

UNIVERZITA PAVLA JOZEFA ŠAFÁRIKA V KOŠICIACH

# Book of Abstracts NEW TRENDS IN CHEMISTRY

Trends in chemistry, research and education  
at Faculty of Sciences of P.J. Šafárik University Košice

Edited by: Renáta Oriňaková



Faculty of Sciences

Košice 2016



# BOOK OF ABSTRACTS

## NEW TRENDS IN CHEMISTRY

**Trends in chemistry, research and education at Faculty of  
Sciences of P.J. Šafárik University Košice**

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## Analytical Chemistry and Nanomaterials

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Unique and advantageous properties of different nanomaterials are frequently used in many areas of technology and daily life including methods and procedures of analytical chemistry. Nanoparticles of metals, nanorods and nanotubes, fullerenes, and quantum dots help analytical chemistry at an improvement of selectivity and sensitivity of wide spectrum of methods for theseparation, detection and determination of number of analytes of chemical, clinical, pharmaceutical, environmental and technological interest [1, 2]. Examples will be given and evaluated with special attention devoted to bioanalytical chemistry and biosensors.

Two main aspects of the basic analytical chemistry research are typically considered:

- a) how nanoparticles can be used to improve analytical procedures,
- b) how to purify, characterize and detect nanoparticles in industrial bulk materials as well as in complex matrices such as environmental and biological samples.

The needs of analytical chemistry towards nanotechnology have been also indicated:

- a) to make reproducible nanomaterials for analysis, it is critical to be able to perform analyses at the nm scale,
- b) new tools for analyzing targets in living cells and even in whole animals [3].

On the other hand, nanotechnology and engineered nanomaterials require from the analytical chemistry correlation between results on for geometry and interface, interpretation on a nanoscale, and identical information obtained by individual techniques. Together with the nanotechnology advantages, methodologies for nanomaterials analysis in environment and risk assessment are subject of great interest [4, 5]. New knowledge is required regarding particularly on nanometrology, dispersion, sampling and sample handling, fractionation by ultrafiltration, nanofiltration and dialysis, difference in analysis of particulate and nanoparticulate assemblages compared to conventional analysis of solutes, and validation, measurement uncertainty as well as good laboratory practices [6]. Methods of their evaluation will be mentioned including tests based on interactions with biomolecules such as DNA and enzymes. As far to DNA damage, the comet assay is the most widely utilized method together with, plasmid nicking/agarose gel electrophoresis assay, alkaline precipitation assay and gas chromatography/mass spectrometry (GC/MS) or liquid chromatography/mass spectrometry (LC/MS) [7]. Among bioanalytical tools, DNA-based biosensors have been numerously demonstrated as effective warning devices for the tests of DNA affinity interactions with drugs and chemicals as well as the tests of effects prooxidants and UV light on DNA. Our results on the investigation of quantum dots and metallic nanomaterials regarding an influence the yield of UV irradiation [8] will be reported as well.

### Acknowledgements:

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## Automated Particles Micromanipulation using Holographic Optical Tweezers

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### Micromanipulation exploiting the focussed laser traps

Optical trapping [1] exploits the balanced forces of a laser beam focussed to a microscopic particle. Optical tweezers is a device which controls the laser position pointed by the mouse or joysticks which subsequently moves the trapped particle in desired direction. Devices supplied with the SLM modulator based on the holographic principle are called Holographic Optical Tweezers (HOT). They split the laser beam into several individual ones, each trapping a particle controlled independently on others.

### Semi-automated and automated control of optical tweezers

The semi-automated control of multiple traps requires human navigation through special sensors (e.g. the cameras capturing the operator's fingertips and gaze [2] (Fig. 1 left). On the other hand, the fully automated manipulation requires image analysis where the proper algorithm detects all particles on the microscope image. Then algorithm selects the particle of interest, traps it by the focussed laser beam and moves it to the desired location avoiding obstacles (Fig. 1 right).

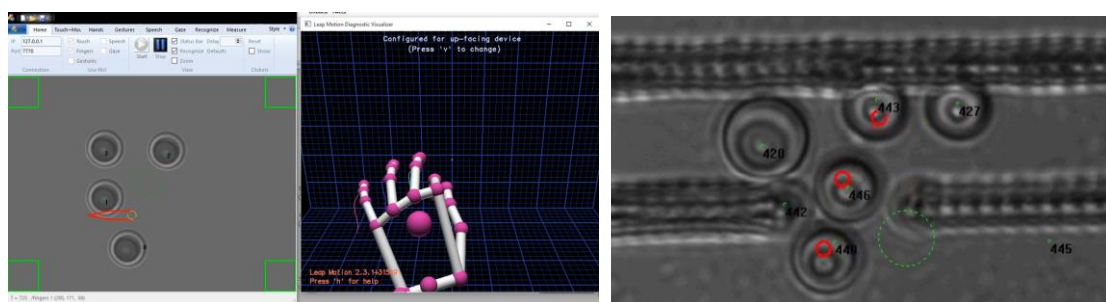


Fig. 1. Control of laser traps by fingertips (left) and movement of particles into sorting container (right).

### Automated cells sorting and analysis

The important application areas of HOT are the cells sorting as well as the analysis of compounds of biological origin. For sorting purposes, we manufactured 3D structures created by two-photon polymerization. They consist of "walls" bounding "containers" that serve as a storage site for particles. For the analysis purposes we tested a method where selected microobjects are measured by Raman spectroscopy or fluorescent technique. The selected particles are sequentially moved to the position where the green laser beam acquires spectrum. Humar et al. describe the construction of the cell lasers [3]. Two types of particles with different shape are present in the intracellular space - liquid crystal droplets or polystyrene microbeads. Depending on the microparticle shape either "cell lasing" or "whispering gallery modes" measurement is applied. It allows the intracellular screening of selected marker.

The proposed interface of HOT device makes possible the development of many interesting applications ranging from micromanipulation to micro/nano robotics [4].

### Acknowledgements:

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### Stereoselective Synthesis of 3-substituted Indolines

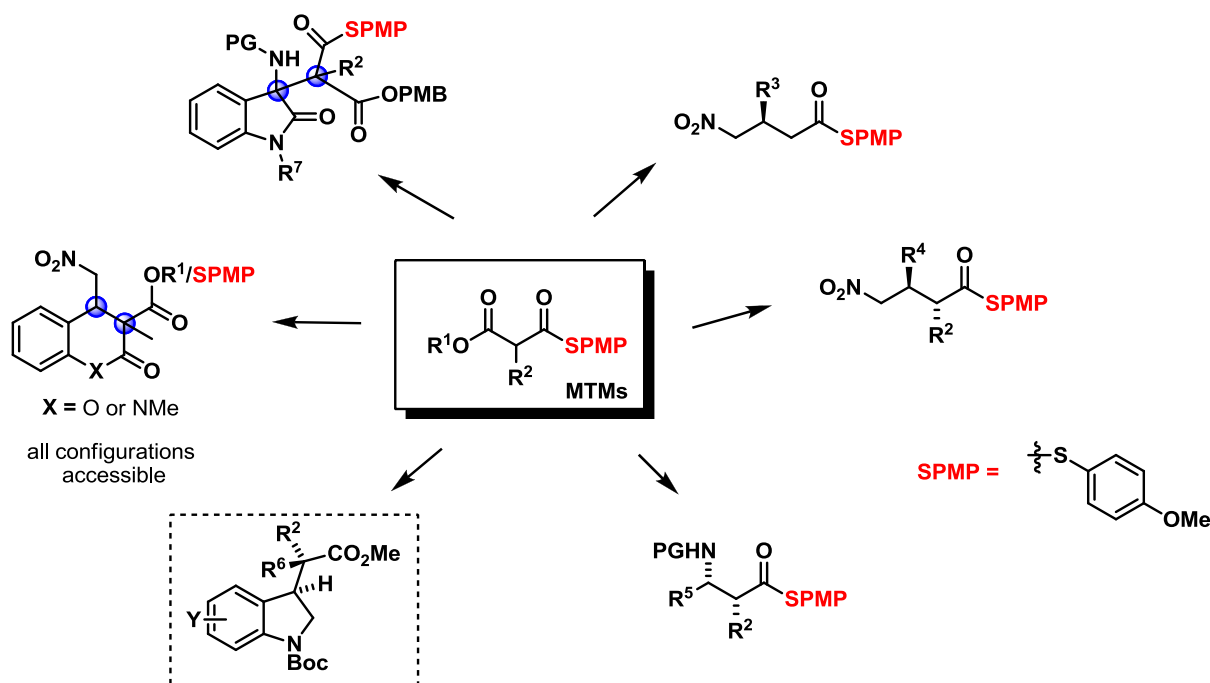
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In nature, malonic acid half-thioesters (MAHTs) serve as thioester enolate equivalents in the biosynthesis of fatty acids and polyketides.<sup>1</sup> The Wennemers group revealed that organocatalysts derived from cinchona alkaloids were suitable for MAHTs activation.<sup>2</sup> Recently Wennemers group introduced monothiomalonates (MTMs) as synthetically even better performing thioester enolate equivalents that allow for stereoselective addition reactions with electrophiles under organocatalytic conditions. In the presence of cinchona alkaloid derived catalysts (1-5 mol %), MTMs proved to be robust, yet readily reacting with a broad range of differently functionalized nitroolefins and imines.<sup>3</sup>



Our synthetic strategy leading to the marked 3-substituted indolines will be presented in detail.

#### Acknowledgements:

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**The use of Flow Cytometry in Testing the Biological Properties of Various Chemicals**

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Flow cytometry (FC) is a laser-based technology that is able to measure simultaneously several physical characteristics of single particles, usually cells. By this method is possible to test whole eukaryotic cells as well as isolated cellular structures such as organelles or prokaryotic cells. Depending on the type of flow cytometer, the particle size should be within range of 0.2 - 150  $\mu\text{m}$ . The individual particles are scanned as they flow in a liquid medium past an excitation light source, usually laser. Principal parameters which are measured in each particle are: size, inside granularity or complexity, and intensity of fluorescence. In addition to the described parameters, the newest machines are able to collect individual images of measured particles. It means that they are combination of both, the FC and fluorescent microscopy [1, 2]. The possibility to measure variety of biochemical, biophysical, and molecular aspects of individual particles within a sample makes this technique a unique and important tool for many scientific disciplines, particularly biological sciences. This technique is most frequently used for immunophenotyping (identification, characterization and quantification of cell subpopulations), discrimination of dead and live cells, identification of intracellular proteins, measuring the membrane potential, analysis of cell cycle kinetics, testing the metabolic activities of cells or analysis of apoptosis.

FC can be successfully used for the testing the biological activity of different chemicals. Biological activity describes the beneficial or adverse effects of a chemical on living matter. Among the various properties of chemical compounds, biological activity plays a crucial role since it suggests uses of the compounds in the medical applications. Mostly, in the first step, new chemicals are characterized by their influence on the growth of different micro-organisms. Subsequently, they are tested on cell or tissue cultures and only after detailed *in vitro* characterization, *in vivo* experiments on animals can be performed. In each of these steps, FC can help to receive precise characteristic of the compound. In the tests of the antimicrobial activity of chemicals, FC is used for counting and statement of viability of microbes. In cell cultures can be measured by FC the influence of chemical on metabolic activity of cells, kinetics of cell cycle, cell death or membrane potential. In the *in vivo* experiments are observed different parameters of immune response after administration of chemicals (phenotyping of immune cells, phagocytic activity, metabolic activity of cells, intracellular production of cytokines and others) or even an impact on host-associated microbial communities which is studied by the help of combination of FC with fluorescent *in situ* hybridization [3].

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**Wireless Technologies in Chemistry Laboratory**

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Latest wired and wireless datalogger solutions for chemistry laboratory developed by company Vernier Software and Technology. General Vernier datalogger system overview. Wired and wireless Vernier chemistry sensors and probes family. Standard (temperature, pH, ORP, conductivity...) and special chemistry sensors (ISE electrodes, colorimeters, spectrometers, gas chromatographs...) for chemistry laboratories. Wireless connectivity upgrade solutions for standard wired sensors. Data share, Wi-Fi and Bluetooth collaboration between Vernier datalogger system and computers and mobile devices (tablets, smartphones). Cooperation of Vernier equipment with various computer (Windows, Mac), mobile (iOS, Android) and Google Chromebook systems.

**References:**

[www.pmsdelta.sk](http://www.pmsdelta.sk)  
[www.vernier.com](http://www.vernier.com)

## What can we learn from Impedance Spectroscopy?

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### Impedance spectroscopy in electrochemistry

Measurement of electrical impedance is a kind of an instrumental method. Over years, with advances of electronics and instrumentation in general, the technique is often available through commercial instruments or add-on modules to such commercial instruments. Impedance, in its simplest form, is an electrical method in which generalized resistance of material to flow of alternating current is measured. The frequency of the applied signal is varied over a wide range, thus the term "spectroscopy" in this method. In the measurement both the ratio of the applied potential and the resulting current, as well as the phase shift between the imposed potential and the resulting current, are measured. Thus, a two parameter result is obtained for each frequency of the applied AC signal. The method, with appropriate mathematical treatment, allows study of materials through evaluation of the two component result - the impedance response - on the applied frequency.

