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Book of Abstracts

29th October 2022
University of Belgrade, Faculty of Chemistry

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Contents

Scientific Program

Time	Program
9:00	*Registration of the participants* Mounting posters for the Poster Session 1 (**ODD POSTER NUMBERS**)
10:00	*Conference opening* Serbian Chemical Society – Dušan Sladić Scientific Committee – Vuk Filipović Serbian Young Chemists' Club presentation – Mihajlo Jakanovski
10:15	*Plenary Lecture* (**PP OP 01**) Ilija Cvijetić *University of Belgrade, Faculty of Chemistry*
11:00	*Oral presentations, Session 1*
	Zorica Novaković (**CMN OP 01**) *University of Novi Sad, Faculty of Sciences*
	Marija Kaluđerović (**OC OP 01**) *University of Montenegro, Faculty of Metallurgy and Technology*
	Marija Milošević (**MS OC 01**) *University Of Belgrade, Faculty of Technology and Metallurgy*
11:35	*Coffee break*
11:50	*European Young Chemists' Network (EYCN) ZOOM presentation* Maximillian Menche – Chair of the EYCN "The European Young Chemists' Network and the Power of Networking"
12:05	*Invited Lecture* (**PPP OP 01**) Ivana Kuzminac *University of Novi Sad, Faculty of Sciences*
12:40	*Oral presentations, Session 2*
	Dušica Jovanović (**TC OP 01**) *University of Belgrade, Institute of Nuclear Science Vinča* *University of Niš, Faculty of Science and Mathematics*
	Milica Đukić (**IAC OP 01**) *University Of Belgrade, Faculty of Technology and Metallurgy*
	Jovana Jovanović (**OC OP 02**) *University of Montenegro, Faculty of Medicine*
	Slađana Đorđević (**TC OP 02**) *University of Kragujevac, Faculty of Science*
13:25	***GROUP PHOTO***
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14:15	*Lunch* Removing posters from Poster Session 1 Mounting posters for Poster Session 2 (**EVEN POSTER NUMBERS**)

15:00	*Invited Lecture* (**PPP OP 02**) Branko Kordić *University of Novi Sad, Faculty of Sciences*
15:35	*Oral presentations, Session 3*
	Dušan Ružić (**MC OP 01**) *University of Belgrade, Faculty of Pharmacy*
	Ana-Andrea Holik (**CE OP 01**) *University of Belgrade, Faculty of Chemistry*
	Aleksa Savić (**BB OP 01**) *University of Belgrade, Faculty of Chemistry*
16:10	*Poster session 2* (**EVEN POSTER NUMBERS**)
17:00	*Break*
17:15	*Closing ceremony* • ***Best Oral Presentation Award*** Board: Vuk Filipović, Ivana Kuzminac, Ilija Cvijetić • ***Best Poster Presentation Award*** Board: Jelena Milovanović, Branko Kordić
17:45	*End of the Conference*

POSTER NUMBER is the last part of contribution code, e.g. XY PP **15**.

VENUE:

- Lectures and oral presentations will be taken place at the **large chemistry amphitheater (VHA)** on the ground floor.
- The Poster sessions will take place in the **hallway in front of the library** on the 1st floor.

Plenary Lecture

PP OP 01

Molecular simulations of 1,5-bis(salicylidene) thiocarbohydrazide bound to ATPase domain of human DNA topoisomerase IIα

Ilija N. Cvijetić[1], Barbara Herlah[2], Andrej Perdih[2]
[1] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
[2] *National Institute of Chemistry, Ljubljana, Slovenia*

1,5-Bis(salicylidene)thiocarbohydrazide (**1**) is a potent antiproliferative agent against leukemia (THP-1) and breast cancer cells (MCF-7). It exhibits a polypharmacological profile and interacts with the DNA replication in a ROS-independent manner. Being structurally similar to **TSC24**, a previously reported catalytic inhibitor of the human DNA topoisomerase IIα (topo II) targeting the ATP binding site on its ATPase domain [1], stimulated us to examine if **1** could inhibit the catalytic activity of topo II. The results of performed topo II-mediated decatenation, cleavage, relaxation, and unwinding assays revealed that **1** is a catalytic inhibitor of topo II and does not act as a DNA intercalator, implying the ATP binding site as a viable target. Here, we will show and discuss results of performed molecular dynamics (MD) simulations (1000 ns in total: three replicas for compound **1** and two for **TSC24**, each 200 ns long) coupled with dynamic pharmacophore analysis and MM/GBSA binding free energy (ΔG_{bind}) calculations. This approach enables a comprehensive examination of both geometric and energetic aspects of **1** and **TSC24** binding in the targeted topo II ATP binding site.

Results indicated that compound **1** is more flexible and interacts more strongly with the ATP site of topo II compared to **TSC24** ($\Delta G_{bind} = -41.75 \pm 3.25$ kcal/mol vs. -29.23 ± 2.86 kcal/mol). The main interactions that stabilize the **1**-topo II complex are hydrogen bonds with Asn95 and Asn120 (part of the adenine binding subpocket) and nonpolar interactions with Ile125, Ile141 and Phe142 (part of the hydrophobic subpocket). The results of MD simulations further suggest that rigidifying the structure and exploiting the available interactions with sugar- and phosphate-binding portions of the ATP binding site could yield more potent catalytic topo II inhibitors possessing the thiocarbohydrazide core scaffold.

References

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Acknowledgments

This work is supported by the Ministry of Education, Science and Technological Development of Republic of Serbia (Contract number: 451-03-68/2022-14/200168), and Slovenian Research Agency (Grant P1-0012 (A.P.) and a Young Researcher PhD Grant (B.H).

Invited Lectures

PPP OP 01

Novel 19-oxygenated steroidal derivatives as potent anticancer compounds

Ivana Z. Kuzminac[1], Sofija S. Bekić[1], Dimitar Jakimov[2], Marija N. Sakač[1]
[1] *University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection, Novi Sad, Serbia*
[2] *University of Novi Sad, Faculty of Medicine, Oncology Institute of Vojvodina, Sremska Kamenica, Serbia*

Hormonal therapy is crucial for hormone-dependent cancers, such as estrogen receptor-positive (ER+) breast cancer. Antiestrogens and inhibitors of enzyme aromatase are used as hormonal therapy for this type of breast cancer. Unfortunately, these compounds can also possess hormonal activity and hence induce side effects. This has motivated scientists to continue their work in order to provide better and more selective hormonal drugs for the treatment of ER+ breast cancer. Herein, is reported design, synthesis, *in silico,* and *in vitro* testing of novel 19-oxygenated steroidal D-homo lactones as potential anticancer compounds. These compounds were designed using the structures of previously known inhibitors of aromatase and the structure of the active center of this enzyme. The first part of the synthesis consisted of three steps and was performed in order to modify the D-ring of dehydroepiandrosterone. After the introduction of D-homo moiety, structural modifications in the A and B rings, as well as the C-19 angular methyl group, were performed. During this multi-step synthetic pathway, steroidal 5,6-halohydrines and 6,19-bridged steroids were also obtained [1, 2]. Further, *in silico* ADME properties were determined for all 19-oxygenated compounds as well as some of their interesting precursors. After that, *in vitro* cytotoxicity of the synthesized steroids was tested on six tumors and one normal human cell line. Additionally, the relative binding affinities of all synthesized compounds to the ligand-binding domains of androgen receptor and estrogen receptor α and β isoforms, as well as the binding of one selected steroid derivative for recombinant aromatase were measured.

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2. I. Kuzminac, D. Jakimov, S. Bekić, A. Ćelić, M. Marinović, M. Savić, V. Raičević, V. Kojić, M. Sakač, *Bioorg. Med. Chem.***2021**, 30, 115935.

Acknowledgments

The authors acknowledge financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-9/2021-14/ 200125) and of Provincial Secretariat for Higher Education and Scientific Research of the Autonomous Province of Vojvodina [Project No. 142-451-2667/2021]. We thank prof. dr. Edward T. Petri and prof. dr. Andjelka S. Ćelić for leading the research regarding *in vitro* testing.

PPP OP 02

Influence of the selected amides on the adsorption of nitro derivatives of phenol on activated carbon

Branko B. Kordić
University of Novi Sad, Faculty of Sciences, Department of Chemistry, Biochemistry and Environmental Protection,Novi Sad, Serbia

In this research influence of selected amides, as a model of Algal organic matter, on the adsorption of nitrophenols from water on activated carbon has been investigated. Research is divided into three parts: investigation of the influence of amide molecule characteristics on the adsorption of nitrophenols, investigation of granulation influence on nitrophenol adsorption in the presence of amide and investigation of nitrophenol characteristics that can influence adsorption in the presence of amides. Activated carbons were characterized using FTIR spectroscopy, SEM analysis, internal surface analysis using nitrogen adsorption at low temperature and determination of the point of zero charges. Geometry optimization of nitrophenol and amide molecules has been carried out and different molecular parameters have been calculated. The influence of amides has been investigated by using diffusion and equilibrium models. Biot number has been obtained in order to establish the limiting step in the adsorption process. Adsorption parameters obtained in two-component adsorption systems were compared to parameters obtained for the adsorption of nitrophenols alone.

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Oral presentations

BB OP 01

Optimization of the expression conditions of fluorescently labeled α-synuclein in *Escherichia coli* by response surface methodology and proteolysis by tobacco etch virus protease

Aleksa D. Savić[1], Marija S. Vidović[2], Jelena Z. Radosavljević[1]
[1] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*
[2] *University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, Belgrade, Serbia*

Alpha-synuclein is an intrinsically disordered protein prone to aggregation and it is involved in the formation of brain tissue amyloids in patients with Parkinson's and other neurodegenerative diseases. By fluorescently labeling recombinantly expressed proteins, the processes of expression and purification of the same can be easily visually monitored. In a previous work, we have constructed three plasmids for the expression of α-synuclein fused C-terminally to His-tagged mCerulean3 through a polyasparagine linker and tobacco etch virus (TEV) proteolytic site. Here we have transformed these vectors into *Escherichia coli* BL21(DE3) and BL21(DE3)pLysS and optimized the expression conditions by response surface methodology (temperature, time after induction, concentration of induction reagent) of the chimeric proteins coded by vectors. Expression of the chimeric protein was tested at optimal conditions in different media and terrific broth gave the highest yield. The obtained chimeric protein was purified by immobilized metal-affinity chromatography (IMAC), yielding ~29 mg of chimeric protein per liter of medium and was shown to be successfully proteolyzed by TEV protease, giving a fragment of α-synuclein of expected electrophoretic mobility. After another round of IMAC, the obtained α-synuclein of native sequence was mainly found to be in the flow-through.

Acknowledgments
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CE OP 01

The effects of using online material for learning about protolytic theory in the first grade of grammar school

Ana-Andrea J. Holik[1], Dragica D. Trivić[1]

[1] *University of Belgrade, Faculty of Chemistry, Belgrade, Serbia*

The effectiveness of online instruction in comparison with traditional classroom-based instruction had been the object of various research studies [1]. The aim of this research study was to examine the effects of using online materials for learning about protolytic theory in the first grade of grammar school. The online material on the protolytic theory was designed in order to enable students: (i) to learn new teaching material in smaller segments; (ii) to check their understanding after each segment of the teaching material; (iii) to make progress through the lesson at their own pace; (iv) to watch videos and illustrations with the aim of relating the macroscopic, submicroscopic and symbolic level of the representations of the contents about acids and bases; (v) to reconsider the correctness of the answers provided. The online material was divided into seven pieces of information. Each piece of information was followed by questions which assessed the achievement in learning that part of the instructional unit and the student-content interaction. The students were also expected to say which segment of information helped them formulate the answer to the question. The research study was conducted in an online environment on the sample of 130 students.

From the pre-test, it can be seen that both groups of students have prior knowledge about acids and bases based on the Arrhenius theory of electrolytic dissociation. Based on the results of the post-test, it can be observed that a high percentage of students successfully mastered the new concepts and definitions presented in the online material, which is reflected in the correct application of newly acquired knowledge.

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CMN OP 01

Synthesis and characterization of ZnO nanomaterials with unique morphologies, structural and optical properties

Zorica Novakovic[1], Snežana Papović[1], Marko Radović[2], Branimir Bajac[2]
[1]*University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia*
[2]*University of Novi Sad, BioSense Institute, Novi Sad, Serbia*

The conducted research compares three different chemical routes for the synthesis of ZnO nanoparticles. Simple sol-gel method was used to synthesize fine nanoparticles with a minimum of laboratory requirements. Ionic liquid assisted method was utilized, aiming to study the influence of a specific solvent, the 1-butyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide on the morphology of the synthesized nanomaterial. For comparison, a conventional hydrothermal method was also investigated due to expected unique flower-like morphology. Before calcination, physico-chemical features of the prepared precursors were studied using the thermo gravimetry and differential scanning calorimetry (TG-DSC). The structural properties of the synthesized materials were characterized by X-ray diffraction spectroscopy and scanning electron microscopy (SEM). Measured XRD spectra revealed that all samples have a wurtzite crystal structure and that no other phases or impurities were present. The sample synthesized with the sol-gel method had the most broader diffraction peaks, indicating the lowest particle size, followed by the sample with sol-gel ionic liquid assisted synthesis, and the sample obtained with the hydrothermal method. SEM micrographs of investigated ZnO samples showed interesting variations in nanostructures and material morphologies, ranging from spherical particles with a highly uniform size to the network of uniform and homogenous flower-like structures and self-assembled nanosheets. Analysis of optical absorption revealed that all synthesized samples have dominant absorption peak at about 370 nm, which is the characteristic band gap absorption of ZnO electronic structure. A comparison of the synthesis methods leads to the conclusion that the sol-gel process yielded lower nucleation and crystallization temperatures. The ionic liquid-assisted method provided an interesting pathway toward the synthesis of ZnO nanomaterials with properties suitable for application in optical technologies. The hydrothermal method revealed that synthesized ZnO material has unique flower-like morphology that is desirable for application in technologies where high active surfaces play a crucial role.

Acknowledgments

I would like to thank my mentors Dr. Marko Radović, Dr. Branimir Bajac, and Dr. Snežana Papović for their support and assistance in conducting this research. Also, many thanks to Andreja Nesterović for recording the XRD and the Biosens Institute for providing the facilities for the experimental research.

IAC OP 01

Thermodynamic behaviour of the system of biomass-derived compounds: Eugenol + 4- propylguaiacol

Milica S. Đukić, Gorica R. Ivaniš
University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

The worrying effects of using fossil fuels, as well as their limited reserves on Earth, have focused the attention of researchers on renewable energy sources. Biomass stood out as an excellent widespread substitute for fossil fuels that can be processed into various platform chemicals [1]. Design and modeling of chemical processes require knowledge of the thermodynamic and transport properties of the compounds involved in the process, both for pure compounds and their mixtures.

Eugenol and 4-propylguaiacol are platform chemicals of similar structure that can be produced from biomass [2]. Density (Fig. 1), refractive index, speed of sound, and viscosity of eugenol, 4-propylguaiacol, and their mixtures, were measured at atmospheric pressure and in the temperature range T = (288.15–343.15) K. Obtained experimental results were used to determine excess molar volumes, refractive index deviations, speed of sound deviations, and viscosity deviations. The obtained results are significant for the further research and also for the application of eugenol and 4-propylguaiacol in ecologically acceptable industrial processes.

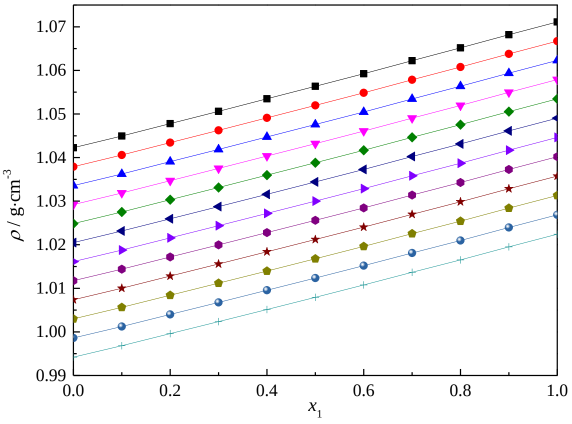

*Figure 1. The density of the mixture of eugenol (1)+ 4-propylguaiacol at atmospheric pressure and in the temperature range T = (**288.15-343.15**) K*

References:

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MS OP 01

Capillarity of plasma treated jute fabrics

Marija Milošević[1], Aleksandra Ivanovska[2], Bratislav Obradović[3], Mirjana Kostić[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia
[2]Innovation Center of the Faculty of Technology and Metallurgy in Belgrade, Serbia
[3]University of Belgrade, Faculty of Physics, Belgrade, Serbia

Jute fibers have a heterogeneous chemical composition that includes cellulose, hemicellulose, lignin, and other minor components. This lignocellulosic fiber is characterized by a complex layered structure with the presence of a hydrophobic surface outer layer consisting of a mixture of waxes and fats. The mentioned hydrophobic surface layer is responsible for fiber's low sorption properties. Therefore, the aim of this study was to enhance the wettability of raw jute fabric by removing the fiber hydrophobic surface layer through a two-step process. The first step includes removing the water-soluble components; raw jute fabric was washed with distilled water at boiling temperature for 30 min and dried at room temperature for 72 h. In the second step, the fabrics were subjected to atmospheric pressure dielectric barrier discharge (DBD) under different conditions (150 Hz and 5.5 kV, *vs*. 300 Hz and 6.0 kV, air as working gas, constant time of 120 s) to remove the hydrophobic layer. Changes in the jute fabrics' surface chemistry were monitored by ATR-FTIR, while the fabric wettability was evaluated by measuring the wetting time and capillarity. The aging effect on the sorption properties of fabrics, in the case of plasma treatment, was investigated up to 28 days following DBD treatment. The obtained results showed that both DBD treatments and aging contributed to the decreased wetting time from 128±8 s for raw jute fabric down to 3.1±0.1 s for a lower frequency DBD treated fabric or even to 1.5±0.1 s after 7 days of aging. Independently on the applied DBD treatment conditions, the jute fabrics' capillarity was significantly improved; *i.e*. their capillary height increased from 87.3 mm for the raw washed jute fabrics up to 138.3 mm and 119.7 mm for a lower and higher frequency DBD treated fabrics, respectively. Although the changes in the fabric surface chemistry were more pronounced for fabric treated with higher frequency DBD, the lower frequency DBD treatment resulted in better sorption poperties. Plasma treated jute fabrics that have improved wettability could be used as geo-prebiotic supports for cyanobacteria growth in a novel solution for damaged land rehabilitation.

Acknowledgments

M.M., A.I., and M.K. would like to acknowledge financial support from the Science Fund of the Republic of Serbia, #7726976, Integrated Strategy for Rehabilitation of Disturbed Land Surfaces and Control of Air Pollution-RECAP.

MC OP 01

Epigenetic drug discovery: fragment-based drug design of novel 1-benzhydryl-piperazine derivatives as selective histone deacetylase 6 inhibitors

Dusan B. Ruzic[1], Nemanja Djokovic[1], Tatjana Srdic-Rajic[2] and Katarina Nikolic[1]
[1] University of Belgrade, Faculty of Pharmacy, Belgrade, Serbia
[2] Institute for Oncology and Radiology of Serbia, Belgrade, Serbia

Selective histone deacetylase 6 (HDAC6) inhibition with small molecules is regarded as a rational strategy to develop safer anti-cancer drugs compared to non-selective HDAC inhibitors[1]. To date, structural motifs that are important for HDAC inhibitory activity and selectivity are defined as: surface recognition group (CAP group), aliphatic or aromatic linker and zinc-binding group (ZBG).

Herein, we describe a comprehensive protocol for the computational fragment search of novel surface-recognition (CAP) groups aimed to design selective Histone Deacetylase 6 (HDAC6) inhibitors (Figure 1)[2]. Identified heterocyclic CAP group, 1-benzhydryl piperazine was employed to synthesize novel HDAC inhibitors with small structural perturbations in the hydrocarbon linker. Enzymatic *in vitro* HDAC screening identified two selective HDAC6 inhibitors (6b, IC_{50} = 186 nM and 9b, IC_{50} = 31 nM), as well as two non-selective nanomolar HDAC inhibitors (7b and 8b). The influence of linker chemistry of synthesized inhibitors on HDAC6 potency was studied using structure-based molecular modelling.

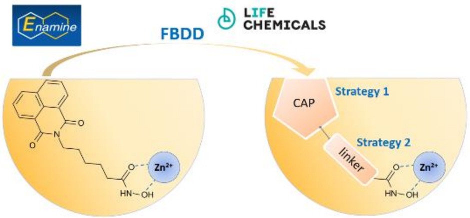

Figure 1. Design of novel selective HDAC6 inhibitors by fragment-based approach

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Acknowledgments

The authors acknowledge a Ministry of Education, Science and Technological Development of the Republic of Serbia Faculty of Pharmacy project (451-03-68/2022-14/200161).

OC OP 01

Synthesis and crystal structure of 1,5-dibenzylidene thiocarbohydrazide

Miljan Bigovic[1], Zeljko Jacimovic[2], Sergiu Shova[3], Marija Kaludjerovic[2]
[1] *University of Montenegro, Faculty of Natural Sciences and Mathematics, Podgorica, Montenegro*
[2] *University of Montenegro, Faculty of Metallurgy and Technology, Podgorica, Montenegro*
[3] *Institute of Macromolecular Chemistry „Petru Poni“, Iaşi, Romania*

Synthesis and synthetic conditions are shown in Figure 1.

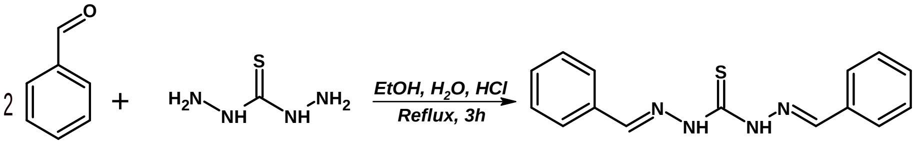
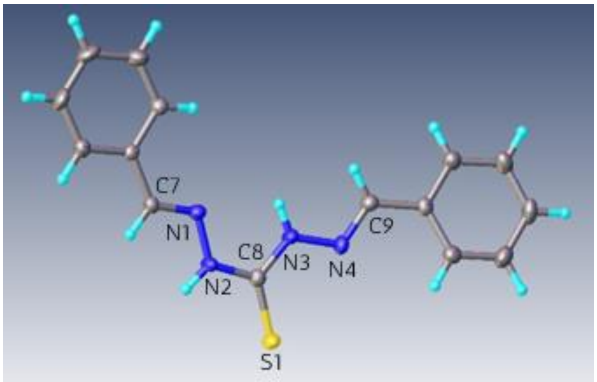


Figure 1. Synthesis of 1,5-dibenzylidene thiocarbohydrazide

IR and NMR spectra were recorded for the obtained product. For a more complete characterization, 1,5-dibenzylidene thiocarbohydrazide, which was obtained in the form of a single crystal by recrystallization from the appropriate solvent, was also successfully examined by X-ray structural analysis. The figure 2. shows its structure. Due to delocalization, the bond lengths C8–N2, C8–N3 have values between the values characteristic of a single bond (1.47 Å) and a double bond (1.29 Å). The situation is similar with the C-S bond, whose length is 1.67 Å [1]. In contrast, the lengths of both the C9–N4 and C7–N1 bonds correspond to a localized double bond.



