

ANALYTICA CHIMICA ACTA

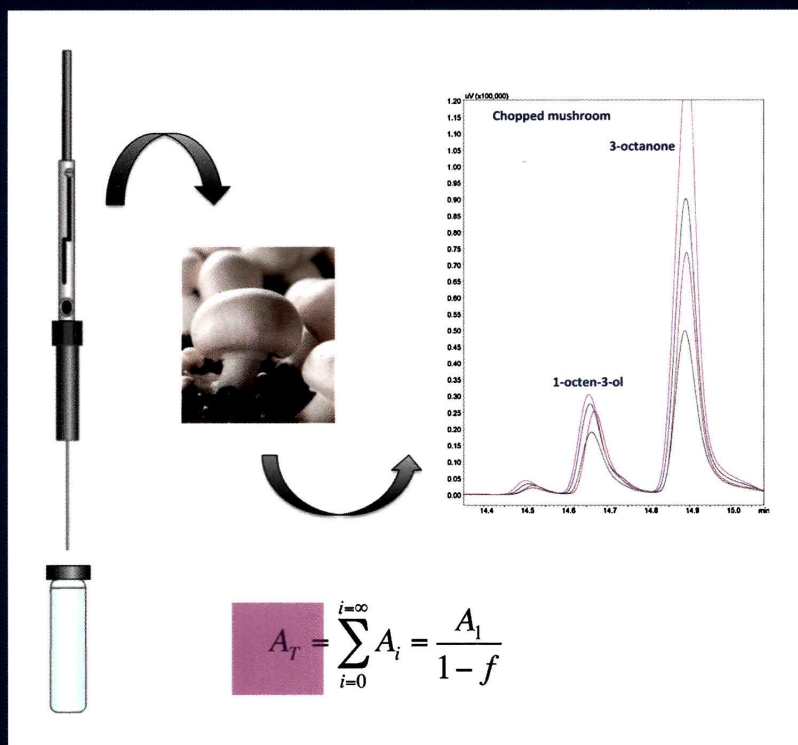
AN INTERNATIONAL JOURNAL DEVOTED TO ALL BRANCHES OF ANALYTICAL CHEMISTRY

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Featured Article

Multiple headspace-solid-phase microextraction: An application to quantification of mushroom volatiles

Rosaria Costa, Laura Tedone, Selenia De Grazia, Paola Dugo and Luigi Mondello

(Published on pp. 1–6 of this issue)

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1 Γ Editorial Board

Page iii

Featured article

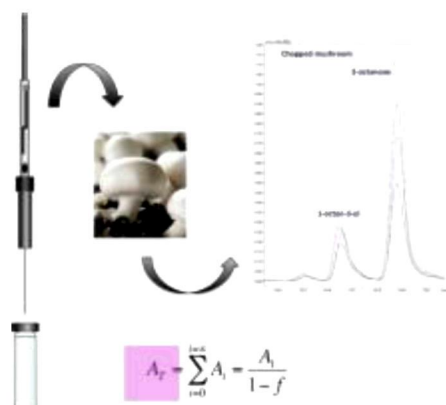
2 Γ **Multiple headspace-solid-phase microextraction: An application to quantification of mushroom volatiles**

Original Research Article

Pages 1-6

Rosaria Costa, Laura Tedone, Selenia De Grazia, Paola Dugo, Luigi Mondello

Graphical abstract



Highlights

► Multiple headspace extraction-solid phase microextraction (MHS-SPME) has been applied to the analysis of *Agaricus bisporus*. ► Mushroom flavor is characterized by the presence of compounds with a 8-carbon atoms skeleton. ► Formation of 8-carbon compounds involves a unique fungal biochemical pathway. ► The MHS-SPME allowed to determine quantitatively 5 target analytes of *A. bisporus* for the first time.

