chromatograms (TICs)

Bhaskaran David Prakash, Kesavan Esuvaranathan, Paul C. Ho, Kishore Kumar Pasikanti, Eric Chun Yong Chan and Chun Wei Yap\*

A fully automated and computationally efficient Pearson's correlation change classification (APC3) approach.

2890

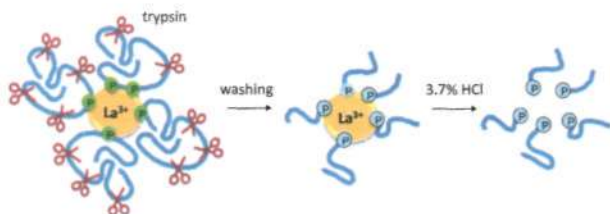


### A tetra-layer microfluidic system for peptide affinity screening through integrated sample injection

Weizhi Wang, Yanyan Huang, Yulong Jin, Guoquan Liu, Yi Chen, Huimin Ma and Rui Zhao\*

A tetra-layer microfluidic system featuring a hexa-unit screening chip with eccentric diffluent layer based pH gradient generators was developed for efficient peptide screening towards target molecules.

2897



### Highly selective recovery of phosphopeptides using trypsin-assisted digestion of precipitated lanthanide-phosphoprotein complexes

Yüksel Güzel, Matthias Rainer,\* Munazza R. Mirza, Christoph B. Messner and Günther K. Bonn

The basic idea of this study was to recover phosphopeptides after trypsin-assisted digestion of precipitated phosphoproteins using trivalent lanthanide ions.

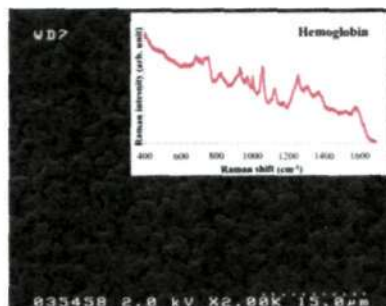


2906

### Hydrophobicity-driven self-assembly of protein and silver nanoparticles for protein detection using surface-enhanced Raman scattering

Mehmet Kahraman,<sup>\*</sup> Ben N. Balz and Sebastian Wachsmann-Hogiu<sup>\*</sup>

We demonstrated a simple sample preparation method for sensitive and reproducible label-free detection of proteins based on hydrophobicity-driven self-assembly of AgNPs and proteins.

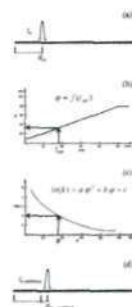


2914

### Gradient stationary phase optimized selectivity liquid chromatography with conventional columns

Kai Chen, Frédéric Lynen, Roman Szucs, Melissa Hanna-Brown and Pat Sandra<sup>\*</sup>

Stationary phase optimized selectivity liquid chromatography (SOSLC) is a promising technique to optimize the selectivity of a given separation.

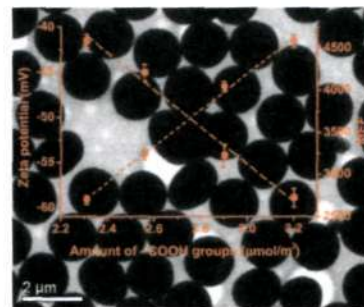


2924

### A rapid method for the assessment of the surface group density of carboxylic acid-functionalized polystyrene microparticles

Shengchao Zhu, Ulrich Panne and Knut Rurack<sup>\*</sup>

Monodisperse polystyrene microparticles with different contents of carboxylate groups have been synthesized and subjected to various direct and indirect methods for functional group quantification.

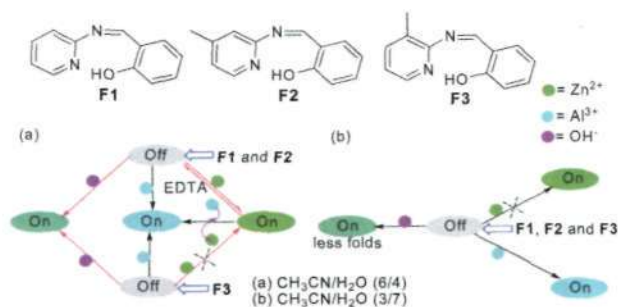


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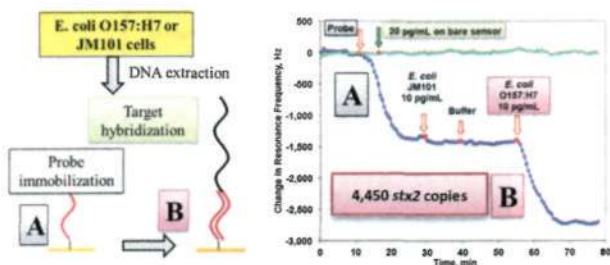
### Simple pyridyl-salicylimine-based fluorescence "turn-on" sensors for distinct detections of Zn<sup>2+</sup>, Al<sup>3+</sup> and OH<sup>-</sup> ions in mixed aqueous media