$C_{15}H_{14}N_4S$,
orthorhombic, Pbca,
a = 8.2436(3) Å,
b = 18.3901(6) Å,
c = 18.6576(7) Å,
V = 2828.49(17) Å^3,
Z = 8,
T = 180 K

Figure 2. X-ray structure of 1,5-Dibenzylidene thiocarbonohydrazide

Reference

1. L. Weiping, *Z. Kristallogr. NCS* **2020**, *235*(1), 99.

OC OP 02

Determination of total organic matter and total organic carbon in Igalo bay peloid

Miljan Bigovic[1], Snežana Pantović[2], Jovanović Jovana[2], Marija Kaludjerović[3]

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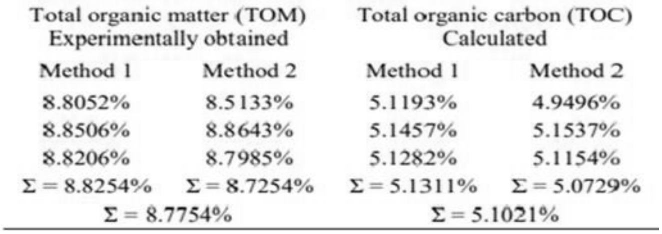
Thermal mud found at coast of Igalo has a long history of therapeutic and cosmetic use. Another property that makes peloid extremly valuable is its closeness to the sea. However, despite its long-term use, the organic composition of peloid, as well as its potential medical properties, have not been examined until recently. In our work, we preformed determination of total organic matter (TOM) and total organic carbon (TOC) in Igalo bay peloid. These two parameters are very significant because their respective quantities can be a precise indicator of the content of organic components in the soil or sediment. Total organic carbon can be measured directly, which is the approach that we have used in our work. Otherwise, it can be determined by the difference of the total carbon content and the inorganic carbon (carbonates, bicarbonates) that is present in the soil. The concentration of total organic matter (TOM) was determined with two different methods. First method is based on combustion of organic and easily volatile materials at high temperatures. After heating, material was cooled in desiccators and the weight change was mesured afterwards. Second method is based on the oxidation of organic matter by hydrogen peroxide with slight heating up. Afterwards, the resulting mixture was placed to solidify the solid phase, the water was separated by decanting, and the solid was transferred to the porcelain cup and evaporated in the dryer to a constant weight. Measurements for both methods were preformed on three samples. The results of the measurements are presented in the table below.



Total organic matter (TOM) Experimentally obtained		Total organic carbon (TOC) Calculated	
Method 1	Method 2	Method 1	Method 2
8.8052%	8.5133%	5.1193%	4.9496%
8.8506%	8.8643%	5.1457%	5.1537%
8.8206%	8.7985%	5.1282%	5.1154%
Σ = 8.8254%	Σ = 8.7254%	Σ = 5.1311%	Σ = 5.0729%
Σ = 8.7754%		Σ = 5.1021%	

Table 1. TOM and TOC in sample of the Igalo peloid

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TC OP 01

Energy landscape of a relaxed amino acid, Glutamine (L), on various undoped and doped TiO_2 surfaces

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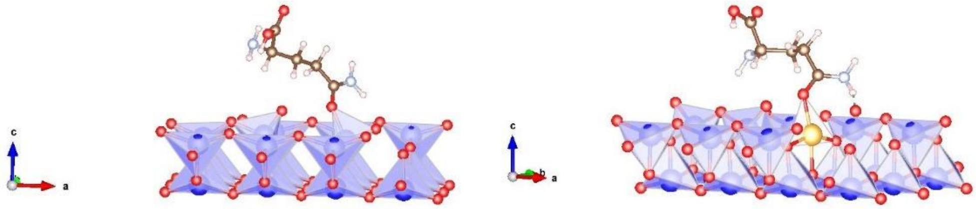
Linking inorganic systems with organic ones is a highly important avenue for finding new drugs and treatment methods. Tumor cells have an increased demand for amino acids due to their rapid proliferation, and several amino acids, such as glutamine (L), have other roles in supporting cancer growth. One of the inorganic materials that can show antitumor properties is titanium dioxide and its crystal modification anatase has shown the highest surface reactivity. In this study we first locally optimized 2D-slab structures of undoped and Au/Ag/Cu doped anatase (001 and 101 surfaces), then similarly optimized a single molecule of glutamine (L) in vacuum. Next, we placed the pre-optimized glutamine molecule in various orientations and on a variety of locations onto the relaxed substrate surfaces, and then performed *ab initio* relaxations of the molecule on the substrate slabs. We employed the DFT method with a GGA-PBE functional, as implemented in the Quantum Espresso code. Comparison of the optimized conformations and electronic structure of the amino acid in vacuum and on the surface, yield useful insights into various biological processes, while several physical interactions between molecule and surface (Figure 1) showed promising applications in biomedicine.



a) b)

Figure 1. Optimized structure of glutamine (L) molecule on: a) undoped anatase slab (001) surface; b) Au doped anatase slab (001) surface, visualized by VESTA program.

Acknowledgments

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TC OP 02

Magnetic properties of *altan*-[n]annulenes

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The altanisation strategy is applied to [n]annulenes to give *altan*-[n]annulenes.[1] In particular, *altan*-[24]annulene and *altan*-[30]annulene were examined in this study. These macrocyclic systems show unique optical, electrochemical, and magnetic properties.[2] The structure of the studied molecules can be rationalized by means of an annulene-within-an-annulene model. The pseudo-π method for current density calculations was performed. In *altan*-[24]annulene, both annulene subunits sustain diatropic (aromatic) character in singlet and triplet states. On the other side, in *altan*-[30]annulene the outer ring sustain paratropic (antiaromatic) currents, but the inner ring sustain diatropic currents in the singlet state, but in the triplet state, both subunits sustain diatropic currents. Calculated *ef* values confirmed more intensive circulations in six-membered rings than in five-membered rings.

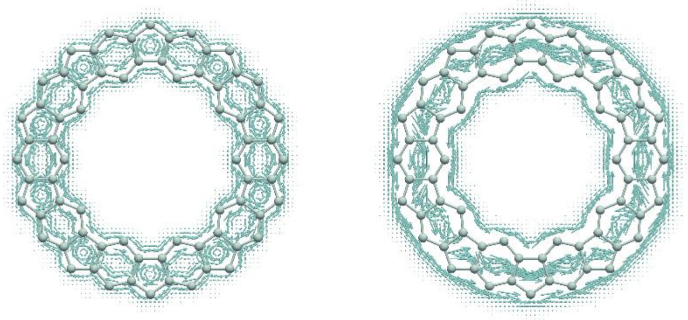

Figure 1. Maps of pseudo-π currents of altan-[30]annulene in singlet (left) and triplet state (right)

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Acknowledgments

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Poster presentations

Analytical chemistry

AC PP 01

Voltammetric detection of chloramphenicol using glassy carbon electrode modified with copper tungstate nanoparticles and molecularly imprinted polypyrrole

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In this study a new voltammetric method for detection of chloramphenicol was developed by modification of glassy carbon electrode with copper tungstate nanoparticles and molecularly imprinted polypyrrole. Four different modified electrodes were constructed using non-imprinted or molecularly imprinted polypyrrole, with or without $CuWO_4$ nanoparticles (GCE|NIP, GCE|$CuWO_4$|NIP, GCE|MIP and GCE|$CuWO_4$|MIP). Copper tungstate nanoparticles used in this research were synthesized by coprecipitation method. The thin layer of polymer on top of the glassy carbon electrode was created by electropolymerization of pyrrole using cyclic voltammetry (CV), in presence of chloramphenicol as template molecule or without it. Determination of chloramphenicol in aqueous solutions was performed by differential pulse voltammetry (DPV) in a three electrode system with a modified electrode as working electrode. It was found that the greatest response to chloramphenicol had GCE|$CuWO_4$|MIP electrode and therefore it was used in further analytical measurements. The linear relationship between current response and concentration of chloramphenicol was estimated in range from 1×10^{-6} M to 5×10^{-5} M with the regression coefficient of 0.995. The detection limit of developed method was 1×10^{-6} M and the sensitivity had value of (255±7) μA/mM. Chloramphenicol eye drops were analysed as real sample and results obtained using DPV were compared to those given by HPLC.

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Acknowledgments

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AC PP 02

The content of selected macro- and microelements in biscuits enriched with beetroot powder

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Fruits and vegetables are important constituents of the diet due to the present high content of nutrients such as vitamins, minerals and fiber. Beetroot (*Beta vulgaris* L.) is an excellent dietary source of essential elements and other bioactive compounds and therefore is one of the agricultural commodities that is very beneficial for human health [1,2]. In this study, biscuits were prepared by substituting spelled flour with beetroot powder at 15%, 20% and 25%, baked at 150 °C, and their mineral composition was evaluated. The selected micro- and macroelements (*Na*, *K*, *Mg*, *Ca*, *P*, *S*, *Fe*, *Zn*, *Se*, *Cu*, *Cd*, *Co*, *As*, *Pb*) were analysed using the optical emission spectrometry with inductively coupled plasma (ICP-OES) technique.

The multi-elemental analysis has shown that the most abundant elements in investigated samples were *P*, *Na*, *S*, *Mg* and *Ca*. In addition, the analysed biscuits also represent a significant source of other biogenic elements such as *Fe*, *Se*, *Zn* and *Cu*. The obtained results indicate that mineral composition depends on the amount of added functional ingredient in biscuits and it increases with an increase in the portion of the beetroot powder. Furthermore, the concentrations of the toxic elements (Pb, As, Cd) were below the method quantification limits in the studied samples. According to obtained results, the analysed biscuits have a high nutritional quality in terms of macro- and microelement content, and beetroot powder has the potential for enrichment of food products.

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AC PP 03

Vitamin *C* content in the sample of black chokeberries (*Aronia melanocarpa* L.)

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Aronia melanocarpa, known as black chokeberry, belongs to the Rosaceae family and has been traditionally used by Potawatomi Native Americans to cure colds [1]. Due to the high content of bioactive compounds such as polyphenols, minerals and vitamins, chokeberry has numerous health-promoting activities, including antioxidative, anticancer, anti-inflammatory and cardioprotective [2]. L-Ascorbic acid is one of the essential vitamins that cannot be synthesized by the human organism. According to data from the US National Institutes of Health, recommended dietary allowance (RDA) of vitamin *C* is 75 mg for adult women and 90 mg for adult men.

In this study, the content of vitamin *C* in aqueous Aronia extract was determined using the high-performance liquid chromatography (HPLC) method. The examined concentration of vitamin C in the analyzed sample was 104,12 mg/100 g of fresh fruit, so it can be considered that Aronia is a rich source of this compound. The obtained result indicates that consuming around 85 g of this fruit could be achieved the daily needs for vitamin *C*. Aronia is usually processed into various products such as juices and jams and it should be noted that the technology of fruit treatments plays an important role in the content of vitamin *C* in of its products.

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AC PP 04

The influence of competing counterions on the solubility of imipramine

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Experimental studies of solubility are important in all phases of drug design and development. Solubility data are used to screen out drug-like candidates, biopharmaceutical classification and formulation optimization. The development of oral and parenteral dosage forms can be challenging, especially when drugs are poorly soluble, ionizable, exhibiting pH-dependent solubility and when multiple counterions are present in drug suspension. The influence of different counterions on the existing equilibria and on pH-dependent drug solubility must be defined in such systems. To investigate the effect of multiple ions on the solubility of a model basic drug – tricyclic antidepressant imipramine (Im), we conducted a systematic study of the Im solubility as a function of pH in the presence of both chloride and phosphate ions as well as in chloride-free and phosphate-free suspensions. The pH–Ramp *shake–flask* method[1,2] was used for solubility determination. The computer program *p*DISOL–X was used for data analysis. It is shown that distinct pH-dependent solubility profiles were obtained in studied systems. Depending on the pH and the total concentration of chloride and/or phosphate ions, Im can precipitate as chloride and phosphate salt or free base. Furthermore, pH values of solid phase transitions (pH_{max}) varied as well. For instance, pH_{max} of solid phase transition of $(ImH)H_2PO_{4(s)}$ to $(ImH)_2HPO_{4(s)}$ change from 5.15 (chloride and phosphate-containing suspensions) to 5.73 (chloride-free suspensions). The intensive self-aggregation of Im in acidic region was suppressed by raising chloride or phosphate ions concentration (I_{avg} 1.42–1.64 M). In that way, solubility of Im was decreased due to the common-ion effect. This study illustrates the influence of competing counterions on Im solubility and on interconversions in solid phase. Hence, such factors must be taken into account during formulation optimization in drug research.

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AC PP 05

Electrochemical determination of mesotrione in river water samples by using boron doped diamond electrode

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Mesotrione is a systemic pre- and post-emergence herbicide for the selective contact and residual control of broadleaf weeds in field corn, seed corn, yellow popcorn and sweet corn. Due to possible contamination of soil and water it is considered to have toxicity potential for human beings [1]. This work presents a simple, rapid, sensitive and accurate determination of mesotrione at unmodified boron-doped diamond electrode, using differential pulse voltammetry in Britton-Robinson buffer (pH 6, oxidation peak at 1.40 V). Under optimized DPV conditions linear calibration curve was obtained for a range of 0.5 to 100 μM. The effect of possible interfering agents is negligible, confirming good selectivity of the method. The method was successfully applied to determination of mesotrione in spiked river water samples. This electrochemical determination of mesotrione represents a favorable alternative to other time-consuming and expensive analytical techniques and procedures.

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Acknowledgments

Ministry of Education, Science and Technological Development of Republic of Serbia Contract number: 451-03-68/2022-14/200168

AC PP 06

Toxicity assessment of nadolol and its photodegradation mixtures using mammalian cell lines

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It is well known that pharmaceuticals may be found in wastewater and ambient surface waters at ng/dm^3 and mg/dm^3 concentrations (Vieno et al., 2007). Indirect photolysis is proven to be one of the efficient methods for their removal from water. The additive, synergistic, or antagonistic effects of compounds or mixtures found in environmental samples can be assessed using bioassays in mammalian cell lines. Bioassays in human colon adenocarcinoma (HT-29) and human fetal lung (MRC-5) cell lines were used as a reliable method for the prediction of single compound or mixtures toxicity towards higher trophic levels organisms and assessment of organ-specific effects (Četojević-Simin et al., 2013). The obtained results were the consequence of the different degradation mechanisms that occurred under different radiation source treatments. Results of the tested samples were depended on the applied radiation source and the type of cell line (Figure 1). The HT-29 cell line was more sensitive towards examined mixtures. Proliferative effects were obtained for the water solution of nadolol (NAD/ultrapure water) and the mixture of NAD and its UV/H_2O_2 photodegradation intermediates.

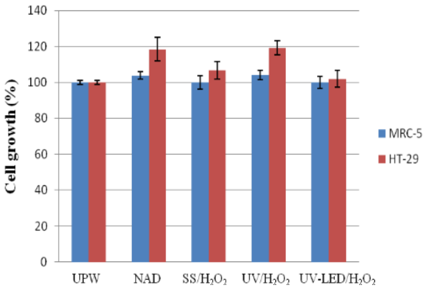

Figure 1. Influence of NAD water solution (0.05 mmol/dm^3) and its degradation mixtures on the selected mammalian cell lines.

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AC PP 07

Determination of heavy metal content in leaves of *Rumex patentia L.* and soil from the industrial area of Pančevo

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With industrial development, heavy metal pollution grows as well. Heavy metals get released in nature from industrial sources and enter ecosystems, where they cause harm to many organisms. The aim of this research was to determine the content of heavy metals in fresh leaves of Rumex patentia and soil from the industrial area of Pančevo. The samples were collected in 8 locations and the content of Al, As, Cd, Co, Cr, Cu, Fe, Hg, Mn, Mo, Ni, Pb and Zn was determined by ICP – OES analysis. The highest observed content was the content of Fe (323.8053 mg/kg in leaves and 6394.9077 mg/kg in soil), Al (176.2411 mg/kg in leaves and 655.6078 mg/kg in soil) and Mn (384.4533 mg/kg in soil). The content of Pb in leaves exceeds the maximum allowed quantity in 2 locations, and the content of Cd in 2 locations as well.

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AC PP 08

Monitoring the status of nitrites in smoked bacon and smoked pork roast

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Nitrites as additives prevent the rancidity of triacylglycerol in meat, prevent the growth of microorganisms and contribute to the taste of smoked meat products. They are registered as official preservatives and additives. The potential dangerous effect on the health of nitrites was discovered in the 1960s and a debate on the safety of cured meat products was initiated, since nitrites are the common additives used in cured meat products. This debate was largely focused on cured meat products, although potable water and vegetables are also considered as substantial sources of nitrites intake. The major concern of nitrites in food is related to the potential ability of nitrites to form carcinogenic N-nitroso compounds. The first half of the 20th century brought a gradual shift to nitrites addition in cured meat products, due to a faster curing time, an increased production capacity and a better knowledge of nitrite chemistry. As nitrite reacts with protein to form carcinogenic compound nitrosamine, which increases the risk of cancer for people who like meat food, so the amount of nitrite added in food has attracted great attention of researchers. This research was conducted in order to monitor the status of nitrites in smoked bacon and smoked pork roast in the period from 2020 to 2022 in Serbia. There are many methods for determining nitrite in food, which can be divided into two categories: spectroscopic methods and chromatographic methods. The spectroscopic method at a wavelength of 538 nm was used for this research. 74 samples of smoked meat were analyzed, of which 33 samples of smoked bacon and 41 samples of smoked pork roast. The test results gave an average level of nitrite content expressed as sodium nitrite ($NaNO_2$) for smoked pork bacon of 32.04 mg/kg, while for smoked pork roast the value was 24.26 mg/kg (maximum concentration 150 mg/kg). Based on this research, it can be concluded that the concentration of nitrites in the tested smoked bacon and smoked pork roast, expressed as $NaNO_2$, was below the established maximum permissible values according to national and European regulations.

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AC PP 09

Total phenolic content and antioxidant capacity of Norwegian plums

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European plum (*Prunus domestica* L.) is a very adaptable fruit species with a large spreading area, but it is mostly grown under the temperate climatic conditions. Plum production has a very long tradition in Norway, which dates back from the Middle Ages. In addition, plum is the second most produced fruit in Norway.[1]

European plum fruits are a healthy food rich in nutrients and phenolics. They are a good source of flavonoids and phenolic acids, as well as vitamins and carotenoids.[2]

Six plum cultivars (Opal, Mallard, Reeves, Jubileum, Avalon and Valon) grown in Norway were used in this study. In total, 56 samples of plum fruits were gathered from two locations and dried after harvest. The total phenolic content and antioxidant capacity were investigated by spectrophotometric tests (*Folin-Ciocalteau* test and $DPPH^{\cdot}$ test, respectively). The content of individual phenolic compounds was analyzed by HPLC. The total phenolic content was in the range 4,43–30,75 g GAE (gallic acid equivalents) per kilogram, while antioxidant capacity was in the range 35,42–262,91 mmol TE (Trolox equivalents) per kilogram dry weight. The results show that all the samples were rich in phenolic compounds and showed high antioxidant capacity.

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Acknowledgments

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AC PP 10

Improving the thermal and electrochemical stability of lithium-ion battery electrolytes safety

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Lithium-ion batteries (LIBs) are becoming increasingly important for electrifying the modern transportation system and, thus, hold the promise to enable sustainable mobility in the future. However, their large-scale application is hindered by safety concerns when the LIBs are exposed to mechanical or thermal abuse conditions. These safety issues are intrinsically related to utilization of highly volatile and flammable organic-solvent-based electrolytes. Improving the thermal stability of electrolytes and the safety of LIBs is one of the imperatives of our investigations. Starting from rather "facile" electrolyte modifications by replacing the organic and/or the addition of functional electrolyte additives, including ionic liquids (ILs) are considered. IL/organic solvent mixtures are investigated as potential optimal electrolytes for LIBs that can combine low flammability, good thermal stability and high electrical conductivity.

In this work, the 1M solution of LiTFSI salt in the mixture containing γ-butyrolacton (GBL) and 1-ethyl-3-methylimidazolium *bis*(trifluoromethylsulfonyl)imide ([C_2C_1im][TFSI])+GBL are investigated, which has shown the most optimal properties. Electrolyte LiTFSI/C_2C_1imTFSI/GBL was used for cycling TiO_2 nanotube arrays electrode as Li-ion anode material. In an attempt to realize LIBs with enhanced safety, herein are investigated electrochemical properties of the LiTFSI/C_2C_1imTFSI/GBL and compared with LiTFSI/$C_2C_1C_1$imTFSI/GBL. It is shown that LiTFSI/C_2C_1imTFSI/GBL electrolyte displayed higher current efficiencies after 350 full (dis-)charge cycles. This is due to hydrogen bond stabilization between the carbonyl oxygen from GBL and H-atom from the C2-position at imidazolium cation of ionic liquid.

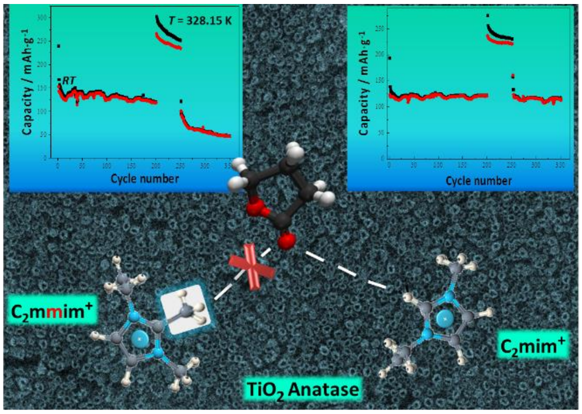

Figure 1. Charge/discharge performance of TiO_2 NTAs in LiTFSI/$C_2C_1C_1$imTFSI/GBL and LiTFSI/C_2C_2imTFSI/GBL electrolyte at different temperatures at a current rate of 3 C

AC PP 11

Iodine number analysis of traditional wood charcoal

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The charcoals analyzed in this research were produced from raw wood, from European Beech (*Fagus sylvatica*, EBC), Oak (*Quercus cerris*, OC), Ash tree (*Fraxinus*, AC), Linden (*Tilia L.*, LC), walnut (*Juglandaceae*, WNC) and cherry (*Prunus avium*, CC) under anaerobic conditions at temperature of 400–500°C by the traditional way, in the brick furnace. The charcoals were additionally dried at 105±5°C for 48 hours, ground and sieved through an ISO sieve with a diameter of 100 µm. The iodine number was determined according to ASTM D4607-94 Standard Test Method for Determination of Iodine Number of Activated Carbon [1]. Iodine number was used to determine the adsorption capacity of activated carbon on the surface of different types of charcoal. The obtained results show that the iodine number is in the following order AC > CC > EBC > WNC > OC > LC which means 214.7 > 256.6 > 577.7 > 868.0 > 954.6 > 1041.1 mg/g, respectively. The iodine number of OC is similar to Saka's results [2].

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AC PP 12

Total phenolic, flavonoid contents and radical scavenging activities of NADES- based propolis extracts

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Propolis is a resinous substance collected by honeybees (*Apis mellifera* L.) from different plant parts such as branches, plant buds, leaves, and exudates partially digested by β-glycosidase from bees' saliva, and after that mixed with beeswax. It is commonly used in folk medicine to prevent and treat colds, ulcers, rheumatism, diabetes, and dental caries. Commercially available products most often comprise ethanolic extracts of propolis. However, high alcohol content and strong residual flavour make such products unsuitable for patients intolerant to alcohol, especially children. Due to mentioned drawbacks, propylene glycolic, aqueous, fructose, or olive oil propolis extracts are commonly found on the market as safer alternatives. These solvents are more appealing options but the extraction efficiency is up to 10 times lower compared to ethanol. Thus, there are high demands for the development of effective and ethanol-free extractions[1,2].

The overall aim of the study is to determine total phenolic, flavonoid content and radical scavenging activity of high-quality and natural-based propolis extract enriched with bioactives using new generation of solvents as Natural Deep Eutectic Solvents (NADES)[1]. Thirty-eight different green NADES have been used for the extraction of phenols from poplar types of propolis. The NADES were prepared by mixing different molar ratios of polycarboxylic acids, amino acids, glycerol, urea, potassium acetate, choline chloride and ethylene glycol. The highest values of TPC, TFC, and DPPH were obtained using following NADES systems: lactic acid/glycerol=1/1; lactic acid/glycine=3/1; glycerol/proline=1/1; choline chloride/succinic acid=2/1 and choline chloride/ethylene glycol=1/4.

