21st Young Investigators' Seminar on Analytical Chemistry

June 25 – 28, 2014, Pardubice, Czech Republic

YISAC 2014

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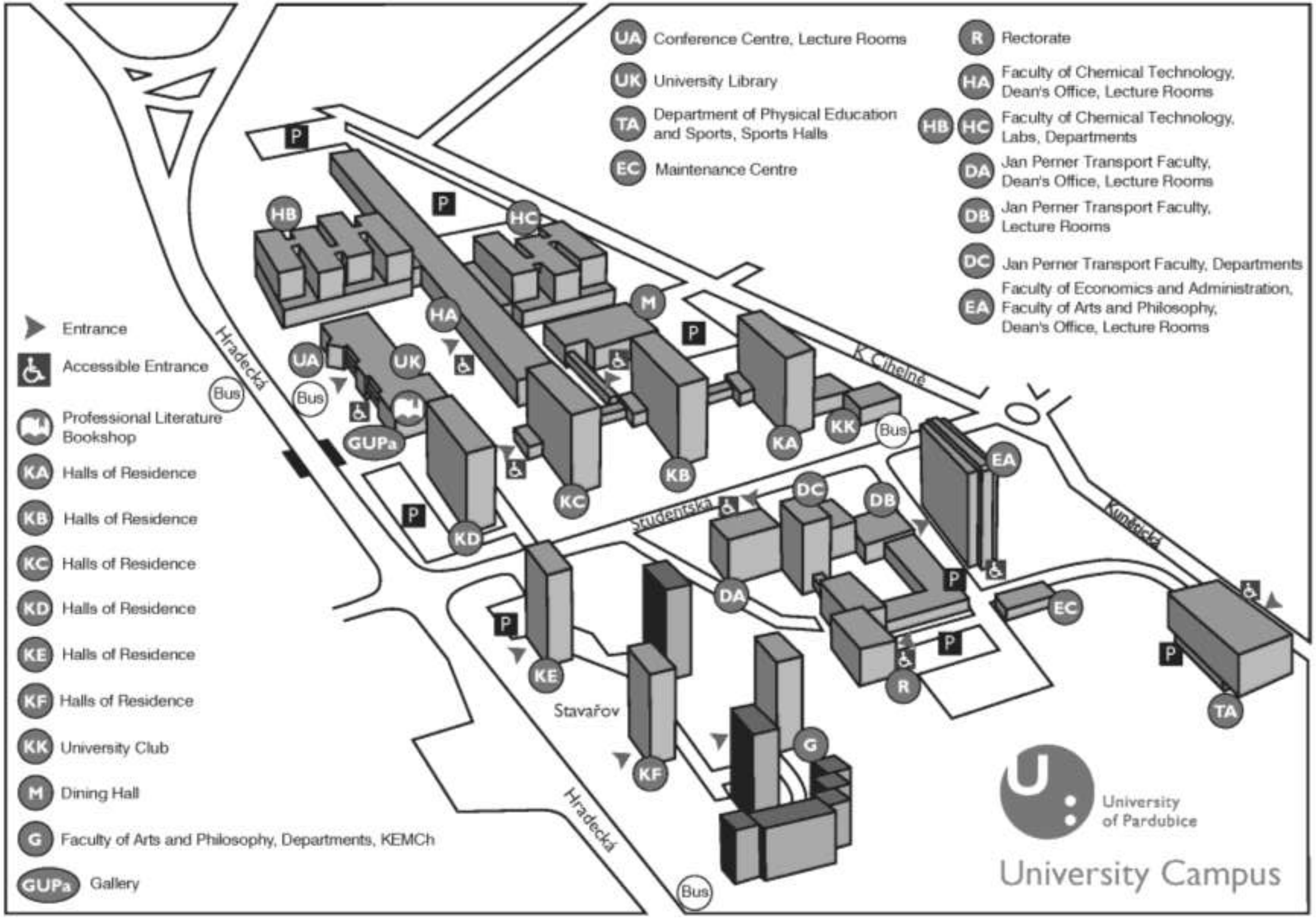
Location and Date

The lectures of YISAC 2014 conference will take place in the C1 lecture hall, located in the first floor of building HA in Faculty of Chemical Technology, University of Pardubice, Studentská 573, Pardubice, from June 25 to June 27, 2014.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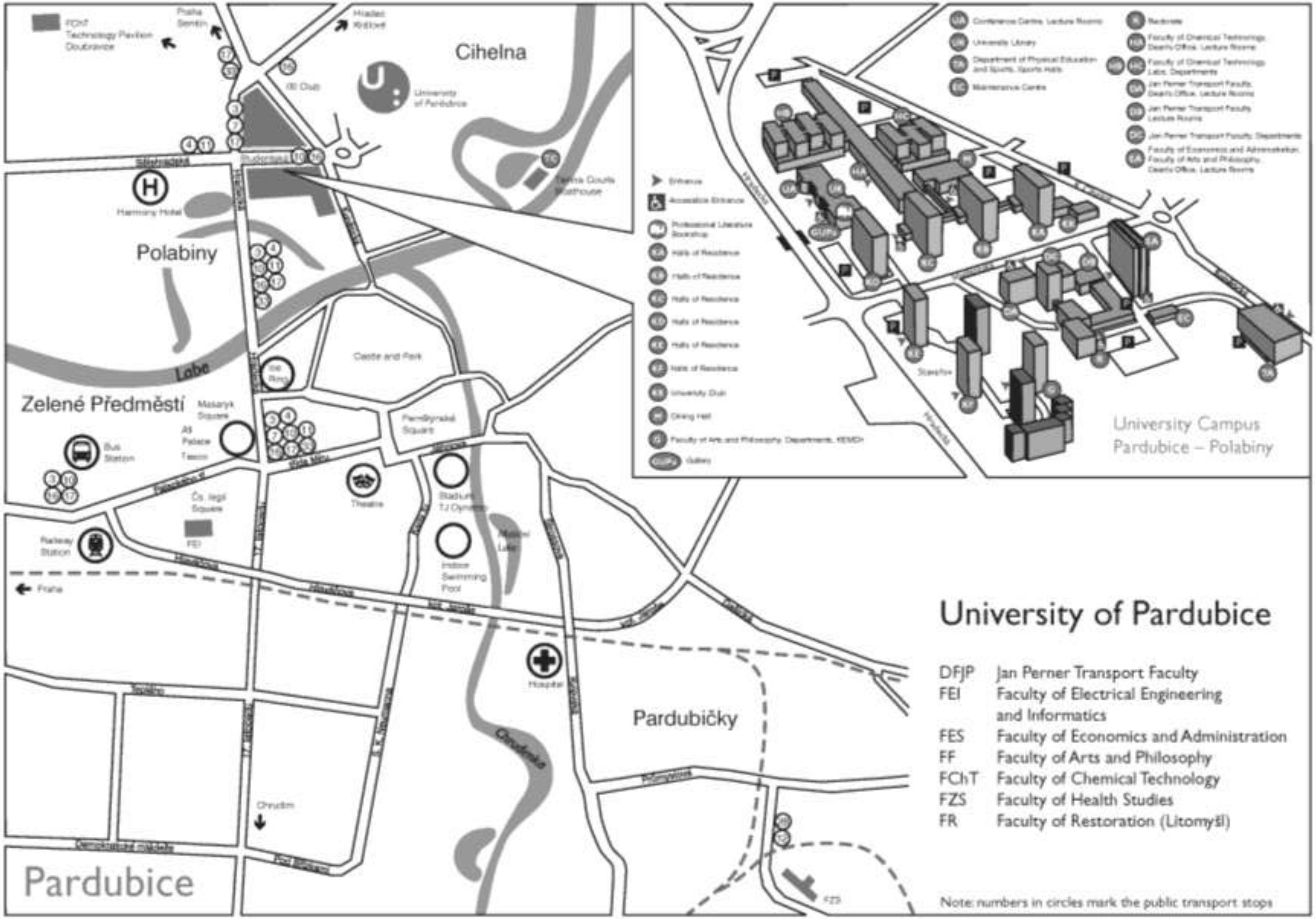

University of Pardubice

DFJP	Jan Perner Transport Faculty
FEI	Faculty of Electrical Engineering and Informatics
FES	Faculty of Economics and Administration
FF	Faculty of Arts and Philosophy
FChT	Faculty of Chemical Technology
FZS	Faculty of Health Studies
FR	Faculty of Restoration (Litomyšl)

Note: numbers in circles mark the public transport stops

YISAC 2014 PROGRAMME

WEDNESDAY, JUNE 25

18:00 REGISTRATION - entrance hall at Faculty of Chemical Technology, Studentská 573, Pardubice (1st floor)

19:00 GET-TOGETHER PARTY

THURSDAY, JUNE 26

8:00 REGISTRATION

9:00 OPENING CEREMONY - lecture hall C1 (1st floor)

SESSION 1, **Electroanalysis I**, Chairman: **Sýs M.**

9:15 **Brycht M.**, Skrzypek S., Smarzewska S., Uslu B., Ozkan S. A.
Voltammetric Investigation of Antidepressant Drug Paroxetine at Boron Doped Diamond Electrode

9:35 **Mehmeti E.**, Stanković D. M., Švorc Ľ., Kalcher K.
Electrochemical Determination of Rauwolfia Alkaloids: Determination of Ajmalicine in Pharmaceutical Formulations Based on a Glassy Carbon Electrode Modified with Gold Nanoparticles