Muthaiah Shellaiah, Yen-Hsing Wu and Hong-Cheu Lin<sup>\*</sup>

Simple pyridyl-salicylimine derivatives are reported for the first time as fluorescence "turn-on" sensors for distinct detection of Zn<sup>2+</sup>, Al<sup>3+</sup> and OH<sup>-</sup> ions in mixed-aqueous media.



2943

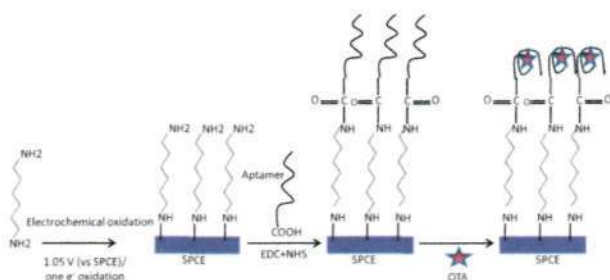


### A method for DNA-based detection of *E. coli* O157:H7 in a proteinous background using piezoelectric-excited cantilever sensors

Kishan Rijal and Raj Mutharasan\*

DNA-based detection of *E. coli* O157:H7 in ground beef wash using *stx2* gene as a marker gene at ~4500 cells.

2951

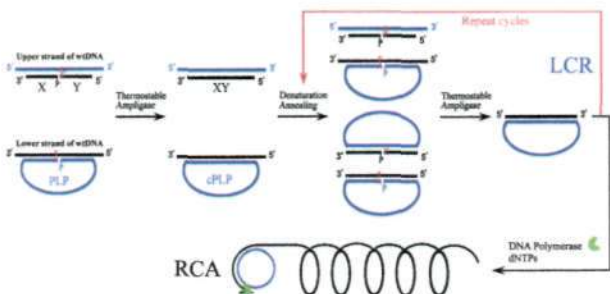


### Electrochemical grafting of long spacer arms of hexamethyldiamine on a screen printed carbon electrode surface: application in target induced ochratoxin A electrochemical aptasensor

Akhtar Hayat,\* Waqar Haider, Marc Rolland and Jean-Louis Marty

A new sensing platform based on the conformational changes of aptamer was developed for the label free detection of small size molecules.

2958

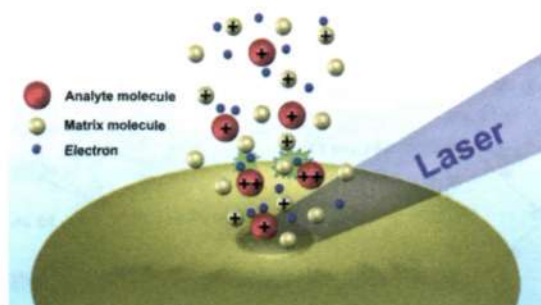


### Ligase chain reaction coupled with rolling circle amplification for high sensitivity detection of single nucleotide polymorphisms

Yongqiang Cheng,\* Jingjing Zhao, Hailian Jia, Zheng Yuan and Zhengping Li\*

Detection of single nucleotide polymorphisms (SNPs) by ligase chain reaction coupled with rolling circle amplification is developed in a label-free and homogeneous manner. The assay provides a new strategy for the detection of SNPs as well as immunoassay, and molecular diagnosis.

2964



### Role of three-body recombination for charge reduction in MALDI process

Yiming Lin, Zhibin Yin, Xiaohua Wang, Weifeng Li and Wei Hang\*

Three-body recombination is suggested to be an important charge reduction mechanism for small molecules in the MALDI events.

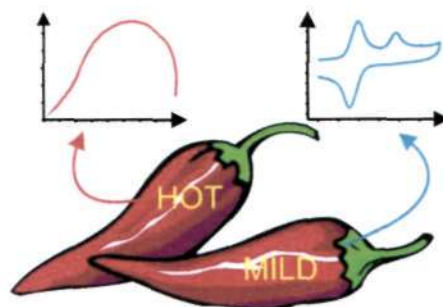


2970

### Electrochemical impedance spectroscopy versus cyclic voltammetry for the electroanalytical sensing of capsaicin utilising screen printed carbon nanotube electrodes

Edward P. Randviir, Jonathan P. Metters, John Stainton and Craig E. Banks\*

Electrochemical impedance spectroscopy is, for the first time, compared to cyclic voltammetry for the electroanalytical detection of capsaicin.