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AC PP 13

Determining the adulteration of paprika powders with Sudan I dye by IR and multivariate classification techniques

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Sweet powder paprika is globally used as a spice for giving taste and colour to meals and it is also very common spice in Serbian cuisine. It is among spices which are often subjected to adulteration mainly using Sudan dyes which are considered suitable for that purpose due to their low-cost and wide availability. Additionally, they are stable compounds which make the appearance of paprika better for longer times since one of the problems of paprika is the degradation of its colour over time [1]. In this study twelve different branded paprika powders were collected from the local market in Serbia. Samples were prepared for analysis using IR spectroscopy with the aim to analyse adultertaion of this spice with Sudan I dye. According to obtanied IR data neither of analysed samples were adulterated with Sudan I dye so for further analysis mixtures of this samples with Sudan I dye were prepared and subjected to multivariate analysis. Differente multivariate classifications models were created for discrimination based on adulterant and powder paprika content in sample mixtures. Principal component analysis (PCA), partial least-squares-discriminant analysis (PLS-DA) and PCA-linear discriminant analysis (LDA) were used in the different spectral ranges. All methods were able to differentiate adulterated from non-adulterated samples with models obtained with PLS-DA being the best.

IR spectroscopy results in combination with multivariate analysis have showed that it is possible to discriminate pure paprika powder samples from paprika powder samples adulterated with Sudan I dye.

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AC PP 14

Investigation of clofazimine acid-base supersolubilization using various weak organic acids

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Nowadays, more than two-thirds of potential drugs currently being discovered are practically insoluble in water with solubility <100 µg/mL. Despite that, compounds with even lower solubility (<0.1 µg/mL) are commonly selected for further development which is very challenging, especially in the pharmaceutical formulation process[1]. Clofazimine (CFZ), an anti-leprosy drug with inhibitory activity against several coronaviruses, has a favourable safety profile[2], but it is poorly soluble in aqueous media. Hence, it is important to develop a method for increasing its solubility. In this work, a relatively novel approach of enhancing solubility of weakly basic drugs by using weak acids that would not form salts with the drug (acid-base supersolubilization (ABS)) has been applied. CFZ aqueous solubility was determined in solutions of tartaric, citric, malic, malonic or maleic acid: in set I acid solutions had the same concentration (2.5 mol/L), and in the set II they were scaled to the same pH (1.0). The drug was added in stirred acid solution until a precipitate was noticed and, after filtration, CFZ concentration in samples was determined by HPLC. Based on set I, it was found that the solubility of CFZ had the highest value in the case of tartaric acid (0.46 mg/mL) compared to other acid solutions of the same concentration. In set II the highest CFZ concentration was determined in the malic acid solution which had the highest concentration (2.8 mol/L) among other acids. On contrary, maleic acid solution at pH=1.0 had the lowest molar concentration (0.5 mol/L) and therefore CFZ was minimally dissolved. Further research will be directed toward the examination of acid structure effect on CFZ solubility.

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AC PP 15

Four radical scavenging activity-HPTLC assays in combination with chemometrics for the assessment of antioxidant activity of *Sempervivum tectorum* L. leaf extracts

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The houseleek (*Sempervivum tectorum* L.) has a wide application in traditional medicine for skin changes treatment, ear, throat and bladder infections, stomach ulcers. Recently, several studies confirmed antioxidative, antimicrobial and anti-inflammatory effects of houseleek [1,2]. Several spectroscopic techniques have been proposed to measure the free radical scavenging capacity (RSC), regardless of the individual compounds which contribute to the total free RSC. On the other hand, high-performance thin-layer chromatography (HPTLC) hyphenated with biochemical detection allows identification of single compounds responsible for radical scavenging activity (RSA). The main aim of current study is to identify single radical scavengers using four HPTLC-based assays such as 2,2-Diphenyl-1-picrylhydrazyl assay (DPPH), 2,2'-Azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) assay (ABTS), potassium hexacyanoferrate(III) total reducing power assay (TRP) and total antioxidant capacity by phosphomolybdenum assay (TAC) in combination with principal component analysis (PCA). The best of our knowledge, HPTLC-TRP and HPTLC-TAC were developed for the first time. PCA was used for the classification of samples with similar RSA and the identification of radical scavengers responsible for classification. HPTLC-DPPH, HPTLC-ABTS and HPTLC-TRP chromatograms showed similar bioactive profiles. Further, HPTLC-TAC fingerprint differs from the others with observed numerous new zones with hR_F at 73, 83, 89, and 98 values. Based on PCA, HPTLC-ABTS and HPTLC-TRP assays showed similar grouping of samples. Phenolic compounds such as gallic acid (hR_F = 48), kaempferol (hR_F = 69) and unknown compound at hR_F = 18 are recognized as markers responsible for the separation between samples.

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AC PP 16

Green extraction of bioactive compounds from chokeberry: screening of Natural Deep Eutectic Solvents and chemical profiling

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Natural Deep Eutectic Solvents (NADES) are new generation of ionic liquids and promising solvents in green extraction. NADES are made by mixing two or more compounds, hydrogen bond acceptor (HBA) and hydrogen bond donor (HBD), at various molar ratios.[1,2] In this paper 28 different NADES are used as eco-friendly alternatives for the extraction of phenolic acids, flavonoids and anthocyanins from chokeberry with the aim of extraction efficiency screening. Twelve different compounds were used for preparation of NADES, among them choline-chloride, proline, urea, glycerol, malic acid, tartaric acid, glucose, fructose, etc. Ultrasound extraction was applied as an eco-friendly and highly-efficient technique for the isolation of phenolics and solid phase extraction (SPE) was used for purification of extracts and removal of NADES compounds. Different extraction parameters were optimized: solid/ liquid ratio, volume of added water and loading volume of extracts on SPE. Repeatability of extraction procedure was assessed. Chemical profiles of the extracts were obtained by applying high-performance thin-layer chromatography (HPTLC) and mobile phase was optimized for simultaneous separation of anthocyanins and other phenolic compounds. Extraction efficiency of NADES was compared to acidified methanol as conventional solvents and 1% citric acid in water (*w/v*) which is a generally recognized as safe (GRAS) solvent. Principal component analysis (PCA) was performed to determine the similarity/dissimilarity between studied NADES and identify the most important compounds (bands) for separation between them. PCA illustrate that extraction greatly depends on the compositions of eutectic mixture and shows that NADES can be “designer solvents”.

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AC PP 17

The effect of methanesulfonic and glutaric acids on the solubility of clofazimine

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In the modern drug research the number of practically insoluble potential drugs is increasing. Poor aqueous solubility can cause poor oral absorption and low bioavailability of drugs. Hence, solubility enhancement is considered as one of the most important challenges in the formulation and development of the dosage forms of drugs. Clofazimine (CFZ) is an antibiotic drug which is used in the treatment of tuberculosis and leprosy. It is recently shown that CFZ has inhibitory activity against certain coronaviruses and can antagonize the replication of SARS-CoV-2.[1] Since CFZ is highly lipophilic molecule with extremely low solubility, it is quite a challenge to find appropriate method for CFZ solubilization. The aim of this work was to investigate the effect of methanesulfonic (MSA) and glutaric (GA) acids on the solubility of CFZ. The effect of MSA on the solubility of CFZ was studied by the pH-Ramp *shake-flask* method (pH-RSF).[2] The solubility of CFZ was determined in the presence of GA in two ways: 1) by melting a mixture of CFZ and GA in different molar ratios, and then dissolving in water; 2) using the pH-RSF method. Interactions between CZ and GA were investigated by IR spectroscopy. It is shown that both MSA and GA increase the solubility of CFZ in acidic suspensions prepared by pH-RSF method. Also, solubility enhancement was observed in the molten CFZ-GA mixtures (molar ratio 1:1 and 1:4) compared to mixtures prepared without melting. Besides that, the IR spectra of these mixtures revealed that characteristic CFZ band was shifted in molted CFZ-GA mixture (molar ratio 1:1) probably due to CFZ-GA interactions. Preliminary results presented in this study illustrate that MSA and GA can be used for solubility improvement of CFZ.

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AC PP 18

Evaluation of antifungal activity of *Origanum vulgare* L. extracts against *Candida albicans* using HPTLC-direct bioautography

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Fungal infections produced by *Candida spp.* include superficial infections of the skin, respiratory system infections, vulvovaginal candidiasis and systemic infections. Treatment of candidiasis is becoming more challenging due to the increasing resistance of *Candida* strains to existing antifungal therapy. Therefore, there is a need to develop fast, simple and effective methods for the detection of antifungal compounds.[1] In this study, the high performance thin-layer chromatography (HPTLC)/bioautography test against *Candida albicans*, as one of the most common causatives of opportunistic infections, was optimized. Ethanol, ethyl acetate and acetone extracts of three samples of *Origanum vulgare* obtained by ultrasound-assisted technique were analyzed. A suspension of *C. albicans* (OD ~ 8.0 McF, in Sabouraud maltose broth with the addition of solid agar at a concentration of 1 mg/mL) in the log phase of growth is used for dipping of HPTLC plates. After incubation with 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) solution, the bioautogram shows two types of active compounds - those that inhibit cell growth as white zones against a purple background, and those that induce growth as intense purple zones. The synergistic effects of the extracts were determined by antibiogram and dot-blot test on HPTLC plate, where the extracts of sample A proved to be the most active against *C. albicans*, while the extracts of sample B have the least activity in terms of growth inhibition. By visual examination of the bioautogram, no significant difference can be observed between samples depending on the applied extraction agent. In addition to other conventional *in vitro* methods, this technique offers the possibility of fast screening of medicinal plants as one of the initial steps in the development of new candidiasis therapy.

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AC PP 19

Comparative analysis of ionization constants determination using spectrophotometry and potentiometry: 3-aminobenzoic acid, 1,3,5-benzenetricarboxylic acid and tyrosine

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The ionization constant (usually expressed in logarithmic form, pK_a) is important physicochemical parameter which is used to characterize the acid-base chemistry of a compound. Since most drugs contain one or more ionizable functional groups, knowledge of pK_a values is necessary in drug research. The most common techniques used for pK_a determination are potentiometry and spectrophotometry. Potentiometry is a method of choice when ionization processes are overlapping, as in such case it is not possible to obtain the absorption spectrum of each species present in solution. The aim of this work was the comparative analysis of pK_a determination using potentiometry and spectrophotometry for model compounds with overlapping ionization processes: 3-aminobenzoic acid, 1,3,5-benzenetricarboxylic acid and tyrosine. The potentiometric titrations were performed with *p*SOL Model 3 instrument (*p*ION) equipped with *p*S software package for titration data analysis.[1] Avdeef–Bucher four–parameter equation was used for electrode standardization.[2] To overcome the above-mentioned limitation of spectrophotometry, the alternative approach was applied in this study. The new aminocaproate phosphate buffer (containing phosphoric and ε-aminocaproic acids) was used for the solutions preparation of the model compounds in pH range 1 – 12. This buffer has numerous advantages like UV-transparency, resistance to pH changes upon standing for several days, useful buffer capacity and constant ionic strength in the wide range of pH values. Absorption spectra were recorded according to specific procedure which was carefully designed to avoid systematic errors. Collected absorption spectra will be used for the development of the algorithm for the spectral deconvolution (using MATLAB). Such software can be very useful tool in the drug research, especially for the analysis of the compounds which pK_a values cannot be determined by potentiometry.

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AC PP 20

Study of interactions between olanzapine and methacrylic, acrylic and acetic acid

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Molecularly imprinted polymers (MIPs) are synthetic polymers with cavities that are complementary in shape and functional groups to the target molecule. The most important step in MIP synthesis is the formation of prepolymerization complex between the template and the functional monomer The analysis of these interactions is thus essential for the preparation of well-performing MIPs[1]. We investigated the interactions of olanzapine (Ola, an antipsychotic drug) with three acidic functional monomers: methacrylic (MAA), acrylic (AA) and acetic acid (AcOH – as a substitute for MAA). Interactions of Ola with different acids (in terms of monomer: template molar ratio) were studied by conductometric titrations in acetonitrile. Additionally, the effect of the ethylene glycol dimethacrylate (EDMA) or divinyl benzene (DVB) as crosslinkers on the determined monomer: template molar ratio was investigated. Ola precipitated in presence of 1.5 equivalents of MAA. The yellow powdery precipitate was analyzed by NMR spectroscopy (1H, 13C, COSY, NOESY, HSQC, and HMBC), and its structure was determined to be a salt of Ola and MAA. ADMET predictor software[2] suggested the imine nitrogen should be protonated (85% chance), but the NMR results showed that it's the piperazine nitrogen that gets protonated. The remaining concentration of Ola in the supernatant was determined by spectrophotometry to be 38% of the original concentration. It was also noticed that the precipitation doesn't occur in the presence of linkers EDMA or DVB, nor did it happen when using AA and AcOH. The results obtained from conductometric titrations vary, depending on the used monomer and linker: ratios obtained with AcOH are considerably higher than those obtained with MAA and AA. The effect of linkers on the determined is visible, but no clear trends could be established. Obtained monomer: template molar ratios could be used to make MIPs with high imprinting factors, selectivity and capacity.

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AC PP 21

Donepezil controlled release in simulated intestinal fluids by molecularly imprinted polymers

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Donepezil is a medication used in the treatment of some symptoms of dementia due to Alzheimer's disease. It is of great importance to find an appropriate delivery system for donepezil keeping in mind the nature of Alzheimer's disease[1]. Molecularly imprinted polymers (MIPs) have many applications, one of which is sustained drug release. MIPs are showing promising results in this field, which aims to achieve desired dosage and therapeutic effect of selected medication. Three molecularly imprinted polymers for donepezil that were previously synthesized[2] were tested for its sustained release. MIPs were synthesized with methacrylic acid as a functional monomer, donepezil as a template (all three MIPs), divinyl benzene (MIP I), and ethylene glycol dimethacrylate (MIPs II and III) were used as cross-linkers in acetonitrile (MIPs I and II) or chloroform (MIP III) as porogenic solvents. Controlled drug release was monitored under physiological conditions in fasted- and fed-state simulated intestinal fluids (FaSSIF and FeSSIF) over a period of 4 h. HPLC with UV-Vis detection was used for donepezil concentration determination. MIP I showed better results and gradual increase in the concentration of released donepezil, while MIPs II and III showed decrease in donepezil concentration over time. Concentration of released donepezil in the case of MIP I was slightly higher in FaSSIF and FeSSIF compared to their corresponding blank buffers. Higher concentrations of released donepezil were also achieved in FeSSIF in comparison to FaSSIF. The highest released concentration of donepezil in FaSSIF was 3,6 mg/g and in FeSSIF 4,8 mg/g.

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AC PP 22

Sorption of testosterone, estrone and β-estradiol on Bovine serum albumin immobilized onto silica particles

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Immobilization of proteins represents one of the leading ways in obtaining new sorbents used for solid phase extraction (SPE) with the aim of detection or isolation of target molecules. Immobilized protein can find application in enantiomer separation technology. Bovine serum albumin (BSA) was immobilized on (3-aminopropyl)triethoxysilane modified silica by the Schiff base reaction mechanism using gluteraldehyde moiety. Considering previously investigated usage of modified sorbents for the determination of progesterone via SPE method[1], the main objective of this paper is to expand the scope and explore the possibility of testosterone, estrone and β-estradiol sorption on prepared sorbents. It has been shown that adsorption of the mentioned target molecules occurs quantitatively. Examined concentration for detecting hormones was 5×10^{-6} M, while the analyte concentration was determined by HPLC-DAD. The binding rate was 98% for testosterone and 100% for estrone and β-estradiol. Immobilized protein was characterized using IR spectroscopy. Obtained results are promising in the scope of possible usage of the immobilized proteins for the detection of low studied steroids concentration.

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AC PP 23

Molecularly imprinted polymer based on silica for benzophenone 4 adsorption

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Benzophenone 4 or 5-benzoyl-4-hydroxy-2-methoxybenzenesulfonic acid (BP4) is one of the many UV filters used in sunscreens formulations and skin care products. Their excessive and improper use in recent decades has led to an increase in their concentrations in aquatic ecosystems. They have been proven to be toxic for many organisms and can form a layer on the surface of the water which prevents light from reaching greater depths, which directly disrupts living ecosystems. The aim of this work was to synthesize molecularly imprinted polymers based on silica, for BP4 template, which could be used for solid phase extraction of BP4 from contaminated water samples. Vinyl modified silica particles were obtained by modification of silica particles (16-32 µm) using vinyltrimethoxysilane. Subsequently, polymer was formed on a vinyl silica surface using 4-vinyl pyridine as a functional monomer and divinylbenzene as a crosslinking reagent. The non-imprinted polymer was synthesized using the same procedure but without template addition in the initial polymerization mixture. After polymerization, the template was removed from the polymer and re-binding of the template was tested using HPLC-DAD. Synthesized polymers showed binding capacities of 92.4 (MIP) and 93.9 µmol (NIP) of template per gram of polymer. Even though no significant difference in template binding between MIP and NIP was obtained, both MIP and NIP showed high selectivity for BP4 binding compared to other UV filters (benzyl salicylate, octyl salicylate, ethylhexyl methoxycinnamate, homosalate, butyl methoxydibenzoylmethane, benzophenone-8, benzophenone-1 and padimate O).

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AC PP 24

Synthesis of molecularly imprinted polymers for UV filter Padimate-O

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UV filters are important component of sunscreens and other skincare products. Because of their property to absorb, reflect and scatter UV light they protect our skin from harmful effects of sunlight. On the other hand, excessive concentrations of UV filters in bathing waters, like lakes or coastal areas prevent sunlight from passing through, thus representing an environmental risk for aquatic ecosystems[1]. Molecularly imprinted polymers (MIPs) are synthetic materials with the ability to selectively bind target molecules, mimicking the characteristics of antibodies and enzymes[2]. The aim of this work was the preparation of MIPs for UV filter Padimate-O. MIPs and non-imprinted polymers (NIPs) were prepared via bulk polymerization method using non-covalent approach for pre-polymerization complex formation. 2-Acrylamido-2-methylpropane sulfonic acid was used as a functional monomer, ethylene glycol dimethacrylate as a cross-linker in dimethylformamide as porogen. Binding capacities of the obtained polymers determined via batch binding experiment method showed greater binding capacity of MIP towards Padimate-O (18.25 µmol of template per gram polymer compared to NIP (4.33 µmol/g) which indicates successful molecular imprinting. Prepared MIP has shown high selectivity towards template UV filter with the binding capacity for template Padimate-O compared to other commercially available UV filters (benzyl salicylate, octyl salicylate, ethylhexyl methoxycinnamate, homosalate, butyl methoxydibenzoylmethane, benzophenone-8, benzophenone-1, benzophenone-4). Obtained results show the potential for prepared MIP application as a sorbent for solid phase extraction used to quantify and monitor UV filters in real aqueous samples.

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AC PP 25

Effect of strawberry crossbreeding on the content of vitamin C

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The term "vitamin C" refers to all compounds that show equivalent biological activity as L-ascorbic acid, including its oxidation products, isomers, esters and synthetic forms. Vitamin C is a powerful reducing agent found in millimolar amounts in plants and plays an important role in removing free radicals. The strawberry represents a relevant source of micronutrients, such as vitamin C, minerals, folate, and phenolic substances, most of which are natural antioxidants and contribute to the high nutritional quality of the fruit.[1] The research was initially conceived to evaluate quality characteristics and nutritional value by analyzing the parental varieties and their progeny - prospective candidates, to check the possibility that, crossing a parent with a high content of vitamin C with a parent with similar or with a lower content of vitamin C, gets a prospective candidate who will have a higher range of this vitamin. In this sense, twenty-four samples of different strawberry genotypes were harvested at the stage of commercial maturity. Of these, 12 samples are parental varieties and 12 are prospective candidates - progeny obtained by crossing parental varieties. In all samples, the content of vitamin C was determined using the HPLC method. Samples were extracted with 3% meta-phosphoric acid. Elution was carried out isocratically, and analysis was done at a wavelength of 265 nm. By analyzing the results obtained for the values of vitamin C content in this work, it was proven that this vitamin's content differs between samples of parental varieties and prospective candidates. The results show that the highest concentration of vitamin C was in the old and standard parent varieties Eva, Alba, and Asia, but there was no clear expression of this trait in the progenies of parent cultivars rich in vitamin C. Even when both parents were very high in vitamin C, no significant amount was found in the progenies. Future investigation is needed to elucidate the inheritance of this trait and its possible use in advanced breeding and selection programs.

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AC PP 26

Synthesis and characterization of polymers for potential controlled release of furosemide

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Furosemide is a compound with strong diuretic effect used in drugs like Lasix®.[1] As elimination half-life of furosemide in human organism is short (up to 100 minutes), it is necessary to develop systems for controlled release. Molecularly imprinted polymers represent smart materials with predetermined selectivity and binding abilities towards selected template present during polymerization.[2] In this research, four polymers were prepared using two monomers (dimethylaminoethyl methacrylate and 4-vinylpyridine) and two cross-linking reagents (divinylbenzene and ethylene glycol dimethacrylate) in acetonitrile as porogen. Following synthesis, polymers were washed with methanol, dried and binding of furosemide was tested, monitored using HPLC-DAD. Polymers were also characterized by FTIR spectroscopy. Polymers showed high binding capacity towards furosemide – 14 mg/g (P1) up to 118 mg/g (P4), thus, it can be concluded that prepared polymers can be potentially used for controlled release. Time dependency of the binding was tested and it was shown that binding of furosemide to polymer reached equilibrium after 6 hours, suggesting controlled release would be possible. Future work will be oriented towards controlled release in physiological-like conditions.

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Biochemistry and biotechnology

BB PP 01

Detection and bioremediation of petroleum pollutants in groundwater of alluvial aquifer of the Sava river, Serbia

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Bioremediation is cheap, efficient, green technology that provides degradation of organic compounds by microorganisms. Products of biodegradation can be less toxic compounds or CO_2 and H_2O, when biodegradation is complete. The aim of this research was detection and biodegradation of petroleum pollutants in the groundwater from alluvial aquifer of the Sava river in the vicinity of one of the largest district heating plants in New Belgrade (Serbia). The heating plant "New Belgrade" has been using petroleum products as fuel for decades. Total Petroleum Hydrocarbons (TPH) were analyzed in 10 groundwater samples collected from boreholes at the depths from 8 to 11 m. From these samples, TPH were isolated using extraction method with *n*-hexane. TPH was further analyzed by gas chromatography with flame ionization detector (GC-FID). In this study bioremediation was applied in order to degrade TPH in the groundwater of the investigated location. This research lasted for one year [1].

In the sample P-5 the initial concentration of TPH was 1.39 mg/L and it was 0.02 mg/L at the end of the bioremediation, with TPH reduction of 98.55 %. In the sample P-6, the initial concentration of TPH was 1.76 mg/L, while at the end of the bioremediation it was 0.03 mg/L, with TPH reduction of 98.30 %. In the sample P-7, the initial concentration of TPH was 1.57 mg/L, and at the end of bioremediation it was 0.03 mg/L with TPH reduction of 98.09 %. It can be concluded that this approach was very successful, with an efficiency of approximately 100 % [1, 2].

