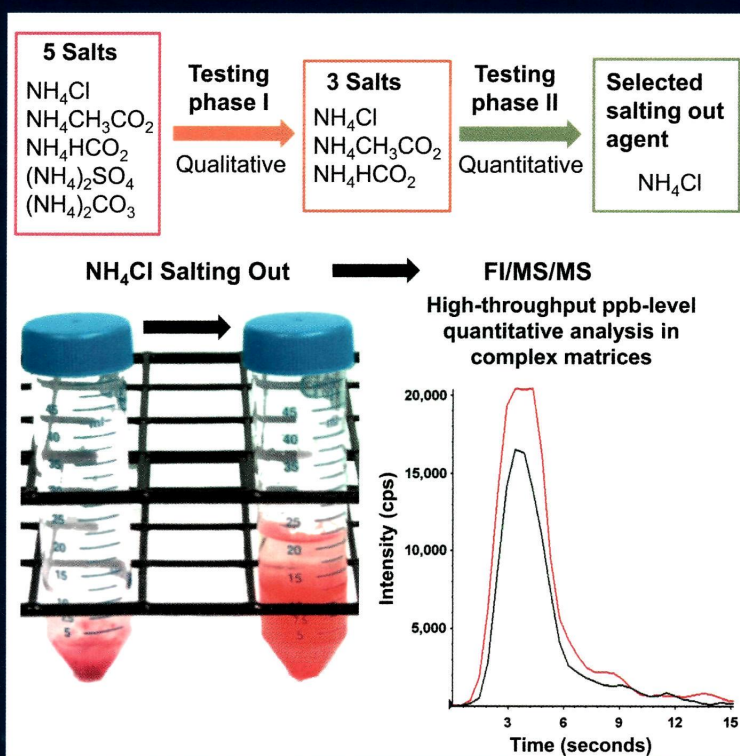


# ANALYTICA CHIMICA ACTA

AN INTERNATIONAL JOURNAL DEVOTED TO ALL BRANCHES OF ANALYTICAL CHEMISTRY



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## Featured Article

Ammonium chloride salting out extraction/cleanup for trace-level quantitative analysis in food and biological matrices by flow injection tandem mass spectrometry

Sergio C. Nanita and Nilusha L.T. Padivitage

(Published on pp. 1-11 of this issue)

# Analytica Chimica Acta

Volume 768, Pages 1-142 (20 March 2013)

## Editorial Board

Page iii

## Featured Article

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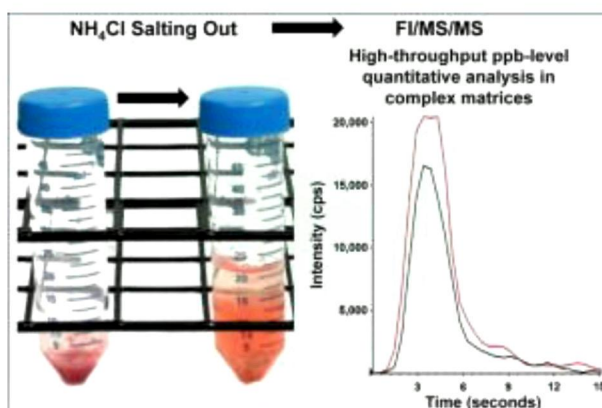
### Ammonium chloride salting out extraction/cleanup for trace-level quantitative analysis in food and biological matrices by flow injection tandem mass spectrometry