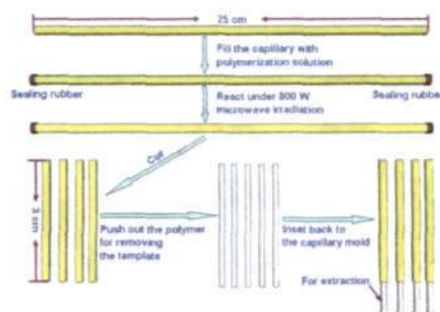


2982

### Microwave-assisted preparation of monolithic molecularly imprinted polymeric fibers for solid phase microextraction

Shuxia Xu, Xinfeng Zhang,\* Yonghua Sun and Dan Yu

A novel microwave-assisted method was developed for fast and batch fabrication of monolithic molecularly imprinted polymer (MIP) fibers, which was based on *in situ* polymerization in a flexible capillary mold under microwave irradiation.

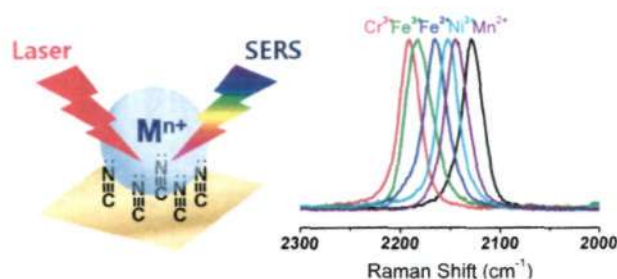


2988

### Cyanide SERS as a platform for detection of volatile organic compounds and hazardous transition metal ions

Kwan Kim,\* Ji Won Lee and Kuan Soo Shin\*

Cyanide adsorbed on nanostructured Au can be used to detect not only VOCs but also transition metal ions *via* SERS.

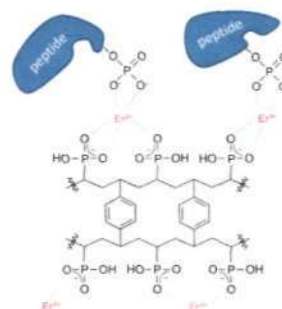


2995

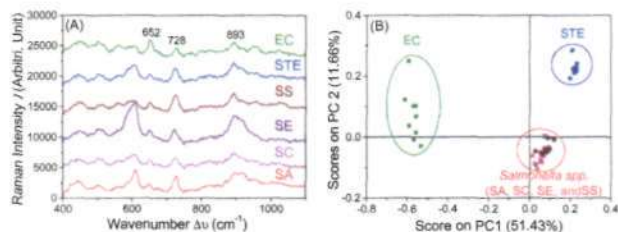
### A new type of metal chelate affinity chromatography using trivalent lanthanide ions for phosphopeptide enrichment

Munazza R. Mirza, Matthias Rainer,\* Christoph B. Messner, Yüksel Güzel, Dieter Schemeth, Taras Stasyk, Muhammad I. Choudhary, Lukas A. Huber, Bernd M. Rode and Günther K. Bonn

A new lanthanide IMAC resin was developed for the specific enrichment of phosphopeptides.



3005

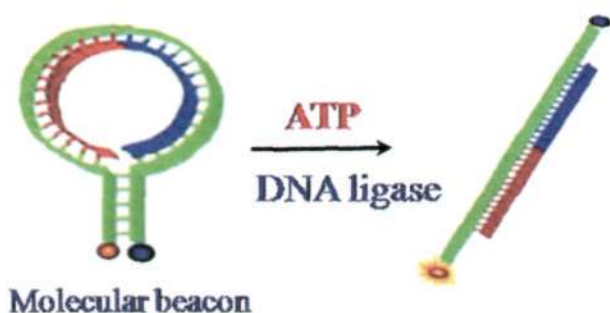


### Detection and differentiation of foodborne pathogenic bacteria in mung bean sprouts using field deployable label-free SERS devices

Xiaomeng Wu,\* Chao Xu, Ralph A. Tripp, Yao-wen Huang and Yiping Zhao

Six different foodborne pathogenic bacteria were identified in mung bean sprouts by label-free SERS with a limit of detection as low as 100 CFU ml<sup>-1</sup> in less than 4 h. They were differentiated between bacterial species and serotypes when chemometric methods are employed.

