

# XXII. WORKSHOP OF BIOPHYSICAL CHEMISTS AND ELECTROCHEMISTS

## BOOK OF ABSTRACTS

29<sup>TH</sup> JUNE 2022

BRNO

MASARYK  
UNIVERSITY



MUNI  
FACULTY  
OF SCIENCE

# **XXII. Workshop of Biophysical Chemists and Electrochemists**

## **Book of abstracts**

**29<sup>th</sup> June, 2022**

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## **THE ORGANIZATION HOSTING THE CONFERENCE**

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**The sponsors of the Workshop of Biophysical Chemists and  
Electrochemists:**

The organizers thank a lot to all this year's sponsors for the support, which enabled to organize this traditional conference: Metrohm Czech Republic s.r.o., Institute of Biophysics of the Czech Academy of Sciences in Brno, Eppendorf Czech & Slovakia s.r.o., Chromservis s.r.o., CHROMSPEC spol. s r.o., KEYENCE INTERNATIONAL (Belgium) NV/SA, LABOSERV s.r.o., MERCK, s.r.o., PRAGOLAB s.r.o., 2THETA ASE s.r.o., TRIGON PLUS s.r.o. and Czech Chemical Society, subdivision Brno.



### *An introductory word...*

Dear friends, dear colleagues,

We warmly welcome you to the 22<sup>nd</sup> year of our traditional conference (WORKSHOP OF BIOPHYSICAL CHEMISTS AND ELECTROCHEMISTS), which takes place again in the Bohunice University Campus (UKB) on June 29, 2022. This year's one-day Workshop will be carried out on the 200<sup>th</sup> anniversary of the birth of a prominent natural scientist, who made famous not only Brno, but the entire Czech scientific community – Gregor Johann Mendel – the founder of genetics and the discoverer of the basic laws of heredity.

The conference is organized under the patronage of the Rector of Masaryk University prof. MUDr. Martin Bareš, Ph.D., the Dean of the Faculty of Science, MU prof. Mgr. Tomáš Kašparovský, Ph.D., and the Director of the Department of Chemistry, Faculty of Science, MU doc. RNDr. Ctibor Mazal, CSc. We welcome friends from Slovakia (Slovak University of Technology Bratislava), Hungary (Faculty of Science, University of Pécs), and the whole Czech Republic. The Workshop program is very rich; in addition to 2 plenary and 5 invited lectures, there will be a total of 23 communications, of which 8 are competition presentations in the Youth Section. The three students with the best presentations of their scientific results will be honored with financial and book awards. Since 2019, the best work in the field of Bioelectrochemistry wins the Emil Paleček Award, which is organized by the Institute of Biophysics of the ASCR, v.v.i. in Brno.

In conclusion, we would like to thank all sponsors (the main sponsor METROHM, Czech Republic, loyal sponsors EPPENDORF Czech & Slovakia, TRIGON PLUS s.r.o., CHROMSPEC Ltd., CHROMSERVIS s.r.o., CZECH CHEMICAL COMPANY and new sponsors KEYENCE INTERNATIONAL, Belgium / LABOSERV s.r.o. and PRAGOLAB s.r.o., MERCK Group). Thanks also go to the Institute of Biophysics headed by the director doc. Eva Bártová (EP Prize) and all who will present and discuss their scientific knowledge. Without you, this conference would not be possible. We wish everyone a stimulating conference that will leave very nice memories in your mind, and that will give you a lot of positive energy for your further scientific and pedagogical work. Welcome to Brno, welcome to Masaryk University, and enjoy this conference!

Libuše Trnková, Iveta Třísková

### **Motto:**

*“The love of science is the love of the truth because honesty is a fundamental virtue of scientists“*

*Ludwig Feuerbach*

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# PLENARY LECTURES

## SINGLE MOLECULE JUNCTIONS WITH REDOX-ACTIVE CENTERS

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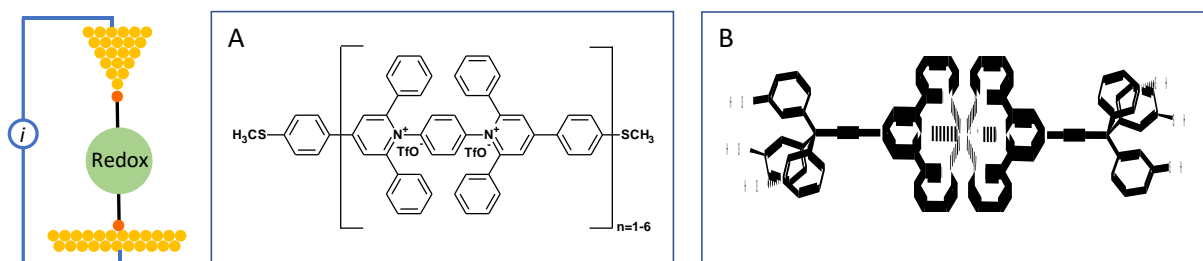
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Organic molecules have been suggested as building blocks of future electronic devices in order to overcome miniaturization limitations of the present-day silicon-based technologies. First electronic circuit based on molecules was demonstrated experimentally in 2003.<sup>1</sup> Since then conductance measurements of individual molecules by methods of the metal-molecule-metal junction formation represent a valuable tool in the field of molecular electronics.<sup>2,3</sup> Such measurements are currently performed in our laboratory on a large number of junctions using either scanning tunneling microscopy break junction (STM-BJ) or mechanically-controllable break junction (MC-BJ) techniques.<sup>4-7</sup>

Some of these results will be discussed in this contribution. The schematic representation of the experimental arrangement and representative selection of molecules are given in Figure 1. The discussion will be focused mainly on the conductance of single molecule junctions containing redox-active centers.



**Figure:** Schematic presentation of a metal-single molecule-metal junction (left) and two types of redox-active molecules (middle and right).

Several aspects of charge transport mechanism like conduction pathway, type and number of anchoring groups will be discussed. Break junction measurements will be complemented by quantum mechanical calculations of the junction evolution geometries and single molecule conductance values. The relationship between the charge transport and charge transfer will be scrutinized experimentally on a group of molecules containing pyridinium-based redox centers. Molecules containing one redox center are suitable for comparison of their charge transfer properties (Marcus theory) and charge transport properties within the metal-molecule-metal junctions (Landauer scattering approach). Experimental findings for selected redox systems will be discussed in terms of the relationship between electron transfer rates and zero-bias molecular conductance of non-adiabatic redox systems as formulated by Nitzan and Ratner.<sup>8</sup>

### ACKNOWLEDGEMENT

The work has been supported by the Czech Science Foundation (21-13458S), the Ministry of Education, Youth and Sports of the Czech Republic (Barrande project 8J21FR016), the French Ministries of Europe and Foreign Affairs (MAE) and of Advanced Education, Research and Innovation (MESRI), PHC Barrande, 2021 project no. 46775VG), Mobility Plus projects between the Czech Academy of Sciences and Hungarian Academy of Sciences (MTA-22-02).

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## SERUM ALBUMIN AS A MULTIFUNCTIONAL AND MODEL MOLECULE IN OUR EXPERIMENTS

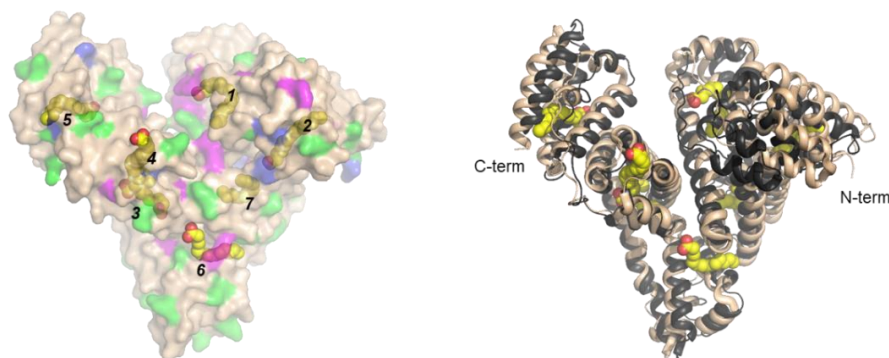
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Serum Albumin is a multifunctional protein with a molecular weight of 67 kDa that carries an overall negative charge at physiological pH. This protein is found in the serum at a concentration of 35–50 g/L. The main functions of this protein include maintaining oncotic pressure, the transport and distribution of fatty acids and thyroid hormones, bilirubin and ions (*e.g.* calcium), and last but not least, it binds a range of drugs. Its half-life is approx. 21 days and it is formed in the liver by the cleavage of preproalbumin. Albumin is used in a number of biochemical and analytical laboratories as a model (reference) protein, blocker of nonspecific binding sites, delivery system, protein component of culture media, molecular weight marker, and applications in clinical practice have been proposed. This protein is very well characterized in terms of its crystal structure, and there is probably no other protein for which we have such an extensive set of structural data and information about its function. For this reason, we have noticed serum albumin to be a "first choice" protein in a number of studies, without having sufficiently assessed its suitability for a given application or being sufficiently acquainted with its physicochemical properties under the given experimental conditions. This can lead to a number of artifacts and misinterpretations. The aim of this paper is to describe and critically assess the applications of mainly human (HSA) and bovine (BSA) serum albumin as model proteins and to discuss the following facts: a) Under native conditions, serum albumin occurs not only in the form of monomers, but also as oligomeric associates. b) Because the protein is isolated, its isolates also differ quite significantly in terms of quality and quantity. The researcher should be aware that he/she is working with a complex of albumin and many other low molecular weight substances. c) Serum albumin can be oxidized to a greater or lesser degree natively, but also during isolation, especially with a single free Cys34. In addition to oxidized forms, its glycosylated form and other oxidative modifications are commonly found in samples. Thus, individual isolates may differ quite significantly in their reactivity to other target molecules. d) The crystal structure (heart-shape) differs from the structure in aqueous solution. e) Also, if serum albumin interacts with surfaces, its structure is subject to local deformations (surface denaturation). Conversely, its global structure changes upon the binding of selected ligands, such as fatty acids, as indicated in the figure below. f) The protein is highly soluble in water, but it also contains hydrophobic domains. From the modest list of points a-f above, it follows that despite the simple isolation and purification of albumin, the standardization and interpretation of the results obtained with it can be quite difficult. Have we gotten used to using serum albumin actively and often routinely in our experiments, without further discussion and critical reflection? The intention of the author of this contribution is to remind us of the dangers that arise from such generalizations, and of specific experimental mistakes that we could make when working with albumin. The multifunctionality of albumin under physiological conditions

suggests that there will be many modalities and variables of this protein in our biochemical or biophysical experiments.



**Figure:** HSA structure with bound oleic acid (PDB 1GNI). (Left) Surface model of HSA. The OA is shown as yellow spheres, lysine (colored in green), histidine (blue) and arginine (pink) residues are shown in stick representation. OA molecules are numbered as in PDB 1GNI. (Right) Superposition of native HSA structure (PDB 1BM0, colored in black) and HSA complex with 7 OA molecules (PDB 1GNI, colored in brown). For more details, see *Int. J. Biol. Macromol.* 203 (2022) 116–129.

## ACKNOWLEDGEMENT

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# LECTURES

## SPECTRO-ELECTROCHEMICAL PROPERTIES OF PHOSPHOLES – MOLECULES FOR ORGANIC ELECTRONICS

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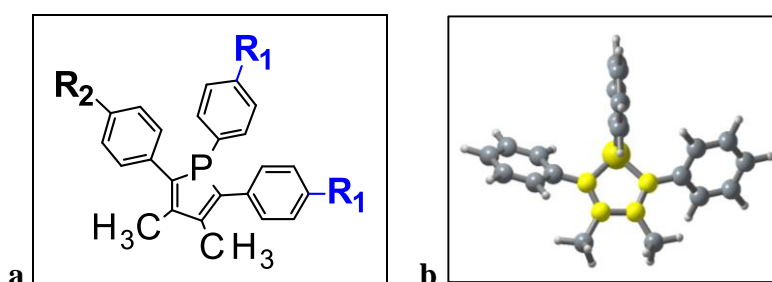
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New candidates for organic electronics, pentasubstituted phospholes with extended  $\pi$ -conjugated arms in positions 1,2 and 5 were synthesized using a new procedure [1] and characterized electrochemically and by UV-vis and EPR spectra. Quantum chemical calculations of redox potentials, optimized structure and HOMO-LUMO energies were performed and successfully correlated with experimental data. Combination of induction and resonance effects of substituents, extension / diminution of the  $\pi$ -delocalized system and steric changes affecting intramolecular electron communication can result in tuning of redox and photophysical properties.

The studied derivatives involve tri-coordinated phosphorus atom with a non-bonding electron pair. Phospholes are non planar, hence they behave rather like dienes [2, 3] and exhibit the lowest aromaticity within the series of analogous pyrrol, thiophene and furan. They are substituted asymmetrically (substituents R1 and R2 in positions 1,2 and 5 – cf. Fig. 1a), whereas in the positions 3 and 4 are methyl groups. The front view (Fig. 1b) shows that the aryl in the position 1 is perfectly perpendicular to the plane of the heterocycle, therefore this substituent is completely electronically isolated. On the other hand, the two aromates in the positions 2 and 5 are partly twisted, therefore some  $\pi$ -overlap with the heterocycle is preserved. The expected application involves solar cells, OLEDs or fluorescent probes [4, 5].



**Figure:** a) Manner of substitution within the series; b) Geometry of the basic derivative.

In this contribution [6] we focus on the first oxidation and the first reduction potentials and their difference, which we call "electrochemical gap" (as an analogy to HOMO-LUMO gap). This value is related to electron delocalization and also to the push-pull abilities of substituents and, in this way, electrochemistry can be interconnected with photochemistry and light absorption or emission. All first reduction and oxidation potentials are reversible or quasi-reversible, therefore they are thermodynamically relevant and thus suitable for correlation with quantum chemical calculations.

The new compounds could be arranged into several individual homologous „series“, where influence of substituents and their position on a) reduction / oxidation potentials; b) changes and extent of electron delocalization; c) absorption / emission of light, was followed and evaluated. The understanding of the structure–properties relationship is the main aim of the study and will be basis of the design of the next series.

### ACKNOWLEDGEMENT

The authors are grateful to the grant support from GAČR No. 18-12150 S and to the institutional support RVO 61388955.

