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PLENARY LECTURES

PL1. **CHAOTROPICS IN RPLC SEPARATION MECHANISM**

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Chaotropic agents (ChA) are weakly hydrated ions (of inorganic or organic nature), with significant charge delocalization, symmetrical conformation (usually spherical), exhibiting lyophilic properties [1]. Chaotropic agents are either anionic or cationic by nature. Accordingly, some ionic liquids can be considered chaotropic or lyophilic.

ChA are used as additives in mobile phases for liquid chromatography (LC) for tuning retention (and consequently selectivity) and peak symmetry for cationic analytes (protonated analytes in acidic environments) separated under the reversed phase (RP) mechanism.

ChA are superior alternative to amphiphilic ion-pairing agents due to their contribution to secondary chromatographic equilibria, without irreversible alteration of the stationary phases surface or retention of neutral compounds. Three different mechanisms were used to describe the action of ChA on separation of basic species under RP mechanism: i) ion association with formation of neutral ion pairs; ii) strong contribution to disruption of the solvation shell of the analyte, resulting in the increase of the intrinsic hydrophobic character of the latter; iii) adsorption of ChA on the stationary phase surface, due to their ability to develop dispersive interactions.

When ionic liquids based on chaotropic counter ions are used, the global scenario increases in complexity. The ChA cations are also adsorbed on the surface of the stationary phase, generating repulsive interactions with the analyte in its ionic form. This may results in a reduction of the chromatographic retention. The ChA cations are also coupling ionized silanols, reducing the stationary phase residual activity and increasing peak symmetry.

Some insights about the retention behavior of some analytes belonging to tricyclic antidepressants, catecholamines and phenethylamines in the presence of chaotropic agents, including ionic liquids, are provided and discussed.

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PL2. **STOCHASTIC MODELLING IN CHEMICAL ENGINEERING-CELLULAR MODELS**

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The practical applications of stochastic processes theory are multiple. This fact is a consequence of the capacity of this theory that can predict the future of a dynamic system by use of its history and its actual state [1]. The prediction of the future by history and actual state is possible for processes where as vehicle of their dynamics it identifies one or more systems with complete random links (SCRL). *The state of a system at time **n** is a random variable* A_n *with values in a finite space (measurable)* (A **A**). *The state evolution at time n+1 results from the appearance of a* B_{n+1} *result which is also a random variable with values in a finite space (measurable)* (B **B**). *The appearance of a result signaling the state evolution could be represented considering a* **u** *application of* AxB *in* A *and introducing the following statement*: A_{n+1}=**u**(A_n, B_{n+1}) *for all* n>=0 . *The* B_{n+1} *probability distribution conditioned by* B_n, A_n, B_{n-1}, A_{n-1},…….B_1, A_1, A_0, *and symbolized as* P(B_{n+1}/B_n,A_n,…A_0), *depends only on the state* A_n. *The group* [(A,**A**),(B,**B**), **u:**AxB→A,P] *defines a SCRL*. The space A represent the **process component** and the space B is the **process connection**. In the case of cellular stochastic models a phenomena results by different structures formation and the passage from one structure to another is made randomly; in this case the structure formation is the "process component" and the passing steps are the "connection process". Two cases are analysed here by mean of cellular stochastic models. The first case refers to acidic cellulose (biomass) hydrolysis. The breakage of the β-1,4-glycosidic bonds by acids leads to the hydrolysis of cellulose polymers, resulting in the sugar molecule glucose or oligosaccharides. Mineral acids, such as HCl and H_2SO_4, have been used in the hydrolysis of cellulose [2, 3]. Here the process component is represented by all fragments with molecular mass under initial cellulose molecular mass, which appear in breaking of molecular structure; the process connection is a Markov type, represented by distribution of the breaking probabilities for all fragments from process component. The effect of temperature and acid concentration in acidic cellulose hydrolysis is very well considered by effect of this parameters on transition frequency in Markov chain connection. The model description, the model mathematical expression, the procedure of model implementation was given in detail. The use of several types of matrix

of transition probabilities is also found in the paper. Uniform distribution for breaking probabilities of cellulose chain was selected in matrix of transition probabilities, which has been used in treatment of hydrolysis evolution for cellulose with low molecular mass. The emphasis in the matrix of the transition probabilities of temperature and environment acidity effect on dynamic evolution of hydrolysis, allowed of model to be expanded and compared with data generated by formal kinetic models. The second case focuses on dynamics of heat transfer in a heat exchanger with two or more passage of hot fluid. The process component is in obtained by building a cellular topology of heat exchanger. The process component respect a Markov connection where de transition frequency is expressed with considering of heat transfer kinetics between cells of considered topology. For the stochastic analysis of dynamics of a multi-pass heat exchanger, it is necessary to start from a concrete case, ie from a dimensioned exchanger or from one in operation. The model development sequences impose: i) the selection of the cellular topology of heat exchanger, ii) the analytical expression of the transition probabilities for the heat exchange between the cells from the selected topology c, iii) the choice of dynamics inputs into the system (flow rate dynamics, temperature dynamics or flow rate and temperature dynamics at the inlet of the fluids in the heat exchanger). In some cases, where the heat exchange dynamics characterizing the heat exchanger can be analysed by phenomenological modelling [4], the obtained results can be compared with those given by the equivalent stochastic model.

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PL3. **ELECTROCHEMICAL SENSORS VERSATILITY IN CONTAMINANTS ANALYSIS**

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Biosensors performances at low concentration levels depend on the sensitivity ensured by the biorecognition element. When analysis of systemic pollutants or secondary plants metabolites are addressed, the measurement sensitivity is the critical issue. The mainly used biorecognition elements are enzymes and whole cells.

Versatility of using enzymes and whole cells for contaminants assessment will be discussed, using two case studies: alkaline phosphatase for heavy metals and radionuclides monitoring and photosynthetic organisms (PS) for halogenated hydrocarbons and endocrine disrupting herbicides.

Development of biosensor based on photosystem II - PSII-NP-SPE biosensor - for chlorinated compounds analysis was based on the PSII susceptibility to modulate its photosynthetic activity in the presence of various pollutants, documented in the past period. The optimum protocol for biosensor design was based on layer-by-layer approach. An amount of 3.2 mg bimetallic nanoparticles Pt@Au was suspended in 500 µL Nafion, 10 µL suspension of bimetallic nanoparticles being dropped on the working electrode surface and allowed to dry. Subsequent conductive layer stabilisation a volume of 10 µL of algal cells suspension in sodium alginate, providing the optimum amount of Chla were deposed, allowed to fast dry, a slight jellifying with calcium chloride was used for whole cells stabilisation. For tetrachloroethylene, PCE the curves dose-response exhibited a domain of linearity for a concentration ranging between 2.47 $\times 10^{-6}$ molL^{-1} to 2.44 $\times 10^{-5}$ molL^{-1}. The developed biosensors were tested on artificial samples obtained by spiking known concentrations of PCE in drinking water, respectively in river water, the recovery from spiked samples was ranging between 98.45% and 103.70%. The use of algal whole cells proved their efficiency both as biosensing elements and in bioremediation strategies, thus demonstrating their versatility.

The alkaline phosphatase (ALP) proved to ensure a high sensitivity of the biosensing devices for radionuclides and heavy metals analysis, the response range of an Au-SPE/polyMB_ALP biosensor being 30 ppb – 160 ppb for Hg(II) and, respectively, U(VI) analysis.

PL4. **OUTCOMES AND IMPACT OF A MASSIVE OPEN ON-LINE COURSE IN OPEN EDUCATIONAL RESOURCES AND E-LEARNING IN TOXICOLOGY: THE TOX-OER PROJECT**

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Due to the lack of European Massive Open On-line Courses (MOOCs) in the field of Toxicology and major differences in the teaching and learning of this important subject at various European chemistry-biology oriented University faculties, we will present the results of our two-years TOX-OER European project which developed a scientific and pedagogical joint between research in the field of toxicology and MOOC pedagogical design [1]. This consisted in a guideline to support partners during: a) the creation of accessible Open Educational Resources (OERs); b) course and module management; c) the implementation, monitoring and evaluation of individual and social learning activities. This procedure contributed to the promotion of using the learning outcomes in the design and delivery of educational programs and activities in favour of pupils, students, young people, trainees, adult learners. Furthermore, the TOX-OER project could create the conditions for the recognition and certification (ECTS) of learning achievements, at least between partners. Finally, throughout the duration of the project the partners involved in the educational tasks managed a virtual space within which the MOOC platform was implemented and where all the OERs are available. TOX-OER project is coordinated by Universidad de Salamanca and its partners are: Università di Bologna, Italy; Universitatea Transilvania din Brașov, Romania; Univerzita Karlova V Praze, Czech Republic; Universidade do Porto, Portugal; Space Research and Technology Institute, Bulgaria; Kymenlaakson Ammattikorkeakoululu Oy, Finland.

[1]. https://toxoer.com/

PL5. **THE DIMETHYLDIHYDROPYRENE PHOTOCHROME: MULTI STIMULI-RESPONSIVE MOLECULES AND THERAPEUTIC APPLICATIONS**

Guy ROYAL

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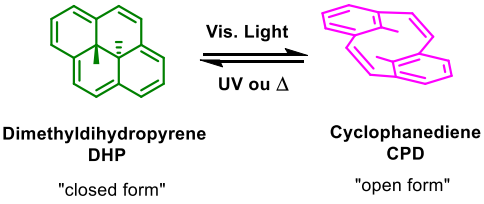
Molecular switches are systems (generally supramolecular architectures) that can exist under several states having different physico-chemical properties and they can be reversibly converted from one state to another using an external stimulus such as an electrical, an optical or a chemical input. These molecules appear particularly interesting for applications in responsive ("smart") materials, electronic devices such as transistors or memory elements or for biologic purposes.

In this context, our objectives are to develop sophisticated molecular switches and to elaborate original responsive molecular materials based on the dimethyldihydropyrene (DHP) photochrome. This organic compound can be readily isomerized under light irradiation into its corresponding cyclophanediene (CPD) form. In particular, we show that, upon chemical modifications, this photoswitch may find interesting uses for the conception of responsive materials and for therapy.