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BB PP 02

The effect of spermidine supplementation on polyamine content in honey bee (*Apis mellifera* L.*)*

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Honey bee (*Apis mellifera* L.), one of the most important pollinators on the planet, provides a vital service to the ecosystem that is essential to maintaining natural biodiversity. However, the number of colonies is decreasing for the last few decades, and the main cause of this problem might be climate change, improper use of agrochemicals and pathogen susceptibility. Polyamines are positively charged molecules found in all living organisms that interact with negatively charged molecules including DNA and RNA and are involved in a wide range of cellular processes such as cell growth, survival and proliferation. The main representatives of polyamines are putrescine, spermidine and spermine, whose concentration is determined by food intake, *de novo* synthesis and microbial synthesis in the gut (Madeo et al., 2018). Spermidine supplementation was previously shown to affect survival and health of many organisms such as *D. melanogaster* and *C. elegans*. The aim of this experiment was to examine the polyamine content in honey bees during ageing and in groups whose nutrition was supplemented with two different spermidine concentrations. Three experimental groups were formed: control C fed with 50% (w/w) sucrose solution, $S_{0.1}$ and S_1 groups named after spermidine concentration in mM, and the experiment lasted for 10 and 17 days. Polyamines were determined in whole body using HPLC, as described by Kebert et al. (2016). When comparing the control groups, the levels of all three polyamines have declined with the ageing of honey bee. In groups supplemented with both concentrations of spermidine, there was an increase in the levels of putrescine and spermidine content, but a decrease in the case of spermine after 10 and 17 days. These results raise questions which require further research.

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BB PP 03

Optimization of extraction conditions of tropomyosin from Mediterranean mussel and its quantification by developed ELISA

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Tropomyosin (TPM) is a major allergen among different shellfish species. Developing sensitive, specific, and reliable methods for quantifying TPM in food products is crucial for persons allergic to shellfish. Commonly used extraction buffers often show shortcomings in their extraction efficiency, which is why sometimes the presence of some allergens can be overlooked in the biological material. Therefore, this work aimed to optimize Mediterranean mussel TPM extraction conditions and develop a sandwich ELISA method for TPM quantification. Several extraction buffers were tested for their efficiency in recovering proteins from fresh frozen and cooked mussels during 2 and 24 hours of extraction. The protein content was quantified using the Bradford protein assay. Protein components of soluble extracts were profiled using SDS-PAGE. TPM presence in soluble extracts was confirmed by Western blot using both monoclonal and polyclonal anti-TPM antibodies. Sandwich ELISA was developed and used to quantify TPM content. None of the extraction buffers showed a significant difference in total protein content between 2 and 24 hours of extraction, indicating that 2 hours is sufficient for protein recovery in both raw and cooked mussels. Significantly fewer proteins were extracted from cooked mussels compared to raw mussels. Densitometrically estimated TPM concentrations indicate that PBS containing 1M NaCl (PBSN) extracts around 40% more TPM than PBS. Carbonate buffers extract even three times higher amounts of TPM than traditionally used extraction buffer PBS. Developed sandwich ELISA has shown not to be reliable for quantifying TPM from mussels, significantly underestimating its concentration, as concluded by comparing TPM concentrations obtained by ELISA with those obtained densitometrically. Therefore, Western blot has been used as an alternative method for mussel TPM quantification. The linear range for TPM quantification using Western blot was between 1.25 and 10 µg/ml. TPM concentrations in mussel extracts estimated using Western blot correlated well with those calculated by densitometric gel analysis. Further work will be aimed at improving the sensitivity of the presented methods and developing new methods for TPM quantification.

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BB PP 04

In vitro analysis of hypoglycemic potential of new grapevine variety *Dionis* wine

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Due to the constant increase in the number of people suffering from Diabetes mellitus type 2, more focus is being put on application of different diets to improve the quality of life. Consumption of red wine has shown positive health effects in numerous studies, manifesting various biological activities [1]. The aim of this study was to determine the hypoglycemic potential of the new wine variety Dionis, grown on Fruska Gora and the well-known variety Cabernet Franc, produced between 2017 and 2021. Their inhibitory potential was evaluated in *in vitro* assays against two enzymes involved in carbohydrate digestion, α-amylase and α-glucosidase [2]. Spectrophotometric methods were used to determine the content of total phenols, tannins, monomeric anthocyanins and flavonoids in wine. All analyzed wine samples manifested some hypoglycemic potential with IC_{50} values ranged 0,825-2,337 mg/mL (α-amylase) and 0,210-0,575 mg/mL (α-glucosidase) for Dionis and 1,543-2,525 mg/mL (α-amylase) and 0,091-1,511 mg/mL (α-glucosidase) for Cabernet Franc. Wine samples of Dionis variety showed higher inhibitory potential to both enzymes compared to Cabernet Franc. One of the Dionis wine samples had a higher inhibitory potential compared to the standard enzymes inhibitor, acarbose [2]. The higher content of investigated monomeric anthocyanins and flavonoids was represented in Dionis wine samples, while the content of total phenols and tannins was similar in samples of both varieties. The obtained results report valuable data about the wine of new grapevine variety Dionis originating from Serbia. They are a helpful starting point in establishing Dionis as a recognisable mark on the global wine market.

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BB PP 05

Pancreatic lipase inhibitory activity of red wines from Vojvodina

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The number of people suffering from obesity and related health complications is growing rapidly worldwide. One of the major causes of obesity and the disease known as metabolic syndrome is consumption of an excessive amounts of food. Excessive intake of triacylglycerols through food leads to their accumulation in adipose tissue. The key enzyme that regulates the metabolism and absorption of triacylglycerol is pancreatic lipase. Inhibition of this enzyme has the potential to reduce the availability of triacylglycerols and prolong the digestive process. Polyphenols are among the potential naturally occurring inhibitors of this digestive enzyme. The aim of this study was to compare the content of total polyphenols, flavonoids, tannins and monomeric anthocyanins in *Dionis* and *Cabernet Franc* red wines and to evaluate their potential to inhibit pancreatic lipase *in vitro*.

The content of total polyphenols, flavonoids, tannins and monomeric anthocyanins was measured by spectrophotometric methods. The lipase inhibitory activity of wine samples was performed using spectroscopy. In the assay 4-nitrophenol palmitate as the substrate was used, which is hydrolysed by lipase to 4-nitrophenol, a yellow colored product that can be monitored at 400 nm[1]. Orlistat was used as a positive control.

Chemical analysis showed that all wines had significant amounts of total polyphenols, flavonoids, tannins and monomeric anthocyanins. All the analyzed wine samples showed inhibitory activity against pancreatic lipase, but slightly lower than the standard inhibitor orlistat.

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BB PP 06

PhaZ expression optimization for improved enzymatic polyhydroxyalkanoates degradation

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Polyhydroxyalkanoates (PHA) are a structurally diverse class of biopolymers biotechnologically produced from renewable resources, which in combination with their biodegradability and biocompatibility renders them a sustainable alternative to petrochemical plastics. Although a cellular form of PHA degrades in a short time as a carbon source, processed biopolymer degradation in an open environment can extend to several months/years, depending on catalytic efficiencies of PHA depolymerases (PhaZs) present in microorganisms[1]. Improvement of PhaZs through directed enzyme evolution can create a recycling route for PHA bioplastics. Enzymatic PHA degradation is advantageous in comparison to thermal decomposition as higher yields of optically pure monomers in an energetically more efficient manner are produced. Further, obtained PHA monomers are valuable in the chemical, cosmetic and especially pharmaceutical industries whose demanding requirements are met by biocatalysis.

Screening for improved PhaZs requires an efficient expression system. *E. coli* is the most extensively developed host system, but oftentimes requires case-specific optimization which was the aim of the present study. Expression conditions for *phaZ* genes from *Comamonas testosteroni* 31A (PHBase), *Pseudomonas fluorescens* GK13 (PHOase) and its computationally predicted mutant with improved thermal stability were optimized in *E. coli* BL21 (DE3) ArcticExpress, pLysS and CodonPlus-RIPL hosts, as gene products turned out to be toxic to the most commonly employed *E. coli* BL21 (DE3) strain. IPTG-induced expression from the pET-22b(+) vector was further optimized by variations in induction temperature and time, cell density and glucose addition. Expression was monitored by SDS-PAGE analysis and PHA degrading activity of both whole cell culture and cellular fractions, as well as a cell-to-cell variation to find the most suitable host for expression of the mutant library. RIPL cells were selected for PhaZ activity screening in directed evolution experiments as they permitted stable expression of all three *phaZ* genes.

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BB PP 07

Antioxidant potential and neuroprotective activity of aerial parts and fruit extracts of hawthorn (*Crataegus* spp.)

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Hawthorn belongs to the Rosaceae family, with 280 species cultivated in Europe, Asia and North America. It possesses antioxidant, anti-inflammatory, cardioprotective, neuroprotective, anti-diabetic activities, and many others, due to the presence of a variety of phytochemicals (polyphenols, flavonoids, lignans, mono- and triterpenoids). In our previous study, we examined the chemical composition of methanol extracts of aerial parts and fruit, and commercial extracts of aerial parts and fruit by total phenolic and total flavonoid assays, as well as by quantitative LC-MS/MS analysis of selected compounds. The initial evaluation of antioxidant activity was examined by DPPH and FRAP assays [1].

In this study, we did further examination of antioxidant potential by lipid peroxidation inhibition assay and ability to neutralize hydroxyl radicals. The neuroprotective activity was examined by acetylcholine esterase inhibition assay [2]. All samples had the ability to inhibit lipid peroxidation with IC_{50} in the range of 0.13-1.20 mg/mL, while IC_{50} for neutralization of hydroxyl radicals ranged from 0.56 to 0.84 mg/mL. It can be concluded that samples that had a higher content of phenols and flavonoids were more active. Extracts of aerial parts had higher activity compared to fruit extracts, and commercial extracts of aerial parts and fruit were more active than corresponding prepared extracts. All samples had the ability to inhibit acetylcholine esterase with inhibition ranging from 27.5 to 38.4% at the concentration of 0.125 mg/mL. Extracts of aerial parts were more active compared to fruit extracts, but there was no difference in activity between prepared and commercial extracts. Based on our results hawthorn is a good source of antioxidant compounds and has moderate inhibitory activity toward the acetylcholine esterase enzyme which can be beneficial for neuroprotection.

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BB PP 08

Antioxidant and neuroprotective activity of extracts of flowers of *Hibiscus* genera

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Hibiscus species from the *Hibiscus* genera, belonging to the Malvaceae family are widely distributed all over the world. They possess antihypertensive, anti-inflammatory, antipyretic, hepatoprotective, anti-diarrhoeic, anti-tumor, antioxidant, antidiabetic, anticonvulsant, and many other activities. Hibiscus contains different phytochemical constituents including flavonoids, alkaloids, saponins, tannins, and polyphenols. In our previous study, we examined two samples of garden hibiscus flowers from 2018 and 2021 year and one commercial sample of hibiscus flowers. Chemical composition was evaluated by total phenolic, flavonoid, and anthocyanin content as well as quantitative LC-MS-MS analysis, while initial antioxidant activity was examined by DPPH and FRAP assay [1].

In this study, antioxidant activity was further evaluated by the inhibition of lipid peroxidation and neutralization of $OH^\bullet$ radical. The neuroprotective activity was investigated by the inhibition of acetylcholine esterase [2]. All samples had the ability to inhibit lipid peroxidation with IC_{50} ranging from 0.24 to 0.95 mg/mL. Extracts of hibiscus flowers can neutralize $OH^\bullet$ with IC_{50} in the range of 0.18-0.37 mg/mL. Extract of garden flowers from the year 2018 showed the highest antioxidant potential, which was expected considering that it had the highest content of phenols, flavonoids, and anthocyanins. All samples had the ability to inhibit acetylcholine esterase, with inhibition of 70.4-74.7% at the concentration of 0.25 mg/mL. The highest inhibition was achieved by extract of garden flowers from the year 2018, while the lowest inhibition was achieved by a commercial sample. Based on these results it can be concluded that flowers of the *Hibiscus* genera have high antioxidant potential, and can exhibit good neuroprotective activity.

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Chemical education and history of chemistry

CE PP 01

Presentation of the processing and use of crude oil and natural gas with hybrid illustrations in the eighth grade chemistry curriculum

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The advantages of using the illustrative-graphic teaching method have been documented in a lot of studies. Hybrid illustrations are a part of this method because they depict abstract elements (geometric shapes, alphanumeric symbols, formulas) combined with realistic images taken from everyday life [1]. Students come across a lot of structural formulas and molecular models while learning the groups of compunds in organic chemistry, which can make the material difficult to understand. The close connection of this branch of chemistry with biology, physiological processes, and industrial use provides many opportunities to represent the abstract content with realistic images.

Crude oil and natural gas are included as a separate unit in the eighth grade chemistry curriculum, emphasizing their role in energy supply and industry. Serbian chemistry textbooks depict the everyday appearance of these materials in different ways but the common feature in each textbook is that there is at least one photo of crude oil mining (tower) and processing (refinery). Some textbooks also include a realistic illustration of the staged refining of crude oil. The mining and processing of natural gas receives less attention in textbooks. The industrial, household and energy supply aspects of both substances are also important, especially in view of the recent energy crisis. In this work, a hybrid illustration is presented that shows the processing and use of natural gas and crude oil, summarizing the knowledge base that students need to know about these substances within the eighth grade chemistry curriculum.

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Chemistry of macromolecules and nanotechnology

CMN PP 01

Mechanical properties and particle size of the waterborne polyurethanes

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In this study, six waterborne polyurethanes (WBPUs) were synthesized based on *α,ω*-dihydroxypropyl poly(dimethylsiloxane) (PDMS), isophorone diisocyanate (IPDI), 2,2-bis-(hydroxymethyl) propionic acid (DMPA) and triethylamine (TEA). WBPUs were prepared without a chain extension step and with various DMPA/PDMS molar ratios (from 0.2 to 0.7). The mechanical features, particle size and particle size distribution, as well as molecular weights of WBPUs were investigated by diverse experimental techniques.

Tensile strength values were in the range from 4.03 to 6.33 MPa, and generally decrease with decreasing PDMS content in WBPUs. This occurs due to the presence of lower degree of microphase separation in WBPUs with lower PDMS content. On the other hand, the incorporation of flexible PDMS led to an increase of elongation at break values (from 0.4 to 58.6%) in WBPUs. The particle size of the prepared WBPU dispersions and molecular weight of WBPU films decrease with increasing DMPA content. Particle sizes of these WBPU dispersions are in the range from 91.4 to 232.3 nm, while the weight average molecular weights (M_w) are in the range from 11900 to 15300 g/mol [1]. Prepared WBPUs are polymer materials with good mechanical features and suitable particle sizes, which enable them to be used as coatings for different purposes.

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CMN PP 02

Green synthesis of nanoparticles: Pulsed Laser Ablation in Liquids

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Laser ablation synthesis in liquid solution (PLAL) is a green technique that allows for the physical formation of ultrapure nanomaterials. In this work, Ag and Au nanoparticles are synthesized by PLAL using two different neodymium-doped yttrium aluminum garnet (Nd:YAG) laser systems. A pure silver/gold target (99.998% purity) was immersed in Milli-Q water and the sample surface of approximately 1 cm^2 in size was continually scanned by a pulsed laser beam to achieve a homogenous ablation. Obtained suspensions were analyzed by ICP-OES, UV-Vis, TEM, and DLS. UV-Vis spectra showed characteristic peaks at 428 nm and 525 nm, which correlate with silver and gold nanoparticles' surface plasmon absorbance. ICP-OES analysis confirmed that these suspensions are free from impurities. Since no stabilizer is added, these nanoparticles tend to agglomerate in time, as TEM and DLS analysis confirmed (Figure 1). Nevertheless, these nanoparticles can be easily functionalized with a variety of ligands such as small molecules, surfactants, dendrimers, polymers, and biomolecules to get desirable functionalities for various applications.

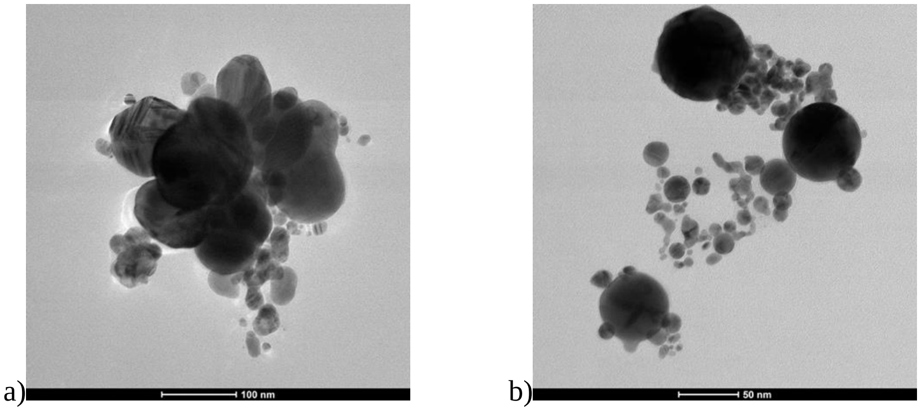

Figure 1. TEM images of a) silver and b) gold nanoparticles

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CMN PP 03

Thermal extraction of pectin from waste apple pomace using choline chloride based eutectic solvents

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Processing of waste by-products of agricultural origin generated by different kinds of industries can entail environmental problems. Waste apple pomace (biomass) could play an important role in pectin production, offering economic advantages and decreasing the environmental impact. Pectin and pectin derived oligosaccharides have many applications in food and pharmaceutical products as gelling agents and stabilizers. Traditional method for pectin extraction involved the use of diluted mineral acids at elevated temperatures, with yields of about 10 to 15%. Because of the relatively long period of exposure to direct heating, thermal degradation of pectin often occurs in this process. The use of deep eutectic solvents could be the solution to this problem. Deep eutectic solvents have shown superior properties when it comes to targeted extraction of certain components from biomass, while providing mild conditions when compared to conventional methods. The aim of this paper is thermal extraction of pectin from waste apple pomace using choline chloride based deep eutectic solvents combined with different acids (oxalic acid, lactic acid and malic acid). Properties of extracted products were examined using FTIR spectroscopy and differential scanning calorimetry.

Acknowledgments

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Green chemistry

GC PP 01

Extraction of active pharmaceutical compound (parthenolide) using aqueous biphasic system based on triblock copolymers and deep eutectic solvent

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The chemotherapeutic parthenolide (PTL) is an exciting new candidate for the treatment of cancer, but like many other small-molecule drugs, it has low aqueous solubility. PTL is a sesquiterpene lactone extracted from the medical herb feverfew (Tanacetum parthenium), (Fig. 1). Therefore, the application of polymer-based micelles as drug delivery systems is a promising technique for increasing the effectiveness of hydrophobic drugs [1]. The reverse pluronic polymers (Pluronics R type) are linear triblock copolymers where the hydrophobic polypropylene oxide blocks are in the external parts of the chains and the hydrophilic polyethylene oxide is in the center, inducing the formation of such different type of structures as reverse micelles.

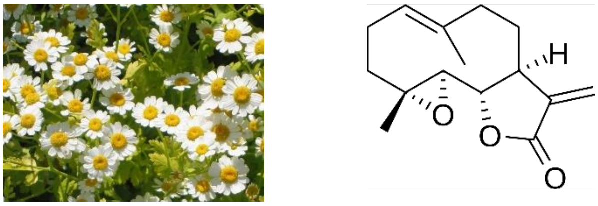

Figure 1. Feverfew (Tanacetum parthenium) and chemical formula of parthenolide.

Accordingly, we describe the green extraction of parthenolide using an aqueous biphasic system (ABS) formed by copolymers and deep eutectic solvent (DES). Copolymers used in this work are Pluronic 10R5 and Pluronic 17R4, also those are compared with polymer PPG 400. Prepared DES is obtained by mixing choline chloride and lactic acid in a molar ratio 1:1. Ternary phase diagrams of the ABSs were determined by the cloud point titration method at 25 °C and atmospheric pressure. A quantitative analysis of PAR was assessed by HPLC with a DAD detector at 210 nm. The partition of PTL in studied ABS systems was expressed through extraction efficiency and distribution coefficient. The trend showed that the hydrophobicity of PTL is responsible for the partitioning of these drugs preferentially into the polymer-rich phase forming micelles.

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GC PP 02

Metal ion separations in polypropylene glycol (PPG400)-based aqueous biphasic systems with functionalized ionic liquids and deep eutectic solvents

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Aqueous biphasic systems (ABS) consist of two immiscible phases formed when certain water-soluble compounds are combined in a predetermined concentration range [1]. Extraction and separation of different metal species for their quantitative regeneration have found a greener way through the use of ABSs [1]. The earliest ABS composed of polymer and inorganic salts have limited application due to low polarity differences between coexisting phases, and viscosity. Ionic liquids (ILs) and deep eutectic solvents (DES) are newer superior solvents applied as phase-forming compounds in ABS. Recently, DESs have been introduced in ABS owing to lower starting material cost, ease of preparation, higher tunability, and biodegradability. On the other hand, ILs could be considered as the parents of DESs. ILs were known to be non-volatile, non-flammable, and stable in air and in water, and were considered as green solvents. Recently, it has been well-known that many of them are, in fact, volatile, flammable, unstable, and even toxic. This situation is attributed to the extensive combinations of cations and anions that meet the definition of ILs, leading to an adverse suite of behaviors. And then DESs were introduced as an alternative to ILs to overcome the drawbacks of ILs [1]. This work aims to compare the extraction of Co, Ni, Cu, In, La, Ce, Nd, and Dy in ABSs based on either DES or IL as salting-out agents. ABSs were built using functionalized IL (cholinium lactate, ChLac) or corresponding DES (Cholinium chloride - lactic acid in molar ratio 1:1) and polypropylene glycol 400 (PPG400). The hydrogen bond donors (HBD, lactic acid) in DES and anion in IL are responsible for the formation of metal complexes, while the hydrogen bond acceptors-HBA in DES (cholinium chloride) and cations in IL are responsible for the formation of ABS and complex extraction. The concentrations of all metals were determined by the ICP-OES method. The results, presented as extraction efficiency, show that the targeted metal ions in higher degree partition in IL or DES-reach phase compared to the PEG-reach phase.

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GC PP 03

Waste to catalyst: Recycling of dental cover waste to boost hydrogen production

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Metals (copper, nickel, zinc, aluminium) and precious metals such as gold and silver, represent a group of very valuable materials with a wide spectrum of possible applications. Catalyst for hydrogen production is one of them. The main problem is their limited quantity, and excessive use can completely deplete the Earth's reserves. Recycling these metals from waste is a promising solution, however, environmental and economic acceptability must be taken into account when choosing recycling methods.

The recycling route of metals from dental powder is presented here, but also its application as a catalyst for the hydrogen evolution reaction (HER). Slurry electrolysis was used as a method of simultaneous recycling of all mentioned metals from HCL, NaCl and H_2O_2 bath. [1] Metals were electrodeposited to the pure nickel cathode, which was directly used as a cathode for hydrogen production. The ability of the deposit to be used in hydrogen evolution reaction was tested using various methods in an alkaline electrolyte (KOH). Cyclovoltammetry, Tafel analysis and electrochemical impedance spectroscopy (EIS) were used for electrochemical characterization. Deposit composition and morphology were examined with XRF and a metallurgical optical microscope.

Results obtained during this research show the possibility of applying the slurry electrolysis as a method of recycling and extracting metals, depositing them on the surface of the electrode and its further use in the production of hydrogen. Compared to the pure nickel electrode, the coating obtained from slurry electrolysis showed better catalytic activity.

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Inorganic chemistry

IC PP 01

Synthesis and characterization of octahedral Ni(II) complex with condensation product of 2-acetylthiazole and thiosemicarbazide

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The ligand (**HL**) was synthetized by the reaction of 2-acetylthiazole and thiosemicarbazide in molar ratio 1:1 in water. In the reaction of ligand (**HL**) and nickel(II) tetrafluoroborate hexahydrate [Ni(**HL**)$_2$](BF$_4$)$_2$ complex was obtained. The Ni(II) ion has octahedral coordination geometry. The tridentate ligand (**HL**) is coordinated to the nickel ion with a NNS set of donor atoms forming two five-membered chelate rings. The ligand (**HL**) and the [Ni(**HL**)$_2$](BF$_4$)$_2$ complex were characterized by elemental analysis, IR and UV/Vis spectroscopy and the structure of the complex was defined by X-ray analysis.

