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SCIENTIFIC COMMITTEE

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PLENARY LECTURES

PL1. PEAK HOMOGENEITY IN LC/DAD AND LC/MS

Andrei MEDVEDOVICI and Dana-Maria PREDA

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The main issues sustaining, during validation, the selectivity of stability indicating HPLC methods using detectors with structural confirmation abilities (DAD or MS) are peak homogeneity and mass balance. Both issues suffer inherently of some drawbacks.

Peak homogeneity (also addressed as peak purity) is generally measured, in software accompanying data processing tools, through the computation of the cosine between the vectors represented in the n-dimensional space describing the spectra acquired during peak elution.

Some questions need to be clarified: a) the influence of the concentration/amount of analyte generating the studied peaks; b) the situation of the perfect peak overlapping; c) potential advantages of spectral manipulation techniques (i.e. first or second derivatives); d) increased spectral similarity between the overlapping peaks.

Authors are discussing a new approach for determining the peak homogeneity based on linear regression, through calculation of the volume of an ellipsoid generated in the 3D-cartesian space through representation of the mean slope, intercept and correlation coefficient and their respective standard deviations resulting from the reciprocal comparison of spectra acquired during peak elution.

The new approach is compared with the commercially available peak purity tool in diode array detection (UV spectrometry) and also applied for MS detection (full scan working mode). Answers to the above mentioned questions are also addressed.

PL2. INFLUENCE OF STRUCTURE OF SUBSTITUTED AZULENES ON FILM FORMATION BY ELECTROCHEMISTRY

Eleonora-Mihaela UNGUREANU

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Azulene can be irreversibly electrooxidated to polymers leading to modified electrodes. The main characteristics of several structures of azulene derivatives ((thiophen-azulen-1-yl)pyridine; azulene-diazenyl-tetrazole, azulene-diazenyl-thiadiazole, azulene crown ethers) were examined in connection to electrochemical experiments performed by cyclic voltammetry, differential pulse voltammetry, rotating disk electrode in view of modified electrodes preparation. The film formation by electropolymerization was examined. The modified electrodes have been tested to prepare sensors for heavy metal (HNM) ions detection in water. Optimum structures to prepare these functional advanced materials and the conditions for HM ions detections using azulene modified electrodes (p*H* of the sample and buffer, complexation time, reduction potential and time) to prepare these functional advanced materials were discussed.

PL3. COUPLED PROCESSES IN BIOFUELS TECHNOLOGY

Tanase DOBRE

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This paper addresses, in a broad sense, the issue of inclusion of anaerobic fermentation biofuels, namely biobutanol, bioethanol, biogas and biohydrogen in the present and future race of energy sources. The paper opens with the general energy problem, showing, in a new form, that we have solar energy, so much that there would be no need for another source. But concretely it is the fact we do not have, yet, one or more technologies that allows the control in takeover and storage of this energy, for consumption requirements of modern society. Because of this fact in emergence and evolution of our five industrial revolutions and especially in transition from one to another, the society was based on technology and on energy resource, characteristic of each revolution [1]. With reference to the predominant energy resource today, namely fossil fuels, the paper tries to give an answer to the question: When do fossil fuels run out?. And even if fossil fuels do not run out [2], an analysis of the fourth industrial revolution and of current state of post-industrial revolution, in terms of global controlling of carbon dioxide excess environmental pollution, imposes restrictions on their use as a basic energetic source. In this context, of the unwritten order to reduce the consumption of fossil fuels, the use of biofuels has come to be regulated worldwide, including in Romania. The part of the paper intended to present biobutanol as a future biofuel shows the processes that can be coupled with ABE fermentation, in order to control it to a higher productivity, not only as a result of limiting of butanol toxicity on the bacterial system that controls this fermentation. A concrete case modelling sustains the advantage of coupling fermentation with in situ separation of fermentation products [3]. In the paper part dedicated to presentation of bioethanol as a high-performance biofuel it insists on the importance of orienting this fermentation process on plant biomass as a primary source of raw material. The put in work of actual fermentation through a coupled process is advantageous and of interest, whatever the generation of bioethanol. Coupled process modelling for fermentation with pervaporation shows promising results [4]. Another part of the paper is dedicated to biogas as a high-potential energy source. Thus, in terms of technological interest, there are aspects of the elementary processes in biogas synthesis, considerations regarding the set of microorganisms involved in this fermentation process and elements regarding the coupled operation of biogas fermenters. Referring to biohydrogen it shows that it can

be produced biologically by biophotolysis (direct and indirect), photo-fermentation and dark-fermentation or by coupling of these processes (such as integration of dark- and photo-fermentation (two-stage process), or biocatalyzed electrolysis, etc.). However, production of hydrogen by these methods at commercial level is not reported in the literature and challenges regarding the process scale up remain. The way of vegetables residues reforming to carbon monoxide and hydrogen remains the most promising technology for hydrogen of near future. More coupled process can be considered for this hydrogen way.

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[3]. B. Ohreac Sandu, T. Dobre, O. Pârvulescu, T. Danciu, Integrations of ABE synthesis with their recovery by gas-stripping, Rev. Chim. (Bucharest) 65 (2014) 581-588.
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PL4. INTUMESCENT MATERIALS BASED ON WASTE GLASS

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Intumescent materials swell when heated with the increase of volume and porosity. This type of materials can be used for passive fire protection in buildings, as coatings which prevent the overheating (especially for metallic structural elements) or as sealants which prevent the fire and smoke spreading.

The paper presents some of the results obtained in our research group regarding the synthesis of intumescent materials by the alkali activation of waste glass powder (WGP) with various additions (borax, sodium carbonate, slag etc.). The activation temperature of the intumescence process, specific for alkali activated materials based on waste glass powder, can be decreased with 100^{o}C up to 400^{o}C when sodium carbonate or borax are added to sodium hydroxide and WGP mixture or it can be increased when slag is present in the binding system.

Coatings based on this type of binding materials (as-such) or mixed with organic binders were applied on steel substrates to assess their ability to mitigate the damages caused by fire.

SECTION A: NATURAL AND SYNTHETIC COMPOUNDS

OA1. CO-RELEASING PROPERTIES, DFT/TDDFT AND DOCKING ANALYSIS OF $[Re(CO)_3(bpy)L]^+$ TYPE COMPLEXES

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Carbon monoxide (CO), known as a toxic gas, is produced in the human body in a certain range during hemoglobin degradation process. The amount of produced CO increases in inflammation [1]. The increase in the concentration of CO in pathological conditions has been the motivation of the research on using CO as a therapeutic agent. As a result of these studies, the CO molecule has been identified as a gasotransmitter such as NO and H_2S. Studies have shown that CO has anti-cancer, anti-bacterial, anti-coagulative activities and also CO has started to be used in vasodilatory treatments [2, 3]. Although inhalation could be thought as first candidate for delivering certain amount of CO to the target tissue, this method is difficult in terms of dose and tissue control. The molecules that designed to deliver CO to a specific tissue in a controlled manner are called CORMs (**CO-R**eleasing **M**olecule**s**). The strongest candidate for CORMs is metal carbonyl complexes in which CO is used as ligand, although many organic species have been used for. Many complexes with different transition metals containing a wide variety of ligands were synthesized for using as CORMs and their activities were investigated [4, 5]. In this study, $[Re(CO)_3(bpy)L]X$ {bpy: 2,2'-bipyridine, L: benzimidazole, azabenzimidazole; X: SO_3CF_3 or PF_6) were synthesized/characterized and CO-releasing activity of these compounds were analyzed. Also, the molecules were optimized and analyzed by common DFT/TDDFT methods and were docked into serum albumin for investigating the interaction of molecules with blood.

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[3]. E. Üstün, A. Özgür, K.A. Coşkun, S. Demir Düşünceli, İ. Özdemir, Y. Tutar, Transit. Met. Chem. 42 (2017) 331-337.
[4]. M.A. Gonzales, P.K. Mascharak, J. Inorg. Biochem. 133 (2014) 127–135.
[5]. S. Pai, M. Hafftlang, G. Atongo, C. Nagel, J. Niesel, S. Botov, H.G. Schmalz, B. Yard, U. Schatzschneider, Dalt. Trans. 43 (2014) 8664-8678.

PA1. NEW CHITOSAN DERIVATIVES WITH N-HETEROCYCLIC SALTS AND INFLUENCE'S FACTORS IN THEIR STRUCTURE

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In last decades, new chitosan derivates solids, semi-crystalline as powders of various granulations were obtained and have variety of applications in medical and engineering fields [1, 2]. We reported here, the synthesis of new N-heterocyclic chitosan derivatives including dibromide of N, N'-bis(phenacyl)-4,4'-bipyridine and dibromide of N, N' bis(phenacyl)-1,2-bis(4-pyridyl) ethane to improve the biological activity (e.g. antimicrobial, antioxidant). Their chemical structures were characterized by elemental analysis (C % and N%) and FTIR spectra. The results show that the polymer's chitosan modification is due to the salt's N-heterocyclic structure, also of reactant's concentrations, temperature, and reaction time between compounds.

Acknowledge: *Financial support from the Doctoral School of Fundamental and Engineering Sciences, "Dunarea de Jos" University of Galati.*

[1]. F. Luan, L. Wei, J. Zhang, W. Tan, Y. Chen, F. Dong, Q. Li, Z. Guo, Molecules 23 (2018) 516.
[2]. K. Gao, Y. Qin, S. Liu, R. Xing, H. Yu, X. Chen, K. Li, P. Li, International Journal of Polymer Science 2018 (2018) e3970142.

PA2. EVALUATING THE BIOLOGICAL POTENTIAL OF SOME NEW COBALT (II) COMPLEXES WITH 3,5-DIMETHYLPIRAZOLE AS LIGAND

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The synthesis and characterization of complexes with azole type ligands and carboxylates has gained a great interest due to their interesting structures and biologic potential, including antimicrobial, antiviral, antidiabetic, anticancer activities.

The versatility of carboxylate allowed to obtain more than one product from the same synthesis route, in the case of some systems formed from copper(II) acrylate/methacrylate and azole derivatives.

In the light of those above mentioned and continuing along our works, we report in this paper the results related to synthesis, structural characterization and biological activity of some new mixed cobalt(II) complexes with metacrylate ion and 3,5-dimethylpyrazole.

Their chemical formulas were achieved correlating the chemical analysis with mass spectrometry data, the ligands coordination modes were assigned by FTIR measurements, and the trigonal bipyramidal geometry of cobalt ion in complexes was assigned by data correlation of NIR-UV-Vis spectra and magnetic moments measurements.

Microbiological assays indicated that Co(II) complexes present a very good activity against *Candida albicans 1760, Enterococcus faecium E5, Bacillus subtillis ATCC 6683* and *Escherichia coli ATCC 25922.*

PA3. SYNTHESIS, PHYSICO-CHEMICAL CHARACTERIZATION, CRYSTAL STRUCTURE AND BIOLOGICAL ACTIVITY OF NEW COPPER (II) COMPLEXES WITH NICOTINAMIDE

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Nicotinamide is a nitrogen donor ligand that was used in treatment of various skin diseases, such as atopic eczema, psoriasis, skin cancer or in prevention against some neurodegenerative diseases as Alzheimer.

A literature survey shows a large number of copper (II) complexes with nicotinamide which can act as monodentate or bridging ligand. Moreover, more than two thirds of all structurally studied complexes contain some carboxylate anions as ligands. Carboxylate anions exhibit a versatile coordination behavior due to their ability to act as unidentate, bidentate chelate or bridging bidentate ligands.

We hereby report the synthesis, structural characterization and antimicrobial activity of two new copper (II) complexes containing both nicotinamide and metacrylate ion as ligands.

In addition, the antibacterial activity of the complexes and the ligand have been evaluated against *Escherichia coli, Staphylococcus aureus* and *Bacillus subtilis.* The results of the antibacterial tests show that copper complexes have higher antibacterial activity compared to the free nicotinamide.

PA4. SYNTHESIS, SPECTRAL AND BIOLOGICAL CHARACTERIZATION OF NEW COPPER (II) COMPLEXES WITH PYRAZOLE TYPE LIGANDS

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The coordination chemistry of pyrazole derivatives received scant attention in the last decade although the pyrazole nucleus is thermally and hydrolytically very stable. The pyrazolate ligand can exhibit three coordination modes, namely unidentate (pyrazole-N), exo-bidentate (pyrazole-N,N') and endo-bidentate.

A literature survey [1] revealed that pyrazole derivatives possess diverse pharmacological activities such as antitumor, angiotensin-converting-enzyme inhibitory, antimicrobial, anti-inflammatory, antiviral, anticonvulsant and antidepressant. Stable, inert and nontoxic metal complexes containing spectroscopically active metal centers are exceptionally valuable as probes for biological systems. Some transition metal complexes with pyrazole derivatives were tested as anticancer agents.

In this context, new copper complexes with mixed ligands, pyrazole derivatives and acrylate ions have been synthesized and characterized by chemical analysis, infrared (IR) and electronic spectroscopies and by thermal analysis. Their influence on the microbial growth was assayed also.

[1]. A. Chauhan, P.K. Sharma, N. Kaushik, Int. J. Chem. Tech. Res. 1 (2011) 11-17.

PA5. COBALT (II) COMPLEXES AS ANTIBACTERIAL AGENTS

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A large number of cobalt (II) complexes with antibacterial properties have been reported in the literature, probably due to their stability, availability, and ease of synthesis. These antibacterial properties could be explained either by the presence of biological active ligands or the stereochemical versatility of metallic ion.

