

# ANALYTICA CHIMICA ACTA

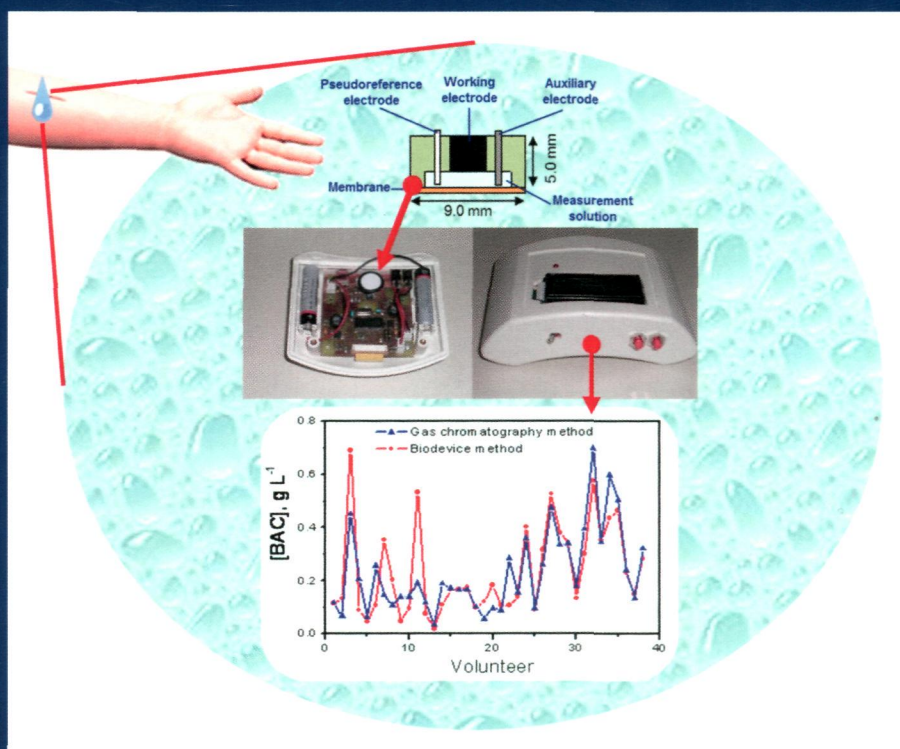
AN INTERNATIONAL JOURNAL DEVOTED TO ALL BRANCHES OF ANALYTICAL CHEMISTRY

## EDITORS:

RICHARD P. BALDWIN  
 NEIL W. BARNETT  
 WOLFGANG BUCHBERGER  
 LUTGARDE BUYDENS  
 PURNENDU K. DASGUPTA  
 ULRICH J. KRULL  
 JAMES P. LANDERS  
 LIANG LI  
 JANUSZ PAWLISZYN  
 PAUL J. WORSFOLD

## REVIEW EDITOR:

MANUEL MIRÓ



## Featured Article

A novel non-invasive electrochemical biosensing device for in situ determination of the alcohol content in blood by monitoring ethanol in sweat

M. Gamella, S. Campuzano, J. Manso, G. González de Rivera, F. López-Colino, A.J. Reviejo and J.M. Pingarrón

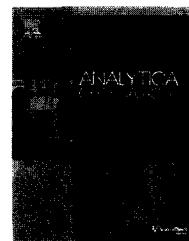
(Reprinted on pp. 1–7 of this issue)



ELSEVIER

available at [www.sciencedirect.com](http://www.sciencedirect.com)

ScienceDirect

journal homepage: [www.elsevier.com/locate/aca](http://www.elsevier.com/locate/aca)

## CONTENTS

Abstracted/indexed in: Aluminium Abstracts; Anal. Abstr.; Biol. Abstr.; BIOSIS; Chem. Abstr.; Curr. Contents Phys. Chem. Earth Sci.; Engineered Materials Abstracts; Excerpta Medica; Index Med.; Life Sci.; Mass Spectrum. Bull.; Material Business Alerts; Metals Abstracts; Sci. Citation Index Full texts are incorporated in CJELSEVIER, a file in the Chemical Journals Online database available on STN International. Also covered in the abstract and citation database SCOPUS®. Full text available on ScienceDirect®.

