
BOOK OF ABSTRACTS

Modern Research Techniques for Physicochemical
Characterization of the Potential Application Systems

PHD STUDENTS SUMMER SCHOOL FOR
May 18-20, 2022
Lublin



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**Modern Research Techniques for Physicochemical
Characterization of the Potential Application Systems**

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Lublin

‘Anything you have learned so far will lose its meaning if you cannot find an application for this knowledge’

Paulo Coelho

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Faculty of Chemistry
Maria Curie-Skłodowska University



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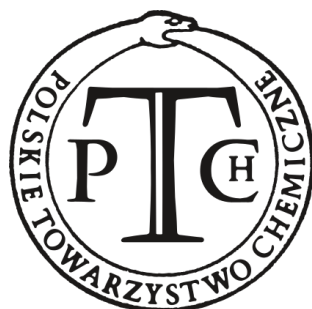
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FOREWORD

The Summer School for PhD Students is organized by the Faculty of Chemistry of Maria Curie-Skłodowska University (MCSU) in Lublin. The aim of the Summer School is to develop the knowledge acquired in the course subjects. PhD students are provided with an opportunity to participate in **lectures** delivered by outstanding lecturers, **workshops**, **discussions**, as well as to present their research results and achievements in the form of **oral** and **poster presentations**.

Among the invited lecturers of the Summer School are scientists and experienced academic teachers:

Prof. Carlos Bravo-Díaz (University of Vigo),

Dr. Agnieszka Brzyska (Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences in Krakow),

Prof. Małgorzata Maciejewska (Faculty of Chemistry MCSU),

Prof. Radosław Zaleski (Faculty of Mathematics, Physics and Computer Science MCSU).

The lectures cover modern research techniques, such as:

- nuclear magnetic resonance (NMR),
- high performance liquid chromatography (HPLC),
- coupling technique of infrared spectroscopy with thermogravimetry (TG-IR),
- differential scanning calorimetry (DSC),
- molecular modelling,
- positron annihilation lifetime spectroscopy (PALS),

and their use for investigations of the systems with a great application potential.

The workshops are closely related to the topic of the lectures. The PhD students divided into small groups have the opportunity to participate in all planned workshops.

The meeting of PhD students from different countries and academic centers ensures the exchange of experiences and good practices in the field of science and research which is the foundation for building international cooperation fostering the implementation of global projects.

INVITED LECTURERS

Prof. Carlos Bravo-Díaz



Prof. Bravo-Díaz is a world-class specialist in micellar catalysis. He graduated in chemistry from the University of Santiago de Compostela in 1986 where he obtained a doctoral degree in 1991. In the years 1991-1993 he carried out research in the team of Prof. Larry Romsted at Rutgers NJ University in the USA. He has been working at the University of Vigo since 1991.

The research interests of Prof. Carlos Bravo-Díaz include: physical chemistry, in particular colloid chemistry, bioorganic chemistry and biophysics. At the beginning, his research focused mainly on the interactions determining the structure and composition of aggregated systems such

as micelles, microemulsions, liposomes, biological membranes, macroemulsions and aqueous solutions of polyelectrolytes. Prof. Carlos Bravo-Díaz deals with issues related to the placement of various antioxidants in natural emulsion systems and their ability to stabilize these systems. The research results find practical application in the food industry. His current research activity focuses on developing a proper composition of parenteral supplements.

He is the author or co-author of over 120 scientific papers published in renowned international specialist journals and book publishing houses as well as a regular reviewer in prestigious chemical journals and a member of scientific societies: Spanish Royal Society of Chemistry and European Colloid and Interface Society. Professor collaborates with many research centers, including: Rutgers, The State University of New Jersey, Universidad de Porto, Universidad de Santiago de Chile and Maria Curie-Skłodowska University in Lublin.

His cooperation with the Faculty of Chemistry at MCSU began in 2008. He visited Lublin many times, presenting the results of his research delivering lectures for students and university scientists. The scientific cooperation resulted in the joint publications in the journals from the Philadelphia list and presentations at international conferences. In 2018 Prof. Bravo-Díaz was awarded the title of Honorary MCSU Professor. The Professor's laboratory in the Department of Physical Chemistry at the University of Vigo is always open to students and workers of the Faculty of Chemistry at MCSU.

Dr. Agnieszka Brzyska



Dr. Agnieszka Brzyska graduated from the Maria Curie-Skłodowska University in 2004. She obtained the doctor's degree in theoretical chemistry at the same university in 2009.

Her scientific interests involve: using quantum chemistry for determination of the fundamental chemical and physical properties responsible for the structure and reactivity as well as spectroscopy of various types of molecular systems; methods of reducing the cost of quantum-chemical calculations (low-scaling QM methods); theoretical design of novel molecular materials; theoretical description of nuclear magnetic resonance spectroscopy and vibration analysis; solvent effects on the NMR and IR spectra.

Her recent research concerns mainly the responses of various molecular systems (such as oligosaccharides, peptides, prospective heterocyclic substitutes for ethanol as biofuels, mechanophores, carbon nanostructures etc.) to mechanical forces. Insight at the molecular level into the nature of changes caused by external forces in the structure of molecules can be obtained through simulations based on theoretical methods.

Dr. Agnieszka Brzyska works as an assistant professor at the Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences in Krakow.

Prof. Małgorzata Maciejewska



Prof. Małgorzata Maciejewska is a specialist in the field of polymer chemistry. She obtained both the master's degree in chemistry in 1997 and the doctor's degree in polymer chemistry in 2002 from the Maria Curie-Skłodowska University. In the years 2002-2015 she carried out research in the team of Prof. Barbara Gawdzik and obtained the habilitation degree presenting the dissertation 'Permanently porous polymer materials - preparation, characterization, selected directions of applications'.

Her research areas involve: polymer synthesis and characterization, porous polymers, functionalization of polymer surface, modification of natural polymers, thermal analysis and application of polymers in separation processes. She focused mainly on the synthesis of polymeric microspheres based on various techniques of heterogeneous free radical polymerization. The current research focused on in-depth characterization and application of porous polymers.

She is the author or co-author over 60 scientific papers published in the journals from the Philadelphia list and other renowned specialist journals as well as many presentations at international conferences. Prof. Maciejewska is also a reviewer in international journals and a member of scientific societies, i.e. The Polish Society of Calorimetry and Thermal Analysis and The Polish Chemical Society. She collaborates with many scientists from Poland and other research centers. Prof. Maciejewska is opened for all kinds of cooperation.

Prof. Radosław Zaleski



Prof. Radosław Zaleski is a worldwide known specialist in positron annihilation. He graduated in physics from the Maria Curie-Skłodowska University in 2000 where he obtained a doctoral degree in 2005 and presented the habilitation dissertation in 2014. In the years 2000-2005 he was a member of the Prof. Tomasz Goworek's team working on an extended model of positronium annihilation.

The model allowed to extend the applicability of positron annihilation lifetime spectroscopy for characterization of mesoporous materials. Prof. Radosław Zaleski had a significant contribution to development of this model, its implementation in a computer code, experimental verification and various studies related to porous materials. He continued this work independently proposing another extension, which enabled using the model for measurements performed in air.

Of his studies those *in-situ* of the processes taking place in the mesopores observed with a microscopic positron probe were particularly interesting: thermal decomposition, adsorption, phase behavior of confined substances, experimental measurements of negative pressure under concave meniscus, etc.

At the same time he focuses on the fundamental issues of positron and positronium and organic materials, as well as applied research on the strengthening of the surface layer of construction materials, food processing, drug delivery, positron emission tomography and material science. He specializes in positron annihilation lifetime spectroscopy being also proficient in various material characterization techniques.

Prof. Radosław Zaleski has authored or co-authored over 90 peer-reviewed papers in reputable journals and reviewed over 60 articles. He is a member of the Polish Physical Society and the International Society for Positron Annihilation and Nuclear Probes. He collaborates with many research centers, e.g. Idaho National Laboratory, Helmholtz Center Dresden-Rossendorf, Slovak Academy of Sciences, etc. He works as an associate professor at the Maria Curie-Skłodowska University. His teaching activities include nuclear physics and energy, automatic measurements and control of measuring apparatus, project management, analysis and presentation of scientific results, etc.

ORAL PRESENTATIONS

Cadmium and lead sorption by exopolysaccharide isolated from *Chlorella vulgaris* culture

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Over the past few years, post-harvest microalgal cultivation medium is being extensively researched for its possible application. One of the components of the medium are extracellular polymeric substances (EPS), represented mainly by exopolysaccharides. EPS exhibits sorption abilities due to the presence of numerous carboxyl, hydroxyl, and amino groups, which are essential for metal binding, in the structure of these macromolecules [1, 2].

The aim of this study is to investigate the cadmium and lead ion sorption capacity of EPS synthesised by *Chlorella vulgaris*.

The sorption properties were analysed in this study according to the procedure described by Dobrowolski et al. [3]. EPS samples were dissolved in a salt solution of cadmium and lead at concentrations of 10, 50, 100, and 150 mg L⁻¹. The final EPS concentration in the prepared sample was 100 mg L⁻¹. The solutions were agitated, centrifuged, and filtered. The filtrates were used for determination of metal content by ICP-OES. Sediments after centrifugation were freeze-dried. The functional groups involved in the EPS-metal interaction were identified with FTIR. Additionally, the content of total sugars, proteins, and uronic acids in the studied EPS was determined.

The results show significant differences in the cadmium and lead affinity for EPS synthesised by *C. vulgaris*. The amount of Pb(II) bound by EPS is approximately twice as high as Cd(II). It was observed that an increase in the metal concentration was accompanied by an increase in the amount of metal ions bound by EPS. Next, the analysis of FTIR spectra allowed identification of functional groups involved in the metal-polymer interaction. As shown by the results, the carboxyl, carbonyl, and hydroxyl groups have the largest share in the sorption.

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Hierarchical self-assembly of tetratopic building blocks

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Supramolecular chemistry is of particular interest over several decades. Many either theoretical or experimental papers have been devoted to various classes of molecules, which are able to self-assemble on solid surfaces. Particularly interesting are rigid organic compounds of diverse architectures that form different molecular networks by means of directional interactions between “active” groups. A good example of such interactions are hydrogen bonds. However, in the systems involving metal atoms, donor-acceptor interactions play a key role. These interactions lead to coordinate bonding between metal and active groups. The capacity to self-assembly could be used in material chemistry and especially for the production of the so-called “smart materials”. They are used in areas such as catalysis, photonics, electronics, and many other fields.

In this work, we present the results of molecular dynamics simulations for tetra-substituted molecules, which can self-assemble into (i) fractals, (ii) porous phases, (iii) one-dimensional lines and (iv) Archimedean tessellation, depending on the symmetry and molecular structure of a building block. These structures have been further characterized by several quantities such as bond order parameter, cluster analysis and other distribution functions.

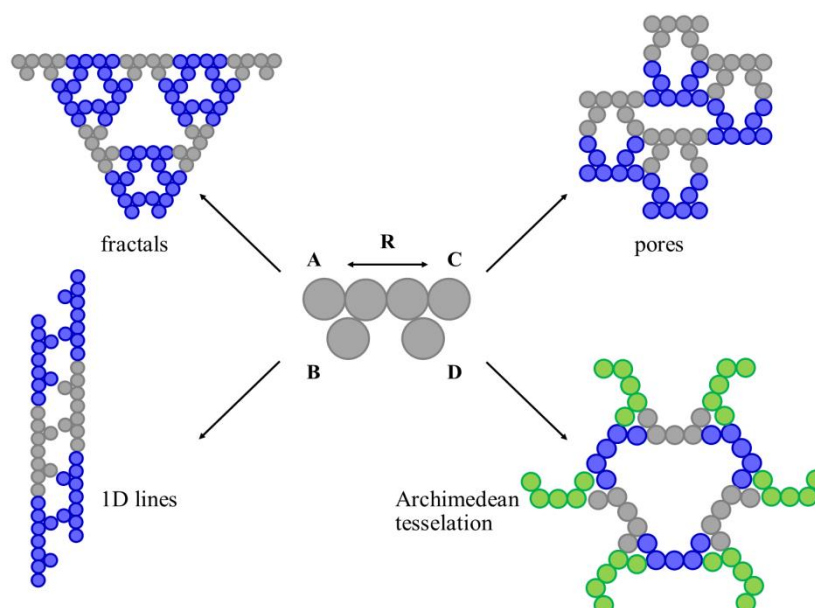


Figure 1. Types of self-assembled networks observed in the systems of tetra-substituted molecules. Coloring on silver, blue and green is used for visualization purposes only

Characterization of the organically modified fly-ash derived zeolite and its sorption properties toward ketoprofen

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The increase of hazardous pollutants in the environment has been observed with rising concern in recent time. Due to their adverse effects both on the environment and living organisms, there is a need to develop effective methods for their capture. Adsorption techniques are the most widely used among known methods applied in pollutants removal. In recent years, low-cost sorbents produced from various types of waste have become very popular. Zeolites from fly ash can be an example. They are crystalline hydrated aluminosilicates with unique properties (catalytic, ion-exchange, sorption), often reported as low cost sorbents in water treatment technologies. In order to improve their sorption ability towards specific pollutants, various methods for their modification have been applied.

The aim of this study was to modify a zeolite obtained from fly ash using β -cyclodextrin, to characterize the zeolite before and after the modification process and to investigate the sorption of ketoprofen on the obtained hybrid material. In this study, a zeolite with NaA structure type was used and then modified using β -cyclodextrin to improve the sorption properties. X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR) were used to characterize the zeolites before and after the modification process. Textural parameters of the materials were determined by nitrogen adsorption/desorption isotherm analysis. The sorption process of ketoprofen on the obtained NaA-CD hybrid material was carried out. The effects of dose, contact time and initial concentration on the sorption process were investigated.