In this paper we report two new cobalt (II) complexes with mixed ligands, picolinate anion and 5,6-dimethylbenzimidazole.

Benzimidazole and its derivatives are bioactive molecules in essential biological systems with a large variety of pharmacological activity. Both benzimidazole derivatives and picolinic acid are proton donors and/or acceptors in enzymatic reactions and were studied for their antibacterial, anti-parasitic, anti-inflammatory and anticancer activity.

Based on these aspects, the new cobalt complexes with mixed ligands, have been synthesized and characterized by chemical analysis, infrared (IR) and electronic spectroscopies as well as by thermal analysis. Complexes exhibit activity against a wide range of bacterial and fungal strains, both on planktonic and biofilm embedded states.

PA6. PHYSICO-CHEMICAL AND BIOLOGICAL CHARACTERISATION OF SOME COBALT(II) COMPLEXES WITH MIXED LIGANDS

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Semicarbazone derivatives exhibit a large spectrum of biologic activity such as anti-inflammatory, antimicrobial, and antitumor and are good ligands that generate stable complexes [1]. On the other hand, cobalt complexes exhibit interesting redox and biological properties that make them suitable for a wide breadth of applications in pharmacology and medicine. As result several Co(II) complexes with multidentate semicarbazones were synthesised and some evidenced a very good antitumor potential based on a nuclease like activity [2].

Having in view these aspects, we extended this field in synthesis of new complexes of Co(II) of type [Cu(vnsc)(N-N)(ClO_4)] (Hvnsc: 2-hydroxy-3-methoxybenzaldehyd semicarbazone, N-N: 2,2'-bipyridine (bipy) or 1,10-phenantroline (phen)) with vnsc as multifunctional ligand and N-N as auxiliary ligand. The features of complexes have been assigned from elemental analyses as well as IR and UV-Vis spectra. The semicarbazone ligand behaves as tridentate species while aromatic amine act as chelate. The distorted octahedral stereochemistry is completed by perchlorate as unidentate ligand.

The antimicrobial assays were performed against Gram positive (*Staphylococcus aureus*, *Bacillus subtilis*), Gram negative (*Escherichia coli*, *Pseudomonas aeruginosa*) and fungal (*Candida albicans*) strains. In all cases it was evidenced that overall antimicrobial potency of ligand was enhanced upon coordination.

[1]. C. Santini, M. Pellei, V. Gandin, M. Porchia, F. Tisato, C. Marzano, Chemical Revue 114 (2014) 815–862.
[2]. A.K. Renfrew, E.S. O'Neill, T.W. Hambley, E.J. New, Coordination Chemistry Reviews 375 (2018) 221-233.

PA7. INSIGHT ON PHYSICO-CHEMICAL AND BIOLOGICAL PROPERTIES OF SOME COPPER(II) COMPLEXES WITH MIXED LIGANDS

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Derivatives bearing 1,2,4-triazolo[1,5-*a*]pyrimidine fused rings exhibit a large spectrum of biological activity such as anti-parasitic, antimicrobial and antitumor [1]. As result several complexes with this kind of ligands were synthesised and some evidenced antitumor, anti-inflammatory, or antimicrobial activity, in most cases these being enhanced in comparison with that of the ligand [2].

Considering these aspects, we extended this field in synthesis of new complexes of Cu(II) with mixed ligands, 5-phenyl-7-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine and 2,2'-bipyridine (bipy) or 1,10-phenantroline (phen). The features of complexes have been assigned from elemental analyses, IR, and UV-Vis spectra. These date evidenced the mononuclear structure of complexes with 5-phenyl-7-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine acting as unidentate and 2,2'-bipyridine or 1,10-phenantroline as chelate species resulting in a distorted square pyramidal stereochemistry.

The antimicrobial activity were assayed against Gram positive (*Staphylococcus aureus, Bacillus subtilis*), Gram negative (*Escherichia coli, Pseudomonas aeruginosa*) and fungal (*Candida albicans*), both planktonic and biofilm embedded strains. In all cases it was evidenced that overall antimicrobial potency of ligand was enhanced upon coordination, the most active being species with phen as ligand.

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[2]. I. Łakomska, M. Fandzloch, Coordination Chemistry Reviews 327-328 (2017) 221-241.

PA8. VANADIUM (V) COMPLEXES WITH BIGUANIDE DERIVATIVES DEVELOPED AS BIOLOGICALLY ACTIVE SPECIES

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Biguanide derivatives are known both for their large spectrum of biologic activity such as hipoglicemiante, antimicrobial and antitumor and as chelate ligands that generate stable complexes [1]. On the other hand, vanadium complexes exhibit interesting redox and biological properties that make them suitable for a wide breadth of applications in pharmacology and medicine. As result several V(IV) and V(V) complexes with multidentate ligands were synthesized. Some species with peroxide as ancillary ligand evidenced a very good antitumor activity based on Reactive Oxygen Species (ROS) generation. A high level of ROS is cytotoxic to the cells and triggers as result the apoptotic mechanisms [2].

In this respect, new vanadium (V) compounds, proposed for use against malignancies, were designed and synthesized by using 1-(*o*-tolyl)biguanide (Htbg) as ligand in presence of ammonium vanadate and hydrogen peroxide. Compounds were formulated as mononuclear species $(NH_4)[VO(tbg)_n(O_2)_m]$ $(n + m = 3)$ based on data provided by microanalytical and thermal data, IR, and UV-Vis spectra. All complexes exhibit a stereochemistry associated with heptacoordination resulting from the chelate behavior of both deprotonated tbg and peroxide anion. The oxoanion acts as unidentate in an apical position.

[1]. R. Olar, M. Badea, D. Marinescu, C.M. Chifiriuc, C. Bleontu, M.N. Grecu, E.E. Iorgulescu, M. Bucur, V. Lazăr, A. Finaru, European Journal of Medicinal Chemistry 45 (2010) 2868-2875.

[2]. E. Kioseoglou, S. Petanidis, C. Gabriel, A. Salifoglou, Coordination Chemistry Reviews 301-302 (2015) 87-105.

PA9. RUTHENIUM (III) COMPLEXES WITH A PURINE ANALOG DEVELOPED AS ANTITUMOR SPECIES

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Triazolopyrimidine derivatives exhibit a large spectrum of biologic activity such as anti-parasitic, antimicrobial and antitumor [1]. As result several Ru(II) and Ru(III) complexes with such ligands were synthesised and some evidenced a good antitumor activity in some cases comparable with cisplatin [2]. The interest for ruthenium anticancer agents was opened by the anti-metastatic activity evidenced both for Ru(II) and Ru(III) complexes with heterocyclic amine such imidazole or indazole as unidentate ligands, the hexacoordination being assured by chloride anions and dimethyl sulfoxide (DMSO) [3].

Considering these aspects, we extended this field in synthesis of new complexes of Ru(III) with mixed ligands, 5-phenyl-7-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine (pmtp) and DMSO of type $[Ru(pmtp)_n(DMSO)_n]Cl_3$ (n = 1, 2; m = 5, 4). The features of complexes have been assigned from elemental and thermal analyses, IR and UV-Vis spectra as well as thermogravimetric analysis. Both 5-phenyl-7-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine and dimethyl sulfoxide behave as unidentate resulting in a distorted octahedral stereochemistry for both mononuclear complexes.

[1]. I. Łakomska, M. Fandzloch, Coordination Chemistry Reviews 327-328 (2017) 221-237.
[2]. J. Wiśniewska, M. Fandzloch, T. Muziol, I. Łakomska, Inorganic Chemistry Communication 109 (2019) 107567.
[3]. G. Golbaghi, A. Castonguay, Molecules 25 (2020) 265.

PA10. PHYSICO-CHEMICAL AND BIOLOGICAL CHARACTERISATION OF SOME COPPER(II) COMPLEXES WITH MIXED LIGANDS

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The copper ion is considered unique from both the point of view of coordinative chemistry and from its biological importance. Some features, such as stereochemical and oxidation state versatility and acid borderline character recommend this ion for the synthesis of complexes with a large variety of ligands, structures and properties.

As result, many copper complexes with antitumor, anti-inflammatory or antimicrobial activity were designed. Most of these complexes contain mixed ligands, one being a N-N-chelating heterocycle such 2,2'-bipyridine (bpy) or 1,10-phenanthroline (phen), chosen both for their chelating ability and intercalative properties. As result several Cu(II) complexes with this kind of ligands were synthesized and some evidenced a very good antitumor potential based on a nuclease like activity [1].

Having in view these aspects, we extended this field in synthesis of new complexes of type [Cu(SCN)(N-N)(X)] (N-N: 2,2'-bipyridine (bipy) or 1,10-phenantroline (phen), X: ClO_4, NO_3) with N-N as auxiliary ligand. The features of complexes have been assigned from elemental analyses as well as IR, UV-Vis and EPR spectra. The thiocyanate ligand behave as bridge while aromatic amine (dipy, phen) acts as chelate. The distorted octahedral stereochemistry is completed by perchlorate and water acting as unidentate and nitrate anions acting as chelate.

The complexes exhibit a good antimicrobial activity both on planktonic and biofilm embedded strains.

[1]. C. Santini, M. Pellei, V. Gandin, M. Porchia, F. Tisato, C. Marzano, Chemical Revue 114 (2014) 815–862.

PA11. NEW BIOLOGICAL ACTIVE COPPER(II) COMPLEXES WITH MIXED LIGANDS

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Pyridine-2-carboxylic acid (picolinic acid, Hpic) was widely used as ligand due its multiple coordination modes and physiological properties, especially insulinomimetic activity. Generally, the reaction between metal (II) salts and picolinic acid provides complexes with the general formula $[M(pic)_2(H_2O)_n]$.

Our work consists in substitution of water molecules with imidazole derivatives. So far, four new complexes of the type $[M(pic)_2(L)]$ (L: imidazole, 2-methylimidazole, 4-methylimidazole, 2-ethylimidazole) were synthetized.

The new compounds were characterized as mononuclear species using elemental and thermal analysis, IR as well as UV-Vis-NIR spectroscopy.

Complexes exhibited activity against a wide range of planktonic Gram negative, Gram positive bacterial strains and fungi.

PA12. GLUCOSINOLATES FROM SOME ROMANIAN SPECIES OF BRASSICACEAE FAMILY

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People ingest a diversity of pharmacologically active chemicals by eating vegetables and fruits. Glucosinolates are biological active compounds with bio-protective effects: antioxidant activity, antimutagenic and antiproliferative activities (chemo preventive agents), antifungal and antibacterial activities and effects on insects and other invertebrates [1,2]. Some extracts of Romanian white cabbage, acclimatized broccoli, black radish, rapeseed and cauliflowers from *Brassicaceae* family are obtained by irradiation in microwave field (2450 MHz) in different media. The antioxidant activities (DPPH, 0.85-1.1 mmol/L Trolox and FRAP assay, 2-20 mmol/L Trolox) and total phenols [3] of extracts were determined (1300-3900 mg GAE/L). Glucosinolates were analyzed by HPLC method, using a Dionex Ultimate 3000 (Dionex Corp., USA) equipped with a PDA 3000 photodiode array detector and a C-18 Acclaim® 120 Silica-Based reversed-phase (4.6x150 mm, 5 μm), at 40°C and flow rate 0.75 $mL \cdot min^{-1}$. The acetonitrile 5% and water 95% as a mobile phase was used.

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PA13. SYNTHESIS AND CHARACTERIZATION OF SOME N-(2-CHLORO-PHENYL)-2-HYDROXY-BENZAMIDE DERIVATIVES

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The inappropriate use of antimicrobial drugs has led to the increasing development of microbial resistance. Nowadays, the resistance has been found in many essential human pathogens and represents a severe risk for public health. 2-Hydroxy-N-phenylbenzamides and their derivatives have been reported to possess an important antibacterial activity even against drug-resistant *Mycobacterium tuberculosis*, Methicillin-resistant *Staphylococcus aureus*, with minimum inhibitory concentrations in micromolar range [1,2]. An advantage of salicylanilides consists in the possibility to act on many targets within the bacterial cells [3].

Salicylanilide entity still represents a studied class of compounds with lots of remarkable pharmacological properties, like antiparasitic [4] and anticancer [5] effects.

Some novel molecules, esters, hydrazides, hydrazones of N-(2-chloro-phenyl)-2-hydroxy-benzamide, were synthesized using classical heating synthesis. The compounds were obtained with good yields (35-96%) after the final purification. All synthesized compounds were characterized using FTIR, ^{1}H and ^{13}C-NMR. Spectral data confirm the proposed structures.

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PA14. ANTHOCYANIN EXTRACTS FROM DIFFERENT PLANT MATRICES AS POTENTIAL NATURAL FOOD DYES

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Color is one of the most important visual attributes of food and has a major influence on the first impression of the consumer [1,2]. Increasing consumer concerns about the adverse effects of synthetic dyes on health, as well as legislative actions limiting their use in the food industry [3], have led to increased interest in the development of food dyes from natural sources. The main classes of natural pigments found in plants are carotenoids, anthocyanins, betalains and chlorophylls. Of these, anthocyanins represent the largest group of natural water-soluble pigments, including more than 635 different anthocyanins identified in plant tissues [4].