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PL6. **PHOTO-INDUCED REDOX CATALYSIS FOR HYDROGEN PRODUCTION IN WATER WITH MOLECULAR COMPOUNDS BASED ON EARTH ABUNDANT ELEMENTS**

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Solar driven water-splitting into hydrogen and oxygen, also referred as artificial photosynthesis, has emerged as a very attractive sustainable approach to produce the fuel H_2 [1]. Molecular approaches to generate H_2 by photo-induced redox catalysis typically involve the association of three-components in homogeneous solution, a light-harvesting antenna (photosensitizer, PS), a H_2-evolving catalyst (Cat), and a sacrificial electron donor (SD) [2, 3]. Ideally these systems should use only earth abundant elements, be cheap, stable and able to operate efficiently in water without addition of toxic organic co-solvents. If much progress has been achieved in recent years in developing H_2-evolving molecular catalysts that fulfill these requirements with the use of Co, Fe, Ni and Mo transition metal complexes, most of the PSs employed for this reduction process still rely on rare and expensive Ru ($[Ru(bpy)_3]^{2+}$, bpy = bipyridine)) and Ir ($[Ir(bpy)(ppy)_2]^{+}$, ppy = phenylpyridine)) complexes. Metal-free organic dyes, only made by abundant elements constitute a very attractive alternative to these transition metal complexes, but the few families of organic dyes, mostly commercial, deteriorate quite readily in the course of photocatalysis [4-6]. Recently, we obtained key results [7] by associating a water-soluble organic dye based on the triazatriangulenium carbocationic motif ($TATA^{+}$) [8] with a very efficient cobalt H_2-evolving catalyst [9-11], and ascorbic acid as SD (Figure 1). The electrochemical, spectroscopic properties of this new dye as well as the photocatalytic performances of this new system will be presented.

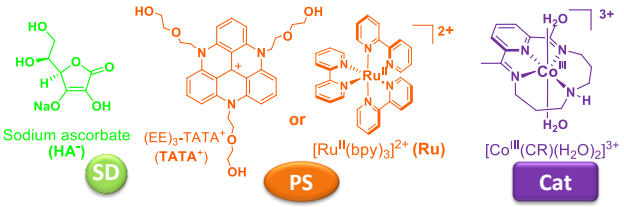

Fig. 1. Molecular photocatalytic system

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SECTION A: NATURAL AND SYNTHETIC COMPOUNDS

OA1. **IN SEARCH OF PROBES OR INHIBITORS OF AMYLOID FIBERS: SYNTHETIC PEPTIDE FRAGMENTS AS FIBERS MODELS**

Camille LAROSA,[1] Carol TSEN YUNG,[2] Laurent LUNVEN,[1] Bianca FURDUI,[3] Rodica DINICA,[3] Isabelle BAUSSANNE,[2] Martine DEMEUNYNCK,[2] and Sabine CHIERICI[1]

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Neurotoxic aggregates and fibers formed from abnormally phosphorylated tau protein are regarded as the main actors involved in the destruction of neurons in tauopathies such as Alzheimer's disease [1, 2]. Yet only a few molecules have shown to efficiently prevent or detect the formation of those aggregates, and the identification of such molecules is still an ongoing interest in a therapeutic and diagnostic context [3, 4]. In line with this objective, we use and develop in vitro models of tau fibers to investigate the inhibitory or probe effect of small library of molecules by means of thioflavin fluorescence assays, circular dichroism and microscopy techniques [5]. Different classes of molecules, including indolizines and the corresponding pyridinium precursors, will be evaluated.

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OA2. **MAGNETIC CHITOSAN COMPOSITE PARTICLES: SYNTHESIS REPRODUCIBILITY AND PARAMETER STUDY**

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The use of magnetic adsorbents in waste water treatment offers the advantage of facile separation from the liquid phase. Expensive filtration equipment and time-consuming sedimentation in industrial environments is thus avoided.

A method for producing magnetite/chitosan composite particles has been previously developed in small scale. The magnetic nanoparticles were synthesized using an innovative approach, by the partial oxidation of ferrous ions initially dispersed within the polysaccharide solution [1].

The innovative adsorbent material has demonstrated superior efficiency towards various heavy metal ions compared to similar materials described in the literature [2, 3]. A potential problem of the existing synthesis method might come from the inherent variability of a natural raw material. The goal of this study is to evaluate its influence upon the product properties to find ways to overcome it. The expected outcome is improving the reproducibility, robustness and ultimately the technology readiness level of the existing synthesis method, while preparing it for scale-up and transfer into an industrial setting.

Acknowledgements. This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation CNCS/CCDI-UEFISCDI PN-III-P2-2.1-PED-2016-0456, within PNCDI III.

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OA3. **POSSIBLE VEHICLES FOR CONTROLLED DRUG DELIVERY BASED ON PMAA-SALECAN-ORGANOMODIFIED CLAY NANOCOMPOSITES**

Raluca IANCHIS,[1] Claudia NINCIULEANU,[1] Catalina GIFU,[1] Tatiana MUNTEANU,[2] Elvira ALEXANDRESCU,[1] Silviu PREDA,[3] Raluca SOMOGHI,[1] Bogdan TRICA,[1] Raluca GABOR,[1] Cristina NISTOR,[1] Sabina NITU,[1] and Cristi PETCU[1]

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Salecan, a water soluble extracellular polysaccharide produced by fermentation from a new strain Agrobacterium sp. ZX09, was proved to assure excellent properties, such as: antioxidative, non-toxic, anti-inflammatory, antimicrobial, antitumoural, antidiabetic [1-3]. Moreover, Salecan provides enhanced mechanical properties to its hydrogels derivatives which is perfectly suitable for applications in pharmaceutical formulations. Our goal was to study the possibility to synthesize semi-interpenetrated systems based on poly(methacrylic acid) and Salecan in the presence of an organomodified clay (Cl 93A). The syntheses were conducted via free radical copolymerization in the presence of ammonium persulfate as initiator and N, N'-methylenebisacrylamide as crosslinking agent. In order to evidence the structural and morphological modifications as a consequence of the various clay concentrations used in the synthesis process, the obtained materials were characterized by several techniques, as follows: FT-IR, TGA, X-ray diffraction and microscopy analyses (SEM, TEM), DMA and swelling studies. The obtained materials are foreseen for drug encapsulation and application in cancer treatment.

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PA1. **COPPER (II) COMPLEXES WITH AROMATIC AMINES AS ANTIMICROBIAL SPECIES**

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Triazolopyrimidine derivatives exhibit a large spectrum of biologic activity such as antiparasitic, antimicrobial and antitumor [1]. As result several complexes with this kind of ligands were synthesized and some evidenced antitumor, antiinflammatory, or antimicrobial activity in most cases enhanced in comparison with ligand [1, 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/ 1,10-phenantroline. The features of complexes have been assigned from elemental analyses, IR, ESI-MS, UV-Vis and EPR spectra, magnetic susceptibility at room temperature as well as thermogravimetric analysis. The 5-phenyl-7-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine behaves as unidentate and 2,2'-bipyridine/ 1,10-phenantroline as chelate species resulting in a distorted square pyramidal or octahedral stereochemistries.

The antimicrobial assays were performed against Gram positive (*S. aureus, B. subtilis*), Gram negative (*E. coli, P. aeruginosa, K. pneumoniae*) and fungal (*C. albicans*), both planktonic and biofilm embedded strains. In all cases it was evidenced that overall antimicrobial potency of 5-phenyl-7-methyl-1,2,4-triazolo[1,5-*a*]pyrimidine was enhanced upon coordination.

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PA2. PHYSICO-CHEMICAL AND BIOLOGIC CHARACTERISATION OF SOME COPPER (II) COMPLEXES WITH PENTAAZAMACROCYCLE LIGANDS

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New complexes of Cu(II) with general formula $[Cu(L)](ClO_4)_2 \cdot nH_2O$, where L: pentaazamacrocyclic ligand obtained by 3,6-diazaoctane-1,8-diamine, an amino acid (L-tyrosine, L-tryptophan, L-histidine or L-phenylalanine) and formaldehyde condensation, have been synthesized and characterized in order to examine their possibility to act as superoxide dismutase mimics. Different spectroscopic techniques (ESI-MS, IR, EPR, UV-Vis spectroscopy) were used to characterize the complexes and to evidence their interaction with superoxide. The *in vivo* superoxide dismutase like activity of the complexes was performed using a method based on the protective effect on a SOD mutant of *Saccharomyces cerevisiae* against free radicals generated by hydrogen peroxide as well as that produced in the cellular respiration process. The results have shown that all complexes exhibited a protective action against the oxidative stress. It is important to be noticed that complexes exhibited also a moderate antimicrobial activity against several bacterial strains, both planktonic and biofilm embedded.

PA3. **SYNTHESIS, SPECTRAL AND BIOLOGICAL CHARACTERIZATION OF NEW COPPER (II) COMPLEXES WITH NICOTINAMIDE**

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Nicotinamide plays an important role in the metabolism of living cells, and some of its metallic complexes exhibit antibacterial activity or act as insulin mimetics. It has often been used as a ligand in the development of treatments for skin disorders such as atopic eczema, psoriasis or even skin cancer. Complex combinations of nicotinamide with various metals and anions have much more intense action than the ligand itself.

Taking into account all these, we report here the synthesis and characterization of new complexes of copper with nicotinamide and methacrylate ion as ligands. The compounds were characterized by chemical analysis as well as IR, UV-Vis-NIR, EPR spectroscopy and magnetic data at room temperature.

All complexes exhibit specific anti-infective properties against Gram-positive (*S. aureus*, *B. subtilis*, *B. cereus*), Gram-negative (*P. aeruginosa*, *E. coli*, *Enterobacter*) and fungal (*C. albicans)* as demonstrated by the low MIC values. Their ability to inhibit the microbial biofilm formation on inert substratum was also assayed.

PA4. **VARIATION OF SALECAN CONCENTRATION IN PMAA-SALECAN-ORGANOMODIFIED CLAY NANOCOMPOSITES**

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In the last decade, clays were intensively used in the synthesis of hydrogels because of their ability to provide increased swelling properties but mainly enhanced mechanical and thermal properties as compared with conventional hydrogels. The objective of the present study was the synthesis and characterization of new hydrogel nanocomposites based on polymethacrylic acid with organomodified clay at different Salecan concentration. A group from China have successfully developed in the last years, a series of Salecan-containing hydrogels proving its significant contribution in several directions. Salecan is a biopolymer, a polysaccharide extracted from algae which can be used in a wide range of applications as: antioxidative, antimicrobial, antitumoural, non-toxic, anti-inflammatory, antidiabetic additive [1, 2]. Based on previous studies with Salecan and on our group experience in the synthesis of polymer-clay nanocomposites we started to develop a new class of Salecan based hydrogel-clay nanocomposites. Free radical copolymerization was used for the obtaining of chemical hydrogel clay nanocomposites. Organomodified montmorillonite with methyl dihydrogenated tallow ammonium was used for the syntheses. The hydrogel nanocomposites obtained with different concentration of Salecan were characterized by FTIR, TGA, XRD, microscopy and swelling studies. The results proved that the presence of Salecan but also its concentration influenced the structure of final nanocomposites. The synthesized hydrogel nanocomposites could find applications in biomedical field.

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PA5. SYNTHESIS AND CHARACTERIZATION OF THE INCLUSION COMPLEX OF β-CYCLODEXTRIN AND [2-(2-BROMO-PHENYLCARBAMOYL)-PHENOXY]-ACETIC ACID ETHYL ESTER

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Cyclodextrins are cyclic (α-1,4)-linked oligosaccharides of α-D-glucopyranose, containing a hydrophobic central cavity and hydrophilic outer surface [1].