9:55 **Zbiljić J.**, Vajdle O., Prlina B., Guzsvány V., Kalcher K.
Monitoring of H_2O_2 Content by MnO_2 Modified Screen Printed Carbon Electrode During Photo-Fenton and Fenton Based Removal of Acetamiprid

10:15 **Zidaric T.**, Jovanovski V., Hocevar S. B.
Preparation of Bismuth Particle Electrode (BiPE) for Electrochemical Trace Analysis

10:35 – 10:55 COFFEE BREAK

SESSION 2, **Electroanalysis II**, Chairlady: **Zbiljić J.**

10:55 **Maczuga M.**, Blum L., Kałus A., Bobrowski A., Królicka A., Zarębski J.
Determination of Pb(II), Zn(II), Ni(II) and Co(II) in Fly Ash Extracts Using Stripping Voltammetry

11:15 **Vajdle O.**, Zbiljić J., Guzsvány V., Avramov Ivić M., Petrović S.
Renewable Silver-Amalgam Film Electrode for Voltammetric Determination of Azithromycin, Roxithromycin and Clarithromycin Antibiotics

11:35 **Cerovac S.**, Guzsvány V., Kónya Z., Ashrafi A. M., Kukovecz Á., Vytřas K.
Determination of Trace Metals and Imidacloprid at Carbon Paste Electrode Surface Modified with Antimony Nanoparticle-Multiwalled Carbon Nanotubes Composite

11:55 **Sýs M.**, Metelka R., Vytřas K.
Amperometric Tyrosinase Carbon Paste Based Biosensor in Food Analysis

12:15 **Zając P.**, Bobrowski A., Kluczniak G., Królicka A., Zarębski J.
Voltammetric Methods for Cr(VI) Determination In Leaching Solutions Of Coal Fly Ashes

12:35 – 14:00 LUNCH

SESSION 3, **Separation Methods I**, Chairlady: **Ovčačíková M.**

14:00 **Staňková M.**, Jandera P., Hájek T.
Monolithic Stationary Phases for Hydrophilic Interaction Chromatography

14:20 **Vaňková N.**, Szlauerová Z., Fischer J., Česla P.
Determination of Fatty Alcohol Ethoxylates in the Elbe and Chrudimka Rivers

14:40 **Huš S.**, Kolar M., Krajnc P., Podgornik A.
Influence of Initiator on the Structure of Poly(Glycidyl Methacrylate) Monoliths

15:00 **Janás P.**, Jandera P., Hájek T.
Comparison of the Separation Properties of Diol Based Columns

15:20 – 15:40 COFFEE BREAK

SESSION 4, **Separation Methods II**, Chairman: **Huš S.**

15:40 **Kristl A.**, Markelj J., Pompe M.
Investigation of Various Separation Mechanisms in Ion-Chromatography

16:00 **Mavrič A.**, Zupančič T., Veber M., Pihlar B.
Coulometric Separation of Chloride before Anion Determination with Ion Chromatography

19:00 SUPERVISORS DINNER

FRIDAY, JUNE 27

SESSION 5, **Mass Spectrometry I**, Chairlady: **Panighello S.**

8:45 **Červená B.,** Cífková E., Lísa M., Chagovets V., Holčapek M., Vostálová J., Galuszka J., Hill M.
Comprehensive Analysis of Lipids in Samples of CVD Patients

9:05 **Weissengruber S.**, Troetzmueller M., Koefeler H., Lankmayr E.
Aspects of Selectivity in Lipidomics by LC-MS Analysis

9:25 **Šmon A.**, Murko S., Repič Lampret B., Battelino T.
Pilot Research for Evaluation of Incidences of Inborn Metabolic Disorders in Slovenia

9:45 **Ovčačíková M.**, Cífková E., Lísa M., Holčapek M.
Comprehensive Two-Dimensional Liquid Chromatography – Mass Spectrometry for Lipidomic Analysis

10:05 **Kremr D.**, Bajer T., Bajerová P., Eisner A., Ventura K.
A Green Method for the Determination of Capsaicinoids from Chilli Peppers

10:25 – 10:45 COFFEE BREAK

SESSION 6, **Mass Spectrometry II**, Chairman: **Šmon A.**

10:45 **Váňová J.**, Česla P., Dinisová P., Česlová L., Fischer J.
Characterization and Quantification of (Poly)Phenols in Sambucus Nigra *L. Infusions using MEKC and LC-MS/MS*

11:05 **Jurković J.**, Kolar M., Muhić-Šarac T.
Acid Mine Drainage from an Abandoned Gold Mine Site

11:25 **Bendakovská L.**, Krejčová A., Černohorský T., Zvoníčková K.
o-TOF-ICP-MS Analysis of Platinum in Algae and Hospital Wastewater

11:45 **Panighello S.**, van Elteren J.T., Orsega E.F. and Moretto M.L.
Application of Laser Ablation ICP-MS Depth Profiling Methods for the Study of Ancient Glass Artefacts

12:05 **Šídová T.**, Husáková L., Urbanová I., Šrámková J.
Matrix Modification for Overcoming the Spectral Effects During oTOF-ICP-MS Analysis of Sulfuric Acid

12:25 – 14:00 LUNCH

SESSION 7, **Separation Methods III**, Chairlady: **Vaňková N.**

14:00 **Čížková A.**, Adam M., Surmová S., Ventura K.
Analysis of Essential Oils in Herbal Teas by Means of Dispersive Liquid – Liquid Microextraction Method

14:20 **Líbalová M.**, Laštovička P., Čermák T., Čegan A.
Determination of the Content of Essential Fatty Acids in EDTA Plasma Type 2 Diabetics

14:40 **Brečko N.**, Kolar M., Košir I. J.
The Dynamics of Higher Alcohol and Ester Formation in Fermented Beverages from Barley, Quinoa and Buckwheat Malt

15:00 **Surmová S.**, Eisner A., Čížková A., Ventura K.
Gas Chromatographic Methods for Analysis of Perfumes

15:20 – 15:40 COFFEE BREAK

SESSION 8, **Other Methods**, Chairlady: **Maczuga M.**

15:40 **Khan Md B.**, Masiol M., Formenton G., Di Gioli A., De Gennaro G., Pavoni B.
Primary and Secondary Carbonaceous Species in Atmospheric Fine Particles in the Veneto Region, Italy

16:00 **Markelj J.**, Veber M., Pompe M.
Modeling of Some Key Properties Related to Secondary Organic Aerosol Formation

19:00 CONFERENCE DINNER

SATURDAY, JUNE 28

9:00 OPTIONAL EXCURSION - sightseeing tour to old city of Pardubice and castle

VOLTAMMETRIC INVESTIGATION OF ANTIDEPRESSANT DRUG PAROXETINE AT BORON DOPED DIAMOND ELECTRODE

Brycht M.[1], Skrzypek S.[1], Smarzewska S.[1], Uslu B.[2], and Ozkan S. A.[2]

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An antidepressant, paroxetine {*Prx*, (3S-trans)-3-[(1,3-Benzodioxol-5-yloxy)methyl]-4-(4-fluorophenyl) piperidine}, is drug of the SSRI type. Paroxetine is normally used in the treatment of clinical depression, obsessive-compulsive disorder, and panic disorder [1].

The aim of this work was to carry out a new method of *Prx* determination at the boron-doped diamond electrode (BDDE) by square-wave voltammetry (SWV) and square wave adsorptive stripping voltammetry (SWAdSV). Experimental conditions, such as pH, frequency, amplitude, step potential, and accumulation potential and time were optimized. Under optimum conditions, the voltammetric determination of *Prx* was performed between the linear ranges of: $1{,}00 \cdot 10^{-6}$ - $1.00 \cdot 10^{-5}$ mol·L^{-1} for SWV and $7.00 \cdot 10^{-7}$ - $3.50 \cdot 10^{-6}$ mol·L^{-1} for SWAdSV. The proposed method was fully validated.

1. Agrawal N., Esteve-Romero J., Dubey N. P., Durgbanshi A., Bose D., Peris-Vicente J., Carda-Broch S., *The Open Analytical Chemistry Journal* **2013**, 7, 1-5.

ELECTROCHEMICAL DETERMINATION OF RAUWOLFIA ALKALOIDS: DETERMINATION OF AJMALICINE IN PHARMACEUTICAL FORMULATIONS BASED ON A GLASSY CARBON ELECTRODE MODIFIED WITH GOLD NANOPARTICLES

Mehmeti E.[1], Stanković D. M.[2], Švorc Ľ.[3], and Kalcher K.[1]

[1]Institute of Chemistry - Analytical Chemistry, Karl-Franzens University, Universitätsplatz 1, Graz, A-8010, Austria.

[2]Department of Analytical Chemistry, Innovation Center of the Faculty of Chemistry, University of Belgrade, Studentskitrg 12-16, Belgrade, 11000, Serbia.

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Simple, sensitive and economically viable electrochemical methods for the determination of some Rauwolfia alkaloids (ajmalicine, reserpine and yohimbine) have been developed. The procedures involve glassy carbon electrodes, bare or modified with gold nanoparticles, and a boron-doped diamond electrode.

In the work presented here gold nanoparticles were attached to the glassy carbon electrode by adsorption. Cyclic voltammetry was used for electrochemical characterization of the analyte, ajmalicine, and differential pulse voltammetry for its quantitative determination. Britton-Robinson buffer solution at various range of pH values served as supporting electrolyte.

The method for the determination of ajmalicine showed a dynamic range for concentrations from 5 μM to 50 μM with a detection limit of (3 σ) 0.45 μM. The procedure could be applied to the determination of ajmalicine in oral solutions for medical applications.