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- [6] to be submitted



## CLINICAL SAMPLES IN ELECTROCHEMICAL ANALYSIS - RECOMMENDATIONS AND BEST PRACTICE

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In recent years, electrochemical analysis (EC) has made a progress towards clinical applications and hospital laboratories. Unfortunately, many EC studies describing various (cancer) biomarker detection are still missing application to clinical samples, although it is known that the clinical samples may due to their complex nature significantly affect overall performance of published assays, especially their efficiency and sensitivity. We observed lower sensitivity in majority of our studied clinical samples in comparison to synthetic target or model cell lines, i.e., when detecting human papillomavirus (HPV) DNA in cervical cancer samples [1,2], or long noncoding RNA e.g. PCA3 in prostate cancer samples [3]. The multicomponent contents of real samples and higher dilution of analyte can be the explanation for these observed effects. Although measurements of real clinical samples often provide lower signals than synthetic or cell line models, we show that sensitivities of our assays are sufficient for given biomarkers, suggesting potential application of biosensors and bioassays into a clinical environment [1-3]. The main reason for relatively small number of published works using real clinical samples can usually be an inaccessibility of clinical samples in research organizations with weak connections to clinicians. These opportunities are available via biobanks, i.e., banks of human biological materials. Masaryk Memorial Cancer Institute serves as a coordinator of National Research Infrastructure of Biobanks and Biomolecular Resources (BBMRI.cz), which is connected to European research infrastructure for biobanking (BBMRI-ERIC). Moreover, biobanks provide not only samples of biological materials (tissue, blood, urine, stool, serum, plasma, primocultures, etc.) from patients with various diagnoses, but also associated data and other services linked with biobanking e.g. usability of samples/data in planned/running project, etc. [4, 5].

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## NANOSCALE ORGANIZATION OF LIPID MEMBRANES

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Biochemical experiments performed more than 20 years ago suggested that plasma membranes of living cells are compartmentalized into small submicroscopic structures (nanodomains) having potentially relevant biological functions. Although this hypothesis has stimulated intensive research in many scientific disciplines, structural features of these nanodomains as well as their importance for the function of biological membranes remain elusive. What exactly are these nanodomains? And do they still exist in 2022? In my lecture, I will look for answers to these questions by introducing a fluorescence microscopy technique MC-FRET developed in our laboratory. I will show that this technique enabled characterization of various types of membrane nanodomains with unprecedented detail and significantly contributed to the current understanding of lipid nanodomains that are formed in simplified models of cellular membranes

### ACKNOWLEDGEMENT

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# THE YOUNG SCIENTISTS SESSION

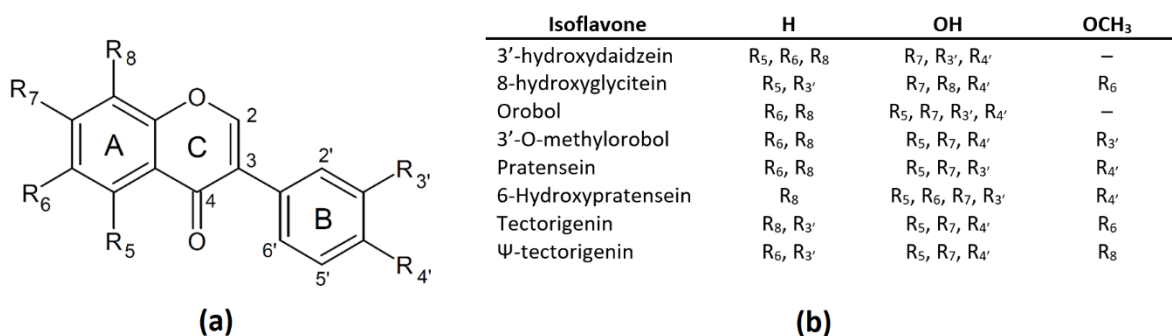
## IMPACT OF SUCCESSIVE DEPROTONATION ON THERMOCHEMISTRY OF RADICAL SCAVENGING EFFECT OF ISOFLAVONES IN WATER

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Isoflavones are sub-group of a large class of flavonoids, which can be found in various plants. They exhibit antioxidant, antiviral, antibacterial or anti-inflammatory effect. Isoflavones consist of main skeleton with two condensed rings (A and C) and phenyl ring (B) attached at C3 atom, and several hydroxy groups attached to rings A and B (see Figure 1) [1]. Hydroxy groups are weakly acidic and can undergo successive deprotonations in aqueous solutions. Thus, one of important factors in observed primary antioxidant action is pH of the environment. With increasing pH, there is higher relative abundance of deprotonated species and enhanced radical scavenging activity is observed [2, 3]. Therefore, two mechanisms of the radical scavenging effect play an important role: Hydrogen Atom Transfer (HAT) and Sequential Proton-Loss Electron-Transfer (SPLET) [4].



**Figure:** (a) isoflavone skeleton with ring labeling and carbon atoms numbering; (b) list of studied isoflavones

Geometry optimizations and thermodynamic calculations were performed in Gaussian 09 [5] program package using B3LYP [6, 7] functional and 6-311++G(d,p) basis set [8]. Optimized structures were confirmed by vibration analysis to be real minima. Solvent effect of water was described using Integral Equation Formalism Polarized Continuum Model (IEF-PCM) [9]. Then, relevant reaction enthalpies were determined from the calculated total enthalpies. Found results are in accordance with weakly acidic nature of phenolic OH groups, because Proton Affinities (PA, first step of the SPLET mechanism) are considerably lower than O–H Bond Dissociation Enthalpies (BDE, representing reaction enthalpy of HAT mechanism). Low PA values suggest the presence of phenoxide anions of isoflavones in aqueous solution at pH = 7 in agreement with experimentally determined pK<sub>a</sub> values. Therefore, reaction enthalpies of the two mechanisms were studied also for phenoxide anions. As it is expected, PA values for isoflavone anions are higher than PA values of non-dissociated molecules. However, only up to 10 kJ mol<sup>-1</sup> increase was identified, when two consecutive deprotonations occur in different aromatic rings, specifically A and B rings. Low enthalpies of dianion formation can be

attributed to 4'-OH and 7-OH groups. For molecules and preferred (poly)anions, Electron Transfer Enthalpies (ETE, second step of SPLET) were studied. We have confirmed that increasing negative charge in anionic species results in the decrease in ETE. Decrease in O-H BDE upon successive deprotonations was observed, too.

Results of this study suggest that consecutive deprotonations of OH groups in isoflavones in aqueous solution result in the lower O-H BDE values, as well as considerable drop in ETE. It is important to note, that the type of scavenged radical and the reaction kinetics may also affect the dominant reaction pathway.

### ACKNOWLEDGEMENT

The work has been supported by Slovak Grant Agency (1/0504/20 and 1/0461/21).

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**ELECTROCHEMICAL IMMUNOSENSOR FOR THE DETECTION OF HMGB1 LEVELS IN SERUM**

Tereza HLAVÁČOVÁ, Petr SKLÁDAL

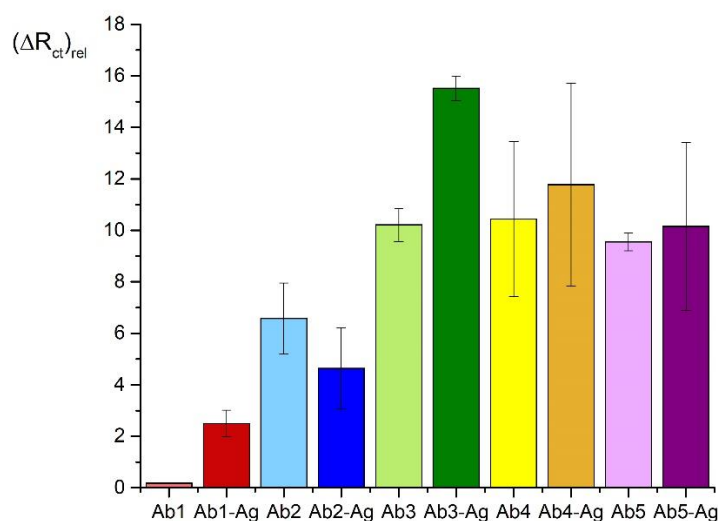
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HMGB1 (High Mobility Group Box1) is a nuclear protein stabilizing nucleosome formation and regulation gene transcription, DNA replication and DNA repair. [1] The protein can be secreted by activated monocytes and macrophages or it is passively released from necrotic and damaged cells.[2] HMGB1 is monitored cancer marker, extracellular forms have been associated with formation, progression, and metastasis of the tumour. [3] HMGB1 stimulates not only tumour growth, but also acts as tumour suppressor depending on interaction with ligands and location. In nucleus it has important role in gene stability and its deficiency causes telomere shortening, thus chromosome recombination and degradation.[4] HMGB1 interacts with DNA, RNA, many proteins, including antibodies, lipids, and other molecules in serum. Pre-treatment of plasma with perchloric acid efficiently removes majority of the interfering contaminants and can overcome short half-life for HMGB1 isoforms in patients if performed after serum preparation. [5]

The most common method for measurement HMGB1 levels is ELISA. It is preferred to use sandwich ELISA for the detection HMGB1. The Western blotting (WB) enables determination of HMGB1 levels in serum as well as detection of its isoforms. [6] However, using WB for determination of the protein is laborious and semi-quantitative, and only in combination with mass spectrometry (MALDI-TOF) enables the detection of isoforms of the HMGB1. Although ELISA is the routinely used method for the determination of HMGB1 levels and can detect 0.2–2 ng/ml of HMGB1, the analysis is time-consuming, and results are not reliable due to the interfering protein from plasma/serum. [5] Hence rapid, cost-effective, and accurate method for determination of HMGB1 levels could be interesting.

Electrochemical immunosensor for the detection of HMGB1 levels, based on disposable sensing elements, is being developed. Electrochemical impedance spectroscopy can follow interaction of HMGB1 with capture antibody immobilized onto gold electrode as change of impedance as formation of the immunocomplex blocks the electrode surface. This enables rapid measurement consisting of 2 min initial impedance, 15-30 min incubation with HMGB1, and 2 min of repeated impedance scan; the impedance measurements can be shortened if single impedance value at chosen frequency is obtained. A higher sensitivity is obtained using secondary antibody conjugated with peroxidase (HRP) resulting in sandwich complex. Afterwards, either amperometric or impedimetric detection of oxidation of 4-chloro-1-naphthol used as HRP substrate is carried out as product of enzyme reaction precipitates on the electrode surface.

The success of the electrochemical immunosensor depends on the specificity of the monoclonal HMGB1 antibodies showed in the Figure, where Ab1 and Ab3 provided, as expected, difference between blank and positive sample. Other antibodies failed with fluctuating and non-specific responses. Further, an advanced version will be constructed enabling simultaneous analysis of a few standards and samples.



**Figure:** Impedance changes depending on the choice of the capture antibody; light colour: blank, dark colour – positive samples of recombinant HMGB1 (Ab-Ag)

## ACKNOWLEDGEMENT

The work has been supported by AZV ČR, Czech Health Research Council grant number NU20-08-00106.

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## HYALURONIC ACID-BASED HYDROGELS WITH TUNABLE MECHANICS FOR IMPROVED STRUCTURAL AND CONTRACTILE PROPERTIES OF CELL

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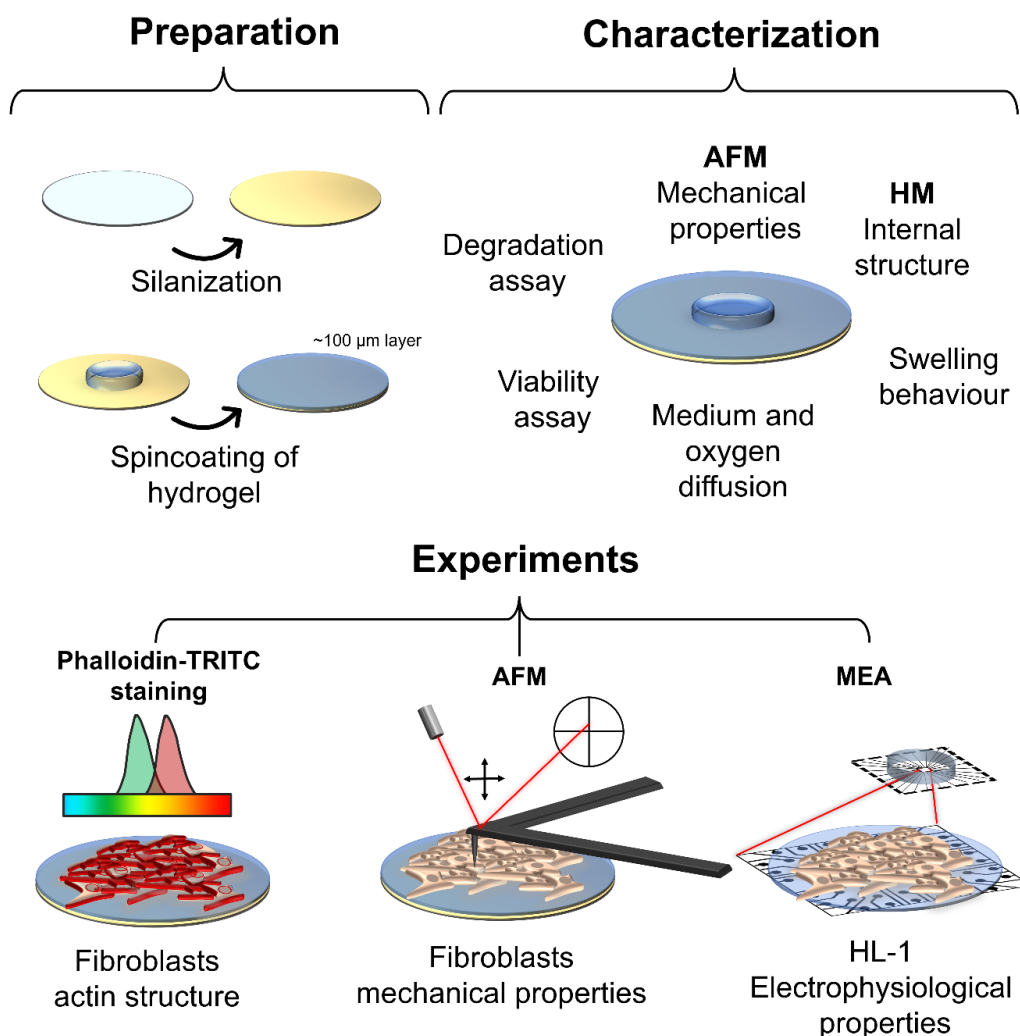
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Cells respond to various cues including chemical signals, protein interactions, and the mechanical properties of the extracellular matrix. Successful development of human *in vitro* model systems depends on the right cellular approach, but in recent years, mechanical properties of cellular surroundings is becoming a crucial factor for the physiological relevance of the given model. Hydrogels are 3D networks of synthetic or biopolymers that have been utilized in medical and research applications for decades now. This study presents a robust hydrogel system with tunable mechanical properties. A Hyaluronic based hydrogel system with tunable mechanical properties was successfully developed, and three separate hydrogels differing by their stiffness were prepared and spin-coated. Characterization showed a correlation between each hydrogel's mechanical properties, internal structure, and swelling capacities. Moreover, viability assay and experiments with the diffusion of Aminophylline, a typical model drug, and electrochemical measurement of oxygen diffusion, proved the usability of the presented hydrogel system for 2D and 3D cellular cultures. Experiments with cells showed vast internal and morphological changes of fibroblasts on hydrogel compared to control, further expanding the insight into mechanosensing cellular capabilities. Lastly, experiments with HL-1 cells showed, that hydrogel coating was associated with improved mechanical and electrophysiological contractile properties.