The distinctive characteristic of cyclodextrins is the capacity to form inclusion complexes with several organic molecules. Through host-guest interactions between the central cavity of cyclodextrin and a nonpolar molecule, the physical, chemical and biochemical properties of guest molecule can be modified, so the application criteria of this guest molecule can also be improved [2].

A β-cyclodextrin inclusion complex containing [2-(2-bromo-phenylcarbamoyl)-phenoxy]-acetic acid ethyl ester as a guest was prepared by kneading method with aliquot addition of ethanol. The product was characterized by FTIR, ^{1}H-NMR, TG/DSC, X-ray diffraction and SEM-Edax analysis which proves the formation of the inclusion complex. The interaction between guest and host molecule was also studied by means of UV-Vis spectrometry. The formation constant was calculated using a Benesi-Hildebrand equation, the obtained value was $8.4 \cdot 10^4$ L/mol. The stoichiometry ratio for the inclusion complex was also determined to be 1:1 based on the linear relationship obtained from the reciprocal plot of 1/A *vs.* 1/[β-Cyd] from the Hildebrand-Benesi equation.

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PA6. MULTIVARIATE ANALYSIS OF THE VOLTAMMETRIC DATA OBTAINED IN ENZYMATIC MODIFICATION REACTIONS OF DIFFERENT LIGNINS THROUGH OXIDATIVE COUPLING WITH HYDROPHILIC COMPOUNDS

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This work reports the principal component analysis on the voltammetric data obtained in the oxidative coupling reactions of four technical lignins with different molecular properties, i.e. Soda Grass/Wheat straw Lignin, Organosolv Hardwood Lignin, Soda Wheat straw Lignin and Kraft Softwood, with glucosamine in acetone/water mixture, using laccase as catalyst. The ability of laccase to facilitate grafting hydrophilic compounds, namely glucosamine to lignin in acetone/water mixtures aiming to obtain grafted novel lignin derivatives with new functionalities was assayed by cyclic voltammetry. The studied lignins behave differently in oxidative coupling reactions due to their origin, different extraction methods and the phenolic content. The aromatic polymer lignin can be modified by grafting the appropriate functional groups to increase the hydrophilicity of the lignin [1]. The whole peak responses were processed using multivariate methods such as principal component analysis (PCA) and partial least squares regression (PLS-R). Also, principal component analysis (PCA) was used to visualize the discrimination capability towards the lignins and the reaction compounds derived from the voltammetric signals acquired, and grouped with a cluster analysis tool to build a preliminary recognition model. This approach can be used to develop simple, rapid and accurate analytical tools to monitor and control the enzymatic coupling reactions of lignin with hydrophilic compounds.

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PA7. **ULTRASOUND AND HEAT STABILITY OF SOME COMMERCIAL ANTHOCYANINS**

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Anthocyanins present a special importance in terms of high potential for their use as natural colorants due to easy incorporation in aqueous media, but also for their nutritional qualities and health benefits. The main difficulty of using these pigments both as food colorants and for their nutritional qualities, is their low stability under the influence of various factors, one of the most important being temperature [1]. Some non-thermal technologies with potential to replace thermal processing of foods include membrane osmotic dehydration, pulse electric field, ultrasound, irradiation, high pressure, etc. [2].

The effect of thermal processing and ultrasound processing on pure anthocyanins (cyanidin-3-glucoside and malvidin-3-glucoside) was investigated in this study. The changes in pigment concentration and antioxidant activity were monitored during both treatments. Anthocyanins concentration and the occurrence of some degradation products were determined through UV-Vis spectrophotometry and HPLC-DAD analysis. Antioxidant activity evaluation was performed by using FRAP (ferric reducing/antioxidant capacity) assay [3]. Also, the degradation kinetic parameters have been evaluated. The obtained results indicate that thermal processing significantly affects the anthocyanins concentration compared to ultrasound treatment. The half-lives were 4.8 h for cyanidin-3-glucoside and 1.9 h for malvidin-3-glucoside, respectively. During both types of treatment, the antioxidant activity was not significantly modified.

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PA8. **AROMATIC PLANT EXTRACTS: INVESTIGATION OF THEIR ANTIOXIDANT AND ANTIMICROBIAL ACTIVITIES**

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Beginning with the discovery of new extraction, processing and purification techniques, the interest in biologically active compounds found in plants increased.

The aim of the paper is to highlight the biologically active compounds present in *Thymus serpyllum*, *Zyzigin aromatica* and *Matricaria chamomilla* species by qualitative and quantitative analysis as well as demonstration of antioxidant and antimicrobial activities by a comparative study.

In this study we used dried plants as plant material and various solvents used to obtain extracts. Analysis of the compounds was performed by chromatographic and spectrophotometric methods. Investigation of antimicrobial activity was performed using the Kirby-Bauer method on reference microbial strains or isolated from patients from Clinical Emergency Hospital for Children "Sf. John "in Galati.

The presence of biologically active compounds as flavonoids and terpenoids was identified in all of the analyzed extracts.The studied alcoholic extracts showed an antioxidant activity which was determined by their action on DPPH, the most significant antioxidant capacity being recorded for the cloves oil.

Antimicrobial activity was determined by the Kirby-Bauer diffusion method. The highest antimicrobial power was found for thyme extract followed by cloves, against *Staphylococcus aureus* and the alcoholic cloves extract had the highest antimicrobial power against *Streptococcus pyrogenis.*

The obtained alcoholic extracts, through their antimicrobial properties, can serve as important sources of biologically active compounds.

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PA9. **NATURAL SOURCES OF ACETYLCHOLINESTERASE INHIBITORS FROM SOUTH-EAST REGION OF ROMANIA**

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Acetylcholinesterase (AChE) inhibitors have been used for the symptomatic treatment of Alzheimer's disease (AD). Plant varieties of *Amaryllidaceae* (*Galanthus* and *Narcissus*) are known to contain galanthamine, a bioactive alkaloid used in antiacetylcholinesterasic therapy.

Two plants from Romania belonging to the *Amaryllidaceae* family have been screened for their anticholinesterase inhibitory activities. The antioxidant activity of plant extracts is an interesting feature for a double mechanism to avoid the deficit of cholinergic system and the oxidative stress in neurodegenerative diseases such as AD so the antioxidant activity of each extract was also evaluated. Of these two plants, *Narcissus pseudo-narcissus* showed the best AChE inhibition.

Additionally, alkaloid extracts of the *Amaryllidaceae* plants were also analyzed by TLC to identify the well-known AchE inhibitor, galanthamine. The two plants root extracts, showed the presence of galanthamine.

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PA10. **SYNTHETIC BIOMATERIALS FOR BIOLOGICAL APPLICATIONS**

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Today main's challenge of tissue engineering is to develop biocompatible materials that mimic general characteristics of natural extracellular matrices (ECMs), and cell – ECM interactions both for biological studies and therapeutic applications [1-3]. In this context we developed azo-materials used as support for biological applications. The material used is a linear polysiloxane with chlorobenzyl groups in the side chain substituted with different azobenzene derivatives. These polymers can provide optically active supports, with tunable properties, to facilitate the understanding of the complex mechanism involved in the interactions between cells and their environment [2, 3]. The optical properties of the materials are presented, as well as preliminary studies showing the materials potential to modify the cell response to the surface.

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PA11. **POTENTIAL OF SYNTHETIC BIOMATERIALS FOR NANOSCALE MANIPULATIONS OF BIOMOLECULES THROUGHT OPTICAL METHODS**

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Developing materials that are capable to bind or trap biomolecule for further nanoscale manipulation is a powerful technique for studying protein motility, dynamic molecular process of proteins, but also for molecular genetics and not only [1]. In both nanomaterials and molecular biology fields, optical methods to manipulate and detect nanoscale objects are highly used [2, 3]. In these sense we developed azopolysiloxanes modified with nucleobases (adenine and thymine) and tertiary amines. First material is capable to bind DNA through hydrogen bonds, and the second one creates strongly electrostatic interactions between substrate and DNA bonds. To further manipulation of biomolecules the stability of the polymeric surfaces in air and in water was tested, and also the mass transport capacity of material, using laser irradiation. Atomic force microscopy and scanning electron microscopy techniques are also used.

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PA12. **CHARACTERIZATION AND MOLECULAR DOCKING STUDIES ON A SERINE PROTEASE INHIBITOR ISOLATED FROM THE SEEDS OF *CITRULLUS VULGARIS***

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Serpins (Serine proteinase inhibitors) continue to attract the attention of researchers due to theirs increased use in medicine and biotechnology. So far, the trypsin inhibitor of watermelon seeds has been studied, together with other plant-derived inhibitors, in order to reveal their structure but not enough to characterize its effects on proteases as mediators in the development of some diseases. We have studied a trypsin inhibitor, previously obtained [1] by isolated and purified *Citrullus vulgaris* seeds (CVTI). By partial enzymatic cleavage of a protein molecule with molecular weight determined by gel electrophoresis under denaturing conditions (SDS-PAGE), several polypeptides were obtained. Two of these, (CVTI-1 and CVTI-2) were selected to evaluate their affinity for tryptase and receptors involved in some cancers and diseases of the cardiovascular, respiratory, gastrointestinal or renal system. Our approach was based on molecular docking simulations. The structures of complexes tryptase-inhibitors have been modeled by energy minimization. The bests results have been obtained for the ligand CVTI-1, produced by enzymatic proteolysis of the inhibitor from *Citrullus vulgaris* seeds, as potential tryptase inhibitory agent by interacting with: TYR (PDB ID: 1AOL) [2], PAR1 (PDB ID: 1NRN) [3], PAR3 (PDB ID: 2PUX) [4] and PAR4 (PDB ID: 2ZPK) [5] receptors.

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PA13. **CHEMICAL COMPOSITION, ANTIMICROBIAL ACTIVITY AND CHEMOINFORMATICS STUDY OF GINGER (*ZINGIBER OFFICINALE*) EXTRACT**

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Ginger is a minor chemical irritant, and has a sialagogue action, stimulating the production of saliva. Mature ginger roots are fibrous and nearly dry. They can be cooked as an ingredient in many dishes. The characteristic odor and flavor of ginger root is caused by a mixture of gingerone, shoagoles and gingerols, volatile oils that make up about 1-3% of the weight fresh ginger [1].

The aim and objective of the present study was to investigate the antibacterial activity and bacterial growth inhibition of ginger extracts and also to realize a cheminformatics study for the major compounds found in ginger. This study is giving us information about molecular targets, bioavailabilty and toxicity according to Lipinski, Vebber, Pfizer etc. rules [1, 2].

Ginger extracts were obtained using solvents, ethanolic soxhlet and water. The results also showed that ginger extracts possesses antibacterial properties and could be used for the treatment of bacterial infections [2, 3].