3013

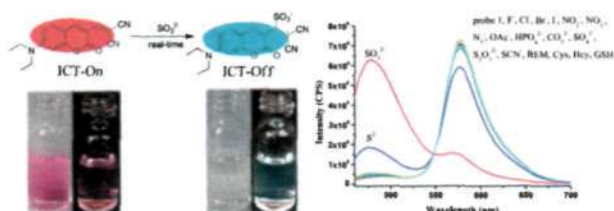


### A novel sensitive and selective ligation-based ATP assay using a molecular beacon

Changbei Ma,\* Zhiwen Tang, Kemin Wang,\* Xiaohai Yang and Weihong Tan

An optical sensor for sensitive and selective ATP detection based on a molecular beacon and DNA ligase has been reported.

3018

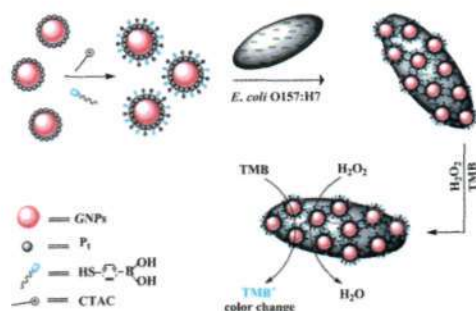


### A real-time colorimetric and ratiometric fluorescent probe for sulfite

Ming-Yu Wu, Ting He, Kun Li,\* Ming-Bo Wu, Zheng Huang and Xiao-Qi Yu\*

A reaction-based colorimetric and ratiometric fluorescent probe based on an ICT-strategy for selective detection of sulfite is presented, and displays high selectivity with more than 100 nm blue shift and 230 fold emission intensity ratio changes.

3026



### Colorimetric detection of *Escherichia coli* O157:H7 using functionalized Au@Pt nanoparticles as peroxidase mimetics

Haichao Su, Han Zhao, Fengmin Qiao, Lijian Chen, Ruihuan Duan and Shiyun Ai\*

Schematic representation of the colorimetric detection of *E. coli* O157:H7 based on the catalase-like activity of MPBA-CTAC-Au@Pt NPs for TMB oxidation.

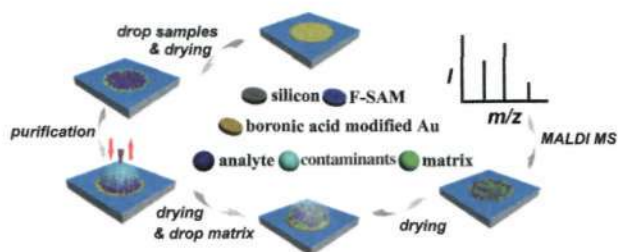


3032

### On-plate glycoproteins/glycopeptides selective enrichment and purification based on surface pattern for direct MALDI MS analysis

Zhoufang Zeng, Yandong Wang, Xinhua Guo,\*  
Ling Wang and Nan Lu\*

On-plate selective enrichment and purification of glycoproteins/glycopeptides is achieved with a surface patterned sample support for direct MALDI analysis.

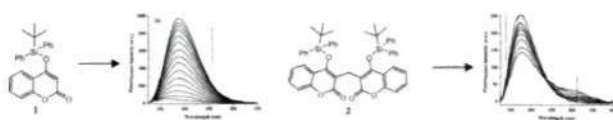


3038

### O-tert-Butyldiphenylsilyl coumarin and dicoumarol: a case toward selective sensing of F<sup>-</sup> ions in organic and aqueous environments

Kumares Ghosh,\* Debasis Kar, Roland Fröhlich,  
Asoke P. Chattopadhyay, Asmita Samadder  
and Anisur Rahman Khuda-Bukhsh

Compound **1** senses F<sup>-</sup> selectively over the other anions examined in CHCl<sub>3</sub> by exhibiting a greater increase in emission. In contrast, **2** shows similar selectivity in CHCl<sub>3</sub> giving ratiometric change in emission as well as color.