AFM – Atomic Force Microscopy, HM – Holographic Microscopy, MEA – Multi-electrode Array

**Figure:** Schematic representation of hydrogel preparation, characterization, and experiments. EDC/NHS crosslinked hydrogels were spin-coated on silanized glass bottom petri dishes. Characterization experiments consists of probing the mechanical properties, internal structure, swelling, diffusion and degradation behavior, together with viability assay. Main experiments included measuring of mechanical properties and structural changes of fibroblast on hydrogels compared to glass, plastic and 0.1% gelatin-covered dishes. Lastly, Electrophysiological properties of HL-1 cells on hydrogels was measured.

## ACKNOWLEDGEMENT

CIISB, Instruct-CZ Centre of Instruct-ERIC EU consortium, funded by MEYS CR infrastructure project LM2018127, is gratefully acknowledged for the financial support of the measurements at the CF Nanobiotechnology.

## ON THERMODYNAMICS OF QUINONE/HYDROQUINONE AND CATECHOL/QUINONE COUPLES AND CONSTRUCTION OF POURBAIX DIAGRAMS

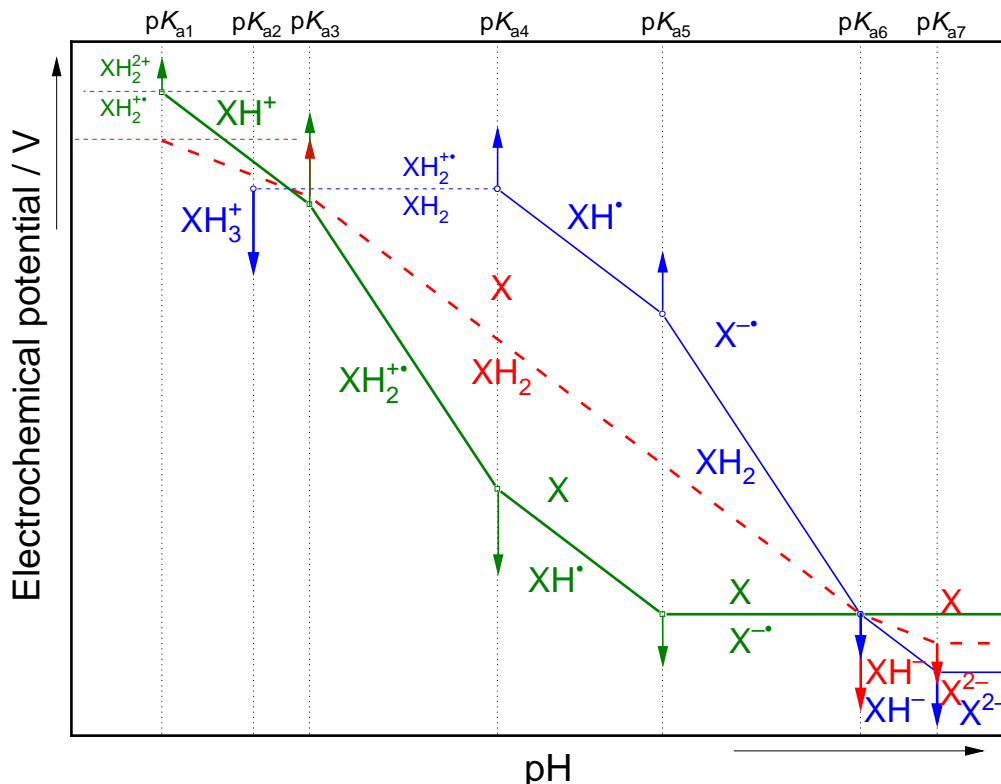
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The electrochemical reduction potentials represent a direct measure of thermodynamic feasibility of oxidation–reduction half reactions. These reactions are fundamentally important in many aspects of organic and environmental chemistry, as well as in materials science and in biology [1]. The high reactivity of many radical species occurring in electrochemical reactions or the mechanistic complexity of redox reactions can make the direct experimental measurement of a corresponding reduction potential difficult. For this reason, the computational chemistry based on the Density functional Theory (DFT) offers a valuable alternative to experiment for the characterization of redox reactions [2]. The critical point of theoretical calculations represents the description of solvent effects. Explicit models are often less computationally economical, but can provide a physical spatially resolved description of the solvent. The second alternative represent implicit solvent models where the solute is encapsulated in a molecular-shaped cavity embedded in a dielectric continuum [3].

Proton-coupled two-electron (PCTE) transfer reactions are of great abundance in plants and living systems. In particular, the PCTE transfers in quinone/hydroquinone redox couples are behind oxidative phosphorylation (ADP-to-ATP) and photosystem [4]. Quinones can successively undergo the first and second electron reduction steps to produce quinone anion ( $X^-$ ) and quinone dianion ( $X^{2-}$ ), respectively. With further accompanying to protonation or deprotonation, it converts among quinone (X)/semiquinone ( $HX^*$ )/hydroquinone ( $H_2X$ ) triad [5].

These redox equilibria are dependent on the pH conditions and they can be depicted using Pourbaix diagrams. These electrochemical potential-pH diagrams consist of three types of lines (see **Figure**). Acid-base equilibria are independent of potential and are represented by a vertical line on the E-pH diagram. Simple redox equilibria are represented on an E-pH diagram by a horizontal line. Finally, the rest lines describe the PCTE transfer.



**Figure:** The general scheme of Pourbaix diagram of studied systems.

In this theoretical study, we have discussed possible acid-base reaction steps occurring during the oxidation of dihydroxybenzene and catechol in water. The Pourbaix diagrams were constructed based on the predicted  $pK_a$  acidic constants values and available experimental or theoretically evaluated electrochemical potentials vs. SHE (Standard Hydrogen Electrode). The calculated results enable the identification of alternative reaction pathways of the radical scavenging abilities of studied molecules. The theoretical limits and chemical precision of used treatments will be also discussed.

## ACKNOWLEDGEMENT

The work has been supported by Slovak Research and Development Agency (APVV-19-0024) and VEGA 1/0461/21.

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## REAGENTLESS CHRONOPOTENTIOMETRIC MEASUREMENT OF ANTIOXIDANT ACTIVITY AT PHYSIOLOGICAL pH

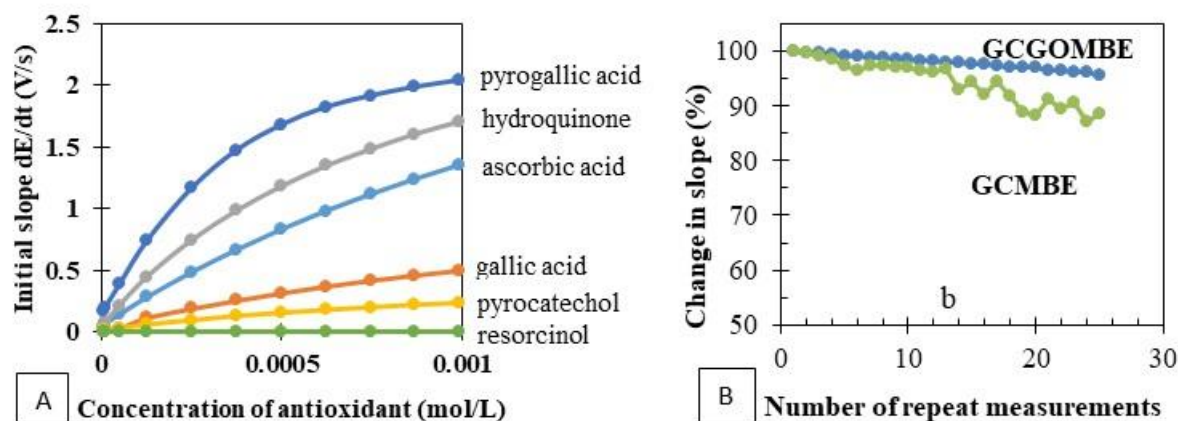
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We recently proposed a novel antioxidant activity measuring method. The method employs a thin redox mediator film immobilized on glassy carbon electrode (GCE). In performing the measurement, first a short controlled potential step is employed where the film is brought to its oxidized state. Upon exposing the electrode to reducing samples, the redox potential changes. The initial slope of the electrode potential – time function is used for assessing the antioxidant activity [1]. Meldola Blue (MB)+(N,N dimethyl-7-amino-1,2-benzophenoxazinium ion) mediator layer was used in the measurement as mediator. Recently using reduced graphene oxide linker layer the stability and activity of the mediator has been considerably improved. The applicability of the method was tested in case of different species, and influence of different parameters on the analytical signal has been investigated. Our recent results obtained with the new method will be presented



**Figure:** (A) The initial slope of various antioxidant concentrations in PBS pH =7 measured using reagentless chronopotentiometric technique. (B) The stability of glassy carbon graphene oxide Meldola blue (GCGOMBE) modified layer compared to glassy carbon Meldola blue layer (GCMBE) during chronopotentiometric measurements of antioxidant activity in PBS PH=7.

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**DESCRIBING 14-3-3 DIMERIZATION: TOOLS TO OBTAIN  $K_D$** Alexandra NÁPLAVOVÁ<sup>1</sup>, Aneta KOZELEKOVÁ<sup>1,3</sup>, Jozef HRITZ<sup>1,2\*</sup><sup>1</sup>. *Central European Institute of Technology, Masaryk University, Kamenice 5, 625 00 Brno, Czechia*<sup>2</sup>. *Department of Chemistry, Faculty of Science, Masaryk University, Kotlářská 2, 611 37 Brno, Czechia*<sup>3</sup>. *National Centre for Biomolecular Research, Faculty of Science, Masaryk University, Kamenice 5, Brno, Czechia*

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The self-association of proteins is one of the cornerstones of cellular processes. The oligomerization is a fundamental way of protein regulation, influencing their functionality and interactome [1]. Therefore, a strong need for quantitative analysis of oligomerization extent arises when studying proteins.

A parameter especially useful for description of self-association is dissociation constant  $K_D$  [2]. Such constant provides us picture of equilibrium between monomers and higher oligomers, at any given concentration. During our research, we focus closely on 14-3-3 proteins. 14-3-3s are regulators ubiquitous in eukaryotic cells, connected to neurodegenerative and oncologic diseases [3]. In their native state, dimers are formed, crucial for proper function [4]. However, it was revealed that phosphorylation at Ser58 of 14-3-3 $\zeta$  leads to monomerization [5,6].

Here, we present an array of biophysical techniques used for oligomeric state quantification of several 14-3-3 $\zeta$  constructs: wild type, phosphorylated at Ser58, monomeric and phosphomimicking mutants [5,7]. Contrary to majority of 14-3-3 studies, dimerization description via  $K_D$  is not biased by used protein concentration. The importance of knowledge of  $K_D$  is demonstrated, as differences in order of magnitude were discovered [5]. Moreover, workflow for  $K_D$  determination via <sup>19</sup>F Trp NMR is presented, exploiting that tryptophan is not only one of the rarest amino acids, but also has a unique role in protein self-association [8].

**ACKNOWLEDGEMENT**

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## PREDICTION OF QM-LIKE PARTIAL ATOMIC CHARGES FOR ALPHAFOLD

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The basic functional unit of all living organisms are proteins. If we want to understand the function of a protein, it is essential to know its structure. Thanks to the AlphaFold algorithm [1], which predicts the structure of proteins based on their sequence, the number of predicted structures is growing very fast. However, due to the high computational complexity of the quantum chemistry apparatus, we are not able to calculate for such large structures another key characteristic, i.e., electron density. A suitable approximation is the concept of partial atomic charges, which describe how much electron density belongs to each protein atom. The most accurate but in our case computationally inapplicable way to obtain partial atomic charges is to derive them directly from the electron density. A significantly faster alternative is to use one of the empirical methods that use only the coordinates of the atoms and information about the bonds between them for the calculation. However, empirical methods must go through a parameterization process, where parameters are searched for such that the resulting empirical partial charges are as similar as possible to those from quantum chemistry.

This paper presents a new empirical method called Split-charge equilibration with parameterized initial charges (SQE+qp) [2] adapted for the AlphaFold Protein Structure Database. Our method can reproduce the partial atomic charges of QM with high accuracy. We also present an implementation of SQE+qp and its parameters via the Atomic Charge Calculator II [3] web application at <https://acc2.ncbr.muni.cz>. Thus, we provide the scientific community with a freely available online tool for calculating QM-like partial atomic charges.

### ACKNOWLEDGEMENT

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## DFT CALCULATIONS OF MICROSCOPIC ELECTRIC PROPERTIES OF MODEL COMPOUNDS POTENTIALLY USED IN ORGANIC ELECTRONICS

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Conjugated organic molecules with suitable optical nonlinearities and spectral characteristics occupy a prominent position in modern research because of their high-cost effectiveness, low dielectric constants, fast non-linear optical response, and easy integration into passive and active devices [1,2]. Whereas the polymeric structures are obtained as highly amorphous materials, their individual oligomers are of particular interest owing to their relatively well-defined structure and easier manipulation (e.g., solubility, purification, film preparation). Another alternative to oligomers represents linear acenes [3].