MONITORING OF H_2O_2 CONTENT BY MnO_2 MODIFIED SCREEN PRINTED CARBON ELECTRODE DURING PHOTO-FENTON AND FENTON BASED REMOVAL OF ACETAMIPRID

Zbiljić J.[1], Vajdle O.[1], Prlina B.[1], Guzsvány V.[1], and Kalcher K.[2]

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Among carbon based electrodes, screen printed carbon electrodes (SPCEs) have been successfully used for the amperometric detection of H_2O_2, especially those modified with MnO_2 as mediator which lowers the oxidation overpotential of H_2O_2 significantly [1]. In this work, the applicability of SPCE bulk modified with MnO_2 (MnO_2-SPCE) was tested for hydrodynamic chronoamperometric monitoring of H_2O_2 during the Fenton and photo-Fenton based removal of acetamiprid, a neonicotinoid insecticide. As first, cyclic voltammetric, differential pulse voltammetric and hydrodynamic chronoamperometric experiments were performed in model solutions for the optimisation of the appropriate analytical method. In the next step, samples were prepared with the following initial concentrations: $3.1 \cdot 10^{-4}$; $2.0 \cdot 10^{-3}$; and $3.0 \cdot 10^{-3}$ mol dm^{-3} of acetamiprid, Fe^{2+} and H_2O_2, respectively [2, 3]. In photo-Fenton experiments the solutions were illuminated with an OSRAM 50 W halogen lamp. All experiments were carried out in a chemical reactor (sample volume 100.0 cm^3) under controlled temperature conditions and at constant stirring. Aliquots for the analysis were taken at the beginning of the experiment and at appropriate time intervals, shorter in the case of photo-Fenton. The only sample pretreatment step was filtration to remove precipitated iron hydroxide after stopping the Fe^{2+} and H_2O_2 based oxidation reactions. Under optimized conditions, with a working potential of 0.4 V, the H_2O_2 contents were determined from the analytical curves based on the standard addition method. Parallel HPLC-DAD measurements were performed to monitor the concentration of acetamiprid.

The authors acknowledge the financial support of the Ministry of Science and Technological Development of the Republic of Serbia (Project No. 172012 and 172059), the Secretariat for

Science and Technological Development, Autonomous Province of Vojvodina, Republic of Serbia (No. 114-451-4418/2013) and CEEPUS III (CIII-CZ-0212).

1. Beyene N.W., Kotzian P., Schachl K., Alemu H., Turkušić E., Čopra A., Moderegger H., Švancara I., Vytřas K., Kalcher K., *Talanta* **2004,** *64*, 1151-1159.
2. Segura C., Zaror C., Mansilla H.D., Mondaca M.A., *J. Hazard. Mater.* **2008**, *150*, 679-686.
3. Guzsvány V., Banić N., Papp Zs., Gaál F., Abramović B., *Reac. Kinet. Mech. Cat.* **2010**, *99*, 225-233.

PREPARATION OF BISMUTH PARTICLE ELECTRODE (BiPE) FOR ELECTROCHEMICAL TRACE ANALYSIS

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Pulsed galvanostatic plating method was applied for the ex-situ preparation of bismuth particles electrode (BiPE), which revealed attractive electroanalytical characteristics for detecting trace (heavy) metal ions. The multiple pulse galvanostatic plating of bismuth particles onto a glassy carbon substrate was investigated and optimised resulting in improved performance of BiPE, e.g. low limits of detection, compared to the ex-situ and in-situ prepared BiFEs, while maintaining favourable electrochemical and mechanical stability. The influence of various variables of bismuth particle-coating preparation, including plating solution, current and duration of pulses, were examined in connection with anodic stripping response for trace concentration levels of cadmium(II) and lead(II). The BiPE was prepared ex-situ from 0.1 M acetate buffer solution (pH 4.5) containing 20 mg/L bismuth(III) together with 40 mg/L NaBr as an auxiliary ligand. After optimisation, the resulting BiPE yielded well-defined and reproducible signals along with a low background contribution. In combination with square-wave anodic stripping voltammetry highly linear response was obtained in the examined low concentration range of 1 µg/L to 10 µg/L with excellent limits of detection, i.e. 0.7 µg/L for cadmium(II) and 0.07 µg/L for lead(II) associated with 5 minutes accumulation, and good repeatability with the RSD of 1.87 % and 1.13 % for 5 µg/L cadmium(II) and lead(II) (n = 12). Evidently, the proposed multiple pulse galvanostatic plating protocol resulted in BiPE with favourable electroanalytical performance which surpasses those of conventionally prepared in-situ and ex-situ BiFEs.

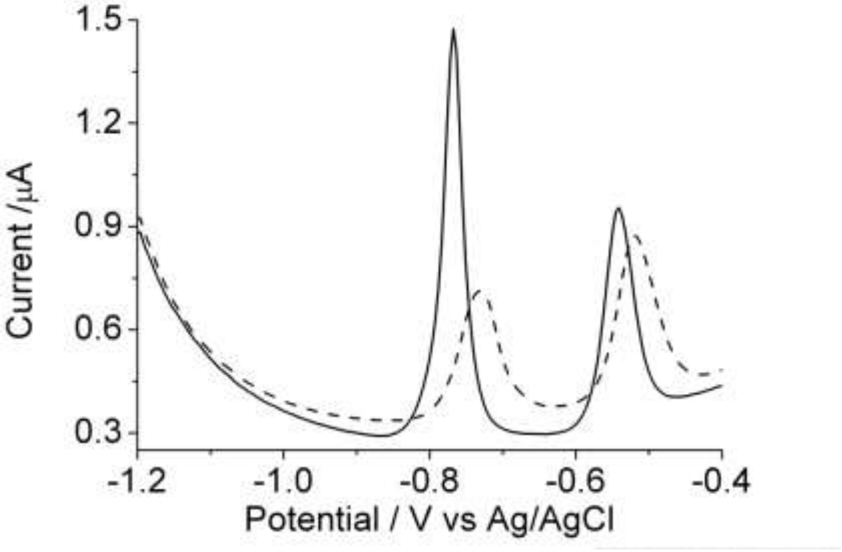

Figure 1: Anodic stripping voltammograms of 5 μg/L cadmium(II) and lead(II) at BiFE (dash line) and BiPE (solid line) in 0.05 M acetate buffer solution (pH 4.5), accumulation potential and time: -1.2V and 120 s.

DETERMINATION OF Pb(II), Zn(II), Ni(II) AND Co(II) IN FLY ASH EXTRACTS USING STRIPPING VOLTAMMETRY

Maczuga M., Blum L., Kałus A., Bobrowski A., Królicka A., and Zarębski J.

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Fly ash is a by-product of burning finely ground coal in a boiler to produce electricity. In power plants, it is removed from exhaust gases primarily by electrostatic precipitators or baghouses, and to a lesser extent by scrubber systems. Fly ash is used as an artificial pozzolan to produce cement or as a replacement for cement in concrete production. Unfortunately, it may contain a variety of toxic elements which under certain conditions can be released from ash and contaminate the soil as well as surface and ground water. Therefore, the estimation of the leaching of toxic substances is important prior to fly ash reuse and disposal.

In this study, three fly ashes originating from different thermal power stations in Poland were examined. The fly ash samples were collected from boilers of two types: a conventional, bituminous coal- fueled boiler, and a fluidized bed lignite- fueled one. The extraction procedure was performed according to EN 12457-2:2002. The obtained extracts were analysed using stripping voltammetry at a hanging mercury electrode. An attempt at the elimination of dissolved organic matter hindering the voltammetric determination was undertaken. Different protocols used to eliminate organic compounds were tested: UV photolysis in the presence of hydrochloric acid, adsorption on fumed silica or Amberlite resin, and microwave digestion with nitric acid.

Financial support from the Polish National Science Centre (Project No. 011/01/B/ST8/07794) is gratefully acknowledged.

RENEWABLE SILVER-AMALGAM FILM ELECTRODE FOR VOLTAMMETRIC DETERMINATION OF AZITHROMYCIN, ROXITHROMYCIN AND CLARITHROMYCIN ANTIBIOTICS

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Azithromycin (AZT), roxithromycin (ROX) and clarithromycin (CLARI), the target analytes, belong to a group of macrolide antibiotics, a relatively new class of compounds, which have been used to treat a wide range of infections in medical and in veterinary practices [1]. For the voltammetric analysis of these antibiotics, renewable silver-amalgam film electrode (Hg(Ag)FE) was applied as working electrode. The preparation of (Hg(Ag)FE) is relatively simple and the renewing of its surface is very easy [2].

Voltammetric characterization and determination of AZT, ROX and CLARI using (Hg(Ag)FE) was performed by cathodic square wave voltammetry (SWV) in aqueous Britton Robinson buffer solution as supporting electrolyte. Three reduction peaks of CLARI were obtained with peaks maxima at around 0.05 V, between -0.25 V and -0.66 V, and from -1.60 V to -1.70 V. One reduction peak was obtained in the case of AZT and ROX with peak maxima in the potential range from -1.75 V to -1.90 V, and between -1.45 V and -1.70 V, respectively. The highest intensity of the reduction peaks was registered at the pH 4.0 and pH 9.0 in the case of ROX, and at pH 8.0 and pH 6.0 in the case of AZT and CLARI, respectively. Relative good linearity in the model solutions of these antibiotics were obtained in the lower μg mL^{-1} range. The reproducibility of the analytical signals was characterized by the relative standard deviation (RSD) less than 5.0 % in all cases.

The developed SWV methods were applied for determination of AZT and ROX in the spiked river water samples.