For the extraction of anthocyanins, native vegetable sources (fruits, vegetables, flowers) were chosen, namely: black mulberries, black currants, cherries, red onions, red radishes, purple potatoes, wild poppy, and red peony. Anthocyanins extraction was carried out with acidified alcohol in ultrasonic condition (59 kHz, 30 min., 25°C). The concentrated extracts were analyzed for anthocyanin composition (HPLC-DAD), anthocyanin content (pH differential), total phenolics (Folin-Ciocalteu), and antioxidant capacity (DPPH, FRAP). The highest anthocyanins content were obtained for the extracts of wild poppy petals (9.031±0.062 mg/g plant material), cherries skin (3.959±0.204 mg/g plant material) and red onion skin (2.714±0.030 mg/g plant material).

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PA15. CHEMICAL COMPOUNDS AND ANTIOXIDANT ACTIVITIES IN TWO FLAVONIC EXTRACTS FROM *HELICHRYSUM ARENARIUM* FLOWERS AND *ROBINIA PSEUDOACACCIA* FLOWERS

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According to literature data, *Helichrysum arenarium* flowers are rich in phenolic compounds including flavonoids, chalcones, phenolic acids, coumarins, and pyrones. *Robinia pseudoacaccia* flowers are also useful sources of flavonoids, important compounds for the defense against reactive oxygen species.

Dried flowers of *Helichrysum arenarium* and *Robinia pseudoacaccia* were used to prepare two flavonic extracts as follows: the dried flowers were extracted in 50% ethanol for 6 hours at room temperature. The alcohol was removed at an evaporator Royeyov IKA RV10 at 50ºC, 200 mBarr.

Chemical analysis of the extracts consists in: identification and cuantification of the flavonic compounds using High Performance Thin Layer Chromatography (HPTLC); total polyphenolic content using Folin-Ciocalteu method. For antioxidant activities assessment there were used the DPPH and FRAP assay. For the two extracts the sun protection factor (SPF) was determined using a Spectra Manager TM soft.

In the *Helichrysum arenarium* extract were identified: apigenin, rutin, caffeic acid, chlorogenic acid. In the *Robinia pseudoacaccia* extract was identified luteolin 7-glycoside. Both extracts presented high antioxidant activities measured by the two methods. The sun protection factor was high mainly in *Helichrysum* extract.

As conclusion, the chemical composition of the analyzed extracts justify the high antioxidant activities as well as the screen effect against the UV radiations (SPF).

Our results recommend the two plant extracts as good active principles for cosmetic industry.

PA16. CELLULOSE FIBER EXTRACTION FROM *ULVA LACTUCA* ALGAE BY CHEMICAL TREATMENT

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In this study, cellulose extraction from *Ulva Lactuca* specie was realized by chemical treatment. Cellulose is a homogeneous biopolymer made of β-(1,4) linked D-glucose, being the most common in nature.

This biopolymer presents many advantages for the composite materials production because it can be used in the food industry as packaging materials, provided that the biopolymer used is compatible with foodstuffs, but also in other areas of activity depending on the properties of the material obtained.

Freshly harvested seaweed was dried at 50 ℃ for 2 days, crushed and made into a very fine powder in order to increase the contact surface in the Soxhlet extraction process. The extracted analytes were concentrated in the boiling flask which contains 100 ml of ethanol as the extraction solvent.

The ulvan from the solution were removed with 100 mL of ammonium oxalate (0.05 % v/v) after another hour of boiling. Afterwards, the algae were bleached in a solution consisting of 200 ml acetic acid (5 % v/v) and 100 ml NaClO (2 % v/v) heated to 60 °C.

After the powder was brought to pH = 7, it was introduced into a NaOH solution (0.05M) for 12 hours. Subsequently, it was washed to neutrality and heated to boiling point in a hydrochloric solution (5%). Finally, cellulose fibers extracted were dried in the oven at 105 °C [1].

Thus, a yield of 41,85% cellulose per d.m. was obtained proving that *Ulva Lactuca* specie is a viable alternative resource in cellulose production.

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PA17. DRUGLIKENESS PARAMETERS FOR LUTEOLIN DERIVATIVES: A COMPUTATIONAL APPROACH

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The present paper reports predicted physical and chemical parameters derived from structural descriptors and features of Luteolin and its derivatives (Luteolin 5-O-glucoside, Luteolin 7-O-glucoside, Luteolin 6-C-glucoside, Luteolin 8-C-glucoside and Luteolin-7,3'-di-O-glucoside) to assess their druglikeness. Toxicological information as ADME profile (absorption, distribution, metabolism, and excretion) parameters and pharmacokinetic properties are obtained using SwissADME tools [1]. Results are given in terms lipophilicity, water solubility and accordance to Lipinski [2] and Weber's [4] rules for druglikeness assessment. Evaluation of gastrointestinal absorption and brain penetration of investigated structures is resulted from the brain or intestinal estimated permeation model (BOILED-Egg diagram) [4] related with lipophilicity (the water-octanol partition coefficient's values) and polarity (the topological surface area). These predictive findings based on semi-empirical models could serve as preliminary biopharmaceutical evaluation of Luteolin derivatives for further optimization as therapeutical compounds.

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PA18. DESIGN, SYNTHESIS AND MOLECULAR DOCKING STUDIES OF SOME SULFONAMIDE DERIVATIVES

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Sulfonamide derivatives are biodegradable chemicals producing herbicide or growth regulating auxinic effects, lacking of toxicity to humans, animals, bees, and fish. Some sulfonamide compounds were designed and synthesized and the influence of the nature of the substituents on the molecular properties and on the biological activity was studied. The DFT/B3LYP/6-31G* level of basis set was used for the computation of molecular structure of optimized compounds. The calculations of characteristics and molecular properties were performed using Spartan'14 Software from Wavefunction, USA. The frontier molecular orbital energies, global reactivity descriptors, various thermodynamic parameters and dipole moment were predicted to examine the molecular properties of sulfonamides. Molecular docking studies were realized to identify and visualize the most possible interactions between ligands and the protein receptor. The score and hydrogen bonds formed with the amino acids from group interaction atoms are used to predict the binding modes, the binding affinities, and the orientation of the docked ligands in the active binding site. The protein-ligand complex was realized based on the X-ray structure of "loopless" GH19 chitinase (PDB ID: 3WH1) [1] using CLC Drug Discovery Workbench 2.4 software. The molecular docking study was conducted using two reference compounds (BCO-2 and BCO-4) [2, 3].

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PA19. BIOLOGICAL ACTIVITY OF SAGE ESSENTIAL OIL

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Sage essential oils are applied in the treatment of a range of diseases and has been shown to possess antioxidant, antimicrobial, viricidal, cytotoxic, antimutagenic, anti-inflammatory and antifungal activities [1, 2].

Studies show that *Salvia officinalis L.* contains a wide range of constituents including: alkaloids, carbohydrates, fatty acids, glycosidic derivatives, phenolic compounds, poly acetylenes, steroids and terpenes/terpenoids [3,4].

Considering the data from scientific literature the *S. officinalis* essential oil was analyzed through the determination of the total polyphenolic content using the Folin-Ciocâlteau spectrophotometric method and the evaluation of the antioxidant capacity using DPPH Radical Scavenging test.

The obtained results are similar with previous published researches concerning the total phenols concentration and antioxidant activity for sage essential oils [5-7].

The study was followed by the antibacterial activity testing of sage essential oil against 20 Gram positive and Gram negative bacterial strains isolated from clinical specimens. Sage essential oil showed significant but variable antibacterial activity with inhibition zones ranging from 4 mm to 9.5.mm. The effect was stronger on Gram positive (*Enterococcus, Staplylococcus*) than Gram negative bacteria (*Escherichia sp, Proteus sp, Kleksiella sp*).

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PA20. QUANTITATIVE ANALYSIS OF POLYPHENOLS AND BIOLOGICAL ACTIVITY OF BLACK POPLAR BUDS ALCOHOLIC MACERATES

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Literature data regarding black poplar buds indicates a high content of bioactive compounds with a wide range of applications in cosmetics, in the treatment of various dermatitis, respiratory diseases etc. Therefore, we found interesting to determine the main bioactive components of black poplar bud's crude alcoholic macerates and to establish their biological activity in order to assess the use for dermato cosmetic products formulation.

Three black poplar bud's alcoholic macerates were analysed by Folin-Ciocâlteau method in order to determine the total phenolic compounds and by HPLC-DAD method for identification and quantification of the individual phenolic compounds. The results for total phenols values indicate that *Populus nigra* buds macerates present high concentration of phenolic compounds between 1387.5 and 2872.5 mg GAE/100g dw. The antioxidant activities were established by DPPH Radical Scavenging test and the results indicates that the analyzed samples exhibited high antioxidant activity. Antibacterial activity of black poplar bud's alcoholic macerates has been tested against two groups of Gram-positive bacteria (*Enterococcus* and *Staphylococcus*) by using the difusimetric method. The *in vitro* inhibitory activities results were good and ranged from 8.6 to 10 mm inhibition zone in case of *Enterococcus* strains, and from 8.2 to 9.4 mm in case of *Staphylococcus*, respectively.

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PA21. SYNTHESIS, SPECTRAL CHARACTERIZATION AND MOLECULAR DOCKING STUDY OF NEW 2,6-PYRIMIDINEDIONE DERIVATIVES WITH POTENTIAL BIOLOGICAL ACTION

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Based on literature data on alkylating agents in the class of alkyl or aryl sulfonamides and sulfonates, we considered useful a specific docking study on enzymes involved in the proliferation of tumor cells located in the colon.

Thus, we formulated several molecular structures that we investigated in connection with the inhibition of the activity of cyclin-dependent kinases and then we synthesized them. From the compounds tested following the docking study, two were selected: 2,6-dioxo-1-phenyl-1,2,5,6-tetrahydropyrimidin-4-yl-4-amino-benzenesulfonate (C-1) and N - (2,6-Dimethylphenyl) -2- (2,6-dioxo-1-phenyl-1,2,5,6-tetrahydropyrimidin-4-yl-oxy) acetamide (C-2).

The biological targets used for screening were several isoforms of the cyclin-dependent kinase class.

The compounds were characterized by electronic excitation spectrometry (UV-Vis), vibration-rotation spectrometry (FT-IR) and proton nuclear magnetic resonance spectrometry (1H-NMR). Purity was verified by HPLC chromatography (UV-Vis detector).

The molecular docking study revealed a possible inhibitory effect of the two compounds on certain enzymes in the class of cyclin-dependent kinases, but in silico research is preliminary, indicative tests that offer only starting points in structural modeling and obtaining new valuable molecules from pharmacologically.

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PA22. SYNTHESIS, SPECTRAL CHARACTERIZATION AND MOLECULAR DOCKING STUDY OF SOME NEW N3-ARYLBARBITURIC ACID DERIVATIVES WITH POTENTIAL LOCAL ANESTHETIC ACTION

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Azoles (pyrazole and imidazole), as well as their derivatives are of special pharmacological interest due to their properties and the numerous structure-biological activity relationships in which they are involved. Structures are already used in therapy, including azole rings with bactericidal / bacteriostatic, antifungal, analgesic, antipyretic, antitumor, β-blocking, antihypertensive, antihistamine or local anesthetic action. On the other hand, progress is being made in the field of drug design of local anesthetics due to the elucidation of mostly complex membrane structures that include voltage-gated sodium channels.

The paper presents the synthesis, spectral characterization and a molecular docking study of new compounds containing in the molecule an ester-type anesthetic chain, substituted with an azole ring, with a hydrophilic role (pyrazoles or imidazoles) and a pyrimidine ring, as a lipophilic group (2,5-dioxo-pyrimidinedione).

The molecular docking study was performed using the crystal structure of the voltage-dependent sodium channel NavAb, obtained from the RCSB PDB database (PDB ID: 6MVX). The structures of the ligands and the receiving macromolecule were properly optimized, and the virtual screening was performed with PyRx 0.8, which uses AutoDock Vina as the docking algorithm. The physicochemical properties were calculated using the SwissADME online server. Binding energies between -8.9 and -7.8 kcal / mol were obtained for the conformations with maximum score, and the ligands interacted with the sodium channel, at the level of its pore. According to the prediction, the newly synthesized molecules follow Lipinski's rule.

Further studies are needed to confirm the biological activity of the tested compounds.

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PA23. FUNCTIONALIZED ZINC OXIDE NANOPARTICLES OBTAINED IN GREEN SEAWEEDS EXTRACTS

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The synthesis of nanomaterials by "green chemistry methods" has become progressively important in recent years. The metal oxide nanoparticles are increasingly more obtained by the green synthesis to avoid the production of unwanted or harmful by-products. Besides this, the presence of biomolecules as capping agents improve the properties of nanomaterials and enhance the range of their applications. The utilization of plant extracts, which control the particles growth, is probably the most facile and inexpensive method for obtaining inorganic nanomaterials by green synthesis [1]. Zinc oxide, an indispensable material in practice, can be obtained in a wide variety of plant extracts [2]. We obtained ZnO nanopowders in green seaweeds (*Ulva lactuca*) extracts by using chemical precipitation and hydrothermal synthesis. ZnO nanopowders were characterized by X-ray diffraction (XRD), UV–visible and Fourier transform infrared (FTIR) spectroscopy. The XRD patterns revealed the synthesis of zinc oxide with the hexagonal wurtzite structure. The crystallites dimension calculated from XRD patterns confirms the synthesis of nanoparticles. The band gap energy was calculated from UV-vis spectra by using the Tauc equation. FTIR spectra confirmed the synthesis of ZnO with wurtzite structure, and also the presence of capping agents. The photocatalytic properties were tested in the degradation of Congo red solutions and very high values of photocatalytic efficiency (around 80% after 120 min) were obtained.