### Types of frequency dependence

From the introduction it should be obvious that with changing the excitation frequency the impedance *response* is changing. This can lead to the notion that the impedance of the *system* (not just the impedance *response*) is changing. This may be a subtle difference, but it is not and it deserves a bit of explanation. A good example of a frequency dependent impedance (resistance in this case) is the physical chemistry textbook example of the Debye-Falkenhagen effect [1]. In the process, associated with solution conductivity, the motion of ions is involved, requiring readjustment of the position of neighboring ions. This leads to a frequency-dependent conductivity and permittivity.

Most experiments involving impedance measurements, however, study systems whose fundamental response to alternating electric current or field is independent of the applied frequency. In fact, the software typically used to evaluate the response is predicated on the assumption that the system remains unchanged during the frequency impedance scan. A good example of a component with constant property and changing impedance response is a capacitor. An ideal capacitor will have infinite impedance at zero frequency (DC current) and zero impedance at very high (infinite) frequency. Its fundamental characteristics, capacitance, will be, however, constant throughout the measurement frequency range. In the case of solution conductivity, displaying the Debye-Falkenhagen effect, the conductivity will be higher at very high frequencies, where the effect is more significant.

### Examples of studies benefitting from electrochemical impedance measurements

From the author's collection of work there will be presented a few examples of studies in which impedance measurements can play important role. For example in the physico-chemical studies of the interface between two immiscible electrolytes, the structure of the double-layer between the two phases is of an utmost importance. Impedance, used to measure electrical capacitance in this case, is an irreplaceable tool. In another research the measurements of doped ceramics at high temperature give a direct indication of the activation barriers, a parameter needed for characterization and successful development of materials for such applications as solid oxide fuel cells or high temperature sensors.

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**Enantioselective Sorbents in LC**

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Chromatographic separations based on enantioselective sorbents are widely used for analysis and preparation of various biochemicals (drugs, fragrances, pollutants). The overview of the most important concepts of chiral stationary phases broadly used for direct enantiomeric LC separations including the recognition mechanism, advantages and limitations are presented together with the newest types of chiral selectors and examples of their application.

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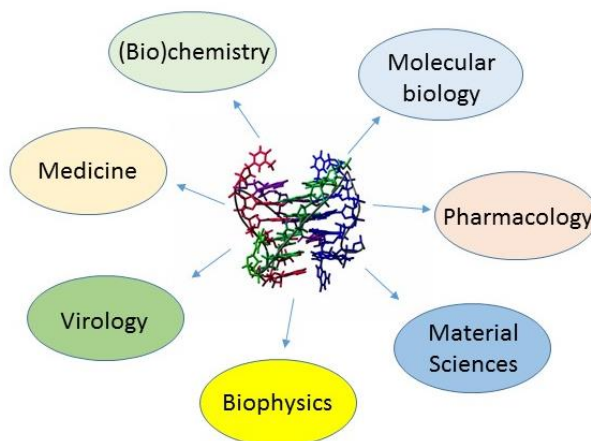
## G-Quadruplexes: Occurrence, Properties and Applying in Biomedical Sciences

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Nucleic acids in living systems do not occur in linear polymeric forms but they adopt complex architectures – wrapped DNA duplex and a variety of other folds. A fascinating structure is the G-quadruplex motif. G-quadruplexes are a family of peculiar three-dimensional arrangements adopted by G-rich DNA and RNA molecules, resulting from the stacking of several *G-quartets*, and stabilized by cations such as sodium and potassium. This structural motif shows some unusual properties newly found in other topological forms. The self-assembly of guanine derivatives has been known for more than a century, and the formation of G-quartets was proposed in the 1960s. Research into the relevance of G-quadruplexes has maintained an important momentum because these structures are stable under physiological conditions and there is increasing evidence pointing to biological roles of these conformations. G-quadruplex formation is significantly associated with oncogenes, tumor suppressors and somatic copy number alterations related to cancer development [1]. The G-quadruplexes may therefore represent promising targets for cancer intervention. A remarkable quantity of information has been obtained since the discovery of the G-quadruplex motif, which has made this field to grow from basic science to various applications, e.g. specific drug development inhibiting cancer growth or virus proliferation, receptor moiety of biosensor based on G-quadruplex aptamers, development of artificial antibodies [2]. The pace of progress took another leap during the last decade, and quadruplexes changed status from laboratory curiosity to hot topic within a few years thanks to seminal contributions from several laboratories. Now we can say, G-quadruplex motif is more attractive object and frequency of quotations increases by day; some remarks about it can be found in heterogeneous scientific areas, e. g. molecular biology, biochemistry, medicine, pharmacy, virology, biomaterials, biophysics and bioimaging.



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## Mechanism of Thermocatalytic Conversion of Methane to Hydrogen over Zn/Cu MWCNT's Catalysts

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An excellent catalytic activity has been observed with Zn/Cu MWCNT's catalysts in conversion methane to future carrier – hydrogen. MWCNT base has been doped with Zn, Cu or both Zn/Cu. This represents cheaper version to the catalysts with noble metals. Detailed mechanism of catalysis is not clear yet. Zn plays multifunctional role and affects dispergation and distribution of the Cu particles and improves overall catalytic activity. Zn can also act as precursor for dehydrogenation of many structures to hydrogen. The increase in selectivity with increasing copper loading could be explained by the necessity to have a specific stoichiometric ratio of zinc to copper present on the catalyst surface in order to ensure best possible functionality.

The higher conversion rate of ZnMWCNT's was 17.3%, CuMWCNT 's 14% and for bimetallic Zn/CuMWCNT 's 49% of hydrogen at 900°C, 1.2 mg of catalyst and 1 mL of methane. Conversion rate has been monitored by pyrolysis gas chromatography.

By TOF SIMS analysis it was confirmed that Zn oxidizes itself to form ZnO which is responsible for catalytic activity. Mechanism of action, based on structure of the catalyst in this multicomponent system will be discussed. Detailed TOF SIMS analysis showed interesting fragments: Cu<sup>+</sup>, CCu<sup>+</sup>, CuO<sup>+</sup>, CCuO<sup>+</sup>, ZnOCuO<sup>+</sup>, CZnOCuO<sup>+</sup>. Both kind of particles are bound to carbon nanotube skeleton in oxides form or via bridge of oxidized forms of Zn or Cu(Fig.1).

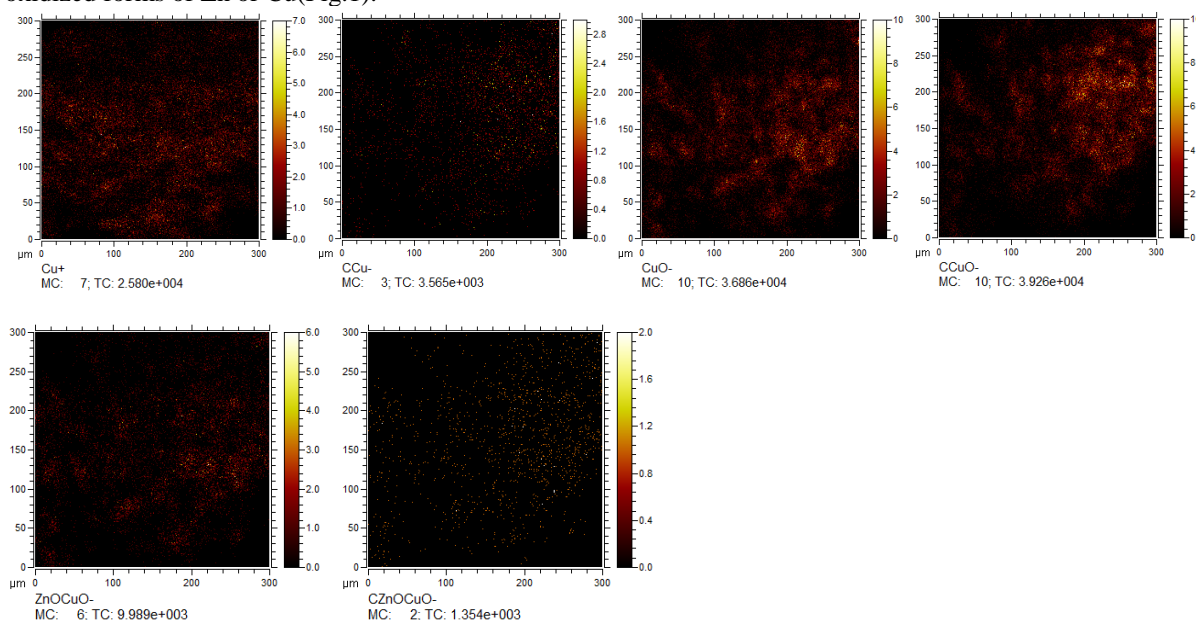


Fig. 1 TOF SIMS images of Zn/CuMWCNT's catalysts for different fragments. Surface analysis.

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**Preparing Chemistry Teachers for Teaching for the 21st Century**

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The aim of the contribution is to inform about Inquiry-Based Science Education (IBSE) as a concept of science education for the 21st century. Graduates of the 21st century need skills to be applied to the labor market. Inquiry based teaching seems effective to meet these requirements. It is necessary to prepare teachers and future teachers for application IBSE.

How are graduates of teaching ready for IBSE? At the undergraduate training of chemistry teachers at the Faculty of Sciences of Pavol Jozef Šafárik University in Košice training for IBSE is the part of the contents of our teaching subjects of Special practice of school experiments I, Didactic of Chemistry I and Didactic of Chemistry II. The results of our research indicate the differences in the opinions and attitudes of future chemistry teachers at IBSE before and after training. Future chemistry teachers inclined to IBSE, but they need to be acquired by competencies to the implementation of IBSE.

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**Application of Switchable Solvent for the Homogeneous Liquid-Liquid Microextraction  
of Palladium prior to Determination by FAAS.**

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Increased risk of exposure of population to palladium is closely related with rapid expansion of automotive industry, because automobile catalysts are mobile sources of palladium. Therefore the effective method for monitoring of palladium are most desirable. In proposed work the unique properties of green solvent, N, N-dimethylcyclohexylamine, was exploited for homogenous liquid-liquid microextraction of palladium, in order to isolation and preconcentration of palladium from environmental samples followed by determination by flame atomic absorption spectrometry. Hydrophobic form of extraction solvent, N, N-dimethylcyclohexylamine, was changed to hydrophilic form after reaction with carbonated water to achieve the best possible contact surface between extraction solvent and solution of sample. High concentrated sodium hydroxide solution was used as trigger for separation of palladium enriched N, N-dimethylcyclohexylamine phase. 4-(5bromo-2-pyridylazo)-5-(diethylamino)-phenol (Br-PADAP) was used as a complex agent for Pd(II). After optimization of condition the calibration curve was found with linear range from 6.7 to 1200  $\mu\text{g L}^{-1}$ . A limit of detection 2.0  $\mu\text{g L}^{-1}$  was calculated by following equation  $\text{LOD}=3S_a/b$ , where  $S_a$  is the standard deviation of  $y$ -residuals of regression line and  $b$  is the slope of the calibration curve. Proposed method was successfully applied for determination of palladium in catalytic converter and environmental water samples.

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**Comparison of Solid Phase Extraction to Novel Dispersive Liquid-Liquid  
Microextraction for the Determination of Free Estradiol in Human Urine**

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In estrogen analysis, sample-pretreatment is a crucial step due to low concentrations of these hormones in complex biological samples. Extraction procedure is important not only for the pre-concentration of analytes, but also for the reduction of matrix effect on the following analytical method. Solid-phase extraction (SPE) has been for long time considered to be "standard" extraction method for biological samples, however, it is being replaced by novel microextraction techniques offering simple operation and reduction in time and organic solvent consumption, such as dispersive liquid-liquid microextraction (DLLME) introduced in 2006 by Rezaee's group [1]. In this work, DLLME procedure was optimized and results were compared with those obtained with SPE extraction. The results were evaluated by means of thin-layer chromatography with chemical and densitometric detection and HPLC-UV.