Original Research Article

Pages 1-11

Sergio C. Nanita, Nilusha L.T. Padivitage

## Graphical abstract



## Highlights

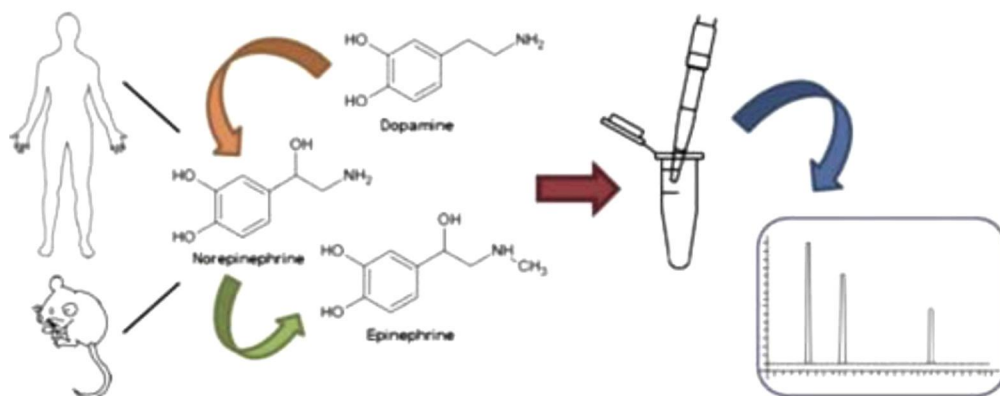
► A novel sample extraction/cleanup method for trace-level analysis in food and body fluids. ► NH<sub>4</sub>Cl salting out allows high-throughput part-per-billion analysis by FI/MS/MS. ► Flow injection tandem mass spectrometry improves pesticide residue analysis.

## Review Article

3

### Liquid chromatographic methods for the quantification of catecholamines and their metabolites in several biological samples—A review

### Graphical abstract



### Highlights

► HPLC methods for quantifying catecholamines and their metabolites are reviewed. ► The collection, handling and treatment of biological samples are analyzed. ► Chromatographic variables are discussed and detection systems are compared.

### Atomic Spectrometry

41

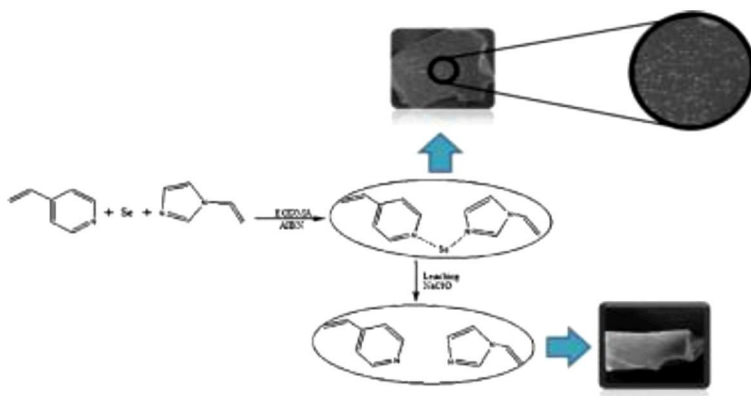
#### Determination of selenium using atomically imprinted polymer (AIP) and hydride generation atomic absorption spectrometry

Original Research Article

Pages 35-40

Grazielle Cabral de Lima, Ayla Campos do Lago, Arley Alves Chaves, Pedro Sergio Fadini, Pedro Orival Luccas

## Graphical abstract



## Highlights

- Atomically imprinted polymers (AIP) was synthesized for the first time.
- The material exhibited adequate sensitivity expressed by high preconcentration factor.
- A method for on-line selenium determination by HG-AAS in food samples was developed.

Chemometrics

5

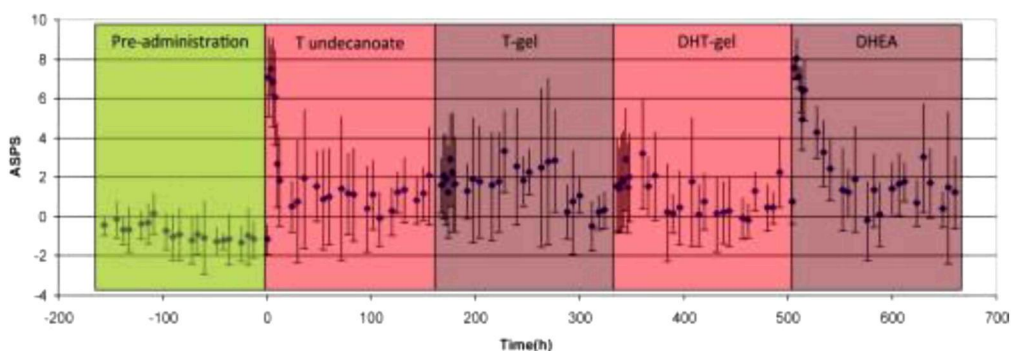
## Statistical discrimination of steroid profiles in doping control with support vector machines