XRD results revealed the absence of destructive effect of modification on the NaA zeolite structure. FTIR study confirmed the effectiveness of the modification and showed functional groups of the obtained hybrid material. The analysis of nitrogen adsorption/desorption isotherms showed a significant decrease in S_{BET} value (from 33 to 7 m²/g) for the material after modification. The micropores area was reduced by 96.5 % and the external surface area decreased by about 59.0 %. Drug removal study revealed that the sorption capacity of NaA-CD towards ketoprofen was 12.3 mg/g and the optimum contact time was 90 min. Smiljanić et al. [1] obtained a similar sorption capacity value for the clinoptilolite-cetylpyridinium chloride composite towards ketoprofen (13.6 mg/g) [1].

Acknowledgements

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Physicochemical, structural, and adsorption properties of chemically and thermally modified activated carbons

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Activated carbons are a good deal of research due to their unique physicochemical properties. Activated carbons are non-hazardous materials with a well-developed porous structure and usually with a significant share of micropores [1]. Activated carbon surface consists of three major sections: carbon basal planes (above 90% of the surface composition), heterogeneous sites (oxygen-containing groups mostly situated at the edges of basal graphite planes), and inorganic ash [2]. The well-developed surface of activated carbons in combination with thermal, chemical, and mechanical resistance makes these materials excellent adsorbents for water or wastewater purification, especially from organic compounds that are hard to decompose in water [3]. Despite these valuable features of activated carbons, surface functionalization is often a desirable operation as it may improve the sorption uptake, and makes the adsorbent much more selective from which the oxidation process is one of the most commonly used because of its simplicity [4].

In this work, activated carbons were chemically and thermally modified to diversify their acid-base character. The main aim of this work was to assess the efficiency of surface modifications of activated carbons concerning studying the differentiation of their affinity towards selected aromatic organic compounds. For this purpose, the comprehensive characteristics of modified activated carbons were analyzed using several analytical techniques: scanning electron microscopy, low-temperature nitrogen sorption, potentiometric titration of suspension, X-ray photoelectron spectroscopy, thermal analysis to provide knowledge of the textural, structural, acid-base, and thermal properties of samples. In addition, to verify the applicability of adsorbents for removing selected organic compounds, the equilibrium and kinetic experimental data were measured and analyzed by applying various equations and models.

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Arsenic removal using the iron oxide sorbent modified with lanthanum(III) ions

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Removal of arsenic compounds from the groundwater is an important issue of environmental protection. Several methods such as precipitation, oxidation, coagulation, ion exchange, adsorption and membrane filtration have been elaborated for arsenic removal from water. Unfortunately, many of these technologies are not sufficient to meet drinking water requirements. They are simply expensive or too complicated to handle. Adsorption seems to be the most appropriate way to combat the problem of arsenic contaminated aquatic systems. In recent years considerable work has been done on developing novel composite materials containing binary iron-metal oxides.

In this research, the commercially available iron oxide sorbent with quaternary ammonium groups (Ferrix A33E) was successfully modified with lanthanum(III) ions for removing arsenate(V) from water. This was confirmed by the scanning electron microscopy SEM, Fourier-transform infrared spectroscopy FTIR and X-ray photoelectron spectroscopy XPS. After the La(III) modification the surface area and the total pore volume increased. Moreover, the maximum sorption capacity towards As(V) ions increased from 34.41 to 53.33 mg/g. A33E-La(III) was characterized by better sorption capacities at the initial As(V) concentrations 25, 50 and 100 mg/dm³. The time needed to reach equilibrium was practically identical.

The Freundlich and Halsey isotherms described arsenic(V) sorption behaviour the best and this process was mainly chemisorption due to the energy larger than 8 kJ/mol. Moreover, thermodynamic studies revealed spontaneous and exothermic nature of the As(V) adsorption. As for the sorption mechanism, at optimal pH 6 the arsenate(V) ions were adsorbed through the formation of inner-sphere monodentate or bidentate complexes as well as lanthanum arsenate precipitation. However, in the alkaline environment the adsorption could still proceed due to the inner-sphere complexation with lanthanum hydroxide. Moreover, even after 3 cycles of adsorption-desorption, A33E-La(III) had still larger As(V) adsorption capacity than that of A33E.

It was found that the presence of lanthanum on the surface of the ion exchanger plays a great role in the adsorption of As(V) from the contaminated water due to changing the mechanism of the process. The exceptional As(V) removal capability of lanthanum-modified A33E-La(III) leads to its potential application for not expensive treatment of arsenic-contaminated water.

The synthesis of calcium phosphate based materials using agricultural waste as a calcium donor for environmental applications

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Owing to the growing demand for biocompatible, bioavailable and bioresorbable materials, the challenge is to find new and effective methods of synthesizing calcium phosphate bioceramics as well as to improve them [1]. A major component of human hard tissue, hydroxyapatite (HA), is considered as a material of a great potential in accordance medical, environmental and agricultural purposes [2]. The natural material being the product of the biomineralization process, possesses characteristic properties and composition. It was also widely proved that the biphasic calcium phosphate materials (BCP), composed of both calcium phosphates- HA and β -TCP forms, combines the beneficial properties of both forms [3]. Due to the economical and environmental aspects, the use of common biowaste- eggshells as a calcium donor during hydrothermal synthesis procedure is an effective solution [1,4]. The reduction of energy input is also a crucial factor determining the application of the procedure on a commercial scale.

In the presented research, the environmentally friendly procedure with the use of raw, uncalcined eggshells as the calcium ions precursor was analysed. The material was obtained at various initial pH values and analysed by means of the SEM, XRD and FTIR techniques. The microwave irradiation as a synthesis stage was employed and the changes in the composition and morphology of the obtained materials were underlined. The materials were also examined in the terms of biomedical applications as an enrichable additive to mouth daily care products supporting the biomineralization process. In this purpose the calcium ions release profiles were determined in the ultrapure water as well as in the Artificial Human Saliva solution. Then, the copper ions adsorption process on the chosen product was studied through fitting obtained data to the most common adsorption models including Langmuir and Freundlich concepts.

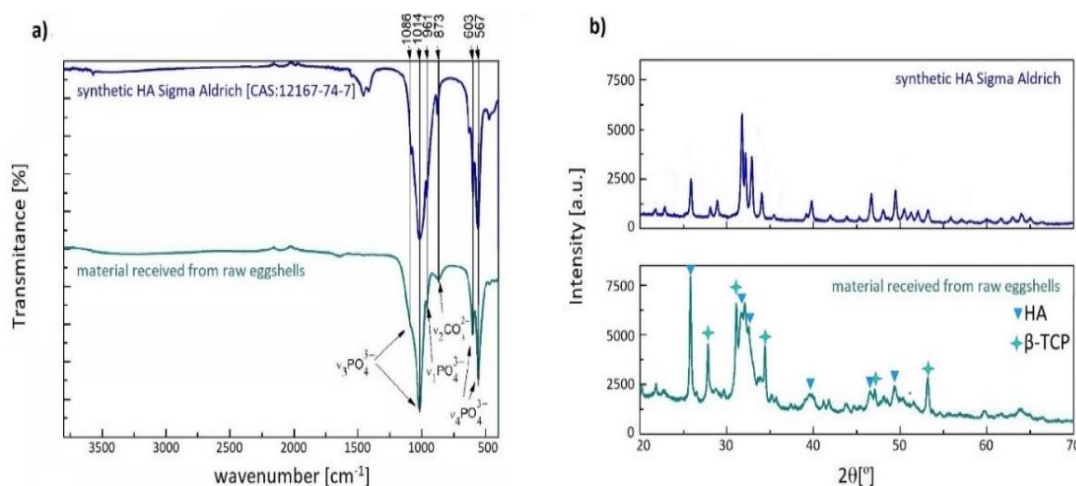


Figure 1. The FTIR (a) and XRD (b) spectra of the obtained material using eggshells as a calcium donor

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Supplementation of *p*-coumaric and 4-hydroxybenzoic acids enhances antioxidant properties of gluten proteins

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Consumer interest in healthy food and its beneficial effects on the body is growing. Wheat bread, as a staple part of the daily diet, is essential for human nutrition. As a result, supplementing wheat bread with substances known to have healthy benefits could be a useful method to enhance and diversify personal diet. Polyphenol extracts or free polyphenols can be added to wheat bread. Phenolic acids are present in a variety of foods, including fruits, vegetables, cereals, and other grains [1]. Benzoic and cinnamic acid derivatives are two types of phenolic acids. The skeletons of hydroxybenzoic derivatives are C6-C1. The hydroxycinnamic derivatives have a nine-carbon skeleton (C6-C3). The aim of the study was to assess the antioxidant properties of gluten proteins modified by 4-hydroxybenzoic acid (a hydroxybenzoic acid derivative), and *p*-coumaric acid (a hydroxycinnamic acid derivative).

Model dough samples with selected phenolic acids were prepared in a farinograph in concentrations 0.05 %, 0.1 % and 0.2 %. The mixing process of the supplemented dough was stopped just before the farinograph peak indicating the destruction of the gluten network (dough breakdown). Gluten samples were prepared by washing out the gluten from the model dough and lyophilized. Phenolic acids were extracted from gluten samples in methanol. UV-VIS spectroscopy was used to measure acid concentrations and antioxidant properties in methanolic extracts. Phenolic acids present in the gluten network were extracted according to method described by Sivam et al. (2013) with some modifications. 7.5 mg of gluten samples were extracted for 16 h with 1.5 mL of methanol [2]. In the next step, the extracts were centrifuged (14,000 × g, 3 min.). UV-VIS spectroscopy was used to measure acid concentrations and antioxidant activity in methanolic extracts. ABTS and FRAP assays were used to determine antioxidant properties.

After supplementation, 4-hydroxybenzoic and *p*-coumaric acids are detected in the gluten network. Coumaric acid has the highest level of extraction, according to UV-VIS spectra. Because of its high extractability, this acid may be the least linked to the gluten network. When compared to control gluten samples, supplemented samples had higher antioxidant properties in both ABTS and FRAP experiments. The antioxidant activity of extract from 4-hydroxybenzoic supplemented gluten was lower than that of samples supplemented with *p*-coumaric acid, according to the results of ABTS and FRAP experiments. The CH=CH-COOH group in hydroxycinnamic acids is regarded to be key in explaining why they have a far higher antioxidative efficacy than hydroxybenzoic acids, which has -COOH group. According to the results, phenolic acids could be employed to make health-promoting wheat products that have stronger antioxidant properties.

Acknowledgements

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Antimicrobial activity of the LL-37 peptide as a result of interaction with *Legionella gormanii* phospholipids

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Legionella species are Gram-negative intracellular pathogens of various protozoan species, such as amoebae and ciliates. Upon transmission to the respiratory tract through contaminated aerosol, the bacteria replicate within alveolar macrophages [1]. Among *Legionella* species, which are recognized to be pathogenic for humans, *L. gormanii* is the second prevalent causative agent of community-acquired pneumonia after *L. pneumophila* [2].

The aim of the study was to investigate the antimicrobial activity of human LL-37 cathelicidin against *L. gormanii*, determination of the minimum inhibitory concentration and the mechanism of peptide interaction with the bacterial cell membranes.

The results of the colony-forming unit (CFU) assay revealed that the LL-37 peptide inhibited *L. gormanii* growth in a dose-dependent manner. Bacteria cultured on medium with exogenous choline were more sensitive to the peptide than bacteria grown on medium without choline. The Langmuir monolayer technique coupled with the Brewster angle microscope (BAM) and the surface potential sensor was used to study the interaction of the LL-37 peptide with phospholipids (PLs) isolated from *L. gormanii* cultured with (PL+choline) and without choline (PL-choline). The presence of LL-37 in PL-choline and PL+choline monolayers induced a shift of the surface pressure-area (π -A) isotherms towards larger mean molecular areas (Mma) due to the LL-37 accumulation at the liquid/gas interface and interaction with PLs. As the concentration of the LL-37 in the subphase increased, the area per molecule and the surface potential also increased while the compression modulus (C_s^{-1}) values, calculated from the π -A isotherms, decreased indicating less condensation of the PL monolayers. Besides, BAM images revealed the different morphology of the PL-choline and PL+choline membranes which affected the LL-37 action. Moreover, interactions of the peptide with the PL resulted in a reduction of the membrane thickness due to disturbance in molecular packing and ordering.

To conclude, the LL-37 peptide destabilized the PL monolayers especially derived from *L. gormanii* cultured on medium with exogenous choline, suggesting a bactericidal effect.

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Formaldehyde and water adsorption on functionalised graphene surfaces – a theoretical investigation

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Everyday human activity exposes him to constant contact with potentially dangerous substances. Their elimination is a research challenge today. Understanding the mechanisms of interaction of the adsorbent with the adsorbate molecules is a valuable source of information needed to design effective methods for the detection and removal of undesirable substances. Therefore, an attempt was made to determine the interactions of functionalized graphene surfaces with molecules of formaldehyde belonging to the group known as indoor pollutants and with water molecules ubiquitous in the air [1].