**Acknowledgements:**

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**Enantioselective Analysis of Novel Bioactive Compounds Using HPLC with  
Cyclofructan Chiral Stationary Phases**

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Normal phase HPLC methods were developed for the enantiomeric separation of new spirobrassinin analogs with potential biological activity on cyclofructan-based chiral stationary phases (CSPs) containing isopropyl carbamate (CF6-IP), R-naphthylethylcarbamate (CF6-RN), or dimethylphenylcarbamate (CF7-DMP) as chiral selectors [1]. The effects of the mobile phase composition, the nature and concentrations of the polar and acidic modifiers on the resolution and retention were investigated. The best results were achieved using n-hexane and 2-propanol with trifluoroacetic acid as mobile phase modifiers. The effect of different column temperature on the enantioseparation was studied in the temperature range 5-40 °C. Thermodynamic parameters values were calculated from plots of  $\ln k$  versus  $1/T$ . It was found that studied chiral separations were enthalpy driven. The elution sequence of the enantiomers was determined in all cases. Better results were achieved on CF6-RN chiral stationary phase which was able to separate all nine but one analytes and provided six baseline separations. The developed methods were used for enantiomeric excess determination of the individual enantiomers in scalemic mixtures.

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**Identification of Platinum Forms Using Various Possibilities of Analytical Signal Enhancement. Determination of Platinum by AAS and UV-VIS.**

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Various possibilities of analytical signal enhancement were used for Pt determination as ion associate (IA) with  $\text{SCN}^-$  and 1,3,3-trimethyl-2-[3-(1,3,3-trimethyl-1,3-dihydroindol-2-yliden)-propyl-1,3-dienyl]-3H-indolium chloride more known as Astraphloxine FF (APFF). The conversion of platinum IA allows the extraction of Pt from samples containing many elements such as Cu, Cd, Ni, Co, Cr, Pb, In, Ag, Pd, Ir, Rh, and Ru. In this case, platinum (II) is extracted in the form of IA under standard conditions, whereas platinum (IV) is extracted only after the initiation of IA formation by force of various sources of energy (thermal treatment, ultrasonic and microwave energy) in the test sample. In comparison with thermal treatment the use of ultrasonic power reduces the needed time from 30 min up to 5 min and microwave energy up to 45 s. Optimized conditions of IA formation enabled the suggestion of speciation analysis of Pt(II) and Pt(IV). Species can be determined simultaneously in the concentration ratios from 1:5 to 5:1. IA are extractable by toluene or amylacetate up to volume ratio  $V_{\text{aq}} : V_{\text{org}} = 50 : 1$ . This fact decreases the LOD from  $90 \mu\text{g L}^{-1}$  to  $5 \mu\text{g L}^{-1}$  and from  $7.1 \mu\text{g L}^{-1}$  to  $0.3 \mu\text{g L}^{-1}$  (as Pt) of UV-VIS and AAS determination respectively. Proposed methods were used for Pt determination in artificial and real samples with reliable results.

**Acknowledgements:**

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**Isolation, Purification and Analysis of Microbial Exopolysaccharides Produced by  
*Lactobacillus Reuteri***

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Exopolysaccharides, exocellular polymers present in the surface of many bacteria, including *Lactobacillus* strain, were isolated, purified and analysed for determination of total sugar content [1]. Two strains of *Lactobacillus reuteri* have been examined for their exopolysaccharide production capacity, L26 (isolated from a pig) and SL16 (isolated from a hen). They were investigated in semi-defined medium (SDM) with addition of sucrose, by different isolation methods. Both strains produced exocellular polymer, but in different ratios. The production kinetics and exopolysaccharides yields were strongly dependent on the fermentation conditions. Physical factors (temperature, pH) and chemical factors (medium composition, initial sucrose concentration) were of utmost importance. Exopolysaccharides yields were analysed by colorimetric procedure described by DuBois et al., using glucose as standard [2]. Based on the measured absorbance values for the samples, the concentration of all the carbohydrate components was determined according to the calibration curve of glucose. The results indicate that strain SL16 produce more EPS than strain L26. Optimal conditions for the maximum production of EPS by strain SL16 were 10% sucrose in culture medium, temperature 31°C and pH 6,2.

**Acknowledgements:**

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## Trace Analysis of Sulfur and Phosphorus Utilizing Quadrupole-based ICP-MS

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This work presents development of analytical method for trace phosphorus and sulfur contents in environmental and biological matrices utilizing quadrupole based inductively coupled plasma mass spectrometry (ICP-QMS) with octopole collision-reaction cell. Determination of sulfur and phosphorus remain challenging according to relatively high first ionization potentials [1,2] and also according to the spectral-, matrix-, and physical-based interferences that are difficult to remove using conventional quadrupole-based ICP-MS. The one of the preferred method for elimination of spectral interferences in quadrupole ICP-MS is octopole collision-reaction cell (ORC) that is employed throughout this work.

The optimization of experimental conditions for ORC in collision operating mode using He as the collision gas is presented in this work. According to the development of the analytical method He flow rate was optimized. The impact of He pressure on the background equivalent concentration (BEC) of interesting isotopes in mass range for <sup>34</sup>S  $m/z=34-74u$  and for <sup>31</sup>P  $m/z=31-79u$  was monitored. With regard to the optimization measurements isotope of <sup>31</sup>P was calibrated in the 2 linear calibration ranges: 10-200  $\mu\text{g L}^{-1}$  (1<sup>st</sup> range), and for 75-750  $\mu\text{g L}^{-1}$  (2<sup>nd</sup> range), and the optimal helium flow rate of 3  $\text{mL min}^{-1}$  for the both calibration ranges of <sup>31</sup>P was evaluated. Linear working range for sulfur determination was estimated in the interval of 0-1000  $\mu\text{g L}^{-1}$  and for the higher concentration levels of 0-5000  $\mu\text{g L}^{-1}$  was suitable quadratic calibration function. Helium flow rate of 2  $\text{mL min}^{-1}$  was evaluated as optimal for sulfur analysis. The basic validation and calibration parameters for both elements were estimated, and throughout the experiments external analytical calibrations could be used.

Optimization of ORC conditions meant improvement of BEC and validation parameters of investigated elements. Accuracy was evaluated as recovery (Rec) of laboratory reference material (LRM) (Rec= 95-100% for <sup>34</sup>S; and Rec= 97-100% for <sup>31</sup>P). Precision was evaluated as repeatability, relative standard deviations (RSD) were in the range of 0.1-2.6% for <sup>34</sup>S and 0.4-5.8% for <sup>31</sup>P. The LOD ( $3\sigma$ -criterion) was 96  $\text{ng L}^{-1}$  for linear and 321  $\text{ng L}^{-1}$  for non-linear working range for <sup>34</sup>S and for <sup>31</sup>P were 4  $\text{ng L}^{-1}$  in 1<sup>st</sup> calibration range and 6  $\text{ng L}^{-1}$  in the 2<sup>nd</sup> range.

### Acknowledgements:

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- 2) VEGA 1/0253/16; Project - Development of the analytical techniques suitable for the on-line dynamic control.
- 3) Slovak Spectroscopic Society, member of the Association of Slovak Scientific and Technological Societies.

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### Characterization of Half and Full Heusler Alloys based on NiFeZ (Z = In, Sn, Sb)

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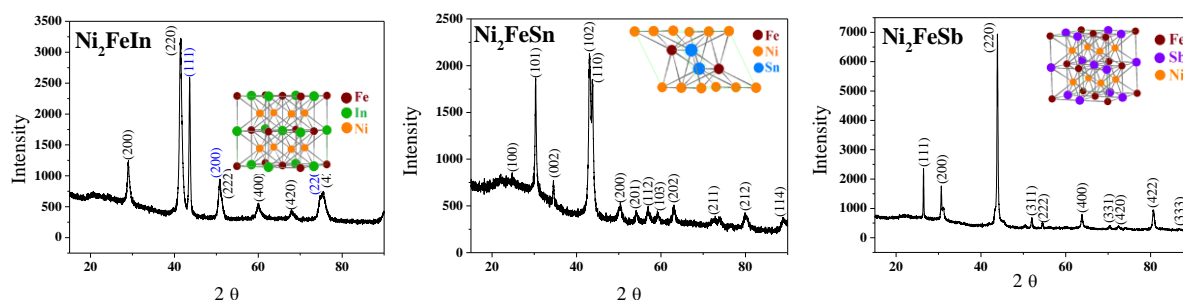
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Heusler alloys are increasingly more known alloys with promising technological applications (like sensors, magnetocaloric cooling, shape memory devices, spintronics etc.). In general, Heusler alloys are ternary alloys divided into two groups: half Heusler alloys XYZ (with stoichiometry 1:1:1 and C1<sub>b</sub> structure) and full-Heusler alloys X<sub>2</sub>YZ (with stoichiometry 2:1:1 and L2<sub>1</sub> structure) [1].

One of the few disadvantages of Heusler alloys is their complicated production process that consist of melting pure elements together and further long-term thermal treatment at elevated temperature in order to get correct structure with proper chemical short range order. Heusler alloys in the form of ingots are usually produced by melting the constituent metallic elements in Ar atmosphere. This method is deficient for correct structure and homogeneous system. Melt spinning is one of the most popular methods of preparation of Heusler alloys in the form of ribbons, providing with cooling rate 10<sup>5</sup>-10<sup>6</sup> K/s in a single step. In last years, the rapid quenching is employed to produce a high quality of these alloys [2].

Currently, there is a lot of Heusler alloys based on nickel. Regular example of Heusler alloy in spin polarized materials is the alloy with chemical composition of NiMnSb. Large attention is attracted by alloys NiMnZ (Z=Ga, In, Sn, Sb) due to the multifunctional properties. However, system based on NiMn has some drawbacks, which is the loss of Mn during the melting process [3]. Based on this drawback, we substituted the Mn with Fe and we prepared the set of half and full Heusler alloys.

In this article we studied a structural, chemical and magnetic properties of NiFeZ and Ni<sub>2</sub>FeZ (Z=In, Sn, Sb) Heusler ribbons produced by melt-spinning method. SEM/EDX analysis shows the correct chemical composition of all examined alloys. Structural characterization was provided by X-ray powder diffraction (XRD) method. In all cases we can observe the multiphase system. But this alloy Ni<sub>2</sub>FeSb crystallizes in L2<sub>1</sub> structure, corresponding to the structure of full Heusler alloy. Ferromagnetic character of alloys was observed from the magnetic measurements. Hysteresis loops were measured in the parallel and perpendicular orientation of magnetic field with respect to the ribbon plane at room temperature. It confirms the easy axis in the plane of the ribbon and hard axis perpendicular to the ribbon's plane. Small influence of anisotropy is observed from hysteresis loops of Ni<sub>2</sub>FeSb alloy.



**Fig. 1** X-ray diffraction profile of Ni<sub>2</sub>FeZ (Z=In, Sn, Sb) ribbon

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### Silver Complexes and their Potential Bioapplication

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Increasing antimicrobial drug resistance encourages chemists, namely in the field of bioinorganic chemistry, to suggest search for and effective treatments toward pathogenic microorganisms. The underlying idea is to connect antimicrobial metal (zinc(II), copper(II), silver(I)) and efficient organic ligand into a new synergic drug.

Remarkable antimicrobial properties exhibited by silver complexes with N-heterocyclic carbenes (NHCs), phosphines, N-heterocycles and with a variety of pharmaceutical agents were summarized in the review [1]. Investigation of zinc (II) and silver(I) carboxylates represents another significant contribution to research of new drugs. It is evident that silver(I) carboxylates show more effective antimicrobial activity (mainly antifungal) than their zinc(II) analogues [2]. Moreover, silver(I) complexes with imidazole ligands are attractive in the field of antimicrobial antiresistance treatments because imidazole-containing drugs (ketoconazole, clotrimazole) are commonly used to treat infections caused by fungus or yeast. Moreover imidazole-based medications based on nitroimidazole have excellent activity against anaerobic microorganisms [3].

In addition, silver complexes have become attractive as anticancer therapeutics in the last decades. A few review articles focus their attention on silver(I) complexes containing various types of ligands such as carboxylic acids, amino acids, nitrogen, phosphorus or sulphur donor ligands which exhibit selective effects against variety of cancer cells [4]. As Ortego described [5], several silver(I) derivatives with O-, N-, P- or S- donor ligands or N-heterocyclic carbene ligands have shown high cytotoxic behaviour against diverse human tumor cells.

Silver pyridinecarboxylate/phosphonate/sulfonate and silver complexes with bioactive ligands were prepared and characterized by X-ray crystallography, elemental analysis, IR spectroscopy and thermal analysis in solid state. Their stability was verified by UV and NMR spectra in DMSO solution. Comparison of structural, spectral, thermal, and biological properties is described and correlated.