Original Research Article

Pages 41-48

Pieter Van Renterghem, Pierre-Edouard Sottas, Martial Saugy, Peter Van Eenoo

## Graphical abstract



### **Highlights**

► Support vector machines classifies steroid profiles in doping analysis. ► A general detection model was developed with satisfying detection windows. ► Good diagnostic performance was achieved. ► In combination with the concept of the biological passport, this model is a promising anti-doping strategy.

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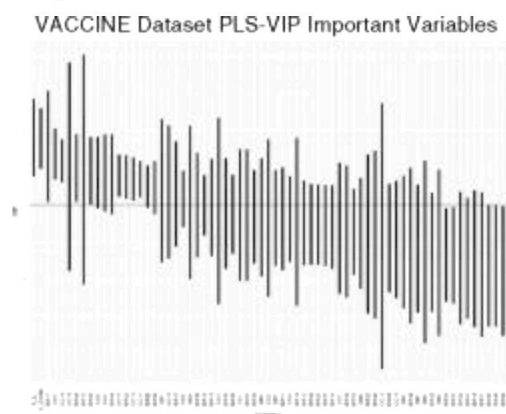
### **Use of the bootstrap and permutation methods for a more robust variable importance in the projection metric for partial least squares regression**

Original Research Article

Pages 49-56

N.L. Afanador, T.N. Tran, L.M.C. Buydens

### **Graphical abstract**



### **Highlights**

► A more robust variable importance in the projection metric (VIP) is explored. ► Bootstrap and permutation methods in relation to VIP robustness are presented. ► The selective performance of the VIP vs. the proposed method is assessed.

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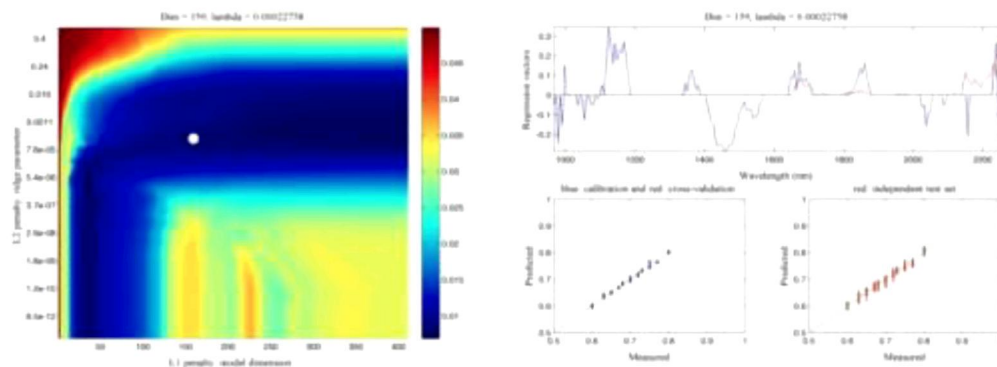
### **Parsimonious and robust multivariate calibration with rational function Least Absolute Shrinkage and Selection Operator and rational function Elastic Net**

Original Research Article

Pages 57-68

P. Teppola, V.-M. Taavitsainen

## Graphical abstract



## Highlights

- ▶ A unique approach using rational functions and Elastic Net.
- ▶ Chemometric preprocessing not needed when using rational functions.
- ▶ Building parsimonious models in an automated way.
- ▶ Automated variable selection.
- ▶ A full continuum of feasible solutions with parsimony and/or smoothness.