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PA14. **OPTIMIZATION OF A MICROWAVE-ASSISTED EXTRACTION METHOD FOR THE ISOLATION OF NATURAL COMPOUNDS FROM THE *ANTHRISCUS SYLVESTRIS* AERIAL PARTS**

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Microwave-assisted extraction (MAE) is a process that uses microwave energy and solvents to extract target compounds from various matrices. The highly localized heating of the substrate can cause selective migration of target compounds from the matrix at faster rate and with better extraction yield compared to conventional extraction methods. In this paper the influence of extraction temperature, irradiation time and nature of the extraction solvent on the microwave-assisted extraction of polyphenols and lignans from the aerial parts of *Anthriscus sylvestris* (wild chervil) was investigated. The responses considered were the total phenol content, total flavones, as well as the individual concentration of the main polyphenolic derivatives (chlorogenic acid and luteolin-7-O-glucoside) and lignans (podophyllotoxin and deoxypodophyllotoxin). The quantitative determination of the main derivatives of the *A. sylvestris* aerial parts extracts was performed by HPLC, using a 0.1% trifluoroacetic acid: acetonitrile gradient as mobile phase. Out of the three investigated factors, temperature and extraction solvent had the biggest impact on the overall extraction process. In terms of individual components, the polyphenol content was mostly dependent on the extraction temperature, whereas the extraction solvent nature influenced the most lignans extraction. Adjustment of the dielectric constant and of the dielectric loss constant of the extractive solution by using a mixture of solvents allowed an approximately 5 fold increase of the lignan content and 10 fold increase of the polyphenol content of the resulting extracts in comparison with the extraction in pure solvents.

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PA15. **CHEMICAL AND MOLECULAR OBSERVATIONS OF SOME PLANT-SOURCE EXTRACTS**

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In the last few years the use of natural products has gained a major interest. This is due to their potential in treating many skin disorders. In addition they reduce the penetration of the radiations into the skin and decrease inflammation, oxidative stress and DNA damaging effects [1,2]. Today, we can find on the market an enormous variety of skin care products. For example, gels are becoming more popular due to their easy application, better percutaneous absorption (when compared with other semisolid preparation) and resistance to the physiological stress caused by skin flexion, blinking and mucociliary movement, adopting the shape of applied area [3]. Another type of organic cosmetics with solid impact are the organic waters or facial mists.

In order to pinpoint the advantages of 100% plant-source dermato-cosmetics, we developed in this paper many chemical and molecular observations upon four organic cosmetic waters obtained from two plant species: sea buckthorn (*Hippophae rhamnoides*) and birch (*Betula pendula*), using different parts of the plants. The sea buckthorn waters were obtained individually from the fruits, seeds and peel. The birch water was obtained from the sprouts. The pH and ORP (oxido-reduction potential) values, together with the stability, density and molecular analysis will also be presented.

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PA16. **DETERMINATION OF THE POLYPHENOLIC COMPOUNDS IN ALCOHOLIC EXTRACT OF *LAVANDULA AUGUSTIFOLIA L.* BY HPLC/DAD**

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The essential oil of *Lavandula augustiofolia L.* isolated by hydro-distillation is more studied that alcoholic macerate extracts of lavender.
By maceration of lavender plant in alcohol can be extracted other polyphenols compounds than in hydro-distillation method.

Aerial part of *Lavadula augustifolia L.* was macerated in methanol and the extract was analyzed by HPLC/DAD. Five individual polyphenolic compounds were identified and quantified. Significant concentrations of chlorogenic acid, gallic acid, ellagic acid, cinnamic acid and *p*-coumaric acid were found in the studied alcoholic extract of lavender.

The highest amount of polyphenolic compounds found in alcoholic extract of lavender reaches the value of 213.396 mg ellagic acid/100g d.w., 209.981 cinnamic acid/100g d.w. and 131.709 gallic acid/100g d.w.

From the obtained data we concluded that the antioxidant properties of the plant tissues of lavender may represent an alternative to synthetic antioxidants in preservation of food, as well as in the pharmaceutical industry and cosmetics.

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PA17. **ANTIOXIDANT CAPACITIES AND PHENOLS COMPOSITION OF WILD AND CULTIVATED BERRIES**

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It is well known that the consumption of controlled diets high in berries, increases significantly the human body capacity to maintain the health, protecting human organisms against oxidative stress induced by free radical species.

The study presents original results concerning analytical characterisation of alcoholic extracts from four wild berries (blueberries, blackberries, red currants and raspberries) and two cultivated berries (black cherries and strawberries). Total and some individual polyphenols concentrations were determined using molecular absorption spectrometry (modified Folin Ciocalteu method) and respectively HPLC-DAD. To analyse lipid-soluble antioxidant capacity (ACL) the photochemiluminescence method using trolox as standard has been used.

The highest total phenolic content was registered in blueberries (543.5 mg/100g f.w.) and black cherries (518.5 mg/100g f.w.), while the lowest was found in raspberries (344.5 mg/100g f.w.).

HPLC – DAD analysis indicate the presence of six individual polyphenolic compounds in different concentrations: gallic acid exists in all studied berries in variable concentrations (62.664 - 178.821 mg/100 g f.w); chlorogenic acid (30.152 - 243.923 mg/100g f.w.); 3-O-methyl-gallic acid (2.035 - 4.907 mg/100 g f.w.); caffeic acid (0.401 - 5.665 mg/100 g f.w.); *p*-coumaric acid (4.252 mg/100 g f.w.) in raspberries and 10.806 mg/100 g f.w. in blackberries) and cinnamic acid (0.958 mg/100 g f.w. in strawberries and 0.661 mg/100 g f.w. in red currant). ACL results show values between 54.00 and 1152 µmoles trolox/100 g f.w. All obtained results indicate that all studied berries extracts are rich in antioxidant compounds and can be used in diets or to get health benefits.

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PA18. **CHITOSAN EXTRACTION FROM EXOSKELETON OF *PACHYGRAPSUS MORMORATUS* CRAB FOR APPLICATION IN THE PHARMACEUTICAL INDUSTRY**

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Chitosan is a linear amino polysaccharide obtained by chemical extraction from crab shell waste. This process involves the partial deacetylation of chitin. Chitosan is known to be a versatile natural compound with many important properties that make this polimer suitable for different biomedical applications. After cellulose is the second most abundant natural polymer. Chitosan is biocompatible, biodegradable and non toxic, properties that are used for the formulation of conventional pharmaceutics as a potential excipient. In this research the main focus is the synthesis of chitosan from the exoskeleton of the stone crabs, *Pachygrapsus mormoratus* found in the Black Sea shores and the physico-chemical characterization of the parameters.

PA19. BIOLOGICAL ACTIVE COMPOUNDS FROM *CAPSICUM ANNUUM* AND *PIPERUM NIGRUM* USED IN THE FORMULATION OF ANTIREUMATIC PHARMACEUTICAL FORMS

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Since ancient times, plants have been considered important sources of pharmaceutical compounds, civilization being indissolubly linked to the plant world. They have been for millennia the major source of bio-products essential to the survival of the entire animal kingdom. The paper aims to achieve an extraction of active principles from two native vegetal species, *Capsicum annuum* (pepper) and *Piperum nigrum* (black pepper) in order to formulate pharmaceutical forms with anti-inflammatory action in rheumatic diseases.

We used native dry fruits of *Piperum nigrum* and *Capsicum annuum*, harvested in mid-August. The plants were subjected to ethanol extraction and the active principles were highlighted by thin layer chromatography and separated using column chromatography.

The extracts were analyzed using UV-Vis spectrophotometry. Subsequently, two pharmaceutical forms, ointment and cream, were made, using extracts from the two plants and other active substances with anti-inflammatory and analgesic action such as methyl salicylate, camphor or *aetheroleum eucalipti.*

Thin layer chromatography revealed bioactive compounds such as β-carotene, capsaicin or piperine in the hot pepper and black pepper extract. By separating the compounds, capsaicin (0.06%) from *Capsicum annuum* and piperin (1.2%) from *Piperum nigrum* were isolated on the chromatographic column.

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SECTION B: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

OB1. **VOLTAMMETRIC APPLICATIONS OF PENCIL GRAPHITE LEADS**

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Voltammetry is largely applied in different fields of analysis due to its inherent advantages like simplicity, rapidity and lower costs in comparison to other common used analytical techniques. Another important aspect of voltammetry is related to its ability to help understanding some of the charge transfer processes occurring in living organisms. On the other hand, its sensitivity and very often also the selectivity are very good and nevertheless they are continuously improved by the development of new types of working electrodes. The widespread pencil graphite leads (a composite of graphite, clay and a binder) constitute an electrode material more and more employed in the last 30 years in the so called Pencil Graphite Electrodes (PGEs) [1]. The use of PGEs as cheap, disposable working electrodes eliminates the time-consuming polishing step absolutely necessary to clean the active area of solid electrodes in order to obtain reproducible results. Besides their economic aspects, bare or modified PGEs present high sensitivity, stable and reproducible signals, being thus adequate for the analysis of a variety of analytes and matrices [2].

The present work makes a review of the voltammetric methods based on PGEs developed by our group for the study of various analytes including pollutants (alkyl-phenols), drugs (vitamins, famotidine, carprofen, propranolol, metamizole) and polyphenolic antioxidants (gallic acid, elagic acid, caffeic acid and its derivatives, naringenine and its derivatives) from different samples (water, beverages, pharmaceuticals).

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OB2. **EVALUATION OF MAGNETIC CHITOSAN COMPOSITE AS A GREEN ADSORBENT FOR REMOVAL OF REACTIVE ORANGE 16 FROM SIMULATED WASTEWATER**

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Partial oxidation of ferrous ions dispersed in the polymer solution was used for preparing a novel magnetic chitosan composite (MagCS) [1]. The obtained material was used for removal of Reactive Orange 16 dye from aqueous solutions. Towards this purpose a series of batch studies were carried out. The adsorption process was optimized with respect to various experimental parameters such as pH, initial dye concentration, adsorbent mass, contact time and temperature. Physicochemical characterization of MagCS before and after adsorption experiments was performed by EDX analysis. Three kinetic models were taken into consideration to fit the sorption data: pseudo-first order, pseudo-second order and intra-particle diffusion. Langmuir, Freundlich and Dubinin-Radushkevich models were used to analyze the adsorption isotherms. The results showed that MagCS is an efficient adsorbent for the removal of the anionic dye from wastewater.

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OB3. **COPPER (II) IONS REMOVAL FROM SIMULATED WASTEWATER USING A CHITOSAN COMPOSITE ADSORBENT-STUDY OF PROCESS EQUILIBRIUM, KINETICS AND THERMODYNAMICS**

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Heavy metals contribution to the major pollution in water has attracted significant attention since they are not biodegradable and tend to accumulate in living organisms, being potentially toxic at very low concentrations. To overcome this issue, a novel chitosan/magnetite adsorbent has been previously prepared by our team by an in-situ method using chitosan and ferrous chloride as raw materials, nitrate ions as a mild oxidizing agent and glutaraldehyde as crosslinker.