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PA24. THE FIRST STEP OF BIOETHANOL PRODUCTION - EXTRACTION YIELD OF CELLULOSE FROM SOFTWOOD SAWDUST

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Current trends are to reduce the use of fossil fuels and their impact on the environment and to obtain energy from solar, wind and biofuels. Because in nature there are huge quantities of lignocellulosic materials, biofuels, especially bioethanol, could be produced by utilizing lignocellulosic biomass. Therefore, the first step to be taken into account for obtaining bioethanol is the processing of lignocellulosic biomass by various pretreatment methods: physico-chemical, mechanical or biological.

The purpose of this work was to extract the cellulose fraction from lignocellulosic biomass (softwood sawdust) by physical-chemical pretreatment. The sawdust of different granulosity was pretreated acid and alkaline using different concentrations of sulfuric acid, respectively sodium hydroxide. In this study, the temperature, the solid-liquid ratio and the cellulose extraction time were also taken into consideration. This step is very important because it has as main purpose the removal of lignin but also of the other components existing in lignocellulosic biomass.

After the application of the two pretreatments (acid and alkaline), higher yields in cellulose were obtained for the alkaline pretreatment. Some of the components released after the two pretreatments were analyzed by spectrophotometric and HPLC methods.

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SECTION B: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

OB1. TRACE METALS MONITORING IN EXTRACTIVE INDUSTRY WASTES

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The goal of this study is to develop a comparative evaluation of wastes and wastes leachates generate in extractive industry in order detect the migration of contaminants from hard rock mining operation in ground waters and soils. The study is performed using different types of rocks from different stone quarries located in the Dobrogea area of Romania. The wastes are generated from exploitation of limestone rocks, green systems and granite. The leaching test are realized using 2 l/kg [1] and 10 l/kg [2] ratios. The monitored parameters are chosen in accordance with the legislation in force and are analyzed using standard test methods. The chemical parameters monitored are total suspended solids, dissolved organic carbon, total organic carbon, chlorides, sulphates, trace metals such as lead, cadmium, total chromium, copper, nickel, barium, molybdenum, zinc [3].

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[3]. SR EN ISO 17294-2:2017- Water quality - Application of inductively coupled plasma mass spectrometry (ICP-MS) - Part 2: Determination of selected elements including uranium isotopes

OB2. THE ELECTROANALYTICAL PERFORMANCE OF NANO-CRYSTALLINE GRAPHENE ELECTRODES

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Graphene based nanomaterials are expected to possess properties that make them very efficient tools for the development of electrochemical sensors due to the excellent mobility of electrons in honeycomb sp^2-hybridized carbons, being well known that electro-catalysis readily occurs on graphene [1].

Nano-crystalline graphene (NCG) shares electrical characteristics matching few-layered graphene in terms of sheet resistance, meanwhile the electrochemical features, reflected by the heterogeneous electron transfer rate constant, are closer to the highly oriented pyrolytic graphite (HOPG - basal plane). In aqueous based electrolytes the redox transfer at NCG electrodes is promoted through an increase of the availability of edges, obtained under a pre-activation step, thus obtaining redox features comparable with the glassy carbon electrode (GC). In organic solvent-water mixtures electrolytes the electrochemical pre-activation process was unnecessary for improving the redox features of NCG electrodes.

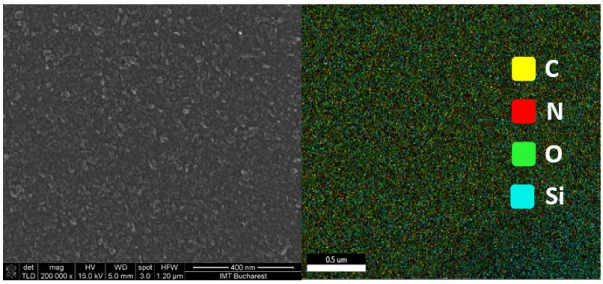

Figure 1. Micrographs illustrating the morphology of the PECVD grown nano-crystalline graphene (NCG) – top view and cross-section; the EDAX profile is also presented.

Plasma-enhanced chemical vapor deposition (PECVD) allowed growth of graphene and N-doped graphene domains on SiO_2, consisting of densely packed nano-sized islands [2]. The Raman spectrum of the nano-crystalline

film, made of graphene domains, showed peaks at 1349 cm^{-1} (D band), 1590 cm^{-1} (G-band), 2682 cm^{-1} (2 D band) and 2942 cm^{-1} (D + D' bands), suggesting crystalline arrangement of graphene domains, and a certain degree of disorder.

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OB3. ABIOTIC REDUCTIVE DECHLORINATION OF A-HEXACHLOROCYLOHEXANE BY IRON SULFIDE NANOPARTICLES. OBSERVING THE INFLUENCE OF pH ON THE DEGRADATION RATE

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In this study, a new method for the synthesis of FeS nanoparticles was developed in order to be used in the reductive dechlorination of α-hexaclorocylohexane (α-HCH), mimicking its transformation pathways in anoxic environments. The FeS nanoparticles were synthesized by adding 250 mL 0.2 M Na_2S over 250 mL 0.2 M $FeSO_4$, under a N_2 flow. The experiments with FeS were carried out in three 250 mL anaerobic bottles screwed gas-tight by butyl septa, at 3 different pH values: 2.4, 5.3 and 11.8. α-HCH was added from a stock solution in acetone to a final concentration in water of about 20 μM. The dechlorination reaction was performed for 32 days in an incubator at 30 ℃ and 125 rpm. For sampling, 14 mL aliquots of α-HCH solution were taken with syringes at regular intervals for gas chromatography-mass spectrometry (GC-MS) characterization. The GC-MS measurements were performed on a Varian 450 GC-240 MS using an ion trap mass analyzer. The results of the dehalogenation experiment shown that α-HCH was completely degraded in the anaerobic bottle with pH of 11.8, while for those with pH 2.4 and pH 5.3, α-HCH was only partially degraded, confirming the previously observed pH influence [1] on degradation of γ-HCH by FeS nanoparticles. The degradation products identified tentatively by GC-MS were: β - pentachlorocyclohexene (β - PCCH), 1,2,4-trichlorbenzene, 1,2-dichlorobenzene and benzene. Overall, the results of this dehalogenation experiment showed the potential of FeS nanoparticles in dehalogenation of HCH isomers, while various dehalogenation reaction mechanisms are yet to be investigated.

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PB1. COMPARATIVE STUDY ON THE PHYSICO-CHEMICAL AND ELECTRICAL PROPERTIES OF ABO_3 PEROVSKITES

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Perovskite-type materials constitute a wide family of inorganic compounds showing related crystallographic structures and diverse chemical composition, which are based on the general ABO_3 formula. During the past few years, perovskites have received considerable attention from diverse scientific disciplines such as chemistry, materials science or physics because of their multiple also for technological development due their moderate production costs [1]. Another key feature of these materials, which makes them attractive for research purposes, is the possibility of tuning their composition and morphology to show (or to improve) electrical conductivities [2], optical band gaps [3], or catalytic properties [4].

In this paper, a comparative study between Al doped $LaMnO_3$ compounds synthesized by the sol-gel method and ultrasonic method with immersed sonotrode in the reaction medium followed by annealing at 600˚C, for 6 h was performed. The obtained materials were studied morpho-structural by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), specific surface (BET), transmission electron microscopy (TEM) and semi-quantitative analysis (EDX). Also, the electrical measurements were performed at room temperature in order to investigate the conduction mechanisms and the influence of Al substitution in $LaMnO_3$ materials.

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PB2. RECYCLING VEGETABLE WASTE, WOOD ASH AND SAWDUST BY COMPOSTING

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Sustainable economic development requires the implementation of processes with limited negative impact on the environment and identification of wastewater treatment technologies applicable at industrial level, for pollutants removal up to the limit accepted by standards for their discharge into the emissary. The new economic requirements request researches with high applicability and technologies with low pollution, which determines the obtaining of new ecological and "economic" materials that can be used in the processes of water depollution.

Municipal waste is a growing concern in the world through the large quantity produced every year, the environmental problems and the costs of their storage. Composting is a technique frequently used to recycle a large variety of organic by-products, transforming them into fertilizers for the soil. Recycling process of biodegradable organic waste by composting may represents an ecological solution to obtain new materials used as bio-fertilizers or as ecological adsorbent substrates for toxic metals present in polluted waters. Adsorption is an effective and economical method, used to remove toxic metal ions from aqueous solution due to its simple management, less waste and possible reuse of the adsorbent material. The good results obtained by using, as adsorbent material, the compost obtained by recycling domestic waste, wood ash and sawdust waste seems to confer to composting process new contribution as a sustainable, environmental remediation technology in the future.

The composts obtained during our studies were used for Ni^{2+} and Cu^{2+} removal from wastewater. The adsorbent compost structure and morphology was investigated, before and after adsorption process from used water, by FTIR, AFM, SEM techniques. The adsorption parameters (contact time, the ratio of wastewater volume: adsorbent compost mass) were optimized and both, kinetic and thermodynamic adsorption mechanisms were established. Adsorption of heavy metals on compost substrate represents a sustainable, low-cost process useful in wastewater treatment.

PB3. COMPARATIVE THERMODYNAMIC STUDY OF RETENTION ON VARIOUS STATIONARY PHASES IN REVERSED-PHASE LIQUID CHROMATOGRAPHY

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The retention behavior of some aromatic hydrocarbons on octyl, octadecyl and phenyl silicagel stationary phases was studied for the temperature interval between 20°C and 50°C. The van't Hoff plots were studied for some mobile phase compositions, using acetonitrile or methanol as organic modifier. The linear regression parameters obtained were used in the calculation of important thermodynamic parameters of the retention process, such as the standard enthalpy variation and standard entropy variation associated with the transfer process of analytes from the mobile phase to the stationary one.

The variation of the standard enthalpy was calculated from the slope of these linear plots and its dependence on the mobile phase composition was rather different for the two organic modifiers. The variation of the standard enthalpy was very small for the four aromatic hydrocarbons in case of using acetonitrile, while for methanol used as organic modifier the variation of the standard enthalpy changed significantly from benzene to propylbenzene.

The variations of the standard entropy and Gibbs free energy change for the hydrocarbons were estimated considering a phase ratio of 0.25 for the columns used.

PB4. METAL NANO-OXIDE BASED COLORIMETRIC SENSORS FOR THE DETERMINATION OF SOME POLYPHENOLS IN PLANTS

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This work presents a novel method for determining the composition of mixtures of natural polyphenolic compounds. The method is based on the formation of colored spots by these compounds upon reaction with different nano-oxides e.g.: CeO_2, TiO_2, MoO_3, MgO, etc. impregnated on filter paper and constituting a colorimetric sensor array.

The image of the colored spots was analyzed, and the intensity of the blue color (BCI) component has shown maximum sensitivity in relation to polyphenolic compounds. The inverse of BCI was linearly correlated with the logarithm of the individual polyphenolic compound concentrations.

By using partial least squares regression for chemometric analysis of 1/BCI values of synthetic binary mixtures of several polyphenolic compounds measured with the colorimetric sensor array, it has been demonstrated good correlation between the actual and the predicted concentration of several polyphenols.

For more complex mixture containing 5 polyphenolic compounds (caffeic acid, gallic acid, quercitrin, ellagic acid, and rosmarinic acid), it was demonstrated that a good correlation between the actual and the predicted concentrations was only in the case of quercitrin. For the other phenols, the colors measured with the colorimetric sensor array were greatly influenced by the concentration of the other components in the mixture. The proposed method for polyphenol determination has advantages that include simplicity, low cost and portability.

PB5. SPECTROFLUORIMETRIC DETERMINATION OF CIPROFLOXACIN AND NORFLOXACIN IN PHARMACEUTICAL FORMULATIONS. APPLICATIONS TO STABILITY STUDIES

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Ciprofloxacin (CIP) and norfloxacin (NOR) are two synthetic fluoroquinolones (FQ) containing α-carbonyl carboxylic acid configuration and belonging to the bacteriophage family [1]. These antibiotics are broad-spectrum antibacterial agents widely used against *Gram-negative* and *Gram-positive* bacteria. CIP is an active drug after oral or intravenous administration,─extensively used for the clinical treatment of human infectious diseases [2]. NOR is administrated in urinary infections with a good localized action on affected sites [3]. Due to long-term *in-vivo* accumulation of residual drugs in human body, CIP and NOR may have carcinogenesis, teratogenesis, mutagenesis potential.

In this work, two fluorimetric methods for the determination of these FQ are presented, based on their intrinsic fluorescence (1) and on fluorogenic chelates formed between analytes and Al(III) (2). For both antibiotics, after performing a spectrometric study, the optimum excitation and emission wavelengths were set at 275 nm and 445 nm, respectively. It was observed that in the presence of Al(III), the fluorescence intensity of the analyte increases and in the emission spectrum, the signals shape is improved. Both developed methods can be used to detect the pure form of CIP and NOR at *sub-ppm* levels with a good reproducibility (RSD < 1 %), to quantify these antibiotics in pharmaceutical tablets and also, to study their stability under different stress conditions (acidic, alkaline, oxidative, photolytic and thermal conditions according to ICH guidelines).

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PB6. ELECTROCHEMICAL APPROACHES FOR ELLAGIC ACID DETERMINATION IN DIETARY SUPPLEMENTS

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Ellagic acid ($C_{14}H_6O_8$, EA) is a polyphenol dimeric derivative of gallic acid, usually present in ellagitannin and in small quantities as free form [1, 2]. It is abundant in many red fruits but also found in large amounts in wood, nuts and medicinal plants. Extracts from sources containing EA high levels are used as ingredients in traditional medicine, dietary supplements, food and beverages. The EA redox properties might be related to its antioxidant power that retard the progress of many chronic diseases. This work presents a voltammetric approach for EA determination in dietary supplements containing pomegranate extracts.