## Electrochemistry

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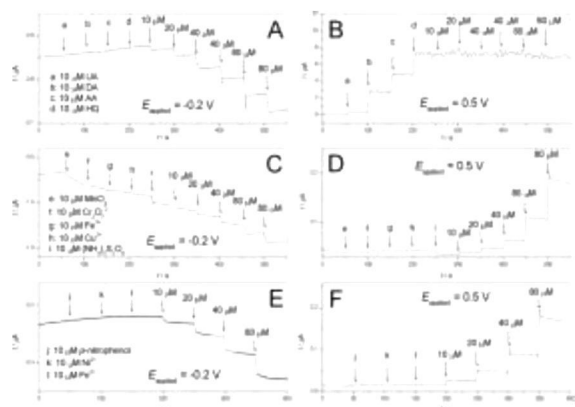
### Preparation of cobalt-tetraphenylporphyrin/reduced graphene oxide nanocomposite and its application on hydrogen peroxide biosensor

Original Research Article

Pages 69-75

Longzhen Zheng, Dan Ye, Leyan Xiong, Jingpeng Xu, Kun Tao, Zhijun Zou, Danlin Huang, Xiaowei Kang, Shaoming Yang, Jian Xia

## Graphical abstract



## Highlights

► CoTPP/RGO nanocomposite was prepared by a  $\pi$ - $\pi$  stacking interaction. ► CoTPP/RGO showed electrocatalytic activity for both oxidation and reduction of  $\text{H}_2\text{O}_2$ . ► The high sensitivity was due to the synergy effect between CoTPP and RGO. ► The CoTPP/RGO electrode showed good anti-interfering ability.

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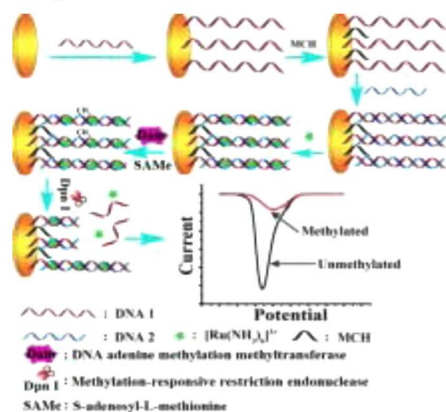
### Electrochemical strategy for sensing DNA methylation and DNA methyltransferase activity

Original Research Article

Pages 76-81

Gang Lin Wang, Long Yin Zhou, Hong Qun Luo, Nian Bing Li

#### Graphical abstract



## Highlights

► An electrochemical strategy for sensing DNA methylation and DNA methyltransferase activity was proposed. ► A methylation-responsive DNA biosensor was fabricated. ► This assay was based on electrostatic adsorption of  $[\text{Ru}(\text{NH}_3)_6]^{3+}$  on the anionic DNA biosensor. ► A low detection limit ( $0.18 \text{ U mL}^{-1}$ ) was obtained without any amplification. ► This strategy can be applied to qualification of activity of other methyltransferases.

Extraction and Sample Handling

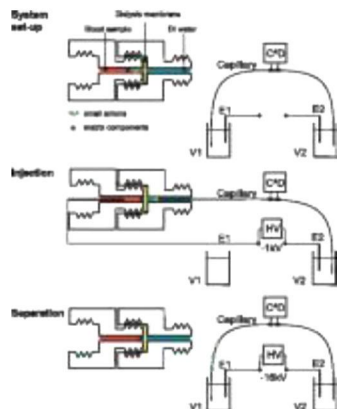
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### Direct analysis of formate in human plasma, serum and whole blood by in-line coupling of microdialysis to capillary electrophoresis for rapid diagnosis of methanol poisoning

Original Research Article

Pages 82-89

### Graphical abstract



### Highlights

- In-line coupling of microdialysis to CE-C<sup>4</sup>D is presented
- Formate is directly analyzed in plasma, serum and whole blood samples
- Electrokinetic injection across dialysis membrane ensures efficient sample clean-up
- Formate, as a marker of methanol intoxication, is determined in less than 4 min
- Significant formate levels were found in serum of a methanol poisoned patient.