The aim of this study is to evaluate the applicability of the novel material as a highly efficient, environmentally friendly and cost-effective adsorbent for Cu^{2+} ions removal from simulated wastewater. The adsorption behavior of chitosan composite microparticles for Cu^{2+} was investigated as a function of pH, contact time, initial metal ion concentration and temperature. The adsorption isotherms were analyzed using the Langmuir, Freundlich and Dubinin–Radushkevich models.

The adsorption and desorption mechanisms were discussed. The adsorption kinetics was tested for the pseudo-first order and pseudo-second order kinetic models. The results show that our novel material is a promising adsorbent for removal of Cu^{2+} from contaminated water.

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PB1. **ANALYTICAL METHODS APPLIED FOR CHARACTERIZATION OF ARCHAEOLOGICAL ARTEFACTS FROM AMBER**

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In the present work, we report the experimental results that refer to the analytical methods applied for physico-chemical characterization of amber samples in order to discriminate between two different types, Baltic amber and Romanian amber (romanite) and to expertise artefacts found in archaeological sites. These are two raw material presumptive available for jewelry manufacturers in our country. The originality of the study is the use of non-destructive and/or minimally invasive analytical methods (FTIR, Raman, XRF, SPME-GC-MS, LC-MS) when structural and compositional characterization of archaeological objects of amber have to be performed. The results of LC-MS analysis concluded that the concentrations of succinic acid in sample extracts could play as a criterion for distinguishing between the two amber geological specimens. The SPME-GC-MS can distinguish between romanite and succinite based on the ratio borneol/ camphor which is higher in Baltic amber compare to Romanian amber. Also, artificially ageing experiments were performed in five different media on two sources of geological amber. These were analyzed before and after the ageing experiment by spectroscopic methods and the acquired spectra were statistically processed by multivariate data analysis (PCA). The results confirm that the two categories of amber have different behavior in terms of direction and degree of alteration during the experiments, and Romanian amber is the most affected by the hostile environment. During the ageing experiment the Baltic amber turns into something very close to romanite. This observation confirms some hypothesis of Stout *et al.* that romanite is thermally altered Baltic amber. All four analytical methods developed have potential application in structural characterization of resins from different sources making them applicable to expertise archaeological artefacts.

PB2. **DETERMINATION OF PARABENS IN COSMETICS USING A DISPOSABLE GRAPHITE ELECTRODE**

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Parabens are hydroxybenzoic esters with antimicrobial and antioxidant activity, widely used as preservatives in drugs and cosmetics. The name "paraben" originates from *p*-hydroxybenzoic acid [1].

In the present work the voltammetric behavior and the quantitative determination of methyl-paraben (MP) and propyl-paraben (PP) were investigated for the first time using the pencil graphite electrode (PGE). Due to its good conducting properties and its economic advantages the disposable PGE was often applied for rapid voltammetric determinations of various analytes [2]. Cyclic voltammetric studies demonstrated that MP and PP are irreversible oxidized at the PGE and involves diffusion controlled and pH-dependent electrode processes that implies an equal number of protons and electrons. For quantitative determinations the more sensitive differential pulse voltammetry (DPV) method was employed. The influence of several chemical (electrode material, pH and supporting electrolyte) and instrumental (pulse amplitude and step potential) parameters on the voltammetric response of PP was studied. Under the optimized conditions (pencil leads B-Laco, phosphate buffer solution pH 7.00), PP was quantitatively determined by DPV from 6×10^{-7} M to 9.6×10^{-4} M. The developed method was applied to the determination of the total parabens content (TPC) in cleansing milk, expressed as g equivalent MP or g equivalent PP per kg cosmetic product (g EMP/kg or g EPP/kg). The obtained results of 3.96 g EMP/kg or 4.92 g EPP/kg indicated that the TPC in the investigated cleansing milk was within the limits set by the Scientific Committee on Consumer Safety [3].

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PB3. **RETENTION STUDIES FOR VARIOUS PEPTIDES IN LIQUID CHROMATOGRAPHY BASED ON HYDROPHILIC INTERACTION MECHANISM**

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This study reports the retention behavior of several highly polar peptides on hilic and zwitterionic sulfobetaine stationary phases under different elution conditions. Both mechanisms are currently used in the separation of very polar compounds that are difficult to be retained on reversed-phase stationary phase, such as saccharide and glycosides, nucleosides and nucleobases, flavonoids, or acidic agricultural compounds [1]. The influence of mobile phase composition was investigated for two organic modifiers (acetonitrile, methanol), by their ratios in mobile phase, and the nature and the content of ionic salts used as additives. For these purposes, some mathematical models used in order to differentiate between partition and adsorption processes were applied to the experimental dependences of the retention factor on mobile phase composition [2]. Influence of temperature on the retention of studied compounds was also investigated by means of van't Hoff plotts, which were used in estimating thermodynamic parameters of the chromatographic process (variation of standard enthalpy and entropy) [3]. The obtained results can be assigned to a mixed retention mechanism relying on both partition and adsorption processes.

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PB4. **VOLTAMMETRIC INVESTIGATION OF NARINGIN**

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Naringin (NG) is a flavanone glycoside present in citrus fruits, especially grapefruit, being responsible for their bitter taste. NG has antioxidant activity and some other benefic effects on health [1]. Due to the presence of the HO-groups polyphenols are electroactive and thus their redox behavior can be investigated by electrochemical methods. To the best of our knowledge there are no literature data explicitly related to NG voltammetry. Therefore, the present work describes the cyclic voltammetric (CV) behavior of NG on a disposable pencil graphite electrode (PGE) and the development of a differential pulse voltammetric method (DPV) for its quantitative determination. The influence of the following parameters on the NG voltammetric response on PGE has been investigated: electrode material type, electrode surface pretreatment, pH, supporting electrolyte, NG solution stability and analyte concentration. The best signals were recorded on pretreated HB Rotring pencil leads. CV studies emphasized that NG presents two irreversible oxidation waves, only that appearing at potentials of about 700-800 mV being well defined and having thus analytical importance. This NG oxidation was pH-dependent, controlled by a mixed diffusion-adsorption process and implied $1e^-$ and $1H^+$. Using DPV at pretreated PGE and 0.05 M potassium hydrogen phthalate as supporting electrolyte, NG can be determined quantitatively in the concentration range 1.4-140 μM. The repeatability of the NG electrode response, expressed as percentage relative standard deviation (RSD%), was evaluated at three NG concentration levels. All the RSD% values were within the accepted limits. The developed method was applied with good results to NG determination in grapefruit samples.

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PB5. **APPLICATION OF THE PENCIL GRAPHITE ELECTRODE TO THE DIPYRIDAMOLE DETERMINATION**

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Dipyridamole (DIP), 2,6-bis-2,6-bis(diethanolamino)-4,8-dipiperidino [5,4-d] pyrimidine, is a drug used for the treatment of different cardiovascular diseases, having also antioxidant activity. Sometimes it is illegally used to increase the efficiency in some sports and, on the other hand, its uncontrolled consumption may have dangerous side effects on human heath [1]. Thus, the development of a rapid voltammetric method can offer a versatile tool for understanding the DIP biological action based on its redox reactions as well as for its sensitive quantitative determination.

The present work describes for the first time the voltammetric investigation of DIP on a disposable pencil graphite electrode (PGE). DIP presents two well-defined separated oxidation peaks, whose intensities are concentration dependent. For the quantitative determination of DIP a differential pulse voltammetric method was optimized with regard to the type of the working electrode (bare or electroactivated), the supporting electrolyte (nature, concentration and pH) and the instrumental parameters. Under optimized conditions the developed DPV on PGE method presented a linear range of more than 3 orders of magnitude ($7.5 \times 10^{-7} – 2.5 \times 10^{-3}$ mol L^{-1} DIP). The standard addition method was employed to evaluate the DIP content of some pharmaceutical preparations. The good agreement between the results obtained using the described DPV method and the amounts declared by the pharmaceuticals producer demonstrates the applicability of the method.

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PB6. **VOLTAMMETRIC METHOD FOR CAPTOPRIL DETERMINATION**

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Captopril (CAP), 1-(3-mercapto-2-D-methyl-1-oxopropyl) proline, is used as a drug being the first discovered orally active inhibitor of the angiotensin-converting enzyme (ACE). This medication work to block an enzyme system, which causes artery walls to relax, lowering of blood pressure, and thus enhances the pumping efficiency of a failing heart and improves cardiac output in patients with heart failure [1]. Accordingly, CAP has been widely used for the treatment of hypertension, congestive heart failure, and left ventricular dysfunction after myocardial infarction, as such or in combination with other drugs [2, 3].

A novel voltammetric assay for captopril determination based on an electrochemically pre-treated pencil graphite electrode (PGE*) was developed. The electrochemical behavior of CAP at the surface of PGE* was investigated by using cyclic voltammetry and linear sweep voltammetry (LSV). Whereas at the surface of the unmodified electrode no electrochemical activity of CAP can be observed, a very sharp anodic wave with the peak potential about 200 mV (versus Ag/AgCl) is obtained using the pre-treated electrode. The LSV peak currents increased linearly with the corresponding CAP concentration in the range of 2.5×10^{-5} M – 7.5×10^{-4} M; the estimated detection limit was $2.34 \cdot 10^{-5}$ M CAP. Finally, the sensor was examined as a selective, simple, and precise new electrochemical disposable tool for the determination of CAP in real pharmaceutical samples, with good results.

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PB7. **RAPID VOLTAMMETRIC ANALYSIS OF DIPYRONE IN PHARMACEUTICALS**

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Dipyrone (DYP) or sodium metamizole, well-known on the Romanian market as Algocalmin, is a non-opiate and non-steroidal anti-inflammatory and analgesic drug having also antipyretic activity. DYP is actually a prodrug. Administrated orally or intravenously, it is effective only after its hydrolysis into its active metabolites. Despite its popularity, this drug is prohibited in some countries due to its severe side effects [1]. DYP is not very stable, so that the development of a simple, rapid and cost-effective voltammetric method for its routine assay could be of interest.

The aim of the present work was the voltammetric investigation of DYP using for the first time cheap, disposable pencil graphite electrodes. Cyclic voltammograms emphasized a complex irreversible process of DYP, presenting two well-defined separated oxidation peaks and some other ill-defined anodic waves. The main oxidation peak, situated at potentials of about 0.550 V, is due to a diffusion controlled, pH-dependent electrode process. The most intense differential pulse voltammetric (DPV) peaks were obtained in Britton-Robinson Buffer pH 1.81 when using HB Auchan graphite leads as working electrode. Under optimized conditions the intensity of the DPV peak varied linearly with the DYP concentration in the range $1 \times 10^{-6} – 2 \times 10^{-3}$ mol L^{-1}. The repeatability of the electrode response, expressed as percentage relative standard deviation, was evaluated at three concentration levels. The obtained values were within the accepted limits for the respective concentration levels. The developed method was successfully applied to the determination of the DYP content of pharmaceutical tabets and injections using the standard addition method.

