

ANALYTICA CHIMICA ACTA

AN INTERNATIONAL JOURNAL DEVOTED TO ALL BRANCHES OF ANALYTICAL CHEMISTRY

EDITORS:

MANUEL MIRÓ

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:

COO. COO. -00C Gd³⁺ 000 .00C poc COO COO COO. Gd³⁺ COO -00C-COO 000 Gd³⁺ **G**d³⁺ ОН -00C

Review Article

Determination of Gadolinium-Based MRI Contrast Agents in Biological and Environmental Samples: A Review

Lena Telgmann, Michael Sperling and Uwe Karst

(Published on pp. 1-16 of this issue)

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Analytica Chimica Acta

Volume 764, Pages 1-92 (18 February 2013)

Editorial Board

Page iii

Review article

2

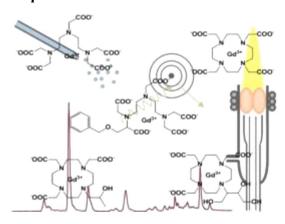
Determination of gadolinium-based MRI contrast agents in biological and environmental samples: A review

Review Article

Pages 1-16

Lena Telgmann, Michael Sperling, Uwe Karst

Graphical abstract



Highlights

► All major methods for the analysis of Gd-based MRI contrast agents are discussed. ► Biological and environmental samples are covered. ► Pharmacokinetics and species transformation can be investigated. ► The figures of merit as limit of detection and analysis time are described.

Chemometrics

3

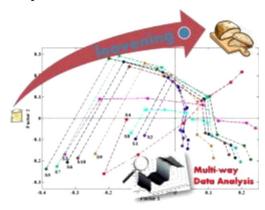
Near infrared spectroscopy and multivariate analysis to evaluate wheat flour doughs leavening and bread properties

Original Research Article

Pages 17-23

Mario Li Vigni, Marina Cocchi

Graphical abstract



Highlights

Dough leavening is studied by means of multi-way methods and NIR spectroscopy. ► Trends of variability of the NIR signal with time (leavening profiles) are obtained. ► Bread properties (e.g. volume) can be predicted from its behavior during leavening. ► Model interpretability is improved through nested mode biplots of PARAFAC loadings.

4

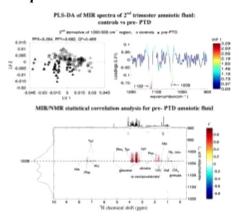
Mid-infrared (MIR) metabolic fingerprinting of amniotic fluid: A possible avenue for early diagnosis of prenatal disorders?

Original Research Article

Pages 24-31

Gonçalo Graça, Ana Sofia Moreira, Ana João V. Correia, Brian J. Goodfellow, António S. Barros, Iola F. Duarte, Isabel M. Carreira, Eulália Galhano, Cristina Pita, Maria do Céu Almeida, Ana M. Gil

Graphical abstract



Highlights

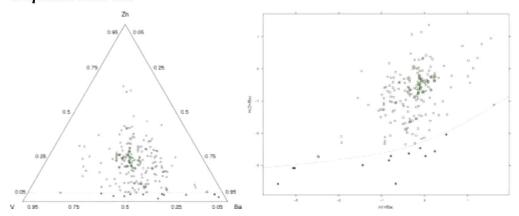
► First profiling study of amniotic fluid by MIR and multivariate analysis. ► MIR/MIR and MIR/NMR correlation for IR assignment of disease-related metabolites. ► MIR profiling changes related to fetal malformations and preterm delivery. ► Putative interpretation of MIR signatures of fetal malformations/preterm delivery.

5

Values below detection limit in compositional chemical data Original Research Article Pages 32-43

J. Palarea-Albaladejo, J.A. Martín-Fernández

Graphical abstract



Highlights

▶ Less-than replacement methods for compositional chemical data. ▶ New model-based univariate multiplicative replacement method. ▶ Evaluation of competing methods performance. ▶ Computer code implementing the methods provided.

6

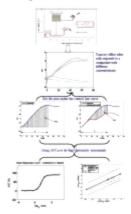
Cytotoxicity assessment based on the AUC_{50} using multi-concentration time-dependent cellular response curves

Original Research Article

Pages 44-52

Tianhong Pan, Biao Huang, Weiping Zhang, Stephan Gabos, Dorothy Yu Huang, Vignesh Devendran

Graphical abstract



Highlights

▶ Dose- and time-dependent cellular responses are used to evaluate the cytotoxicity. ▶ The CI can reflect the cell number, cell viability and morphological change, etc. ▶ AUC is more relevant to the intensity of the cell treatment. ▶ AUC_{50} can be used for cytotoxicity assessment. ▶ AUC_{50} combined with RTCA HT assay can achieve a high-throughput screening.