Atomic Spectrometry

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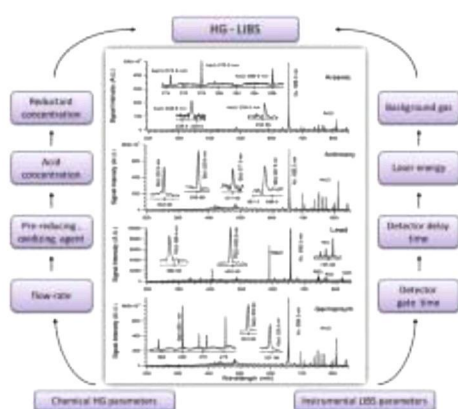
Optimization of chemical and instrumental parameters in hydride generation laser-induced breakdown spectrometry for the determination of arsenic, antimony, lead and germanium in aqueous samples

Original Research Article

Pages 7-17

Semira Ünal Yeşiller, Şerife Yalçın

Graphical abstract



Highlights

- ▶ Continuous flow hydride generation technique for LIBS detection of As, Sb, Pb and Ge. ▶
- Optimization of chemical and instrumental parameters in HG-LIBS. ▶
- Quantitative determination of As, Sb, Pb and Ge in aqueous samples. ▶
- Enhancements in LOD values compared to direct liquids analysis by LIBS. ▶
- Investigation of the effect of carrier gas on LIBS signal strength.

Chemometrics

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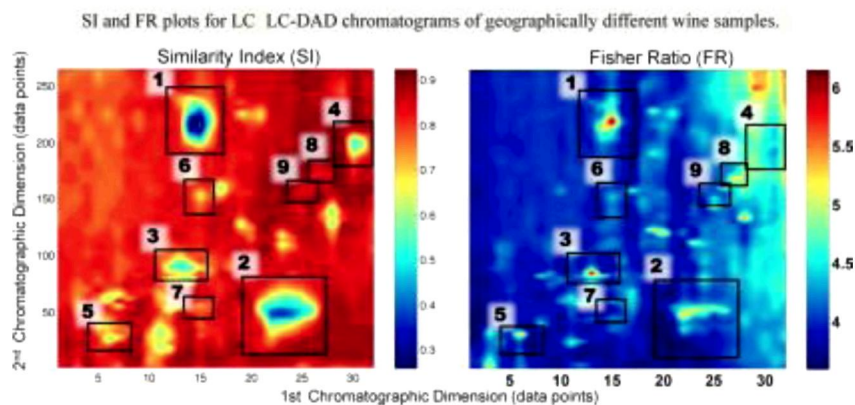
Comparison of chemometric methods for the screening of comprehensive two-dimensional liquid chromatographic analysis of wine

Original Research Article

Pages 18-28

Hope P. Bailey, Sarah C. Rutan

Graphical abstract



Highlights

► We compare two chemometric techniques for rapid screening of LC × LC-DAD. ► The Fisher ratio and similarity index methods were compared. ► Significant concentration differences of peaks between sample types were determined. ► Various chromatographic conditions were found to have an effect on both methods.

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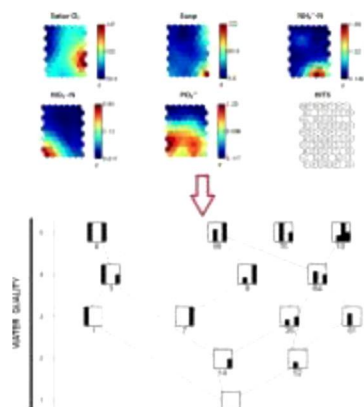
Hasse diagram technique as a tool for water quality assessment

Original Research Article

Pages 29-35

Tsvetomil Voyslavov, Stefan Tsakovski, Vasil Simeonov

Graphical abstract



Highlights

► Pre-selection procedure by self-organizing maps technique to reduce irrelevant information. ► Supervised pattern recognition to reveal specific patterns of pollutions along the river flow using Hasse

diagram technique. ► Risk assessment combining chemometric techniques and local ecological legislation.

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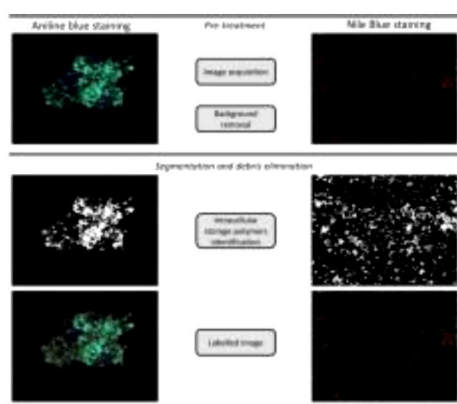
Prediction of intracellular storage polymers using quantitative image analysis in enhanced biological phosphorus removal systems

Original Research Article

Pages 36-44

Daniela P. Mesquita, Cristiano Leal, Jorge R. Cunha, Adrian Oehmen, A. Luís Amaral, Maria A.M. Reis, Eugénio C. Ferreira

Graphical abstract



Highlights

► Fluorescence staining and image analysis were used to monitor an EBPR system. ► Intracellular storage polymers were measured in anaerobic and aerobic stages. ► Partial least squares (PLS) were used to model the polymers concentrations. ► Previous stage identification improved the assessment of the polymer concentrations. ► A novel method for intracellular storage polymers assessment was established.