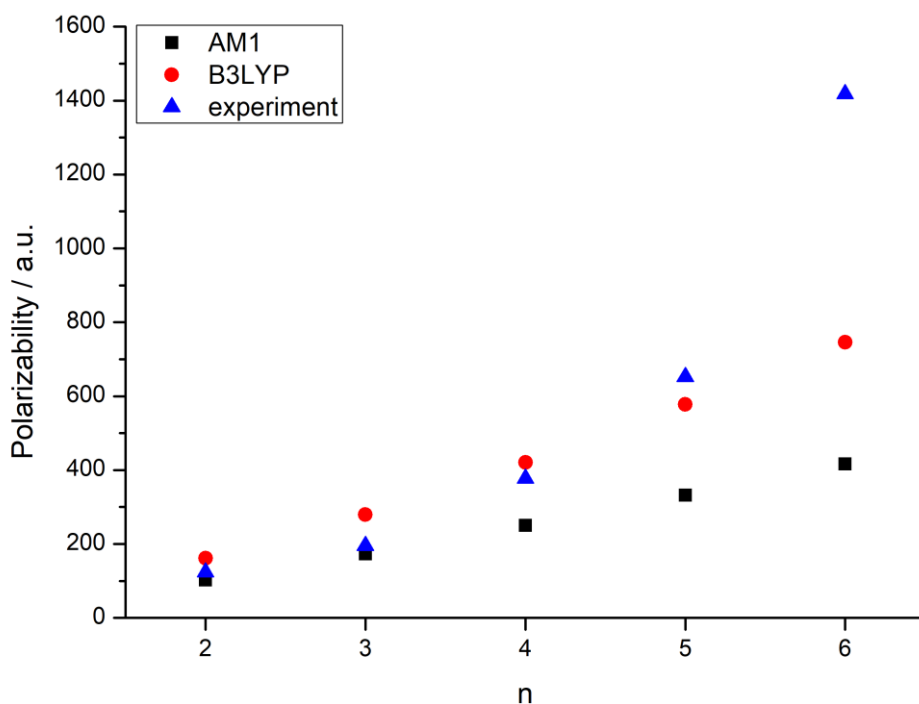
An important microscopic electrical parameter for dielectrics is polarizability or coefficient of polarization  $\alpha$ . Polarizability expresses the ability of atoms, molecules, or groups of a dielectric material to be polarized in the presence of external electric field. This quantity can be expressed as follows [4]:

$$\mu_i(E) = \mu_i(0) + \alpha_{ij}E_j + \frac{1}{2}\beta_{ijk}E_jE_k + \frac{1}{6}\gamma_{ijkl}E_jE_kE_l \dots \quad (1)$$

where  $m_i$  is the component of dipole moment vector in absence of external electric field and  $a_{ij}$ ,  $b_{ijk}$  and  $g_{ijkl}$  are components of polarizability, first and second hyperpolarizabilities tensors, respectively. The electric field is expressed by the components of electric intensity vector  $E$ . Experimentally the mean value of polarizability tensor  $(a_{xx}+a_{yy}+a_{zz})/3$  is usually determined from the refractive index or from dielectric measurements.

Identifying the relation between optical properties and molecular structure is the key tool for a rational design of new electronic fabrics. The experimental data for the linear and non-linear optical properties reveal the initial strong increase with chain length, too. The mean value of polarisability ( $a_{av}$ ) measured by Zhao et al. [5] (in tetrahydrofuran solutions at 589 nm) and extrapolated to the static limits by Champagne et al. [6] are: 124.2 au for T2, 195.8 au for T3, 377.7 au for T4, 652.1 au for T5 and 1418.0 au for T6. The corresponding B3LYP(SMD)/6-31G(2d,p) values are slightly lower than experimental one. The similar trends exhibit also the values predicted using the semiempirical AM1 method [6].





**Figure:** The dependence of B3LYP, AM1 [6] theoretical and experimental averaged polarizabilities on the number of repeating units for oligothiophenes.

In this theoretical study, we have next investigated the influence of the molecular length and molecular symmetry on the electronic and vibronic contributions of polarizabilities for 5 various model oligomers and condensed acenes. The theoretical limits and chemical precision of used treatments were also discussed.

## ACKNOWLEDGEMENT

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# POSTERS

## LINEAR REGRESSION IN ANALYTICAL LABORATORY USING PROGRAMMING LANGUAGES PYTHON AND R

Adam BŘEZINA<sup>1\*</sup>, Vojtěch VRÁNA<sup>1</sup>, PŘEMYSL LUBAL<sup>1</sup> and Marta FARKOVÁ<sup>1</sup>

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Analytical laboratories generate large amounts of experimental data that need to be evaluated. The data processing can be done using applications which can automate this process, simplify data manipulation and reduce errors in comparison with manual procedures. They also make the evaluation faster and more accurate which leads to better results. In this work, programming languages Python and R were used because they are free, explicit, productive, easy to use and have strong communities.

Python is a programming language for general purposes. It is widely used in the scientific sphere because it allows to create applications with many features in relatively short time. For example, library *PyQt5/PySide2* is used for constructing GUI (graphical user interface), *matplotlib* for drawing charts, *NumPy* and *pandas* for efficient data processing and *SciPy* consists of statistical functions and tools. Prepared codes can be converted to executable files (*.exe*), which run without the need to have Python installed.

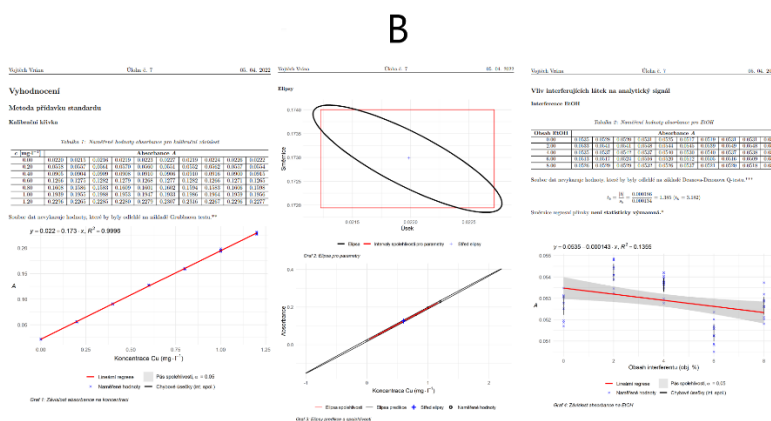
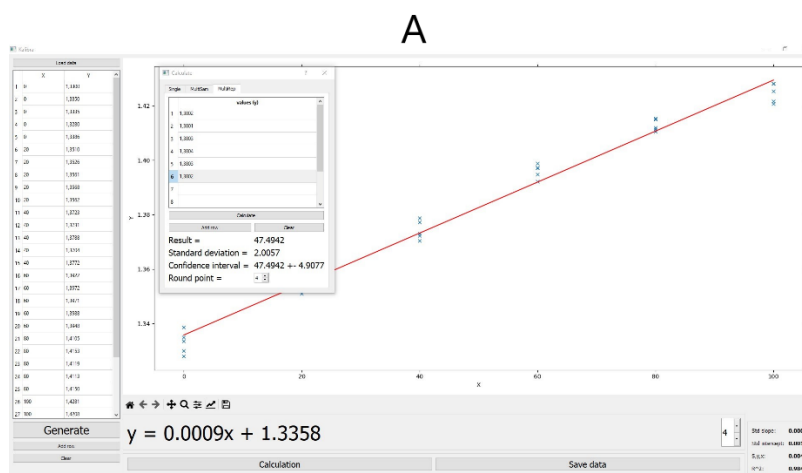
R is a programming language and environment for statistical computing and graphics. It is meant mostly for statistical and mathematical computing; therefore, its syntax is easier to read and write. It offers a wide range of libraries and packages, which makes development of applications much faster. However, R scripts cannot be currently converted to standalone programs (such option may be available in the future), and there are numerous limitations in creating the GUI. The potential of R to view objects and operate with them can be enhanced using integrated development environment *RStudio*. *R Markdown* is an *RStudio*-included package which compiles *R Markdown* outputs into different formats, such as *.pdf*, *.html*, or *.docx*, which makes the results clearer and better looking.

In Python, we created an application called *Kalibra* (Figure A), which is intended for easier manipulation with calibration data than for example in MS Excel. In *Kalibra*, the user can upload data from various data files – text file (*.txt*), comma-separated-values (*.csv*) or MS Excel file (*.xlsx*). The program calculates parameters of calibration curve, tests if the slope and intercept are statistically significant, and constructs a graph for easy visualization of the data. All calculated statistical characteristics are shown inside the *Kalibra* window. It is also possible to easily calculate the corresponding *x* value for the measured signal, standard deviation and confidence interval.

Furthermore, a script in R Markdown was developed, which evaluates data measured in an analytical chemistry practical's task conducted at Masaryk university (*Measurement of copper in wine sample by AAS*) and generates a complete protocol. The data from AAS software are saved in a *.pdf* file which is then imported into the R script and transformed into a more easy-to-read MS Excel spreadsheet. Firstly, the outlier values are removed from dataset using Grubb's T-test and a table with marked outliers is created. Then the graph of linear regression and the corresponding equation is added, and the concentration of copper in the wine sample is determined. The obtained results are statistically evaluated by calculating the standard

deviations, confidence intervals, limits of detection (LOD) and quantification (LOQ). The significance of interferences was also tested. All outputs are exported in a .pdf file. Example of the final file is shown in the Figure B.

Both prepared applications work efficiently and are easy to use. They show that Python and R programming languages are suitable for developing programs for data evaluation. This makes work in the analytical laboratory faster, more effective, easier, and more productive. The saved time enables to measure more data.



**Figure:** A – example of window of *Kalibra* application;  
B – example of output from R application

### ACKNOWLEDGEMENT

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## STUDY OF RONS FORMATION IN AQUEOUS SOLUTIONS USING DIELECTRIC BARRIER DISCHARGE AND ITS BACTERICIDAL EFFECTS

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The recent trend of cold plasma liquid activation research comprises an increasing number of relevant publications dealing with a variety of devices and applications. Plasma activated liquids (PAL) contain species responsible for oxidative stress in bacterial cells. The most important in case of bactericidal effects is believed to be hydrogen peroxide. H<sub>2</sub>O<sub>2</sub> itself isn't able to cause much damage in the bacterial cell, however the secondary reaction between H<sub>2</sub>O<sub>2</sub> and cellular Fe<sup>2+</sup> ions create hydroxyl radicals, which are extremely reactive species that directly oxidize all cellular biomolecules. When H<sub>2</sub>O<sub>2</sub> concentration is high enough, the oxidation will provide lethal effects [1,2]. The bacterial cells can be also damaged by a nitrosative stress, which is in the case of PAL mainly caused by nitrites at low pH values. The acidification of NO<sub>2</sub><sup>-</sup> produces a complex mixture of nitrogen oxides as well as nitrous acid, which is unstable and is spontaneously decomposed to produce NO and nitrogen dioxide [3,4]. Chemical and bactericidal effects induced by plasma in aqueous solutions upon the dielectric barrier discharge (DBD) in air were investigated. For plasma treatment, distilled water and a fertilizer (Start-r, Mills, USA) were used. Inactivation of *Escherichia Coli* TOP10 strain was determined in dependence on pH and chemical changes induced in the studied solutions. Effect of PAL preparation time on the production of H<sub>2</sub>O<sub>2</sub>, NO<sub>2</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup> was studied, the concentrations of RONS were determined spectrophotometrically (see Table).

**Table:** Concentrations of RONS, pH values and *E. coli* log reduction according to PAL preparation time

Sample		H <sub>2</sub> O <sub>2</sub> (mg/l)	NO <sub>3</sub> (mg/l)	NO <sub>2</sub> (mg/l)	pH	Log reduction
Distilled water	0 min	0.00	0.00	0.00	6.50	-
	2 min	0.78	3.47	1.15	4.47	2.79
	5 min	0.95	19.48	2.09	3.68	3.48
	10 min	0.88	49.68	4.17	3.33	4.66
Fertilizer	0 min	0.00	85.76	0.04	7.20	-
	2 min	0.31	96.00	1.93	4.60	2.97
	5 min	0.34	104.72	3.58	4.10	3.44
	10 min	0.34	109.31	4.11	3.80	6.11

For each experiment, a fresh bacterial suspension in Luria Broth (LB) medium with concentration ~ 10<sup>8</sup> CFU/ml was used. 1 ml of this suspension was mixed with 9 ml of each sample of PAL and after 10 minutes, 100 µl was transferred to LB agar plates. After the 24 h incubation at 28°C, number of CFU was determined. Obtained results are summarized in Table. The best result for *E. Coli* inactivation was shown by the sample of fertilizer after the 10 min activation in DBD, even though smaller concentration of H<sub>2</sub>O<sub>2</sub> was detected in this sample.

This result points out the importance of  $\text{NO}_2^-$  presence together with low pH for the bactericidal effects of PAL.

### ACKNOWLEDGEMENT

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**AMPHIPHILIC SUBSTANCES AS HYDROGEL MODIFIERS**Richard HEGER<sup>1\*</sup>, Miloslav PEKAŘ<sup>1</sup>

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Nowadays, hydrogels are an indispensable material that is occurring in countless different industries where they hold a huge number of functions and applications. Due to biodegradability and biocompatibility, a solution for the potential application is often sought in the physically crosslinked hydrogels.

Physically crosslinked hydrogels are formed by molecular entanglements and secondary forces including ionic, H-bonding, or hydrophobic forces. They have several advantages compared to chemically crosslinked hydrogels. Specifically, can be highlighted their ability to absorb a large amount of water, and their reversibility, homogeneity, or occurrence of hydrophilic and hydrophobic areas lead to a very high interest in the incorporation of bioactive substances. However, many of their advantages are overshadowed by their poor mechanical properties due to their reversible physical interactions [1]. Therefore, to support their advantages, and bolster their disadvantages, this study deals with modifying the hydrogels by additions of amphiphilic substances into their structure. One of many ways to manoeuvre and control the hydrogel structure and its properties is to incorporate hydrophobic moieties with self-assembly capability into the aqueous environment. Domains formed by the self-assembly impart hydrogel's properties from the mechanical but also from the functional point of view [2].

The structure and properties of all hydrogel samples were modified by the addition of differently charged surfactants which after overcoming the critical micellar concentration form micelles. Physically crosslinked hydrogel systems were subjected to the complex characterization in their swollen form. The evaluation of viscoelastic properties was carried out by rheology tests consisting of strain and frequency sweep tests, as well as three interval thixotropy tests. The transport properties were evaluated by release dye experiments using a different array of model dyes with different structures and charges.

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## ELECTROCHEMICAL BEHAVIOUR OF NEW PSYCHOACTIVE SUBSTANCES 3-FLUOROPHENMETRAZINE AND 4-METHYLPENTEDRONE

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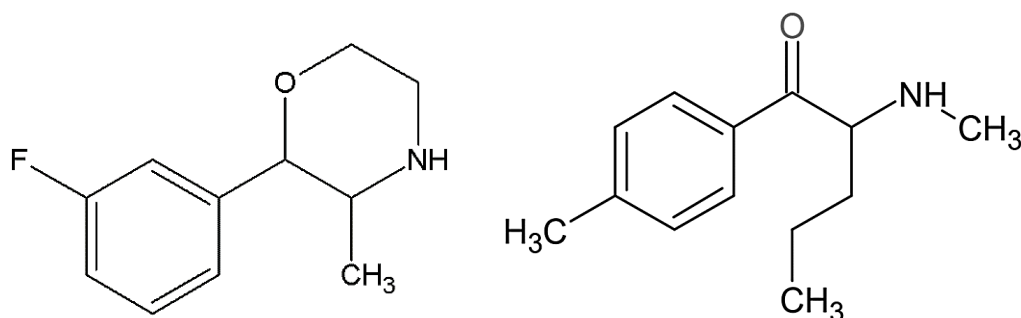
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New psychoactive substances (NPS) are used as an alternative to classical drugs. These types of drugs aren't usually controlled by current legislative and data about its toxicity are limited. European Monitoring Centre of Drug and Drug Addiction and the United Nations Office on Drug and Crime newly report many derivatives every year [1].

