Souhrny prací soutěže o Cenu K. Štulíka

S. Baluchová and K. Schwarzová-Pecková *(Charles University in Prague, Faculty of Science, Department of Analytical Chemistry, UNESCO Laboratory of Environmental Electrochemistry):* **Voltammetric Determination of Vanillylmandelic and Homovanillic Acid at Boron Doped Diamond Electrode**
Keywords: boron-doped diamond electrode, homovanillic acid, vanillylmandelic acid, voltammetry

The electrochemical oxidation of two main catecholamine metabolites vanillylmandelic and homovanillic acid at anodically oxidized boron-doped diamond electrode using voltammetric techniques was investigated. Their behavior in aqueous media depends significantly on pH; the highest and best developed voltammetric signals were obtained in an acidic medium when both organic compounds occur in their non-ionized form. Calibration dependences are linear for both studied compounds in phosphate buffer pH 3.0 in the concentration range from 4 to 100 μmol l^{-1}. Using differential pulse voltammetry limits of detection for homovanillic acid (LOD = 0.57 μmol l^{-1}) and for vanillylmandelic acid (LOD = 0.41 μmol l^{-1}) were achieved. The possibility of their simultaneous determination at boron-doped diamond was also verified.

Š. Havlová and V. Prokopec *(Department of Analytical Chemistry, University of Chemistry and Technology, Prague):* **Application of Surface-enhanced Raman Spectroscopy for The Detection and Identification of Gallic Acid**
Keywords: surface-enhanced Raman spectroscopy, gallic acid, gold, silver, substrate

Gallic acid was analyzed using surface-enhanced Raman spectroscopy in presence of gold and silver large area SERS active substrates. For these metal substrates adsorption of gallic acid was studied at various concentrations and Raman spectra were measured at two excitation wavelengths (785 nm and 1064 nm) which are compared with each other for each concentration especially in terms of total surface enhancement, band positions and band shapes.

K. Kudláček[a], K. Nesměrák[a], and J. Babica[b] *([a] Department of Analytical Chemistry, Faculty of Science, Charles University in Prague, Prague; [b]Czech Pharmaceutical Museum, Faculty of Pharmacy, Charles University in Prague, Kuks):* **Analysis of Historical Pharmaceutical Preparations of Quinine and Theophylline**
Keywords: quinine, theophylline, long-term stability, degradation, RP-HPLC

Pharmaceutical preparations of quinine (injection solutions) and theophylline (suppositories) about seventy years old were analyzed using RP-HPLC. The composition of mobile phase was optimized. The samples of quinine injection solutions consist of 92% or 87% of declared quinine content. Quinotoxine has been identified as the product of quinine degradation. The quantification of theophylline in suppositories did not show any degradation after more than 67 years from their manufacturing.

N. Ladislavová, O. Vyhnálek, Š. Urban, V. Škeříková, and P. Cinková *(Department of Analytical Chemistry, Faculty of Chemical Engineering, UCT Prague):* **Creation of Special MS Library for Human Odour Analysis**
Keywords: human odour, special MS libraries

Universal MS libraries commonly used for GC/MS analysis and experiments do not suffice for decoding of the patterns of human odour. First qualitative analysis of human odour samples revealed that critical amount of chemical compounds, which were found in odour samples, were not registered in commercial libraries. However, a specialized MS library is crucial for decoding human odour patterns for generic and individual identification. The main idea for identification is cross-correlation between characteristics of experimental subject (such as sex, health condition, smoker/non-smoker etc.) and qualitative and quantitative aspects of chemical compounds which are present in its odour sample, therefore compact and reliable spectra database is elemental tool for further experiments. Issues of creating user library are described in the text above.

S. Lupínková[a], M. Benkocká[a], J. Braborec[a,b], J. Matoušek[a], K. Kolářová[c], M. G. S. Londesborough[b], and Z. Kolská[a] *([a] J. E. Purkyně University in Ústí nad Labem, Materials Centre and Department of Physics, [b] Academy of Sciences of the Czech Republic, Institute of Inorganic Chemistry, Husinec-Řež, [c] University of Chemistry and Technology in Prague, Department of Solid State Engineering):* **Analysis of Chemically Modified Polymer Surfaces**
Keywords: polymers, surface properties, borane compounds, XPS, electrokinetic analysis, contact angle, mikrobial testing

In this work we studied surface properties of different surface-modified polymers. Polymers were firstly activated by Piranha solutions. Activated polymer surfaces were grafted by amino-compounds and subsequently with borane compounds. Surface properties were characterized by X-ray photoelectron spectroscopy, goniometry and electrokinetic analyses. Selected samples were tested for toxicity.

K. Matějková, A. Kaňa, and O. Mestek *(Department of Analytical Chemistry, University of Chemistry and Technology, Prague):* **Determination of Trace Elements in Czech Honey**
Keywords: honey, inductively coupled plasma – mass spectrometry, principal component analysis, honey origin

Honey is generally considered as nutritionally valuable food. The aim of this study was (a) determination of the content of selected (both essential and toxic) metal elements in the Czech honey samples using the inductively coupled plasma – mass spectrometric method, (b) evaluation of the data obtained considering the influence on human health and (c) elucidation of the relationship between the elements contents and geographic origin of the honey employing the principal component analysis. The results show that the contents of elements do not represent any health risks for adults. The geographic source is somewhat reflected in the honey composition but the relationships are too complex to allow us the determination of the honey origin based on the information about metal elements contents.