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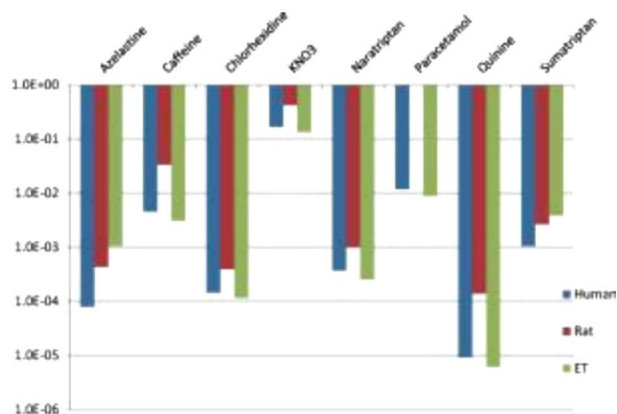
Assessment of bitter taste of pharmaceuticals with multisensor system employing 3 way PLS regression

Original Research Article

Pages 45-52

Alisa Rudnitskaya, Dmitry Kirsanov, Yulia Blinova, Evgeny Legin, Boris Seleznev, David Clapham, Robert S. Ives, Kenneth A. Saunders, Andrey Legin

Graphical abstract



Highlights

- ▶ Chemically diverse APIs are studied with potentiometric “electronic tongue”.
- ▶ Bitter taste of APIs can be predicted with 3wayPLS regression from ET data.
- ▶ High correlation of ET assessment with human panel and rat in vivo model.

Electrochemistry

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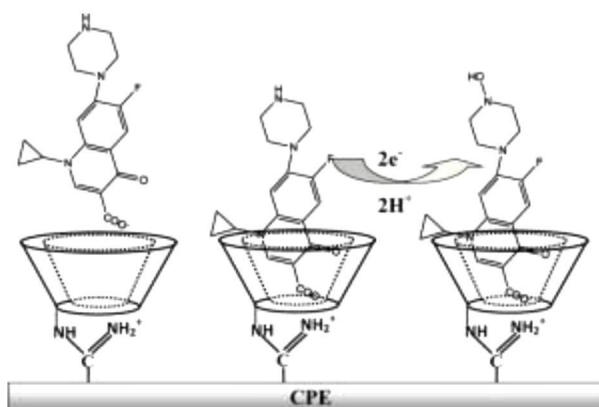
A novel sensor based on electropolymerization of β -cyclodextrin and L-arginine on carbon paste electrode for determination of fluoroquinolones

Original Research Article

Pages 53-61

Fenfen Zhang, Shuqing Gu, Yaping Ding, Zhen Zhang, Li Li

Graphical abstract



Highlights

► Electropolymerization of β -cyclodextrin and l-arginine on carbon paste electrode. ► The electrooxidation and reaction of FQs on the modified CPE were surmised. ► The sensor is used to detect ciprofloxacin, ofloxacin, norfloxacin and gatifloxacin. ► Determine FQs drugs in pharmaceutical formulations and human serum samples. ► It showed high stability, repeatability, reproducibility, good sensitivity.

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Construction of label-free electrochemical immunosensor on mesoporous carbon nanospheres for breast cancer susceptibility gene

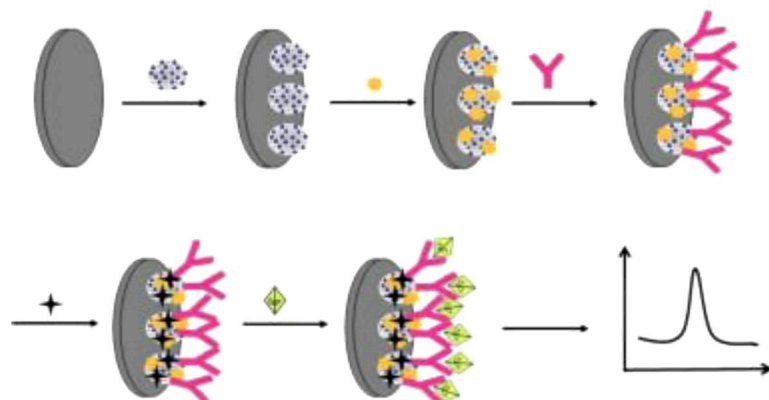
Original Research Article

Pages 62-67

Haixia Fan, Yong Zhang, Dan Wu, Hongmin Ma, Xiaojing Li, Yan Li, Huan Wang, He Li, Bin Du, Qin Wei