There are four main groups of NPS: synthetic stimulants, synthetic cannabinoids, synthetic hallucinogens, and synthetic depressants. Both studied substances are synthetic stimulants. Synthetic stimulants induce feelings of happiness, euphoria, relaxation, because it usually increases the level of serotonin and dopamine [2]. 3-fluorophenmetrazine (3-FPM) was first notified in 2014. It has similar effects as phenmetrazine known for the obesity treatment in 1950s under commercial name Preludin [3]. 4-methylpentedrone is one of the synthetic cathinones. These substances are associated with activity called 'chemsex', which is using chemicals during sex. It can cause health problems, in addition to risky behaviour (HIV transmission) it also has a lot of side-effects, mental and physical [4].



**Figure:** Chemical structure of 3-FPM (left) and 4-MPD (right).

The aim of the work is to identify possible metabolic pathways in human organism. Part of the reaction scheme can be an electron transfer coupled with chemical reactions. Therefore, this work is focused on the electrochemical behaviour of both substances by means of cyclic voltammetry and UV-Vis and IR spectroelectrochemistry [5].

The stability of substances was verified by UV-Vis spectrophotometry. Compounds 3-FPM and 4-MPD in the form of white powder were obtained from the Institute of Forensic Medicine and Toxicology, 1<sup>st</sup> Faculty of Medicine in Prague. Their purity was confirmed using HPLC. The voltammograms were recorded in aqueous medium at different pH values, using three-electrode

electrochemical cell with glassy carbon electrode as a working electrode. The advantage of the spectroelectrochemical technique is in the detection of short-living reaction intermediates [6]. The spectroelectrochemistry was measured in aqueous and nonaqueous medium and indicated the formation of the intermediates. Theoretical calculations of frontier orbitals energies and their spatial distribution supported the research. Oxidation and reduction mechanism of 3-FPM and 4-MPD was proposed.

### ACKNOWLEDGEMENT

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## LABEL-FREE IMPEDIMETRIC BIOSENSING AND CONCENTRATION OF REDOX PROBE

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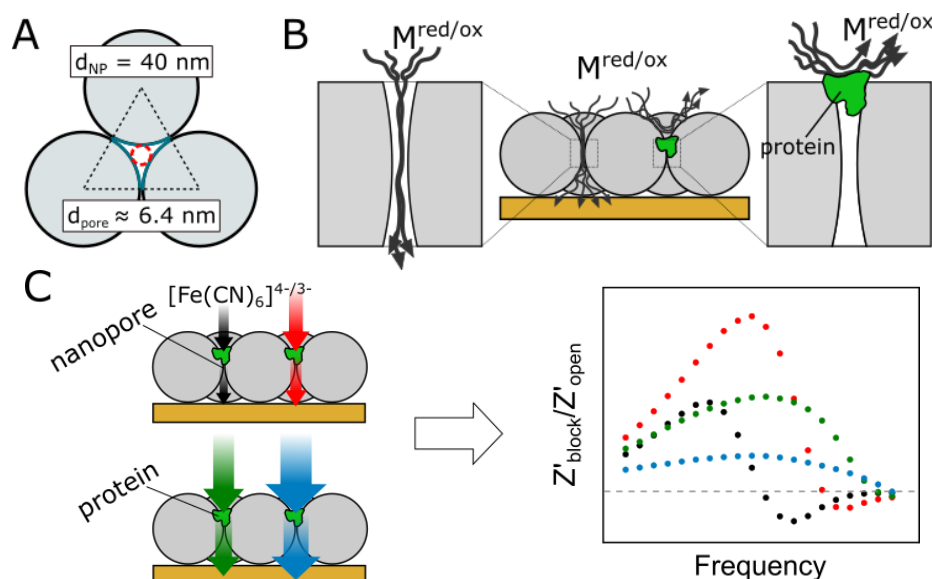
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We have previously designed and tested a label-free biosensing platform based on nanopores. [1-3] The nanoporous matrix is formed directly on the electrode surface using simple immobilization of spherical nonconductive (polystyrene) nanoparticles in a dense monolayer. The open interstitial space among three neighbouring spherical NPs in the densest planar hexagonal arrangement forms a nearly triangular nanopore (Figure A, B). In such arrangement, if close surroundings of the nanopore are modified with antigen, affinity interaction with corresponding antibody will result in nanopore blocking. Nanopores impermeable for the present redox probe will substantially increase the measured electrochemical impedance. However, this design does not work as simply as was described [1], extensive work must be devoted to set the concept working and various parameters must be studied in detail on various model cases.

For this reason, in our model affinity biosensor, covalent attachment of albumin protein on top of 40 nm polystyrene nanoparticles represents a capture of an analyte resulting in blockage of the nanopores. [4]

Different bulk concentrations of the ferro/ferricyanide redox pair were probed by Faradaic electrochemical impedance spectroscopy. The character of the redox probe permeation towards the electrode surface differed in dependence on its concentration. Not surprisingly, the bulk concentration of the redox probe affected the performance of the electrochemical detection, demonstrating the importance of controlling this parameter in immunosensing applications.



**Figure A:** three neighbouring spherical NPs in the densest planar hexagonal arrangement form nearly triangular nanopore, **B:** nanopore blockage with a protein causes increase of impedance, **C:** different concentrations of ferro/ferricyanide exhibit different electrochemical behaviour.

### ACKNOWLEDGEMENT

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## DEVELOPMENT OF ELIMINATION VOLTAMMETRY WITH LINEAR SCAN USING $[\text{Fe}(\text{CN})_6]^{3-/4-}$ SYSTEM

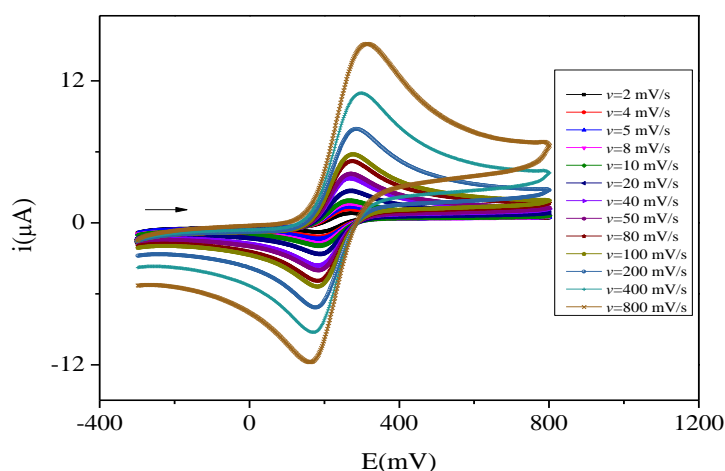
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Cyclic voltammetry (CV) is one of the most widely used electrochemical methods for the study of electroactive substances. It is a versatile technique that allows investigating the mechanisms of redox and transport properties of the electrochemical system [1-3]. The cathodic and anodic polarization of the electrode provides information not only about the reduction and oxidation steps of the studied depolarizer but also about its behavior in the electric double layer.

The aim of electrochemical research is a deeper understanding of the influence of electrode surface morphology and chemistry on the redox and adsorption behavior of the investigated analyte. Further information beyond the CV can be provided by elimination voltammetry with linear scan (EVLS), which is mainly applicable to reversible and quasi-reversible processes [4-6]. For this purpose, we studied the redox system  $[\text{Fe}(\text{CN})_6]^{3-/4-}$ , which is very often used as a redox probe and subject to undergoing electron transfer *via* a simple outer-sphere mechanism [7]. The  $[\text{Fe}(\text{CN})_6]^{3-/4-}$  complex is the studied redox mediator and homogeneous one-electron electrocatalyst [8]. As a result, it is critical to undertake in-depth research on this ferro-ferri redox couple. Our voltammetric studies with carbon electrodes demonstrate that the electron transfer (ET) in this system is related not only to the electrode surface (material, morphology, chemistry) but also to the concentration of the supporting electrolyte in the system. In other words, the ET is influenced by the invisible activation or passivation layer created on the electrode surface, resulting in a more complicated ET than a simple outer-sphere mechanism [9-11].



**Figure 1:** Cyclic voltammograms of  $[\text{Fe}(\text{CN})_6]^{3-/4-}$  (0.1mM) in 0.1M KCl on a polymer pencil graphite electrode (pPeGE, Tombow) for different scan rates (from 2mV/s to 800mV/s).

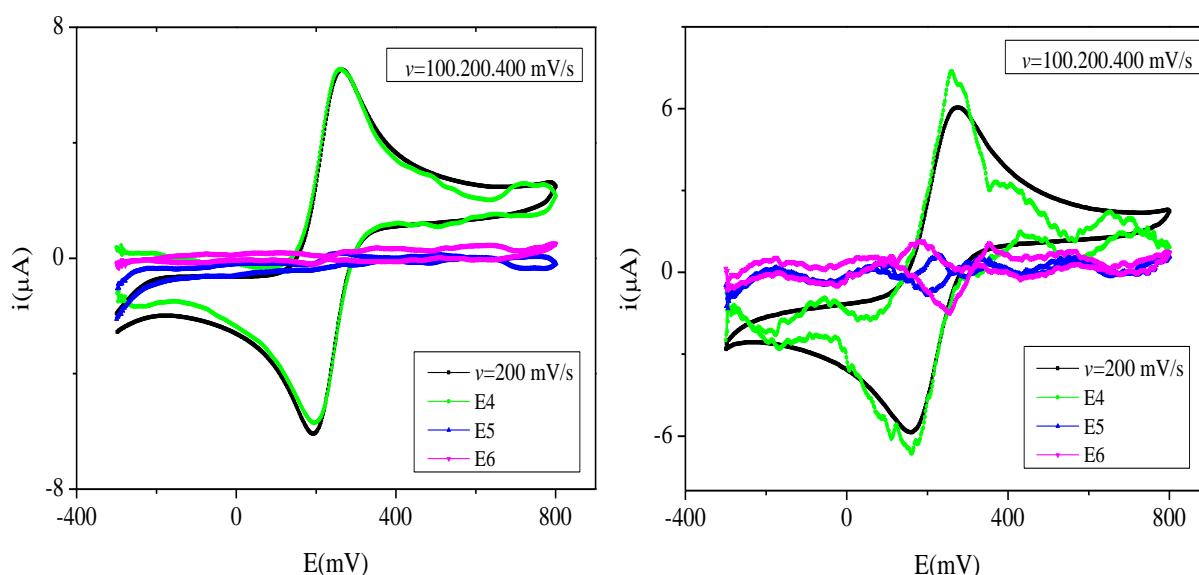
Common CV records (current-potential curves) of a redox pair  $[\text{Fe}(\text{CN})_6]^{3-}/[\text{Fe}(\text{CN})_6]^{4-}$  on the polymer pencil graphite electrode (pPeGE) at different scan rates are shown in Fig. 1. Cyclic voltammograms show overall electrode processes and indirectly provide some evidence of the

effects of different experimental parameters, but the EVLS can analyze and solve this process in detail. EVLS is a novel approach for processing electrochemical data collected by voltammetry that can remove some individual selection currents from total voltammetric currents measured at various scan rates. EVLS is a powerful data processing tool, according to many published publications [4]. The following three equations are commonly used in EVLS [5,6]. We used three EVLS functions ( $I$  is the reference scan rate,  $I_{1/2}$  and  $I_2$  are one-half and double of the reference scan rate, respectively):

**E4**  $f(I) = -11.6570I_{1/2} + 17.4850I - 5.8284I_2$ , which eliminates simultaneously charging and kinetic currents with retaining the diffusion current,

**E5**  $f(I) = 6.8284I_{1/2} - 8.2426I + 2.4142I_2$ , which eliminates simultaneously charging and diffusion currents with retaining the kinetic current, and

**E6**  $f(I) = 4.8284I_{1/2} - 8.2426I + 3.4142I_2$ , which eliminates simultaneously the kinetic and diffusion currents with retaining the charging current.



**Figure 2:** Comparison of CV and EVLS (**E4**, **E5**, **E6**) of  $[\text{Fe}(\text{CN})_6]^{3-/4-}$  (0.1mM) in 0.1M KCl on a pPeGE (the reference scan rate of 200 mV/s) with two different reference electrodes.

The EVLS can also detect a defective function of the reference electrode or its circuit. In Fig. 2A, both EVLS functions E5 (the elimination of the diffusion current component  $I_d$  and the conservation of the kinetic  $I_k$ ) and E6 (the elimination of the diffusion current component  $I_d$  and the conservation of charging current component  $I_c$ ) carefully follow the zero current line. This trend is not observable in the case of the other reference electrode (Fig. 2B), where EVLS E5 and E6 show a deviation from the zero current line.

The EVLS procedure is able to experimentally point out changes in the ET process with a change in the scan rate, potential window, supporting electrolyte concentration, and working electrode type. In this study, different initial potentials, scan rates window, scan, and the stability of sample solution are all discussed with respect to previously published results [8-11]. At the same time, we use EVLS to study different scanning numbers and different potential windows of the  $[\text{Fe}(\text{CN})_6]^{3-/4-}$  system on the cyclic voltammogram. It is the first time to use

EVLS to eliminate the corresponding current, trying to explore the “secret” of the reaction inside the cyclic voltammetry.

### ACKNOWLEDGEMENT

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## THE NEW SOLID-CONTACT ION-SELECTIVE ELECTRODE BASED ON DODECABENZYLAMBUS[6]URIL FOR PERCHLORATE ANALYSIS

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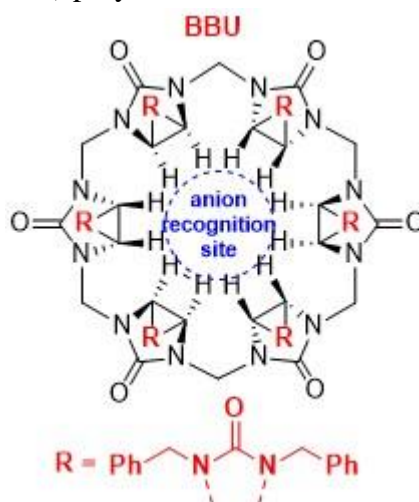
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Dodecabenzylambus[6]uril (Bn<sub>12</sub>BU[6] – see Figure) is an anion receptor that binds the perchlorate ion the most tightly (stability constant  $\sim 10^{10} \text{ M}^{-1}$ ) of all anions due to the excellent match between the ion size in relation to the receptor cavity [1-3]. This new bambusuril compound was used as an ionophore in the ion-selective membrane (ISM) to develop ion selective electrodes (ISEs) for determination of perchlorate concentration utilizing the poly(3,4-ethylenedioxythiophene) (PEDOT) polymer film as a solid-contact material.