The research was carried out on the basis of an *in silico* experiment with the use of the DFT/B3LYP computational method [2]. In order to obtain a reasonable quality to computational time ratio, calculations were carried out with a gradual increase of the size of the graphene surface fragment. Next, the surface was modified by introducing functional group(s) (e.g., Figure 1a) attached to the edge of the chosen graphene fragment, called a representative fragment. The so-called "mixed" basis set B1/B2 was used. The larger basis set B1 (being 6-311++G**) and smaller one B2 (being 3-21G) were adopted as indicated in Figure 1b [3, 4]. Due to the variety of possible interactions between the adsorbent and adsorbate molecule the systematic compact notation has been proposed (see Figure 1c).

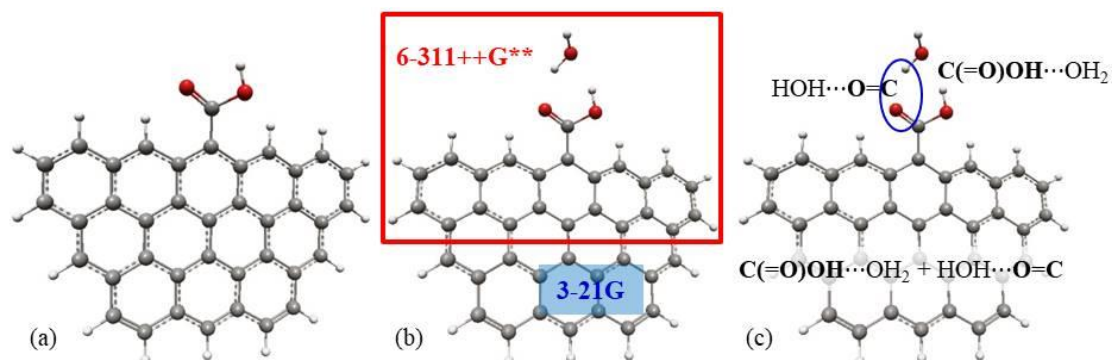


Figure 1. (a) Representative fragment of a graphene surface with the attached carboxyl group, (b) 6-311++G** and 3-21G basis set regions, (c) Notation used for denoting adsorbent – adsorbate interactions

The calculations clearly show the cooperative character of a hydrogen bonds. In addition, they show that the physical adsorption of water molecules is competitive against formaldehyde. However, in addition to the physical adsorption considered here, chemisorption – leading to the C-N bond formation in the case of formaldehyde – is also possible indicating that formaldehyde can be effectively eliminated using functionalized graphene surfaces.

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Application of LC-QTOF in lipidomic profiling of cold pressed seed oils

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Lipidomics, which is a branch of metabolomics, is an explosively developing field of science in which research is focused on the identification of lipids, their biological functions and interactions with other molecules [1]. The identification of a large number of lipids is an extremely demanding task due to the structural diversity of the lipids as well as the diverse composition of the matrix.

The increased interest in lipidomic research in recent years was related to the introduction to analytical practice new methodological and apparatus solutions in the field of liquid chromatography and mass spectrometry. MS-based methods ensure very high sensitivity while requiring minimal sample preparation and barely small amounts of samples. The popularity of these methods can be attributed to several advantages over other techniques, for example reduced ion-suppression effects [2]. Lipidomics has been accepted among others, as a lipid-related research tool in drug development trials or clinical biomarker discovery [3]. Furthermore, it is a discriminant technique successfully used in nutritional research aimed at differentiating and authenticating food products.

In recent years unrefined, cold-pressed seed oils have been gaining popularity due to the high content of various bioactive compounds and favourable nutrition properties. During the process of cold pressing the seeds, the temperature does not exceed 60 °, which guarantees the maintenance of the original aroma, taste and nutrients such as tocopherols and carotenoids [4]. Together with increase of interest in this products cold-pressed seed oils quality and authenticity control has become an issue of great importance to consumers.

Acknowledgements

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Crystalline host-guest complexes of pillar[n]pyridiniums and *p*-sulfonatocalix[4]arene

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The introduction of charge into the molecule in supramolecular chemistry is an attractive approach to building water-soluble complexes. Such charges bear many supramolecular macrocycles: calix[*n*]arenes, Stoddart's blue box, "Texas-sized" molecular box *etc.* Depending on the macrocycle's structure and properties, they have found numerous applications in the host-guest systems, sensing, catalysis, and design of porous materials. An interesting class of negatively charged molecules is anionic *p*-sulfonatocalix[4]arene. With an electron-rich basket-like cavity is a well-known water-soluble supramolecular host, capable of forming various types of assemblies, such as bilayer clay-type structures, capsules, nanometer tubules or spheres [1].

Here, we demonstrate our approach toward design of molecular crystalline assemblies using oppositely charged macrocyclic building blocks, anionic *p*-sulfonatocalix[4]arene and cationic pillar[*n*]pyridiniums. Pillar[*n*]pyridiniums are a new family of water-soluble inherently cationic host molecules of prismatic electron-deficient cavities [2]. These two types of macrocyclic hosts are complementary in terms of charge, shape and symmetry. Their self-assembly is guided mainly by the electrostatic attraction between anionic sulfonate groups of calix[4]arene and the positive charge on the pyridinium rings of the cationic macrocycles. The crystallization in gel and liquid-liquid diffusion methods have been used to obtain suitable crystals build from mixed macrocycles for single-crystal X-ray diffraction analysis. Moreover, *p*-sulfonatocalix[4]arene protects pillar[*n*]pyridiniums from deprotonation and irreversible structure changes that limit their application. This ability of supramolecular supersalts to improve the chemical stability of pillar[*n*]pyridiniums makes them promising repositories for chemically pregnable charged entities.

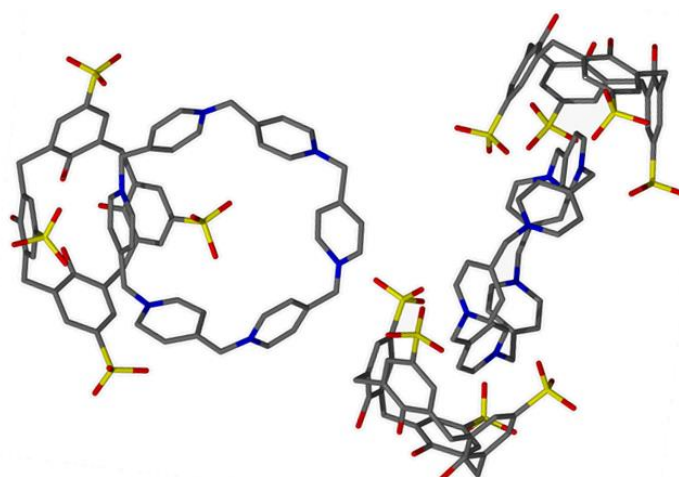


Figure 1. Complexes formed by *p*-sulfonatocalix[4]arene and pillar[6]pyridinium

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Visual discrimination of α,ω -alkanedicarboxylic acids

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Dicarboxylic acids of the general formula $\text{HOOC}-(\text{CH}_2)_n-\text{COOH}$ have wide use in our daily life [1]. They are applicable in industry and many biochemical processes such as energy production and storage. However, increased amounts of these compounds may cause inflammation and more serious metabolic disorders. Accordingly, their detection and recognition are of high importance for environmental protection and public health. The discrimination of these acids is challenging because of their very similar physicochemical properties [2,3].

Here, we present an absolutely new method that recognizes the sequence of linear saturated carboxylic diacids by taking advantage of the difference in length and utilizing plasmon coupling. The interactions between these diacids and gold nanoparticles, the surface of which is covered by cationic pillar[n]pyridinium macrocycles, produce a multilevel response, including a color that can be watched with a naked eye. The color develops from purple to red and back to purple, gauging the length, flexibility as well as the odd-even character of the diacid chain.

To sum up, we presented handy nanoreceptors for the visual detection of linear fatty diacids. These receptors are simple aqueous ensembles of gold nanoparticles and pillar[n]pyridinium macrocycles. Cross-linking of these constructs with carboxylic diacids produce small interparticle gaps that allow plasmon coupling, and hence, the color change.

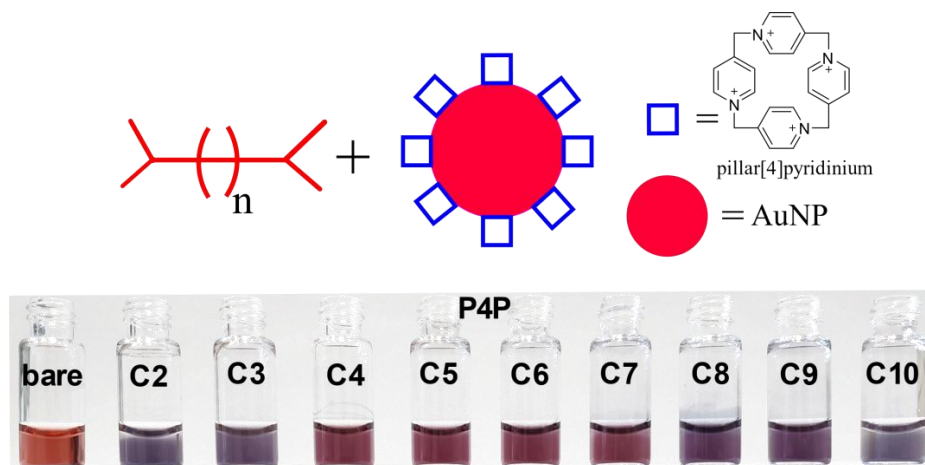


Figure 1. Supramolecular nanosensor in the presence of α,ω -alkanedicarboxylic acids

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Influence of gallic acid and its derivatives on the structure of the gluten network in wheat gluten dough

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Bread for many of us is an important element of the diet, so it can be used as a carrier for nutrients. There is a possibility of supplementing wheat dough with compounds characterized by "pro-health" properties. However, supplementation of wheat dough with different substances disturbs a proper structure of the gluten network and thus deterioration of the bread quality. Phenolic acids are non-flavonoid plant compounds present, for example, in cereals, fruits, vegetables and herbs and belong to compounds that can positively affect human health. They are characterized by antioxidant, antibacterial and anti-inflammatory properties as well as can eliminate reactive oxygen forms and block free radicals. Thus, as "pro-health" ingredients, they can constitute an appropriate addition to bread and enrich it [1].

The quality of the bread and its texture are greatly influenced by the physicochemical properties of gluten proteins (gliadin and glutenin). These proteins influence the quality of the wheat flour and therefore also the quality of the wheat dough. Glutenins and gliadins are able to form a high-molecular complex – gluten – in the presence of water. It has the form of a viscoelastic mass, which in molecular terms is composed of polypeptide chains. These chains are stabilized with disulphide bridges, hydrogen bonds and hydrophobic interactions, which are extremely important in the process of dough mixing process [2].

The aim of the research is to determine the influence of gallic, ellagic and tannic acid on the structure of gluten proteins in gluten dough (without starch), the changes in disulphide bridges conformations and environment of two amino acids: tyrosine and tryptophan. Gluten dough supplemented with selected polyphenols was prepared in the vibrating kneader. The polyphenols contents were 0.05 %, 0.1 % and 0.2 % (w/w). The gluten was washed out from the gluten dough, freeze-dried for 24 h and pulverized. Next, the samples were studied by using FT-Raman spectroscopy [3].

Analysis of the FT-Raman difference spectra in the amide I band showed that gallic acid and their derivatives induce changes in the structure of gluten proteins. The observed changes concern mainly β structures, which are dominant structures in glutenins. As for gallic acid, the percentage of g-g-g conformation remains at a similar level comparing with the control sample. In the case of ellagic and tannic acid, the percentage content of the most energy-stable conformation is higher compared to the control sample and does not change with increasing percentage content of these acids. The results suggest that the presence of phenolic compounds can prevent the protein complexes from changing the conformation of the disulphide bridges to less stable ones.

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The effect of physical aging on the contents of polycyclic aromatic hydrocarbons and their derivatives in biochars

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Biochar (BC) is a stable, carbon, porous material obtained via thermal decomposition of various types of biomass (plant material, agricultural waste, animal manure, sewage sludge, food residues, wastewater, hardwood, softwood) under an oxygen-limited atmosphere [1]. Pyrolysed material acquires special properties, so it can be used in different branches of industry. Among all possible biochar applications, a large part constitutes agricultural use of BC. The biochar addition to soil improves soil fertility, water retention, and vegetation yield as well as stimulates bacterial growth [2-5]. However, BC can also introduce into the environment some hazardous substances (e.g. polycyclic aromatic hydrocarbons, PAHs and their derivatives). Moreover, their fate during short- and long-term BC application into the soil is not well elucidated. Therefore, in our studies, the contents of bioavailable and total fractions of PAHs and their derivatives in straw-derived biochars (obtained at 500°C, BCW500; 600°C, BCW600; and 700°C, BCW700) were determined. Furthermore, biochars were subjected to a physical aging process to simulate and accelerate some environmental phenomena which affect BC during agricultural application. The contents of the studied contaminants in biochar before and after aging (BCW500-PA, BCW600-PA, and BCW700-PA) are given in Table 1.