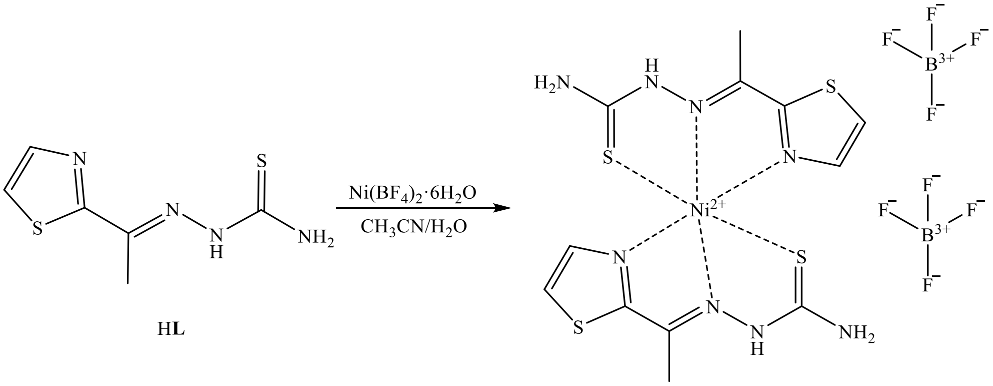

*Figure 1. Synthesis of [Ni(**HL**)$_2$](BF$_4$)$_2$ complex.*

Acknowledgments

This research was supported by the Science Fund of the Republic of Serbia, #7750288, Tailoring Molecular Magnets and Catalysts Based on Transition Metal Complexes – TMMagCat.

IC PP 02

Synthesis and characterization of the Cu(II) complex with the Schiff base of aminoguanidine and 2,4-dihydroxybenzaldehide

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The versatility of coordination chemistry of 2,4-dihydroxybenzaldehyde derivatives has been proven by the search of the Cambridge Structural Database. Complexes of these compounds with 3d, 4d, and 5d-metals, but some s-, and p-elements as well, are structurally characterized. Having in mind the well-known significance of aminoguanidine [1], it is of interest to examine the possibility of syntheses and characterization of metal complexes containing these two compounds.

The reaction of an aqueous solution of $Cu(OAc)_2 \cdot H_2O$ with the chloride salt of the Schiff base of aminoguanidine and 2,4-dihydroxybenzaldehide (L), in molar ratio 1:1, yielded in formation of single crystals of the complex $[Cu(L–H)Cl] \cdot 3H_2O$. The complex is poorly soluble in water and alcohols, and well soluble in DMF. The molar conductivity of the synthesized complex in DMF shows its non-electrolytic nature (11 S cm^2/mol). The ligand is coordinated in ONN manner, through oxygen atom of the deprotonated hydroxy-group in position 2, azomethine and nitrogen atom of imino group of aminoguanidine residue. Copper(II) is situated in a square-planar environment (τ_4=0.07) of three ligators of the chelating ligand and one chlorido ligand forming one five-membered and one six-membered metallocycle (Fig 1).

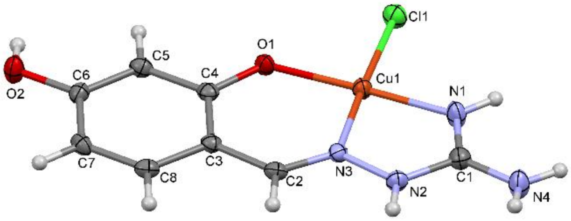

Figure 1. Molecular structure of the complex $[Cu(L–H)Cl] \cdot 3H_2O$.

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Acknowledgments

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IC PP 03

Synthesis and characterization of new [Ru(η^6-*p*-cymene)Cl_2(L)] complex

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In this report, we have synthesized a complex of Ru(II)-*p*-cymene and 3-amino-2-cyano-*N*-phenyl-3-(4-phenyl-1-piperazinyl)-2-propenethioamide ligand. The new complex was synthesized according to the method described elsewhere with slight modifications.[1] To a solution of [Ru-(η^6-*p*-cymene)Cl_2]$_2$ (0.0998 g, 0.1630 mmol) in methanol (15 mL) and 3-amino-2-cyano-*N*-phenyl-3-(4-phenyl-1-piperazinyl)-2-propenethioamide (**L**) (0.36348 g, 1 mmol) was added at room temperature (Fig. 1). The resulting mixture was heated and refluxed for 3 h. The solution was evaporated on a vacuum evaporator to a volume of 3 to 4 ml and then left at room temperature to slowly evaporate further. An orange powdery precipitate was separated. The precipitate was filtered off under a vacuum and washed with diethyl ether. The characterization of the synthesized complex [Ru(η^6-*p*-cymene)Cl_2(**L**)] was performed using IR and NMR as well as by determining the melting point. The interactions of the new complex with CT-DNA and HSA molecules were examined, as well as its cytotoxic activity on certain cell lines.

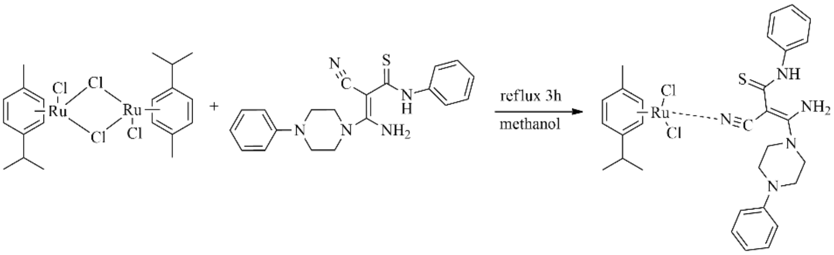

Figure 1. Synthetic route of new Ru(II) complex.

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This work was supported by the Serbian Ministry of Education, Science and Technological Development (Agreement No. 451-03-68/2022-14/ 200122).

IC PP 04

Synthesis and characterization of octahedral Ni(II) complex with condensation product of 2-acetylpyridine and Girard's P reagent

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The ligand ([**HL**]Cl) was synthetized by the reaction of 2-acetylpyridine and Girard's P reagent in molar ratio 1:1 in ethanol. In the reaction of ligand ([**HL**]Cl), nickel(II) tetrafluoroborate hexahydrate and sodium azide [Ni(**HL**)$(N_3)_3$] complex was obtained. The Ni(II) ion has a distorted octahedral coordination geometry. The tridentate ligand (**HL**) is coordinated to the nickel ion with an NNO set of donor atoms forming two five-membered chelate rings and the other three coordination sites are supplemented by azido ligands. The ligand (**HL**) and the [Ni(**HL**)$(N_3)_3$] complex were characterized by elemental analysis, IR and UV/Vis spectroscopy and structure of the complex was defined by X-ray analysis.

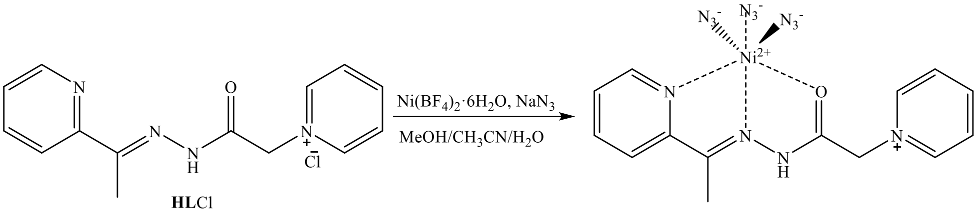

*Figure 1. Synthesis of [Ni**HL**$(N_3)_3$] complex.*

Acknowledgments

This research was supported by the Science Fund of the Republic of Serbia, #7750288, Tailoring Molecular Magnets and Catalysts Based on Transition Metal Complexes – TMMagCat.

IC PP 05

Synthesis and characterization of platinum(II) complex with 2-amino-6-methylbenzothiazole

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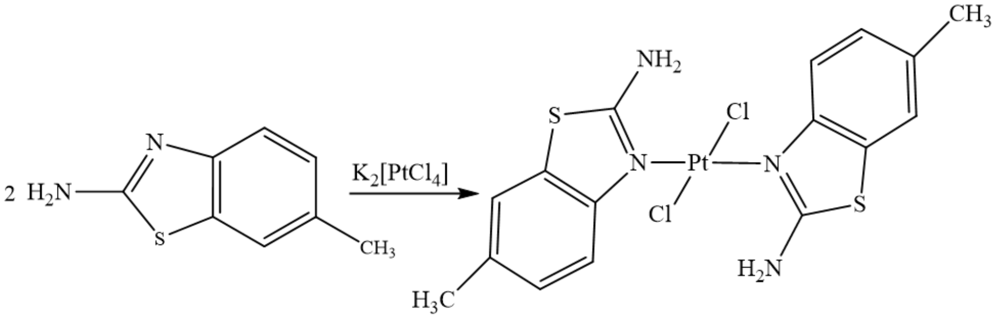
This paper examines the synthesis of new complex of platinum(II) ion with 2-amino-6-methylbenzothiazole (general formula [PtL_2Cl_2]). The new complex was synthesized according to the method described earlier [1]. $K_2[PtCl_4]$ (0.05 g) was dissolved in 10 mL of water and placed on a magnetic steerer. An appropriate amount of the ligand 0.038 g was dissolved in methanol and was added to $K_2[PtCl_4]$ water solution in portions. Pt(II) ion and ligand reacted in a molar ratio 1:2 (Scheme 1). The reaction lasted for 3h at room temperature. The obtained yellow precipitates were filtered, washed with water and dried on air. Characterization of the synthesized complex [PtL_2Cl_2] was performed by using IR and NMR spectroscopy.



Scheme 1. *Procedure for the synthesis of new Pt(II) complex*

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Acknowledgments

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IC PP 06

Silver(I) complexes with clinically used azoles: synthesis and structural characterization

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Recently, various antifungal azoles, namely clotrimazole, econazole, tioconazole and voriconazole were used for the synthesis of new gold(III) complexes of the general formula [$AuCl_3$(azole)], which have shown good to moderate antibacterial and antifungal activities, being, in most cases, more active than the respective azole ligands [1]. Moreover, we synthesized and biologically evaluated a silver(I) complex with the known antifungal drug itraconazole (itraco) as a ligand, $[Ag(itraco\text{-}N)_2]NO_3 \cdot H_2O$, which has manifested an improved anti-*Candida* potential and therapeutic safety compared to itraconazole [2]. Inspired by these results, in this study, we used the same method to prepare two new silver(I) complexes with clinically used azoles, econazole (ecz) and voriconazole (vcz), $[Ag(ecz)_2]PF_6$ (**Ag1**) and $\{[Ag(vcz)_2]PF_6\}_n$ (**Ag2**). These complexes were synthesized by the reaction of $AgPF_6$ with an equimolar amount of the corresponding azole in ethanol at room temperature. The characterization of the synthesized complexes was done by spectroscopic (NMR, IR, UV–Vis) methods, and cyclic voltammetry, while its crystal structures were determined by single-crystal X-ray diffraction analysis.

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IC PP 07

Platinum(II) complexes with different 2-substituted pyridine-4,5-dicarboxylate esters: structural characterization and interaction with biomolecules

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Cancer is one of the most important health problems in the world. Platinum-based drugs are widely used as chemotherapeutic agents, especially cisplatin. The antitumor activity of cisplatin is based on its ability to bind to DNA preventing replication of this biomolecule and thus inhibiting the growth of tumor cells in living organisms.[1] In the present study, different 2-substituted pyridine-4,5-dicarboxylate esters were used as ligands for the synthesis of new platinum(II) complexes, [$PtCl_2$(py-2tz)] (**1**), [$PtCl_2$(py-2metz)] (**2**), and [$PtCl_2$(py-2py)] (**3**) (py-2tz is dimethyl 2-(thiazol-2-yl)pyridine-4,5-dicarboxylate, py-2metz is dimethyl 2-(4-methylthiazol-2-yl)pyridine-4,5-dicarboxylate and py-2py is dimethyl 2,2′-bipyridine-4,5-dicarboxylate). The synthesized complexes were characterized by spectroscopic and electrochemical methods, while the structure of complex **1** was determined by single crystal X-ray diffraction analysis, which confirmed chelating bidentate coordination of py-2tz ligand to Pt(II) ion through the heterocyclic nitrogen atoms. The interaction of these complexes with calf thymus DNA (ct-DNA) and bovine serum albumin (BSA) was studied to evaluate their binding affinities towards these biomolecules for possible insights into their mode of action.

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IC PP 08

Synthesis and characterization of novel triphenyltin(IV) complex with 2-(4-methyl-2-oxoquinolinyl)ethanoic acid

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Among the nonplatinum metal complexes with antitumor activity, organotin(IV) complexes have gained considerable attention due to their promising biological activities [1]. These compounds induce cell death at low doses and, in some cases, show even higher anticancer potential compared to clinically used *cisplatin* [2]. Herein, the synthesis of 2-(4-methyl-2-oxoquinolinyl)ethanoic acid and its triphenyltin(IV) complex has been performed (Fig. 1). The ligand precursor has been obtained by the hydrolysis of methyl ester synthesized in the reaction between 4-methyl-2-quinolone and methyl 2-bromoethanoate. In the reaction of the deprotonated ligand with an equimolar amount of Ph_3SnCl the desired complex was precipitated as a white solid. The synthesized compounds have been characterized using standard analytical methods. The following research on synthesized compounds will be focused on examining their antitumor activity against various cancer cell lines.

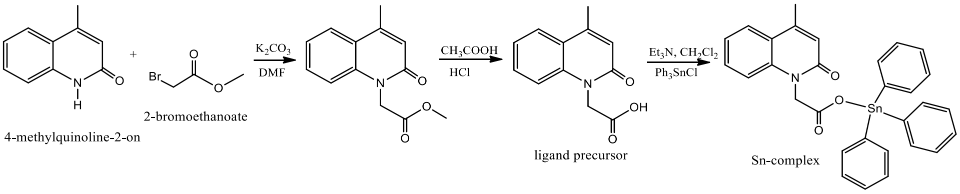

Figure 1. Synthesis of the ligand and its triphenyltin(IV) complex

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Acknowledgments

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IC PP 09

Synthesis and structural characterization of gold(III) complex with clinically used isoconazole

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There is an increasing demand for design of novel metal complexes with biologically relevant molecules for potential use in technology and medicine. Isoconazole (iso) is a well-known antifungal drug and belongs to a family of *N*-substituted imidazole derivatives, which have shown potent activity against a variety of fungal and yeast infections and have been widely used in the medical treatment of humans and animals.[1] Considering this, in the present study, isoconazole nitrate is used for the synthesis of mononuclear gold(III) complex, [$AuCl_3$(iso)]. This complex was obtained by reacting equimolar amounts of potassium tetrachloridoaurate(III) and iso nitrate in ethanol under reflux conditions for 3 h. The characterization of [$AuCl_3$(iso)] complex was done by spectroscopic (NMR, IR, UV-Vis) methods,cyclic voltammetry, and single-crystal X-ray diffraction analysis. The obtained spectroscopic and crystallographic results revealed that in this complex, the isoconazole is monodentately coordinated to the Au(III) center through the nitrogen atom of the imidazole fragment, while the remaining coordination sites are occupied by chlorido ligands resulting in a square-planar geometry around the Au(III).

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IC PP 10

Oxorhenium(V) complexes in the drug combination study

Tamara Petrović[1], Nevenka Gligorijević[2], Ferdinand Belaj[3], Sanja Grgurić-Šipka[1],
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Rhenium complexes merit particular attention in the area of metallodrug design due to rhenium's broad spectrum of oxidation states and consequently, the possibility to design compounds of a great structural diversity. Thus, the synthesis, chemical characterization and antitumor activity in vitro of the three Re(V) complexes is described. Novel compounds were obtained via reaction of $[ReOCl_3(PPh_3)_2]$ with corresponding ligands (pyridine-2-carboxylic acid, 3-methylpyridine-2-carboxylic acid and 6-methylpyridine-2-carboxylic acid) in acetonitrile at 78 °C for 3h. The complexes were fully characterized using NMR, IR, MS and elemental analysis. Their octahedral geometry with bidentate *NO* ligand was confirmed by X-ray diffraction analysis. Antiproliferative effect was determined by MTT assay and only the complex with pyridine-2-carboxylic acid (**1**) showed dose-dependent cytotoxic potential, particularly toward triple-negative breast adenocarcinoma cells MDA-MB-231 with IC_{50} 68.90 ± 1.73 µM and pancreatic adenocarcinoma cells PANC-1 with IC_{50} 69.8 ± 2.3 µM. Drug combination studies in PANC-1 cells with **1** and Verapamil hydrochloride (VRP) showed slight arrest of cell cycle in the S phase and also it increase its antiproliferative potential to IC_{50} 51.4 ± 2.8 µM. Part of the research included a depletion of the glutathione (GSH) level by L-buthionine-sulfoximine (L-BSO) at sub-toxic concentrations (100 µM) in PANC-1 cells which caused an increase of activity of **1** to the IC_{50} 57.67 ± 6.51 µM.

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IC PP 11

Novel Pt(II) complexes with Schiff-base ligands: synthesis and characterization

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Platinum complexes have a great application in medicine, but their use for clinical purposes is limited due to side effects (resistance, vomiting, cardiotoxicity, etc.). Well knownmetal-based drug is cisplatin or *cis*-diamminedichloridoplatinum(II), *cis*-$[PtCl_2(NH_3)_2]$. One of the ways to avoid unwanted effects is the synthesis of novel Pt(II) complexes with bidentate coordinated Schiff bases, which will have a stimulating effect and less harmful impact.[1,2]

Novel Pt(II) complexes with the general formula $[PtCl_2(L)]$, where L are propyl or butyl amine of 2,2''-dihydroxy-4-methoxybenzophenone have been synthesized and characterized by elemental analysis and ^1H and ^{13}C NMR spectroscopy (Fig. 1).

Spectroscopic data support square-planar coordination geometry of synthesized complexes, with coordination of Schiff-base ligand *via* nitrogen and oxygen donor atoms. The cytotoxic activity complexes Pt(II) will be evaluated.

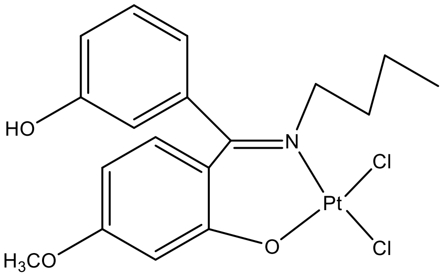

Figure 1. Structures of Pt(II) Schiff-base complex $[PtCl_2(L)]$ *(* L *is butyl amine of 2,2''-dihydroxy-4-methoxybenzophenone)*

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Material sciences

MS PP 01

Microcomposite based on magnetite modified with silicon dioxide and titanium dioxide: synthesis and photocatalytic activity investigation

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Various organic compounds which can be found in wastewaters represent a serious threat to the living organisms and the environment. That is why it is necessary to remove these pollutants from wastewaters efficiently. One of the effective and frequently used methods for degradation of organic pollutants is photocatalysis [1]. As an economical, environmentally friendly and photocatalytically active material, titanium(IV) oxide is used as an efficient photocatalyst. However, its removal after finished photocatalysis often causes difficulties. Although centrifugation and filtration were used so far, they have been proven to be complicated and expensive [2].

In this research, a microcomposite of magnetite modified with silicon dioxide and titanium dioxide was synthesized by a combined method. Its catalytic effect on photodegradation of brilliant green dye was investigated at various pH values. The investigation was performed by monitoring the absorbance of the dye solution during irradiation with UV light in the presence of the synthesized composite. The synthesized composite has shown a catalytic effect on the photodegradation of brilliant green dye in neutral and basic solution. It was shown that the efficiency of the synthesized microcomposite on the photocatalytic degradation increseas with the increase of pH value. The most important advantage of the synthesized composite when compared to commercially available ones is the possibility of quantitative separation by a magnet after the photocatalytic degradation process.

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MS PP 02

Development of macroporous bioceramic material based on calcium-hydroxyapatite doped with magnesium, strontium and fluorine ions and coated with chitosan

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Natural bone and dental tissues contain calcium-hydroxyapatite crystals (HAp) as the main inorganic component. Small amounts of various cations and anions can be incorporated into calcium-phosphate materials and affect their microstructure, mechanical and biological properties mimicing the properties of normal biological tissues [1]. The aim of this research was the synthesis and examination of the mechanical properties, as well as the bioactivity of bioceramic scaffolds based on hydroxyapatite doped with strontium, magnesium and fluorine ions, uncoated and coated with polymer chitosan. The influence of doped fluorine ions and chitosan on the properties of bioceramic scaffolds was also investigated. Hydroxyapatite (HAp) powders were synthesized and doped by hydrothermal process. The content of Mg and Sr doping ions was constant in amount of 3 mol% related to calcium, while the content of F ions was 0.5, 1 and 2 mol%. Powder with 1 mol% F was calcined at a temperature of 1000 °C for 2 hours. The polymer sponge replica method was used to obtain scaffolds. The scaffolds were subsequently coated with a thin layer of chitosan. The elemental analysis of the synthesized powders was determined by energy dispersive spectroscopy (EDS). EDS confirmed the presence of doping Mg and Sr, while the amount of doping F ions was 0, 0.24 and 1.34 at%, respectively. X-ray diffraction analysis determined the phase composition of the powders and scaffolds, which showed the presence of HAp and additionally β-tricalcium phosphate phase in scaffolds. In the compressive strength test, the synthesized scaffolds withstood a maximum force of 0.38 N, while the chitosan-coated scaffolds withstood 3.9 N. Bioactivity was investigated by keeping the scaffolds in simulated body fluid for a period of 28 days. Scanning electron microscopy was used to examine the morphology of nanostructured powders, microstructures of macroporous scaffolds and the bioactivity of the scaffolds. The uncoated scaffolds showed satisfactory bioactivity, but low amount of newly formed HAp crystals. Lower bioactivity occurred in coated scaffolds due to the slow degradation of the chitosan polymer. It was observed that the addition of F ions and chitosan polymer resulted in significant changes to the properties of the synthesized scaffolds, which indicates their potential application in tissue engineering and controlled drug release.

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MS PP 03

Development of controlled-porous bioceramic materials based on calcium-phosphate, doped with magnesium, strontium and fluorine ions in the form of inserts

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Hydroxyapatite is the main inorganic component of human bone and teeth, and therefore numerous researches are being carried out in order to improve its properties for application as bioceramic material in bone and tooth tissue engineering. After installation, dental inserts are exposed to the aggressive effect of the environment and saliva. It is necessary to synthesize a biocompatible material that would find application in dentistry as a substitute for dentin [1,2]. The aim of this work is to process, characterize and test the mechanical properties of dental inserts based on hydroxyapatite doped with strontium, magnesium and fluoride ions. Hydroxyapatite powder was synthesized and doped by hydrothermal method. The content of doped Mg, Sr ions was constant in all samples in amounts of 3 mol% related to calcium, while the content of F ions in the powders was 0.5, 1 and 2 mol%. Energy dispersive spectroscopy confirmed the proportion of doped F ions in the synthesized powders was 0, 0.24 and 1.34 at%, respectively. The Ca/P molar ratio in the powders was 1.16, 1.17 and 1.18 respectively, which indicates calcium-deficient powders. The inserts were pressed with a uniaxial press at 100 MPa and isostatic press at 400MPa then sintered at 1200 ºC for 2 hours. X-ray diffraction analysis of the sintered materials showed the presence of HAp and β-tricalcium phosphate. Scanning electron microscopy was used to examine the morphology of nanostructured powders and the microstructure of controlled porous inserts. Doped particles have similar dimensions and needle structure. While examining the microstructure of the inserts, it was noticed that with an increase in the proportion of F ions, there is an increase in the number and size of pores inside the insert, which is reflected in their mechanics. Examining the hardness and fractured toughness of the inserts, showed that with an increase in the proportion of F ions, the hardness of the inserts decreased, while the proportion of F ions has no significant effect on the fracture toughness. The values of hardness and fracture toughness showed potential for application in dentistry as dental inserts.