The EA electro-oxidation mechanism was studied in methanol aqueous media using cyclic voltammetry (CV), differential pulse voltammetry (DPV) and amperometry (AMP). CV was performed to select the best working electrode (vs Ag/AgCl) and to study the scan rate influence on anodic peak intensity (I_{aEA}), for EA determination. Good results were obtained on glassy carbon electrode (GCE) when an EA characteristic anodic peak was observed between 750–800 mV, which separated into two distinct peaks at higher scan rates. The influence of supporting electrolyte pH (1.8–8.8) on EA oxidation was performed using DPV and satisfactory signals were recorded in methanol/H_2SO_4 0.1 N media = 1/4 (v/v). Under the optimized experimental conditions, I_{aEA} was linearly dependent on EA concentration in the ranges 0.1–7.5 μM in DVP and 0.1–9.78 μM in AMP, respectively. The developed voltammetric method was applied to the EA content determination in commercial available dietary supplements. The obtained results were in good agreement with those of the manufacturer.

Acknowledgements: *This work was supported by University of Bucharest, research grand number 1490/2020.*

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PB7. SIMULTANEOUS ELECTROCHEMICAL DETECTION OF CATECHOLAMINE NEUROTRANSMITERS AT ACTIVATED PENCIL GRAPHITE ELECTRODE

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The selective simultaneous determination of epinephrine (EP) and norepinephrine (NP) by cyclic square wave voltammetry (CSWV) was investigated at electrochemical activated pencil graphite electrode (PGE*).

Based on the electrochemical reversibility of these catecholamines, the reduction peaks of EP and NP oxidation products were taken into consideration for this study. Thus, in 0.1 M PBS (phosphate buffer solution) pH 7.4, one voltammetric peak was obtained at –0.25 V for epinephrine and two well-separated peaks were observed at about +0.15 V and –0.25 V for norepinephrine. Therefore, NP determination in the presence of EP is possible by monitoring the peak that appears at +0.15 V, where there is no electrochemical signal for EP. On the other hand, EP detection can be done applying the well-known standard addition method exploiting the signal appearing at –0.25 V. EP can be also quantified as the difference between the total content (EP+NP) determined using the peak obtained at –0.25 V and the NP content found as was previously mentioned.

The reduction of all oxidation products was pH dependent, an equal number of protons and electrons being involved in the electrochemical processes. Interference studies showed that the activated electrode has excellent selectivity toward EP and NP in the presence of potential interferents like ascorbic or uric acids.

The developed voltammetric method has been successfully applied to the simultaneous determination of EP and NP from injectable pharmaceutical formulations, obtaining acceptable recoveries.

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PB8. VOLTAMMETRIC INVESTIGATION OF DIOSMIN

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The flavonoide glycoside diosmin (DIO) has anti-inflammatory, antioxidant and numerous other beneficial effects on human health. It was introduced in 1969 to treat lymphedema and varicose veins, but it was also employed as a chemopreventive agent in urinary-bladder and colon carcinogenesis [1]. Usually, flavonoids are electroactive compounds and yet there are still few reports on the electrochemical behavior of DIO [2, 3]. This work presents a voltammetric investigation of DIO on the disposable pencil graphite electrode (PGE). Cyclic voltammetry at PGE in acidic media emphasized that in the first potential scan DIO presents two irreversible oxidation signals (~0.85 V and ~1.3 V vs. Ag/AgCl) and one reduction wave (~0.62 V). In the next two cycles one can observe two supplementary pairs of peaks (at ~0.46 and ~0.66 V) corresponding to pH dependent, quasireversible electrode processes that involve an equal number of electrons and protons. Using the signal from ~0.85 V in 0.1 M H_2SO_4, DIO can be determined by differential pulse voltammetry in the concentration range 1×10^{-6} – 1×10^{-5} M with detection (LoD) and quantification limits (LoQ) of 3.40×10^{-7} M and 1.13×10^{-6} M DIO, respectively. Using adsorptive stripping differential pulse voltammetry (t_{ac} = 60 s, E_{ac} = 0, 0 V) DIO can be quantified between 1×10^{-7} M and 2.5×10^{-6} M with LoD and LoQ of 7.42×10^{-8} M and 2.47×10^{-7} M DIO, respectively.

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PB9. ELECTROCHEMICAL STUDY OF CHLOROGENIC ACID

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Chlorogenic acid (CA) is a polyphenolic compound commonly found in the human diet, present in many fruits, vegetables and in some beverages. CA influences the color, aroma, bitter taste and astringency of foods [1].

A simple, inexpensive, sensitive and rapid voltammetric method was developed using PGE (pencil graphite electrode) as the working electrode. PGE has the major advantages of being single-use, commercially available and inexpensive, also presenting a good reproducibility.

The influence of the solution pH on the electrochemical signals of CA was investigated using cyclic voltammetry (CV) and square wave voltammetry (SWV). The best results were obtained in strong acidic media and it was established that the oxidation process involves an equal number of transferred protons and electrons. The appropriate supporting electrolyte was found to be Britton Robinson buffer pH 1.81.

The voltammetric behavior of the CA was studied by CV on PGE at different scan rates between 10 and 1000 mV/s. The applied diagnosis criteria led to the conclusion that the anodic peak is generated by a quasi-reversible process, controlled by diffusion.

In order to perform the CA quantitative determination, the working parameters in SWV were optimized: pulse amplitude (50 mV), amplitude of the potential step (1 mV) and duration of the potential step (0.02 s). The intensity of the peak current varied linearly with the CA concentration in the range $1 \cdot 10^{-7}$ M - $1 \cdot 10^{-4}$ M. The limit of detection ($9.55 \cdot 10^{-8}$ M) and the limit of quantification ($2.89 \cdot 10^{-7}$ M) were calculated.

The developed method was successfully applied to the analysis of real samples (commercially available Green Coffee food supplements), the results obtained by SWV on PGE being in good agreement with the values declared by the manufacturer.

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PB10. SIMPLE AND SENSITIVE VOLTAMMETRIC DETERMINATION OF LAMOTRIGINE

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Lamotrigine (LTG), a phenyltriazine derivative, is an anticonvulsant used in the therapy of patients with epilepsy, bipolar disorder or dementia [1]. In the present study the electrochemical method for the determination of lamotrigine at activated pencil graphite electrode (PGE*) was optimized. Cyclic voltammograms of LTG in Britton-Robinson buffer (BRB) solution pH 4.6 exhibited an oxidation signal at +0.35 V and a reduction response at –0.96 V (vs. Ag/AgCl).

The oxidation peak, attributed to the LTG molecule dimerization, was used to develop a simple linear sweep voltammetric (LSV) method for the drug quantification. A dynamic linear range of $2.5 \cdot 10^{-5}$ – $1 \cdot 10^{-3}$ M LTG was obtained. The detection and quantification limits were calculated as $1.94 \cdot 10^{-5}$ M and $5.89 \cdot 10^{-5}$ M, respectively. The practical application of the sensor was demonstrated by determining the concentration of LTG in pharmaceutical samples with good precision and acceptable recoveries.

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PB11. MONITORING OF PHYSICO-CHEMICAL PARAMETERS OF GROUDWATERS FROM DOBROGEA AREA

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One of the most important environmental issue is groundwater contamination [1-3]. The aim of the work was to estimate the quality of some groundwaters from the Dobrogea area. Physico-chemical parameters like: pH, chlorides, nitrites, hardness, turbidity, alkalinity, conductivity, ammonium and nitrates were analyzed. The values of the parameters: chlorides, conductivity, hardness and nitrates for certain analyzed samples exceed the maximum levels allowed by the legislation. The metal content in chromium, cadmium, copper, iron, manganese, nichel, lead and zinc was also determinate using atomic absorption spectrometry with graphite furnace. The concentrations of the eight studied metals were within the maximum allowed limits established by the Romanian legislation. The Health Risk Index (HRI) was also estimated as the ratio of daily metal intake (MRI) to mean reference metal dose (RfD).

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PB12. OPEN EDUCATIONAL RESOURCES FOR LEARNING WASTE MANAGEMENT IN RURAL COMMUNITIES

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The organisations involved in the waste management can be of three different types: (i) as organisations acting in the waste management sector (either public or private) (ii) as institution with activity of public interest carried out by administration authorities and (iii) as ordinary waste-producing organisations (almost any organization).

Starting with 2019 the EU Commission Decision no. 2019/61 was launched, "on the best environmental management practices, sector environmental performance indicators and benchmarks of excellence *for the public administration sector"*. Further, in 2020 a new EU Commission Decision no. 2020/519 was launched, "on best environmental management practices, sector environmental performance indicators and benchmarks of excellence *for the waste management sector"*. Both decisions were under the Regulation (EC) no. 1221/2009 "on the voluntary participation by organisations in a Community eco-management and audit scheme (EMAS)". The harmonization of the two decisions is needed, so that their effective implementation should avoid the overload of the activity of the local public administration, which sometimes can be identified in all the three hypostases of organisations dealing with waste management.

Transilvania University of Brasov (Romania) as coordinator, and three more higher educational institutions (HEIs), Reykjavik University (Iceland), Bucharest University of Economic Studies (Romania) and Gheorghe Asachi Technical University of Iasi (Romania) will carry out the project with the title Environmental Education – OERs for Rural Citizens (EnvEdu – OERs). During this project, six modules as Open Educational Resource (OERs) will be developed, of which one module will be Waste Management in Rural Communities.

Thus, the present study aims to highlight the opportunities and barriers identified to the implementation of the two EU Decisions at the level of local rural public authorities.

PB13. SUSTAINABLE COMMUNITIES – LEVELS OF ANALYSIS

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Now-a-days the entire planet is facing with rapid urbanization. The environment provides living opportunities, but if these are altered, constraints on ensuring the living needs are registered. Consequently, challenges in terms of maintaining environmental quality faces politicians, administrative, scientific actors and also regular citizens. Sustainable development, as primary defined four decades ago, guides the anthropic activity to be restrained in between the limits of the planet. Since then, actions and steps were performed, but urban environmental quality remains on discourse agenda.

In 2015, the United Nations (UN) set 17 life-changing goals, known as Sustainable Development Goals (SDGs), and the 11th goal requires to "make cities and human settlements inclusive, safe, resilient and sustainable". Thus, the urban sustainability is a complex concept, it requires new ways of thinking and approaching the actions at different levels of socio-economic system.

The present paper discusses the concept of urban sustainability from the point of view of interaction between individuals and environment, at different spatial levels: micro-level (individual), mezzo-level (neighborhood), macro-level (regional/ national) and global-level. The levels are discussed and exemplified in terms of decisions regarding actions and their environmental impact, in the frame of development of sustainable communities.

PB14. FLUORESCENT DYE REMOVAL FROM WASTEWATER USING SBA-16-BASED NANOCATALYSTS

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Various mesoporous molecular sites have been synthesized using self-assembly of surfactants, with low and/or high molecular weight copolymers. SBA-16 is a porous silica with large mesopores (5–15 nm) similar to cages arranged in centered three-dimensional cubic symmetry [1]. Like SBA-15, it is synthesized under acidic conditions using a non-ionic surfactant – Pluronic, providing a complementary porosity. The mesophase can be created using mixtures of Pluronic P123 and Pluronic F127 [1]. Various catalysts have been applied for the oxidation of organic compounds in water, including the organic dyes. Nile Blue is a fluorescent dye, used in various bio-applications and it is considered a contaminant in water.

In this study, catalysts obtained by immobilization of transitional metals on SBA-16 mesoporous silica were used to oxidize the Nile Blue from wastewater. The obtained silica support and catalysts were characterized by SEM, TG, UV-VIS, FTIR, BET surface area and pore size distribution measurements. The oxidation reactions were carried out in a batch reactor at room temperature and pressure. The de-colorization experiments were monitored by UV-VIS spectrophotometry. The oxidation reactions followed the first order kinetics. The catalysts could be recovered and reused.

The Nile Blue from wastewater can be oxidized by catalysts obtained by impregnation of transitional metals on SBA-16 support, the oxidation products being less harmful for the environment and for the aquatic systems.

Acknowledgements*: The work has been funded by the Romanian Ministry of Scientific Re-search and Innovation, NUCLEU Program-Financing Contract no. 9N/2019, under Project PN 19 11 03 01 "Studies on the obtaining and improvement of the acido-basic properties of the nanoporous catalytic materials for application in wastes valorization".*

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PB15. PHYSICALLY ACTIVATED CARBONS OBTAINED BY PYROLYSIS OF RESIDUAL BIOMASS OR CATALYTIC CLEANING OF SYNGAS

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The global reduction of fossil resources has led to the search and development of new ways of recovery and reuse of materials and / or energy using renewable raw materials in order to reduce dependence on fossil resources and the effect of green house gas on climate changes. In this context, residual biomass that is not recovered is increasingly used for recovery as a material and / or energy vector. This paper investigated the role of the oxidizing agent used in the physical activation of chars obtained by pyrolysis of residual biomass on the resulting activated carbons (ACs) and their efficiency in tar cracking for its removal from syngas. The carbonaceous materials were prepared from a mixture consisting of rapeseed oil cake and walnut shells (1/1 part by weight), which is a local residual biomass. Slow pyrolysis was used to obtain the raw chars. Activated carbons (ACs) were then obtained by physical activation, using steam or CO_2 as activating agents. The carbon materials obtained were physically and chemically characterized before being used in tar cracking tests. The efficiency of carbonaceous materials in tar removing from syngas was studied, and toluene (T) was chosen as a tar model. The toluene cracking efficiency of char and activated carbons was deduced from the degree of toluene conversion compared to the thermal cracking achieved in the absence of carbonaceous materials. The nature of the oxidizing agent affected the porosity and composition of the AC produced: the activation with CO_2 produced AC with a higher carbon content and less ash content. This is due to the fact that the reduction of carbon with CO_2 had a kinetics up to 3-4 times slower than that performed in the presence of steam. CO_2 activation also led to a higher microporosity (87-89%) than steam activation (60-62%), but which provides a larger surface area. Chars resulting from pyrolysis did not show satisfactory efficiency for catalytic cracking of toluene, while activated carbon (AC) showed higher performance. This is probably due to the higher level of porosity and higher ash content. AC obtained by steam activation, which had a higher porosity, produced a much better catalytic effect and in addition was more resistant to deactivation.