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PB8. **PREPARATION OF CONJUGATE OF ANTI-CD45 ANTIBODY WITH FLUOROCHROMES FITC AND ATTO465**

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CD45 is a glycoprotein expressed on the all white blood cells. Determination of cell concentration of CD45+ leukocytes in blood with corresponding antibody – anti-CD45 antibody bound to the fluorochrome, is a very perspective method. For this purpose, two conjugates were prepared anti-CD45 antibody-FITC and anti-CD45 antibody-ATTO465. The isothiocyanate group of FITC and NHS group of ATTO465 were bound with amino groups of the anti-CD45 antibody. Purification of obtained conjugates was carried out by gel filtration chromatography through Sephadex G-25 column. The column flow rate was 0.2 mL/min. The fractions of 2.0 mL were collected. The fraction absorbance was measured with Jenway 6900 UV/Vis spectrophotometer. Anti-CD45 antibody-FITC conjugate was in fraction 4 and anti-CD45 antibody-ATTO in fraction 3. Emission characteristics of the obtained conjugates and fluorescent dyes, FITC and ATTO465, were analyzed. The activity of the conjugates was investigated. The dilute cell samples with total nucleated cell concentration of 1×10^6 cells/mL was mixed with both conjugates separately (anti-CD45 antibody-FITC and anti-CD45 antibody-ATTO) and incubated for 20 min. The stained cells were counted by new fluorescent image cytometry EasyCounter YC from Milkotronic. EasyCounter YC is based on a fluorescence microscopic cell counting technique. Due to the fluorescent dye, LED optics, and CCD capture technologies, cell analysis is accurate, reliable, and fast. The obtained results were compared with results from fluorescence microscope Olympus and proved ability of the conjugates for immunofluorescence microscopic cell counting with new EasyCounter YC.

PB9. **A RAPID METHOD FOR PESTICIDE RESIDUES DETECTION AND MONITORING IN SOME FOODS**

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In order to increase and ensure the security in people nutrition [1-3], we developed a rapid HPLC method for pesticide residues detection and monitoring in some foods like: vegetables (tomatoes, cucumbers, red peppers, white potatoes), fruits (clementine, grapes) and crops (rape, maize, wheat). Samples of tomatoes and cucumbers (Turkey), red peppers (Spain), white potatoes (Greece), clementine (Turkey), grapes (Peru) were obtained from supermarket, and rape, maize, wheat (Romania, Timiș County) were obtained from different small farmers. It was followed some pesticides: imidacloprid, deltamethrin (insecticides), and bromoxynil, amidosulfuron (herbicides). Calibration curves and analyses for pesticide residues were performed using *Pestanal* standards and a HPLC-DAD apparatus, Dionex Ultimate 3000, equipped with a C-18 Acclaim® 120 Silica-reversed-phase column. Extraction and concentration of pesticide residues were made in acetonitrile by QuEChERS method and ultrasonication, at 59 kHz, 30±2^{o}C, during 30 min. Time of analyses was between 5-10 min. The residual pesticide concentrations in samples were compared with MRLs authorized by EU laws [4].

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PB10. **LONG TERM TRENDS OF OXYGEN PARAMETERS IN THE LOWER DANUBE (1996-2014)**

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Monitoring data collected from 1996 until 2014 from nine stations along the Lower Danube were analysed in order to assess long term trends and progress towards the objectives of the Water Framework Directive. Data were retrieved from the TransNational Monitoring Network (TNMN) database of the International Commission for the Protection of the Danube River (ICPDR) [1], and were analysed using a linear model in R, version 3.4.1.

Dissolved Oxygen (DO) concentration has increased during the study period showing that water quality has improved significantly ($p<2e^{-16}$). However, at the confluence with the Arges River DO values have declined between 2010-2014, indicating increasing eutrophication, the Danube basin being under nutrients pressure [2]. Dissolved Oxygen Saturation has also increased in the long term, the only significant decrease being at Sulina ($p=0.0408$).

Biological Oxygen Demand (BOD5) values have decreased and water quality has improved at all monitoring stations except for the confluence with the Arges River where there is a significant deterioration ($p<2e^{-16}$), particularly between 2010-2014.

Chemical Oxygen Demand COD-Mn has an overall declining trend, but COD-Cr has increased along the Lower Danube showing consistent organic pollution from Romanian tributaries.

The results of the analysis show that some of the analysed parameters have improved during the study period and the overall trend is to move from class II to class I according to Romanian standards. The Arges River, discharging insufficiently treated municipal wastewater from Bucharest and Pitesti, has a negative impact on the quality of the Danube water and the organic pollutants load appears to have increased during 2010-2014.

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PB11. **USE OF METALLURGIC COKE AS ABSORBING MATERIAL FOR THE RETENTION OF ANIONIC SPECIES**

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The paper presents a study related to the possibility of using the metallurgic coke as absorbing material in order to reduce the concentration of anionic species in polluted waters. Before use, the metallurgic coke has been structurally analysed through X ray diffraction (XRD) and chemically modified under treatment with KOH, K_2CO_3 and H_2O_2 solutions, of 30% concentration. The diffractometric analyses allowed the roentgenographic deceleration of two diffraction maxims, assigned to the hexagonal structure of the graphite. Following the chemical modification of the coke, the surface properties showed values of the specific surface (>500 m^2/g) which are appreciably higher as regards to the unmodified coke (234.5 m^2/g), being considered active carbonic materials. The retaining capacity of the anionic species has been followed, by using synthetic salts solutions of chloride, nitrite, nitrate and sulphate ions. The determination of the quantity of ions retained by the absorbing materials, has been performed by means of chromatographic technique (Dionex ICS).

The results of the study revealed the increase of the absorbing capacity of the chemically modified metallurgic coke, depending on the chemical agent which is used. The efficacy of the absorbing materials in retaining the anionic materials is different; hence, in case of Cl^- and SO_4^{2-} anions, the highest retaining efficacy was observed in the coke chemically modified by KOH, while in case of NO_2^- and NO^-_3, the highest efficacy was observed in the coke treated with H_2O_2.

PB12. **ANALYSIS OF OCPs AND PCB IN BLACK SEA SEDIMENTS**

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A study was conducted to analyze the organochlorine pesticide (OCPs) and polychlorobiphenyls (PCB) in Black Sea sediments, from Romanian seaside. The sediments samples were collected from 10 sampling sites of Romanian seaside, along 2015 year. Gas chromatography with electron capture detector (GC-ECD) was used to determine the concentrations of OCPs and PCB. The highest concentrations were observed in the warm season, May, June and the lowest values in November. The recorded values were higher in coastal areas receiving Danube River discharges and close to the largest city of the region, Constanta (especially in sampling points in the harbour area). The OCPs and PCB concentrations are not too high, but their presence indicates a significant degree of technical pollution.

PB13. **SIMULATION OF PROCESSES IN A SEQUENCING BATCH REACTOR USING THE STOAT 5.0 PROGRAM**

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The purpose of this paper is to understand the processes that take place in a sequencing batch reactor (SBR).

SBR technology represents a change in the biological activated sludge treatment process that concentrates in a single tank a series of technological stages that take place successively [1].

The SBR procedure is a discontinuous/time-oriented procedure. The spatially separated functional components of an activated sludge treatment plant (biological / post-clarification stage) are built into a separate tank. SBR works at different intervals. The discontinuous / batch operation of SBR comprises the sequence of the following process phases over a cycle: filling phase, the nitrification/de-nitrification, phosphorus removal and carbon degradation reactions phase, sedimentation/decantation phase and transition/idle phase.

Processes simulation was performed using the STOAT 5.0 program. The simulated process corresponds to the Wastewater Treatment Plant in Eforie Sud, the first in Romania which uses the SBR technology.

The SBR process provides any combination of carbon oxidation with nitrogen reduction and phosphorus removal.

SBR technology has the advantage of being more flexible than conventional activated sludge processes in terms of matching reaction times with the concentration and degree of treatment required for a particular wastewater [2].

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PB14. **SAFETY MANAGEMENT OF DRINKING WATER QUALITY**

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This paper presents the necessary steps to be taken to ensure safe drinking water for consumers.

The approach to drinking water quality management is based on the identification of hazards, risks, and their analysis, the probability of occurrence and importance of their consequences. The principles of the Food Safety Management System (which is a preventive risk management system) is based on a method that prioritizes hazards and risks and establishes the necessary control measures to reduce them to an acceptable level [1, 2].

The description of the assessment process of the water supply system should include the entire process from the raw water source to the consumer's tap, including the treatment technology. Drinking water quality varies across the system, so the assessment should aim to verify the drinking water quality at the consumer's tap through comparison with the limit values set by the legal obligations in force [2].

Water supply systems can be described as a series of successive steps that need to be followed to achieve safe, conformable drinking water. To respect the safety of drinking water quality, each step requires careful management that includes:

- Monitoring and control of water sources;
- Appropriate water treatment and monitoring prior to distribution;
- Water storage and provision of water for consumers;
- Safe water distribution through proper maintenance of the distribution system;
- Monitoring the quality of drinking water distributed to consumers [2].

Starting a water safety plan is not an end in itself but a means to achieve a goal. A water safety plan is useful only if it is implemented and reviewed periodically [3].

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PB15. **DETECTION OF PEPTIDE HORMONES AND GROWTH FACTORS IN DRIED URINE MICROSAMPLES: A NEW APPROACH FOR ANTI-DOPING ANALYSIS**

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The alarming prevalence in the use of performance enhancing compounds among athletes highlights the urge to design and develop novel and effective bioanalytical strategies addressed at the fight against doping. In recent years, particular focus has been given by the scientific community to peptide hormones and growth factors for their ability to enhance sport performances [1]. Classic biological fluid sampling and storage for anti-doping purposes still bring complications related to analysis replication and data reliability. Furthermore urine, as the biological matrix of choice, possesses inherent limitations that can affect the stability of doping-relevant peptides such as hormones and growth factors. Indeed, the excreted compounds can undergo post-sampling enzymatic modification by microbial contamination, especially for samples stored and shipped without controlled and certified temperatures to the laboratories accredited by the Wold Anti-Doping Agency (WADA).

The aim of this research work is to establish and implement feasible but reliable protocols for the collection of urine microvolumes and the high-throughput pretreatment and analysis of stably storable miniaturised dried samples [2]. To this aim, dried microsampling strategies coupled to LC-MS/MS analysis are being exploited. Promising preliminary results on test compounds showed how water loss in urine microsamples leads to several advantages and in particular to the enhancement of peptide stability, with consequent improvement of their detection window.