#### Acknowledgements:

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### Analysis of G-quadruplex Putative Sequences in Human Immunodeficiency Viruses

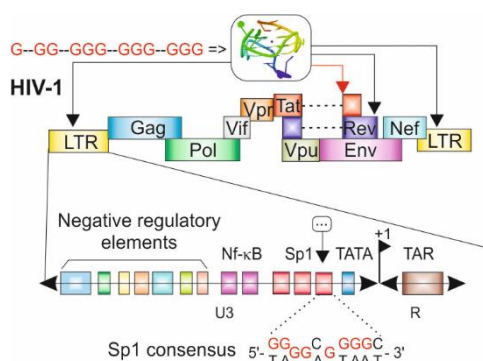
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G-quadruplexes are structures formed from nucleic acids that contain guanine quartets. G-rich sequences able to form G-quadruplex structures were found in eucaryotic telomeres and also in another important regions of human genome, e.g. gene promoters [1]. Formation of G-quadruplexes is often accompanied with telomerase activity. Telomeres in somatic cells are gradually shortened with cell divisions as a consequence of the end-replication effect. In cancer cells the telomerase is still active and prolongs the telomeres which makes the cancer cells immortal. G-quadruplexes folded within the promoter region of target gene cause inhibition of oncogene transcription [2].

The HIV is one of the most studied viruses in the world especially in terms of genetic sequencing, with more than 9500 genomic sequences of HIV isolates sequenced [3]. We have analyzed a series of DNA sequences using modified criteria for identifying sequences which tend to form G-quadruplexes. A number of such sequences were found in various coding and non-coding domains, including the U3 LTR, tat, rec, env and vpx regions. The sequences derived from original isolates were analyzed using standard spectral and electrophoretic methods. Many of these oligomeric sequences were found to form G-quadruplexes, but some of those can preferentially form different non-canonic structures. Targeting the G-quadruplexes or peptide domains located in G-rich coding sequences in HIV offers researchers attractive therapeutic targets which would be of particular use in the development of novel antiviral therapies. The analysis of G-rich regions is a tool to find specific targets of novel antiviral therapies. The analysis of G-rich regions is a tool to find specific targets which could be of interest for specific types of virus.



**Fig. 1** Schematic drawing of the HIV-1 genome organizations and locations of studied sequences.

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### Diarylethene Molecular Switches Containing Crown-Ether Moiety

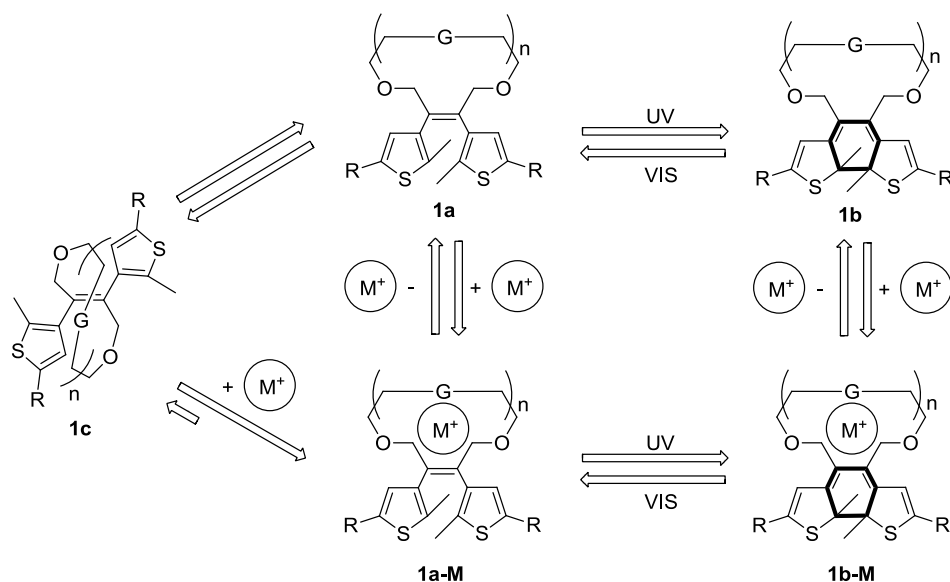
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Diarylethene switches are synthetic organic molecules which contain heterocyclic rings connected with double bond and they have photochromic properties. During photochromic reaction, six membered ring is created and position of double bonds is changed. Photochromism[1,2] can be defined as a reversible phototransformation of a molecular switches between two forms of isomers (closed and open) possessing different absorption spectra. The diarylethene molecular switches with crown-ether units **1** can exhibit novel photochromic and complexation properties due to special position of the crown-ether over central double bond. The crown-ether unit is very flexible and can allow *E*- and *Z*- geometric isomers of the dithienylethene molecular switches. The equilibrium between these two geometric isomers can be shifted to the *Z*- isomer due to complexation with metal ions (Figure 1.).



**Fig. 1** Expected mechanism of molecular switch with crown-ether unit in the presence of metal ions.

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### DNA-binding Properties of Novel Spiro Acridine Isoxazolines

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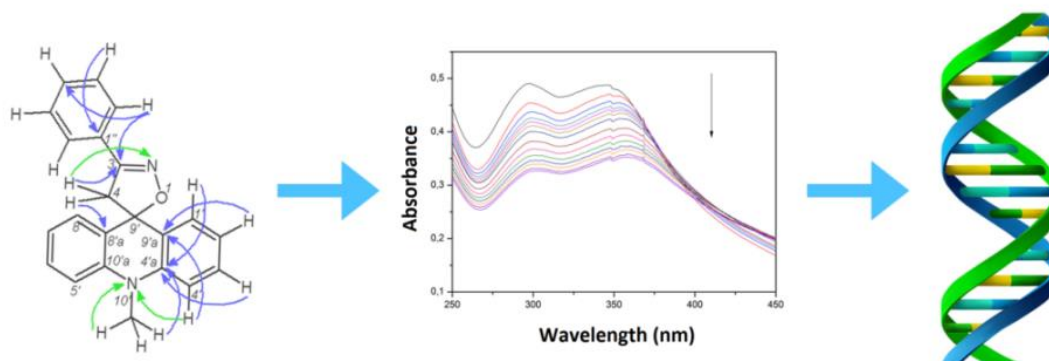
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Acridine and its derivatives are special chemical families with a planar aromatic chromophore which are able to bind into DNA by intercalation mode and thereby inhibit crucial classes of enzymes involved in the regulation of DNA, especially topoisomerases and telomerases. The strong fluorescence properties exhibited by acridine pharmacophores have led to their use in a number of fields of biological research, including as chemiluminiscent agents, DNA intercalators and chemical sensors in fluorescence spectroscopy [1, 2].

Eight new 10'-methyl-3-phenyl-4*H*,10'*H*-spiro[acridine-9',5-[1,2]oxazoles] were synthesized and characterized using elemental analysis, IR, UV-Vis, and NMR measurements. The interactions of acridine derivatives with calf thymus (CT) DNA were extensively studied by various spectroscopic techniques (Figure 1). The data revealed a decrease of peak intensities with the absorbance reduction of approximately 14% to 35% from its initial value. The hypochromism, due to a strong interaction between the electronic states of the intercalating chromophore and those of the DNA bases, was noted to be similar to other reports, suggesting the close proximity of the acridine ring and DNA. The presence of an isosbestic point at 400 nm indicated spectroscopically distinct chromophores, namely, free and bound species. Such spectral behavior is generally associated with the intercalation as a dominant binding mode.



**Fig. 1** UV-vis spectrophotometric titration of 10'-methyl-3-phenyl-4*H*,10'*H*-spiro[acridine-9',5-[1,2]oxazole] with increasing concentration of CT DNA.

The UV-visible and CD measurements implied that these derivatives interact with calf thymus DNA through intercalation. For better information about the DNA binding properties of the investigated spiro acridines we performed competitive binding experiments based on the displacement of ethidium bromide (EB) from CT DNA. From this assay the Stern-Volmer quenching constants were determined and ranged from  $0.126 \times 10^4$  to  $1.394 \times 10^4 \text{ M}^{-1}$ . The experimental results showed that new derivatives bind with DNA *via* intercalation.

#### Acknowledgements:

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### Interactions of Selected 3,6,9-Trisubstituted Acridine Derivatives with DNA and Their Potential Anticancer Effect.

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Acridine/acridone derivatives are known anti-cancer and cytotoxic agents. They also display other forms of bioactivity and are used as biological fluorescent probes, antibacterial, antiprotozoal and antimalarial drugs, in the treatment of HIV and Alzheimer's disease [1,2]. According to recent studies, trisubstituted acridine derivatives capable of binding to G-quadruplexes, exhibit strong anti-tumor effect, which involves several parallel mechanisms, including telomere uncapping, direct or indirect telomerase inhibition with the characteristic induction of senescence and apoptosis. Several structure-activity studies of disubstituted-anthraquinones or acridi(o)nes and trisubstituted-acridines structures have led to the design of a new potent and selective telomerase inhibitor based on 3,6,9-trisubstituted acridine structure, named BRACO-19. Various synthetic methods are focused on the preparation of target acridine skeletons or modifications of naturally occurring compounds, that exhibit promising anticancer activities [1,3,4]. Synthetic or natural acridine/acridone derivatives represent an important class of drugs, which showed the ability to intercalate DNA and inhibit topoisomerase or telomerase enzymes. Intercalation mechanism of these compounds into DNA is based on  $\pi$ -stacking interaction with basepairs of double-stranded nucleic acids. Intercalation of the acridine moiety, with its flat, heterocyclic and polyaromatic structure, into the gap between two chains of polynucleotides, disturbs their crucial role in cell division. The ability of acridine compounds to intercalate into DNA is necessary for their anti-tumor activity and the strength and kinetics of binding acridine to DNA have a crucial impact on the activity of this type of anticancer agent. For the purpose of finding new anti-tumor agents and study of the ability to influence the activity of the enzymes topoisomerase I and II, there were synthesized new 3,6,9-trisubstituted acridine derivatives at the department of organic chemistry [1,5]. Biochemical, biophysical and biological properties of these derivatives were tested using spectroscopic techniques (UV-Vis absorption and fluorescence spectroscopy, circular and linear dichroism) and viscometry. Binding affinity of acridine derivatives with ctDNA (calf thymus DNA) was examined and their binding constants were determined. All of the measurements indicated that the examined compounds behave as effective DNA-interacting agents and also act as effective DNA intercalators.

#### Acknowledgements:

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## Main Differences, Properties and Utilization of Noble Metal Nanoparticles and Nanoclusters

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Materials with nano dimensions have become a part of everyday life and achieve broad spectrum of utilization, for example in aircrafts, energetics, architecture and consumer industry. They are also used in biomedicine as nanovaccines, drug nanocarriers and diagnostic imaging tools. They belong to inseparable components of specialized surfaces, catalysts, sensors and as protection of the environment. General definition of nanomaterials encompasses natural or synthetic materials composed of monodispersed particles or aggregates where  $\geq 50\%$  of particles are with one of the dimension within the length scale 1-100 nm. However, some of their interesting features are typically obtained in dimensions smaller than 3 nm (down to 0,1 nm in case of atomic and molecular manipulations). Nanomaterials have in comparison with bulk materials specific physical, optical, electronic and biological properties, which is mainly effect of high surface-to-volume ratio. Nanoparticles (NPs) and nanoclusters (NCs) are defined as bridges between bulk materials and single molecular or atomic structures. Difference between NPs and NCs is defined by sizes of their cores. Core size of NPs is greater than 3 nm, on the other hand NCs have core size smaller than 3 nm. Noble metal NPs and NCs can be also easily modified on their surface with different biomacromolecules, such as proteins, aptamers, DNA, polymers, dendrimers, etc. Mentioned ligands (alone or with help of other reducing agents) are able to reduce and arrange noble metal atoms into stable NPs and NCs during synthesis. Modified NPs and NCs are finding growing acceptance in biomedicine mainly because of subsequent possibility of functionalization, for example with required functional groups [1-3].

Nowadays, noble metal NCs (mainly Au and Ag) have attracted increasing attention due to their fascinating physicochemical molecular like properties such as quantized charging, photoluminescence, biocompatibility, higher penetration capability and long term stability. It has been demonstrated that capping and stabilizing ligands are dominant factors for acquiring special properties. NCs do not exhibit surface plasmon resonance absorption in the visible region as it is known for NPs, but have fluorescence in the visible to near-infrared region. With these advantages NCs have become interesting sensing and imaging materials [4-6].

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### Regulation of Lysozyme Activity and Stability by the Hofmeister Series Anions

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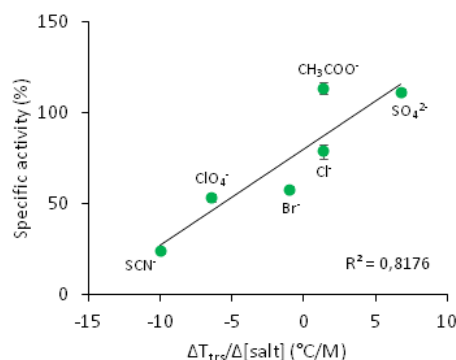
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It was found that the theories that describe electrostatic potential on the interfaces are not able to explain ion-specific phenomenon, the so-called Hofmeister ion effect [1], originally observed in relation to protein precipitation [2]. Since then, Hofmeister effect has been shown to affect number of biophysical and biochemical processes, which include stability, aggregation/fibrilization, enzymatic activity and many others [3]. To examine closely this phenomenon we have studied the effect of six anions ( $\text{CH}_3\text{COO}^-$ ,  $\text{Br}^-$ ,  $\text{Cl}^-$ ,  $\text{ClO}_4^-$ ,  $\text{SCN}^-$ ,  $\text{SO}_4^{2-}$ ) on properties of hen egg white lysozyme (EC 3.2.1.17).