PB16. ELECTROCHEMICAL SENSOR BASED ON CARBON NANOFIBERS FOR DETECTION OF *p*-COUMARIC ACID IN PHYTOPRODUCTS

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p-Coumaric acid (pCA) has an increased applicability in the nutraceutical, pharmaceutical and chemical industries, due to its antioxidant, antibacterial, anti-inflammatory, neuro and cardioprotective properties [1-3].

Given the biological importance of pCA, its detection in various food or pharmaceutical products becomes a necessity.

The present study aims to study the electrochemical characteristics of a carbon nanofibers (CNF-SPE) screen-printed sensor using cyclic voltammetry (CV) and the detection of p-coumaric acid in various phytoproducts. The electrochemical behavior of CNF-SPE was studied in PBS, pH=5.0. Subsequently, the values of the surface concentration of the electroactive species (Γ) were determined by using CV, at different scan rates, and fitting the I vs. v dependence according to the Laviron equation. In the next step, the CNF-SPE sensor was used for the study of pCA acid in PBS solution. It was observed peaks related to the electro-oxidation of pCA acid. The CNF-SPE sensor was used to perform a calibration curve using solutions with different pCA acid concentrations. The low values of LOD and LOQ obtained, demonstrated the sensitivity of CNF-SPE. The p-coumaric acid from three phytoproducts was qualitatively and quantitatively determined using CNF-SPE sensor. Furthermore, the sensor has been shown to have good sensitivity and reproducibility for the detection of p-coumaric acid.

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PB17. NON-INVASIVE TECHNIQUES FOR CHARACTERIZATION OF ORIGINAL ROMAN MOSAIC FRAGMENTS

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In this study, it was reported the preliminary results on the chemical and structural composition of remains of decorative elements of original Roman mosaic fragments collected from the Roman Mosaic Museum, Constanta (Romania). These investigations were carried out by using non-destructive and micro-invasive techniques such as Optical Microscopy, X-Ray Diffraction, Field Emission - Scanning Electron Microscopy - Energy Dispersive X-Ray Spectroscopy, Raman Spectroscopy. The fragments studied in this work, apart from being beneficial to different restoration opportunities of this Roman mosaic, could also be included in its modification through air pollution. The major and minor phase components of the studied mosaic fragments were determined, the crystal structure of the main phases was analyzed, and their three-dimension spatial arrangement was reconstructed. The similar composition of the major phases of all mosaic fragments can indicate a generic recipe for making mosaic elements, but minor phases were presumably added for coloring of mosaic pieces. Some degradation areas inside the volume of the mosaic fragments were found by means of the X-ray diffraction method. These degradation areas are probably related to the formation of iron hydroxides during chemical interactions of mosaic fragments with the sea and urban polluted atmosphere. The results also can offer important information about the original materials that were used in the Roman period.

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PB18. SIMULTANEOUS REMOVALS OF ANIONIC SPECIES BY THE ACTIVATED RED MUD WASTE

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This study presents a novel utilization of the activated red mud waste through the development of a highly selective sorbent for simultaneous removals of anion chloride, nitrite, nitrate, and sulfate from synthetic aqueous solutions.

Red mud is a waste generated by aluminum industries. Raw bauxite residue (red mud) is highly alkaline in nature (pH 10-13) due to Bayer process used for aluminum extraction. Neutralization of bauxite residue is required for safe disposal and utilization purposes. Two modification methods have been used to improve the reactivity of red mud adsorbent to removal of anionic species in the solution: acid treatment (ARM) and activation with cetyltrimethylammonium bromide (MRM).

The morphology, structure and properties of the activated red mud were evaluated using XRD, XRF, EDX and SEM, respectively.

The evaluation of the retention capacity of the anions from the wastewater was performed by modifying the contact time of adsorbent material with synthetic solution with anions known concentration.

The anions concentration was determined by ion chromatography using a DIONEX ICS-2500 chromatograph.

It was found that the modified red mud obtained from industrial waste have adsorbent properties. The highest adsorption capacity was obtained for the modified red mud residue (MRM) for which the maximum retention efficiency for NO_3^- and NO_2^- anions was 72% and 94%, respectively, after 120 minutes of interaction.

PB19. MODIFIED ELECTRODES BASED ON 4-(AZULEN-1-YL)-2,6-BIS((E)-2-(THIOPHEN-2-YL)VINYL) PYRYLIUM PERCHLORATE FOR HEAVY METALS DETECTION

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Human exposure to various dangerous chemicals including heavy metals occurs every day through multiple routes, such as environmental factors, skin contact and even via the umbilical cord to the unborn child. As the amount of fresh water on earth is limited, and its quality is under constant pressure, preserving the quality of fresh water by an integrated monitoring is a very important matter. In this study, a modified electrodes based on a new synthetized azulene-thiophene vinyl pyrylium salt for heavy metals detection from waters is proposed. The 4-(azulen-1-yl)-2,6-bis((E)-2-(thiophen-2-yl)vinyl) pyrylium perchlorate (**L**) was first characterized using electrochemical methods (cyclic voltammetry (CV), differential pulse voltammetry (DPV) and rotating disk electrode (RDE)). Poly**L** films modified electrodes were obtained by successive scanning or by control potential electrolysis (CPE) at different charges and potentials. The new electrodes were applied for the recognition of the following heavy metals ions: Cd(II), Pb(II), Cu(II), Hg(II) [1-3].

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PB20. EVALUATION ON THE CHEMICAL COMPOSITION OF SMOKE FROM HEATED, NOT BURNT, TOBACCO IN ELECTRONIC CIGARETTES

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The smoke produced during the traditional cigarettes tobacco burning or by the electronic cigarettes tobacco heating contains different amount of organic and inorganic chemicals resulting toxic and/or carcinogenic for humans [1, 2].

Based on the claimed lower dangerousness of its smoke, we decided to analyze the chemical composition of both the tobacco and the smoke of a new commercially available electronic cigarette with a temperature regulation software, which heats tobacco without burning it.

Chemical analyzes have been carried out both on tobacco before and after the heating and on the smoke generated both by the electronic and the traditional cigarette.

The analyzed compounds, relevant for human health, were polycyclic aromatic hydrocarbons, metals, aldehydes, benzene and its derivatives, phenols and aromatic amines. In addition, we determined the nicotine content in the pre- and post-heating tobacco and in the smokes.

The analyzes on the cigarettes' smoke were performed by collecting it in a homemade smoke machine and carrying out the smoking process under standard conditions (puff of 2 s and 35 mL of volume; interval between two successive puffs: 30 s). The chemical composition of pre and post heating tobacco was determined by performing various extraction procedures and analysis by chromatographic methods (GC, LC, ICP-MS).

The results obtained by the comparison between the components in the traditional and in the tobacco-heated smoke confirmed that in the latter the content of the searched analytes was reduced in comparison with those contained in the traditional burning derived one. In particular, the concentration of organic compounds such as the various aldehydes and polycyclic aromatic hydrocarbons were of one or two order of magnitude lower.

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SECTION C: PHYSICAL CHEMISTRY

PC1. NUMERICAL MODELING OF MIXED-MODE DELAMINATION FRACTURE IN UNIDIRECTIONAL AS4/PEEK COMPOSITES

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Recently, the *AS4* carbon fiber reinforced poly-ether-ether-ketone (AS4/PEEK) composites became very attractive for orthopedic implants, due to biocompatibility, similar modulus to bone and ability to withstand prolonged fatigue strain [1, 2]. As a consequence of adjacent layers separation, composite laminates suffer delamination failure under static and fatigue loadings, causing an important degradation of the load-bearing property for composite structures [3]. In this paper it was developed a Finite Element Method (FEM) model for the simulation of interfacial failure between two plies of an AS4/PEEK composite sample using Cohesive Zone Model (CZM), under the frame work of Comsol Multiphysics software. Mixed Mode Bending (MMB) method was considered here for the numerical implementation of progressive delamination propagating in composite specimens with pre-existing cracks. Volumetric strain and von Mises stress at the maximum load before fracture have been evaluated at here different ratios between mode II strain energy rate and total strain energy rate G_{II}/G_T = 20 %, 50 % and 80 %.

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PC2. REFRACTIVE INDEX OF L-ALANINE AT DIFFERENT TEMPERATURES: EXPERIMENTAL AND PREDICTIVE CALCULATIONS

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As a continuation of our earliest studies [1], this paper reports experimental refractive index for L-alanine in water and aqueous electrolyte solutions between 293.15 and 323.15 K, at various amino acid and salt modalities. It is noticed an increasing tendency of refractive index with enhanced NaCl and L-alanine concentrations. The rise of temperature induces the decrease of refractive index at constant salt or amino acid molality. Concentration dependence of refractive index was obtained using equation of Koohyar et al., 2011 [2]. As result, the values of refractive index at infinite dilution, are given. Also, discussion related to predictive optical properties of L-alanine in vacuum and in water for equilibrium geometry at ground state, is made. The predictive results of polarizability parameter are realized using Spartan software [3] and Density Functional method (DFT) with Becke's Three Parameter Hybrid Functional using the Lee-Yang-Parr correlation functional theory [4], 6-31 G (d, p) basis set [5]. These findings scientifically contribute to explain intermolecular forces in the given binary and ternary systems.

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PC3. EVALUATION ON DRUG RELEASE KINETICS FROM POLYMERIC NANOPARTICLES LOADED WITH POORLY-WATER SOLUBLE APIS

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Nanotehnology provides solutions to overcome the drawbacks of poorly solubile active pharmaceutical ingredients (APIs). The aim of this research was to investigate the release behaviour of a combination of two poorly-water soluble APIs from poly (D,L-lactide-co-glycolide) (PLGA) nanoparticles. Amlodipine besylate - AML, a calcium channel blocker, and valsartan - VAL, an angiotensin II receptor antagonist drug, were used as poorly-water soluble model drugs.

PLGA nanoparticles loaded with AML-VAL (1:16 w/w) were obtained by nanoprecipitation using an amphiphilic block copolymer - Pluronic F127 as stabilizer. The drugs release from the PLGA nanoparticles was determined by a dialysis membrane method under sink conditions. The whole system was kept under stirring at 150 rpm at 37°C, using 0.1 M sodium phosphate buffer pH 7.4 as release medium. Samples were taken at predetermined intervals for 48 h from the receiver solution and the released drugs in each time point was determined by spectrophotometry.

Nanoparticles provided a slow release for both APIs and an attenuated burst effect compared to free drug. Five kinetics models such as Zero-order, First order, Korsmeyer-Peppas, Higuchi and Hixson-Crowell were applied to predict drug release profiles. The Higuchi model and Korsmeyer-Peppas (R^2>0.97) best described physicochemical release phenomenon for each PLGA formulations.

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PC4. SPECTROSCOPIC AND VOLTAMETRIC TECHNIQUES FOR ASSESSING THE COMPLEXING CAPACITY OF E-5-((5-ISOPROPYL-3,8-DIMETHYLAZULEN-1-YL) DYAZENYL)-1H-TETRAZOLE OF HEAVY METAL CATIONS

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Chemically modified electrodes (CMEs) based on polymeric films of E-5-((5-isopropyl-3,8-dimethylazulen-1-yl) diazenyl)-1H-tetrazole (**L**) deposited on the surface of the glassy carbon electrode have been used for the detection of heavy metal (Me) ions [1]. The investigation of the complexing properties of CMEs with poly**L** film was carried out by chemical preconcentration and anodic stripping. The ability of the **L**-modified electrode to complex metal cations (Cd(II), Pb(II), Cu(II) and Hg(II)) from aqueous solutions of 10^{-8} to 10^{-4} M concentrations was tested. Pb(II) and Hg(II) ions have shown the best signals. The detection limit was estimated at 10^{-8} M for Pb(II) ion. The UV-Vis absorption spectra of **L** solutions in presence of heavy metal ions confirmed the formation of Me(II)$\mathbf{L}_2$ complexes with Pb(II) and Hg(II) [2]. It was shown through voltammetric techniques and UV-Vis spectroscopy that **L** can be used to detect Pb(II) and Hg(II) ions in different water samples.

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SECTION D: PETROLEUM TECHNOLOGY AND MANAGEMENT

OD1. EXPERIMENTAL STUDY FOR OBTAINING QUENCH OIL FROM A RENEWABLE RESOURCE

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The exigencies concerning the quality of quench oils for thermal treatment of metallic parts were recently orientated towards the development of new materials foccusing on costs mitigation and environmental protection [1]. Among other properties, the quench oils are characterized by relatively low viscosity, extremely low water content and high cooling rate [2].