K. Paroulková, V. Škeříková, and P. Cinková *(Department of Analytical Chemistry, Faculty of Chemical Engineering, UCT Prague):* **The Solubility of Odorous Molecules**
Keywords: human odour, fatty acids, esters, GC-MS

Human odour is a very complex chemical mixture; however main components were successfully described. Human odour contains fatty acids and their esters, therefore is rather lipophilic and less volatile. Based on the previous experiment, standard mixture, which consists of Fatty acids and their esters, Aldehydes, Ketones, n-Alkanes and Squalene, was prepared. Three solvents with various polarities were used for extraction of target compounds from glass beads. The main goal of this experiment was to determine differences in the extraction selectivity of solvents used in the GC-MS analysis of the human odour – acetonitrile, ethanol and hexane.

M. Pšenička and P. Kuráň *(J. E. Purkyně University in Ústí nad Labem, Faculty of Environment):* **Study of Kinetics Degradation of Organophosphorus Pesticide Parathion Methyl on Nanocrystals Metals Oxides**
Keywords: degradation, reactive sorbents, parathion methyl

This work was focused on research of parathion methyl kinetics on nanocrystal of metals oxides. Some of prepared reactive sorbents have degradation properties, maximum conversion (66 %) of parathion methyl to 4-nitrophenol was reached within 128 minutes on sorbent 2Ti.8Ce. The use of HLPC-UV-Vis for determination of organophosphorus pesticides by means of quick, robust and sensitive diode array detector was shown to be possible.

F. Smrčka, J. Vaněk, and P. Lubal *(Department of Chemistry&CEITEC, Masaryk University, Brno):* **Dual Sensor based on Eu(III) Complex**
Keywords: makrocyclic ligands, Eu(III) complex, cyclic voltametry, luminiscence spektroscopy, antenna effect

This paper describes the study of the formation of ternary Eu(III) complex with DO2A and DO3A macrocyclic ligands including the picolinate-like ligands serving as the antenna for luminiscence spectroscopy. The luminiscent and electrochemical properties of the ternary Eu(III) complex formed can be used for determination of bicarbonate ions and they can be utilized in order to develop a new dual sensor for bicarbonate anion analysis.

Š. Strnad[a,b], D. Sýkora[a], V. Vrkoslav[b], J. Cvačka[b], L. Maletínská[b], Z. Pirník[b,c,d] *([a] Department of Analytical Chemistry, University of Chemistry and Technology, Prague, [b] Institute of Organic Chemistry and Biochemistry, Prague, [c] Institute of Experimental Endocrinology of the Slovak Academy of Sciences, Bratislava, [d] University of Veterinary Medicine and Pharmacy, Košice):* **Mass Spectrometry Imaging of Metformin in Tissue Sections**
Keywords: mass spectrometry imaging, metformin, MALDI, MALDI MSI

Mass spectrometry imaging is a powerful technique suitable for visualization of the distribution of a wide variety of compounds within tissue sections. The main aim of the study was the development and optimization of a sample preparation procedure allowing determination of the distribution of orally dosed metformin in mice kidney sections. Metformin is the first-line medication for the treatment of type 2 diabetes. The optimization of the sample preparation step before imaging experiments included the selection of a suitable matrix and the optimization of various parameters of MALDI analysis. 2,5-dihydroxybenzoic acid was identified as the best matrix providing highest sensitivity. A sublimation method was successfully used for the matrix deposition. The highest relative concentration of metformin was found in the inner zone of kidney 30 minutes after the drug administration.

L. Šerá[a,b], S. Matějková[b], and O. Mestek[a] *([a] Department of Analytical chemistry, University of Chemistry and Technology, Prague, [b] Institute of Organic Chemistry and Biochemistry CAS, v.v.i., Prague):* **Quantification of Elements in Plant Materials by Electrothermal Vaporization Inductively Coupled Plasma Optical Emission Spectrometry**
Keywords: electrothermal vaporization, optical emission spectrometry, inductively coupled plasma, plants

This paper describes optimization and validation of operating conditions of electrothermal vaporization (ETV) inductively coupled plasma optical emission spectrometry (ICP-OES) method for quantification of Ba, Ca, Co, Cu, Fe, K, Mg, Mn, Na, P, Sr and Zn in plant materials. Besides the optimization of the temperature program, the selection of the gaseous modifier and the spectral wavelengths to be measured, it was studied how the sample quantity affects the result quality of the developed method. During the validation process, the accuracy and precision of the method were checked by analysis of a certified reference material. Limits of detection were estimated by analyses of blank samples. For almost all previously mentioned elements, the method meets requirements commonly applied on analyses by ETV combined with ICP-OES.

D. Šuhajová, M. Adam, K. Adámková, A. Eisner, and K. Ventura *(University of Pardubice, Faculty of Chemical Technology, Department of Analytical Chemistry, Pardubice):* **Analysis of Sulphur Compounds in Garlic Using Stir-Bar Sorptive Microextraction Method**
Keywords: garlic, volatile sulphur compounds, SBSE, GC-ECD

This study is focused on the optimisation of stir-bar sorptive extraction method for isolation of volatile sulphur compounds of garlic followed by gas chromatography coupled with electron impact detector analysis. By the Plackett-Burmanův design the significant experimental parameters affecting the extraction process were evaluated and these parameters were then optimised by central composite design principles.