Supplementary content

Graphical abstract



Highlights

► The immunosensor is designed to determine breast cancer susceptibility gene. ► Mesoporous carbon nanospheres (MCN) have great adsorption capacity. ► MCN could enhance the electroactivity of toluidine blue. ► Room temperature ionic liquid should increase the electrochemical signal.

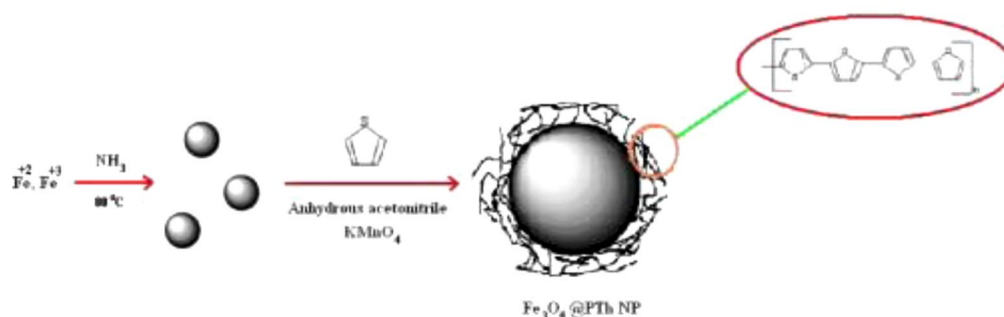
Extraction and Sample Handling

10

Polythiophene-coated Fe_3O_4 superparamagnetic nanocomposite: Synthesis and application as a new sorbent for solid-phase extraction

Original Research Article

Graphical abstract



Highlights

- ▶ A novel polythiophene-coated Fe_3O_4 nanoparticles ($\text{Fe}_3\text{O}_4 @ \text{PTh NPs}$) was synthesized.
- ▶ The synthesized $\text{Fe}_3\text{O}_4 @ \text{PTh NPs}$ were characterized by using different instruments.
- ▶ The $\text{Fe}_3\text{O}_4 @ \text{PTh NPs}$ were applied as a sorbent for extraction of several plasticizers.
- ▶ After extraction, separation of NPs from solution was achieved by a magnetic field.
- ▶ The proposed procedure was applied to analysis of the analytes in real water samples.

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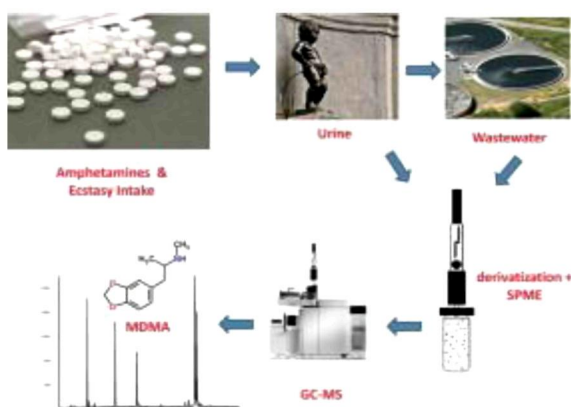
In-sample derivatization-solid-phase microextraction of amphetamines and ecstasy related stimulants from water and urine

Original Research Article

Pages 75-84

Inés Racamonde, Rosario Rodil, José Benito Quintana, Rafael Cela

Graphical abstract



Highlights

► First SPME method for determination of amphetamines and ecstasy in (waste)water. ► In-sample simultaneous derivatization and extraction with *iso*-butyl chloroformate. ► Wastewater (100 mL): LODs: 0.4–2 ng L⁻¹, RSD < 15%; recoveries: 84–114%. ► Urine (1 mL): LODs:<1 µg L⁻¹, RSD < 11%; recoveries: 98–110%. ► Solvent-free and fully automatable method.