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MS PP 04

PANI/TiO_2 nanocomposite: synthesis and application in photocatalytic degradation of organic dyes

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Wastewaters containing organic pollutants from the textile industry represent a serious threat to aquatic organisms. Photocatalysis is one of the most promising methods for decolorizing wastewaters because this process can mineralize toxic organic compounds. As an effective, photostable, reusable, inexpensive, non-toxic, easily available and economically acceptable material, titanium(IV) oxide is frequently used as a photocatalyst. However, its wide band gap limits its visible light utilization, while its low quantum efficiency restricts electron-hole separation which generates reactive oxigen species to degrade organic pollutants [1]. Recently, it has been reported that TiO_2 modified with conducting polymers, such as polyaniline (PANI), can respond to the visible light due to the narrow band gap of the conducting polymers and the quantum efficiency is enhanced due to the good energy level match between TiO_2 and PANI [2]. Due to this, the principle aim of this research was to synthesize PANI/TiO_2 composites with various PANI content and investigate their efficiency in photocatalytic degradation of Red Orange 16 dye.

PANI/TiO_2 nanocomposites were synthesized by radical polymerisation of aniline in the presence of TiO_2 nanoparticles. Synthesized PANI/TiO_2 nanocomposites showed high photocatalytic activity in degradation of Red Orange 16 dye. The most efficient composite degraded 96% of the initially present dye after 90 minutes of irradiation. It was also shown that composites with higher PANI content showed higher photocatalytic activity, but also with increasing PANI to TiO_2 ratio, improvement of photocatalytic activity decreases. In the future, photocatalytic degradation process parameters could be optimized to reach higher efficiency.

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MS PP 05

Extraction of polyphenols from orange peel and their controlled release from pH-sensitive hydrogels

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Several million tons of orange peel are generated annually as a result of the industrial processing of this fruit. Orange peels are rich in polyphenols, that show antioxidant activity. Hence, converting orange peels into antioxidant extract by using green eutectic solvents (GES) would be a good solution. GES represent a mixture of organic substances that are not harmful to human health, environmentally friendly and highly selective towards the targeted active substance. The aim of this work was the extraction of polyphenols from orange peel waste using a GES based on urea and glycerol, their encapsulation into hydrogels based on poly(methacrylic acid) (PMAA), and controlled release from these hydrogels. PMAA are non-toxic, biocompatible and pH sensitive, so they are widely used for the targeted delivery of active substances. Swelling of PMAA and the controlled release of polyphenols from PMAA were monitored in two mediums with different pH values: 0.1 M hydrochloric acid (pH=1) and phosphate buffer (pH=6.8) at 37 °C. The influence of the crosslinker amount and neutralization degree of methacrylic acid (ND) on the PMAA swelling and the release of polyphenols was examined. The kinetics of PMAA swelling and polyphenol release were analyzed using the Peppas model. It was concluded that the swelling degree of PMAA increased with an increase in pH value of medium and ND, and decreased with an increase in crosslinker amount. As a consequence, the cumulative release of polyphenols was around three times higher in pH=6.8 than in pH=1 for both series of the samples. Peppas model showed that diffusion was the primary mechanism of polyphenols release for most samples. Based on the analysis of the results, it is concluded that the sample with optimal characteristics for the controlled release of polyphenols is the sample with 0% neutralized methacrylic acid and 0.4 mol% MBA.

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MS PP 06

Preparation and swelling characterization of P(NiPAM/OPGMA) hydrogels

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For many years now, thermally actuated hydrogels have been the ones most studied and employed in the field of polymeric biomaterials. The monomers, N-isopropyl acrylamide (NiPAM), and oligo(propylene glycol) methacrylate (OPGMA) were selected based on the sharp temperature response of their corresponding hydrogels in a known range of temperatures.[1,2] This research was performed in order to create a new class of P(NiPAM/OPGMA) temperature-responsive hydrogels, and to analyze the influence of different content of monomers on the volume phase transition temperature (VPTT) of the obtained hydrogels. One of the objectives of this study was to provide insight into the effects of applied radiation dose on the swelling and mechanical properties of the hydrogels.

In further work, P(NiPAM/OPGMA) hydrogels were synthesized for the first time by γ-radiation crosslinking of monomers from water/ethanol solution. After the high sol-gel conversion was established, xerogels were subjected to swelling analysis and tested for the mechanism of water diffusion within the hydrogels. The obtained results indicated that new hydrogels based on NiPAM and OPGMA show promising potential for water treatment application due to the relatively high swelling degree of hydrogels and the ability to combine their VPTT close to annual river water temperatures in Serbia.

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MS PP 07

Synthesis of new praseodymium doped phosphate tungsten bronze

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For the preparation of praseodymium doped phosphate tungsten bronze (Pr-PWB), as a starting material is used 12-tungstophosphoric heteropoly acid $H_3PW_{12}O_{40}\times29H_2O$ (PWA) [1]. PWA was first converted into $H_3PW_{12}O_{40}\times6H_2O$ (6-PWA) by heating it to 80 °C in a kiln. The aqueous $PrCl_3\times H_2O$ solution was prepared by dissolving 0.7102 g of $PrCl_3\times H_2O$ in distilled water. This solution is then mixed with aqueous solution of 6-PWA, slightly heated in order to start the crystallization process and left overnight to finish the crystallization. The produced greenish crystals of praseodymium doped phosphate tungsten bronze are created by heating the obtained salt $PrPW_{12}O_{40}\times nH_2O$ in a furnace from room temperature to 600 °C. The conditions for thermal phase transformation of praseodymium salt of 12-tungstophosphoric heteropoly acid to produce new praseodymium phosphate tungsten bronze, have been investigated in the current work. The new material (Pr-PWB), synthesized from Keggin's anion structure as a precursor, is successfully formed. The potential practical application of Pr-PWB is in its installation in batteries and fuel cells, as a catalyst, and due to its specific green color it could also be used as a pigment.

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MS PP 08

A comparative study of two different methods of sample preparation for polyolefins commonly used in medical devices

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Polyolefins (POs) are currently the most widely used engineering plastics due to their relatively low cost, durability, and ease of processing. A feature such as inertness makes polyolefins suitable for applications such as food packaging and medical devices. For the purpose of this study, polyethylene (PE) with good rigidity, hardness, impact strength, environmental stress cracking resistance, and excellent processability, and polypropylene (PP), with high fluidity and very good transparency, were selected polyolefins [1,2]. Knowing that most of the polymer applications are strongly dependent on the initial state of the products, i.e., their morphology, thermal properties, and crystallinity, it is possible to obtain a great variety of morphologies and supermolecular formations by varying different conditions in the preparation process, e.g. cooling conditions during the crystallization process from the melt.

One of the aims of this work was to compare the results obtained for two different methods of sample preparation, quenching, and slow cooling. Initial preparation was performed for selected POs by rapid quenching in ice water and slow air cooling after compression molding. Further, the prepared samples were characterized by SEM, WAXD, FTIR, and mechanical measurements.

The obtained results indicated that PP is much more sensitive to the method of sample preparation than PE, as well as that the initial preparation of samples plays a decisive role in the final properties of materials for polymeric medical devices.

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MS PP 09

Linear and non-linear methods for non-isothermal kinetic curves fitting of dehydration of PAAG hydrogel in equilibrium and non-equilibrium swollen state

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Hydrogels are three-dimensional cross-linked polymeric structures that are able to absorb significant amounts of water, water solutions and biological liquids. The wide applicability of hydrogels is based on their ability to reversibly absorb (swelling) and release (dehydration) water. In present study our aim was to describe the kinetics of non-isothermal dehydration of poly(acrylic acid)-g-gelatin (PAAG) hydrogel, that was swollen in distilled water to different swelling degrees. For this purpose, Weibull distribution function of reaction time was used. PAAG hydrogels were synthesized via crosslinking by free-radical graft polymerization of acrylic acid and gelatin in aqueous media. The non-isothermal thermogravimetric curves were recorded at different heating rates. The comparative analyses of linear and non-linear methods of non-isothermal kinetic curves fitting of PAAG hydrogel dehydration were performed. The influence of linear and non-linear fitting methods on the value of the parameters determined by the Weibull distribution of reaction times, and the quality of fitting, was investigated using different error functions. For all the examined swelling degrees and heating rates, the quality of non-linear fitting was higher than that of linear method fitting. Changes in the values of the Weibull parameters with the degree of swelling of the hydrogel and the rate of heating during dehydration, indicate a change in the state of absorbed water. Based on the obtained results, we have shown that both examined ways of non-isothermal conversion curves fitting allow accurate description of experimental conversion curves of PAAG hydrogel dehydration .

MS PP 10

Highly efficient TiO_2/PPy photocatalysts

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Titanium dioxide is the most suitable semiconductor for photocatalytic application due to its high efficiency, increased stability, low-cost, and non-toxicity. However, it is possible to enhance the photocatalytic activity of TiO_2 by homogenizing it with conductive polymers. One of the most attractive conductive polymers is polypyrrole (PPy) owing to its stability, low-cost, and special redox properties. The aim of this work was to obtain the TiO_2/PPy nanocomposites with a higher photocatalytic activity compared to TiO_2. In order to determine the optimal content of PPy, four TiO_2/x%PPy samples (x = 0, 1, 3, and 5 wt.%) were synthesized and characterized by XRD and TG/DSC analyses. The photocatalytic activity was examined towards the degradation of toxic textile azo dye Reactive Orange 16. It was observed that an increase in PPy content led to better adsorption capacity of the synthesized nanocomposites. Samples TiO_2/1%PPy and TiO_2/5%PPy demonstrated better photocatalytic activity than TiO_2, while TiO_2/3%PPy showed very similar photocatalytic activity to TiO_2. Near complete degradation of the dye (98 %) was reached in 75 min by using TiO_2/1%PPy, comparing to pure TiO_2, which degraded the same amount of the dye in 120 min. Considering all the obtained results, the optimal content of PPy in the composite for degradation of Reactive Orange 16 is 1 wt.%.

MS PP 11

Characterization of pyrophyllite as a potential material for obtaining ceramic membranes

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Pyrophyllite is one of the most common natural clay materials and shows great physicochemical characteristics. Its low electrical and thermal conductivity, low coefficient of expansion, good mechanical strength, as well as excellent stability during heating, make it very suitable for use in different areas. Pyrophyllite is used in many industries, such as the paper and plastic industry, bricks, ceramics, cosmetics, plants, and rubber industry, but also for wastewater treatment. It is a potential material for obtaining ceramic membranes for water filtration [1, 2]. In our study, pyrophyllite was ultrasonically treated in order to remove other impurities, after which pastilles were made under the pressure of 50 MPa, and thermally modified at the temperature of 1050 °C in a time interval of 2-6 h. After the modification, the changes were monitored by different methods: X-ray structural analysis (XRD), infrared spectroscopy with Fourier transform (FTIR), scanning electron microscopy (SEM), Raman spectroscopy, as well as thermal analysis methods, thermogravimetric analysis (TGA) and differential thermal analysis (DSC). It was shown that amorphization and dehydroxylation, as well as homogeneous arrangement of pores, occurred after the thermal treatment. Except for the release of excess water, the thermal treatment led to the removal of certain impurities present in the sample.

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MS PP 12

The removal efficiency of polyethylene isolated from cosmetic products from surface water with a Fe-based coagulant

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A large number of cosmetic products such as toothpastes, soaps, shampoos, conditioners, deodorants, sunscreens and face creams potentially contain microplastic particles. By studying the available cosmetic products that contain microplastics, it was concluded that 70% of cosmetic products contain polyethylene. When using cosmetic products, small plastic particles are washed away and end up in municipal wastewater, so a large number of microplastic particles are discharged into the water treatment plant [1,2]. Water treatment plants represent a barrier that prevents polluting substances, such as microplastics, from reaching the recipients, but at the same time they have been identified as a potential source of environmental pollution. Coagulation and flocculation are one of the most common methods used in water treatment, so the aim of this work was to determine the efficiency of microplastics removal from surface water by coagulation and flocculation. The concentration of microplastics in this work was 100 mg/L. Iron-based coagulant ($FeCl_3$) was used to remove polyethylene isolated from cosmetic products from surface water (Danube river), with concentrations of 20-220 mg Fe/L. The characterization of the samples after treatment of coagulation and flocculation was performed, and the values for pH, electrical conductivity, turbidity and TOC were determined. Based on the obtained results, it can be concluded that $FeCl_3$ proved to be effective in removing polyethylene isolated from cosmetic products from surface water, as indicated by values of 41-94%. Future research should be directed towards improving the process of coagulation and flocculation to remove microplastics from the water as well as possible, but also to possibly change the environmental conditions in which the experiment was conducted.

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MS PP 13

Synthesis of $Cu(OH)_2$ nanobelts with control over particle size and morphology

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The preparation of metal–organic frameworks (MOFs) as thin films with controlled thickness and preferential orientation is a key challenge that could enable their application to device fabrication in different fields such as optoelectronics and sensing. Recently, the use of pre-formed ceramic nanostructures as sacrificial templates for the growth of MOF crystals has been introduced as a promising strategy to control the orientation and morphology of MOF particles and films [1]. For instance, highly aligned $Cu(OH)_2$ nanobelts (NBs) films can be converted to different Cu-MOFs by exposure of the substrate to a solution containing the appropriate organic linker [1]. It has been shown that the size and orientation of the ceramic particles determine that of the resulting MOF crystals [2]. Thus, designing synthetic strategies to control the morphology and size of the precursor $Cu(OH)_2$ nanobelts is of high importance for the progress of MOF-based devices. In this work, $Cu(OH)_2$ NBs were synthesized following a procedure based on the literature [1], where different parameters were varied, such as addition time of the reagents, temperature treatment, and the use of different nitrogen bases. The influence of these parameters on the chemical composition, crystallinity, and morphology of the particles was studied by FT-IR spectroscopy, X-Ray Diffraction and Atomic Force Microscopy (AFM). Interestingly, it was found that the use of DABCO as a nitrogen base partially substituting NH_4OH can induce a change in the aspect ratio of the nanostructures (DABCO-NB). To study the influence of the different synthetic conditions on the resulting NB film quality, aligned NBs were deposited on a silicon substrate using a dip coater, according to the reported semi-automatic protocol [2]. We observed that the DABCO-NB coatings under high humidity (50% RH) show a better coverage and homogeneity than the standard samples. Thus, the use of a different nitrogen base seems to improve the adhesion of this film to a silicon substrate in high humidity conditions. These results could be beneficial for the fabrication of highly oriented MOF films.

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Acknowledgment

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Medicinal chemistry

MC PP 01

Copper(II) complexes with 4-(diethylamino)salicylaldehyde and *α*-diimines: Cytotoxic activity

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The cytotoxic activity of two copper(II) complexes with 4-(diethylamino)salicylaldehyde and α-diimines (2,2'-bipyridine and 1,10-phenanthroline) is presented in this work. Complex **1** is a mononuclear Cu^{2+} complex containing 2,2'-bipyridine, while complex **2** is binuclear and contains 1,10-phenanthroline as a co-ligand. The cytotoxicity of these complexes and their precursor compounds has been tested against five human malignant cell lines: HeLa, A375, A549, PC-3, and MCF7, as well as against normal human keratinocyte cell line HaCaT. Both tested Cu(II) complexes demonstrated remarkably stronger cytotoxic activity against all malignant cell lines in comparison to the cytotoxic activity of their precursor compounds, with the intensities of cytotoxic activity of complex **2** being higher comparing to those of complex **1**. Furthermore, complex **2** showed better cytotoxic activity than cisplatin, which was used as a positive control. Cytotoxic effects of tested complexes were not associated with production of oxidative stress. All obtained results are encouraging for the design and synthesis of new Cu(II) complexes as potential chemotherapeutic drugs.

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MC PP 02

Synthesis, antiproliferative activity and *in silico* testing of 17α-(pyridin-2-yl) estrane derivates

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Steroidal compounds with the heterocyclic system show significant biological activity, ex. antitumor, antiparasitic, antibacterial, etc. Because of that, the design and synthesis of potential antitumor agents for the treatment of hormone-dependent diseases is often based on modifications involving heterocyclic rings. With this in mind, we synthesized 17α-(pyridin-2-yl) derivates of estra-1,3,5(10)-triene starting from estrone and its C3 analogs. Furthermore, *in silico* ADME profiles were determined by comparing physiochemical properties obtained by the SwissADME web tool with five different sets of criteria and using the BOILED-Egg model. This model was used to predict the possibility of gastrointestinal absorption and brain penetration. Also, the antiproliferative activity of the synthesized compounds was tested on a panel of six cancer cell lines(MCF-7, MDA-MB-231, PC3, HeLa, HT-29, A549), and one healthy cell line (MRC-5) using the standard MTT assay.

Acknowledgments

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MC PP 03

Cleistanolate analogue: synthesis and antiproliferative activity

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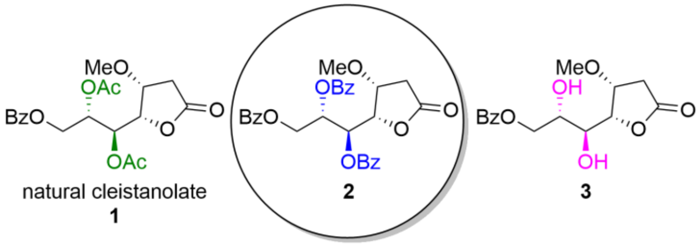
In 2017, natural cleistanolate **1** was isolated from methanol extract of *Cleistichlamys kirkii* (Annonacae).[1] This year, our research group published the first synthesis of natural cleistanolate, revision of its stereochemistry and preliminary cytotoxicity.[2]

Herein, we will present the synthesis of tri-*O*-benzoyl cleistanolate analogue **2** starting from D-xylose. Antiproliferative activity of compound **2** is evaluated. Its cytotoxicity will be compared with natural cleistanolate **1** and mono-*O*-benzoyl cleistanolate analogue **3** (Scheme 1).



Scheme 1. Chemical structures of natural cleistanolate and its analogues.

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MC PP 04

Ferrocenyl analog of valproic acid: a new inhibitor of glutamate decarboxylase

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Valproic acid (2-propylpentanoic acid) is one of the most widely used antiepileptic drugs in the world which, among other things, elevates the level of γ-aminobutyric acid in the brain [1]. Previous studies have shown that if a part of the structure in the starting biologically active molecule is replaced with a ferrocene unit, it could be obtained as a new molecule with improved activity and/or pharmacokinetic properties. Therefore, this research aimed to obtain 2-(ferrocenylmethyl)pentanoic acid by malonic ester synthesis and to spectrally characterize synthetic intermediates and the final product (NMR, MS, UV-Vis, and/or IR). Moreover, the action of 2-(ferrocenylmethyl)pentanoic acid on the glutamate decarboxylase, one of the key enzymes in the biosynthesis of γ-aminobutyric acid, was also studied, and it was found to display the opposite (inhibitory) effect in comparison to valproic acid [2].

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MC PP 05

5-*O*-Benzyl derivatives of C-6 epimers goniofufurone and 7-*epi*-goniofufurone: synthesis and cytotoxic activity

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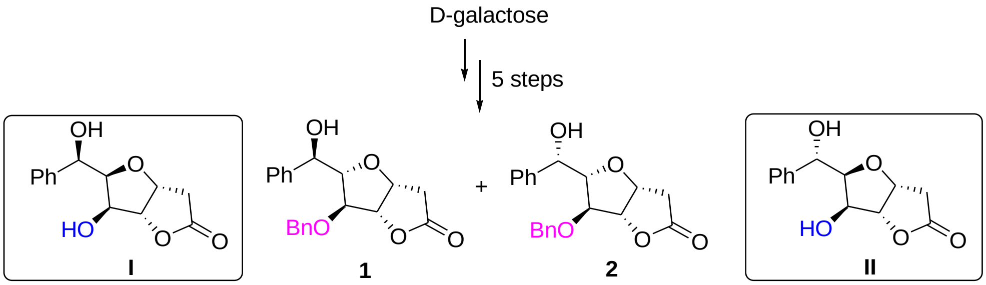
(+)-Goniofufurone (**I**) and 7-*epi*-goniofufurone (**II**) are naturally occurring styryl lactones that showed significant in vitro cytotoxicity against several human tumors (*Scheme 1*).[1] 5-*O*-Benzyl derivative of (+)-goniofufurone also showed very promising biological activities.[2] Herein, we report on a synthesis of epimers **1** and **2** (*Scheme 1*) of these natural products starting from D-galactose. The *in vitro* antiproliferative activities of synthesized molecules will be briefly discussed. This could provide information about the influence of stereochemistry at the C-6 position on the cytotoxic activities of these types of styryl lactones.



*Scheme 1. Naturally occuring lactones **I** and **II** and the corresponding analogues **1** and **2**.*

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MC PP 06

Synthesis and cytotoxicity of Cu(II) complexes with salicylaldehyde derivatives and α-diimines

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In this work we are presenting the synthesis and cytotoxic activity of two new Cu(II) complexes. The complexes were obtained in the reaction of $Cu(BF_4)_2$ $6H_2O$, methyl 3-formyl-4-hidroxybenzoate and an α-diimines (2,2'-bipypiridine or 1,10-phenanthroline) in molar ratio 1 : 1 : 1. The cytotoxic activities of the complexes and its precursor ligands were examined against five human malignant cell lines: cervical adenocarcinoma HeLa, melanoma A375, breast adenocarcinoma MCF7, prostate adenocarcinoma PC-3, and lung carcinoma A549, as well as against normal human keratinocyte cell line HaCaT. The both synthesised complexes showed stronger activity against all tested malignant cell lines than its precursors. The stronger activity was achieved with the complex with 1,10-phenanthroline. Furthermore, that complex exerted even stronger activity than cisplatin, with IC_{50} values ranged from 0.31 µM to 0.44 µM. These results may suggest the promising anticancer effects of Cu (II) with methyl 3-formyl-4-hidroxybenzoate and 1,10-phenanthroline.

Acknowledgments

The authors are grateful to the Ministry of Education, Science and Technological Development of the Republic of Serbia for the financial support (451-03-9/2021-14/200043).

MC PP 07

Synthesis and antitumour activity of a novel conformationally restricted analogue of (+)-muricatacin

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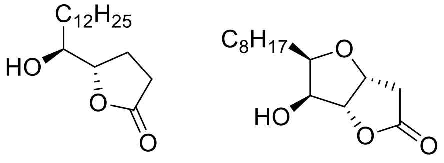
(+)-Muricatacin (**1**) is a natural product that exhibits significant antitumor activity.[1] In this work, the synthesis of a novel conformationally restricted (+)-muricatacin analogue, **6** *(Scheme 1)*, with a furano-furanone ring system was achieved, starting from D-xylose. Analogue **6** was evaluated for its *in vitro* antitumor activity against a panel of tumor cell lines and one healthy cell line (MRC-5).



(+)-muricatacin **1** **6**

*Figure 1. Structures of (+)-muricatacin (**1**) and novel analogue **6**.*

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MC PP 08

A variation in the initial step in the synthesis of halogenated goniofufurone/tiazofurin analogs and *in silico* search for their receptors

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We introduced a minor variation in the synthesis of thiazole goniofufurone analog (**7**), and present a planned two-phase extension that could yield halogenated analogs **1a-d**. We screened potential receptor candidates for the lead compound **1** using pharmacophore mapping via *PharmMapper*.[1] Finally, we docked compounds **1** and **1a-d** via *AutoDock VinaXB* to 25 proposed receptors, and some of the best rotamers will be presented and compared (Fig. 1).[2]

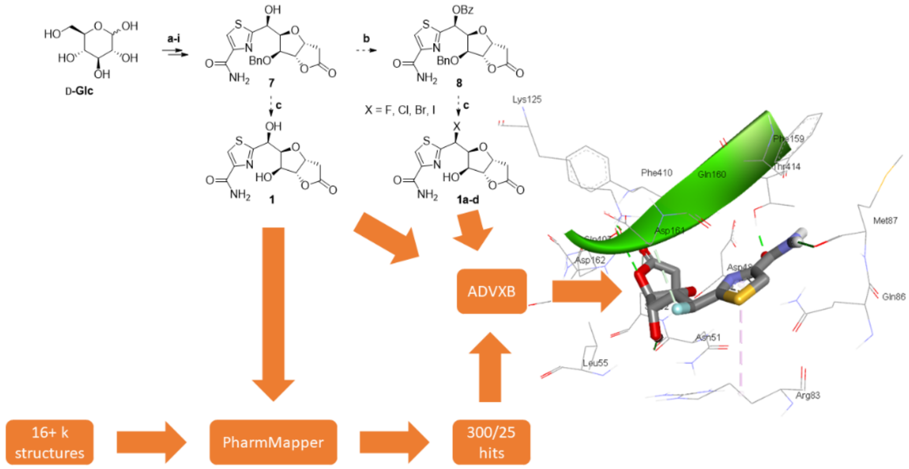

Figure 1. Complete workflow.