This research was carried out within the project *Enhanced urinary stability and detection window of peptide hormones and growth factors by dried urine microsampling* funded by WADA [Research project reference number 17A20LM].

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PB16. **TOX-OER FOR LEARNING ENVIRONMENTAL MONITORING THROUGH OPEN EDUCATIONAL RESOURCES**

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The "Learning Toxicology through Open Educational Resources – TOX-OER" project was developed due to the identification of a lack of Massive Open On-line Courses (MOOCs) in Europe in the toxicology domain. Seven partners developed and shared their toxicology-related knowledge and skills, the partnership being formed by Universidad de Salamanca (Spain) as coordinator, Space Research and Technology Institute (Bulgaria), Univerzita Karlova V Praze (Czech Republic), South-Eastern Finland University of Applied Sciences (Finland), Università di Bologna (Italy), Universidade do Porto (Portugal) and Universitatea Transilvania din Brasov (Romania).

The project consortium developed 7 modules, as Open Educational Resources (OERs): Module 1: General Concepts; Module 2: Pharmaco-Toxicokinetics; Module 3: Principal Groups of Xenobiotics – Prescription Drugs and Drugs of Abuse; Module 4: Environmental Pollutants; Module 5: Target Organ Toxicity and Biomarkers; Module 6: Environmental Toxicology; Module 7: Patents and Patent Application. During the project lifetime (from September 2015 to February 2018), a Massive Open On-line Courses (MOOC) platform was installed, where all seven OER modules are available in 8 languages (of all partners and English): video presentations, supporting texts, additional documentation, evaluation tests. The main beneficiaries or the TOX-OER project are our students, from very diverse study programs, they were already involved in OERs testing, as a first step of project implementation in our universities.

The aim of this presentation is to share part of the TOX-OER outcomes developed by the project partnership, especially the modules related to the pollutants and their environmental monitoring.

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SECTION C: PHYSICAL CHEMISTRY

PC1. **PREDICTION OF REACTIVITY PARAMETERS USING DENSITY FUNCTIONAL THEORY (DFT) CALCULATIONS FOR SULPHUR CONTAINING AMINO ACIDS**

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In this work, an attempt to evaluate global chemical reactivity of Methionine and Cysteine by computational approach using Density Functional Theory (*DFT*), was made. The predictive calculations were achieved with Spartan software from Wavefunction, Inc. Irvine CA USA [1], hybrid algorithm B3LYP (the Becke's 3-term functional; Lee, Yang, Parr exchange Hybrid) [2, 3] and polarization basis set 6-31G (d, p) for equilibrium geometry at ground state in vacuum and in water, after energy minimization and geometry optimization. Starting from frontier molecular orbitals (*FMOs*) energy diagram, other global reactivity parameters were calculated by applying Koopmans' theorem [4]: ionization potential *(I*), electron affinity (*A*), electronegativity (χ), chemical hardness (η), global softness (σ), chemical potential (μ) and global electrophilicity index (ω). The results were compared with those obtained for other amino acids, with different functional groups (e.g. serine).

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PC2. **MODELS FOR THE ESTIMATION OF VOLUMETRIC AND TRANSPORT PROPERTIES OF DIESEL FUEL + BIOALCOHOLS BLENDS**

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Recent researches [1, 2] proved that the addition of bioalcohols to diesel fuel decreases harmful emissions like particulate matters and smoke due to the oxygenated nature and specific physicochemical properties of the alcohols. The engine performance can be improved using diesel fuel + bioalcohol blends as a result of the higher percentage of premixed combustion due to low cetane number of alcohol and improved spray characteristics of diesel fuel + alcohol blends that decrease viscosity and density compared to fossil fuel [3]. Even the literature presents studies regarding emissions characteristics of diesel fuel + alcohol blends [4], more research work is needed to characterize the physicochemical properties of these blends in order to find the optimum blend composition to be used as fuel for diesel engine.

The aim of this study is to report density and viscosity data for diesel fuel + alcohol blend over the entire composition range and to evaluate the accuracy of different models to predict these blend properties. Due to the polar nature of the alcohol molecule, density and viscosity dependency on composition of diesel fuel + alcohol blends differ from that of diesel fuel + biodiesel blends. A nonlinear density variation with composition was observed. With respect to viscosity, only models that take into account the interaction between fuel molecules can accurately predict viscosity variation with composition for diesel fuel+bioalcohol blends.

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PC3. **COLLAGEN-SODIUM CARBOXYMETHYLCELLULOSE SPONGIOUS MATRICES LOADED WITH NON-STEROIDAL ANTI-INFLAMMATORY DRUG FOR BURN HEALING**

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The goal of this work was to design and assess some topical collagen-sodium carboxymethylcellulose (NaCMC) sponges loaded with mefenamic acid as a non-steroidal anti-inflammatory drug model, usable in burn wounds healing. Type I fibrillar collagen gel was extracted from calf hide. The spongious forms were obtained by lyophilization of hydrogels with the same amount of drug and different ratios between collagen and NaCMC. All samples were cross-linked with glutaraldehyde for 24 hours at 4°C. The collagen matrices were investigated by optical microscopy, FT-IR spectroscopy, water absorption, enzymatic degradation and drug release kinetics analysis. Preliminary *in vivo* experiments were carried out for the collagen composites on small rodents to study the therapeutic potential in burn healing. All tests revealed proper morphological structure, adequate swelling ability and degradation profiles. The kinetic patterns recorded (i) an initial fast drug release that reduces inflammation and pain associated to a burn wound, and (ii) a progressive and sustained release securing the protective anti-inflammatory and analgesic effect for a longer period of time. The wound healing effect was faster for animal groups treated with collagen sponges and drug-loaded collagen sponges compared to non-treated control group. The complex physical-chemical, biopharmaceutical and pharmacological evaluation of the designed collagen spongious matrices indicate their potential use for burn wounds healing.

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PC4. **DFT CALCULATIONS OF PROTON AFFINITIES OF NATURAL DYES USED IN SOLAR CELLS**

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Dye sensitized solar cells (DSSC) rely on a successful combination of several materials like TiO_2, electrolyte (I_3^-/I^-), dye, a thin film of platinum and conducting glass. The natural dye used in the present study is extracted from *Hibiscus Sabdariffa L.* harvested in the flora of Senegal. We notice that the efficiencies of DSSC depend strongly on the pH of solution 0.23% and 0.13% for pH 3.5 and 5, respectively. The UV-Visible absorption spectra of red *Hibiscus* were characterized in the region from 200 nm to 900 nm. A red shift is observed upon dye adsorption on substrate and upon increase of pH value in aqueous solutions. The peak has a maximum at 519 nm for pH=2.5, this value being in agreement with those obtained by Time Dependent-Density Functional Theory (TD-DFT) calculations. The TiO_2 nano powder paste was spread on fluorinated-tin oxide (FTO) layers. All DFT and TD-DFT calculations were performed using GUASSIAN 09 program package with the B3LYP exchange-correlation functional and the DGDZVP basis set. The electronic structure and electronic spectrum of the dyes in fully protonated and partially deprotonated forms is studied. We make a prediction about the proton affinity and the pKa of the dye molecule based on energies at optimized geometry in vacuum and in solvent, employing the conductor-like polarizable continuum model (C-PCM).

PC5. **FEM MODELLING OF MASS TRANSFER IN ELECTRODIALYSIS DESALINATION**

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In this study it was developed a bi-dimensional Finite Element Method (FEM) based on electrodialysis unit cell model formed by two concentrate compartments bordering two ion exchange membranes (anionic and cationic), a diluate compartment being considered in the center. This model, implemented with Comsol Multiphysics software, take into consideration a variable current density along the flow direction at a constant voltage drop due to a variation of salt concentration [1]. Ion and charge transport, current density and potential profile along the cell have been modeled using Nernst-Planck equation with three modes of mass transport (diffusion, migration, convection) and Navier-Stokes equation, along with Faradays law and Nernst- Einstein equation [2]. Total flux distribution for Na^+ and Cl^- species, ion concentration distribution and electrolyte current density have been numerically computed at different operating conditions: channel inlet velocity between 0.01 - 0.1 m/s and cell potential between 0.5 – 1.5 V. Interpolymer ion exchange membranes of different thickness, with different specific conductivities at NaCl concentrations of 0.1 M and 0.5 M have been considered in this simulation study [3].

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PC6. **INFLUENCE OF FACTORS ON NICKEL ELECTROPLATING**

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Nickel plating is widely used in industry for corrosion control, resistance to wear and decorative purposes [1, 2].

This research work investigated the influence of the pH, temperature and deposition time on nickel electroplating of copper. Operating temperature was varied from 40^0C- 100^0C and the electroplating time was between 30 minutes and 60 minutes. Deposition time has a great influence on the electroplating process. It was observed that amount deposited increases with increase in the plating time. After deposition, the corrosion rates in acidic media were calculated.

Optimum conditions for a uniform appearance, finer grained structure and dendrites free were observed at pH 4 electrolyte solution, deposition time 30 minutes and temperature 60^0C.

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PC7. **KINETIC STUDY OF SOME COMMERCIAL PHARMACEUTICAL FORMULATIONS OF ACETYLSALICYLIC ACID**

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The kinetic analysis of the reaction that a drug may have in aqueous solution may serve to establish objective criteria for assessing its stability in solution at a certain temperature [1, 2].

The aim of the study was to determine the amount of salicylic acid (SA) resulted from the hydrolysis reaction of acetylsalicylic acid (ASA) from different commercial pharmaceutical formulations using a spectrophotometric method and to determine the amount of degradable acetylsalicylic acid over time. The method was linear over the SA concentration range: 1-80 µg/mL with R^2=0,9996. In dilute aqueous solution the rate equation for the hydrolysis of acetylsalicylic acid is reduced to the first-order kinetics. The influence of pH and temperature on the rate of hydrolysis have been investigated. The kinetic parameters, the constant rate (k), the activation energy (E_a) for ASA hydrolysis as well as the Arrhenius pre-exponential factor (A) have been determined.

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PC8. **THERMAL DECOMPOSITION OF ZINC OXIDE NANOPOWDERS FUNCTIONALIZED WITH ANTHOCYANINS**

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The functionalized semiconductor nanoparticles obtained in vegetal matrix are innovative hybrid materials with interesting properties (*i.e.* optical, catalytic, and antimicrobial) [1]. The presence of organic compounds on inorganic materials surface influences their properties but, for some applications, including photocatalysis and DSSCs, the removal of organic template from functionalized nanomaterials can be useful.

The blue zinc oxide nanopowder was obtained by functionalization of ZnO nanoparticles with anthocyanins, using one-pot synthesis. The sensitization of ZnO nanopowder, obtained by chemical precipitation, with pigments from red cabbage extract, was also performed [2]. The thermogravimetric analysis of blue zinc oxide nanopowders revealed that for both nanomaterials the thermal decomposition occurs in four steps. A stronger bonding of organic pigments in the blue ZnO nanopowder obtained by one-pot method was evidenced by their loss at higher temperature. The morphology, cell parameters, lattice strain, and crystallite size of pristine zinc oxide nanoparticles obtained by thermal degradation of functionalized ZnO nanopowders were studied by transmission electron microscopy and electron diffraction. The photocatalytic activity was determined in the degradation of Congo red azo dye.