**Figure:** The chemical structure of dodecabenzylambus[6]uril (Bn<sub>12</sub>BU[6] = ionophore)

Variation of the content of Bn<sub>12</sub>BU[6] and tridodecylmethylammonium chloride (TDMACl) in the plasticized poly(vinyl chloride)-based ISM was also tested. All the prepared solid-contact ISEs and their analytical performance were characterized by potentiometry, cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and chronopotentiometry. The ISEs showed rapid response and a sub-Nernstian slope ( $\sim 57 \text{ mV/decade}$ ) during potentiometric measurements in perchlorate solutions in the concentration range from 0.10 to  $10^{-6} \text{ M}$  simultaneously with their high stability and sufficient selectivity to other common inorganic anions like bromide, chloride, nitrate and sulphate. The function of the ISE was further verified by analysis of real water samples (lake, sea, and mineral water), which gave accurate and precise results. Other experimental details are given elsewhere [4].

### ACKNOWLEDGEMENT

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## ELECTROCHEMICAL STUDY OF 3D PRINTED TITANIUM ALLOY SURFACE WITH SECM

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Additive manufacturing that also called 3D printing is a rapidly developing technique. It has essential advantages over traditional ways of making products of specific shapes and size. It is particularly so when certain metal objects are fabricated. In certain 3D printing technologies used for producing metal items the cooling rate of the newly formed layers is much higher than in conventional casting. It can be as high as  $10^3$ - $10^5$  K/s. In addition the anisotropy of thermal gradient during fusion and solidification can result in anisotropic microstructure and mechanic stress. It can result in substantial differences between certain properties of the 3D printed and that of the traditionally made ones.

Owing to its high specific strength and excellent corrosion resistance TiAl6V4 alloy made with conventional technology is a broad scale used material. It is applied in aerospace industry as well as in making implants for biomedical application.

Recently in our work a 3D printer has been constructed that employs a wire and arc additive manufacturing technology. It can be used for printing TiAl6V4 alloy items. It is hoped that the 3D printing technology worked out will be appropriate for producing biomedical implants of personalized shape and size. High corrosion resistance is one of the most important properties that a biomedical implant must have.

In our recent work the corrosion resistance of 3D printed TiAl6V4 alloy samples have been studied using scanning electrochemical microscopy (SECM). The action and stability of the spontaneously forming TiO<sub>2</sub> protective layer have been investigated. Furthermore the formation rate of it has been measured and self-healing kinetics studied. In the Conference the employed SECM method, as well as the results obtained will be presented



## ELECTROCHEMICAL DETECTION OF H<sub>2</sub>S PRODUCED IN MUST DURING FERMENTATION

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Hydrogen sulphide (H<sub>2</sub>S) is a naturally occurring poisonous gas. Analysis of it in environmental, living organs or in the process of fermentation H<sub>2</sub>S containing samples has an important task.

Hydrogen sulfide (H<sub>2</sub>S) is a volatile sulfur-containing compound that occurs as an activity of microorganisms in foods. Its presence in beers, ciders and wines is clearly the result of a fermentation defect.

The reasons for the production of hydrogen sulfide during winemaking can be traced back to the activity of yeasts. All yeasts, whether spontaneous (autochthonous) or selected species, produce hydrogen sulfide. However, in addition to the genetic coding of yeasts, this property is mainly related to the elemental sulfur and sulfur-containing compounds (sulphates, sulphites) in grape must and to the deficient in nutrient and vitamin content of the grapes. The sulfur content of the must consists of the pesticide residues used in the plant protection of the grapes and the potassium metabisulphite used in the crushing of the grapes.

H<sub>2</sub>S gas can be found in 20 µmol/dm<sup>3</sup> concentration in the tissues of living animals at pH=7.4 or 90ppb at pH=3.6 in fermentation of must. Recently the involvements of H<sub>2</sub>S in numerous physiological processes have been proved. This generated a rapidly increasing interest in studying its interaction with enzymes and with flavor compounds of must. Its role as a bad smell signaling molecule of the must fermentation systems has been proved. New investigations are dealing with the role of H<sub>2</sub>S in must or in the readymade wine after a certain fermentation, and its studies are going supporting the wine making production. Most of the wine celeries have applied H<sub>2</sub>S treatment since hundred years back, based on simple methods based on folk observations, using materials and tools that are also used in grape production and have been classified as standard procedures over the years. The very sensitive electrochemistry can give indication of the H<sub>2</sub>S content and the change of H<sub>2</sub>S producing reaction. The H<sub>2</sub>S is a redox-sensitive unstable molecule, and its concentration is relatively small in the complex chemical composition of must or wine. On the poster the worked out amperometric method and the H<sub>2</sub>S sensor developed will be introduced. The concentration changes appropriate measuring method and apparatus are needed. The dynamic concentration range, the lower limit of detection, the selectivity, stability of the cell are presented in this study

### ACKNOWLEDGEMENT

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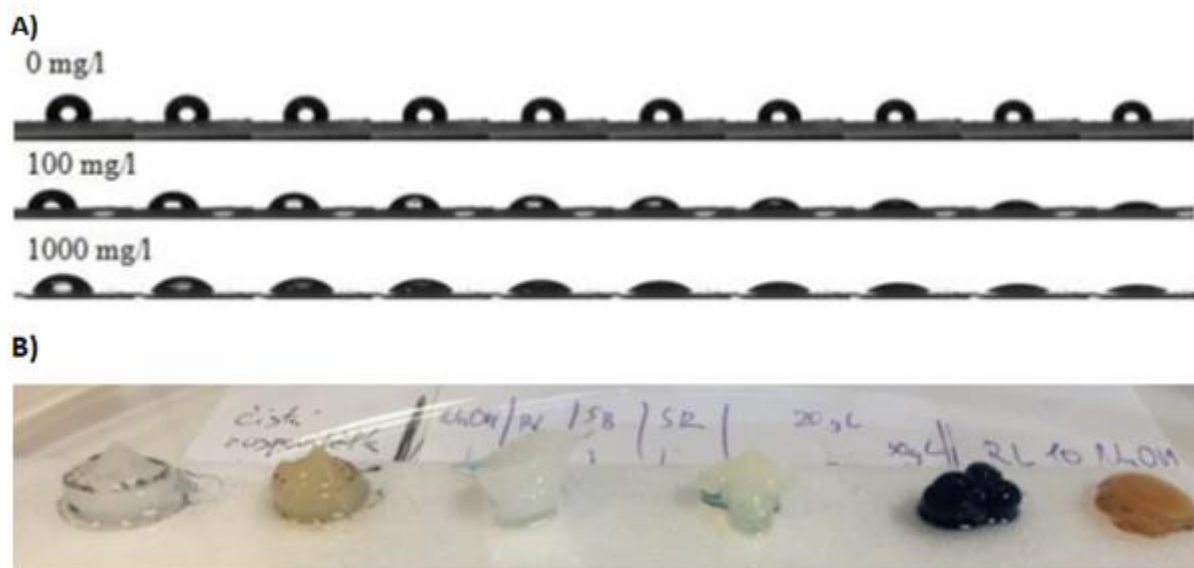
## THE CONTRIBUTION OF PHYSICAL CHEMISTRY TO RESEARCH AND DEVELOPMENT OF BIOSURFACTANTS AND THEIR POTENTIAL USE IN CARRIER SYSTEMS

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The presented study deals with the very topical issue of biosurfactants. A battery of methods of physico-chemical and colloidal analysis was utilized in complex characterization of studied molecules. The model biosurfactants were first characterized by standard methods used to study these kinds of compounds (biocomponents, saccharides, proteins, etc.). Fourier transform infrared spectrometry was used as a standard technique of structural analysis. Tensiometry was chosen as a common representative of methods used in study of aggregation behavior, in determination of critical aggregation concentration of rhamnolipids [1]. Furthermore, alternative techniques were designed and optimized as a cheap and fast substitute of tensiometry in a routine microbiological labwork. These were based mainly on a microplate assay and its modified alternatives. These methods were found of a low sample consumption and of satisfactory effectivity in confirming the presence and semi-quantitative determination of biosurfactant content in the solution. The result of this part is a few simple methods that have been proven effective in fundamental research of (bio)surfactants.

In the next part of the study, the previous methods were interconnected with another current topic – the hydrogel-based carrier systems [2]. Since the biggest problem is the passage of hydrophobic drugs through the bloodstream, or through universal body barriers (e.g., blood-brain), it is necessary to chemically modify these carriers in order to be able to administer hydrophobic substances effectively. Based on literature research, several systems were designed and subsequently studied, in which there is a presumption of possible use for carrier systems and at the same time they have biosurfactants incorporated in them due to their ability to solubilize hydrophobic molecules. This part of the study was dealing with the possibility of biosurfactants (mainly rhamnolipid) used in hydrogel carrier systems intended for the administration of hydrophobic compounds [3]. At the same time, the individual carrier systems, the procedure of their preparation, and the possibilities of their use were described, and their advantages and disadvantages were also compared. The screening of both individual substances (biosurfactants and gelation agents) and their mutual interactions, as well as methods used to study the emerging structures, was performed. The indirect investigation of molecular interactions in the system was based on the technique of dynamic light scattering. The next part describes the optimization of hydrogel formation with incorporated biosurfactants in their structure and then the formed gels were subjected to rheological and solubilization tests. The study of the internal structure of these gels in a dry state was performed by scanning electron microscopy.



**Figure:** Study of rhamnolipid biosurfactants A) contact angle measurements in correlation to concentration B) use of rhamnolipids in chitosan hydrogels with dyes (hydrophilic and hydrophobic)

### ACKNOWLEDGEMENT

The work has been supported by the University Specific Research, project No. FCH-S-22-7909; Faculty of Chemistry, BUT.

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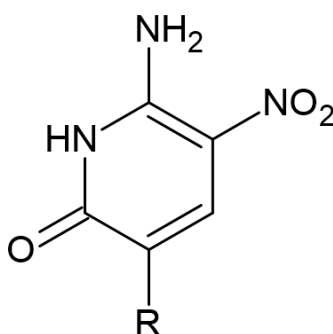
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## VOLTAMMETRY OF DNA OLIGONUCLEOTIDES CONTAINING SYNTHETIC COMPONENTS

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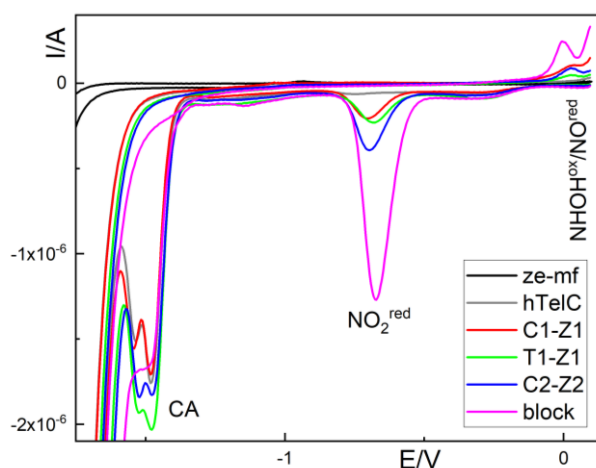
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**Figure 1:** Chemical structure of the unnatural base Z (6-amino-5-nitro-2(1H)-pyridon).

One of the important directions of synthetic biology has been the development of new unnatural DNA bases (UDB), which can not only form a stable and continuous DNA double-helix but can also be replicated and transcribed. The primary purpose of the UDB development is expansion of the genetic alphabet, and the main intention behind the development of unnatural DNA bases is the addition of new genes and proteins as e.g. carriers of medicinal drugs or to help the progress of new approaches to diagnostics of various diseases [2]. The unnatural base pairs often differ in their chemical properties from the canonical DNA bases which stimulates the development of analytical methods for their determination [1]. They can be also utilized in the design of new methods for DNA analysis in general.



**Figure 2:** First scans of nucleotides containing base Z in their sequence.

In the case of base Z (structure shown in Fig. 1)) we have identified electrochemical processes to differentiate them from natural bases, such as the reduction of the nitro group in the structure [3], which is visible in the Fig.2 as the peak marked  $\text{NO}_2^{\text{red}}$ . As a result, we have been able to

differentiate among oligonucleotides containing a single base Z in its sequence (C1-Z1 and T1-Z1), two residues of base Z (C2-Z2) and the oligonucleotide containing ten base Z moieties (block) from the unmodified sequence of a C-rich human telomere (hTelC), which does not contain any base Z, as shown in Fig.2.

### ACKNOWLEDGEMENT

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## THE NEW QUANTUM DOT FRET-BASED LUMINESCENT PROBE FOR CASPASE-3/7 IMAGING INSIDE CELLS

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Nowadays luminescent semiconductor quantum dots (QDs) are widely applied in different areas due to their unique optical properties. QDs can be used as photoluminescent labels with excellent possibilities for high-throughput detection and diagnostics. For most of such applications QDs must be coupled to biomolecules, which often represents a fundamental challenge.

High-sensitivity and high-selectivity analyses are more widely used not only as tools of investigation in biology and medicine, but also in diagnostic practice. Modern technologies and instrumentations of laser-induced fluorescence or bioluminescence offer the possibility to study biological phenomena at a cellular or even molecular level. The progress of bioanalytical techniques has accelerated the deep understanding of cellular processes [1,2].

Our research is focused on biologically active molecules, such as caspases, which play important roles in cell signaling regulation in normal and diseased states and are attractive targets for biological diagnosis and also for medical therapy[2,3]. Deregulations of the mediators in apoptotic pathways are linked to a wide range of pathological conditions such as cancer, autoimmune or neurodegenerative diseases, and viral infections. Since the down-regulation and decreased activity of caspase-3/7 is a prognostic indicator of different tumors, an improvement in screening of this enzyme in individual cells proved to be of a diagnostic importance [4-6].

Recently, luminescent semiconductor QDs are widely applied in different areas due to their advantages over organic low molecular mass luminescent dyes. In addition, QDs are suitable as Förster resonance energy transfer (FRET) donors in optical sensors [7,8]. According to the Förster definition [9], FRET is a photophysical process by which the energy of the donor luminophore in excited state is nonradiatively transferred to the acceptor and then emitted as a longer wavelength photon. The immediate nonradiative process is based on dipole–dipole interactions between a donor and acceptor in distance of 1–10 nm [10,11]. The implementation of QD as donors brings several advantages [12]. High brightness, quantum yields, and long photoluminescence times are prerequisites of extraordinary energy transfer rate. Similarly, the energy transfer rate is increased by the attachment of multiple acceptors to the large surface area of QDs. The size tunability of luminescence spectra is advantageous for the optimization of spectral overlap between donor and acceptor. The broad absorption bands allow an effective excitation of QDs at a wavelength low enough not to directly excite acceptors and lead to development and applications of FRET sensors with QD.