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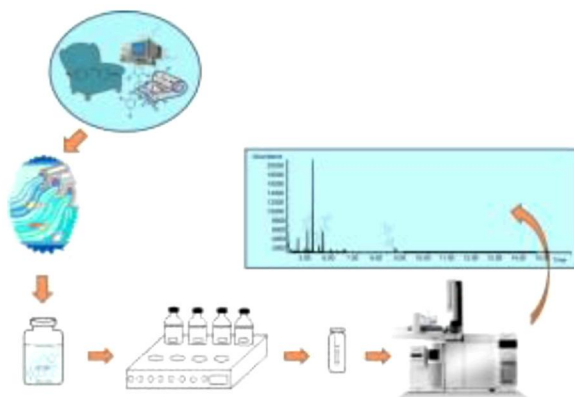
Application of polydimethylsiloxane rod extraction to the determination of sixteen halogenated flame retardants in water samples

Original Research Article

Pages 85-93

Carme Valls-Cantenys, Eugenia Villaverde-de-Sáa, Rosario Rodil, José Benito Quintana, Mònica Iglesias, Victòria Salvadó, Rafael Cela

Graphical abstract



Highlights

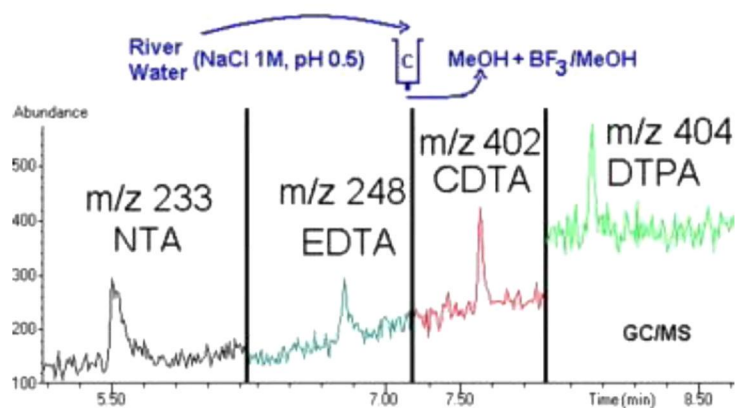
► Simultaneous determination of nine BDEs and seven non-BDE flame retardants. ► Disposable polydimethylsiloxane (PDMS) is an efficient tool for flame retardants extraction. ► Enrichment factors between 108 and 840 were obtained. ► Detection limits obtained were in the range from 0.4 to 10 ng L⁻¹. ► The method has been successfully applied in the analysis of complex matrix waters.

13

Determination of aminopolycarboxylic acids in river water by solid-phase extraction on activated charcoal cartridges and gas chromatography with mass spectrometric detection. Method performance characteristics and estimation of the uncertainty

Original Research Article

Graphical abstract



Highlights

- ▶ SPE of aminopolycarboxylic acids without preparing iron complexes is studied.
- ▶ Adjusting water sample conditions the retention on activated charcoal is feasible.
- ▶ There is not any significant matrix-effect in the quantification by GC/MS.
- ▶ Method performance characteristics are given. Robustness and uncertainty are evaluated.

Flow Analysis

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Influence of material transition and interfacial area changes on flow and concentration in electro-osmotic flows

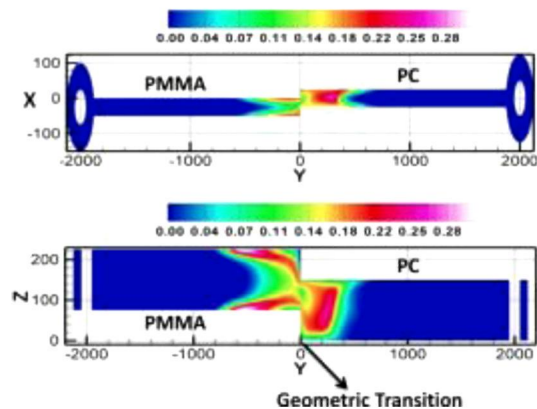
Original Research Article

Pages 103-110

Sudheer D. Rani, Byoung-Hee You, Steve A. Soper, Michael C. Murphy, Dimitris E. Nikitopoulos

Supplementary content .

Graphical abstract



Highlights

- ▶ Combined material and geometrical transition in electrokinetic flows was studied.
- ▶ Material and geometrical transition resulted in dispersion and reduced flow rates.
- ▶ Effect of only geometrical transition on species was less compared to material transition.
- ▶ Sample dispersion was quantified with standard metrics.
- ▶ Correlations were developed to estimate the reduction in flow rates.