Table 1. The contents of polycyclic aromatic hydrocarbons and their derivatives in studied materials

Sample	The concentrations of bioavailable fraction of PAHs ± SD* [ng/L]	The concentrations of bioavailable fraction of PAHs derivatives ± SD* [ng/L]	The contents of the total fraction of PAHs ± SD* [µg/g]	The contents of the total fraction of PAHs derivatives ± SD* [µg/g]
BCW500	3.51 ± 0.20	0.25 ± 0.01	151.55 ± 6.94	1.48 ± 0.07
BCW500-PA	11.66 ± 0.61	0.62 ± 0.03	191.92 ± 8.35	2.42 ± 0.11
BCW600	3.17 ± 0.15	0.48 ± 0.02	181.08 ± 8.29	1.92 ± 0.09
BCW600-PA	14.16 ± 0.73	0.40 ± 0.02	239.25 ± 11.44	2.23 ± 0.11
BCW700	3.53 ± 0.17	0.48 ± 0.02	158.02 ± 7.23	4.31 ± 0.20
BCW700-PA	12.38 ± 0.65	0.55 ± 0.03	205.83 ± 8.96	6.79 ± 0.30

* SD – standard deviation

The results indicate that the contents of the studied contaminants were affected by the physical aging processes. The concentration of bioavailable fraction of PAHs increased significantly as well as the total fraction of analytes. The contents of PAHs derivatives in studied biochars also increased in almost all cases. Due to the toxic, mutagenic, and carcinogenic properties of PAHs, the results are disturbing and the topic needs some additional investigations.

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Comparison of physicochemical, release and antioxidant properties of ascorbyl palmitate-loaded polysaccharide/gelatine edible films

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Many compounds present in food undergo oxidation, which leads to deterioration of the sensory attributes and nutritional value of a product. Consequently, the concept of active packaging that prevents or slows down the degradation of oxy-labile compounds has attracted growing interest. The effectiveness of active packaging depends on the ability of an active substance to penetrate into or to stay in the reaction site. This in turn depends on the properties of the carrier material, including the type of interactions between the active substance and the carrier. For this reason the selection of appropriate carrier is extremely important step in packaging development. Currently, renewable biopolymers, especially plant polysaccharides, are considered as a promising material for production of eco-friendly packaging.

Ascorbyl palmitate (AP) is an ester of palmitic acid and ascorbic acid (AA) used as a food additive. It is a strong amphiphilic antioxidant intended for the fat-containing foods. Compared to water-soluble AA, AP is more stable (the esterification reduces the hydrolysis of AA) and not sour. Therefore, AP can be a potentially more beneficial component of active packaging systems, than the AA. Nevertheless, because of partially hydrophobic character of AP, the obtaining homogenous biopolymeric carrier systems is extremely difficult and requires addition of emulsifiers and ethanol as a co-solvent. Proteins (e.g. gelatine (GEL)) and some polysaccharides, such as gum Arabic (GAR), starch modified with octenyl succinic anhydride (OSA), and water soluble soy polysaccharides (WSSP) may be used as effective emulsion stabilisers. We hypothesized, therefore, that the mixtures of these polysaccharides with GEL can be preferable carriers for AP terms of ensuring good emulsification.

This study aimed to characterize the physicochemical, release, and antioxidant properties of edible films obtained from bi-polymeric emulsions (GAR/GEL, OSA/GEL, and WSSP/GEL) incorporated with increasing concentrations (0, 1, 2 %) of AP. The microscopic images showed that AP was present in the emulsions both in the form of longitudinal crystals and microglobules. The incorporation of AP slightly decreased the pH of emulsions. Likely due to the amphiphilic character, the incorporation of AP into the carrier films increased the moisture content, but reduced the solubility in water. In the case of GAR-containing system, the AP improved water vapour barrier properties and tensile strength. In turn, the AP in did not affect the water vapour permeability and mechanical strength of the OSA-based system. The increase in AP concentration improved the UV-blocking properties of the films. The Makoid-Banakar model with time lag was the best tool to predict the release kinetic of AP release from the carriers into ethanol (lipophilic food simulant). Based on the time required for 25 % release, at the highest concentration of AP (2 %), the OSA-based system offered 2.2 and 16.2 times faster release compared to the WSSP- and GAR-based carriers, respectively. Consequently, the OSA/GEL film had the best initial antiradical activity. In summary, the GAR-based system offered the slowest release of AP and, consequently, the most prolonged antiradical activity.

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Aging studies of crosslinked polymeric composites

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Degradation of synthetic polymers is defined as all the changes that occur in their physicochemical properties, due to the chemical reactions taking place. They cause disruption of the main chain of macromolecules. In the case of biopolymers, in addition to the destruction caused by chemical reactions, there are changes caused by physical transformations, leading to damage to higher order structures. For this reason, the degradation of biopolymers is usually referred to as thermodynamic denaturation [1].

Degradation of polymers causes changes in their structure, which are usually irreversible. They are the result of chemical reactions such as crosslinking, oxidation or chain scission. The changes appearing in the structure of the polymer may be the result of physical or chemical transformations. The fastest observable symptoms are changes occurring on the surface of the material, such as a colour, gloss. In order to minimize the risk of significant effects of external factors on the properties and structure of polymers, they are modified, for example, by using additives (stabilizers, UV-absorbing substances or antioxidants) [2].

Chemical degradation is caused by chemical agents, i.e. acids, bases, solvents or reactive gases, which are in direct contact with the polymer material. This type of degradation occurs when the chemical reaction is initiated by low molecular weight chemicals [3].

UV polymerization of composites containing bisphenol A diacrylate (BPA.DA) and methyl methacrylate (MMA) in a weight ratio of 7:3 was carried out. UV initiator in the form of Irgacure 651 (IQ) was used. The respective amounts of monomers were mixed and then vented in a heating chamber at 65°C. A filler in the form of zinc oxide (ZnO) and benzethonium chloride (BEN) at 0, 1, 2, 5 % was added to the mixture. The mixture was stirred, then 1 % by weight of UV initiator was added. The mixture was transferred into 10x12x2mm glass molds with a teflon spacer. The composites were placed in a chamber equipped with 160W mercury lamps and exposed for 30 minutes.

For aging tests, the composites were cut into 10x10 mm samples, their thickness was 2 mm. They were placed in tightly capped tubes that were filled with solvents such as water, acetone, sodium hydroxide and hydrochloric acid. The aging process was carried out for 6 months at ambient temperature. The samples were also exposed to sunlight. To evaluate the changes taking place, the samples were weighed weekly for 12 weeks, then at 16, 20 and 24 weeks. Before weighing, the samples were dried at 85°C for one hour to remove adsorbed solvents. After each weighing, photographs were taken of the samples to visually assess the changes occurring in the structure. ATR/FTIR analyses were also performed before and after ageing to evaluate chemical structure of the samples.

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Bio-profiling of plants *via* effect directed analysis coupling high-resolution mass spectrometry

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A combination of effect-directed analysis (EDA) and high-performance thin-layer chromatography (HPTLC) screening is suitable for searching and investigating new biologically active substances of plant origin. These substances can potentially treat Alzheimer's and Parkinson's diseases, diabetes, obesity, depression, osteoporosis, and bacterial infections. The great advantage of EDA based on HPTLC is the possibility of analyzing many samples even in complex matrices and comparing the composition of the samples in one run. Moreover, the additional advantage is connected with the possibility of identification and isolation of the target substances. The detection of antibiotics, antioxidants, enzyme inhibitors, genotoxic compounds, estrogen and androgen activity, can be performed directly on the HPTLC plate [1,2].

In our present study, HPTLC screening and profiling were applied to determine bioactive substances in 15 supplement preparations of *Rhodiola rosea* L. root, in fruits and leaves of *Akebia quinata* Decaisne, and flower of *Clitoria ternatea* L.. For this purpose, the enzyme inhibition assays such as acetylcholinesterase, butyrylcholinesterase, tyrosinase, lipase, α/β -glucosidase, α -amylase, and β -glucuronidase were used. Antibacterial properties were investigated using Gram-positive bacteria *Bacillus subtilis* and Gram-negative bacteria *Avilibrio fischeri* assays. Additionally, the plants were tested for estrogen, antiestrogen, androgen, and antiandrogen activity. Moreover, samples were tested for genotoxic activity. The active bands were detected by bioassays directly on the HPTLC plate and were identified using high-resolution mass spectrometry using the TLC-MS interface.

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Application of nanomaterials as a solid contact in ion-selective electrodes

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Ion-selective electrodes with solid contact, due to their significantly better analytical parameters compared to their classic predecessors with an internal solution, have gained in popularity in recent years. In order to miniaturize the sensors and improve their operation, internal solutions were removed and attempts were made to obtain constructions in which it was possible to place the membrane directly on the electrode surface. However, this caused blockage of the flow at the interface and problems with the stability and reproducibility of the electrode potential. Therefore, an additional layer of solid contact was placed between the electrode and the ion-selective membrane, which, characterized by both electronic and ionic conductivity, significantly improved their work and improved service life [1].

The first materials used as solid contact were substances from the group of conductive polymers [2]. In the following years, various nanomaterials were also used for this purpose, the most common of which are carbon nanomaterials (nanotubes [3], nanofibers [4], fullerenes [5], carbon black [6]). There are also available in the literature electrodes for the construction of which nanoparticles, for example of gold [7] or platinum [8], were used.

The work describes the use of various types of nanomaterials as a solid contact in ion-selective electrodes sensitive to potassium and nitrate ions. In the former, nanoparticles of various metal oxides (zinc oxide, copper oxide and iron oxide) were used for the construction of sensors, while in the latter - polyaniline nanofibers doped with chloride and nitrate ions (PANINFs-CL AND PANINFs-NO₃) [9] and multi-walled carbon nanotubes-ionic liquid nanocomposite [10]. The basic analytical parameters of the tested sensors (such as the slope of the characteristic curve, linearity range, detection limits) were determined and compared with the unmodified sensors (containing only a membrane layer placed directly on the electrode). The influence of the modification on the stability and reversibility of the electrode potential as well as the influence of variable measurement conditions on the operation of the electrodes was also investigated. The electrodes were obtained and then successfully used to determine the appropriate ions in natural water samples.

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Adsorption of rhamnolipid and surfactin from mixed water-ethanol solvent

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Biosurfactants are natural surface-active compounds produced by microorganisms. They are characterized by amphiphilic build (with hydrophilic head and hydrophobic tail) which allows them to create micelles and to adsorb on different interfaces. Biosurfactants are biodegradable and non-toxic, they exhibit similar or better physicochemical properties than synthetic surfactants (low CMC, high surface activity, wide tolerance for pH and temperature change). This is why biosurfactants are of interest when it comes to various industries (e.g. cosmetics, food, pharmaceuticals).

In many products as well as industrial processes, biosurfactants are used in various solvents. One of the most often used solvents is ethanol. As a short chain alcohol, in the concentration called critical aggregation concentration (CAC), it is able to create aggregates [1]. For this reason, modification of surfactant behaviour in the bulk phase and their adsorption on the solution-air interface by ethanol will depend on the form that it attains in the solution.

As it is very difficult to find data concerning biosurfactant properties in the presence of the alcohol, the research's goal was to determine changes of adsorption properties of chosen biosurfactants (surfactin and rhamnolipid) in mixed water-ethanol solution in the whole range of ethanol concentration [2,3]. The research was based on the solutions surface tension measurements in 293 K. Basing on thermodynamic analysis of obtained results, it was concluded that ethanol influences on surfactin adsorption in the bigger extent than vice versa. In the low ethanol concentration and rhamnolipid concentration corresponding to unsaturated adsorption monolayer, the rhamnolipid adsorption was more favourable than in case of ethanol.

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The effect of boron concentration on the electrical, electrochemical, morphological and optical properties of boron-doped diamond sheets

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Diamond sheets are a highly attractive material for future flexible electrochemical sensors [1-3]. Unfortunately, there is a significant lack of knowledge regarding the effects of boron incorporation on the electrical, electrochemical, morphological and optical properties of free-standing, nanocrystalline diamond sheets.

In the following work, we describe the electrical, electrochemical, morphological, and optical properties of free-standing nanocrystalline diamond microsheets (thickness ~ 1 micron) as a function of boron doping. For this purpose, the boron-doped diamond sheets were deposited on a mirror-polished tantalum substrate using the microwave plasma-enhanced chemical vapour deposition technique (MPECVD). Each sample was grown with a different [B]/[C] ratio (up to 20 000 ppm) in the gas phase. As a result of the lattice mismatch between two materials and thermal-induced stress, the diamond sheets delaminate from the tantalum substrate.

The highest doped samples with [B]/[C] = 20 000 ppm in the gas phase exhibits the metallic conductivity, while the lower doped samples show typical p-type semiconductor character. The charge transport at room temperature is dominated by the thermally activated nearest-neighbour hopping between boron acceptors through impurity band conduction, while at low temperatures (< 300 K) a crossover towards variable range hopping is observed. With increasing boron concentration, a shift of the position of the diamond peak towards lower frequencies is noticeable. A decrease in the diamond phase is accompanied by a lowering of the optical band gap. Additionally, the cyclic voltammetry studies revealed the electrochemical activity and current density increase for higher doping levels.

Our research can be a stepping stone in the production of flexible electrochemical devices based on diamond sheets.

Acknowledgements

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Surface analysis of polymer-made implants

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Polyethylene terephthalate (PET) is a polymer which, due to its mechanical and plastic properties, is becoming more and more popular in reconstructive medicine (prostheses, implants) and tissue engineering (artificial organs) [1,2]. However, its surface of inert and hydrophobic nature requires modification to avoid the risk of implant rejection [3]. In order to improve the biocompatibility of the polymer, thin films of biological substances can be deposited on its surface.

The aim of the study was to investigate the physicochemical properties of the PET surface, activated by low temperature air plasma and covered with the phospholipid – 1,2-dioleoyl-*sn*-glycero-3-phosphocholine (DOPC), immunosuppressant – cyclosporine A (CsA), and/or antioxidant – lauryl gallate (LG), by means of the Langmuir-Blodgett method. One component or mixed monolayers of varying LG amounts were employed. Selected techniques were used for the surface examination, i.e. atomic force microscopy (AFM), secondary ion mass spectrometry with a time-of-flight analyser (TOF-SIMS), and wettability measurements. Based on the contact angle values the surface free energy and its components were calculated from Lifshitz-van der Waals-Acid-Base (LWAB) approach.