The authors acknowledge the financial support of the Ministry of Science and Technological Development of the Republic of Serbia (Project No. 172012 and 172013).

1. Omura S. (Ed.), *Macrolide Antibiotics: Chemistry, Biology and Practice*, Academic Press, Orlando, FL, 1984.
2. Piech R., Bás B., Kubiak W.W., *J. Electroanal. Chem.* **2008**, *621*, 43-48.

DETERMINATION OF TRACE METALS AND IMIDACLOPRID AT CARBON PASTE ELECTRODE SURFACE MODIFIED WITH ANTIMONY NANOPARTICLE-MULTIWALLED CARBON NANOTUBES COMPOSITE

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Antimony nanoparticle-multiwalled carbon nanotubes composite (SbNPs-MWCNT) was obtained by modified way of earlier reported synthesis[1] and was characterized by TEM and XRD. The applicability of such type of material was tested as surface modifier of carbon paste electrode (SbNPs-MWCNT-CPE). The sensor was used for determination of Pb(II) and Cd(II) by square-wave anodic stripping voltammetry, and for measurement of organic compound imidacloprid with nitroguanidine electroactive functional group reducible in fairly negative potential range. Key operational parameters such as deposition potential and time as well as the supporting electrolyte composition (hydrochloric acid pH 2.0 for target metals ions and Britton-Robinson buffer pH 7.0 for imidacloprid) were optimized. The electrode of interest exhibited well-developed signals and pretty linear calibration plots for both metal ions tested, in the concentration range from 3.0 to 50.0 µg L^{-1}. For the neonicotinoid insecticide the concentration range was from 1.41 to 32.769 µg mL^{-1}. In the case of all investigated target analytes the relative standard deviation of measurements was lower than 4.5 %.

This document has been produced with the financial assistance of CEEPUS III (CIII-CZ-0212) network.

1. Ashrafi, A.M., Cerovac, S., Mudrić, S., Guzsvány, V., Husáková, L., Urbanová, I., Vytřas, K., *Sens. Actuators, B* **2014**, *191*, 320-325.

AMPEROMETRIC TYROSINASE CARBON PASTE-BASED BIOSENSOR IN FOOD ANALYSIS

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Carbon paste electrode with surface modification by carbon nanotubes was chosen as an electric transducer, on which tyrosinase was immobilized using conductive copolymer Nafion to develop a final biological sensor. The tyrosinase is a copper containing metalloenzyme which catalyzes oxidation of polyphenols (present in food) to corresponding quinones [1]. Electrochemical reduction of these quinones at constant potential is a principle of the amperometric biosensor [2]. Qualitative representation of each polyphenol in analyzed foodstuffs cannot be realized without the use of chromatographic techniques. Using an appropriate biosensor, only total phenolic content can be determined. This nutrition value is expressed as a mass equivalent of water soluble analog of vitamin E which is known as Trolox [3]. Commonly used spectrophotometric methods based on reducing properties of analyzed polyphenols can be replaced by this more sensitive electrochemical sensor. The biosensor can be applied in analyses of food with low content of vitamin C such as wines, beers [4], teas [5], selected fruits etc. Thus, it can be used to monitor food freshness and to control technological processes as well.

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VOLTAMMETRIC METHODS FOR Cr(VI) DETERMINATION IN LEACHING SOLUTIONS OF COAL FLY ASHES

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Fly ash, a product of burning coal in power plants is used as an additive to Portland cement or as an admixture for concrete. To evaluate the potential hazard of Cr(VI) released from coal fly ashes to the environment, voltammetric procedures of its quantification in water extracts from ashes were elaborated. For this purpose two approaches were undertaken:

- adaptation of a well-known catalytic adsorptive stripping voltammetric (CAdSV) method of the determination of Cr(VI) in the presence of diethylenetriaminepentaacetic acid (DTPA) and nitrate ions [1].
- implementation of a metallic film electrode for the quantification of Cr(VI) exploiting its reduction to Cr(III) in strongly or moderately acidic solutions.

An example of the quantification of Cr(VI) in the extract from the selected fly ash is shown in Fig. 1.

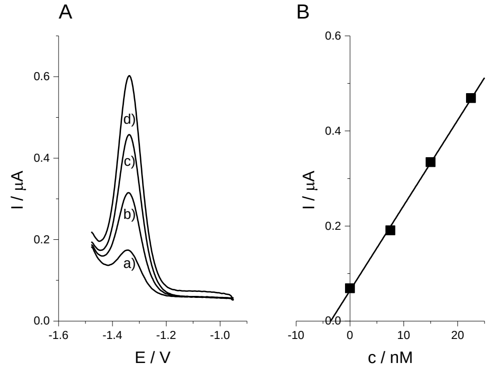

Figure 1. A. DP-CAdSV curves recorded in fly ash extract without (a) and after Cr(VI) standard additions (b-d). Examined solution: sample diluted 400 times, 0.1 M acetic buffer, 0.025 M DTPA and 0.25 M KNO_3. E_{acc} = -1.2 V for 30 s. B. Standard addition plot.

The amounts of Cr(VI) determined in the extracts of various fly ashes ranged from 50 to 100 ppb in the presence of a comparable concentration of Cr(III). The above results were validated by means of the classical spectrometric method with diphenylcarbazide. During preliminary studies concerning the second approach the best voltammetric response was obtained at the ex-situ plated gold film electrode.

Financial support from the Polish National Science Centre (Project No. 011/01/B/ST8/07794) is gratefully acknowledged.

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MONOLITHIC STATIONARY PHASES FOR HYDROPHILIC INTERACTION CHROMATOGRAPHY

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Reversed-phase is the most commonly used system in the liquid chromatography, employing a non-polar stationary phase and polar mole phases. Hydrophilic interaction chromatography makes use of polar stationary and polar mobile phase. For micro liquid chromatography conventional columns filled with spherical particles or monolithic columns can be used. Monolith is formed by a single piece of highly porous material which contains flow pores. They can be either inorganic monolithic stationary phases or organic polymers. Organic monoliths were prepared by in-situ radical polymerization in fused silica capillaries filled by polymerization mixture, which contains a functional monomer, crosslinking monomer, porogenic solvents, and thermal initiator of polymerization reaction.

Monolithic capillary columns for hydrophilic interaction chromatography were prepared by using a polar functional monomer N,N-dimethyl-N-methacryloxyethyl-N-(3-sulfopropyl) ammonium betaine together with seven different crosslinking monomers: ethylene dimethacrylate, tetramethylene dimethacrylate, hexamethylene dimethacrylate, dioxyethylene dimethacrylate, pentaerythritole triacrylate, bisphenol A dimethacrylate, and bisphenol A glycerolate dimethacrylate, with porogenic solvents: 1-propanol, 1,4-butanediol, and water and with azobisisobutyronitrile as a initiator of polymerization reaction.

The effect of crosslinking monomers on the efficiency was determined from van Deemter plots. Columns prepared with dioxyethylene dimethacrylate and bisphenol A glycerolate dimethacrylate showed efficiency up to 70 000 theoretical plates/m. These columns provide good run-to-run and batch-to-batch repeatability of the elution volumes with relative standard deviation of 1.3 % or lower on both columns. The columns provided a dual retention mechanism and were used for isocratic separation of model mixture of phenolic compounds both in acetonitrile-rich mobile phases in HILIC mode and in the mobile phases with higher concentrations of water in the reversed-phase mode.

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DETERMINATION OF FATTY ALCOHOL ETHOXYLATES IN THE ELBE AND CHRUDIMKA RIVERS

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Fatty alcohol ethoxylates (FAEs) belong to a group of nonionic surfactants. They are composed of alkyl chain (hydrophobic tail) and ethoxylate chain (hydrophilic head). The most commonly used FAEs contain carbon chain with an average length of carbon chain 12 – 18 C atoms and with an average number of ethoxy units 0 - 18. Alcohol ethoxylates are manufactured by the reaction between aliphatic alcohol and ethylene oxide. This reaction is catalysed by sodium hydroxide or potassium hydroxide. [1, 2]

FAEs are widely used as substitution for highly toxic nonylphenol ethoxylates. They are often used in laundry detergents, cleaning agents, cosmetics, herbicides etc. Fatty alcohol ethoxylates toxicity was tested on water organisms for example daphnia magna, algea, fish and after these tests, their water toxicity was setted as relatively high, but lower than toxicity of nonyl ethoxylates. That is why it is important to control FAEs concentration in the water. [3]

In this work we have analysed samples from the rivers Elbe and Chrudimka. Solid phase extraction was used to extract FAEs from water samples. Octadecyl silica gel based sorbent and the mixture of methanol:dichlormethane (9:1 (v/v)) as the elution solvent were used. After extraction step the samples were derivatized using phenyl isothiocyanate reagent with addition of triethylamine as the catalyst. Derivatives were separated by reversed phase liquid chromatography with gradient elution and detected with UV-VIS detector at 280 nm.

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INFLUENCE OF INITIATOR ON THE STRUCTURE OF POLY(GLYCIDYL METHACRYLATE) MONOLITHS

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Monoliths with high level of porosity and interconnected structure can be prepared using a wide variety of techniques. One of the most established techniques is the polymerisation of high internal phase emulsion (HIPE), where the internal phase exceeds 74 % of the total emulsion volume [1].

Among other applications, polyHIPEs can be used in chromatography [2-5]. Especially interesting are polyHIPEs prepared from glycidyl methacrylate (GMA), which is a reactive monomer and could be further functionalized. With optimized morphology of GMA-based polyHIPEs, the use in chromatography could even expand.