Mass Spectrometry

15

Inter-laboratory trials for analysis of perfluorooctanesulfonate and perfluorooctanoate in water samples: Performance and recommendations

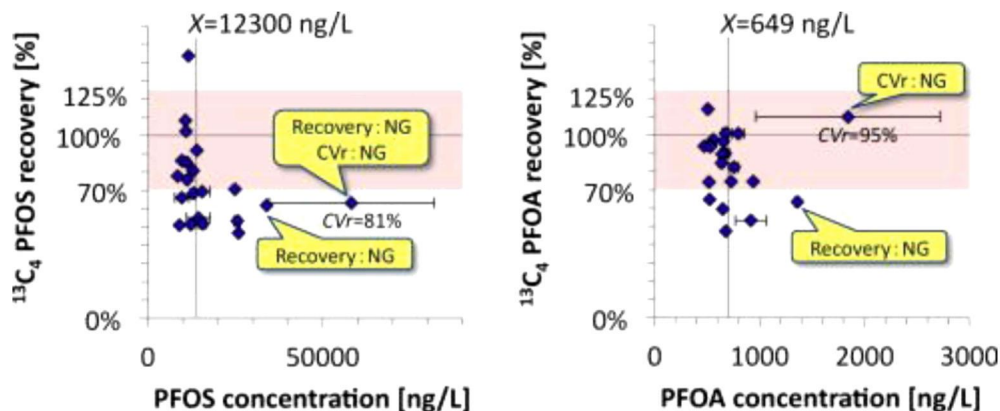
Original Research Article

Pages 111-120

Sachi Taniyasu, Kurunthachalam Kannan, Qian Wu, Karen Y. Kwok, Leo W.Y. Yeung, Paul K.S. Lam, Brock Chittim, Takafumi Kida, Takumi Takasuga, Yoshiteru Tsuchiya, Nobuyoshi Yamashita

[Supplementary content](#)

Graphical abstract



Highlights

- ▶ Three inter-laboratory trials were conducted to validate perfluorochemical analysis in water samples.
- ▶ Provision of SOPs and standards improved the precision and accuracy of analysis. ▶ The repeatability and reproducibility coefficients of variation were below 35%. ▶ Accuracy was improved with the use of appropriate labeled internal standards.

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Detection and identification of drugs and toxicants in human body fluids by liquid chromatography–tandem mass spectrometry under data-dependent acquisition control and automated database search

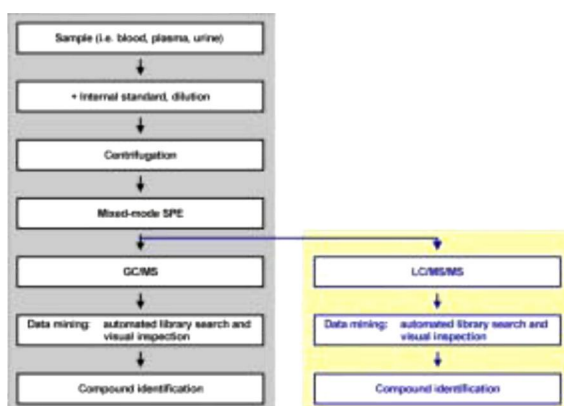
Original Research Article

Pages 121-131

Herbert Oberacher, Birthe Schubert, Kathrin Libiseller, Anna Schweissgut

Supplementary content

Graphical abstract



Highlights

- ▶ Untargeted LC/MS/MS screening for drug identification in blood, plasma and urine. ▶ The assay shares the sample preparation workflow with established GC/MS screening. ▶ Compound identification with the “Wiley Registry of Tandem Mass Spectral Data”. ▶ Selectivity, detection capability and reliability of identification are discussed. ▶ Parallel screening with LC/MS/MS and GC/MS offers utmost reliability.