The AFM imaging provided information on the nanoscale topographical characteristics of the PET supported biological layer, such as the roughness and height profiles. The TOF-SIMS analysis confirmed that monolayers were transferred from the liquid subphase onto the solid substrate quantitatively and helped determine the relative positions of the molecules in the films. The wettability results indicated the increase in surface polarity with increasing the LG molar ratio in the monolayer due to the specific interactions between the particular components (DOPC, CsA, and LG).

Designing surfaces with defined topography and hydrophilic-hydrophobic properties can significantly contribute to the formation of highly biocompatible systems that could be used in medicine as artificial organs or implants.

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Copper-catalyzed tandem halogen exchange/C-P cross-coupling of (cyclo)alkenyl/aryl bromides and secondary phosphine oxides

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We report on a protocol for copper-catalyzed tandem halogen exchange/C-P cross-coupling between cycloalkenyl bromides and secondary phosphine oxides [1]. The method utilizes the catalytic system based on CuI and DMEDA, and NaI additive. The use of the iodide salt reduces the required amount of organic bromides to near-stoichiometric by promoting *in situ* halogen exchange which was shown in a kinetic study to be faster than the cross-coupling.

The method shows good efficacy for diarylphosphine oxides including sterically hindered ones, lower efficacy was observed with the introduction of an alkyl or electron-deficient aryl substituents at phosphorus atom (Figure 1). The procedure can also be used for acyclic alkenyl bromides and aryl bromides albeit with lower generality.

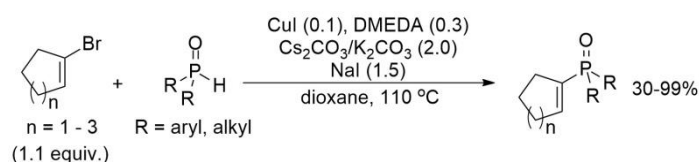


Figure 1. Tandem halogen exchange/C-P cross-coupling of cycloalkenyl bromides and secondary phosphine oxides

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Characterization of photocatalysts based on activated carbons used for photodegradation of pharmaceuticals

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Pharmaceuticals are substances produced by human, they are commonly used for medical purposes as well as people and animal healthcare. Unfortunately, more and more of these kind of compounds are treated as potential bioactive chemicals which may have a negative impact on the natural environment and human health. These compounds may be introduced to the aquatic environment, for instance, through domestic or industrial wastewater. Nowadays, there are many different methods used to remove the contaminants from aqueous solutions, including adsorption processes. However, advanced oxidation processes, e.g. photocatalytic degradation in the presence of visible light, are becoming more and more popular. As effective photocatalysts, one can use, activated carbons doped with nanoparticles characterized by photocatalytic properties.

The main aim of the presented research was to obtain effective activated carbon based photocatalysts doped with bismuth vanadate (BiVO_4), nanoparticles used for photocatalytic degradation of pharmaceuticals in the presence of visible light. Spruce cones were used as a precursor for obtaining activated carbons. The pyrolysis process was carried out in the CO_2 (100 mL/min) or N_2 (150 mL/min) atmosphere. In the heating stage at 800°C the samples were annealed for 2 hours. The obtained activated carbons were used for synthesis of BiVO_4 /activated carbon composites. The photocatalysts were prepared by wet impregnation and hydrothermal method. In both methods activated carbons were doped with 40 wt.% of BiVO_4 nanoparticles. The photocatalytic activity of the obtained samples was tested at the visible light. The sulfamethoxazole ($C_0 = 5 \text{ mg/L}$), a commonly use bacteriostatic antibiotic, was applied as a model pollutant.

On the basis of the research it was found that both wet impregnation as well as the hydrothermal method can be used for the synthesis of photocatalytic materials. All obtained materials were active at the visible light. However, the material obtained by wet impregnation was characterized by the highest photocatalytic activity – about 80 % of the antibiotic was degraded.

POSTER PRESENTATIONS

Metal sorption by exopolysaccharide from green microalgae *Parachlorella kessleri*

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Microalgae are cultured mainly for the wide use of their biomass, whereas the culture medium is very often unexploited, although it can be rich in many valuable metabolites. Exopolysaccharides (EPS), i.e. macromolecules secreted outside cells, are one of the components of the culture medium. One of their functions is to protect cells from unfavourable environmental conditions, including the toxic effects of heavy metals. Due to this property, EPS can be used in the process of removing heavy metals from aqueous solutions [1].

The aim of the study is to determine the sorption capacity of exopolysaccharides derived from unicellular microalgae *Parachlorella kessleri*.

The sorption properties were analyzed in this study according to procedure described by Dobrowolski et al. [2]. EPS samples were dissolved in a salt solution of cadmium and lead at concentrations of 10, 50, 100, and 150 mg L⁻¹. The final EPS concentration in the prepared sample was 100 mg L⁻¹. The solutions were agitated for 30 min, centrifuged, and filtered. The filtrates were used for determination of metal content by ICP-OES. Based on the results obtained, the removal efficiency and sorption capacity were calculated.

The results indicate that lead ions are removed more efficiently than cadmium ions. This was confirmed by sorption calculations. The highest efficiency of lead ion removal was observed in the sample containing 10 mg L⁻¹ Pb(II), then the efficiency of this process decreased with the increasing metal content in the sample. The elemental analysis of EPS showed high contents of Ca, Mg, and S. These elements were present in the highest amounts in the nutrient solution.

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Local and global crystallization observed in Janus particle systems under confinement

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Janus particles are entities that are composed of at least two chemically or physically distinctive surfaces. Therefore, the interactions between Janus particles depend on their spatial separation and orientations. Anisotropies in the molecular properties and/or geometry give rise to a variety of different phase transitions and self-assembled structures. The self-assembly of Janus-like particles can be used to fabricate new materials with unique physical properties. This process is an important topic of research due to promising applications of these materials in nanotechnology, biotechnology, electronics, photonics, drug delivery, and others.

There are plenty of papers devoted to the investigation of Janus-like molecules in bulk, however, it is very little known on how they behave under confinement. Therefore, we wanted to fill this gap and in this work, we have employed Monte Carlo simulations with square-well interparticle potential to investigate the influence of confinement effects in two types of walls, that is, (i) symmetric walls and (ii) anti-symmetric walls. In the former, the walls have attracted and repelled the repulsive and attractive parts of the Janus particle, respectively. In the latter case, one wall was the same as for the symmetric wall and the second one was opposite to that. We have found out that depending on the pore width, on the strength of the interactions between Janus particles with the walls and the nature of the wall we observe the formation of nanoclusters with a local crystalline structure, 2D crystallization, and 3D crystallization. These structures have been characterized by various order parameters such as 2D or 3D bond order parameter. Additionally, we have evaluated the distribution of the clusters and their average size.

Sulfamethoxazole sorption onto modified zeolite material

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Pharmaceuticals are widely used to treat and alleviate the symptoms of infections in humans and animals and as growth promoters. Many of these compounds are only partially metabolized by human and animal organisms. The great majority of drugs are excreted through urine and feces, and consequently enter wastewater. Wastewater treatment plants are only slightly able to treat wastewater from pharmaceuticals, so consequently they enter the environment and can adversely affect humans and animals. In light of these facts, it is necessary to develop effective methods to capture pharmaceuticals from water and wastewater. Numerous methods are known to remove organic pollutants from water and wastewater. Among them, adsorption techniques are the most widely used because of their numerous advantages, which include the multiplicity of available adsorbents, high removal efficiency, relative simplicity of operation and the lack of influence of the potential toxicity of the removed compounds on the removal process. In recent years, sorbents for which waste materials (e.g. fly ash) are used have become very attractive. An example of such a sorbent can be zeolite obtained on the basis of fly ash. In the case of zeolites, there is a need to modify their surface so that they can be used as sorbents of organic compounds (e.g. pharmaceuticals).

The aim of this study was to evaluate the sorption potential of zeolite with NaX structure type obtained from fly ash modified with β -cyclodextrin against sulfamethoxazole (SMX). The zeolite with NaX structure type used in this study before and after the modification process was characterized using X-ray diffraction (XRD) and scanning electron microscopy (SEM). The NaX-CD hybrid material was then used as a sorbent for sulfamethoxazole. The effects of various factors on the sorption process, including the effects of dose, contact time, and initial concentration, were investigated.

The results obtained allowed to determine the optimum dose of NaX-CD hybrid material, the optimum contact time and mechanism of sorption process, and to determine adsorption isotherms. The optimum material dose is 0.5 g/L, and the sorption capacity decreases with increasing material dose. The equilibrium state between sulfamethoxazole solution and NaX-CD material was established after 180 min, and the sorption process follows the pseudo-first order model. The analysis of the equilibrium sorption data allowed to conclude that the Freundlich adsorption isotherm best describes the sorption process.

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Composite hydroxyapatite/iron oxide – significant information

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The composite hydroxyapatite/iron oxide (particularly magnetite or maghemite particles) is a popular topic of research. Combination of hydroxyapatite and iron oxide properties, i.e. large specific area, adsorption properties, reactivity, stability, magnetism and eco-friendliness allows obtaining versatile material, which can be used in many branches. According to Scopus database the trend of composite studies is increasing.

The material can be synthesized by several of methods, e.g. wet (co-precipitation, hydrothermal, sol-gel), dry, high temperature (combustion, pyrolysis), from natural sources and combined methods. Each of these techniques influences the composite characteristics, i.e. surface area, shape of particles. However, the wet methods are commonly used in laboratories and industry due to their simplicity and low cost.

The composite hydroxyapatite/iron oxide adsorption properties were examined. It was proved that the material can remove metal ions, including heavy metals, e.g. cadmium, lead, copper, nickel, uranium, but also anions, dyes and organic substances, i.e. humic acid, parabens, proteins and enzymes. Binding of compounds on the composite surface can occur through various mechanisms, e.g. electrostatic, complexations and ion exchange reactions. Thus, one specific mechanism cannot be identified.

It is worth to notice that the composite exhibits also a catalytic activity. It was proved that it can be used as a catalyst in synthesis processes, activation, transformation, oxidation reactions or in biofuels production. Such a material is an eco-friendly catalyst, which meets green chemistry principles.

Another important area where the composite may find potential use is medicine. Due to its biocompatibility, proper size, durability and magnetic properties the material can be applied as a contrast agent in magnetic resonance imaging method. Similar compound requirements are used in hyperthermia method, which allow destroying cancer cells. Thus, composite hydroxyapatite/iron oxide can be a potential medium in this technique. Moreover, tissue compatibility and adsorption properties provide an opportunity to use it as a drug carrier. Due to hydroxyapatite abilities, the compound can also be applied in orthopaedics, e.g. in bone regenerations processes or implants.

To summarize, hydroxyapatite/iron oxide composite proved to be a multifunctional material. It can be used in adsorption processes including cations and anions, dyes and organic compounds removal, medicine in a wide range (MRI, drug transport, cancer treatment, and orthopaedics) or as a catalyst. However, there is still a lack of knowledge concerning removal of some ions, e.g. barium, iodine, aluminium or cesium and strontium. This area of research is not fully investigated. The results so far are promising. Nevertheless, more thorough studies are needed to confirmed and expand information regarding its properties and potential applications [1].

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Structural, textural, physicochemical, and kinetic release of bioactive substances characteristics of kaolin-carbon-plant materials

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Clay is an abundant raw material with different applications and possibilities depending on the mineral texture, structure, composition, and other factors. The mineral properties result from the presence of non-clay components, organic materials, exchangeable ions, or soluble salts [1]. One of the interesting and intensively researched clays is kaolin. The kaolin is known as porcelain clay or china clay because it is the basic raw material for the fabrication of china or porcelain, however, the mineral is also widely used in obtaining paper, paints, rubbers, or cosmetics. The kaolin name originates from the hill in China (Kao-ling), where this mineral has been mined for centuries. The kaolin consists mainly of kaolinite, but usually also contains quartz and mica. The kaolinite, a main ingredient of kaolin is a layered clay mineral from the group of silicates. The kaolinite is built of a tetrahedral sheet of silica linked by oxygen atoms to the octahedral sheet of alumina. The kaolinite layers stick together because of Van der Waals and hydrogen bonds. The kaolinite is a relatively soft mineral with a Mohs hardness scale value in the range of 2.0-2.5 [2-4].

In this work, multiphase kaolin-carbon-plant materials were obtained by mechanochemical activation using a knife, or planetary-ball milling that ensures a high degree of phase dispersion. The influence of the different compositions of kaolin-based materials on the textural, structural, thermal properties was examined by the usage of X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FT-IR) techniques. Moreover, the kinetic release of bioactive substances (anthocyanins, chlorophylls, or carotenoids) studies was performed.