In this study, type of initiation and initiator concentration proved to be an important factors regarding resulting polyHIPE morphology. Depending upon the used initiator, the morphology resulted in either the formation of small and interconnected pores or big pores, which were rather closed. Surface area evaluation of resulting polymers was done by nitrogen adsorption / desorption. Typical polyHIPE morphology was determined using scanning electron microscopy.

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COMPARISON OF THE SEPARATION PROPERTIES OF DIOL BASED COLUMNS

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The effect of the mobile phase composition on the retention of phenolic compounds and derivatives of phthalic acid was investigated on three different diol-based stationary phases. All showed dual retention mechanism, HILIC at highly-organic while RP in highly-aqueous mobile phase. Experimental data were described by a four parameter equation, which involves contribution of both HILIC and RP mechanisms [1]:

$$\log k = a + m_{RP} \cdot \varphi_{H2O} - m_{HILIC} \cdot \log(1 + b \cdot \varphi_{H2O}) \qquad (1)$$

The range of mobile phase, where HILIC conditions predominates was compared between columns. The separation selectivity was determined by calculating the separation factors, α, which signify the relation of the retention factors of phenolic acids to the retention factor of 4-hydroxyphenylacetic acid and the retention factors of flavonoids to the retention factor of flavone in the HILIC mode. The results were then compared between individual columns. Columns with simply bonded glycerol groups, YMC-Triart Diol HILIC and LiChrospher Diol showed higher retention, due to stronger polar interactions of solutes with stationary phase, and better selectivity than Luna HILIC with crosslinked oxyethylene-hydroxy groups.

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INVESTIGATION OF VARIOUS SEPARATION MECHANISMS IN ION-CHROMATOGRAPHY

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Ion-exchange chromatography is becoming an often applied analytical method in determination of biogenic amines because of its simplicity, sensitivity, selectivity and speed [1, 2]. While measuring retention times of most common biogenic amines present in food [3], we observed strong affinity of 2-phenylmetylamine and tryptamine to the stationary phase. The results obtained by log-log plots could not be explained by pure ion-exchange interaction. Even though the applied cation-exchange stationary phase was designed to prevent hydrophobic interactions [4], observed outcomes indicate presence of additional interaction that governs separation.

Therefore the aim of our research was to isolate the individual separation mechanisms to enable their identification. Modifications of the separation conditions were tested, which eliminates individual interaction between analytes and stationary phase, that is, the addition of organic solvents would prevent possible hydrophobic interactions.

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COULOMETRIC SEPARATION OF CHLORIDE BEFORE ANION DETERMINATION WITH ION CHROMATOGRAPHY

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Anion chromatography is widely used for anion determination in biological samples. When determining anions in trace amounts such as oxalate in urine, blood serum or sea water, the much higher concentration of matrix anion such as chloride can interfere with retention. It was found that high concentration of matrix anion which elutes prior to analyte can increase retention times due to self-elution effect and on-column changes in eluent composition [1].

Current methods for chloride removal such as precipitation of silver chloride with silver nitrate, silver acetate or silver oxide or using cation-exchange column with silver cations can cause blockage of separation column with colloidal silver chloride [1, 2], introduction of another interfering anion or dilution of sample [3]. Coulometric formation of silver cations and precipitation of silver chloride on porous silver anode was suggested previously as an appropriate matrix separation method [3].

To increase the electrical current and consequently, the speed of separation, high ratio between electrode area and electrochemical cell volume is desired. The foregoing was achieved in two ways using flow-through cell packed with silver micro wires and silver nanoparticles. Both types of working electrode were tested. Flow rate through the cell and potential of electrolysis were optimized in buffers that are suitable as mobile phase for ion chromatography (borate, hydrogen carbonate/carbonate). The problems with electrocrystallization of silver chloride, formation of colloidal silver chloride and formation of silver oxide were considered. The results and application on samples with high chloride concentration will be presented.

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COMPREHENSIVE ANALYSIS OF LIPIDS IN SAMPLES OF CVD PATIENTS

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Lipids include diverse range of compounds like fatty acids and their derivatives, cholesterol, bile acids, etc. They serve as a source of energy, building blocks of cell membrane, hormones, etc. Due to their important role in human organism, their dysregulation or unbalance could be reason of onset of some pathological state like cardiovascular diseases (CVD), cancer or Alzheimer disease.

Methods with a single internal standard and response factors were used for the separation and quantitation of lipid classes. Polar lipid classes (phosphatidylethanolamines, phosphatidylcholines, sphingomyelines and lysophosphatidylcholines) were measured using hydrophilic interaction liquid chromatography in ultrahigh-performance liquid chromatography (UHPLC) setup coupled with electrospray ionization mass spectrometry. Normal-phase UHPLC coupled with atmospheric pressure chemical ionization mass spectrometry was used for the quantitation of nonpolar lipids (cholesteryl esters, triacylglycerols, cholesterol, diacylglycerols and monoaclyglycerols).

Matrix-assisted laser desorption/ionization mass spectrometry was used for fast measurement of lipidomic profiles in total lipid extracts of plasma and erythrocytes. Gas chromatography with flame ionization detection was used for the identification of fatty acid profiles. The comprehensive lipidomic profiles of CVD patients and healthy volunteers were obtained, however no significant differences were observed in the quantity of polar and nonpolar lipids.

The orthogonal two dimensional partial least square was used for the separation of 5 groups (healthy, obese and 3 types of CVD). The most important lipid molecules, which contribute to the separation of healthy group *vs.* groups of CVD patients in score plot graphs, were identified. The main goal of our study is find potential differences between CVD patients and healthy volunteers, which could be useful in better understanding of the role of lipids in the pathological state of organism and contribute to earlier diagnostic or treatment of CVD.

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ASPECTS OF SELECTIVITY IN LIPIDOMICS BY LC-MS ANALYSIS

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Lipidomics is a rapidly expanding research field that studies the metabolism of biological systems. The recognition of the role of lipids in many metabolic diseases is coupled with the rapid advances in the chemical analysis technology.

Besides various other techniques in complex lipid analysis, mass spectrometry has emerged as an indispensable tool for characterization, identification and quantitation of lipids, often coupled to electrospray ionization (ESI) as the ionization technique of choice. In addition, a variety of different chromatographic separation techniques has been developed to best analytical performance with respect to precision, accuracy and sensitivity. Thus, liquid chromatography coupled to mass spectrometry (LC-ESI/MS) based methods has emerged in the past decade, particularly as this setup is able to alleviate ion suppression effects in electrospray and allows also detection of less abundant lipids.

Compared to direct infusion systems, HPLC adds separation and retention time as further levels of selectivity resulting in increased specificity for lipid identification and quantitation. However, every recorded spectrum has still to be regarded as a single event with unique matrix effects and solvent composition. In the context of LC-MS analysis, these interferences are attributed to ion suppression effects.

Due to its sensitivity and selectivity, mass spectrometry occurs preferentially with ultra high mass resolution (mass resolution > 100 000) including fragment ion information (MS/MS), which is the method of choice for qualitative and quantitative lipidomic analysis. An adequate sample preparation technique including methods like solid phase extraction (SPE) or “simple” liquid-liquid extraction is often still necessary to additionally increase the selectivity of the analytical workflow especially in complex samples. Although it is not yet possible to detect and quantify all individual lipids in a given cellular system, the aim of lipidomic analysis is to determine correctly as many individual lipids as possible.

PILOT RESEARCH FOR EVALUATION OF INCIDENCES OF INBORN METABOLIC DISORDERS IN SLOVENIA

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Inborn errors of metabolism are rare; phenylketonuria has an incidence of 1:10,000, while most of the others are rarer [1]. In Slovenia we routinely screen for two inborn metabolic disorders, phenylketonuria and congenital hypothyroidism. In our pilot research we would like to expand the number of screened diseases with the use of tandem mass spectrometry (MS/MS). MS/MS is a method of choice with high selectivity and sensitivity and allows us to screen for several disorders in the one run (less than 2 minutes) [2]. To screen for disorders quantification of different acylcarnitines and amino acids in dried blood spots is performed. A specific deviation of one or more metabolites from the normal concentration range is a sign of a possible metabolic disorder. In such cases further conformational tests are needed. One patient with an abnormal concentration of 3-hydroxyisovaleryl carnitine (C5OH) has already been detected. C5OH is a metabolite that is associated with different metabolic disorders and to confirm or reject the possible diagnosis additional tests are needed [3]. First will be the measurement of organic acids in urine by gas chromatography, coupled with mass spectrometry. Further genetic testing and/or determination of enzyme activity will be necessary.

Our research will be the first to evaluate the incidences of inborn metabolic disorders in Slovenia. It will help in planning the expansion of screened metabolic disorders in Slovenia.