Enzymatic activity and thermal stability of lysozyme in the presence of salts have been investigated by fluorescence spectroscopy and differential scanning calorimetry, respectively. The effect of sodium salts of the anions on lysozyme properties depends on anion concentration as well as on position of anion in the Hofmeister series. The parameters describing its activity and stability in the presence of salts show positive correlation, i.e. relative increase in stability is accompanied by similar relative increase in activity of the enzyme (Figure 1).



**Fig. 1** Correlation between the specific activities of lysozyme in 0.5 M salts (pH 5.2, 35 °C) and the values of  $\Delta T_{\text{trs}}/\Delta[\text{salt}]$  expressing de/stabilization effect of the corresponding salts. Specific activity in the absence of salts was taken as a reference for relative specific activity calculations.

Kosmotropic anions (sulfate and acetate) increase stability and activate the enzyme while chaotropic anions (bromide, thiocyanate and perchlorate) including chloride decrease stability and inhibits the enzyme activity. Strong correlation between stability and activity of lysozyme suggest the interdependence of its properties in the presence of salts. The fact that the properties of lysozyme correlate with partition coefficients of anions at nonpolar hydrocarbon surface as well as polarizability of monovalent anions indicates that Hofmeister effect of anions is intermediated by interaction of anions with nonpolar surface of the enzyme.

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### Study of Binding Interaction between Selected Ferrocenyl Chalcones and Bovine Serum Albumin

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Serum albumins are the most abundant proteins in the circulatory system of a wide variety of organisms, which play a dominant key role in the binding and transport of numerous endogenous and exogenous ligands. Serum albumin often enhances the apparent solubility of hydrophobic drugs in plasma and modulates their delivery, disposition, efficacy and distribution to cells *in vivo* and *in vitro*. The drug-protein interaction may result in the formation of a stable protein-drug complex, which has significant effect on the delivery, distribution, free concentration and metabolism of drugs in the blood circulatory system. Thus, the drug–albumin complex may be considered as a model to gain fundamental insights into drug–protein interactions and explore its applications [1].

As an effective bioisostere, ferrocene is becoming a potential platform for drug design due to its redox properties, high lipophilicity, and three-dimensional metallocene unit. Many ferrocenyl compounds display interesting antimalarial, antifungal, cytotoxic, or antitumor activities. Ferrocene can act as a one-electron donor undergoing oxidation to the ferricenium ion ( $\text{Fe}^{3+}$ ) or as a source of reactive oxygen species which induce oxidative DNA damage. Furthermore, the combination of ferrocenyl moiety may increase their biological activity. Chalcones are naturally occurring derivatives of the parent compound 1,3-diphenyl-2-propen-1-one. Among the naturally occurring chalcones and their synthetic analogues several compounds displayed a broad range of biological activities such as antimalarial, antibacterial, antiviral, antiangiogenic, and anticancer effects [2].

In our recently published article [2], was determined that selected ferrocenyl chalcones **A–D** and non-chalcones ferrocene analogue **E** have affect on the tumour cells viability. For these reasons, we focus on identification type of binding interaction between bovine serum albumin (BSA) and ferrocenyl chalcones. Drugs-BSA interactions were studied using fluorescence spectroscopy. The binding constants were determined from fluorescence spectroscopic titration.

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### The Effect of Perturbation of Heme Region on Peroxidase-like Activity of Cytochrome *c*

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Physiological function of cytochrome *c* (cyt *c*) involves electron shuttle between respiratory complexes III and IV in mitochondria. To perform this task, cyt *c* has to adopt its native, fully folded state. Cyt *c* as an example of moonlighting protein plays important role in unrelated physiological process such as in initiation of mitochondrial apoptosis [1]. However, this assumes different conformational properties of cyt *c*, in which cyt *c* has increased peroxidase activity [2]. In this work we have studied how perturbation of heme region induced by chemical denaturation affects cyt *c* peroxidase-like activity.

This small globular protein is often utilized as a good model for study local conformational changes in heme proteins. Native state of cyt *c* is a form when the sixth ligand of heme iron is occupied with Met80. Due to natural dynamics of the heme region, which includes residues 70-85 of the polypeptide chain, cyt *c* protein can switch between the native form (6-coordinated low spin Fe) and the so-called open form cyt *c* (6-coordinated and/or 5-coordinated high spin Fe). The rate of the dynamics and thus the fraction of the opened form of cyt *c* can be modified by denaturants such as urea or guanidine hydrochloride.

The peroxidase-like activity of cyt *c* was measured at neutral and acidic pHs in the presence of urea. The rate constant of the reaction increased with increasing concentration of urea at both neutral and acidic pHs. Interestingly, the increased peroxidase-like catalytic activity of the protein was not accompanied by significant conformational change. The conformational properties of cyt *c* have been monitored by absorption spectrometry at Soret region sensitively monitoring the heme region and by fluorimetry that reflects changes in tertiary structure of protein.

Our previous study suggests that the rate of interaction of heme iron with small external molecules (as CN<sup>-</sup>) is controlled by the polypeptide chain flexibility as a result of anion action on the water/protein arrangement [3,4]. In the present work, we show a correlation between bindings of cyanide to heme iron with peroxidase-like activity monitored by guaiacol oxidation. The properties of heme region of cyt *c* are modified by increased urea concentration in the range from 0 to 6M at neutral and slightly acidic pH.

Our results of urea effect on conformational properties of cyt *c*, its ability to bind cyanide as well as its peroxidase-like activity indicate that the peroxidase-like activity of cyt *c* is not accompanied by conformational change. On the other hand, the correlation between rate constant of cyanide binding and peroxidase-like activity of cyt *c* strongly indicate an involvement of dynamics in inducing of peroxidase-like activity in cyt *c*. We believe that our model may explain certain properties of cyt *c* at the membrane interface.

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### The Study on Glucose Oxidase Deflavinization Reversibility

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Glucose oxidase (GOX) is an enzyme acting as a redox carrier in oxidation of beta-D-glucose leading towards production of hydrogen peroxide, reaction, which is the basis of glucose biosensor currently used in medicine. Relatively complex structure of GOX as well as its application potential makes it an interesting protein for structural studies [1, 2].

From structural point of view, GOX is homodimeric glycoprotein with one molecule of flavinadeninedinucleotide (FAD) cofactor noncovalently but strongly bound to each one of protein subunits [1, 2]. Molecules of carbohydrates, mainly D-mannose, D-galactose and D-glucosamine, are bound to protein surface representing 16-25% of its structure [1]. Carbohydrate content is higher (up to 60%) when the recombinant protein is produced in yeast [3].

The aim of our study is to compare the properties of wild-type GOX with its apo-form as well as reconstituted protein, with molecule of FAD bound back in structure to determine how cofactor affects the properties of GOX. For such study one has to use suitable method of deflavinization.

Four different deflavinization methods were examined experimentally. These methods differ in the type of salt, pH and time of incubation being utilized. Akhtar et al. [4] used the presence of divalent cations, calcium and magnesium, (ii) Zlateva et al. [5] were able to prepare the apo-GOX by the effect of nucleophilic agents such as KCN, KOCN and KSCN, (iii) Massey et al. [6] used 3M KBr, and (iv) Swoboda [7], in which the author used the saturated ammonium sulphate at very acidic pH, pH 1.4, as deflavinization agent. Upon binding FAD cofactor to protein molecule analysis of structural changes, stability and activity was done by absorption, fluorescence and CD spectroscopy, differential scanning calorimetry and SDS-PAGE.

We concluded, that the best way to prepare the apo-GOX has been reported by Swoboda [7]. Upon interaction with FAD, its binding back to protein structure has been observed, when upon dialysis to remove free FAD, protein regained its yellow colour. Spectral analysis confirms the successful reconstitution of protein structure, even though the SDS-PAGE electrophoretogram shows that upon deflavinization the dissociation of GOX to its subunits occurs. Activity measurements further indicate that after refluorination GOX regains its ability to oxidize β-D-glucose. Stability of native and refluorinated GOX is almost identical, while the stability of defluorinated protein is significantly lower and this form of GOX has tendency to aggregate.

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### Tioflavin T- G-quadruplex DNA Interaction

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G-quadruplex structure is one of the most studied secondary motif occurred in nucleic acids [1]. This motif influences the activity of transcription factors and cells differentiation as well as it participates in the development of neurogenesis [2]. G-quadruplex putative sequences are located in various important genomic, e.g. telomeres and oncogene promoter regions. These loci are promising therapeutic target for anti-cancer drugs because G/quadruplexes are closely related to carcinogenesis, cell aging and genetic instability [3]. Although G-quadruplex is considered to be functionally an important regulating element in mammalian genome, details of its all possible functions remain unexplained [4]. Currently, there is an effort to identify low-molecular drugs stabilizing the G-quadruplex motifs. Many of them have a relatively low cytotoxicity to normal cells and selectively inhibit the growth of the rapidly proliferating cancers [5]. The macrocyclic structures are particularly attractive to design G-quadruplex ligands because they show a much lower affinity to double-stranded DNA than to the G-quadruplexes [6]. The current trend is the development of highly-selective ligands, which would be able to distinguish different topological variants of G-quadruplexes and deactivate only a specific number of genes which are essential for gene expression of tumour cells, as well as infected cells [7,8]. Tioflavin T (ThT) has an excellent affinity to G-quadruplexes. ThT and its derivatives are promising for applying in new functional bio-materials and biosensors [9]. The main objective of this study was to clarify the impact and a way how ThT interacts with different structural DNA motifs, and especially with different topological forms of G-quadruplex. Moreover, the ligand ThT-DNA complexes show a high fluorescence, whereas the structural selectivity for different forms of G-quadruplexes has not yet been clarified, as demonstrated by the absence of relevant literature sources. This study is focused on the interaction of ThT with various structural motifs of DNA. For this purpose, the spectral methods, UV-Vis absorption spectroscopy, circular dichroism and spektrofluorescence have been used.

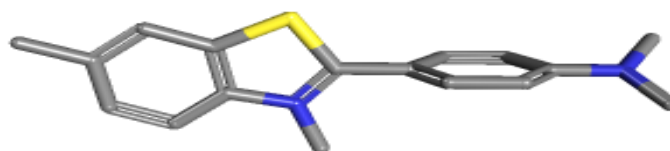


Fig. 1 Structure of ThT

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Chemistry and Cytotoxicity of 3,6-bis(imidazolidinone)acridines

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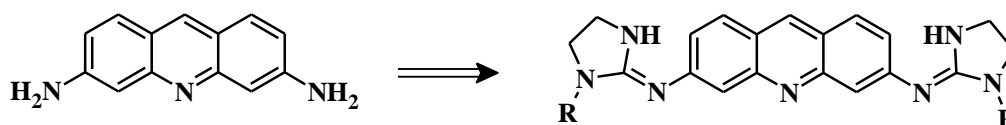
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New acridine derivatives bearing two symmetrical imidazolidinone rings, 3,6-bis((1-alkyl-5-oxo-imidazolidin-2-ylidene)imino)acridines (alkyl = ethyl, *n*-propyl, *n*-butyl, *n*-pentyl, *n*-hexyl), were prepared and their biological properties were studied. A binding of imidazolidinones to calf thymus DNA was examined by UV-Vis, fluorescence, and CD spectroscopy. The binding constants determined by UV-Vis spectroscopy were found in the range  $1.9 \times 10^5 - 7.1 \times 10^5 \text{ M}^{-1}$ . Electrophoretic separation proved that imidazolidinones inhibited topoisomerase I in 40  $\mu\text{M}$  concentration although only those with longer alkyl chains were able to penetrate the membranes and efficiently suppress the cell proliferation. The most active in cytotoxic tests was 3,6-bis((1-*n*-hexyl-5-oxo-imidazolidin-2-ylidene)imino)acridine with  $\text{IC}_{50} = 2.12 \pm 0.21 \mu\text{M}$  (HL 60 cell line) after 72 h incubation. Molecular dynamics simulations and solvent-accessible surface areas (SASAs) calculations were used to explore an intercalation mechanism. Molecular dynamics simulations favor stacking between adjacent C:G base pairs from a minor groove side and SASAs calculations predict a loss of entropy as the driving force for the complex stability [1].



R : ethyl, *n*-propyl, *n*-butyl, *n*-pentyl, *n*-hexyl

Fig. 1 Imidazolidinones of acridine.