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Enhanced arsenic(V) removal by commercially available ion exchanger modified with La(III) ions

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Arsenic has long been recognized as a toxin and carcinogen. Chronic exposure to arsenic may occur through natural sources such as weathering reactions, volcanic emissions as well as human activities like mining. Of the various risks, exposure to arsenic through contaminated drinking water is probably the greatest threat to human health. Therefore, it requires to look into the problem of arsenic(V) adsorption more intensely to find out an appropriate adsorbent with affinity to arsenate(V) ions. The commercially available adsorbent containing inbuilt iron nanooxide molecules of the goethite structure, Purolite Arsen X^{np} (X^{np} in short), was chosen to this study. Modification of this sorbent with lanthanum(III) ions lead to obtaining the new material X^{np}-La(III). The modification process itself was tested for optimal pH, kinetics, and equilibrium adsorption isotherm study. The sorbent characteristics were made using, among others, SEM, FTIR, and nitrogen adsorption/desorption isotherms. Then, several tests were conducted to compare the adsorption properties of the modified and unmodified material. It was found that X^{np}-La(III) was able to completely remove arsenate(V) from water with an initial concentration of up to 50 mg/dm³. Without modification, it was not possible to reach the WHO recommended 10 µg/dm³ arsenic limit even at an initial concentration of 25 mg/dm³. Moreover, the maximum sorption capacity increased threefold after modification. Such La(III)-based adsorbent can be successfully applied in wastewater purification and used many times after proper regeneration what leads to cost reduction.

The initial pH value influence on the calcium phosphate ceramics originated from eggshells

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As long as the orthopaedics and dental implants are used for effective treatment, the growing demand for new biocompatible materials is observed. The ideal material for human hard tissue replacement should present a number of properties such as biocompatibility, osteoconductivity, bioavailability and non-toxicity [1]. Owing to numerous advantages calcium phosphates are commonly studied not only for biomedical applications but also as a fertilizing agent, drug delivery system and adsorbent for environmental purposes. Despite the evidence, that calcium phosphates are biocompatible, bioadsorbable and bioavailable, obtaining the material with desired mechanical, antimicrobial and surface properties and reasonable costs of production are still unattainable challenge [2]. Avian eggshells are agricultural wastes which can provide calcium during the calcium phosphate synthesis with double benefit - reducing the waste amount and lowering the production costs. It was proved that the residues composed mainly of calcium carbonate can be an efficient calcium ion donor [3,4].

The purpose of the studies was finding an environmentally friendly synthesis procedure using raw eggshells with elimination of the most energy demanding stages. Using the raw material allowed to avoid the calcination process. The composition and morphology of the obtained product was analysed with respect to the initial pH value of the reacting mixture using the SEM, XRD and FTIR techniques. In the acidic environment the product was composed mostly of the more soluble in the aqueous media CaP forms: DCPD and OCP whereas in alkaline HA and β -TCP the biphasic material was obtained. Moreover, at the pH₀ value equal to 10.6 the most desirable HA/ β -TCP ratio was obtained in terms of biomedical application. Moreover, the calcium ion release profiles were determined in the artificial human saliva (ASH) as well as in the saline solutions and composition changes after soaking were found out.

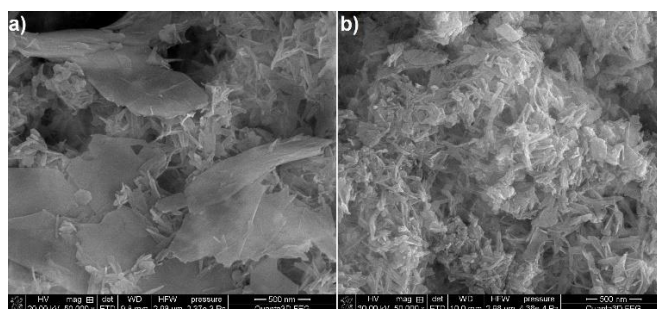


Figure 1. SEM pictures of the product obtained at pH₀=10.6 before (a) and after (b) soaking in AHS solution

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Effect of hydroxybenzoic acids on the antioxidant properties of gluten proteins

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Plant phenolics are an important part of the human diet because they have powerful antioxidant properties as well as other health advantages. According to epidemiological studies, a diet rich in antioxidant fruits and vegetables lowers the risk of numerous oxidative stress-related disorders, such as cancer, diabetes, and cardiovascular disease. The antioxidant capacity of phenolic compounds varies depending on the number and position of hydroxyl groups. Phenolic acids have structural differences due to the number and position of hydroxyl or methyl groups on the aromatic ring. Phenolic acids are aromatic natural compounds containing phenolic ring and carboxylic group. Hydroxybenzoic acids are derived directly from benzoic acid and contain a C6–C1 structure [1].

The aim of the research was to evaluate antioxidant properties of gluten proteins after supplementation with hydroxybenzoic acid derivatives (4-hydroxybenzoic acid, protocatechuic acid, vanillic acid, syringic acid). Model dough samples enriched with phenolic acids at concentrations of 0.05 %, 0.1 %, and 0.2 % were made in a farinograph. The dough gathering time was determined by subtracting four minutes from the average of three DBD times obtained from farinograms. The subtraction of 4 minutes ensures that the collected dough had the proper structure for all repetitions. Because the time necessary for "dough breakdown" varies depending on the type of phenolic acids used, control samples were taken at two distinct times: 22 minutes (CTL22) for PCAT samples, 36 minutes (CTL36) for 4XY, SYR, VAN. All samples were prepared in triplicate. Gluten samples were washed out from model dough and lyophilized.

Phenolic acids present in the gluten network were extracted based on the method described by Sivam et al. (2013) with some modifications. 7.5 mg of gluten samples were extracted for 16 h with 1.5 ml of methanol [2]. In the next step, the extracts were centrifuged ($14,000 \times g$, 3 min.). UV-VIS spectroscopy was used to measure acid concentrations and antioxidant activity in methanolic extracts. ABTS and FRAP assays were used to assess antioxidant properties.

Benzoic acid derivatives are detected in the gluten network after supplementation. According to UV-VIS spectra protocatechuic acid has the lowest degree of extraction, indicating that it is the most strongly attached to gluten proteins. Higher antioxidant properties of supplemented samples were detected in both ABTS and FRAP assays when compared to control gluten samples. According to the results of ABTS and FRAP assays, extract from 4-hydroxybenzoic supplemented gluten had the lowest antioxidant activity. The highest antioxidant activity was found in extracts from vanillic and syringic supplemented gluten. The antioxidant activity appears to be influenced by functional groups on the benzoic ring. According to the data, hydroxybenzoic acid derivatives could be used to produce health-promoting enriched wheat products.

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Physicochemical characteristics of the *Legionella gormanii* lipids

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Bacteria from the family *Legionellaceae* are Gram-negative bacilli associated with water environments: either natural or man-made systems. Inhalation of contaminated aerosol leads to proliferation of *Legionella* within a variety of eukaryotic cells, including human monocytes and alveolar macrophages. The most important of the numerous virulence factors, which enable the bacteria to colonize the host organism are associated with the cell surface. The utilization of exogenous choline by *Legionella* spp. results in changes in the composition of lipids and proteins, which influences the physicochemical properties of the cell surface.

The aim of the study was the characterization of physicochemical properties of the lipids isolated from *L. gormanii* cultured with (PL+choline) and without choline (PL-choline).

Lipids were extracted from *L. gormanii* cells using a modified Bligh and Dyer method [2]. The Langmuir monolayer technique was used to study the physicochemical properties of the lipid membranes at the liquid/air interface. The PL-choline and PL+choline formed stable monolayers at 20 and 37°C. A difference concerned the shape of surface pressure-area (π -A) isotherms, “lift-off” and limiting area as well as the film compressibility and morphology. The π -A isotherm of PL+choline monolayer exhibited a continuous increase in the surface pressure with compression while that of the PL-choline monolayer showed an inflection at the surface pressure of 20 mN/m, followed by a shift towards the lower areas. The compression modulus as a function of surface pressure ($C_s^{-1} = f(\pi)$) determined for the PL-choline monolayers showed the presence of two distinct maxima separated by a minimum which corresponds to a discontinuity on the π -A isotherm. This indicates a change in the organization of the monolayer as an effect of appearance of heterogeneity (more condensed domains and less condensed patches) due to limited miscibility or immiscibility. Such a transition in the PL-choline monolayer morphology was confirmed by means of Brewster angle microscopy. It was not observed in the case of PL+choline monolayers.

The results point out that the choline supplementation in *L. gormanii* induces further alteration in the physicochemical properties of the membrane lipids.

Acknowledgments

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Effect of the carbonyl group and the selected heteroatoms on the frequencies of group vibrations of methyl and methylene groups – a theoretical study

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The presence of certain groups and some heteroatoms in the structure of the compound often has a significant impact on the force field of the molecule, which translates into changes in the frequency of group vibrations, e.g., of the CH₃ and CH₂ groups. Experimental studies often do not contain complete information on this topic. In this case, computational quantum chemistry may prove helpful. Theoretical research related to the analysis of the influence of the carbonyl group and the oxygen and silicon atoms in the immediate vicinity of the CH₃ and CH₂ groups on the frequencies of their stretching (ν) and bending (δ) vibrations (Figure 1) was carried out. There were (often significant) shifts in the frequency ranges relative to the isolated groups, i.e., adjacent only to other CH₃ and CH₂ groups. A training set of molecules was selected to investigate the above mentioned effects. The calculations were carried out using DFT method with the B3LYP exchange-correlation functional and the 6-31G** basis set [1,2]. Only harmonic frequencies were analyzed (see, e.g., [3]).

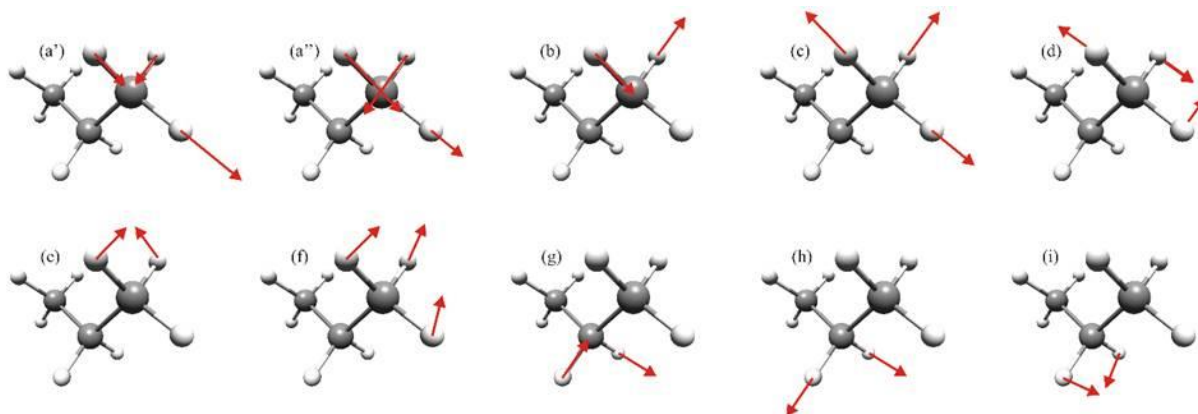


Figure 1. Displacements of atoms of methyl and methylene groups: (a'), (a'') $\nu^{\text{asym},\Lambda}(\text{CH}_3)$, (b) $\nu^{\text{asym},\text{B}}(\text{CH}_3)$, (c) $\nu^{\text{sym}}(\text{CH}_3)$, (d) $\delta^{\text{asym},\Lambda}(\text{CH}_2)$, (e) $\delta^{\text{asym},\text{B}}(\text{CH}_3)$, (f) $\delta^{\text{sym}}(\text{CH}_3)$, (g) $\nu^{\text{asym}}(\text{CH}_2)$, (h) $\nu^{\text{sym}}(\text{CH}_2)$, (i) $\delta^{\text{sym}}(\text{CH}_2)$

The effect of the selected groups or heteroatoms on the frequencies of group vibrations depends on their type and the type of the considered vibrations. The carbonyl group in the vicinity of the CH₃ group significantly differentiates the frequencies of both types of asymmetric stretching vibrations. On the other hand, the frequencies of all bending vibrations of both groups are slightly lower. The presence of the oxygen atom in the vicinity of the CH₃ and CH₂ groups causes a significant widening of the frequency ranges of the stretching vibrations. This effect is much smaller for bending vibrations. The influence of the silicon atom in the vicinity of the CH₃ and CH₂ groups on their stretching vibrations is negligible, while a much greater influence was observed in the case of bending vibrations, especially symmetric one.

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Comparison of lipidomic profiles of unrefined, cold-pressed camelina and hemp seed oils

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The global production of edible oils is increasing annually, and new oils of plant origin are entering the worldwide market. Plant oils contain mainly triacylglycerides and diacylglycerides, free fatty acids, phospholipids, glycolipids, phytosterols and carotenoids, as well as antibacterial and ant-inflammatory ingredients [1]. The content of individual compounds generally depends on the species, growing conditions and the method of oil production. One of the conventional methods of extracting vegetable oils is cold pressing, which is a rapid mechanical process. Cold pressing is a technology that does not involve the use of heat treatment or organic solvent. Moreover, it is a very simple, environmentally friendly technology that does not require large amounts of energy or large outlays investment [2]. Besides the extra virgin olive oil, cold-pressed oils from flax, hemp, camelina seeds and others have been growingly marketed. These oils link good nutritional properties and a pleasant flavour and scent that may fulfil consumer preferences. Camelina (*Camelinasativa L.*) is an annual plant, originating from Eastern Europe and Western Asia, in which the oil content in seed ranges from 30 to 40 % [3]. Due to the good balance of fatty acid profile and other bioactive components camelina seed oil plays an important role in the healthy diet. Hemp (*Cannabis sativa L.*) is one of the most widely cultivated plants mainly for fiber and oil. As a result of high amount of α -linolenic and γ -linolenic acids hemp oil has high nutritional and pharmaceutical values [4].