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COMPREHENSIVE TWO-DIMENSIONAL LIQUID CHROMATOGRAPHY – MASS SPECTROMETRY FOR LIPIDOMIC ANALYSIS

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Lipids have numerous important functions in cells, tissues and body fluids, such as the formation of lipid bilayer, cell signaling, energy storage, etc. Lipidomics is a subset of metabolomics, which is aimed on the complex analysis of cellular lipid molecules isolated from cells, tissues or biological fluids and their biological roles with respect to health and disease states. Lipidomics contribute to the understanding how lipids work in a biological system (cellular physiology and pathology) [1]. One part of this work is focused on off-line two-dimensional liquid chromatography - mass spectrometry (2D-LC/MS) analysis of plasma samples, where the total lipid extract of plasma was separated into individual fractions of polar and nonpolar lipid classes. In the first dimension, 6 classes of polar lipids and 3 classes of nonpolar lipids were isolated by hydrophilic liquid chromatography (HILIC), where compounds are separated according to their polarity. Individual fractions were subsequently measured in the second dimension by reversed-phase high-performance liquid chromatography (RP-HPLC), where the polar lipids are separated according to the acyl chain length and the number of double bonds. Nonpolar lipid fractions are separated according to the value of an equivalent carbon number [2]. Another part of this work is focused on the development of on-line two-dimensional ultra high-performance liquid chromatography mass - spectrometry (2D-UHPLC/MS) method for the analysis of lipids. For this purpose, RP-LC mode is used in the first dimension, while HILIC is used in the second dimension of comprehensive 2D-LC/MS setup. Lipids were identified from extract of plasma sample using this comprehensive on-line 2D-UHPLC with ESI-MS in positive ion mode.

This work was supported by ERC CZ grant project LL1302 (Ministry of Education, Youth and Sports of the Czech Republic).

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A GREEN METHOD FOR THE DETERMINATION OF CAPSAICINOIDS FROM CHILLI PEPPERS

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Chilli pepper is the fruit of plants from the genus *Capsicum* containing a group of pungent chemical analogues – capsaicinoids. The main aim of this work was an introduction of Pressurised Hot Water Extraction (PHWE) as a method that fills up the principles of green analytical chemistry. As an extract reagent, hot water under high pressure is used. PHWE was employed for an extraction of the capsaicinoids from the chilli peppers. At first, PHWE was optimised for extraction time and extraction temperature. A central composite experimental design was used in the optimisation of the extraction conditions. The amount of extracted capsaicinoids showed the optimal extraction at temperature of 200 °C and extraction time of 10 + 20 minutes. Separation, identification and quantification of four capsaicinoids (capsaicin, dihydrocapsaicin, nordihydrocapsaicin and nonivamide) were performed using Reversed Phase High Performance Liquid Chromatography with Mass Spectrometry (RP-HPLC/MS).

CHARACTERIZATION AND QUANTIFICATION OF (POLY)PHENOLS IN *SAMBUCUS NIGRA* L. INFUSIONS USING MEKC AND LC-MS/MS

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Elderberries are rich in flavonols, phenolic acids, anthocyanins, carotenoids, vitamins and minerals [1]. Bioactive compounds from elderberries have potent antioxidant, anticancer, antimicrobial and anti-inflammatory properties [2]. Extracts of elderflowers are used in cold, fever and sinusitis [3]. They are used for their diuretic and perspiratory properties.

In this work, micellar electrokinetic chromatography and liquid chromatography were used for the characterization and quantification of phenolic acids and flavonoids in *Sambucus nigra* L. infusions. The aims of this work were to optimize the conditions of separation and to compare the results obtained using micellar electrokinetic chromatography and liquid chromatography-tandem mass spectrometry. Micellar electrokinetic chromatography was carried out in a non-coated fused silica capillary. Sodium decyl sulphate was used as a micellar agent. For the analysis of polyphenols, application of sodium decyl sulphate yielded better resolution than sodium dodecyl sulfate. Using sodium decyl sulfate, selectivity of the separation is also higher and time of the separation is lower [4]. The second method, liquid chromatography-tandem mass spectrometry, was based on separation in reversed-phase mode using octadecyl silica gel column packed with fused-core particles. The compounds were identified based on the multiple reactions monitoring of characteristic transitions in the mass spectra.

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ACID MINE DRAINAGE FROM AN ABANDONED GOLD MINE SITE

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Acid mine drainage (AMD) is a well-known environmental problem arising from both working and abandoned mines. This process happens when minerals, especially sulphide minerals, are exposed to environmental atmospheric or water oxidation. This oxidation causes sulphide ions to oxidise to sulphate ions whereby their generation causes water pH decrease, and therefore increases the releasing of toxic metals from a mine site. AMD can cause high concentrations of metals and other pollutants in water. The more common sulphide mineral used during the mining of valuable metals such as Cu, Pb, Zn or Au, is pyrite - FeS_2. The gold-bearing form of this mineral was used during mining activities at the biggest gold deposit in Bosnia and Herzegovina, the Bakovići mine.

The chemical parameters that were selected for the research and for determining the AMD process in water were: pH, electrical conductivity, red-ox potential, concentrations of sulphates, and the amounts of Fe, Al, Pb, Cd, As, and Cr. ICP –MS was used for the purposes of metal analyses, and chromatography for the water analysis of anions' ions. Additionally, standard parameters for water quality were measured for five samples taken from the River Gvožđanka, which passes the gold mine site, one sample of drinkable water - underground source, and three water samples that were drawn directly from the mine's body. The results showed that the River Govožđanka and water source were uncontaminated by AMD products, but the water from the mine's body was highly contaminated, especially by sulphates, iron, and aluminium.

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o-TOF-ICP-MS ANALYSIS OF PLATINUM IN ALGAE AND HOSPITAL WASTEWATER

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Platinum is a very resistant precious element, which can be found as isolated metal, in alloys (with Ir, Rh, Ru etc.) and in various industrial applications. Platinum and its compounds caused „platinosis“ (excitement, oversensitivity – rash, nasopharyngitis, photophobia). A very important application area represents platinum cytostatics (cisplatinum, carboplatinum), which are widely used to treat cancer. These cytostatics are mutagenic and are regarded as suspected of carcinogenicity in humans. Platinum complexes are also considered as indicators of wastewater and surface water pollution. A pollution of wastewaters coming from various hospital workplaces is largely removed in a wastewater treatment plant. Anthropogenic Pt enters into water ecosystems and can be accumulated in river plants, organisms and sediments. For analysis of platinum classical methods (chelatometry, gravimetry) or instrumental methods as atomic absorption spectrometry, spectrophotometry or electrochemical methods can be used. The most frequently used methods are ICP-MS, ICP-OES and ET-AAS.

Our study was dedicated to bioaccumulation experiments and related analytical methods for determination of platinum in algae. Algae (*Chlorella kessleri*) were cultured (30 days) in a growth medium with the addition of platinum (the final concentration 100 μg·l^{-1}) and in hospital wastewater. Algae were centrifuged, washed, dried and decomposed (the microwave oven MWS-2, Berghof, Germany; nitric acid). Simple and reliable ICP-MS and ICP-OES methods for the processing and determination of platinum in algae were developed. Three isotopes of Pt ($^{194\,195\,196}$ Pt, LODs 0.0241; 0.0249; 0.0338 μg·l^{-1}) were monitored by the ICP-MS (Optimass 9000, GBC Australia) using internal standard Rh (10 μg·l^{-1}). For the ICP-OES analysis (Integra XL2, GBC, Australia) the spectral line 214.42 nm was used (LOD was 11.90 μg.l^{-1}). The repeatability was comparable for the ICP-MS and ICP-OES; the ICP-OES seemed to be easier and more laboratory comfortable. The accumulated Pt in algea was estimated (21 - 47 % of the originally added amount). Contamination problems during the bioaccumulation experiment as well problems connected with a small sample preparation were solved.

APPLICATION OF LASER ABLATION ICP-MS DEPTH PROFILING METHODS FOR THE STUDY OF ANCIENT GLASS ARTEFACTS

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The analysis of archaeological glass is often challenging because of the occurrence of physical and/or chemical damage to the surface of the artefact. In particular, chemical damage as a result of long-time exposure to adverse conditions may have led to corrosion of the artefact's surface. Although LA-ICP-MS is able to remove superficial layers by performing pre-ablation passes, severe degradation of the surface, which is often not evident even with microscopic inspection, may lead to inaccurate bulk analytical data if undegraded glass has not been reached. LA-ICP-MS in line-scanning mode usually leads to retrieval of elemental data from a depth of between 1-2 μm and is thus not the appropriate tool to retrieve bulk elemental information from severely degraded glass.

In this study the focus is on understanding the merits of two depth profiling procedures (single/multiple spot drilling) and their results investigated by drilling different artifacts. The drilling approach by single spot was developed and well discussed by Van Elteren et al., 2013 [1] for the study of corroded artifacts by multi-elemental 3D mapping. The procedure in a single point is based on 50 laser pulses per point at a pulse rate of 1 Hz and it is useful to investigate the top surface layer of the glass (ca. 5 μm). The shallow depth and the time consuming by this method are not the appropriate tools to retrieve bulk elemental information from degraded glasses. This method was improved with the multi spot drilling which is based on 50 or 100 laser pulses per point at a pulse rate of 10 Hz to retrieve information from deeper layers (ca. 50 μm), to obtain a depth profile of the glass and an estimation of the bulk composition not affected by the degradation.

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MATRIX MODIFICATION FOR OVERCOMING THE SPECTRAL EFFECTS DURING oTOF-ICP-MS ANALYSIS OF SULFURIC ACID

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Direct multi-element analysis of sulfuric acid by inductively coupled plasma mass spectrometry (ICP-MS) using a low resolving power instrumentation is strongly complicated especially due to the spectral effects from different polyatomic ions. For the quadrupole based mass spectrometers being the most widely used in analytical practice a collision/reaction cell technology enables to overcome these problems. To this date, however no method is available enabling analysis of diluted sulfuric acid using inductively coupled plasma orthogonal acceleration time-of-flight mass spectrometry (ICP-oa-TOF-MS). For this purpose, a simple technique employing barium salt for precipitation of sulfates as $BaSO_4$ prior to analysis by ICP-oa-TOF-MS was introduced in this work. Matrix modification [1] resulting in the separation of sulfates enables the elimination of spectral interferences originating from different sulfur containing species like $^{32}S^{16}O^+$, $^{32}S^{16}O^1H^+$, $^{32}S_2^+$, $^{32}S^{16}O_2{}^1H^+$, $^{34}S^{16}O_3^+$, which hamper the determination of $^{48}Ti^+$, $^{49}Ti^+$, $^{64}Zn^+$, $^{65}Cu^+$ and $^{82}Se^+$. After that, direct and simultaneous determination of 16 elements (Be, Ti, V, Cr, Mn, Ni, Co, Cu, Zn, Ga, Ge, As, Sb, Te, W, Re) can be performed in 10% (w/w) H_2SO_4 with Rh as an internal standard and using external calibration with matrix matched standards. Accuracy and precision was confirmed by the analytical recovery study and by the comparison of the results with those obtained by high resolution ICP-MS method.