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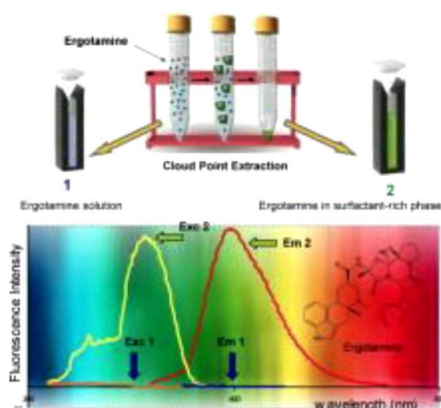
### Sensitive ergotamine determination in pharmaceuticals and biological samples using cloud point pre-concentration and spectrofluorimetric detection

Original Research Article

Pages 90-95

Chien C. Wang, Liliana P. Fernández, María Roxana Gómez

### Graphical abstract





## Highlights

► A highly efficient cloud point extraction method was developed for ergotamine. ► Direct gel-state fluorescence determination was performed after extraction. ► Emission advantages of undiluted surfactant rich phase were explored for the first time. ► A total enhancement factor of 1325 was achieved for ergotamine determination. ► The simple, low cost, non-toxic methodology was successfully applied to real samples.

## Flow Analysis

127

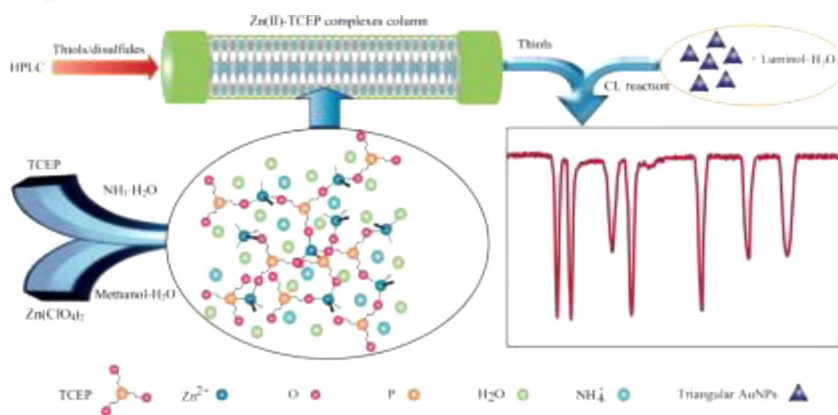
### Automated high performance liquid chromatography with on-line reduction of disulfides and chemiluminescence detection for determination of thiols and disulfides in biological fluids

Original Research Article

Pages 96-101

Shouli Bai, Qingshuo Chen, Chao Lu, Jin-Ming Lin

## Graphical abstract



## Highlights

► An on-line Zn(II)-TCEP reduction column for disulfides is fabricated. ► This reduction column is coupled with HPLC-CL system for assay of thiols and disulfides. ► The optimum pH for disulfides reduction is compatible with that of the HPLC mobile phase. ► The proposed method has been applied to analyze real samples.

## Mass Spectrometry

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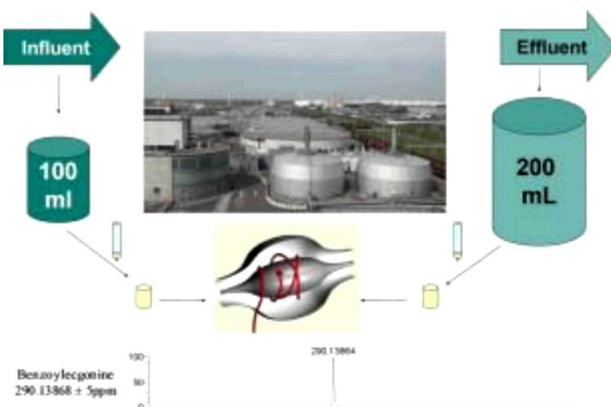
## Performance of the linear ion trap Orbitrap mass analyzer for qualitative and quantitative analysis of drugs of abuse and relevant metabolites in sewage water