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### Total Stereoselective Synthesis of a Novel 7a-hydroxymethyl Substituted Tetrahydropyrrolizidine

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Polyhydroxylated pyrrolizidine alkaloids isolated from various plant families represent an impressive structural motif that has proven to be a rich source of glycosidase inhibitors [1]. Although a number of members of this compound class have been studied at a clinical level, none of them have been approved as a drug. Attempts to improve the selectivity and efficiency of these inhibitors with minimal side effects have been made to develop several analogues of the naturally occurring heterocycles to meet the aforementioned challenges [2]. For most pyrrolizidines isolated from natural sources, the presence of the hydroxymethyl side chain at the C-1 or at the C-3 position is typical. On the other hand, only a few alkaloids possess the substituted 7a-hydroxymethylpyrrolizidine skeleton [3].

Herein, we report stereoselective synthesis of (1*S*,2*R*,6*R*,7*S*,7*aR*)-7a-hydroxymethyl-1,2,6,7-tetrahydropyrrolizidine [4], using isothiocyanate prepared by *aza*-Claisen rearrangement of appropriate D-glucose derived allylthiocyanates [5].

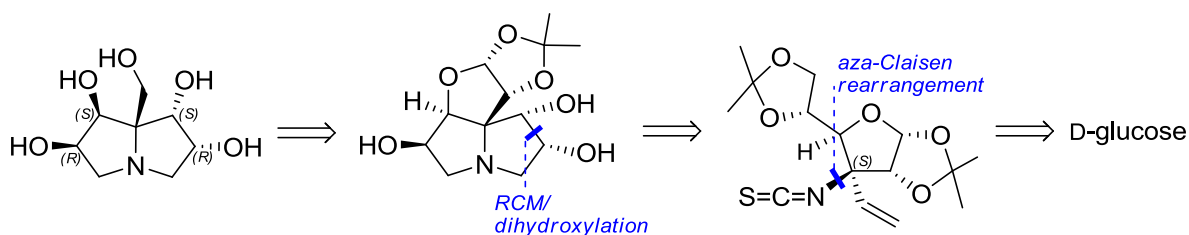


Fig. 1: Retrosynthesis of target compound starting from D-glucose

#### Acknowledgements:

The present work was supported by the Grant Agency (Nos. 1/0398/14 and 1/0568/12) of the Ministry of Education and by Slovak Research and Development Agency (No. APVV-14-0883).

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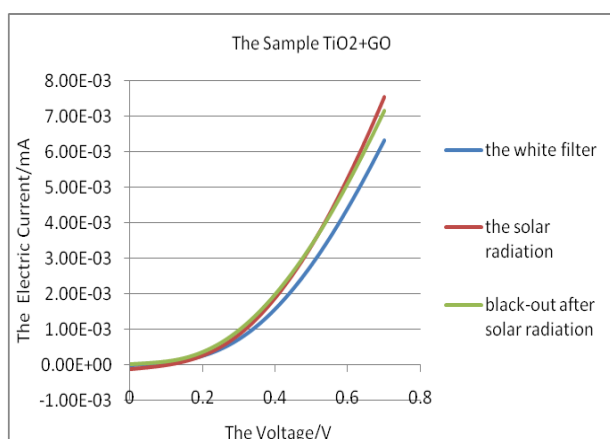
### Composite Materials for Solar Energy Conversion

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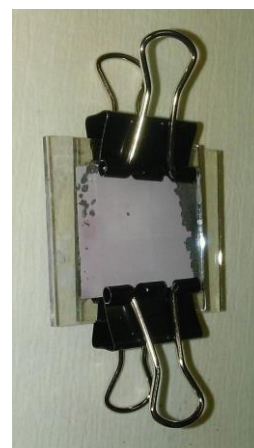
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The demand for simple and inexpensive materials that have suitable properties for conversion and storage of energy is increasing. Our article deals with composite materials for solar energy conversion, which can be used in dye-sensitized solar cells. Our aim of thesis was preparation and testing of the carbon based composite materials. These materials were prepared by adding nanotubes (MWCNTs) and / or the graphene oxide (GO) to an active cathode or anode material or to the electrolyte. Electrochemical characterization methods as current-voltage characteristics and electrochemical impedance spectroscopy were used and structure of the samples, was observed by scanning electron microscopy. The solar cells were illuminated by a halogen lamp where the colour filters can be changed or by the solar radiation and the cells were measured by black-out too. We found that the addition of GO and MWCNTs to an active electrode improved the results of the cells compared to the samples the carbon-based materials directly to the electrolyte were applied. The addition of GO to an anode (the sample  $\text{TiO}_2+\text{GO}$ ) showed the best values of current (see Fig.1) and therefore improved fill factor and significantly reduresistance.



**Fig. 1.** Current – voltage characteristics of the sample  $\text{TiO}_2+\text{GO}$



**Fig. 2.** The sample of the dye synthesized solar cell

#### Acknowledgements:

This work was supported by the Projects APVV-0677-11 and APVV-14-0103 of the Slovak Research and Development Agency and VVGS-PF-2016-72645 of Pavol Jozef Šafárik University.

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## Degradation Behaviour of Porous Iron Materials with Polymer Coating in Simulated Body Fluid

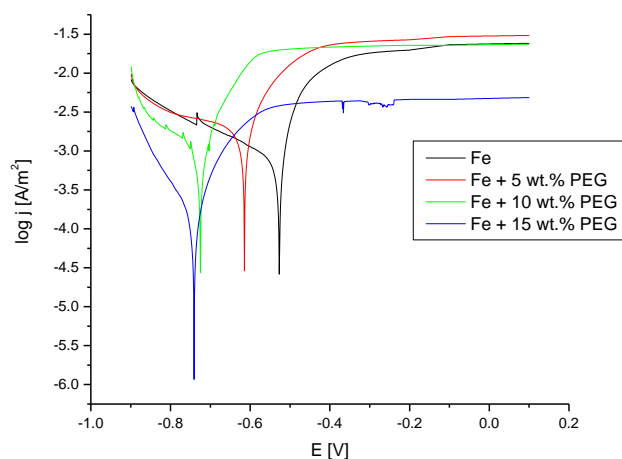
L. Markušová-Bučková<sup>a\*</sup>, R. Oriňaková<sup>a</sup>, A. Oriňak<sup>a</sup>, M. Kupková<sup>b</sup>, M. Hrubovčáková<sup>b</sup>,  
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Degradable biomaterials represent a new class of materials to help in the treatment of damaged tissue by mechanical support and promote cellular proliferation. They gradually degrade with increasing tissue repair [1]. These materials resolve some problems caused by permanent implants, such as chronic inflammation, stress shielding, number of surgical interventions and so on [2]. In this work the corrosion behaviour of degradable materials based on carbonyl iron powder with polyethylene glycol (PEG) film have been studied for their potential use as orthopedic implants. The surface of porous samples was more compact and homogenous with increasing amount of polymer. Corrosion resistance of these materials was evaluated by potentiodynamic polarization curves and electrochemical impedance spectroscopy (EIS) method in Hank's solution. The addition of PEG has increased the corrosion potential in Hank's solution (Figure 1). The Nyquist plots obtained by EIS measurement with samples before and after 24 and 48 hour immersion in simulated body fluid indicate that the impedance value of tested samples decreases as the following: Fe, Fe + 5 wt.% PEG, Fe + 10 wt.% PEG, Fe + 15 wt.% PEG. The results of 12-week static immersion test show that PEG coated specimens exhibit higher mass losses compared to uncoated bare iron sample. We can conclude that the PEG coated iron based samples have better degradation behaviour than the uncoated ones and they seem to be promising temporary implant material for bone applications. Consequently, the cytotoxicity and the hemocompatibility of prepared materials must be verified.



**Fig. 1** Potentiodynamic polarisation curves of carbonyl iron samples with and without PEG film obtained in Hank's solution at pH 7.4 and 37°C at scan rate 0.1 mV/s.

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## Electrocatalytic Hydrogen Evolution at Electrospun Carbon Fibers Decorated with Nickel and Nickel Phosphide Nanoparticles

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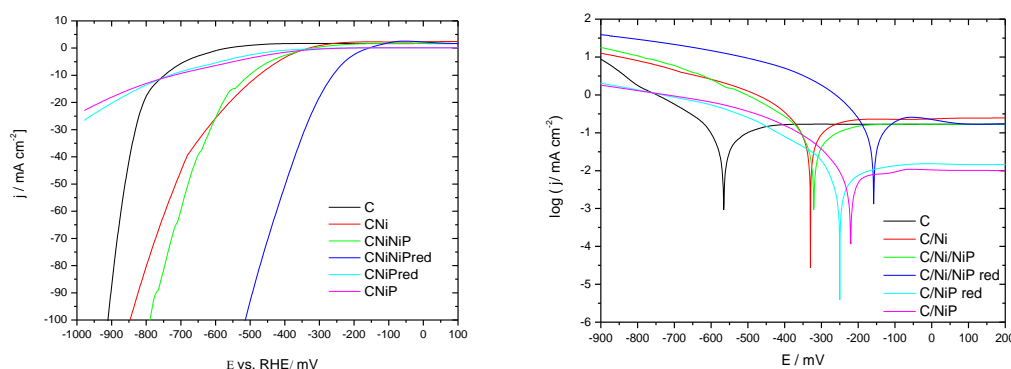
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The hydrogen evolution reaction (HER) acquired by the electrocatalytic reduction of water may provide a sustainable energy supply for the future, but this technique is currently limited due to a high price and resource scarcity of the used noble metals such as Pt. A lot of activities were therefore focused on the fabrication of electrodes enabling the effective and economically viable HER. At present, the electrodes from noble metals are preferentially replaced with various cheaper electrode materials with a comparable efficiency such as Ni and Ni-based alloys, for example, Ni/NiO core/shell nanosheets [1] or NiS<sub>2</sub> [2].

In this work, the carbon microfibers decorated with nickel, nickel/nickel phosphide and pure nickel phosphide nanoparticles were successfully prepared by means the simple needle-less electrospinning method as perspective electrode materials for an efficient hydrogen catalytic reaction. The polyacrylonitrile (PAN) was used for precursor fibers formation. The final morphology, porosity and position of the incorporated nickel or nickel phosphides nanoparticles can be designed by the calcinations temperature and used atmosphere. The linear sweep voltammetry and Tafel slopes measured in 0.5M H<sub>2</sub>SO<sub>4</sub> solution confirmed that the highest HER activity exhibit carbon fibers containing the nickel and nickel phosphide nanoparticles after the heat treatment in the hydrogen reduction atmosphere (Fig. 1).



**Fig. 1** LSV curves (a) and Tafel plots (b) of HER in 0.5 M H<sub>2</sub>SO<sub>4</sub> for fibrous samples with nickel and nickel phosphide nanoparticles and bare carbon fibers.

### Acknowledgements:

This work was supported by the Scientific Grant Agency VEGA of the Slovak Republic (Project 1/0074/17).

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### Electrochemical Degradation of Metallic Biomaterials

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Metallic biomaterials are required to interact with the body, promote the healing process, provide mechanical support for a certain time and progressively degrade. Materials such as stainless steel, titanium and its alloys and cobalt-based alloys represent the category of inert biomaterials. The Fe based alloys are one of the classes of metals that have been proposed as potential biodegradable materials [1]. But the mechanical properties of pure iron are modest and not particularly well suited for the use as biomaterial. To accelerate degradation and improve mechanical properties, the iron was alloyed with manganese. The manganese has been chosen because it is less noble than iron, it is known as an austenite-forming element, and from a biological point of view, the excess of manganese is not reported to be toxic in the body system [2]. Many studies have proved the potentiality of Fe-Mn alloys to be used in cardiovascular applications.

Pure Fe samples and samples from Fe-Mn alloys were prepared by a powder metallurgy from elemental iron and manganese powders. Powders were mixed in a turbula mixer for 20 minutes. The mixtures with 25, 30 and 35 wt.% Mn were prepared. All samples were prepared by blending, compressing and sintering with the aim to study their dimensional changes, microstructure, microhardness distribution and primarily the electrochemical corrosion behaviour in a simulated body environment.

The microstructure of specimens was investigated using optical microscope and scanning electron microscope coupled with the energy dispersive spectrometer. Corrosion properties were investigated using a potentiodynamic polarization method. Measurements were carried out with a conventional three-electrode arrangement by the use of the Autolab Potentiostat 302N. Corrosion of samples in the Hank's solution was investigated. In all experiments, the temperature was maintained at 37°C.

Before the polarization tests, the samples were kept immersed in the electrolyte for one hour and the evolution of the open-circuit potential (OCP) was recorded. The OCP corresponds to the difference in potential between the reference electrode and the metal immersed in a corrosive medium [3]. The corrosion potential of a freely corroding iron sample persistently decreased with time, while the corrosion potentials of Fe-Mn samples are therefore a smoother function of time. This indicated the localised corrosion of iron sample and more uniform corrosion of Fe-Mn samples.