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ANALYSIS OF ESSENTIAL OILS IN HERBAL TEAS BY MEANS OF DISPERSIVE LIQUID – LIQUID MICROEXTRACTION METHOD

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This work deals with the optimization and the application of two microextraction methods for isolation of essentials oils in herbal teas. These two approaches are Dispersive Liquid-Liquid Microextraction (DLLME) and Dispersive Liquid-Liquid Microextraction Based on the Solidification of Floating Organic Drop (DLLME-SFO).

Based on the preliminary experiments the solvent systems (i.e. extraction and dispersive solvents) were selected. The optimizations of individual experimental conditions for both mentioned methods were performed with the use of orthogonal central composite design (CCD). Namely, volumes of both extraction and dispersive solvents, and sonication time, were optimised. Evaluation of optimal parameters was realised by the response surface modelling (RSM) approach where the desirability of individual parameters were tested.

The optimized procedures were applied for the extraction of essential oils from real herbal tea samples. The analytical separation was performed with the usage of gas chromatography with the flame ionization detector. The results obtained by these methods were compared. Moreover, both tested extraction methods were compared to each other as such. This comparison included the method applicability, compatibility with the analysis of essential oils, and consumption of environmentally not-friendly chemicals.

DETERMINATION OF THE CONTENT OF ESSENTIAL FATTY ACIDS IN EDTA PLASMA TYPE 2 DIABETICS

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This study examines the composition dependence of essential fatty acids in EDTA plasma of type 2 diabetes on the degree of glycemic expressed by the concentration of glycated hemoglobin (HbA1c). The main objective of this pilot study is to contribute to the development of diabetes diagnosis and expand knowledge of the pathogenesis of this disease.

Lipid extracts from deproteinated plasma samples were separated by preparative thin-layer chromatography into five fractions (phospholipids, diacylglycerols, free fatty acids, triglycerides and cholesterol esters). All fractions were isolated and after the addition of internal standard (cis-13,16,19-docosatrienoic acid, concentration 10 µg / ml) hydrolyzed and converted to corresponding methyl esters of fatty acids. Thus prepared samples were analyzed using a gas chromatograph. Thirty-seven anonymized plasma samples randomly selected type 2 diabetic patients were processed in this study. These samples of biological material were also used for verification of analytical method. Furthermore, there were used 27 healthy blood donors plasma samples as a control group. For purposes of the study, samples were categorized into three groups according to level of glycosidic hemoglobin (HbA1c). This indicator appears to be most reliable because it is affected by poor conditions (such as non fasting) prior to collection, and highlights the development of blood glucose in the last 4 to 6 weeks.

For studied diabetic patients was found to decrease the concentration of essential fatty acids in dependence to the increasing concentration of HbA1c. Besides, it was found to increase in diabetics concentration of saturated fatty acids depending on the increasing concentration of HbA1c. As previously described lipotoxicity saturated fatty acids can be found changes in the plasma concentrations of acids give rise to insulin resistance and the consequential metabolic complications leading to the development of metabolic syndrome followed by type 2 diabetes.

THE DYNAMICS OF HIGHER ALCOHOL AND ESTER FORMATION IN FERMENTED BEVERAGES FROM BARLEY, QUINOA AND BUCKWHEAT MALT

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The purpose of this work was to develop and validate the GC method for determining higher alcohols and esters in beer and gluten-free beer-like beverages, as a function of raw material and successive fermentation. Higher alcohols and esters are mainly by-products of the fermentation process and contribute to the beers' flavours in both positive and negative senses. Some important higher alcohols were analysed: methanol, 1-propanol, isobutanol, 2-methylbutanol, 3-methylbutanol, and 2-phenylethanol. In addition some important esters were determined such as: ethyl acetate, isoamyl acetate and 2-phenylethyl acetate. All these compounds, together with acetaldehyde, form the common set of volatile compounds that are regularly observed during beer analysis. In addition, we also tried to determine two vicinal diketones, i.e. 2,3-butanedione (diacetyl) and 2,3-pentanedione and one aldehyde *trans*-2-nonenal, which are very important representatives of beer aroma. Finally, the method was used for following the content of all the mentioned volatile compounds in wort and beer prepared from different raw materials (barley, buckwheat, and quinoa) and each of them fermented successively eleven times.

The results showed that both the raw material and successive fermentation influenced the final concentrations of the volatile substances, as well as the profiles of their production during fermentation. For buckwheat, differences in regard to barley were not so significant that they would essentially affect the quality of the final product. On the other hand, the quinoa beverage deviated from a typical barley beer substantially and for this reason it could not simply be used as a gluten-free substitute for barley beer. The yeast used in all the experiments (*S. pastorianus* TUM 34/70) was, in terms of volatile compounds, proved to be suitable for the sequential fermentation of barley, buckwheat, and quinoa wort.

GAS CHROMATOGRAPHIC METHODS FOR ANALYSIS OF PERFUMES

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Nowadays, perfumes are produced from natural or synthetic substances. The most of perfumes contain a lot of compounds. This research deals with the analysis of volatile organic compounds in natural perfumes such as Praga Alchymica, which is produced by Rafaella. Rose Taif and Rose Josefina are additional samples. There are the starting materials for the manufacture of perfumes. For analysis of volatile substances headspace and gas chromatography-mass spectrometry (GC/MS) have been used as these are frequently used methods for perfume analysis.

The results indicate that nature of pure perfume like Rose Natura and Rose Taif has different compounds without 1-linalool as both of them have different smells. Moreover, on the aforementioned basis such information can be used for determination of basic compounds in mixed perfume like Rose Josefina. The same substances from Rose Taifa and other aromas were measured in this perfume. Praga Archnica was mixed from Rose nature and unknown flavor. This research also proved that for small amount of samples it is better to use GC/MS compared to headspace GC. Research will also entertain using "heart-cut" MDGC system with using chiral columns in the second dimension.

PRIMARY AND SECONDARY CARBONACEOUS SPECIES IN ATMOSPHERIC FINE PARTICLES IN THE VENETO REGION, ITALY

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Airborn carbonaceous particulate matter is classified into two main types, i.e. elemental carbon (EC) and organic carbon (OC). EC is primary pollutants released from the incomplete combustion of carbon-containing fuels, while OC may be emitted directly from sources (primary OC) or derive from chemical transformation of volatile organic compounds (VOC) as secondary OC. Secondary organic aerosol (SOA) was found to account for 85% of particulate organic matter in the warm season and 25-28% of the $PM_{2.5}$ mass in an important district of the Po Valley, Milan [1]. Therefore, both primary and secondary OC are important fractions of carbonaceous particulate matter. Organic and elemental carbon concentrations were examined from April 2012 to February 2013 at six provinces in the Veneto region, to determine the secondary organic carbon (SOC) in order to understand the contribution of SOC to the total organic carbon (TC). Sixty samples per station were collected for analyses in every alternate month (April, June, August, October, December and February): 10 samples per station in 10 consecutive days of the months selected. The OC concentration ranged from 0.98 $\mu g\ m^{-3}$ to 22.34 $\mu g\ m^{-3}$, while the mean value was 5.48 $\mu g\ m^{-3}$, contributing almost 22% to the total $PM_{2.5}$ and 81% of the total carbon. EC concentrations fluctuated from 0.19 to 11.90 $\mu g\ m^{-3}$ with a mean value of 1.31 $\mu g\ m^{-3}$, contributing for 5 % of the total $PM_{2.5}$ and 19 % to the total carbon. The monthly OC concentration gradually increased from April to December, but EC remained rather constant during the warm months. Although there were concentration differences in OC among the stations, these were not statistically significant as confirmed by Kruskal–Wallis one-way analysis of variance test. The OC/EC ratios ranged between 0.71 to 15.38 with a mean value of 4.54, which is higher than the values observed in most of the other European cities. Statistically significant correlations between EC and OC (r value less than 0.80) were found in all the months except October and December. The SOC was calculated from the EC tracer method. Based on EC/OC minimum ratio, the secondary organic carbon (SOC) contributed for 65 % of the total organic carbon during the study period, while SOC for 56 % of the total OC as evaluated by a by regression analysis. The contribution of the secondary fraction to the TC was higher during the colder months compared to the warmer ones, likely as a consequence of a lower temperature and stable conditions favoring the accumulation of pollutants and the condensation or nucleation of volatile organic compounds.