Electrochemistry

7厂

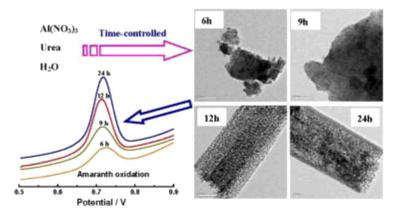
Morphology-controlled electrochemical sensing amaranth at nanomolar levels using alumina

Original Research Article

Pages 53-58

Yuanyuan Zhang, Tian Gan, Chidan Wan, Kangbing Wu

Graphical abstract



Highlights

▶ A facile way to tune morphology and sensing properties of alumina was developed. ▶ Oxidation activities of amaranth on alumina surface were morphology-dependent. ▶ Alumina microfibers were more active and greatly increased the signal of amaranth. ▶ Sensitive, rapid, selective and accurate method was developed for amaranth detection.

8

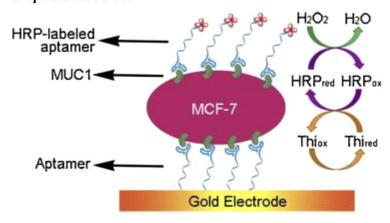
Sensitive detection of human breast cancer cells based on aptamer-cell-aptamer sandwich architecture

Original Research Article

Pages 59-63

Xiaoli Zhu, Jinghua Yang, Min Liu, Yao Wu, Zhongming Shen, Genxi Li

Graphical abstract



Highlights

► An electrochemical biosensor for the detection of MCF-7 cells was fabricated. ► An aptamer–cell–aptamer sandwich architecture was constructed on an electrode. ► Dual-recognition and enzyme-linked amplification were well integrated. ► Favorable sensitivity and selectivity can be achieved.

Molecular Spectrometry

9

Iodine and creatinine testing in urine dried on filter paper

Original Research Article

Pages 64-69

Theodore T. Zava, Sonia Kapur, David T. Zava

Graphical abstract



Highlights

▶ Dried urine iodine and creatinine extract quantitatively correlates well with liquid urine.
 ▶ Filter paper strips can be easily shipped and stored.
 ▶ Urine iodine and creatinine are stable at ambient temperature when dried on filter paper.
 ▶ Dried urine iodine and creatinine are run using a 96-well format.

10┌

Development of a generic assay for the determination of total trihydroxybenzoate derivatives based on gold-luminol chemiluminescence

Original Research Article

Pages 70-77

Dimosthenis L. Giokas, Dionysios C. Christodouleas, Ioanna Vlachou, Athanasios G. Vlessidis, Antony C. Calokerinos

Graphical abstract

Highlights

► Gold is used as an alternative oxidant to luminol under mild conditions. ► Trihydroxybenzoates are selectively determined in complex mixtures. ► The method is straightforward without any interim steps.

11厂

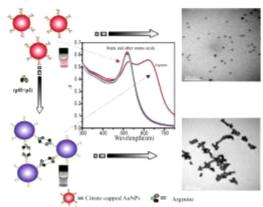
Visual detection of arginine based on the unique guanidino group-induced aggregation of gold nanoparticles

Original Research Article

Pages 78-83

Wendan Pu, Huawen Zhao, Chengzhi Huang, Liping Wu, Dan Xu

Graphical abstract



Highlights

► A simple, fast and novel colorimetric method for arginine detection was developed. \blacktriangleright This method showed high sensitivity and selectivity. \blacktriangleright As low as 0.4 μ M arginine could be easily detected by the naked eye. \blacktriangleright This method was successfully used to detect arginine in real samples.

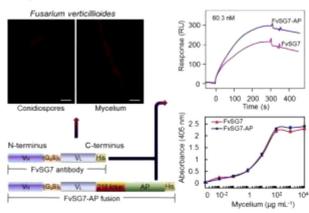
A phage-displayed chicken single-chain antibody fused to alkaline phosphatase detects *Fusarium* pathogens and their presence in cereal grains

Original Research Article

Pages 84-92

Zu-Quan Hu, He-Ping Li, Jing-Bo Zhang, Tao Huang, Jin-Long Liu, Sheng Xue, Ai-Bo Wu, Yu-Cai Liao

Graphical abstract



Highlights

► Generation of a highly reactive scFv antibody against *F. verticillioides*. ► Localization of the antibody binding to the surface target of *F. verticillioides*. ► Expression of the antibody–alkaline phosphatase (AP) fusion linked by a 218 linker. ► The antibody–AP fusion has a higher affinity than the parental antibody. ► The antibody–AP fusion detects toxigenic *Fusarium* pathogens in cereal grains.