Degradation rates of iron and Fe-Mn alloys immersed in the Hank's solution were examined by polarisation method. Polarisation curves were obtained by varying the applied potential from - 700 mV to - 300 mV at the scan rate 0.1 mV/s. The corrosion potential and corrosion current were calculated from the intersection of the anodic and cathodic Tafel lines extrapolations. From the polarisation measurements is evident, that the addition of Mn particles to the iron material causes a shift of corrosion potential towards to negative values. Thus the corrosion resistance of Fe samples was much higher than that of the Fe-Mn samples. The corrosion current density of Fe sample was approximately ten times lower than corrosion current density of alloy samples. The corrosion rates of Fe-Mn porous samples are higher than the ones reported for nonporous iron based samples. This could be affected by the higher surface area, roughness, and penetrable structure of material.

The iron based alloys prepared by powder metallurgical methods seem to be promising candidates for degradable biomaterials. The control of the biocorrosion rate, the improvement of mechanical properties and the reduction of the cytotoxicity are the subjects of future studies.

#### Acknowledgement:

This work was supported by the Slovak Grant Agency VEGA under project No.1/0211/12 and by the project APVV-0677-11.

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**Electrochemical Preparation and Characterization of PPy, Ag/PPy and Ni/PPy Layers  
as Electrocatalysts for Hydrogen Evolution.**

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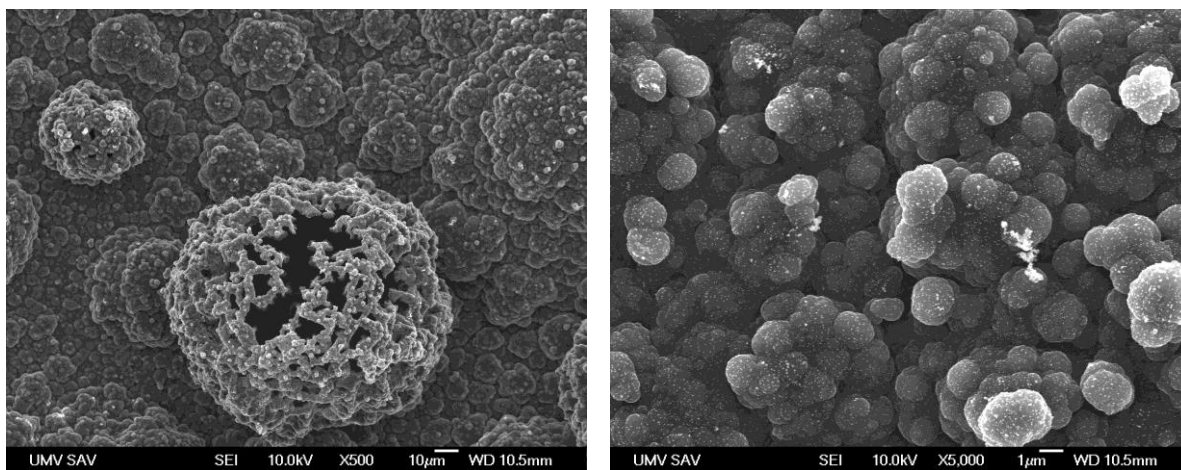
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Hydrogen, the most abundant element on earth, is the cleanest and ideal fuel. Therefore, hydrogen is increasingly considered as the fuel of the future [1]. The techniques such as electrolysis, photocatalysis and thermolysis are employed to produce hydrogen [2].

This work presents the electrochemical preparation and characterization of nanostructured layers and study of their electrocatalytic activity in the hydrogen evolution reaction. The influence of experimental conditions of pyrrole polymerization on the surface morphology and electrocatalytic activity of polypyrrole films was studied. The results showed that the best morphology as a matrix for nanostructured metallic layer exhibited the PPy layer prepared at the highest concentration of polypyrrole monomer, the lowest pH value, and lower scan rate without stirring.

Moreover, the deposition of nanostructured silver and nickel layers on polypyrrole substrate using cyclic voltammetry was studied. The effect of experimental conditions, such as potential range and number of deposition cycles on surface morphology of Ni and Ag layers was examined. The performance of prepared layers in electrocatalytic hydrogen evolution reaction was evaluated. Owing to higher surface area of active material dispersed on PPy matrix, hybrid layers exhibited better electrocatalytic activity in hydrogen evolution reaction. The higher electrocatalytic activity and stability of Ag/PPy hybrid layer was observed compared to Ni/PPy hybrid layer. The highest electrocatalytic activity showed hybrid layer produced after 10 cycles of Ag electrodeposition (Ag10/PPy) (Figure 1).



**Fig. 1** SEM images of Ag10/PPy layers obtained by electrodeposition in the range of potential from -350 mV to +250 mV.

**Acknowledgements:**

This work was supported by the Scientific Grant Agency VEGA of the Slovak Republic (Project 1/0074/17).

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### Hydrophobicity of Silver Layers Induced by Microparticle Geometry

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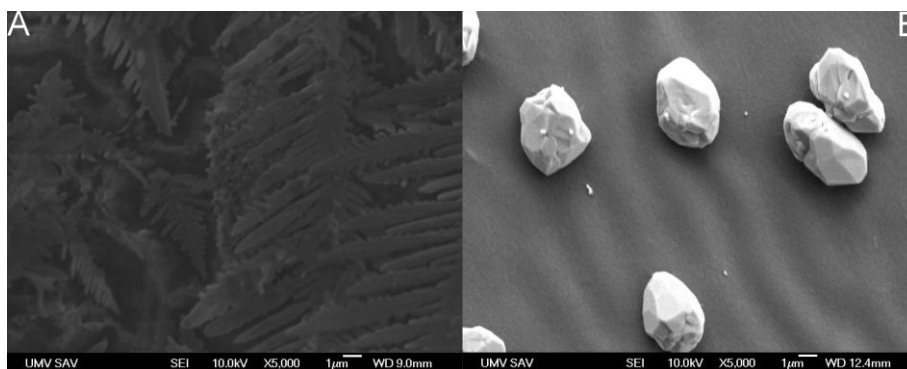
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We have employed an easy and inexpensive methods of electrochemical deposition to prepare a set of silver surfaces. The focal point of this study was investigation of the effect of the duration of the current deposition cycle and the number of current pulses on the geometry of silver microstructured surfaces and on the free surface energy, polarizability, hydrophobicity and thus adhesion force of the silver surfaces. We have observed that the changes in surface hydrophobicity were primarily influenced by the size and density of the microparticles on the surface. The results have shown that morphology of the silver microparticles was related to number of current pulses mainly, while the duration of one current pulse has only a minor effect on the final surface microparticle geometry and thus on the surface tension and hydrophobicity. We have found out that the surface hydrophobicity depended predominantly on the length of the dendrites not on their width. The highest silver surface hydrophobicity was observed on a surface prepared by 30 current pulses with a pulse duration of 1 s (Fig. 1A), the lowest hydrophobicity was observed when deposition was performed by 10 current pulses with a duration of 0.1 s (Fig. 1B). We have calculated the partial surface tension coefficients  $\gamma^D_s$ , polarizability  $k_s$  of the silver surfaces, we have transformed the conventional geometry of the silver microparticles to the fractal dimension  $D$  and we have also derived the relation for adhesion strength determination [1]. All calculated parameters can be applied in future applications in living cells adhesion prediction and spectral method selection. Silver films with microparticle geometry showed a lower variability in final surface hydrophobicity when compared to nanostructured surfaces [2]. The comparisons could be used to modify surfaces and to modulate human cells and bacterial adhesion on body implants, surgery instruments and clean surfaces.



**Fig. 1** Representative SEM micrographs of electrochemically prepared silver microparticles; A – particles prepared by 30 pulses with duration of 1 second; B – particles prepared by 10 pulses with duration of 0.1 second.

#### Acknowledgements:

This work was supported by the Projects VEGA 1/0074/17 of the Scientific Grant Agency of Ministry of Education SR, APVV-0677-11 and APVV-0280-11 of the Slovak Research and Development Agency.

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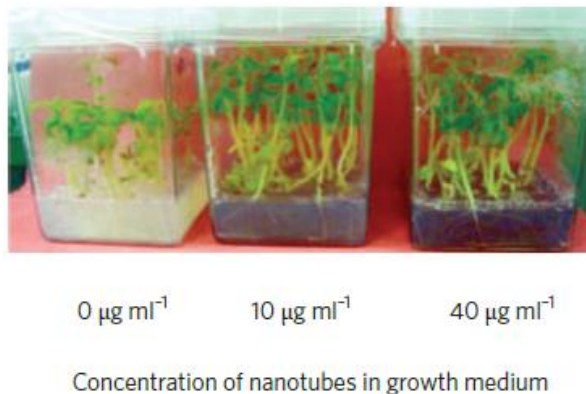
### Intelligent Nanofertilizers

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The present work deals with the intelligent nanofertilizers using for increasing demand for food, biomass, biofuel production and decreasing economical and environmental implications. Nitrogen, which is a key nutrient source for food, biomass, and fibre production in agriculture, is by far the most important element in fertilizers when judged in terms of the energy required for its synthesis, tonnage used and monetary value. However, compared with amounts of nitrogen applied to soil, the nitrogen use efficiency (NUE) by crops is very low [1]. Numerous attempts to increase the NUE have so far met with little success, and the time may have come to apply nanotechnology to solve some of these problems. Carbon nanotubes were recently shown to penetrate tomato seeds [2], and zinc oxide nanoparticles were shown to enter the root tissue of ryegrass [3] (Figure 1). This suggests that new nutrient delivery systems that exploit the nanoscale porous domains on plant surfaces can be developed. The potential use of nanotechnology to improve fertilizer formulations, however, may have been hindered by reduced research funding and the lack of clear regulations and innovation policies. Current patent literature shows that the use of nanotechnology in fertilizer development remains relatively low (about 100 patents and patent applications between 1998 and 2008) compared with pharmaceuticals (more than 6,000 patents and patent applications over the same period) [4]. A nanofertilizer refers to a product that delivers nutrients to crops in one of three ways. The nutrient can be encapsulated inside nanomaterials such as nanotubes or nanoporous materials, coated with a thin protective polymer film, or delivered as particles or emulsions of nanoscale dimensions. Owing to a high surface area to volume ratio, the effectiveness of nanofertilizers may surpass the most innovative polymer-coated conventional fertilizers, which have seen little improvement in the past ten years [5].



**Fig. 1** Nanomaterials can enter plants. Improved growth of 27-day-old tomato seedlings grown in a medium containing carbon nanotubes [3].

#### Acknowledgements:

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### Nanostructured Surfaces for Biomedical Applications in Diagnostics

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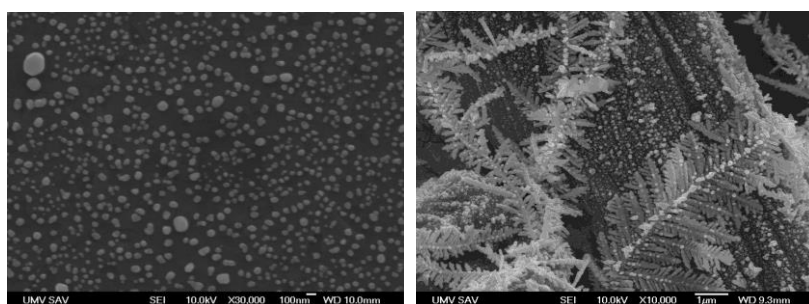
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In today's advanced age, there is very actual need to search more effective and more sensitive diagnostic methods. Surface enhanced Raman spectroscopy is a very promising diagnostic technique providing an accurate image of the composition of analyzed biological samples. The success of this method of analysis involves the use of the most suitable SERS active substrate that will give us the highest analytical signal enhancement. Existing research shows the sensitivity of SERS at one molecule with an enhancement factor of  $10^{14}$  [1]. This fact supports all efforts to study changes on molecular level and differences in the composition of body fluids. SERS becomes an excellent diagnostic tool for differentiation of biological samples from healthy and oncological patients by detection of changes in SERS spectra and by final statistical measurements [2].

Our aim is to prepare the most suitable nanostructured substrate for blood serum SERS analysis, which will be used as a detecting chip for diagnostic microfluidic device. We have chosen two types of solid supports for SERS substrates – ITO glass and filtration paper. Nanostructured substrates were prepared electrochemically by potentiostatic method. We were able to modulate shape, size and density of deposited nanoparticles by changing of input parameters of electrodeposition. Figure 1 shows different shapes of nanostructures deposited on ITO glass (a) and on conductive filtration paper (b) at the same conditions of electrochemical deposition.