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MODELING OF SOME KEY PROPERTIES RELATED TO SECONDARY ORGANIC AEROSOL FORMATION

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Secondary organic aerosol (SOA), oxidized particulate organic matter formed by atmospheric transformation, comprises a large fraction of tropospheric aerosol (20-90% of aerosol mass in the lower troposphere) [1,2]. Because of the impact of atmospheric aerosol on health, visibility, and climate on the one hand and the large uncertainty in the formation and evolution of SOA on the other hand, further research is needed on both: experimental and theoretical part [3]. Quantitative structure-activity relationship (QSPR/QSAR) is important for evaluation and prediction of the key properties in SOA formation, since experimental measurements are not available. Especially suitable descriptors are topological indices because they are easily calculated, which is important when modelling large data set due to large computational time. At the same time these indices usually give good correlations with the modelled property.

For our work, we have created user friendly software MACI (Molecular Activity Characterization Indices) which offers creation and validation of models using variable connectivity indices. The key advantage of the selected indices is possibility of structural interpretation, which enables better understanding of mechanism that governs modelled property [4-6]. MACI will be freely available for research purposes. Here we present several developed models for the prediction of some key properties related to SOA formation: atmospheric reaction rates of volatile organic compounds with hydroxyl radical, vapour pressure and the octanol-air partition coefficient K_{OA}.

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University
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Since its founding in 1950, the Faculty of Chemical Technology, University of Pardubice, has become a renowned institution of higher education in a variety of chemistry related areas. At present, the Faculty provides courses leading to Bachelor, Master and Doctoral degrees.

The backbone of the study programme is represented by the two-level five-year Master degree course in Chemistry and Technical Chemistry. The students of the first level cover the basic areas of technical chemistry such as general, inorganic, organic and analytical chemistry; mathematics; physics; physical chemistry; computing; chemical engineering supplemented by the study of toxicology; ecology; and technically oriented foreign language training. The follow-up course extends the first level and students' knowledge. The students can also participate in a scientific research at the Faculty departments or gain the first experience in the leading companies in the country or abroad. The offered specialisations are: Inorganic and Bioinorganic Chemistry, Inorganic Technology, Chemical Technology of Paper and Pulp, Chemical Engineering, Material Engineering, Environment Protection, Organic Chemistry, Economics and Management of Chemistry and Foodstuff Industries, Process Control, Technical Physical and Analytical Chemistry, Technology of Organic Specialities, Technology of Polymers Manufacturing and Processing, Theory and Technology of Explosives, Fibres and Textile Chemistry, Environmental Engineering. The second level is concluded by the defence of the diploma thesis and the Final State Examination leading to the Master degree (Ing.).

Another five-year course in Chemistry and Technology of Foodstuffs offers the study specialisation in Evaluation and Analysis of Foodstuffs. Beside the subjects of technical chemistry and language training, the first study level comprises general and foodstuffs microbiology, biochemistry, and the basis of food-processing technologies. The advanced programme offers subjects such as food analysis and enables the students to become acquainted with the standard methods of food assessment, trace analysis of the food chain using modern instrumental methods, and computing.

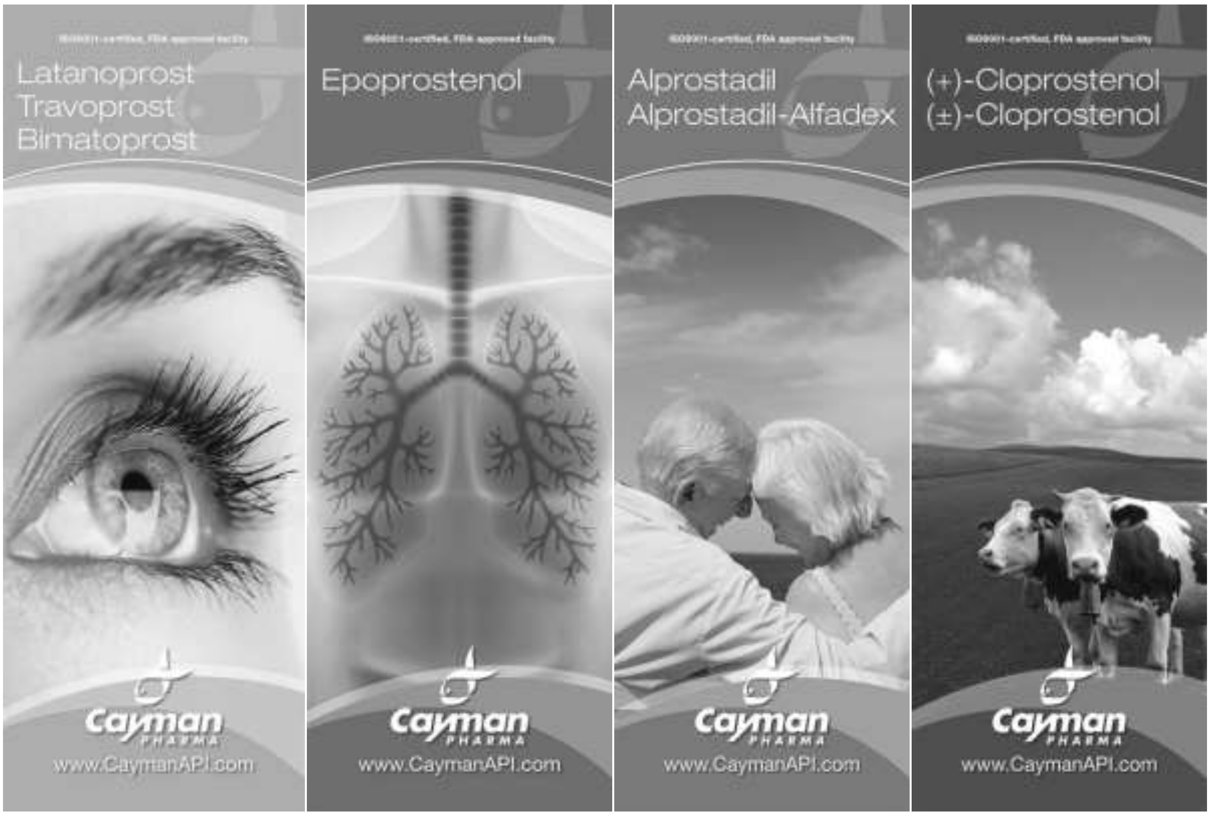
Master study course in the Special Chemical and Biological Programmes consists in the first study level of the specialisation in Clinical Biology and Chemistry. The course comprises - besides the chemistry-oriented subjects and mathematics - biostatistics, physics, computing, general and clinical biochemistry, general biology, physiology, general microbiology, genetics, immunology, toxicology and medical information technology. The course leads to the Bachelor degree (Bc.) and is followed by the second level course in Analysis of Biological Materials extending the students' knowledge of clinical biology and chemistry and leading to the Magistr (Master - Mgr.) degree.

The Faculty as the only one in the Czech Republic offers higher education in the field of Graphic Arts, both in the Bachelor, and Master degree courses. Graduates of the three-year Bachelor programme are knowledgeable in printing techniques and materials; they are able to use computer techniques for pre-printing operations, electronic publishing and multimedia communication. Acquired knowledge can be extended in the follow-up two-year Master course that prepares students for both managing positions in the large companies, and private entrepreneurship, too.

The three-year Bachelor study programme in Chemical and Process Engineering specialising in Chemical Process Control is also taught on the basis of special needs of the chemical industry. The graduates assert themselves as a middle company management and technical workers in plants of chemical, pharmaceutical and food industry. They can also continue their study in some of the two-year Master courses in Chemistry and Technical Chemistry.

After the Master courses, the successful graduates can continue their studies in the three-year postgraduate Doctoral courses leading to the PhD. degree. The Doctoral study programmes, which are closely connected to Chemistry and Technical Chemistry courses, progressively extend the gained knowledge and put a stress on the independent research activities. It is common that a part of the Doctoral studies can be carried out at one of the well-known universities abroad in close co-operation with the Faculty and its research laboratories. The scientific activities of the Faculty aim at both elementary and technological research. The postgraduate Doctoral programmes are consequently focused on the following fields: Inorganic Chemistry, Organic Chemistry, Analytical Chemistry, Physical Chemistry, Inorganic Technology, Organic Technology, Technology of Polymers, Chemistry and Technology of Inorganic Materials, Chemical Engineering, Technical Cybernetics, Economics and Management and Applied and Landscape Ecology.

A number of successful technical projects were completed in co-operation with the industrial sector and a wide range of scientific papers was published and met with an excellent scientific response. The growing reputation of the Faculty is also indicated by many international conferences and congresses held at the University every year. The Joint Laboratory of Solid State Chemistry of the Academy of Sciences of the Czech Republic and the University of Pardubice, the Research Centre of New and Perspective Inorganic Compounds and Materials, as well as the shared laboratories at other research institutions and the Pardubice Hospital also contribute to the high reputation of the Faculty.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SYSTEM FOR DETECTION OF PRESENCE OF LEAKAGE OF OILS

DETECTOIL

DETECTOIL is a unique device for detecting and monitoring the presence of oils and related liquids on the surfaces of waters. It is applicable in various branches of industry (power plants, wastewater purification stations), in oil separators, in care of environment, etc., for control and security purposes.

DESCRIPTION

The system consists of a sensor (size 70x70x30 mm) and of a measuring unit (size 220x50x150 mm) fed by 12 V from a voltage source (either d. c. from a battery or a. c. from a transformer), with an output for connection to a signalling unit (bell, buzzer, light) or to a regulation, recording or other systems.

The principle of the device allows a reliable operation with practically no maintenance. Its installation is simple and can be carried out even in media threatened by risk of explosion. With the small dimensions of the sensor the detector can be installed even in wells, drill holes or side-branch pipes.

Basic technical data

220 V; 3.5 mA a. c. (or from car battery 12 V; 70 mA d. c.); gross weight 1.9 kg.

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