Sensors and Bioselective Reagents

Core-shell Fe_3O_4 -Au magnetic nanoparticles based nonenzymatic ultrasensitive electrochemiluminescence immunosensor using quantum dots functionalized graphene sheet as labels

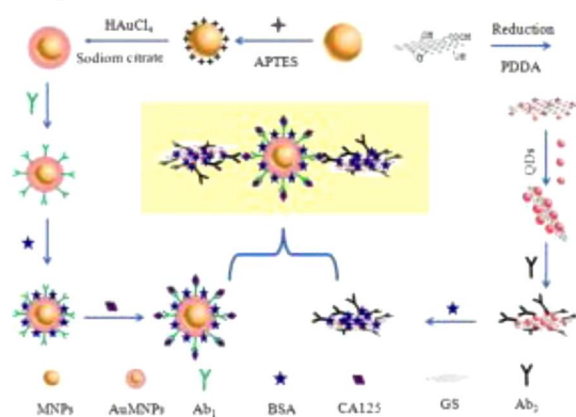
Original Research Article

Pages 132-139

Weiyang Liu, Yan Zhang, Shenguang Ge, Xianrang Song, Jiadong Huang, Mei Yan, Jinghua Yu

[Supplementary content](#)

Graphical abstract



Highlights

- ECL immunosensor for CA125 based on a microfluidic strategy with a homemade ECL cell was proposed.
- Core-shell Fe_3O_4 -Au magnetic nanoparticles were employed as the carriers of the primary antibodies.
- CdTe quantum dots functionalized graphene sheet were used for signal amplification.

Facile preparation of glutathione-stabilized gold nanoclusters for selective determination of chromium (III) and chromium (VI) in environmental water samples

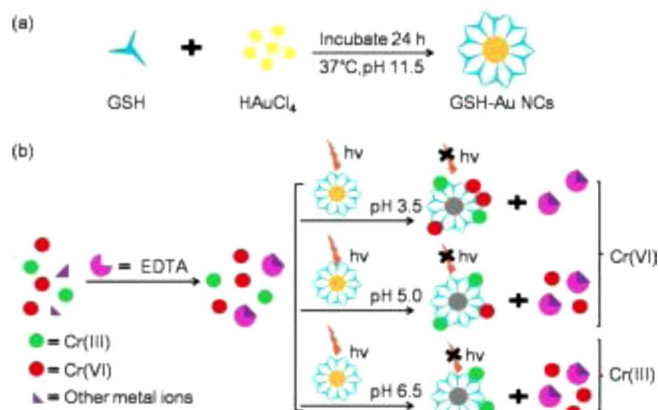
Original Research Article

Pages 140-146

Haiyan Zhang, Qian Liu, Thanh Wang, Zhaojun Yun, Guoliang Li, Jiyan Liu, Guibin Jiang

[Supplementary content](#)

Graphical abstract



Highlights

► Facile and rapid preparation of fluorescent glutathione-stabilized gold nanoclusters. ► New method for selective determination of Cr(III) and Cr(VI) using GSH-Au NCs. ► The detection method possessed simplicity, high throughput, high selectivity and sensitivity.

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Design of a sensitive aptasensor based on magnetic microbeads-assisted strand displacement amplification and target recycling

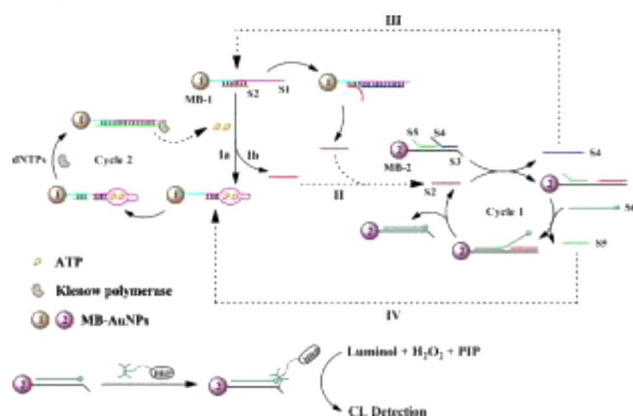
Original Research Article

Pages 147-152

Ying Li, Xiaoting Ji, Weiling Song, Yingshu Guo

[Supplementary content](#)

Graphical abstract



Highlights

► An aptasensor is fabricated by strand displacement amplification and target recycling. ► The reaction efficiency is greatly improved by cross-circular amplification. ► Sensitive detection of other targets can be achieved by using different aptamers.