Original Research Article

Pages 102-110

Lubertus Bijlsma, Erik Emke, Félix Hernández, Pim de Voogt

### Graphical abstract



### Highlights

- ▶ A methodology was developed for the determination of 24 drugs of abuse in sewage waters. ▶
- Quantitative analyses were performed using liquid chromatography–HR Orbitrap mass spectrometer. ▶
- Compared to QqQ results, Orbitrap is almost equally sensitive. ▶
- Accurate mass full scan data allowed retrospective analysis.

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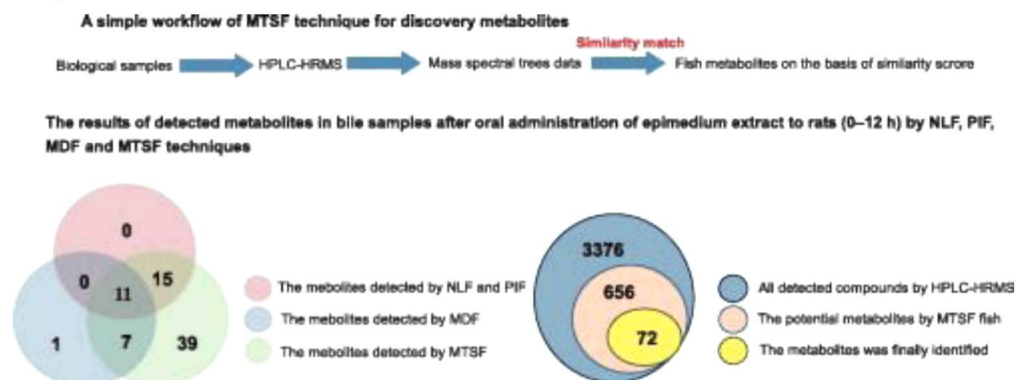
## A new strategy for the discovery of epimedium metabolites using high-performance liquid chromatography with high resolution mass spectrometry

Original Research Article

Pages 111-117

Ying Jin, Cai-Sheng Wu, Jin-Lan Zhang, Ying-Fei Li

## Graphical abstract



## Highlights

- ▶ A new metabolite discovery strategy was established using HPLC–HRMS and MTSF technique. ▶
- Metabolites of epimedium extract, a well-known TCM were successfully discovered and identified by the new strategy. ▶
- A total of 115 metabolites with 11 structural skeletons were reported. ▶
- The MTSF technique showed superior efficiency and selectivity than NLF, PIF and MDF.

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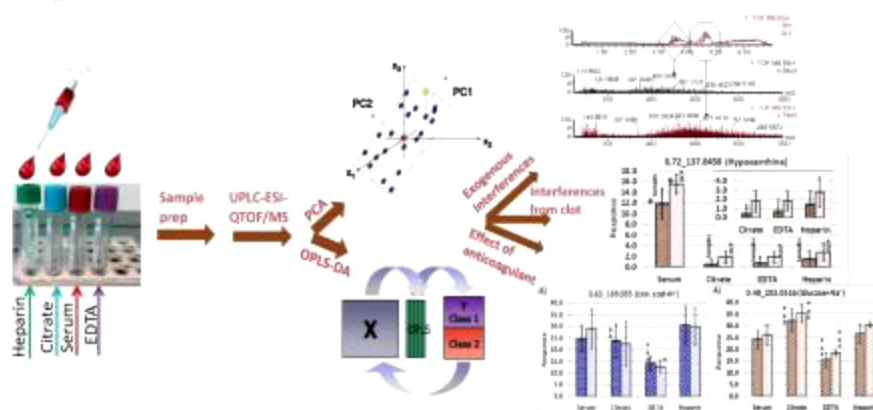
## UPLC-ESI-QTOF/MS and multivariate data analysis for blood plasma and serum metabolomics: Effect of experimental artefacts and anticoagulant