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Organic chemistry

OC PP 01

The electrochemical characterization of newly prepared ferrocene-containing tetrahydropyrimidin-2(1*H*)-ones

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Herein, we report the preparation and electrochemical evaluation of novel ferrocene containing tetrahydropyrimidin-2(1*H*)-ones.[1, 2] Starting with the matching 3-arylamino-1-ferrocenylpropan-1-ols, sodium cyanate (NaOCN), and glacial acetic acid, the synthesis was accomplished. The reaction's potential application to seventeen 1,3-amino alcohols bearing ferrocene core has been investigated, and the desired 1-aryl-4-ferrocenyltetrahydropyrimidin-2(1*H*)-ones were produced in good to excellent yields (up to 93%). All items have been well purified (>95% purity). The electrochemical evaluation has been done utilizing cyclic voltammetry. Obtained results showed that all prepared molecules exhibit one well-defined oxidation wave on the forward-potential sweep (0.662 – 0.696 V) and one reduction wave during the back-potential sweep (0.485 – 0.552 V). We attributed them to the oxidation of the ferrocene core during the forward-potential sweep, and the reduction of the obtained ferricenium ion at the back-potential sweep. Additionally, CV measurements offer an extra level of purity assurance for the samples under investigation.

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OC PP 02

Optimization of the reaction conditions for synthesis of 3-etoxycarbonylmethyloxyimino androstane derivate

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Oximes represent a group of organic molecules that is very interesting from the point of view of synthetic chemistry. The characteristic functional group of these molecules contains two nucleophilic atoms (nitrogen and oxygen), which allows them to build *N*- and *O*-substituted derivatives. Compounds in which the oxygen atom of the oxime group is attached to a hydrocarbon residue are called oxime ethers.[1] Oxime ethers are used in organic synthesis to obtain various compounds such as amino alcohols, hydroxylamines and amines, and under certain conditions heterocyclic compounds. In addition to synthetic applications, this group of molecules has shown a wide range of biological activities. Therefore, the development of efficient methods for the synthesis of these compounds is significant in synthetic chemistry.[1,2]

For these reasons, by optimizing the reaction conditions, we have achieved an efficient synthesis of a new 3-carboxymethyloxiimino derivative in the 17α-(pyridine-2-ylmethyl)androstane series, which will be used as a precursor for further chemical transformations and obtaining biologically active molecules.

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OC PP 03

Nitric oxide scavenging effect of immortelle essential oils and two synthetic italidiones

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Herein, the in vitro NO-scavenging ability of two *Helichrysum italicum* (Roth) G. Don (Asteraceae; immortelle) essential oils and two synthetic italidiones, 4,6-dimethyloctane-3,5-dione and 4,6,9-trimethyldec-8-ene-3,5-dione (β-diketones found only in immortelle), was evaluated. The essential oil at non-cytotoxic concentrations (≤ 10 μg/mL) is known to significantly suppress NO production in rat peritoneal macrophages. A chromatographic fraction of the oil containing italidiones displayed similar activity (ca. 65%) at all tested concentrations [1]. Some β-diketones could act as potent NO scavengers, hinting at the possible reason for the observed decrease in NO production. In this work, the cell-free assay where NO was generated from sodium nitroprusside and quantified by the Griess reaction was used. At higher concentrations, the effect of both β-diketones and the oils was negligible, while at 1 μg/mL they reduced the amount of released NO by ca. 10%. The antioxidant capability of β-diketones is associated with the corresponding keto-enol tautomer, and the poor NO-scavenging effect of the herein studied β-diketones could be explained by the low equilibrium relative amount of the keto-enol form under physiological conditions. Quercetin, used as the positive control, manifested a similar effect at lower concentration (5%), while at 10 μg/mL displayed considerable NO-scavenging ability (46%).

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OC PP 04

Detection of biomarkes of adulterated *Allium ursinum* with *Convallaria majalis* and *Arum maculatum*

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A. ursinum and poisonous adulterants *C. majalis* and *A. maculatum* were used as a model for detection of adulterants in edible plant. *A. Ursinum* samples were spiked with *C. Majalis* and *A. Maculatum* to mimic adulteration. Metabolomic fingerprinting of all samples was performed using ^{1}H NMR spectroscopy (1D zgpr pulse sequence), and the resulting data sets were subjected to multivariate data analysis. As a result of this analysis, signals of adulterants were extracted from the data, and the structures of biomarkers of adulteration from partially purified samples were elucidated using 2D NMR. Thus, isovitexin and vicenin II, azetidine-2-carboxylic acid, and trigonelline indicated adulteration of *A. Ursinum* samples with *C. majalis*. Isovitexin was also recognized to be an indicator of adulteration of *A. Ursinum* with *A. maculatum*. In conclusion, the case study of *A. Ursinum* suggested that plant metabolomics approach could be utilized for identification of low molecular weight biomarkers of adulteration in edible plants.

Acknowledgments

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OC PP 05

Novel imidazole-based dyes: synthesis and investigation of various types of chromism

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Substituted dimers of triphenylimidazole have drawn attention during past few years as substances that change their color under the influence of various factors, such as light, temperature and mechanical pressure. Furthermore, such compounds can exhibit solvatochromic and halochromic behavior, which additionally widens the area of their possible application [1, 2]. In this research two novel pigments were synthesized, dimethyl and dinitro derivatives of 2,2',4,4',5,5'-hexaphenyl-2H,2'H-2,2'-biimidazoles. Synthesis of each pigment was done through two steps: condensation of benzil and substituted benzaldehydes in the presence of ammonium ions yealding substituted triphenylimidazoles and their oxidative dimerization. It was shown that both sythesized compounds show solvatochromic, halochromic, thermochromic and piezochromic characteristics. Pigment with nitro substituent showed solvatochromism of higher intensity, which is a consequence of more intensive interactions of nitro group with basic chromophore in comparison with the methyl group. With an increase of pH value of the solution, heating or applying mechanical pressure, the pigment with methyl substituent changes color from pale yellow to purple, while the pigment with nitro substituent changes color from yellow to red. As pigments that show different types of chromism, newly synthesized compounds have potential wide application in making photographs, as a photosensitive component of solar cells, for initiating polymerisation reactions and many others, which is why they are of great interest for further investigation.

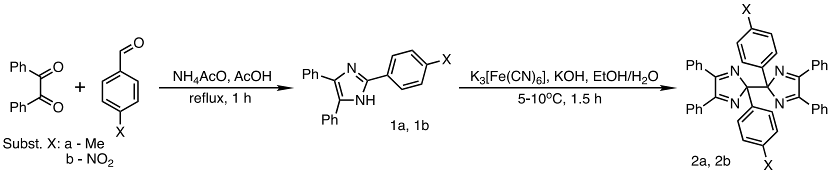

Figure 1. Synthesis of substituted 2,2',4,4',5,5'-hexaphenyl-2H,2'H-2,2'-biimidazoles

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Acknowledgments

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OC PP 06

Complete spectral characterization of shiobunone and isoshiobunone isolated from *Acorus calamus* L.

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In this study acorenone- and asarone-type *Acorus calamus* L. (Acoraceae) rhizome essential oils were analyzed by GC-MS. Most of the samples were obtained by hydrodistillation, while few were purchased from local stores. Those that have been determined to be the acorenone-type oils were further individually subjected to dry-flash chromatography. The following pure sesquiterpenoids were isolated by subsequent silica-gel column chromatography: preisocalamendiol, isocalamendiol, shiobunone, isoshiobunone, and acorenone. Structures of shiobunone and isoshiobunone were elucidated by spectral means (MS, 1D- and 2D-NMR). Also, a complete assignment of ^{1}H- and ^{13}C-NMR spectra of these compounds was performed, as well as a total spin simulation of ^{1}H-NMR spectra, which allowed their relative configuration to be confirmed, as well as their most stable conformation determined. The biosynthesis of these compounds was also proposed and discussed.

Acknowledgements

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OC PP 07

Serum biomarkers of schizophrenia

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Schizophrenia is a widespread mental disorder that leads to significant functional impairments and premature death. The state of the art indicates gaps in the understanding and diagnosis of this disease, but also the need for personalized and precise approaches to patients through customized medical treatment and reliable monitoring of treatment response. In order to fulfill existing gaps, the establishment of a universal set of disorder biomarkers is a necessary step.

The investigation of serum samples of Serbian patients with schizophrenia (51) and healthy controls (39), based on NMR analyses based on detection and of low molecular weight components in samples can be difficult due to overlapping signal caused by line broadening characteristics of macromolecules. A way of overcoming this problem could be the exploitation of the difference in relaxation between small molecules and macromolecular species, such as the application of a T2 filter by using the Carr–Purcell–Meiboom–Gill (CPMG) spin-echo pulse sequence, which led to the identification of 26 metabolites/biomarkers for this disorder.

The established biomarker set includes aspartate/aspartic acid, lysine, 2-hydroxybutyric acid, and acylglycerols, which are identified for the first time in schizophrenia serum samples by NMR experiments. The other 22 identified metabolites in the Serbian samples are in accordance with the previously established NMR-based serum biomarker sets of Brazilian and/or Chinese patient samples. Thirteen metabolites (lactate/lactic acid, threonine, leucine, isoleucine, valine, glutamine, asparagine, alanine, gamma-aminobutyric acid, choline, glucose, glycine and tyrosine) that are common for three different ethnic and geographic origins (Serbia, Brazil and China) could be a good start point for the setup of a universal NMR serum biomarker set for schizophrenia.

Acknowledgments
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OC PP 08

Synthesis of *para*-nitro fentanyl

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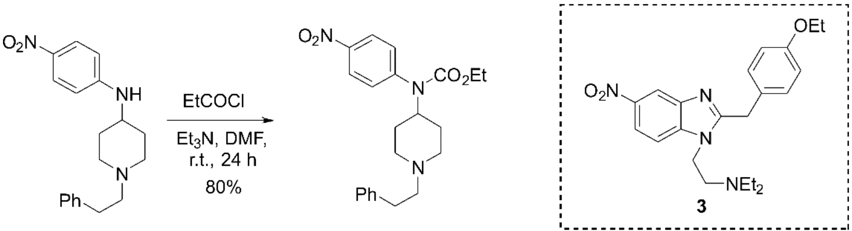
4-Anilidopiperidines represent an important class of opioid analgesics. Several highly potent compounds in clinical use are fentanyl, sufentanil, alfentanil, lofentanil, and remifentanil. Since the discovery of fentanyl, many modifications were made in order to obtain the best structure-activity relationship. Among other fentanyl derivatives, *para*-nitro fentanyl **2** was recognized as a worthwhile target compound due to its similarity with potent analgesic etonitazene **3**. So far, attempts to synthesize **2** by means of acylation of secondary amino group in **1**, eluded organic chemists because of the extremely low nucleophilicity of *para*-nitro aniline nitrogen atom.[1] Previously we described successful synthesis of tertiary carboxamides by propyonilation of low nucleophilic secondary amino groups.[1,2] Here, propionyl chloride (EtCOCl) or bromide (EtCOBr) were used in polar, aprotic solvent *N*,*N*-dimethylformamide (DMF) with or without addition of *N*,*N*-dimethylpyridine-4-amine (DMAP) as a catalyst. The developed protocol was successfully applied for the synthesis of **2** (Scheme 1). *Para*-nitro fentanyl was synthesized for the first time and in high yield.

As a part of our future endeavor, **2** will be pharmacologically evaluated for the analgesic activity.



1 **2**

*Scheme 1. Key reaction step for the synthesis of para-nitro fentanyl **2** and structure of etonitazene **3***

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OC PP 09

Antioxidant potential, total phenolic and anthocyanin contents of new raspberry cultivars

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Raspberry fruits (*Rubus idaeus L.*) are essential for health because they contain a large range of minerals, vitamins and phytochemicals. The most important phytochemicals are phenolic compounds as a class of secondary metabolites. The yield of bioactive compounds from plant sources depends on solvent properties, nature of the plant material and extraction temperature and time.[116] In the green chemistry approaches, natural deep eutectic solvents (NADES) were typically used as a substitute for organic solvents in order to preserve the environment. The NADES was selected based on literature data and prepared in 1:2 ratio of choline chloride and urea with 15 % water added. These compounds act like antioxidants which stop or slow damage to cellular DNA, lipids and proteins caused by reactive oxygen species (ROS).[0] Total phenolics, anthocyanins and antioxidant capacity were determined for five lyophilized raspberry cultivars: Amira, Cascade Harvest, Glen Fine, Glen Ample, and Tulamin. Total phenolic content was evaluated by standard Folin-Ciocalteau method and ranged from 3.38 to 4.75 mg of gallic acid equivalents/1 g of fresh weigh. For antioxidant activity of the NADES extracts 2,2-diphenyl-1-picrylhydrazyl hydrate (DPPH) assay was applied. The lowest IC50 value was obtained for the Amira variety, followed by Glen Fine, Cascade Harvest, Glen Ample and the highest for the Tulamin variety (2.17, 2.27, 2.46, 3.01 and 3.38 mg/mL, respectively). Total anthocyanin content was measured with pH differential method and calculated using molar extinction coefficient for cyanidin-3-glucoside. The highest anthocyanin content shows Glen Ample variety followed by Amira, Cascade Harvest, Glen Fine and the lowest for Tulamin (4.19, 2.78, 2.02, 1.94 and 1.41 mg/ml, respectively). A growing number of scientific papers suggest that berries rich in anthocyanins exhibit a wide range of protective effects with potential benefits for human health.

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OC PP 10

Supramolecular architectures of selected xanthenedione derivatives

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The wide range of pharmacological activities (e.g. antiviral, antifungal, antibacterical, antiinflamatory, leishmanicidal and antidepresant) has already been attributed to the xanthenediones, a group of synthetic heterocyclic compounds possessing a pyran nucleus fused on either side with cyclohex-2-enone rings [1]. In this work, two 3,3,6,6-tetramethyl-9-substituted-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-diones (Figure 1) were synthesized and their crystal stuctures were determined by single crystal X-ray diffraction. The main structural feature in compound **1** is a supramolecular chain along the *a*-axis formed by O4–H4···O2 hydrogen bond and C13–H13···O4 and Br1···Br2 interactions between the adjacent asymmetric units, while the formation of supramolecular network is further achieved by C–H···π interactions between the adjacent chains. The main motif in **2** is a dimer formed *via* O4–H4···O2 hydrogen bond and Cl1···π interactions. The neighbouring dimers are connected through strong C7–H7A···π interactions, thus resulting in formation of a zigzag chain parallel to the *c*-axis. Weak C–H···π interactions link the adjacent chains into a supramolecular layer. This work may provide a basis for design of new biologically active xanthenediones both at the molecular and supramolecular level.

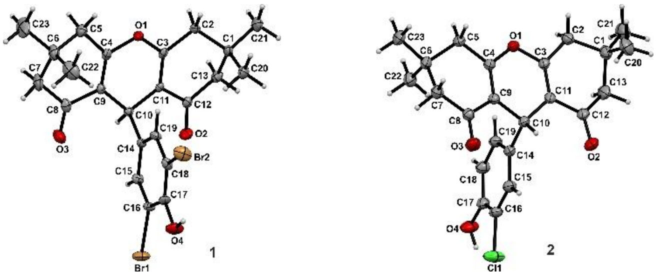

*Figure 1. The asymmetric unit of **1** and **2** showing 30% displacement ellipsoids (the H atoms are presented as small spheres of arbitrary radii).*

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OC PP 11

Application of the reacton *p*-cymene with hydrogen peroxide in trfluoroacetic acid for the identification of secondary metabolites of *Doronicum columnae* Ten.

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Essential oils of many plant species contain phenolic compounds, among which the best-known ones are the regioisomeric monoterpenes thymol and carvacrol, present in a large number of taxa of the families Asteraceae and Lamiaceae. The essential oil of *Doronicum columnae* (Asteraceae), in addition to these two compounds, contains other regioisomers of isopropylmethylphenols and various derivatives, ethers and esters. The goal of this work was the identification of these compounds in the mentioned essential oil, as well as the synthesis of some of the possible regioisomeric phenols, their ethers and esters. Due to the complexity of the essential oil of *D. columnae,* the oil was initially directly chemically transformed and the products were further analyzed. For the synthesis of regioisomeric phenols, and their derivatives, a reaction of *p*-cymene with trifluoroperacetic acid, obtained *in situ* from trifluoroacetic acid and hydrogen peroxide, was used, as it yielded a mixture of isomers of isopropylmethylphenols present in the essential oil. All of the products, and constituents of the essential oil, as well as the obtained derivatives, were analyzed by GC-MS and NMR spectroscopy.

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OC PP 12

Mechanistic investigation of cobalt-catalyzed deallylation

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The significant expansion of the literature on cobalt catalysis in the past decade stems from modern tendencies within the chemistry community toward developing simple and efficient synthetic methods that are also environmentally benign and sustainable. Our group is interested in cobalt-based catalytic methodologies that utilize inexpensive and stable cobalt sources. Recently, we developed an efficient deallylation protocol using $CoBr_2$ as a catalyst (Figure 1). Based on the experimental results the reaction mechanism was proposed. The mechanism investigation included control experiments and identification of side products and intermediates.

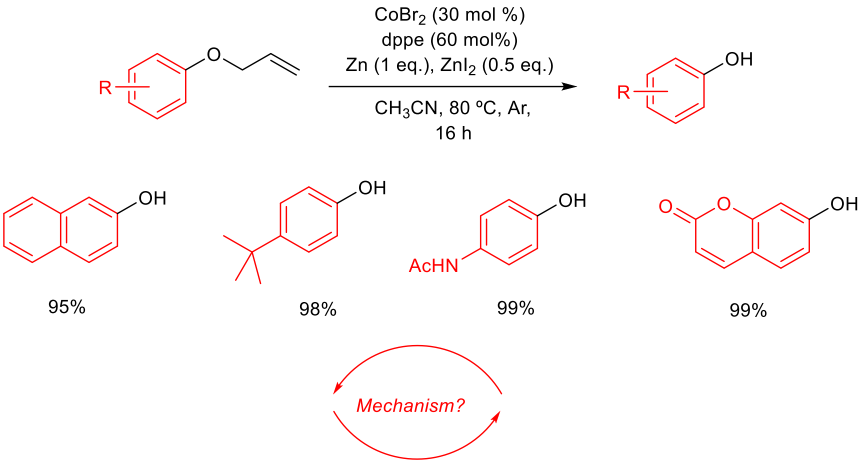

Figure 1. Cobalt-catalyzed deallylation

Acknowledgments

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OC PP 13

Amide derivatives of 4-aminoquinoline as reversible inhibitors of acetylcholine- and butyrylcholine-esterase

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Cholinesterases are extracellular enzymes found primarily in the central nervous system and at peripheral neuromuscular junctions. Two enzymes in the cholinergic nervous system are acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). AChE and BChE inhibitors are neurotoxic compounds capable of inducing central and/or peripheral cholinergic crises. A number of these compounds have also found use as drugs to alleviate AD symptoms. They are based on the premise that increasing the availability of acetylcholine for receptors in the brain leads to better signal transport between neurons, which will improve cognitive function. The results of our study indicate that the introduction of the adamantyl group has a favorable effect on inhibitory activity. It was hypothesized that the introduction of a polar group into the side chain of the compound could increase the activity of the new derivatives, for two reasons. The first is an increase in the polarity of the molecule, which leads to an increase in bioavailability. The second is the realization of additional interactions in the active site of the enzyme. It was hypothesized that an amide group, as part of the side chain, would be a good starting choice for a polar group. Then, the preliminary modeling of a selected set of derivatives containing an amide group in a sequence, which differ from each other in the length of the sequence, the orientation of the amide group in relation to the quinoline core, and the substituent on the terminal amino group of the side chain, was performed. By heating 4,7-dichloroquinoline in 1,4-diaminobutane, at 130 °C, in an argon atmosphere, corresponding 4-aminoquinolines were obtained. HOBt and EDC were used as reagents to obtain the activated *N*-Boc-glycine derivative and the deprotection of the *N*-Boc protected amino group was carried out by a standard procedure, using trifluoroacetic acid in methylene chloride, at room temperature. Further modifications of the terminal amino group by reductive amination yielded two series of derivatives that have *N*-benzyl or *N*-adamantyl moieties.

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Physical chemistry

PC PP 01

Holographic method as a powerful tool for investigating chemical reactions: experimental setup

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Holography, i.e. holographic interferometry, is a method that records the deformation, i.e. the dynamics of the process between two or more moments of exposure. [1] The presented work defined the holographic method with an appropriate experimental setup. The experimental setup consists of optical components specially designed for measuring chemical reactions. This setup is specific because it has the possibility of so-called triple recording [2]. The possibility of observing the process without disturbing it is of great importance for the investigation of very sensitive chemical reactions, such as oscillatory reactions. This kind of experimental setup opens up possibilities for exploring the profiles of various chemical reactions on the nanoscale; especially iodate-based oscillatory reactions for which the exact mechanism is still unknown.

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PC PP 02

Ab initio study of electronic spectra of complex ion iron(II)phenanthroline, $[Fe(phen)_3]^{2+}$

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The vertical electronic spectrum and excitation energies of the singlet, triplet and quintet states $[Fe(phen)_3]^{2+}$ (Fig. 1) are computed by the means of the single reference time-dependent DFT method and the multireference state-average complete active space self-consistent field (CASSCF) with N-electron Valence State Perturbation Theory (NEVPT2) methods. In all calculations, the ZORA relativistic approximation and RI approximation were used, together with the appropriate basis set of triple-zeta quality. The geometry optimizations and vibrational frequencies calculations of $[Fe(phen)_3]^{2+}$ complex ion were done with B3LYP functional. The computations were carried out using the ORCA program package. Analysis of the spectrum showed that there are three types of excitations: (i) ligand-field or metal-centered (MC) transitions involving electron transitions within Fe-3d orbitals; (ii) metal-to-ligand charge transfer transitions (MLCT) in which an electron is transferred from Fe to an orbital on the ligand and (iii) excitations entirely localized on the ligands, the ligand centered (LC) transitions. Several different active spaces were used in order to describe these types of excitations. The spectrum is in good agreement with the experimental data.[1,2]

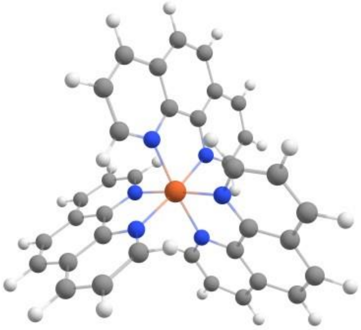

Figure 1. Ball and stick representation of complex ion studied in this paper

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PC PP 03

Solvothermaly synthesized copper doped bismuth vanadate

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Photoeletrochemical (PEC) water splitting is a promising method for clean energy production and different oxide materials have been explored to find the right solution. Among them, as one of the most promising photoanode materials, bismuth vanadate ($BiVO_4$) has attracted a lot of attention due to the suitable band gap edge alignment, low-cost synthesis method and great visible light harvesting features. Nowdays, research related to the $BiVO_4$ is mostly oriented towards repairing poor charge transfer properties which exist due to the high rate of electron–hole recombination. Metal doping is one of the strategies to improve these intrinsic drawbacks. Herein, we report physicochemical properties of solvothermaly sinthesized pristine $BiVO_4$, 1%-, 2.5%- and 5%- Cu-doped $BiVO_4$ powders at 180 ºC for 8 h. X-ray diffraction (XRD) study indicates that, depending on the degree of doping, material exists in monoclinic or tetragonal scheelite phase. Pure monoclinic phase was formed in a case of pristine, 1%- and 2.5%- Cu doped samples. After doping with 5 %, phase transition occurred and material showed tetragonal phase. Scanning electron microscopy (SEM) reveals that samples with monoclinic phase consists of worm-like and prismatic structures while tetragonal samples exhibited spherical shape. Furthermore, structure was examined with Raman and FTIR spectroscopy. The results were in accordance with diffraction study where band positions were well matched with phase composition. Optical properties were characterized with UV–Vis diffuse reflectance spectroscopy (DRS) and photoluminescence (PL) spectroscopy. Monoclinic samples showed band gap around 2.4 eV, while sample with tetragonal phase has band gap around 2.8 eV. PL showed that that monoclinic samples possess better recombination features than tetragonal ones. Photoelectrochemical measurements suggest that material is sensitive towards visible light and, after doping, improved its performance towards oxygen evolution reaction.