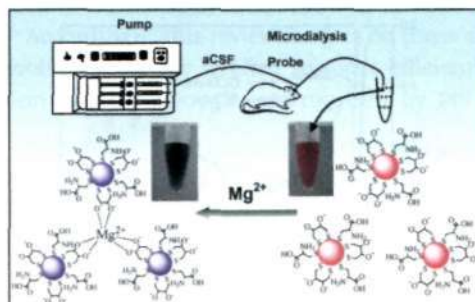


3046

### Cysteine-modulated colorimetric sensing of extracellular Mg<sup>2+</sup> in rat brain based on the strong chelation interaction between dithiothreitol and Mg<sup>2+</sup>

Xuming Zhuang, Dalei Wang, Lifen Yang, Ping Yu,\*  
Wei Jiang\* and Lanqun Mao\*

Simple and effective measurement of Mg<sup>2+</sup> in the brain of living animals is of great physiological and pathological importance.

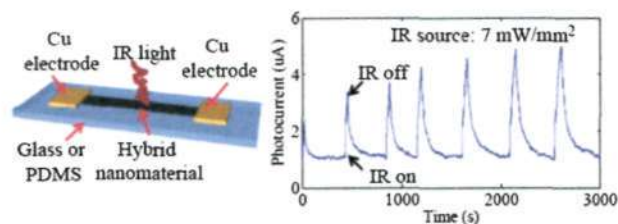


3053

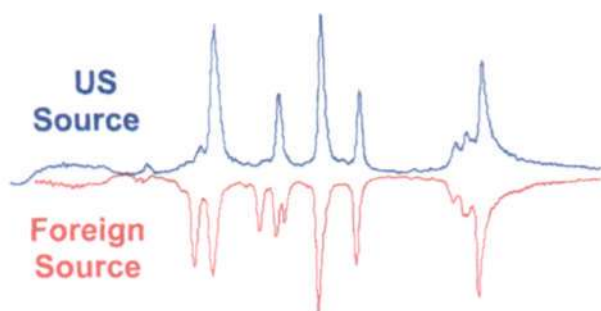
### Ultrasensitive thin film infrared sensors enabled by hybrid nanomaterials

Yi-Hsuan Tseng, Yuan He and Long Que\*

IR sensors based on single-walled carbon nanotube-copper sulfide nanoparticle hybrid nanomaterial thin films offer ultrasensitivity and very low detection limit.



3058

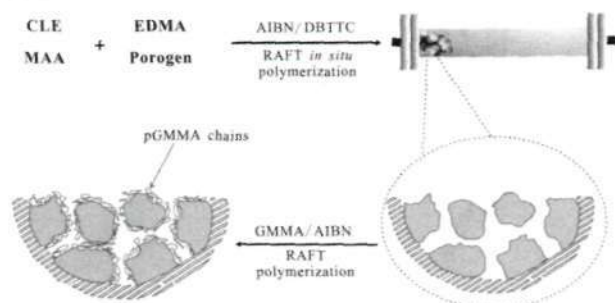


### Structural comparison of two anti-CD20 monoclonal antibody drug products using middle-down mass spectrometry

Bo Wang, Ashley C. Gucinski, David A. Keire, Lucinda F. Buhse and Michael T. Boyne II\*

Middle-down LC-MS analysis can be used to identify structural heterogeneities between a monoclonal antibody from different sources.

3066

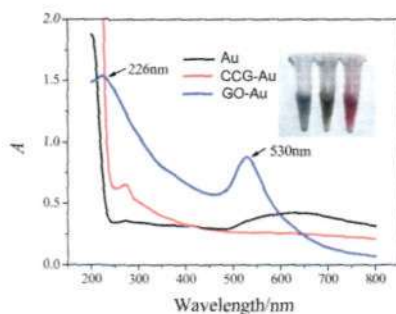


### Preparation of clenbuterol imprinted monolithic polymer with hydrophilic outer layers by reversible addition-fragmentation chain transfer polymerization and its application in the clenbuterol determination from human serum by on-line solid-phase extraction/HPLC analysis

Xiaobing Li, Man Zhou, Mamat Turson, Shen Lin, Ping Jiang and Xiangchao Dong\*

The preparation of clenbuterol imprinted monolithic polymer and its application in human serum analysis.

3075



### One-pot green synthesis of graphene oxide/gold nanocomposites as SERS substrates for malachite green detection

Wen Liang Fu, Shu Jun Zhen\* and Cheng Zhi Huang\*

In this contribution, graphene oxide/gold nanoparticle (GO/AuNPs) hybrids were *in situ* fabricated through a green one-pot procedure by using tyrosine as an environment friendly and biocompatible reducing agent, which can be used as highly efficient surface enhanced Raman scattering (SERS) substrates with the enhancement factor at  $3.8 \times 10^3$ .