The present work was dedicated to obtaning quench oil from rapeseed oil, through thermal cracking, at 300-375 ^{o}C, in advanced vacuum (10^{-3} mbar), and residence time between 2 and 20 min. Important yields of pyrolitic oil were obtained at 300-310 ^{o}C , between 61% and 87%.

Even though the viscosity of the raw oil diminished during the process by only 2-3.3 cSt measured at 100 ^{o}C, the cooling rate at 200-400-600 ^{o}C of the pyrolitic oil was much higher, even better than that of the usual commercial oil. This indicates that the heat transfer was favoured by lower viscosity and recommends the pyrolitic oils for the rapid cooling (quench) of steel parts during their thermal treatment.

The Rockwell hardness tests on carbon-steel 25CD4 specimens proved that the pyrolytic oils obtained in this experiment are prone for use as quench oils, since the values of the hardness degree are close (43-45 HRC) to the comercial mineral oil (45 HRC).

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OD2. NEW TECHNOLOGY FOR ETHERS MANUFACTURING BY REACTIVE DISTILLATION PROCESS

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It is well known that ethers are components used in gasoline formulation to increase the performance of spark ignition engines by increasing the octane number and reducing the impact on the environment.

The reactive distillation is a process gaining ground in front of conventional synthesis methods.

Thus, an experimental study of *in situ* etherification of catalytic cracking light gasoline through a reactive distillation process was carried out.

The experimental laboratory plant consists in a fractionation column equipped with Rashig packing, and a catalyst layer interspesed in the packing. The catalyst is an acid-functionalized ion exchange resin, with sulfate ions (commercial name Purolite) which is commonly used as a catalyst at the synthesis of MTBE and TAME.

The aim of this study was to achieve *in situ* etherification of isoolefins and olefins from catalytic cracking light gasoline with different alcohols: methanol, ethanol, isopropanol and n-butanol, at temperatures in range of 60-70^{o}C, at atmospheric pressure, in a reactive distillation system.

Based on the chromatographic analysis of the etherification products corroborated with the mass balance of components, the conversions of the different olefins were calculated. From here, more detailed interpretations of the etherification results could be made.

Another important conclusion, based on the experimental data obtained in this work and in previous works, was that a process of increasing the octane number of petrol can be developed by *in situ* etherification of isoolefins and olefins in the reactive distillation system.

OD3. PREPARATION OF SULFONATED PVA-PVP-HPA MEMBRANES FOR FUEL CELL APPLICATIONS

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A novel ionic polymer membranes of different thicknesses based on polyvinylpyrolidone (PVP), polyvinyl alcohol (PVA), sulfosuccinic acid and heteropolyacids such as silicotungstic acid (SiWA) and phosphotungstic acid (PWA) with or without silica have been synthetized for polymer electrolyte membrane fuel cells (PEMFCs). The chemical characterization of the membranes has been studied by Fourrier Transform Infrared Spectroscopy (FT-IR). The thermal stability of the membranes has been studied using the techniques of thermogravimetric analysis (TGA) and differential Scanning Calorimetry analysis (DSC).The water uptake, ionic conductivity, ionic exchange capacity and fixed ion concentration of these membranes were determined. The results showed that the ionic conductivity and the water uptake of the nanocomposite membranes PVA-SSA-PVP-HPA-SiO_2 were higher than that of the PVA-SSA-PVP-HPA membranes due to hydrophilic nature of SiO_2 nanoparticles. PVA-SSA-PVP-HPA-SiO_2 membranes containing 5 wt.% Of silica nanoparticles have demonstrated the best physicochemical characteristics, water uptake reaches 77 %, an ionic conductivity of $7.55.10^{-3}$ $S.cm^{-1}$ and ion exchange capacity of 3,67 mmol $.g^{-1}$. This value is much higher than those of membranes Nafion® 117 (0,93) and Nafion®112 (0,99) which do not exceed 1 $mmolg^{-1}$. The results suggest that the obtained membrane shows good thermal stability, excellent mechanical property and high ionic conductivity, and the low-cost hybrid membrane can be a promising candidate for future applications related to proton exchange membrane fuel cell (PEMFC).

PD1. HYDROCONVERSION OF PYROLYTIC BIO-OIL OVER Cu/Mo CATALYST

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Conversion of pyrolytic oil into deoxygenated liquid fuels is made in order to obtain biofuels components and green bitumen solvents. These processes are dependent on the nature of the catalyst tested and the reaction conditions. Therefore, the deoxygenating process is accompanied by other secondary reactions such as hydroisomerization, dehydrogenation and cyclization, which occur simultaneously [1]. The hydroconversion study was carried out on pyrolytic bio-oil obtained by pyrolysis of the digestate conditioned with lipid fraction. The granular Cu-Mo/gama alumina catalyst was prepared by impregnating with an aqueous solution of copper nitrate and ammonium molybdate using the pore filling method. The catalyst was characterized by textural analysis and acidity measurements. The textural characteristics of the catalysts tested were: specific surface area, pore volume, average pore diameter, pore size distribution. The specific surface area was calculated using the BET equation in the linear part of the adsorption isotherm. For evaluation of pore distribution and pore size, the hysteresis isotherms desorption branch was applied using the BJH method. The acidity measurements were done by thermodesorption of diethylamine. Experiments were carried out on a laboratory equipment in continuous system using a fixed bed catalytic reactor at 275-325°C, pressure from 10 bar to 40 bar and the liquid hourly space velocity from 0.8 h^{-1} to 1.5 h^{-1}. The main compounds resulting from the process are hydrocarbons and oxygenated compounds.

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PD2. BIOPENTANOL, A POSSIBLE FUEL FOR TRANSPORTATION DOMAINE

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The growing demand for transport fuels in correlation with the need for environmental protection has led to the trend of diversification of biofuels used as fuels for internal combustion engines. The introduction of new biofuels on the transport fuels market requires a detailed knowledge of both the properties of new biofuel and the properties of their blends with conventional fuels.

Biopentanol can become a candidate either as an additive or as a substitute of conventional fuels. In order that blends of conventional fuels with 1-pentanol to be used in the field of transportation, their properties must be known, respectively how the addition of pentanol influences the properties of the basic fuel. One of the properties that influence both the combustion process from diesel engine, but also transport and storage operation, is density. The aim of this study is to report density data for diesel fuel+1-pentanol and biodiesel+1-pentanol blends over the entire composition domain and for temperature ranging from 20 ºC to 40 ºC and to evaluate the accuracy of different models to predict these blends properties.

The decrease of the density of the blends with the increase of the alcohol content was observed both for the blends of pentanol with diesel fuel and biodiesel. It was noted that the dependence of density on the composition of the blends is not linear. Such behavior is usually typical to systems characterized by differences in the chemical structure of the components. The density decrease with the increase of temperature was observed for the two studied blends. The prediction of the density of the blends with 1-pentanol have quite small values of the absolute and relative error when using Kay rule. However, a third degree polynomial equation has a slightly higher accuracy in density estimation. On the other hand, Kay rule is easier to be used because its application only requires knowing the density of the pure components of the pseudo-binary blends of fuels.

SECTION E: FOOD CHEMISTRY AND ENGINEERING

OE1. STUDIES OF ELECTROCHEMICAL BEHAVIOR AND SOME BIOLOGICAL EFFECTS PRODUCED AT CELLULAR LEVEL OF MONOSODIUM GLUTAMATE FOOD ADDITIVE

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Monosodium glutamate (E-621, abbreviated MSG) is a food additive widely used in the food domain as a flavor and taste enhancer. The present study aims to evaluate MSG electrochemical behavior, its detection in food products and its biological effects on RAW 264.7 murine macrophage cells.

Both cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) experiments were performed using three types of screen-printed electrodes (DropSens) having carbon, gold or platinum as non-enzymatic working electrode. Aqueous solutions of single MSG solute as well solutions with added supporting electrolyte (KNO_3, $NaNO_3$ or KCl) were prepared. The CV results showed signal appearance for MSG as cathodic peaks or shoulders with a linear dependence between the current and MSG concentration. The electrode process of glutamate ion is irreversible, and diffusion controlled. Layered double hydroxides (hydrotalcite) films containing Ni and Al formed by laser deposition improved the cathodic reduction of glutamate anion, mostly for carbon screen-printed electrodes. EIS plots recorded at open-circuit potentials as Nyquist or Bode diagrams can give valuable information on the electrode/electrolyte interface behavior. We noticed that the charge transfer resistance (diameter of Nyquist semicircles) decreased in MSG solutions prepared with supporting electrolyte; this can be attributed to the enhanced electron transfer in cathodic process. Also, Bode plots showed lower values for the maximum of phase angles thus evidencing a better electrical conductivity of the interface.

We demonstrated the possible detection of MSG from food products by means of CV method using the aqueous extracts from bologna sausage (PA), frankfurter hot dogs (CF), hot dogs with cheese (CB) and vegetable soup concentrate cubes (SM). In the case of carbon screen-printed electrode, the linear correlation between cathodic peak current and MSG concentration suggests the possible use of CV for its direct determination for food industry.

On the basis of this calibration curve we have found the concentration order of MSG in food samples as the following: CF < PA < CF < SM.

The *in vitro* study of antiproliferative effect, cytotoxicity and proinflammatory activity of MSG using the RAW 264.7 murine macrophage line was conducted in 3 complementary directions: first, establishing the ability of monosodium glutamate to induce cell mortality, by using the MTT assay to determine cell viability; second, establishing by its oxidizing activity if MSG is toxic for cells inducing oxidative stress, measured by the Griess test for determination of extracellular NO; third, to observe whether MSG presence induces an immune response quantified by the secretion of proinflammatory cytokines, tumor necrosis factor (TNFα) in this case, measured through the immunoenzymatic ELISA technique. Tests regarding the viability of MSG on the murine macrophage tumor cell line suggest that its toxicity is due, in part, to the increase in oxidative stress. The low levels of TNFα suggest that MSG does not act by inducing inflammation but causes cellular damage through nitrogen oxide production. Regarding the cytotoxic effects induced by MSG on murine macrophages at concentrations similarly to native biological conditions, we observed a uniform decrease of TNFα secretion for exposure of RAW cells in more concentrated MSG solutions (higher than 25 mM), a fact which is apparently contrary with some literature data that indicated an increases of this cytokine levels following MSG intake.

PE1. CHEMICAL COMPOSITION AND TEXTURE EVALUATION OF FOOD EMULSIONS

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Emulsions represent an important class of semisolid foodstuff; many food products exist as emulsions at some phase throughout production process. The emulsion can be defined as a mixture of two immiscible phases, one of the phases being dissipated as small round droplets in the other one. The emulsion samples analyzed in this research were represented by butter with different fat content. The butter's physicochemical parameters analyzed were as follows: moisture content, fat content and color parameters. For samples firmness measurements a texture analyzer was used (Mark 10 Corporation, ESM 301, USA) fitted with 100 N load cell. Also a gas chromatograph (Shimadzu Corporation) was used for fatty acids determination.

The fat content of analyzed samples ranged between 81.5% and 59.3% while the water content increased with the decrease of the fat content from 16.82% to 38.78%. The butter brightness varies from 89.50 to 95.15 the highest values being recorded by the samples with the lowest fat content. All a* color parameters were in the negative part of the green – red axis with the values ranged between -7.33 and -6.41; instead the b* color parameters are all in the positive part of the yellow–blue axis more towards yellow. The b* color parameter varied from 19.28 to 31.42, the highest value being observed for butter samples with the highest fat content. Pearson correlation highlighted a positive correlation between fat content and samples firmness (r = 0.883*) and also a negative correlation between moisture content and firmness (r = 0.904*).

Both mechanical and color parameters of the analyzed samples were influenced by the fat and water content. A high fat content causes a high firmness, adhesiveness and a low cohesiveness.

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PE2. DESIGN AND CHARACTERIZATION OF AERATED CONFECTIONERY PRODUCTS

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The confectionery industry is a unique and diverse food sector, involving a wide range of ingredients and technologies to produce innovative and special sweet products. Generally, the desired structure of the bakery products and especially of confectionery ones depends on the aeration process. The purpose of this study was to develop new aerated confectionery products using different raw materials and techniques and also to characterize them in terms of chemical composition, porosity, texture properties and appearance. For chemical characterization of the confectionery samples the protein content, moisture, fat content, total acidity, water activity and the concentration of soluble substances were measured. The texture profile analysis is a double compression test which can quantify a large number of texture parameters in a single analysis and it was used for texture measurements of the design samples. The aeration process was performed by mechanical whipping with a planetary mixer.

One factor analysis of variance - ANOVA highlighted that the samples concentration of soluble substances express as º Brix differ significantly ($p < 0.01$); the confectionery samples with vegetable cream showed the highest concentration of soluble substances (26.75). The fat content ranged between 14.50 % and 21.05 %, while the protein content was in the same range (10.40 - 9.55 %). The aeration process of confectionery products leads to a lower caloric intake by increasing the final volume of the product and by reducing the amount of ingested food. As regarding the texture parameters, the protein content influences the samples fracturability, while the air introduced into the product influences the samples hardness.

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PE3. EVALUATION OF THE RHEOLOGICAL PROPERTIES OF THE DOUGH AND THE CHARACTERISTICS OF THE BREAD WITH THE ADDITION OF PURPLE POTATO

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The aim of this study was to determine the rheological characteristics of the dough at the addition of purple potato paste in different quantities (0-100 g). The wheat flour type 480 and 1250 were used. The rheological characteristics of the dough were determined with the help of Chopin Alveograph analyzing the tensile strength. The rheological measurements were made with the HAAKE RheoWin Mars 40 rheometer and the dough's visco-elastic modulus was analyzed at the frequency of 1-20Hz. The bread samples were analyzed in terms of volume, porosity, color, and texture. The textural parameters determined with the help of the texturometer were the elasticity, adhesiveness and stickiness of the bread crumb. It has been found that the addition of purple potato dough does not adversely alter the rheological properties of the dough. The elasticity and stickiness of the bread core increases with the increase of potato addition in the case of whole-grain flour. The color of the bread intensifies as the dose of purple potato paste increases.