The aim of the study was to compare the lipidomic profiles of camelina and hemp seed oils. The sample preparation procedure involved liquid-liquid extraction by organic solvents. Analyses were carried out by high-performance liquid chromatography coupled to high-resolution quadrupole time-of-flight mass spectrometry (LC-QTOF 6500 Agilent Technologies). Lipidomic profiling was performed using Mass Profiler Professional (Agilent Technologies) and Simca (Sartorius). The results of the analyses showed differences in the composition of lipidomic features between the samples of camelina and hemp seed oils.

Acknowledgments

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Electrostatic self-assembly of organic crystals from charged macrocycles

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Macrocyclic host molecules are versatile building blocks in the supramolecular chemistry and crystal engineering. Depending on their structure and properties, macrocycles have found numerous applications in the host-guest systems, sensing, catalysis, design of porous materials, *etc.* We report here an aqueous self-assembly driven by complementarity in charge and shape between two families of oligocharged macrocyclic hosts - cationic pillar[*n*]pyridiniums and anionic *p*-sulfonatocalix[4]arene. *P*-Sulfonatocalix[4]arene with electron-rich basket-like cavity is well-known water-soluble supramolecular host, capable of forming various types of assemblies, such as bilayer clay-type structures, capsules, nanometer tubules, spheres or Russian-doll assemblies [1]. Pillar[*n*]pyridiniums are new family of water-soluble permanently charged cationic macrocycles of electron-deficient cavities, now available in two sizes - rigid square-shape tetramer and flexible roughly hexagonal hexamer [2]. These two types of macrocyclic hosts are complementary in terms of charge, shape and symmetry. Their self-assembly is guided mainly by the electrostatic attraction between anionic sulfonate groups of calix[4]arene and positive charge on the pyridinium rings of the cationic macrocycles. The crystallization in gel and liquid-liquid diffusion methods have been used to obtain suitable crystals built from mixed macrocycles for single crystal X-ray diffraction analysis. The structural aspects of the supramolecular architectures and main non-covalent interactions guiding the assembly will be discussed.

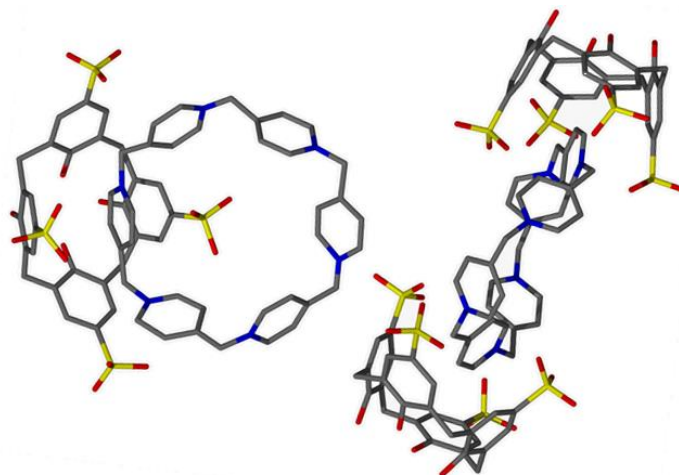


Figure 1. Complexes formed by *p*-sulfonatocalix[4]arene and pillar[6]pyridinium

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Probing E/Z isomerism by pillar[4]pyridinium/gold nanoparticle ensembles and their photoresponsive behaviour

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Geometric isomers are compounds that contain either double bonds or else ring structures that prevent functional groups from freely rotating around a chemical bond. They are important and applied in many fields. Among them, wide employment has butendioic acid, trans form of which (fumaric acid) is used as the intermediate in Krebs cycle while cis isomer (maleic acid) is abiotic. Other important geometrical isomers are azobenzene-4,4'-dicarboxylic acid (ADA) and stilbene-4,4'-dicarboxylic acid (SBDA) which regulate mechanical properties of thin films, macroscale motion of MOFs [1].

Despite the fundamental importance and broad application of these dicarboxylic acids, their recognition remains challenging and greatly unexplored. Although, several reports on detecting butendioic acid, the general strategy for the detection of E/Z dicarboxylic acids has not yet been developed.

Here, we present a general approach for the recognition of E/Z diacids using supramolecular interactions coupled with a plasmonic response. We developed a new supramolecular nanosensor [2,3] consisting of gold nanoparticles/pillar[4]pyridinium ensembles. In the presence of E/Z dicarboxylic acids, the nanoparticles approach one another to the distance of single diacids, resulting in plasmon coupling. The strength of plasmon coupling is proportional to the relative distance between carboxylic groups. The method allows one for the discrimination of both single isomers as well as their interconversion. Such a molecular recognition coupled with responsive nanoscale self-assembly resembles natural mechanisms and may be another brick to building artificial complexity.

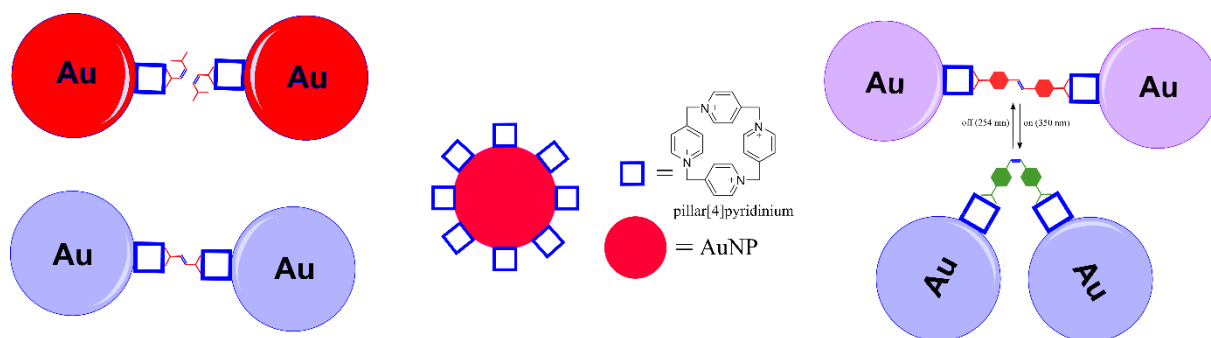


Figure 1. Supramolecular nanosensor in the presence of E/Z diacids

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Study of the influence of flavonoids and their glycosides on the secondary structure of gluten proteins using FT-IR spectroscopy

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The most frequently consumed grain product in the daily diet is bread. In addition to providing energy, depending on the type of flour used for its preparation, it can be an excellent source of fiber and other compounds that have a beneficial effect on the human body. In addition, it is also possible to enrich bread with various types of "health-promoting" substances and thus provide additional health benefits.

Phenolic compounds are secondary plant metabolites, among which two large groups of compounds have been distinguished: phenolic acids and flavonoids. They have a variety of beneficial bioactive properties, including anti-allergic, anti-viral, anti-inflammatory and antimutagenic properties [1]. Therefore, these compounds can be used as supplements enriching wheat bread. In addition to health benefits, supplementation may worsen the qualitative properties of the bread. These properties are closely related to the structure of the gluten network in wheat flour, which consists of gliadins and glutenins. These proteins combine with each other in the presence of water by means of various kinds of interactions [2].

The aim of the research is to determine the effect of selected polyphenols from the group of flavonoids (quercetin, naringenin) and their glycosides (rutin, naringin) on the secondary structure of gluten proteins in the model dough using FTIR spectroscopy [3].

Analysis of the difference spectra in the amide I band showed that both flavonoids and their glycosides induced changes in the secondary structure of gluten proteins. The difference spectra in the amide I band can be divided into two spectral regions. The range from 1570 to 1650 cm⁻¹, contains negative bands, whereas the range from 1650 to 1720 cm⁻¹ contains positive bands. A similar arrangement of the bands in the positive range, related to β -sheets and anti-parallel β -sheets after the addition of flavonoids and their glycosides, indicates that these compounds react with gluten proteins with the OH group present at the B ring. Furthermore, analysis of the difference spectra of the gluten - polyphenols samples in the amide III band revealed a distinct negative band in the region characteristic for β -sheets and positive bands in the spectral regions characteristic for random coils.

Acknowledgments

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The effect of chemical aging on the physicochemical characteristics of sewage sludge-derived biochars

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Biochar (BC) is an eco-friendly material obtained via pyrolysis of biomass. The final parameters of BC depend mainly on the applied pyrolysis temperature and type of feedstock [1,2]. The BC characterization was presented in several scientific papers. The temperature affects the cation exchange capacity, polarity, mass, energy yield, degree of aromaticity, and carbon, oxygen, and hydrogen contents [1,2]. Higher pyrolyzing temperature increases pH [1]. On the other hand, the characteristic of BC is changing under the influence of environmental conditions during the agricultural application of pyrolyzed material (as soil addition).

The study aimed to determine the selected physicochemical parameters of biochars obtained from sewage sludge via pyrolysis at 500°C (BCZ500), 600°C (BCZ600), and 700°C (BCZ700). Subsequently, the biochars were subjected to chemical aging processes (CA) at 60°C (BCZ500-CA60, BCZ600-CA60, and BCZ700-CA60) and 90°C (BCZ500-CA90, BCZ600-CA90, and BCZ700-CA90), and the physicochemical characterization of aged BC were done. Then, the results were compared (Table 1). The chemical aging processes were performed by the exposure of biochar to temperatures mentioned above in airtight stainless steel containers for 6 months. This period was chosen because the most significant changes in BC oxidation, physicochemical characterization, and losses of volatile compounds took place during 6 months [3] (further aging did not lead to major alterations). During all aging experiments, the 40 % WHC (water holding capacity) was maintained.

Table 1. The selected physicochemical parameters of biochar

The selected parameters	Biochars before aging			BC after CA at 60°C			BC after CA at 90°C		
	BCZ500	BCZ600	BCZ700	BCZ500-CA60	BCZ600-CA60	BCZ700-CA60	BCZ500-CA90	BCZ600-CA90	BCZ700-CA90
S _{BET} [m ² /g]	78.04	79.56	94.00	72.81	74.36	85.91	69.95	95.32	116.36
C [%]	24.96	24.45	24.14	23.15	24.06	23.29	22.98	23.25	21.77
H [%]	1.35	0.86	0.76	1.29	0.92	0.80	1.35	1.03	0.67
N [%]	3.38	2.24	1.39	2.79	2.22	1.39	2.85	2.32	1.32
H/C	0.054	0.035	0.031	0.056	0.038	0.033	0.059	0.044	0.031

To characterize biochars before and after chemical aging processes several parameters were set out. For each biochar, the percentage contents of carbon, hydrogen, nitrogen, oxygen, and ash were determined as well as the pH value, specific surface area, and porosity. Moreover, the hydrophobicity, polarity, and aromaticity were specified. The X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) were also applied.

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The effect of water-soluble astaxanthin on the physicochemical, release, and antioxidant properties of polysaccharide/gelatin blend films

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Astaxanthin (ASX) is one of the natural carotenoid present in *Haematococcus pluvialis*, yeast as well as in hydrobiontes, such as crab, shrimp, and salmon. With its unique antioxidant power, superior to vitamin E, β -carotene, and coenzyme Q10, the ASX has attracted great attention in the scientific world. Natural ASX has greater antioxidant capacity than the synthetic ASX. Nevertheless, the latter is more popular on the market as it is about three times cheaper, more stable, oil-free, and water-soluble.

Since food products contain many oxidation-susceptible substances, active packaging materials with incorporated antioxidants arouse great interest. In this study we hypothesized that owing to its natural red colour and capability of scavenging free radicals, ASX is the preferred choice for the active antioxidant packaging development specific applications, e.g. edible coatings for cheese, nuts, red meat, surimi sticks, etc.

The objective of this study was to compare the effects of increasing concentrations (0, 0.25, 0.5, 1 % w/w) of a commercial water-soluble AstaSana astaxanthin (AST) on the physicochemical, release, and antioxidant properties of blend films based on carboxymethyl cellulose (CMC), gum Arabic (GAR), starch modified with octenyl succinic anhydride (OSA), water-soluble soy polysaccharides (WSSP) and gelatin (GEL). The films were obtained from aqueous film-forming solutions (FFSs) containing polysaccharide/GEL blends at the ratio of 75:25 (5 % w/w), glycerol (1 % w/w), and AST.

The AST contributed to slight acidification of the FFSs. Microscopic images showed that the CMC/GEL and OSA/GEL films were phase-separated systems, whereas GAR/GEL and WSSP/GEL films were homogenous. The AST-supplemented films were intensive red and exhibited reduced transparency as a result of their grainy microstructure caused by presence of granular starch (the carrier in the AST formulation). Likely due to the low quantity of AST in the systems, the Fourier-transform infrared spectra of the control (AST-free) and AST-supplemented films were similar. With the exception of OSA/GEL film, the incorporation of AST into films significantly decreased their swelling ability. In turn, apart from the CMC/GEL film, the incorporation of AST significantly decreased the solubility.

Regardless of the AST concentration, CMC yielded films with the best mechanical strength and stiffness. The OSA/GEL films were the most stretchable. AST decreased tensile strength of the CMC/GEL film, but improved the mechanical cohesiveness of the GAR/GEL film.

Depending on the carrier type and AST concentration, ~35–100% of the AST was released from the films during the 4-h dissolution test. Based on the quarter-release times, the WSSP-based film offered the slowest release rate of AST ($t_{25\%} = 31.68\text{-}87.54\text{min}$). The rapid AST diffusion process ('burst effect') was observed for the CMC-containing films ($t_{25\%} = 1.20\text{-}1.74\text{ min}$). In general, the WSSP75/GEL25 film displayed the most linear (the Zero-order similar) release profile. So, this carrier has potential for release of AST at a quasi-constant speed. The gradual increase in the concentration of AST in films resulted in a gradual increase in the antiradical properties in the films

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Synthesis of composites based on acrylate monomers

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In general definition, composites are materials that are formed from at least two phases (components). These phases have different properties. Thus, a composite material takes on properties that are different, and usually better, than components that are used separately or properties that result from adding them together. The components of a composite should be connected at the macroscopic level. At the microscopic level, they form compositions composed of many components, while at the macroscopic level they adopt the behaviour typical of homogeneous materials [1].