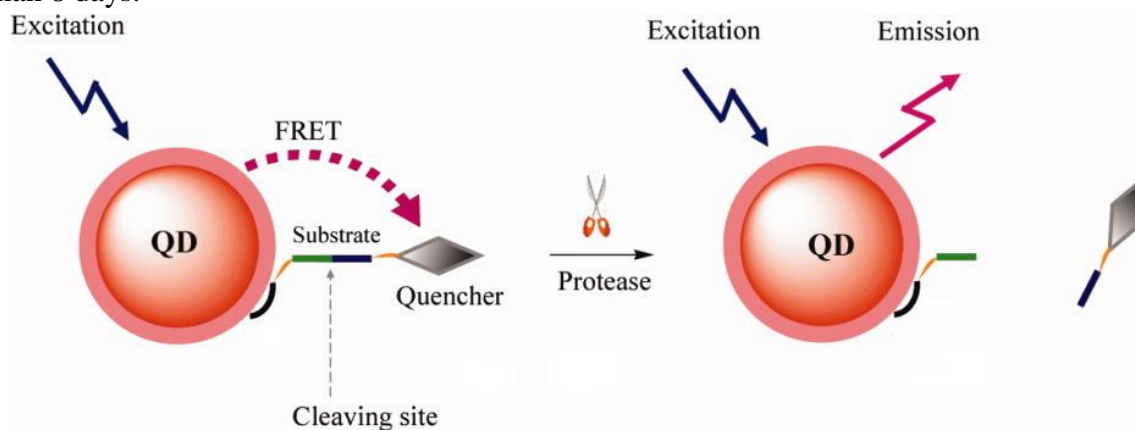
Recent studies have shown that electron transfer between quantum dots and attached fluorophores increases the FRET efficiency in this system [13]. This enables real-time monitoring of enzymatic activity of peptide cleaving enzymes (**Figure 1**).

The aim of our research was developing of the new quantum dot luminescent probe for caspase 3/7 imaging inside cells. The two step synthesis of luminescent probe based on ligand-exchange

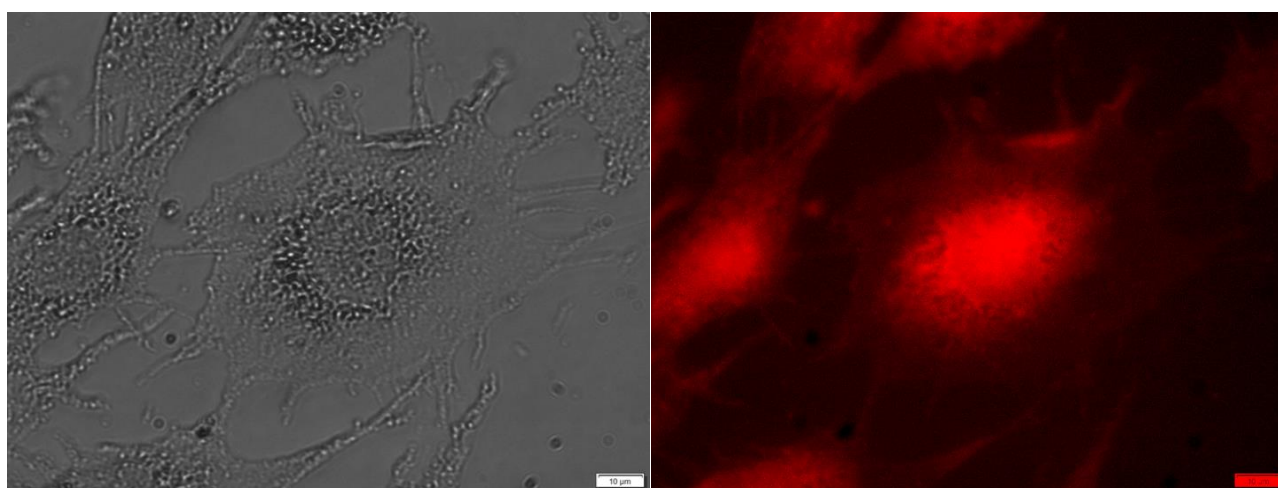


in the first step and the specific reaction of amino group in the second step was optimized. The QDs and their conjugates after first step of synthesis were analyzed by the laboratory built CE-LIF system. Optimal conditions for quantitative separation of the native quantum dots and their conjugates with peptide by using capillary electrophoresis were found and checked. In this work, testing of novel quantum dot luminescent probe is presented for a long-time monitoring of caspase 3/7 distribution in apoptotic and nonapoptotic osteoblastic cells.

The luminescence properties of the novel quantum dot luminescent probe were checked by monitoring of the reaction inside the MC3T3-E1 cells treated with camptothecin (**Figure 2**). The fluorescent probe reaction inside the cells was monitored by microscope Olympus IX 71 with Xe-lamp. The fluorescence emission was observed at 600 nm with excitation light at 530 nm. The cells were incubated with the fluorescence probe for 24 hours at 37°C and 5% CO<sub>2</sub>. The synthesized luminescent probe proved to enable much longer imaging of active caspases than commercially available probes. Stability of the fluorescence signal inside the cells is more than 8 days.



**Figure 1:** Scheme of the quantum dot FRET-based luminescent probe reaction with cleaving enzyme.



**Figure 2:** Comparison of the white light microscope picture (in the left) and the fluorescence microscope picture (in the right) of the MC3T3-E1 cells treated with camptothecin 24 hours after incubation with fluorescent probe.

## ACKNOWLEDGEMENT

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## RHEOLOGY OF AGAROSE HYDROGELS MODIFIED BY SILK FIBROIN

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Agarose is linear polysaccharide derived from seaweed that forms biocompatible hydrogels widely used in medical applications and tissue engineering. In similar applications, silk fibroin is also used for its properties, which is a fibrous protein derived from silkworm cocoons and can also form hydrogels in a suitable environment. By combining these two materials, a hydrogel is formed, which can be considered as a simple model of the extracellular matrix. It has a very complex structure and has the character of a hydrocolloid. However, it can be simplified to an amorphous part (proteoglycans and glycosaminoglycans) and a fibrous part (collagen and elastin).

Rheology is one of the main tools for the characterization of hydrogel materials. The viscoelastic properties of hydrogels can be determined by oscillating rheology tests and the main goal of such experiments is to determine what changes in mechanical properties occur, whether in terms of materials used (agarose, fibroin), their concentration and combination. The mechanical properties of hydrogels, such as gel network elasticity and crosslink density, are also related to their diffusion properties.

Silk fibroin was extracted using Ajisawa's reagent [1]. Samples were prepared with two different concentrations of agarose (0,5 and 1,5 wt. %) and two different concentrations of silk fibroin (2,0 and 5,0 wt. %). Rheology properties were studied by amplitude and frequency sweep tests (Anton Paar MCR 72). Amplitude sweep test were used for determination of LVR and frequency for frequency sweep tests. Main result of frequency sweep test is determination of mesh size of the hydrogels.

Viscoelastic modules were decreasing with decreasing agarose concentrations and decrease with the fibroin presence. High concentrated fibroin enhances the mechanical properties of low concentrated agarose, on the other hand, fibroin weakens mechanical properties of high concentrated agarose. For agarose hydrogels, the mesh sizes were decreasing with increasing agarose concentration. The same trend was shown by fibroin samples but with a larger mesh size. The presence of fibroin in agarose reduced mesh size, decreasing with increasing agarose and fibroin concentrations. The results correspond to the diffusion coefficients found in the previous study [2].

### ACKNOWLEDGEMENT

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## UPGRADE OF FLUOROMETER FOR REAL-TIME MEASUREMENT OF ENDOTHELIAL BARRIER AND LIPOSOMES DIFFUSION

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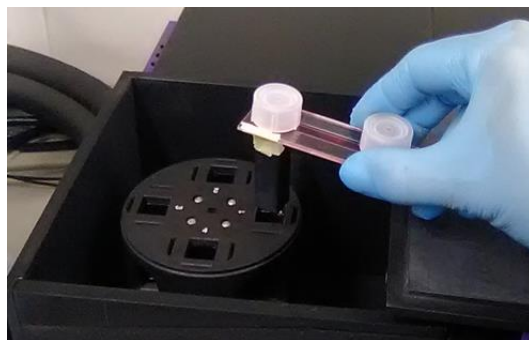
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### BACKGROUND

Vascular endothelium play important role in many physiological and pathological states and it is also pivotal structure allowing effective drug transfer in vivo – both in form of soluble macromolecules or in form of encapsulated molecules (liposomes or another nature or synthetic nanovesicles). Endothelial cells (ECs) form layer with specific permeability, which react to different biophysical and biochemical state during. Fluorescent dyes and spectrometer traditionally help to quantify leakage kinetics across the the model layer of ECs in vitro under normal or some pathological conditions (infection, hypoxic, acidic condition). We have focused to construct innovative two-compartments in vitro model and to test leakage kinetics of modern liposomes with miRNA cargo and to measure accelerating effect of ultrasound stimuli on ECs.

### METHOD OF SETUP PREPARATION

(A) Preparation of ECs and basal lamina: Endothelial cells were prepared as described in [1] using gelatine-coated culture flasks, after 3rd passage the ECs were seeded onto polycarbonate mesh (mesh opening 1  $\mu\text{m}$ , open area 2%). (B) Preparation of liposomes: We have prepared synthetic liposomes using components DOTAP/DOPE/Cholesterol/PEG (ratio was 50/10/38,5/1,5), moreover Rhodamine-B and synthetic miRNA-30 were encapsulated inside the liposomes using previously published methodology [2]. The liposomes were characterised as negative and 90-nm spheres. (C) Assembling of ECs into in vitro model: Our in vitro model of ECs monolayer and two compartments mimick real in vivo situation of diffusion from intracapillary to extracapillary space. Our setup geometry was not traditional setup used in many publication - some upper compartment (with high concentrated diffusive molecules; without any hydrostatic or hydrodynamic pressure) and lower compartments (target). Our setup was prepared as “vertical sandwich model” with one compartment on the left site and one compartments the right site of the ECs monolayer. Left compartment was constructed as fluidic microchannel (volume 800  $\mu\text{L}$ , circulating fluid via micropump), the right compartment was constructed as reservoir (volume 800  $\mu\text{L}$ ) with main part in the cuvette. The cuvette were compatible with sample stage of ChronosBH spectrometer (ISS, Germany), detail on Fig.1. Moreover, our in vitro model was upgraded heat and gas input (for long-time experiments of the cells for 12 hours and longer time).



**Figure:** Sample holder of spectrometer and in vitro fluidic setup with live cells.

## METHOD OF MEASUREMENT

In vitro endothelial permeability was measured by ChronosBH spectrometer (ISS, Germany) as time-lapse measurement of diffusion of (i) FITC-labeled dextran (10 kDa) across the confluent ECs (ii) by diffusion of rhodamine labelled liposomes (green and red fluorescence in one time). The spectrometer measurement were designed as 12-hour continual measurement. Transendothelial transfer of dextran and liposomes were measured without ultrasound stimuli and after ultrasound pulses with injection of SonoVue (cavitation agent). Additional resistance measurement was integrated by assembling of special evaporated gold microelectrodes in series with a gold counterelectrode near ECs layer. Resistance across the ECs monolayer was measured using cell-substrate impedance-sensing system (Applied Biophysics).

## RESULTS

The setup was optimized for user-friendly 12-hour continual time-lapse measurement. Initial resistance across ECs layer was  $1450 \pm 190 \Omega$  (recomputed per  $1\text{cm}^2$ ), the change of resistance on ECs without activated microfluid was stable, with microfluid was decreased to  $1250 \pm 240 \Omega$  and sono-stimuli shifted to  $350\text{--}650 \Omega$ . Basal fluorescence detected by fluorometer in the cuvette was minimal and relatively stable during 12 hours (green RU = 25000; red RU = not measurable), sono-pulses caused significant leakage of green-fluorescent molecules (shift to 200 000 in 2 minutes; reached plateau in 10 minutes) and gradual opening for larger liposomes (increased to average RU = 95000 in first 5 minutes and RU = 175000 after 2 hours). In vitro diffusion kinetics should be complemented and correlated also with microscopic scan of opening pores in ECs layer in future.

## ACKNOWLEDGEMENT

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## ACCESSING THE ORGANIC MATTER IN BIOCHAR USING CHEMICAL FRACTIONATION

David ŠIRŮČEK<sup>1\*</sup>, Michal KALINA<sup>1</sup>, Martina KLUČÁKOVÁ<sup>1</sup>

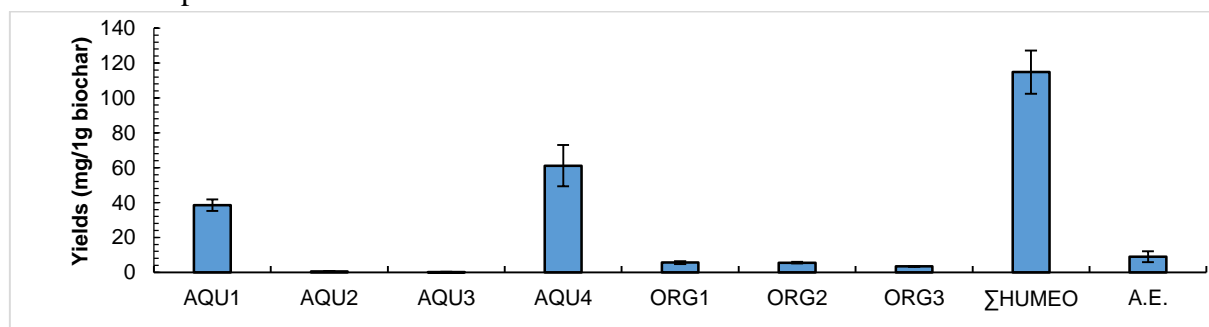
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This contribution is focused on utilization of a sequential chemical fractionation method for determination of organic matter content, its distribution in biochar and the possible use of biochar as a soil conditioner in agriculture. For these purposes the optimized chemical fractionation procedure was used to reveal the content of organic matter in different biochar samples with different properties (samples with European biochar certification for usage in agriculture) which depend significantly on the temperature used during a pyrolysis of biomass residues in the process of biochar production. These samples were also fractionated by classic alkaline extraction to obtain the so-called extractable fraction of organic matter (NOM).

Biochar is one of the important soil conditioners, known for having positive effect on crop yield, soil quality, nutrient cycle, and carbon sequestration due to the transfer of organic carbon from it to the soil. However, the effect depends on the properties of the biochar, its doses to the soil, but also on the properties of the soil itself. Surprisingly, some authors point to the fact that biochar does not always have a positive effect on soil, plants, or microfauna. Therefore, it is necessary to perform its depth characterization to be able to predict its role in soil and its optimal application dose.