PE4. OSMOTIC DEHYDRATION OF APPLE AND PEAR SLICES: COLOR AND CHEMICAL CHARACTERISTICS

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Osmotic dehydration is the pre-treatment method of preservation the fruit and vegetable to increase its shelf-life in which these are immersed in concentrated salt or sugar solutions.

The effect of osmotic dehydration was investigated on the color and chemical characteristics of dehydrated fruits (apple and pear) in fructose osmotic solutions. Difference in CIE-LAB, chroma - C^* and hue angle H^* were performed with a Chroma Meter CR-400/410. Apple *(Malus domestica 'Jonathan')* and sweet autumn pear variety *(Pyrus comunis)* were osmotically dehydrated in three aqueous solution of fructose (40, 60 and 80%), during 3 h of process at temperatures of 20 ^{0}C, with fruit/osmotic agent ratio of 2:1. Water loss and solids gain showed significant differences depending on the concentration of the osmotic agent and process time. The use of highly concentrated osmotic solutions induced losses of phenolic content (TPC) and ascorbic acid in sliced apple and pears. Fructose concentration and osmosis time induce significant increase of a* and b* colorimetric parameters but did not affect the lightness (L*) of pear slices.

PE5. LIFE CYCLE ASSESSMENT OF FERMENTED MILK: YOGURT PRODUCTION

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Yogurt is a fermented milk product, resulted through milk acidification by lactic acid bacteria, highly appreciated worldwide. In this study, life cycle assessment (LCA) methodology was applied for modelling of environmental impacts associated with yogurt production. The system boundaries include the following activities: milk processing, transport, solid waste and wastewater treatments. Functional unit set for this study is 1 kg of produced yogurt. The input and output data were collected from various sources like reports, databases, legislation and others. All these data were used further in the impact assessment stage performed with GaBi software which includes LCA methods like CML2001 -Jan. 2016, ReCiPe 1.08, UBP 2013, EDIP 2003 and others. Results showed that the global warming potential (GWP) determined for yogurt was 2.92 kg CO_2 eq. per kg of yogurt, while acidification potential (AP) was approximately 0.014 kg SO_2 eq. per kg of yogurt. It was observed that the main contributor to all impact categories is consumption of electricity during the yogurt production, mainly in the pasteurization, evaporation and cooling stages. 61.4% of the emissions resulted from transportation of raw materials contributes to GWP, while 38.3% to photochemical ozone creation potential (POCP). Emissions from wastewater treatment are contributing especially to the eutrophication potential (EP), while emissions from solid waste landfilling are contributing mainly to POCP.

PE6. PRODUCTION OF BETA GLUCAN FROM SPENT BREWER'S YEAST

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Yeast cells (*Saccharomyces cerevisiae*) have been widely used in many branches of industry, not only in baking and alcohol production. Interest in yeasts has gradually increased with the possibility of being used as a source of nutrients, functional foods with potential biological activities or in bioremediation.

In the beer industry for example, yeast *Saccharomyces cerevisiae* exhibit a finite replicative lifespan after which, due to a high amount of polysaccharides, amino acids, polyphenols, and mineral compounds they can be reused in obtaining new valuable compounds. World-wide spent yeast is still underutilized, a significant amount of yeast are mostly used for swine and ruminant feed. Only in the brewery about 2.1 million tons/year of spent yeast could represent an alternative source of bioactive compounds such as beta glucan, a β-1,3/1,6 polysaccharide found in the yeast cell wall.

On this basis, for this study spent yeast slurry from brewery with an 18% solid content was subjected to extraction in order to obtain β-glucans. After the autolysis by endogenous enzymes a further alkaline acid treatment was applied to break the cell wall, followed by successive washings for isolation and characterization the water insoluble glucan.

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PE7. THE CORRELATION BETWEEN QUALITY PARAMETERS AND MINERAL CONTENT OF FRUIT JUICES

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Fruit juices are a rich source of nutrients and valuable components [1-2]. The aim of this study was to investigate the quality parameters such as total acidity, vitamin C, total phenolic compounds, total nitrogen, protein content, Brix index, free CO_2, carbohydrates from fruit pulp, fresh juice and different brands representative for the Romanian market of orange, lemon, grapefruit, kiwi, apple and pear juices. It was also studied the content of iron, copper and chromium in order to calculate Pearson correlation coefficients. The highest amounts of total phenolic compounds, respectively total nitrogen and carbohydrates were detected in grapefruit fresh juice. The results showed that correlations for all the studied fruit juices samples between total phenolic compounds, respectively protein content and mineral content are positive. The total phenolic content is closely correlated with iron ($r = 0.9428$) and copper ($r = 0.9873$) for all of juices samples. A significant correlation was statistically observed between the total phenolic content and the concentration of copper ($p = 0.01 < 0.05$). No significant correlation was observed in the case of chromium (Pearson coefficient is negative in all cases). Also, no correlation was observed in the case of vitamin C. Consequently, the correlations of total polyphenols and protein content with mineral content suggested the influence of these compounds on mineral bioavailability.

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PE8. QUALITY CONTROL OF WHITE AND ROSÉ WINES

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Physico-chemical analyzes are a valuable tool in knowing the composition of grapes, must and wine in different stages, but also of the finished wine subject to bottling. One of the parameters, volatile acidity analysis was probably the first measure of wine quality and is routinely used as an indicator of wine spoilage. The sulphur dioxide was indispensable in winemaking due to conservation properties and the alcohol concentration acting as antiseptic for yeasts, reducing the total acidity and contributing to the wine bouquet [1,2]. The aim of this study was to investigate the quality parameters such as: pH, volatile acidity (VA), total acidity (AT), sulphur dioxide (SO_2) and alcohol concentration (CA) for white and rosé wines and one of homemade rosé wine. The GlassChem oenological system was used to determine SO_2, VA and CA. AT was determined by acid-base titration and the pH was measured with a pH220 pH-meter from Extech Instruments. VA and AT were maximum for the home-made rosé wine. For the white wines the pH values ranged between 2 and 2.7 and between 3 and 3.5 for the rosé wines, respectively. Physico-chemical parameters studied for white and rosé wines were within the maximum limits allowed by the actual legislation, except for one white wine, whose sulphur dioxide content exceeds the maximum limit allowed. Volatile acidity value obtained for homemade rose wine exceeds the permitted limit.

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PE9. DOSAGE OF SULFUR DIOXIDE IN SOME FRUIT JAM AND JELLY

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Sulphur dioxide (SO_2), labelled E220 on food packaging, is used as a preservative for certain dried fruits, canned vegetables and fruits, natural juices and in wine production, as an antimicrobial and antioxidant agent. Sulphur dioxide present in small amounts of food is tolerated by most people, but in some cases it can cause allergic reactions or other side effects, such as headaches. In the experimental part of the paper were analysed seven samples of jam and six samples of jelly from different fruits sold on the Romanian market in order to dose the total sulphur dioxide content. Total sulphur dioxide was determined by the optimized Monier-Williams method, which is a distillation-titration procedure (the sulphur dioxide distillation from complex matrixes followed by iodine titration). The experimental results showed high concentrations of sulphur dioxide above the maximum limits allowed in all the jam samples analysed and in five of the six jelly samples studied. The highest concentration of sulphur dioxide was recorded in currant jam (320 mg/kg) and cherry jelly (242.04 mg/kg), well above the maximum allowed limits (by over 6, respectively 4 times higher).

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PE10. NITRATES AND NITRITES OCCURRENCE IN FRUITS

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Toxic substances in food have always been a source of concern for specialists, especially since in recent years the excessive use of various chemicals in agriculture, environmental pollution, increasing industrialization of food, have taken this issue to a higher level with direct implications on the health of consumers. The presence of toxic substances takes on increasingly varied and increasingly complex forms. The present study aims to determine nitrates and nitrites concentrations from different varieties of apples and pears sold on the Romanian market by small farmers.

Samples were taken for analysis from 10 varieties of apples and 7 varieties of pears sold by small farmers on the Romanian market. The following apple varieties were analysed: Mutsu, Red Delicious, Ionatan, Golden, Idared, Starkrimson, Florina, Russet, Granny Smith and Renet. The pear varieties subjected to the analysis were: Abate, Xenia, Jambon, Red, Williams, Conference and Bergamote. Nitrates and nitrites were measured by molecular absorption spectrometry. Following the analysis of the results obtained, it was found that: all varieties of apples and pears have nitrates in very high concentrations, above the safety limit. The highest concentration of nitrates was recorded in the apple variety Starkrimson of 210 mg NO_3^- / kg and in the Bergamot pear variety of 260.54 mg NO_3^- / kg. Traces of nitrites were also recorded in all varieties of analysed fruits.

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PE11. CONSIDERATIONS ON GOAT MILK BIOCHEMICAL COMPOSITION

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The nutritional quality of goat's milk is superior to cow's milk, between them there are significant differences in lipid composition; thus, goat's milk being richer in butyric acid (C4: 0), caproic (C6: 0), caprylic (C8: 0), capric (C10: 0), lauric (C12: 0), myristic (C14: 0)), palmitic (C16: 0), linoleic (C18: 2) and lower in stearic acid (C18: 0) and oleic acid (C18: 1) [1]. The high amount of medium chain fatty acids, characteristic of goat's milk, has many benefits for human health. About 20% of the fatty acids in goat's milk are short-chain fatty acids, which are easier to digest, and the concentration in medium-chain fatty acids (55%) is relatively high [2]. The fat content is one of the most important technological, nutritional and dietary parameters of goat's milk. Our data show that the percentage of milk fat increases immediately after parturition, then decreases for most of the lactation. This is due to two phenomena: a diluting effect, due to an increase in the volume of milk up to the peak of lactation and an effect of decreasing lipid mobilization, which leads to decreased plasma levels of non-esterified fatty acids, especially C18: 0 and C18: 1, necessary for lipid synthesis in the mammary gland. Starting with the third month of lactation, the average amount of milking milk/day undergoes only slight variations. Also, the fat and protein percentage remains relatively constant during June-August. The levels of monounsaturated, polyunsaturated fatty acids and conjugated linoleic acids in milk increased during the summer months compared to the spring months, and the level of saturated fatty acids decreased during the summer months. Our data indicate that Carpathian breed females, whose food comes mostly from grazing, produce milk during the summer with an omega-6 / omega-3 ratio below 4. In conclusion, grazing has a major beneficial effect by decreasing the level of saturated fatty acids and increasing the level of fatty acids in goat's milk, considered to have a favorable effect on human health (C9-18: 1, C18: 3n-3, C9t11-CLA), compared with the winter diet of animals, especially that based on concentrates and corn silage [3].

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PE12. THE FIRST STEP OF BIOETHANOL PRODUCTION - EXTRACTION YIELD OF CELLULOSE FROM SOFTWOOD SAWDUST

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Current trends are to reduce the use of fossil fuels and their impact on the environment and to obtain energy from solar, wind and biofuels. Because in nature there are huge quantities of lignocellulosic materials, biofuels, especially bioethanol, could be produced by utilizing lignocellulosic biomass. Therefore, the first step to be taken into account for obtaining bioethanol is the processing of lignocellulosic biomass by various pretreatment methods: physico-chemical, mechanical or biological.

The purpose of this work was to extract the cellulose fraction from lignocellulosic biomass (softwood sawdust) by physical-chemical pretreatment. The sawdust of different granulosity was pretreated acid and alkaline using different concentrations of sulfuric acid, respectively sodium hydroxide. In this study, the temperature, the solid-liquid ratio and the cellulose extraction time were also taken into consideration. This step is very important because it has as main purpose the removal of lignin but also of the other components existing in lignocellulosic biomass.

After the application of the two pretreatments (acid and alkaline), higher yields in cellulose were obtained for the alkaline pretreatment. Some of the components released after the two pretreatments were analyzed by spectrophotometric and HPLC methods.

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PE13. DEVELOPMENT OF BIODEGRADABLE AND EDIBLE MATERIALS FOR PACKAGING MEAT PREPARATIONS

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The food industry is one of the major generators of plastic waste derived from conventional synthetic petroleum-based polymers which are non-biodegradable. A concern of specialists is to replace these materials with those based on biopolymers that can protect food, extend shelf life and increase their nutritional value, improve organoleptic characteristics such as taste, smell, appearance by adding additives to the base matrix. The biopolymers used in film formulation were sodium alginate, agar, and glycerol was used as a plasticizer. The study was focused on finding the optimal ratio between the biopolymers that form the packaging matrix and the barrier and physical-mechanical properties of the materials used. The lowest membrane water transfer rate and the lowest amount of water transferred in 48 hours was recorded in membranes with double alginate content compared to agar, as well as the lowest value of water activity a_w (of 0.2886 at 25.05°C) which demonstrates that the membrane ensures the preservation of the product in the absence of the development of microorganisms. Also, the same membranes had the highest hardness values (HL), ensuring the product against external mechanical actions. The color of the samples evaluated using a colorimeter (Chroma Meter CM-700, Konica Minolta, Japan) varied from slightly yellow to slightly green, without influencing the consumer's perception.

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