The matrix and reinforcement are mentioned as the basic components of composite materials. The matrix is the continuous component of the composite material structure. It is in the matrix that the reinforcement elements are placed. It is a homogeneous material that fills the space and provides a bond for the filler elements. An additional function of the matrix is to protect the filler material from external influences, to give shape to the manufactured composite, and to transfer external stresses to the filler. Typically, the matrix makes up 10 to 80 % of the volume of the entire composite. Reinforcement is also referred to as filler and also as dispersed phase. It is the load-bearing element, which is responsible for shaping the other properties of the composite [2].

Polymer composites are widely used in many fields. In medicine, they are used to produce prostheses, but their big disadvantage is their short service life, which is 7-10 years. They are also used to create vascular implants, vascular prostheses, or organ walls, cartilage, and joints [3]. Structural composites are used to create parts and housings of machines, building elements, car bodies, airplanes, power plants, means of sea transport, or chemical apparatus. They are used to build bridges, canals, tanks, and space equipment [3].

The aim of the work was the polymerization reaction of composites derived of bisphenol A diacrylate (BPA.DA.) and active diluents. The reaction was carried out in the presence of a UV initiator (Irgacure 651, IQ) and filler in the form of benzethonium chloride (BEN). In the first stage, appropriate amounts of bisphenol A diacrylate and one of three used active diluents (2-ethylhexyl acrylate (AEH), butyl acrylate (BA), or methyl methacrylate (MMA)) were measured into a 50 ml beaker in a 7:3 weight ratio. The monomer mixture was placed in a heating chamber to deaerate (65°C). Then, appropriate amounts of filler in the form of BEN (0 %, 1 %, 2 % and 5 %) were added to the mixture. The whole mixture was mixed and UV initiator was added at 1 % by weight, calculated with respect to the amount of monomers. The polymerization mixture was poured into a 12x10x2 mm glass mould which consisted of two non-stick coated glass plates, and a teflon spacer. Then, the moulds were placed in a chamber equipped with 160 W mercury lamps and the samples were exposed to UV light for 30 minutes. In a further step, the composites were transferred to a heating chamber for 4 hours (85°C) for crosslinking. The obtained composites were tested by spectroscopic (ATR/FTIR) and thermal (DSC and TG) analyses.

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Effect directed analysis of biologically active compounds present in *Rhodiola rosea* L. root and rhizome by HPTLC/bioassay/MS

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Rhodiola rosea (*R. rosea*) has been used in Complementary and Alternative Medicine (CAM) for many years. The root and rhizome of *R. rosea* contain adaptogens, which help to increase nonspecific resistance to stress by enhancing our ability to adapt and survive. In the study, fingerprint profiles followed by detection of bioactive compounds through thin-layer chromatography-direct bioautography (TLC-DB) were acquired. The fingerprint can be used as a quality control tool to authentic and compare subtle differences among samples of identical plant resources. TLC-DB is an effective and inexpensive assay for the fast and precise detection of biologically active substances in complex mixtures such as plant extracts. The biological activity of preparations of *R. rosea* root and rhizome were compared. The samples were prepared as 70 % methanol extract. The silica gel 60 F₂₅₄ plates with applied samples were developed with the optimized mobile phase (ethyl acetate: methanol: water – 77:13:10 v/v). Then, fingerprint profiles were obtained by derivatization with general reagent AS for detection of terpenes, Thymol and PABA reagents for detection of sugars, bromocresol green reagent for acids, and NP-PEG reagent for detection of polyphenols. The antioxidant (DPPH reagent), antibacterial (*Bacillus subtilis*), and enzyme inhibition (lipase, tyrosinase, α -glucosidase, and acetylcholinesterase) activities of extracts were tested by TLC-DB. All the tests were done directly on the TLC plate under the same chromatographic conditions. The results show that the investigated samples differed in their chemical composition and biological activities. The *Rhodiola* root and rhizome standard were ampler on active compounds in comparison to supplements. Additionally, all preparations showed antioxidant activity, antibacterial activity against *Bacillus subtilis*, and enzyme inhibition of lipase, tyrosinase, and α -glucosidase. The compounds detected by bioassays directly on the TLC plate were isolated and identified using liquid chromatography-mass spectrometry [1,2].

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Influence of the structure of the nanocomposite used for membrane preparation on the parameters of nitrate selective electrodes

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Nanomaterials have recently become very popular thanks to their unique properties, both physical and chemical, due to their small dimensions. They are used in many fields of science and industry, including energy conversion and energy storage [1]. They are also often used in analytical chemistry for the construction of biosensors [2] and potentiometric sensors [3], and in particular they have the function of solid contact in ion-selective electrodes with solid contact (SC-ISEs). Carbon nanotubes, single-walled (SWCNTs) and multi-walled (MWCNTs) are perfect for this role. However, in order to further improve the analytical parameters of sensors, new materials are sought, which can also be successfully used in the construction of electrodes. For this purpose, scientists synthesize various types of nanocomposites that could combine the advantages of the ingredients from which they were made, and even exhibit much better properties. In the scientific literature, there are many examples of the use of nanocomposites as a solid contact in ion-selective electrodes, including ionic liquid-multiwalled carbon nanotubes nanocomposite in electrodes for the determination of copper ions [4], or multiwalled carbon nanotubes - poly(3-octylthiophene-2,5-diyl) nanocomposite in electrodes for the determination of potassium ions [5].

The work describes extensive research on nitrate all solid state ion-selective electrode based on different types of multiwalled carbon nanotubes-ionic liquid nanocomposite [6]. Potentiometry, electrochemical impedance spectroscopy and chronopotentiometric techniques were used to compare the properties of the produced electrodes. The electrodes were constructed using nanocomposites containing various types of nanotubes that differ in structure (length, diameter, homogeneity). The obtained sensors differed in the slope of the calibration curve and its linearity range. They were resistant to changes in the redox potential of solutions and able to work in a wide pH range. In addition, significant differences depending on the type of carbon nanotubes were obtained in the case of the electrical parameters of the electrodes.

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Usefulness of contact angle measurements for determination of solid surface tension

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Wetting is a very important phenomenon that results from intermolecular interactions between the liquid and the solid body. It is very common in nature and occurs in everyday life, environmental protection, agriculture and plays an important role in, e.g. biomaterials [1], powder production [2], flotation or textile manufacturing [3].

The angle that is measured at the point where liquid-gas interface and solid phase meet each other with plane tangent to the surface of the liquid drop and they are at equilibrium, is called a contact angle. Taking into account Young equation, the contact angle depends on the liquid and solid surface tension as well as solid-liquid interface tension. To solve this equation, adhesion work of the liquid to the solid surface, solid and liquid surface tension as well as surface tension of the solid body should be known. According to van Oss, the solid and liquid surface tension can be represented as Lifshitz-van der Waals and Lewis acid-base components. Moreover, the Lewis component can be shown as a function of geometric mean from electron donor and electron-acceptor parameters. To obtain values of the components and parameters of solid surface tension, there's a need to use three reference liquids from which one is apolar and two are polar [4].

Zisman et al. [5] proposed a parameter known as critical surface tension of solid wetting which equals the surface tension of the liquid that completely wets the solid. In this way, taking into account apolar low energetic solids, critical surface tension can be obtained both basing on the cosine of contact angle and liquid surface tension, and basing on the relationship between adhesion and liquid surface tension.

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Characteristics of multi-component stent coatings

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Cardiovascular diseases are the most common cause of death worldwide. Arterial stenting has emerged as a promising slightly invasive stent-based therapy. The stent biocompatibility determines the immune response of the human body that settles the integration of the foreign body [1]. Since most cardiovascular stents are built of stainless steel and metal alloys, corrosion plays a key role in the results of implantation [2,3]. For diminishing this side effect and enhancing stent biocompatibility with the surrounding living tissue, there can be used various techniques of material surface modification [4,5]. One of them is deposition of an additional protective layer that will screen the stent surface from the attack of environmental factors capable of disturbing the stent integrity and its function. This coating can be gold and/or biological substances.

The purpose of our study was to prepare and characterize the multi-component Langmuir monolayers and Langmuir-Blodgett (LB) films on gold. The compounds, such as: 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), which is a building component of cell membranes, cyclosporine A (CsA) – a strong immunosuppressant widely used in transplantology, and lauryl gallate (LG) – an antioxidant, were employed in the form of monomolecular films to modify properties of the gold substrate. Then, quality of the obtained LB films was analysed using various techniques.

To estimate the mass of deposited films and support coverage the quartz crystal microbalance (QCM) was used. Experimental mass was smaller than calculated (theoretical) one which evidenced that all compounds deposited onto QCM substrate did not form strictly packed LB films and their molecules were inclined. This could be related with some defects in the monolayers. To confirm above observation, cyclic voltammetry (CV) was applied. The CV data showed that the more compact was the monolayer the smaller number of defects was obtained. To study the surface nanostructure atomic force microscopy (AFM) was employed. Furthermore, to examine the hydrophilic-hydrophobic character of modified gold surface the contact angles (CA) of water were measured.

The obtained data showed that all studied monolayers were homogeneous, with molecules inclined in respect to the surface normal. Additionally, ternary DOPC-CsA-LG monolayer at 1:1:2 molar ratio was the most packed film.

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Intramolecular nucleophilic substitution in ω -haloalkylphosphine derivatives

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Complexes of transition metals with organophosphorus compounds are one of the most important catalysts in carbon-carbon and carbon-heteroatom bond formation reactions [1,2]. P-Heterocyclic phosphines and phosphines with cycloalkyl substituents are good σ -donors with moderate steric bulk which makes them suitable ligands for the catalytic transformations of less activated or deactivated substrates [3-5]. We have developed a method of the synthesis of cyclic phosphines through haloalkylation of simple alkyldiaryl- and dialkylarylphosphine derivatives followed by α -metalation which led to intramolecular cyclization through the nucleophilic substitution of halide at the terminal carbon atom. This provides an easy access to a variety of tertiary phosphines containing a cycloalkyl substituent or cyclic phosphine derivatives (Scheme 1).

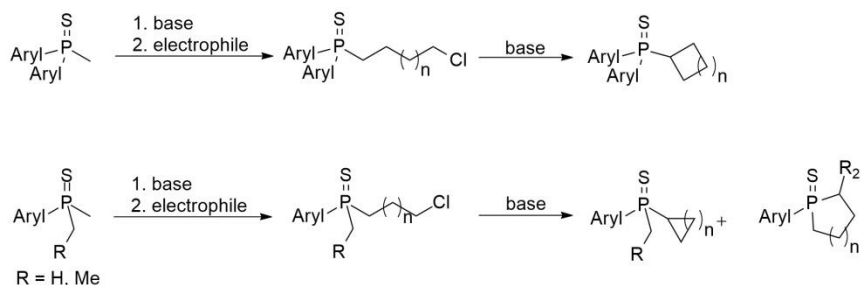


Figure 1. The synthesis of cycloalkylphosphine sulfides via haloalkylation and cyclization

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Synthesis and characterization of novel $\text{CoFe}_2\text{O}_4/\text{TiO}_2/\text{AC}$ nanocomposites used for photocatalytic degradation of organic dyes

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People have been struggling with the problem of water pollution for a long time. Water is the most important compound on the Earth which is necessary for human life. Even trace amounts of water pollution can be dangerous for environment as well as to human and animal health and even life. Due the intensive development of industry and economy dyes constitute a large group of water pollutants. These compounds are often toxic and carcinogenic, moreover are not biodegradable in the environment. The number of methods used to water treatment is numerous. Unfortunately, many of them are not advantageous for the environment in effective time and cost consuming and often result in dangerous and toxic by-products formation. Advanced oxidation processes play an important role in water purification, including photocatalytic degradation of dyes in the presence of visible light, which enables the complete mineralization of organic pollutants to simple inorganic compounds.

One of the method of photocatalysts production which not resulting in by-products is mechanochemical synthesis. The term "mechanochemistry" refers to the chemical and physico-chemical reactions carried out in various types of ball mills. During the collision of the grinding balls, the powder particles are repeatedly crushed, flattened and re-welded. Mechanochemical synthesis does not require the use of solvents, high temperature and pressure. The mechanochemistry reactions enable to preparation of new compounds create novel properties and reduction of particle size.

One of the most commonly used photocatalysts are semiconductors. An example is TiO_2 . This oxide is characterized by a high band gap energy which makes it highly photocatalytic in the presence of UV radiation. The reduction of the band gap energy of the semiconductor by introducing an appropriate dopant can result in the possibility of effective application of titanium (IV) oxide in the presence of visible light (Vis).

The aim of the research was to obtain novel composite capable of photocatalytic organic dyes degradation at the visible light. $\text{CoFe}_2\text{O}_4/\text{TiO}_2/\text{AC}$ nanocomposites were prepared using the high-energy planetary mill Pulverisette 7 Premium Line (Fritsch). To characterize the obtained materials, the low-temperature nitrogen (N_2) adsorption/desorption, X-ray diffraction (XRD) and thermogravimetric (TG, DTG, DTA) methods were used. The photocatalytic activity of the composites was tested regarding to Safranin T.

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