### Featured article

- A novel non-invasive electrochemical biosensing device for in situ determination of the alcohol content in blood by monitoring ethanol in sweat  
M. Gamella, S. Campuzano, J. Manso, G.G.d. Rivera, F. López-Colino, A.J. Reviejo and J.M. Pingarrón ..... 1

### Tutorial

- Second- and higher-order data generation and calibration: A tutorial  
G.M. Escandar, H.C. Goicoechea, A. Muñoz de la Peña and A.C. Olivieri ..... 8

### Review articles

- Ion chromatography-mass spectrometry: A review of recent technologies and applications in forensic and environmental explosives analysis  
L. Barron and E. Gilchrist ..... 27
- Trends and challenges of refractometric nanoplasmonic biosensors: A review  
M.-C. Estevez, M.A. Otte, B. Sepulveda and L.M. Lechuga ..... 55
- Ultrasound: A subexploited tool for sample preparation in metabolomics  
M.D. Luque de Castro and M.M. Delgado-Povedano ..... 74

### Atomic Spectrometry

- Direct determination of sodium, potassium, chromium and vanadium in biodiesel fuel by tungsten coil atomic emission spectrometry  
S.E. Dancsak, S.G. Silva, J.A. Nóbrega, B.T. Jones and G.L. Donati ..... 85
- Determination of trace sulfur in biodiesel and diesel standard reference materials by isotope dilution sector field inductively coupled plasma mass spectrometry  
R.S. Amais, S.E. Long, J.A. Nóbrega and S.J. Christopher ..... 91
- Determination of hafnium at the 10<sup>-4</sup>% level (relative to zirconium content) using neutron activation analysis, inductively coupled plasma mass spectrometry and inductively coupled plasma atomic emission spectrometry  
M. Smolik, H. Polkowska-Motrenko, Z. Hubicki, A. Jakóbk-Kolon and B. Danko ..... 97
- Development of a simple method for the determination of nitrite and nitrate in groundwater by high-resolution continuum source electrothermal molecular absorption spectrometry  
G.C. Brandao, G.D. Matos, R.N. Pereira and S.L.C. Ferreira ..... 101
- Advanced recognition of explosives in traces on polymer surfaces using LIBS and supervised learning classifiers  
J. Serrano, J. Moros, C. Sánchez, J. Macías and J.J. Laserna ..... 107

### Chemometrics

- An efficient algorithm coupled with synthetic minority over-sampling technique to classify imbalanced PubChem BioAssay data  
M. Hao, Y. Wang and S.H. Bryant ..... 117

### Electrochemistry

- Amplified impedimetric aptasensor based on gold nanoparticles covalently bound graphene sheet for the picomolar detection of ochratoxin A  
L. Jiang, J. Qian, X. Yang, Y. Yan, Q. Liu, K. Wa and K. Wang ..... 128

---

Sensitive and selective electrochemical determination of quinoxaline-2-carboxylic acid based on bilayer of novel poly(pyrrole) functional composite using one-step electro-polymerization and molecularly imprinted poly(o-phenylenediamine) Y. Yang, G. Fang, X. Wang, M. Pan, H. Qian, H. Liu and S. Wang .....	136
<b>Extraction and Sample Handling</b>	
Quantitation of low concentrations of polysorbates in high protein concentration formulations by solid phase extraction and cobalt-thiocyanate derivatization J. Kim and J. Qiu .....	144
Two highly stable and selective solid phase microextraction fibers coated with crown ether functionalized ionic liquids by different sol-gel reaction approaches J. Shu, P. Xie, D. Lin, R. Chen, J. Wang, B. Zhang, M. Liu, H. Liu and F. Liu .....	152
<b>Mass Spectrometry</b>	
Sequential photocatalyst-assisted digestion and vapor generation device coupled with anion exchange chromatography and inductively coupled plasma mass spectrometry for speciation analysis of selenium species in biological samples Y.-n. Tsai, C.-h. Lin, I.-h. Hsu and Y.-c. Sun .....	165
Liquid chromatography tandem mass spectrometry determination of free and conjugated estrogens in breast cancer patients before and after exemestane treatment Y. Zhao, J.M. Boyd, M.B. Sawyer and X.-F. Li .....	172
<b>Molecular Spectrometry</b>	
Validation of an in-line Raman spectroscopic method for continuous active pharmaceutical ingredient quantification during pharmaceutical hot-melt extrusion L. Saerens, N. Segher, C. Vervaet, J.P. Remon and T. De Beer .....	180
Silver overlayer-modified surface-enhanced Raman scattering-active gold substrates for potential applications in trace detection of biochemical species K.-L. Ou, T.-C. Hsu, Y.-C. Liu, K.-H. Yang and H.-Y. Tsai .....	188
<b>Sensors and Bioselective Reagents</b>	
New competitive dendrimer-based and highly selective immunosensor for determination of atrazine in environmental, feed and food samples: The importance of antibody selectivity for discrimination among related triazinic metabolites M. Giannetto, E. Umiltà and M. Careri .....	197
Label-free amperometric immunosensor based on prussian blue as artificial peroxidase for the detection of methamphetamine L.-Y. Zhang and Y.-J. Liu .....	204