Original Research Article

Pages 118-128

Thaer Barri, Lars Ove Dragsted

## Graphical abstract



## Highlights

- ▶ We studied metabolite profiles in blood serum and different plasma preparations. ▶
- Interferences in serum and plasma samples and anticoagulant effects were identified. ▶
- Serum samples showed

features of polymeric material, peptides, and xanthenes. ► Formate ion clusters and effect of anticoagulants were observed in plasma samples. ► Heparin plasma is advised and serum is a second choice for LC-ESI/MS metabolomics.

Sensors and Bioselective Reagents

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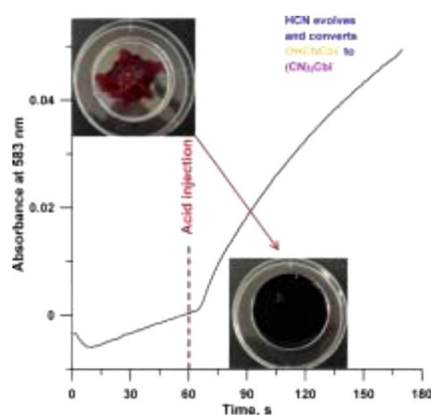
### **A disposable blood cyanide sensor**

Original Research Article

Pages 129-135

Yong Tian, Purnendu K. Dasgupta, Sari B. Mahon, Jian Ma, Matthew Brenner, Jian-Hua Wang, Gerry R. Boss

#### **Graphical abstract**



#### **Highlights**

► Cyanide in blood is determined in ~4 min by an inexpensive sensor. ► As little as 20  $\mu\text{L}$  sample can be used. ► The recommended sample volume, 50  $\mu\text{L}$ , can be obtained by finger prick. ► 50  $\mu\text{L}$  blood sample provides for an LOD of 2.2  $\mu\text{M}$  and upper linear limit of 60  $\mu\text{M}$ . ► With 1 mL sample, baseline cyanide levels in blood can be measured.

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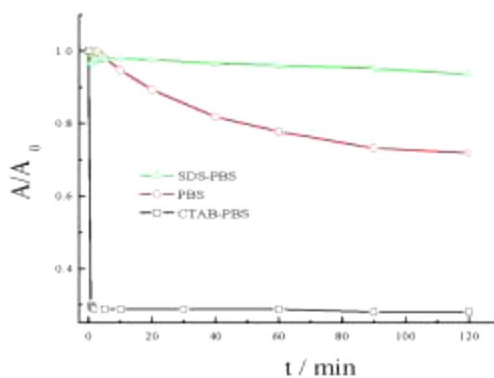
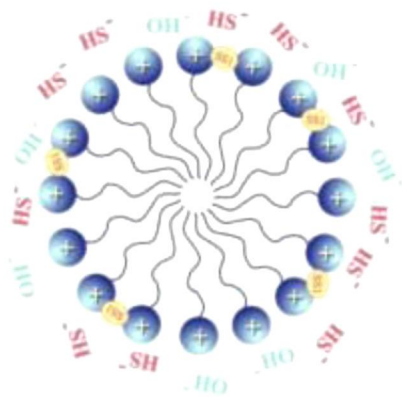
### **Micelle-induced multiple performance improvement of fluorescent probes for $\text{H}_2\text{S}$ detection**

Original Research Article

Pages 136-142

Haiyu Tian, Junhong Qian, Hongyan Bai, Qian Sun, Lingyi Zhang, Weibing Zhang

## Graphical abstract



## Highlights

- ▶ Two new H<sub>2</sub>S probes based on its reducing property were synthesized.
- ▶ Rapid response and high sensitivity (the detection limit as low as 20 nM) towards H<sub>2</sub>S were realized in CTAB micelle.
- ▶ The probes could measure H<sub>2</sub>S levels in fetal bovine serum without any prior sample processing.