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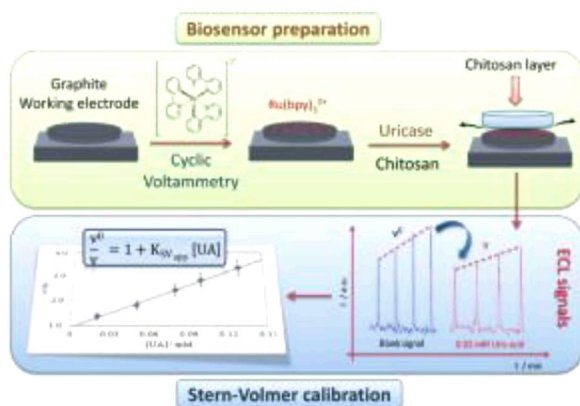
Disposable biosensor based on cathodic electrochemiluminescence of tris(2,2-bipyridine)ruthenium(II) for uric acid determination

Original Research Article

Pages 153-160

J. Ballesta-Claver, R. Rodríguez-Gómez, L.F. Capitán-Vallvey

Graphical abstract



Highlights

► Cathodic ECL offers conventional and non-aggressive analysis conditions. ► The ECL hydrogen peroxide/ruthenium complex system for uric acid determination is novel. ► The ruthenium complex is electrochemically immobilized on graphite screen-printed electrodes. ► The quantification of the uric acid is based on a Stern–Volmer type equation. ► The use of the cathodic ECL working methodology reduces interferences during analysis.

21

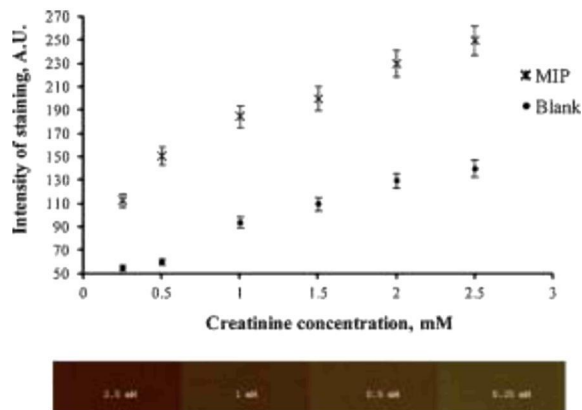
Colorimetric test-systems for creatinine detection based on composite molecularly imprinted polymer membranes

Original Research Article

Pages 161-168

T.A. Sergeeva, L.A. Gorbach, E.V. Piletska, S.A. Piletsky, O.O. Brovko, L.A. Honcharova, O.D. Lutsyk, L.M. Sergeeva, O.A. Zinchenko, A.V. El'skaya

Graphical abstract



Highlights

► A colorimetric test-system for the detection of creatinine in aqueous samples was developed. ► The test-system is based on composite molecularly imprinted polymer (MIP) membranes. ► The colorimetric test-system was characterized with 0.25 mM detection limit for creatinine. ► The linear dynamic range of the test-system for creatinine comprised 0.25–2.5 mM.

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Development and evaluation of a novel nucleic acid sequence-based amplification method using one specific primer and one degenerate primer for simultaneous detection of *Salmonella* Enteritidis and *Salmonella* Typhimurium

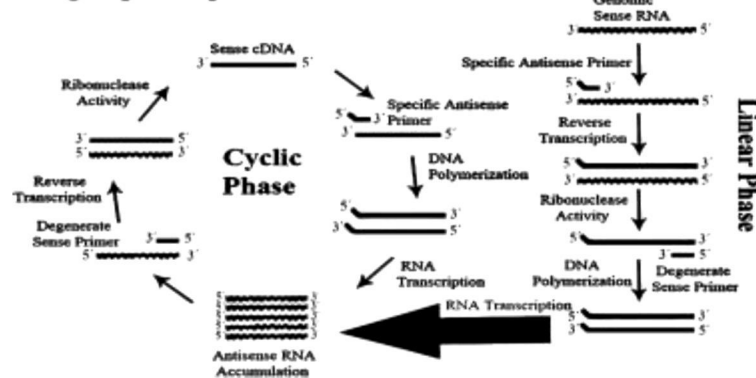
Original Research Article

Pages 169-174

Hamidreza Mollasalehi, Razieh Yazdanparast

Graphical abstract

Single specific primer-NASBA:



Highlights

▶ Development of “single specific primer-NASBA” method. ▶ Designing a highly specific NASBA primer for a segment of 16S rDNA variable region. ▶ Simultaneous detection of *S. Enteritidis* and *S. Typhimurium*. ▶ Achieving the low detection limit of less than 10 CFU mL⁻¹.