PC PP 04

Electrochemical properties of dihydrocaffeic acid coated cobalt-ferrite nanoparticles doped with zinc and gallium

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In this paper, electrochemical properties of dihydrocaffeic acid (DHCA) coated cobalt-ferrite (CFO) nanoparticles doped with zinc (CFO_Zn) and gallium (CFO_Ga) were investigated. CFO, CFO_Zn and CFO_Ga nanoparticles were prepared by the solvothermal method at 180 °C for 8 h with oleic acid as a surfactant. In order to obtain hydrophilic particles, ligand exchange with DHCA was performed. Based on X-ray diffraction analysis positions of all diffraction maxima correspond to the cubic spinel structure. TEM images show that the nanoparticles are non-agglomerated, sphere-like shape with an average particle size of 5±1 nm. Substitution of cobalt with zinc and iron with gallium within CFO structure does not change the size and shape of the nanoparticles. The presence of organic phase on the surface of the nanoparticles was examined by FTIR spectroscopy. FTIR results show that DHCA is bonded to the surface of nanoparticles through carboxyl and catechol groups. Electrochemical properties of nanoparticles were investigated by cyclic voltammetry. Cyclic voltammograms indicate good reversibility of the material. Based on cyclic voltammograms values of specific capacity are calculated. The values of specific capacity at a polarization speed of 5 mV s^{-1} are 4.7 F g^{-1}, 5.8 F g^{-1} and 3.8 F g^{-1} for CFO, CFO_Zn and CFO_Ga, respectively.

PC PP 05

Adsorption and antioxidant properties of tungstophosphates /Y zeolite composite materials

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Nowadays, the significantly increased use of pesticides, caused by enlarged food production, makes the development of removal methods, necessary. Nicosulfuron, a sulfonylurea herbicide, becomes one of the major threats to the environment among the herbicide family. Due to its occurrence, it is important to test its removal by adsorption on environmentally compatible materials, such as zeolites [1]. Zeolite adsorption capacity can be improved by functionalization with heteropoly compounds, as was recently demonstrated [2]. For that purpose, composites of Y zeolite and tungstophosphates (PW) were synthesized using a two-step impregnation method. Prepared zinc, silver, cesium and potassium tungstophosphate salts (ZnPW, AgPW, CsPW and KPW) and their zeolite composites (YZnPW, YAgPW, YCsPW and YKPW) were tested as antioxidants, antimicrobial agents and adsorbents for nicosulfuron pesticide.

HPLC method was employed for pesticide detection and quantification. High adsorption capacities of salts and their composites were established, which could be arranged in the order of participating cation in heteropoly salt: $Zn^{2+}>Ag^{+}>Cs^{+}>K^{+}$. The highest adsorption capacity was obtained for YZnPW (61,7 mg/g). TGA method was used for the investigation of the potential adsorbent regeneration by thermal degradation of nicosulfuron. The antioxidant capacity of the composites was tested using the DPPH method. CsPW and KPW salts are the most efficient antioxidants based on their high inhibition activity (60 % and 40 %). These salts retained high antioxidant activity even with the presence of pesticide. Prepared materials exhibited antimicrobial activity mostly on fungus *C. albicans* and gram-positive bacteria (*S. aureus*, *E. faecalis* and *B. subtilis*). AgPW salt was active for a wide microbe range, and preserved, to a high extent, its antimicrobial activity when incorporated into the composite.

Tested materials are efficient adsorbents of the pesticide nicosulfuron, as well as antioxidants and antimicrobial agents, which makes them prospective candidates for potential environmental applications.

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PC PP 06

Characterization and application of sunflower husk for removing heavy metals from aqueous solution and wastewater

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The industrial wastewater produced from various industries contains a significant amount of pollutants among which are heavy metals and represents one of the leading environmental problems facing public health. Conventional wastewater treatment technologies unsuccessfully remove heavy metals completely. As an alternative to various conventional treatment technologies such as ion exchange, chemical precipitation, and electrochemical treatment which have a lot of drawbacks, biosorption is a process characterized by the use of low-cost and abundant agricultural materials with no significant costs and high sorption potentials of biosorbent due to the presence of carboxylic and phenolic groups in lignocellulose matrix. In Serbia, sunflower is the most common oil plant and grows on about 180 000 ha. After industrial processing between 325, 000 and 360, 000 t of sunflower waste ends up in landfills or is used as a source of energy (1). In this work, the sunflower husk was used to remove Ni from aqueous solutions and wastewater sample. The sunflower husk treated with 1% hydrochloric acid was characterized by Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX). In addition, under optimal conditions, the concentration of Ni in wastewater samplewas obtained and compared by two techniques, induced coupled plasma optical emission spectrometry (ICP-OES) as a standard reference method and laser-induced plasma spectroscopy (LIBS) as a non-standard analytical method. The results of these two methods were compared, to investigate the possibility of using laser-induced plasma spectroscopy as a green alternative for the evaluation of biosorption efficiency.

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PC PP 07

Acetone effects on Briggs-Rauscher oscillatory reaction

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In this work, properties of Briggs-Rauscher (BR) oscillatory reaction[1] in a presence of acetone, as a non-polar solvent, were investigated. The BR reaction itself is oxidation of malonic acid ($CH_2(COOH)_2$) using a mixture of hydrogen peroxide (H_2O_2) and potassium iodate (KIO_3), catalyzed by metal ion (usually Mn^{2+}) in an acidic aqueous solution[1]. It is well-known that BR reaction, as a sensitive matrix, can be used for different analyte properties examination: concentration, antioxidant/antiradical and catalytic activity. As noted, BR reaction occurs in a water medium and therefore the application of these assays is limited to water-soluble samples. Here, the BR reaction is carried out in aceton–water mixture (20 vol%) with the aim to investigate how this non-polar solvent affects the course of the reaction. The influence of solvent can reflect complex phenomena involving many different intermolecular interactions, potentially affecting oscillatory dynamics. Obtained results could be used in a kinetics investigation of the BR reaction and the oscillatory reactions in general.

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PC PP 08

Establishment of DFT model of TiO_2 surfaces for potential application in anodic electrooxidation of organic compounds

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Electrochemical oxidation of organic compounds represents a promising approach in the purification of wastewater and the removal of harmful pollutants. Sophisticated design of innovative electrode materials represents one of the key strategies in achieving the efficiency of this technology. Electrode materials based on titanium dioxide are the subject of the long-term interest of researchers,[1] but there is still much room for development and improvement of electrooxidation efficiency. Targeted adjustment of material properties such as doping, making composites with carbon and metal materials, deposition of thin layers, etc. opens up the possibilities for modification of electrode performance, which requires an understanding of the modification of properties at a fundamental level. Density functional theory (DFT) represents remarkable support to the experimental research, enabling the prediction of the electrode material efficiency, as well as the explanation of the obtained results. In particular, theoretical examination of the interaction of the electrode surface with oxygen-based species is the basis for understanding the efficiency of electrooxidation mediated by the OH-radical[2]and for further guidance of research regarding modifications.

Within this work, optimization of the parameters for the establishment of the TiO_2 (rutile) surface model was performed. In the DFT-GGA approximation, the adsorption of hydroxyl radicals and atomic oxygen on bare TiO_2(110) and TiO_2(100) planes, as well as on Sb-doped and N-doped surfaces, was examined. The adsorption energies were determined and the electronic structure of the surfaces was examined. Obtained results represent the basis for the verification of the model, which will be further applied in the evaluation of the reactivity of modified TiO_2-electrodes in the anodic oxidation of organic pollutants.

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PC PP 09

Periodic mesoporous organosilica nanoparticles for biomedical application and imaging

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Periodic mesoporous organosilica (PMO) nanoparticles are promising new materials for biomedical applications due to their properties such as large specific surface area and porosity as well as organic–inorganic hybrid structure.

Synthesis of a PMO with a novel structure and its capability for two-photon excitation and imaging application is described. This material is synthesized in basic aqueous environment, at room temperature, using cetyltrimethlyammonium bromide as a template for the mesopores and 3,4-diaminobenzophenone as bridged organosilane precursor. The organosilane precursor is first synthesized in THF, in reaction with 3-(triethoxysilyl)propyl isocyanate, to form the bridging bis-silane precursor, which was subsequently used for the synthesis of PMO. Characterization of the prepared PMO was performed by FTIR spectroscopy, Braunauer-Emmett-Teller adsorption method (BET), and two-photon excitation microscopy (TPEF). The band in the IR spectrum at 1030 cm^{-1} proved the Si–O–Si vibrations, while the bands in the range 1530–1660 cm^{-1} arise from C–H bending of aromatic compounds, which proves the composition of the synthesized material. The BET analysis showed specific surface area of 77.5 m^2/g. This material showed promising fluorescent properties upon two-photon excitation at 730 nm, which is a very desirable feature for potential imaging and treatment applications upon exposure to near IR laser. Results from TPEF image of PMO (Fig.1) were acquired with very low laser power 8.58 mW.

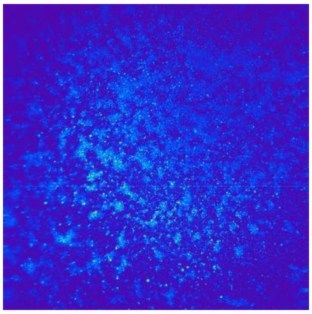

Figure 1. PMO analyzed with TPEF, magnification: ×20, orig.

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PC PP 10

Detection of cherry tomato redox status using EPR imaging

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Electron paramagnetic resonance (EPR) spectroscopy is a noninvasive method of choice in studying the antiradical activity of various biological samples, due to its high sensitivity and selectivity[1]. Despite their great potential, applications of EPR imaging (EPRI) in biology and medicine have been less explored and much slower developed. Due to technical reasons, small samples are more suitable for EPRI. This makes plants the ideal candidates for EPRI experiments.

Cherry tomato contains short-lived free radical species which do not have directly observable EPR signal, and since it is rich in powerful antioxidants, it is very challenging to make this fruit EPR-visible. This problem can be solved by the application of spin probes[2]. These compounds are routinely used in experiments with small animals, but there are no available literature data considering their applications in fruits and vegetables. In this study, we have performed EPRI of the whole cherry tomato fruit using the spin probing EPR technique (and 3-carbamoyl-proxyl as spin probe). The goal of our research was to determine the most efficient spin probe imbibition pathway, and to detect its spatial distribution by the means of EPRI.

The results indicate that spin probing EPRI is a completely noninvasive method for detetermination of the redox status of cherry tomatoes. This procedure could further be applied to other types of fruit and vegetables as well. Since the amount of antioxidants varies depending on the ripening stage of the fruit, the obtained EPR signals could be used in correlating the antioxidant activity of fruit with its ripening stage. The obtained information could be of great significance in increasing the yield of certain cultivars.

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Theoretical chemistry

TC PP 01

An algorithm based on physicochemical fingerprints for measuring chemical similarity of compounds

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The multifaceted nature of molecular similarity makes its quantification difficult and elusive. This is especially true for chemical similarity, a specific kind of molecular similarity. Its manifestation is most pronounced in the case of compounds that exhibit similar physicochemical properties or activities but are structurally rather different. On the other hand, there are structurally similar molecules showing no similar physicochemical properties or activities. Due to all this, the chemical similarity of compounds is rarely examined, causing a lack of new approaches to this issue. In this study, a novel simple algorithm was developed to measure the chemical similarity of molecules with physiological effects. This approach is based on a plain binary fingerprint which was devised by encoding the physicochemical properties of the corresponding compound. Finally, the amount of chemical similarity of molecules is obtained by calculating pairwise and recently introduced extended similarity metrics for cheminformatics data.

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TC PP 02

The chelate complexes as an improved high-energy compounds

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Recent studies in high-energy material design revealed that coordination compounds show excellent detonation performances. Earlier experimental studies found that the nitro-acetylacetonato aluminum (III) complex easily combusts in the air when heated.[1] These findings indicate that the nitro-acetylacetonato metal derivatives may act as potential energetic compounds. The intensive theoretical studies of classical explosives formerly revealed that the impact sensitivity of high-energy molecules could be predicted by analysis of molecular electrostatic potential over the $C–NO_2$ bonds.[2] This concept is applied here.

In order to investigate their energetic properties, we calculated the molecular electrostatic potential and bond dissociation energies for the weakest $C\text{-}NO_2$ bonds for several nitro-tris(acetylacetonato) complexes. The results show good agreement between bond dissociation energies calculated for the weakest $C\text{-}NO_2$ bonds and a slightly positive electrostatic potential above the observed $C\text{-}NO_2$ bonds. The bond dissociation energies for studied complexes are close to the BDE value calculated for the 1,3,5-triamino-2,4,6-trinitrobenzene classified as a significant low-sensitive explosive. We also noticed that the metal ion replacement may be used for fine-tuning of the electrostatic potential above the middle regions of the nitro-chelate rings. However, the presented results show that these compounds have moderate sensitivity, and that the positive electrostatic potential above the central area of the nitro-chelate rings could be used for the assessment of detonation properties of chelate energetic molecules.

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TC PP 03

Influence of the presence of halogen substituents on high-energy properties of nitroaromatic molecules

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Sensitivity towards detonation of high energetic materials (HEMs) and the positive potential in the central regions of their molecular surfaces are directly related. The presence of halogen atoms in HEMs creates the possibility for halogen bonding which can be used for modifying of electrostatic potential values [1]. Also, it has been noticed that the substitution of hydrogen atoms by halogen atoms in molecules like nitromethane leads to a decrease of bond dissociation energy values (BDE) for the C–N bond [2].

In this paper, the geometries and potentials in the central regions of molecular surfaces of 1,4-dihalo-5,8-dinitronaphthalene and 2,3-dihalo-5,8-dinitronaphthalene were analyzed. Optimal geometries and maps of electrostatic potential (MEP) were calculated using PBEPBE/6-311G** level of theory. The WFA-SAS program was used to obtain MEP for the mentioned molecules. Bond dissociation energies for optimized geometries were calculated using SAPT program.

Results showed that the potentials above the central regions of molecular sufaces in the 2,3-dihalo-5,8-dinitronaphthalene molecules are higher than in the case of 1,4-dihalo-5,8-dinitronaphthalene analogues. The most significant difference was detected in the case of molecules with chlorine as a substituent (up to 3 kcal/mol). However, the dissociation energies of C–N bonds are higher for all 2,3-substituted dinitronaphthalenes compared to 1,4-substituted analogues. There is a decrease in BDE values in both cases, but it is more significant for the 1,4-substituted dinitronaphthalenes, where the BDE value for 1,4-difluoro-5,8-dinitronaphthalene is more than 7 kcal/mol higher compared to the BDE for iodine analogue.

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TC PP 04

Modeling of interactions of *N*-benzyl derivatives of long-chained 4-amino-7-chloro-quionolines with the RhIR receptor of *Pseudomonas aeruginosa*

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In this investigation, we examine interactions of synthetic ligands with one of the quorum sensing protein receptors of *Pseudomonas aeruginosa*, RhIR, in order to identify amino acids that are responsible for interactions with potential inhibitors of receptor activity. Figure 1 shows interactions of ligands with 5% and 60% inhibition rates respectivly. Potential amino acids that are involved in interactions with inhibitors are TYR-72, TRP-96, ASP-81, which, depending on the interaction type, contribute differently to the share of inhibition. It was found that with decreasing in intensity of interaction with TRP-68, the inhibition increases and the highest inhibition is reached when there is no interaction with TRP-68.

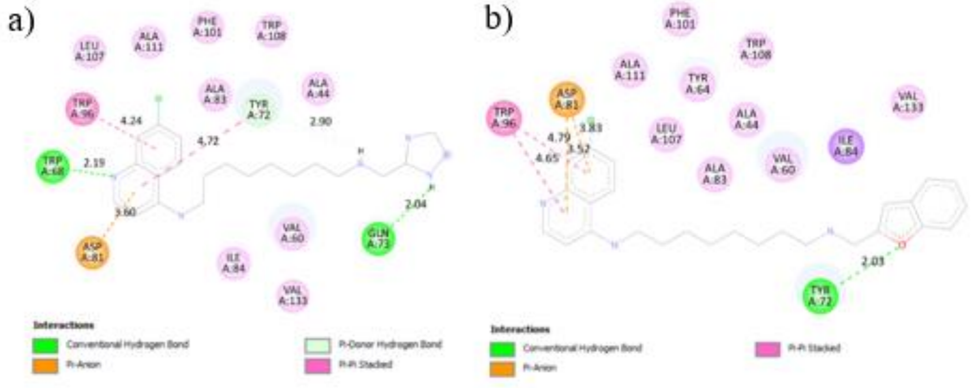

Figure 1. Interactions of 2 ligands a) with low inhibition rate and b) with high inhibition rate

Structures of inhibitors were generated in ChemDraw. Ligand structures were saved in the appropriate format using AutoDockTools. The RhIR protein, which has 241 amino acids in 1 chain, was prepared in AutoDockTools while the docking was done in AutoDock Vina. Conformations were selected using USCF Chimera software, interaction schemes were generated using Discovery Studio 2021 Client.

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TC PP 05

Theoretical study of chelate-aryl stacking interactions between nickel *bis*(dithiolene) and benzene

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Chelate–aryl stacking interactions between nickel *bis*(dithiolene) and benzene were studied by the means of quantum chemical calculations. The calculations were performed at CCSD(T)/CBS level, which is a gold standard in quantum chemistry, as well as the ωB97X-D/6-31+G(d) level, which was shown to be in good agreement with the reference method for these interactions. The calculations have shown that nickel *bis*(dithiolene) forms chelate-aryl stacking that reaches the CCSD(T)/CBS interaction energy of −5.60 kcal/mol (Figure 1), which is of similar strength as chelate-aryl stacking of nickel *acac* complex.[1] Energy decomposition analysis performed at SAPT0/def2-TZVP level showed that the dominant energy component of this interaction is dispersion; however, due to cancelation of most of the dispersion by exchange, electrostatic component is the one responsible for the strength of these interactions, as well as the geometries of minima at potential energy curves.[2] The results of the calculations are in good agreement with electrostatic potentials of nickel *bis*(dithiolene) and benzene (Figure 1).[1,2]

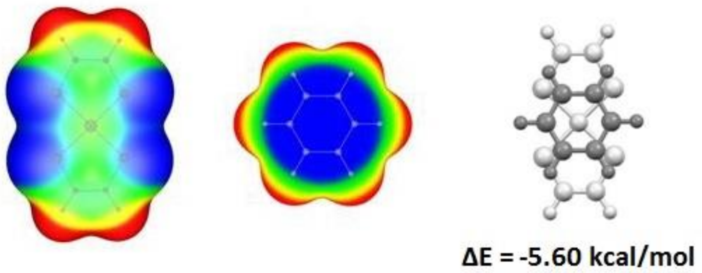

Figure 1. Electrostatic potentials of nickel bis*(dithiolene) and benzene, plotted on the contour of electron density of 0.001 a.u., and the top view of their most stable stacking interaction, with denoted CCSD(T)/CBS interaction energy. Electrostatic potentials lower than −6.3 kcal/mol are blue, between −6.3 and 0.0 kcal/mol green, between 0.0 and +6.3 kcal/mol yellow, and higher than +6.3 kcal/mol are red.*

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TC PP 06

Three types of hydrogen bonds of free and coordinated amino acids with water molecule

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The strength of the hydrogen bond between two water molecules is increased when water molecules interact with the metal ion. This was confirmed from the analysis of crystal structures in the Cambridge Structural Database (CSD), where the shortening of d_{OH} distances was observed, and the increased strength of hydrogen bonds of coordinated water molecules. Three types of hydrogen bonds of free amino acids as zwitterions and coordinated amino acids with water molecules were investigated by analyzing the data deposited in CSD and performing DFT calculations. In NH/O hydrogen bond type the amino acid acts as a hydrogen donor and the nitrogen belongs to the α-amino group. In O_1/HO and O_2/HO hydrogen bond types, where oxygen O_1 is the hydroxyl oxygen, and the oxygen O_2 is the carbonyl oxygen of the α-carboxyl group, the amino acid is a hydrogen acceptor. For free amino acids as zwitterions, the two oxygen atoms are identical, so only one O/HO hydrogen bond was investigated. The data from searches of free amino acids as zwitterions showed the peak on hydrogen donor-acceptor distance distribution in the 2.8 – 2.9 Å range for NH/O, and 2.7 – 2.8 Å for O/HO hydrogen bond. The peak on the hydrogen bond angle distribution was in 160 – 170° range for both hydrogen bonds of free amino acids as zwitterions. The coordinated amino acid CSD searches resulted in hydrogen donor-acceptor distance and hydrogen bond angle distribution peaks in 3.0 – 3.1 Å and 110 – 120° range for NH/O, 2.8 – 2.9 Å and 120 – 130° range for O_1/HO, and 2.7 – 2.8 Å and 160 – 170° range for O_2/HO hydrogen bond. DFT calculations were performed for glycine (Gly), cysteine (Cys), phenylalanine (Phe), and serine (Ser), both free and coordinated in octahedral complexes of cobalt(III) with varying charge of the complex (+2, +1, 0, −1). Interaction energies between free amino acids as zwitterions and water were in the range from −8.6 to −10.5 kcal/mol for NH/O, and from −6.9 to −7.6 kcal/mol for O/HO hydrogen bonds. In coordinated systems, the interaction energies were from −2.2 to −16.9 kcal/mol. All interaction energies are in good agreement with electrostatic potential (Vs) values on interacting atoms in amino acids. The results showed small dependence of interaction energy on type of amino acid, and very large dependence on charge of the complex.

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TC PP 07

Molecular docking of porphyrin-like complexes to SARS-CoV-2 main protease

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Molecular docking method, which was recently modified to allow traditional and covalent docking of organometallic compounds [1], was used to theoretically investigate the potential binding of 15 copper(II) complexes with porphyrin-like ligands to main protease of SARS-CoV-2 virion (CLpro). Method was implemented by importing published parameters into the program GOLD from the CCDC package. Target of the docking experiments was active site of the CLpro. Method was validated by redocking of N3 inhibitor, and by comparing obtained results with published crystal structure [2]. Structures of investigated complexes were obtained by filtering Cambridge Structural Database for porphyrin-like compounds with copper(II) ion. Each structure was refined using semi-empirical PM6 method implemented in MOPAC 2016 and subsequently modified for docking experiments with dummy hydrogen atoms that simulate metallic d-orbitals. Docking experiments were performed with 50 genetic algorithm runs for each investigated complex, GoldScore function was used to score fitness, no early termination was set, and rest of the settings were left at the default values. Obtained scores were then compared to the scores derived from experiment with known inhibitor to rank inhibitory potential of investigated compounds.

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