**Fig. 1:** Potentiostatic deposited silver nanostructures at the -0,05V potential and 120 s from  $\text{Ag}_2\text{SO}_4$  electrolyte on a) ITO glass (mag. 30 000x) b) conductive Ni-filtration paper (mag. 10 000x)

SERS analysis was performed on the ITO glass with deposited silver nanostructured film using model analyte – rhodamine 6G with different concentration. The highest signal enhancement was evaluated at  $8.18 \times 10^6$  for sample potentiostatically deposited at 800s and -0.04 V. We have prepared substrate which enhanced analytical signal 8 million times, compared to reference measurement of rhodamine 6G with the same concentration on non-nanostructured silver surface. Now we are optimizing conditions of electrochemical deposition of nanostructured silver on the conductive filtration paper to increase its hydrophobicity, what is important for preconcentration of sample on the substrate surface. This ensure detailed SERS spectras and much higher signal enhancement.

#### Acknowledgements:

This work was supported by the Scientific Grant Agency VEGA of the Slovak Republic (Project 1/0074/17).

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## Novel MWCNTs-based Composite Catalysts in Direct Thermal Decomposition of Methane

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Hydrogen is considered as a clean, viable alternative fuel and “energy carrier” of future. It is also of great industrial interest and is used in chemical processes, as for the desulphurization or hydrogenation, in production of ammonia and fertilizers. The major problem in utilization of pure hydrogen as the fuel is its unavailability in nature and the need for inexpensive production methods [1]. 95 % of hydrogen is produced from fossil fuel but current methods emit large amounts of carbon dioxide. Pyrolysis is more ecologic and has lowest environmental impact from methods which use fossil fuels as hydrogen precursor, in the total production of carbon dioxide emission and consumption of energy [2]. An advantage of the pyrolysis is that resulting products are in two phases, specifically solid carbon and gaseous hydrogen, therefore the latter mentioned can be directly used in fuel cells and this will eliminate the need for different carbon oxides separation and sequestration processes altogether. In addition high quality carbon obtained in this process [3]. The application of catalysts decreases an energetic requirement of process. In general, for thermal decomposition of methane the most studied are Ni, Co, Cu and Fe-based catalysts, very often on some kind of support [4]. The multiwalled carbon nanotubes (MWCNTs) satisfied requirements for support because they had large surface area and are very stable at higher temperature. Only few studies deals with this issue and therefore we studied performance of the metals, mentioned above, attached on MWCNTs in pyrolysis of methane. In a preparation of MWCNTs-based catalysts first the MWCNTs had to be activated (creation of functional groups, mainly carboxyl, where metal particles are formed) and purified in strong acids. A mixture of nitric and sulfuric acid was used (3:1) and mixture was refluxed 2 h. Next the MWCNTs were filtered off and dried. Then activated MWCNTs were used in method known as electroless deposition of metals. The electrolyte solution comprised typical components i.e. precursors of each metals (Ni, Co, Cu, Fe) in form of nitrates, buffer (pH 9.5; NaOH and Na<sub>2</sub>CO<sub>3</sub>) and reducing agent (formaldehyde and NaH<sub>2</sub>PO<sub>2</sub>). The attachment of metal particles was confirmed with TOF-SIMS, SEM and TEM. The best results with all catalyst were obtained at 900°C. The best conversion of methane to hydrogen (87%) was obtained with of Ni/MWCNTs. The Co/MWCNTs had the conversion rate 85%, and Fe/MWCNTs had value of 19%. The Cu/MWCNTs had lowest conversion 14%.

### Acknowledgements:

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## Plasmonic Nanostructured Surfaces Prepared by Colloidal Lithography

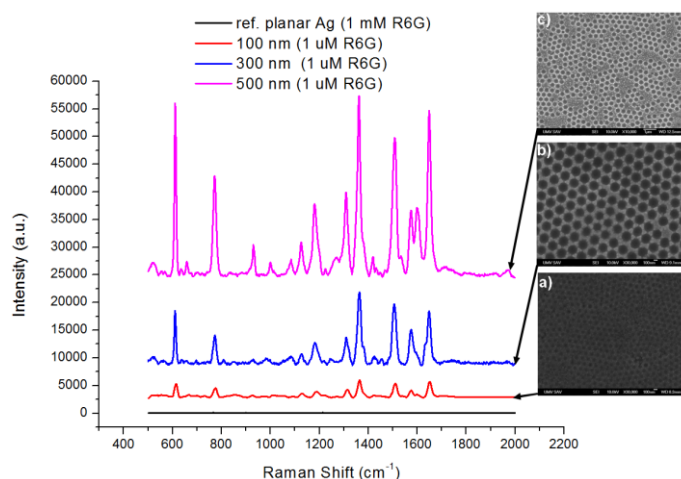
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Surface enhanced Raman spectroscopy is now widely used to characterize the functionality of plasmonic nanostructured surfaces. The main characteristic of plasmonic surfaces is the analytical signal enhancement, which ideally can lead to the detection of a single molecule [1]. The nanocavity metallic film prepared by the colloidal lithography and electrochemical deposition has advantages such as simplicity of the preparation, homogeneity of the surface, as well as the reproducibility of measurement results. In our work we focus on the SERS characterization of the Ni/Ag nanocavity films with different thickness and diameters. The preparation of a nanocavity film consists of three steps: the first step is the preparation of polystyrene beads monolayer with different diameter (100 nm, 300 nm, 500 nm) on hydrophilic glass slide, transfer onto the water surface and finally picking it up on the ITO electrode. Next step is electrochemical deposition of Ni from modified Watt's solution followed by dissolution of the polystyrene spheres. The last step is deposition of Ag from silver sulfate solution. These nanocavity films were tested as plasmonic substrate for Surface enhanced Raman spectroscopy with 532 nm excitation laser. Rhodamine 6G was used as a model analyte with different concentration for samples and reference which consist of planar Ag target for SIMS measurement. Fig.1 Shows representative SERS spectra of Rhodamine 6G and as can be seen, the intensity dramatically increased when the diameter of nanocavities was increased from 100 nm to 500 nm. The enhancement factor was calculated from the most intensive peak at  $610\text{ cm}^{-1}$  from spectrum measured at 500 nm nanovacity film and was established at value  $5,49.10^5$ . These results predict the use of hybrid Ni/Ag nanocavities films as a plasmonic substrate for detection of low concentrations of molecules in biodiagnostics, drug analysis, etc.



**Fig.1** SERS spectrum of  $1\mu\text{mol}\cdot\text{dm}^{-3}$  R6G measured on different nanocavities substrate with comparison on planar Ag target  $1\text{mmol}\cdot\text{dm}^{-3}$  concentration of R6G. Inset SEM images shows Ni/Ag nanocavities plasmonic films a) 100 nm nanocavities, 30 000x, b) 300 nm nanocavities, 30 000x, c) 500 nm nanocavities, 10 000x

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### References:

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### Preparation of Alginate Capsules for Pancreatic Cells Encapsulation

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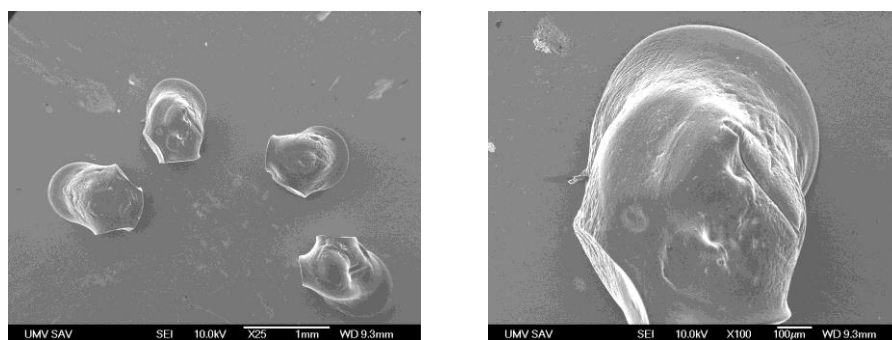
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Diabetes mellitus is heterogeneous metabolic disease characterized by sustained increase of glucose in blood called hyperglycemia [1]. Several types of diabetes are recognized, such as diabetes mellitus type I, diabetes mellitus type II, gestational diabetes mellitus and other specific types of diabetes. All these types of diabetes are caused by destroying or decreased function of  $\beta$ -cells.  $\beta$ -cells are part of the Langerhans islets presented in pancreas and represent 60 – 65% of Langerhans islets [2]. A problem with transplantation of Langerhans islets is autoimmune system that destroys transplanted  $\beta$ -cells immediately after transplantation. The solution of this problem is to create polymer capsule which works as polymer membrane. Polymer capsules can be formed from various polymers like sodium alginate, polyethylene glycol, chitosan etc. The main function of this polymer is to avoid the immune system destroy to encapsulated islet cells. Encapsulated islets of Langerhans would be able to produce sufficient amount of insulin and control the blood glucose level [3].

Size of about 800  $\mu\text{m}$  is considered to be optimal. It was found from other studies that the capsules of smaller size have been overgrown with tissue too quickly after transplantation. For this reason insulin cannot be transported through polymer capsules to the patient body. The aim of this work was to find suitable conditions for alginate capsules formation with adequate size for cells encapsulation. Alginate capsules were prepared by syringe pump. The size of capsules was affected by the size of the needle used (27G - 0.4 mm diameter, 25G – 0.5 mm diameter, 22G – 0.7 mm diameter and 21G – 0.8 mm diameter). The most appropriate size of capsules, about 800  $\mu\text{m}$  (Fig. 1) was obtained using 27G needle. The blood glucose level after 24, 48 and 72 hours encapsulation will be determined at gold screen printed electrode surface using cyclic voltammetry.



**Fig. 1** SEM images of prepared Alginate gel capsules prepared using 27G (0,4mm diameter) needle.

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#### References:

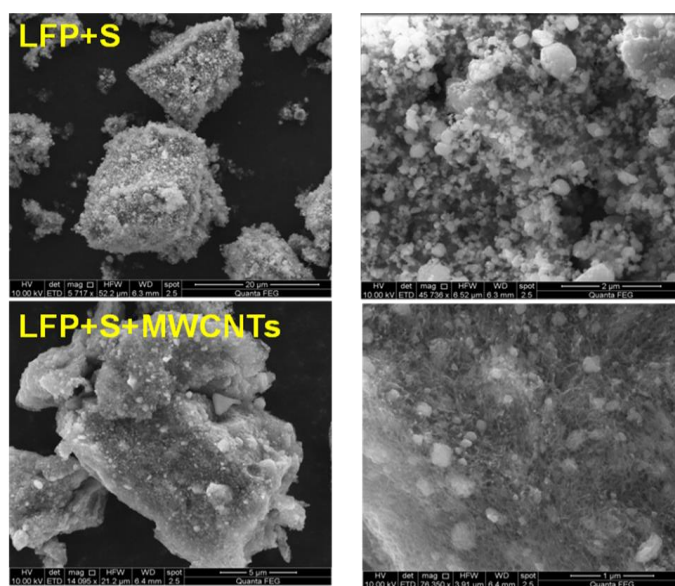
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## Sulfur Based Cathode Composites with MWCNTs Additives for High Performance Batteries

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Elemental sulfur is considered to be one of the most promising candidates as a material for the positive electrode of a high-performance lithium secondary battery, because sulfur has a high theoretical specific capacity of 1672 mAh g<sup>-1</sup> [1,2]. The higher energy density of the lithium-sulfur battery is due to the fact that each sulfur atom can bind two lithium ions, whereas, in the case of conventional battery types, less than one lithium ion is “captured” on average [3,4]. The advantage of lithium-sulfur batteries is primarily their superior storage capacity (energy density), but they also excel in economic and environmental terms. Sulfur is a relatively inexpensive and abundant raw material, unlike expensive elements, such as cobalt, which are used in lithium-ion batteries. This is important because material costs make up a very large proportion of the total cost of a battery. S-LiFePO<sub>4</sub>-PPy cathode material was synthesized using a solid-state method in ball mill. The preparation technique, composition and electrochemical performance of carbon-coated and MWCNTs coated S-LiFePO<sub>4</sub>-PPy nanoparticles were investigated. The S-LiFePO<sub>4</sub>-PPy cathode with MWCNTs additive showed an initial capacity of 1100 mAh/g at 0.1 C. Morphology of this sample is also very homogeneous and distribution of the pores and MWCNTs on the surface of the cathode particles is very well organized. The results suggest that the S-LiFePO<sub>4</sub>-PPy with MWCNTs additive can be used as a cathode material of lithium-ion batteries for large-scale application.



**Fig. 1** SEM images showing the morphology of the S-LiFePO<sub>4</sub> sample (up) and S-LiFePO<sub>4</sub>-MWCNTs sample (down).

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## LIST OF POSTERS

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- P9** Tioflavin T- G-quadruplex DNA Interaction, A. Halaganová, E. Demkovičová, P. Krafcíková, V. Víglaský
- P10** The Effect of Perturbation of Heme Region on Peroxidase-like Activity of Cytochrome c, M. Berta, N. Tomášková, R. Varhač, E. Sedlák
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**New trends in chemistry, research and education at Faculty of Sciences  
of P. J. Šafárik University Košice 2016**

**BOOK OF ABSTRACTS. NEW TRENDS IN CHEMISTRY**

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