Individual fractions obtained from sequential chemical fractionation as well as NOM samples were characterized by methods of elemental analysis (determination of organic elements content), thermogravimetry (contents of ash, organic matter, and moisture). Based on the obtained yields (**Figure 1**) it can be said that the largest fraction is AQU4, however, most of it are NaHCO<sub>3</sub> and Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> used during the fractionation. On the other hand, the AQU1 fraction, which consists of unbound or only weakly bound molecules, is significantly higher than other samples obtained. A similar trend can be observed with the ORG (organo-soluble) samples. Comparing the humeomics ( $\Sigma$ HUMEO) and the alkaline extraction (AE) we notice that AE yield is several times smaller but still we must take in account the elemental analysis and thermogravimetry data to calculate the organic matter content which is much more significant and eliminates the content of salts introduced into the individual fractions during the fractionation procedures.



**Figure 1:** Average yields obtained by both sequential chemical fractionation and alkaline extraction related to 1 g of biochar used during both processes.

The results showed how much, and which organic elements are contained in the biochar sample related to 1 g of it. The assumptions about the solid structure were confirmed according to the fact that, despite the use of strong and relatively aggressive solvents, it has been impossible for us to extract a significant amount of total organic matter contained. Nevertheless, the biochar has a great potential for use in agricultural sector as a soil supplement as biochar is likely to be retained in the soil matrix for a relatively long time and thus contribute to the stabilization of soil organic matter.

Overall, the analyses show that the investigated biochar is a rigid and durable material that, even after using of aggressive reagents and high temperatures, still contains a high amount of organic matter. The structure couldn't be cleaved at a level where strongly bound organic matter could be extracted, which is indicating the high resistance of organic matter in biochar structure. To be able to make more detailed description we will perform chromatographic analysis (GC-MS and LC-MS) which will provide us information on the molecular level of fractions or structural analysis methods (e.g., FTIR, NMR).

### ACKNOWLEDGEMENT

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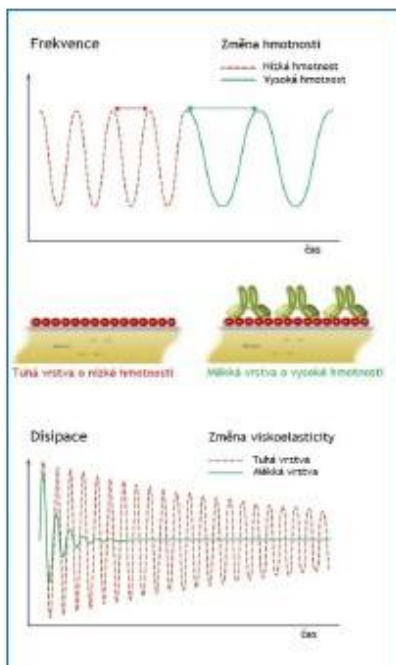


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## METODA QCM-D MĚŘENÍ HMOTNOSTI, TLOUŠTKY A STRUKTURNÍCH VLASTNOSTÍ MOLEKULÁRNÍCH VRSTEV



### Metoda QCM

Základem měření QCM je AT-štěpený křemenný krystal, připojený ke zdroji střídavého napětí pomocí dvou elektrod a pokrytý tenkou vrstvou kovu. Adsorbce molekul na povrch krystalu vyvolá změnu rezonanční frekvence, na které krystal kmitá. Z této změny lze vypočítat změnu hmotnosti. Jedná se o velmi citlivou metodu umožňující sledovat rozdíly hmotností v řádu nanogramů, interakce molekul a kinetiku probíhajících reakcí a to v reálném čase a bez nutnosti značení.

### QCM-D

Patentovaná technologie stanovení disipace neboli ztráty energie umožňuje měřit rychlost, kterou vrstva látky na povrchu krystalu pohlcuje energii. Je zaznamenána poté, co je krátce přerušeno buzení křemenného krystalu střídavým proudem, probíhající v krátkých intervalech v průběhu celého měření. Jako výsledek dostaneme spolu s křivkou změny rezonanční frekvence také křivku disipace energie. Ta vypovídá o viskoelastických vlastnostech adsorbované vrstvy.

### APLIKACE:

- Adsorpční a desorpční kinetika
- Příprava a uchování léčiv
- Solární články nové generace
- Imunokompatibilita implantátů
- Polyelektrolytické vrstvy
- Interakce protein-DNA
- Tvorba lipidových vrstev
- Korozní palivových článků
- Strukturální změny proteinů
- Účinnost detergentů
- Aktivita enzymů
- Interakce Ab-Ag
- Degradace celulózy
- Nanotoxikologie
- Analýza toxinů
- Buněčná adheze
- DNA hybridizace
- Pokovování



### Q-Sense E4 Auto

- 4 paralelní automatická měření
- Moduly: elektrochemický, elipsometrický, mikroskopický, atd.



### Q-Sense Omega Auto

- 2 x 4 paralelní automatická měření
- Zabudovaný termostat
- Mikrotitrační destička s autosamplérem



### ZAŘÍZENÍ PRO PŘÍPRAVU A TESTOVÁNÍ BATERIÍ



**MTI Corporation**  
www.mtixtl.com

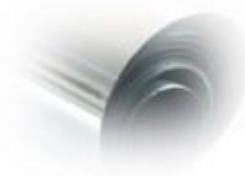
MTI Corporation (USA) je předním výrobcem zařízení a spotřebního materiálu pro výzkum a výrobu baterií. Komplexní nabídka zahrnuje přístroje pro přípravu elektrolytů a elektrod ale také pro kompletaci a testování baterií různých typů (knoflíkové baterie, tužkové baterie, akumulátory). Většina zařízení je vhodná pro provoz v rukavicovém boxu s inertní atmosférou dusík/argon.

- Vysokoteplotní pece a sušárny
- Vakuové mixéry, mlýny, drtiče
- Zařízení pro nanášení tenkých filmů
- Válcové lisovací a krimpovací zařízení
- Vysekávače elektrod
- Testovací držáky baterií



### SPOTŘEBNÍ MATERIÁL PRO PŘÍPRAVU BATERIÍ

- Pouzdra
- Pružiny
- Distanční disky
- Separátory
- Fólie
- aj... [www.mtixtl.com](http://www.mtixtl.com)

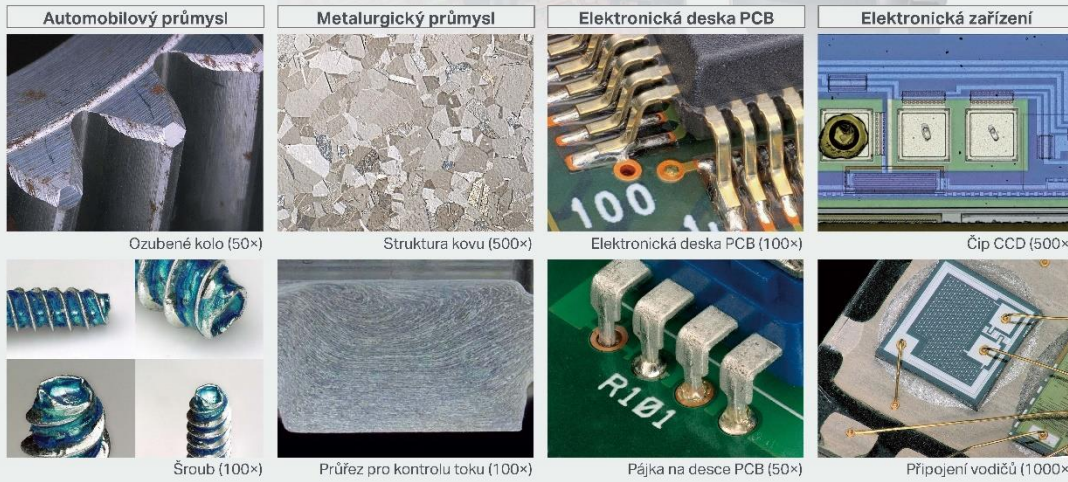


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 CHNSO analýza AAS analýza částic HPLC  
 hmotnostní SPEKTROMETRIE centrifugy EXTRUZE  
 ICP-MS SERVIS termická analýza AIR monitoring  
 XPS widefield TEXTURA spotřební materiál NMR  
 DLS automatické dávkování iGC TOC analýza RVC

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## 2 THETA

### Analytical standards equipment

2 THETA ASE s.r.o.  
Jasná 307, 735 62 Český Těšín, CZ  
e-mail: [2theta@2theta.cz](mailto:2theta@2theta.cz)

Tel: 558 732 122, 602 720 747, 602 240 553, 602 381 940  
[www.2theta.cz](http://www.2theta.cz)

### EcaFlow 150 GLP – analyzátor stopových prvků

Stanovení stopových koncentrací těžkých kovů v různých maticích.  
Speciace, stanovení aniontů, některých organických látek, O<sub>2</sub> a SO<sub>2</sub>...



- analýza včetně kalibrace probíhá plně automaticky a je velmi rychlá
- široký lineární rozsah 0,1 µg/l až několik desítek mg/l
- konkuruje AAS nízkou cenou a provozními náklady
- mobilní verze umožňuje použití v pojezdných laboratořích

### Mikrovlnný mineralizátor MAGNUM II

Tlakové i otevřené rozklady všech typů vzorků

- velmi rychlý rozklad s následným chlazením
- výkon jednotky: 3 ochlazené vzorky za hodinu
- tlakový i otevřený systém v jednom – umožňuje i zakoncentrování vzorku, odkouření kyselin, Kjeldahlizaci, extrakci
- vysoké navážky vzorků - do 2,5 g v tlakovém, do 10 g v otevřeném systému
- měření, regulace a registrace tlaku, teploty a výkonu, měření odraženého výkonu



### Reaktory pro organické syntézy, nanočástice a studium reakcí

### Izotachoforéza, kapilární elektroforéza řady EA

Pro analýzu ionogenních látek ve vodách, zemědělských produktech, potravinách, klinických materiálech...



- dvoukolonové uspořádání umožňuje pracovat metodou ITP i CZE a jejich kombinací
- modulární systém umožňuje měnit konfiguraci
- vodivostní nebo fotometrické detektory
- možnost napojení on-line na MS

Výhody: současné stanovení několika složek s koncentracemi lišícími se až o 6 řádů, nízké limity detekce od 5.10<sup>-9</sup> mol/l, krátká doba analýzy, nízké provozní náklady.

Přístroje: EA 303 – plně automatický s autosamplérem  
EA 102 – manuální dvoukolonový

### Zařízení pro přesný ohřev a chlazení

REGULACE NAPROGRAMOVANÉ TEPLoty S PŘESNOSTÍ 0,1°C, VYSOKÁ VARIABILITA: OBJEMY, PROVEDENÍ (NEREZ, HLINÍK, PLAST) A ROZSAH TEPLot

#### Skříňové termostaty ST, Q-Cell

objem od 70 l do 1460 l

- teplotní rozsah: +3°C až +40°C/ +70°C
- vynucená cirkulace vzduchu, měření teploty v reálném čase
- alarmy překročení nastavené teploty, výpadku napětí, ...



#### Laboratorní chladničky CHL, Q-Cell-CHL

objem od 70 l do 1460 l

- teplotní rozsah: 0°C až +15°C
- nízkoteplotní verze: -10°C až +10°C
- vynucená cirkulace vzduchu



#### Laboratorní mrazničky

Skříňové modely nabízejí objem truhlicové mrazničky objem od

- teplotní rozsah: -25/- 40°C až
- vynucená nebo přirozená

#### ZLN,ZLW, Q-Cell

od 85 - 447 litrů  
200 – 600 litrů.

0°C  
cirkulace vzduchu



#### Sterilizátory SR a Sušárny SL, QSL-1

objem od 15 l (SL), 56 l (SR) do 1005 l

- teplotní rozsah: od 5°C nad teplotou pracovního prostředí do +250°C sterilizátory / do +300°C sušárny
- vynucená nebo přirozená cirkulace vzduchu, přednastavené programy sterilizace, automatické blokování dveří...

#### Klimatické komory KK



objem od 115 l do 1485 l

- teplotní rozsah -10°C. + 60 °C
- rozsah vlhkosti: 30 - 90%
- možnost programování a regulace teploty, vlhkosti a intenzity osvětlení,
- FIT systém – nastavení osvětlení den/noc
- možnost volby barvy světla (LED) panel

### NOVINKA: Přenosný coulometrický analyzátor PCA2

Analýzy těžkých kovů, aniontů, ionogenních organických látek, rozpuštěného O<sub>2</sub>, SO<sub>2</sub>...

- řízen vlastním mikroprocesorem.
- vybaven napájecí baterií pro měření v terénu nebo ve výrobním provozu
- meze stanovitelnosti od 10 µg/l, lineární rozsah koncentrací až 4 řády



### Odběr a úprava vzorků

Nástroje pro odběr plyných, kapalných i pevných vzorků ve výrobě, kontrole, životním prostředí

Více než 40 druhů nástrojů, např.:

- vakuová pumpička pro odběr kapalin ze sudů, cisteren apod. bez kontaminace vzorkovacího nástroje, i pro odběr hořavin do předem evakuovaných lahví
- ventil pro kontinuální odběr vzorků paliv z cisteren
- nástroje pro odběr kapalin z velkých hloubek
- dvouplášťový vzorkovač pro současný odběr několika vzorků sypkých materiálů

Nástroje pro drcení, mletí, tavení a zmenšování vzorků

- čelistové drtiče, laboratorní mlýnky, lisy
- rotační děliče pro definované rozdělení sypkých vzorků
- elektrické tavičky pro přípravu vzorků k RTG analýze



### Dále nabízíme:

#### Laboratorní přístroje

- plamenové fotometry, spektrofotometry
- gelová elektroforéza, osmometry, kryometry
- pH-metry, ionometry, konduktometry, refraktometry – laboratorní i přenosné

#### Příslušenství a spotřební materiály

- elektrody pro měření pH, ISE, konduktometrii...
- pro AAS - výbojky, grafitové kyvety, ICP - hořáky, zmlžovače...

#### Laboratorní potřeby a zařízení, laboratorní nábytek

- homogenizátory, ultrazvukové lázně, laboratorní váhy a termogravimetry
- počítačky kolonií bakterií
- celoplastové digestoře, skříně na kyseliny...

#### Certifikované referenční materiály

- čisté látky, jednoprvkové a víceprvkové roztoky pro kalibraci
- matriční – půdy, hominy, nerostné suroviny, vody, potraviny, rostliny, tkáně, kovy, cement...



## 2 THETA

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### PLÁN AKCÍ 2022

- Hutní a průmyslová analytika 2022**, mezinárodní konference, duben 2022
- Odběry vzorků**, kurz, **září 2022**
- Mikroelementy**, seminář, **září 2022**
- Analýza organických látek**, kurz, **říjen 2022**
- Příprava a užití referenčních materiálů a mezilaboratorního porovnávání zkoušek**, konference s mezinárodní účastí, **listopad 2022**

### ODBORNÁ LITERATURA

Analytická chemie, vzorkování, chemometrie, potraviny, nápoje, gastronomie...

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