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SECTION D: PETROLEUM TECHNOLOGY AND MANAGEMENT

OD1. **PROGRESS IN COLLECTING AND RECYCLING OF USED LUBE OILS**

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Used lube oils are a source of pollution to the environment; they are also a source of energy. Used lube oils must be collected to avoid environmental pollution with hydrocarbons, metals and polycyclic aromatics and also for reevaluation; they can be burnt as fuel oil or re-refined to obtain new base oils. Burning is recommended to be in adequate conditions to avoid pollution with toxic gases, but it is costly. Re-refining is the best re-evaluation of used lube oils.

Collected used lube oils must be analyzed for having a better control on the quality of the final products base oils.

There are many processes for re-refining used lube oils, many of them are obsolete or forbidden because of chemicals used or because of the poor quality of base oils produced or for polluting by-products generated by these processes.

There are 3 processes which are not polluting and produce recycled base oils with quality equivalent to the quality of new base oils from crude oil.

The first one is a pretreatment of used lube oils with chemicals.

The second one is finishing distillates with a hydrogen treatment.

The third one is finishing distillates with a chemical treatment.

The investment cost and the running cost of the hydrogen finishing are higher than those with chemical treatment.

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OD2. **MODELLING THE THERMAL CRACKING PROCESS OF VEGETABLE OILS**

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The thermal cracking of vegetable oils proved to be an alternative for obtaining hydrocarbons in the petrochemical industry. Extensive studies in the laboratories [1, 2] demonstrated that good yields of olefins and aromatics can be obtained, so the scale-up of the process should be performed for industrial applications.

Mathematical models serving this purpose were developed, correlating the products yields with the process parameters.

Based on original experimental data obtained at the thermal cracking of vegetable oils [3, 4], two different models were taken into account and compared: a semi-analytical one (ASEM), developed by the Clean Combustion Technology Laboratory (CCTL), University of Florida, and a another one, obtained by linear regression, and resulting in polynomial functions.

The ASEM model is simple and robust, correlating the products yield with the process temperature and the chemical character of the products to be obtained. The polynomial model predicts the yield by the temperature and the residence time in the reactor.

The parameters of both models were obtained with accuracy. The first model is prone to extension beyond the experiment limits but the second describes the process in more detail.

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OD3. **PREDICTION OF OIL BLENDING PROPERTIES**

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Blending oil is more and more in use in order to have a product with constant time characteristics, absolutely necessary for predictible processing in the refinery.

That is why in this article we analyze the crude extracted in South Sudan and the type of blendings made after the extraction from the Moleta field [1].

The density, the water content and the viscosity variation are studied depending on their mixing rate, and mathematical predictive correlations of these properties are obtained [2, 3].

The differences between the models made in the laboratory and the mathematical methods with the mathematical analysis methods existing in the literature are analyzed.

For all selected linear regression methods (I, II and III polynomial, exponential, logarithmic), the relative errors and the absolute errors are calculated. Also the relative and absolute errors of the model chosen against the models described in the literature are analyzed.

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OD4. **DIESEL BLENDING PROPERTIES PREDICTION**

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In commercial practice, the blending of Euro-compliant diesel is mainly the continuous blending of biodiesel with refined diesel [1].

The paper aimed at:

a. Diesel fuel analysis in terms of marketing;

b. Presentation of the physico-chemical properties of diesel, additives, biodiesel and lamp oil;

c. Analysis of how commercial diesel mixtures are made;

d. Presentation of how to optimize blends of diesel and complementary products.

This material discusses the prediction of the main properties of diesel mixtures (density, cetane number, cetane index, point of congelating, freezing point, 40 to 20 ºC viscosity, distillation curve).

The white spirit effect on diesel is also being analyzed, it being a product that can be used in commercial diesel.

We also wanted to analyze the behavior of two diesel (winter and summer diesel) during mixing: variation of standardized parameters according to mixing rate [2].

Conclusions from laboratory experiments confirm the following:

a. Diesel fuel blends with biodiesel of up to 20% biodiesel may be achieved yet complying with the current standards and therefore it can be used as fuel for the type of engines present on the market;

b. It is possible to make blends of petroleum-based diesel with a maximum of 20% white spirit, because over these values the diesel approaches to a gasoline.

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OD5. **BLACK SEA ALGAE BIOMASS AS AN ALTERNATIVE RESOURCE IN BIOFUELS PRODUCTION**

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The conversion of Black Sea algae biomass into third-generation biofuels appears in the context of European environmental disposition and imperative need to compensate for the depletion of national oil reserves.

Macroalgae are lower plants that accumulate high lipid and protein content along with low-molecular-weight carbohydrates that are the major source of biofuels.

In the context of literature on topic [1], and according to our own works, the following directions of algae recovery resulted for the production of biofuels:

- Obtaining biogas with attractive yields for industrial production (up to 35 m^3 CH_4 / t fresh algae) using algae mixed with sludge from municipal wastewater treatment plants and possibly mixed with other biomass;
- The production of gaseous, liquid and solid fractions by algal pyrolysis, fractions which are biofuels themselves or can be constituents of blending with classical fuels; algae decompose at lower temperatures and provide higher gas yields compared to traditional biomass;
- Bioethanol can be produced from any marine algae species that contain an appreciable amount of polysaccharides. Polysaccharides are decomposed by hydrolysis into simple, fermentable sugars. Conversions of reducing sugars to 89% have been achieved, but the greatest limitation of ethanol yield is given by their low content in total sugars from hydrolysates.

Worldwide, processing applications of industrial algae occupy a fairly low share in the energy sector. Therefore, it may be considered that a high level of innovation is needed to make these processes more economically attractive.

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PD1. **TRANSPORT PROPERTIES OF SOME BIOFUELS BLENDS**

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The continuous growth of energy demand and environment pollution, and the non-renewable nature of fossil fuels resources have led scientists to look for alternatives to fossil fuels for transportation domain. Beside biodiesel that is already used blended with diesel fuel as fuel for diesel engine, other biofuels could be used as additives or replacements for diesel fuel [1-3]. In the last decade, bioalcohols have become interesting as biofuels for internal combustion engines as significant improvements were registered for the yield of bioalcohols production from biomass using sustainable pathways [4, 5].

Viscosity is one of the fuels important properties influencing the behavior of diesel engine. The main objective of this study is to report viscosity data of biodiesel + propanol and biodiesel + butanol blends covering the entire composition range and for temperature varying between 293.15 K and 323.15 K. Based on these data, the optimum alcohol quantity that can be added to biodiesel for the formulation of a fuel with characteristics within the required specifications of diesel fuel quality standard (EN 590), can be determined. The accuracy of different equations to estimate the viscosity of biodiesel + alcohol blends was estimated.

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PD2. **TERNARY FUELS BLENDS WITH APPLICATIONS IN TRANSPORT DOMAINE**

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In order to reduce environment pollution, particular attention has been paid to biodiesel as an alternative fuel for diesel engines due to its advantages compared to diesel fuel. But this biofuel have some drawbacks compared to diesel fuel, such as higher density and viscosity. Fuel density directly influences the performance of the diesel engine, since density influences the mass of injected fuel in the combustion chamber [1]. The high viscosity of biodiesel leads to a poor atomization and this result in incomplete combustion [2].

The addition of an alcohol to diesel fuel + biodiesel blend could solve the problem of high density and viscosity of biodiesel, allowing higher quantities of biofuels to be added to diesel fuel, in order to reduce harmful emissions.

Although density and viscosity data of biodiesel + diesel fuel binary blends at different temperatures are available in the literature [3], for the ternary blends biodiesel + diesel fuel + alcohol, these data are insufficient. The aim of this work was to report experimental density and viscosity data for diesel fuel + biodiesel + isopropanol blend, covering the entire composition range and for temperature varying between 293.15 K and 323.15 K. It was observed that the addition of isopropanol to biodiesel+diesel fuel blends decreases both the density and the viscosity of the formed ternary blend. The use of biodiesel + diesel fuel + alcohol ternary blend as fuel for diesel engine has the advantage of allowing a higher amount of biofuels to be added into the ternary blend and still meeting the requirements of diesel fuel quality standard, EN 590.

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PD3. **THE INFLUENCE OF PHYSICO-CHEMICAL PROPERTIES OF DIESEL-BIODIESEL-ALCOHOL MIXTURES ON THE ENGINE PERFORMANCES**

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The development of technologies for biofuels production has attracted a great deal of interest not only because of the steady rise in oil prices, but also because of the limited fossil fuel reserves. With the rising oil prices, on energy safety and environmental issues, climate change, biofuels have become a major issue around the world. The biofuel is a major renewable energy source to supplement declining fossil fuel resources. Biodiesel is a renewable transportation fuel consisting of fatty acid methyl esters (FAME), generally produced by transesterification of vegetable oils and animal fats.

The paper presents an experimental investigation regarding the use of commercial diesel fuel and different blends of diesel oil with biofuel and alcohol, such as: biodiesel B100 (biodiesel 100%) , B20M10 (20%biodiesel + 10% methanol + 70% Diesel fuel), B20E10 (20% Biodiesel+ 10% Ethanol + 70% Diesel fuel), B20M5 (20%biodiesel + 5% methanol+ 75% Diesel fuel) and B20E5 (20% biodiesel+5% ethanol+75% Diesel fuel). The correlation between the physico-chemical properties and the engine's performances resulted

The use of alcohol additives (methanol and ethanol) in the biodiesel blends reduces the viscosity and density of the resulted blend due to the lower density and viscosity of the additives and affects the engine performances.

PD4. **PERFORMING ESTERIFICATION REACTIONS THROUGH REACTIVE DISTILLATION**

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The reactive distillation is a front-runner of industrial process intensification, by thermal integration of chemical reaction and separation in a single process, with the possibility of increasing the selectivity, in order to obtain preferential products [1]. It can be an alternative to conventional processes, especially for limited chemical equilibrium reactions which typically require one of the reactants in excess. There are numerous applications, such as the esterification reactions.

In this paper, the obtaining of methyl lactate and isopropyl lactate was studied in laboratory, in reactive distillation, by direct esterification and transesterification. The experimental study is based on former studies in literature investigating the kinetics of lactic acid with different alcohols [2, 3] and liquid- vapor equilibria [4]. The influence of the reactants molar ratio and that of the number of theoretical stages in the column were studied. The results show that products yields grow with the molar ratio increasing and with the number of theoretical stages in the column. Using a Raschig rings packed column with an equivalent height of 4.9 theoretical stages and a molar ratio 3/1 alcohol/ lactic acid, the yield in case of methyl lactate was 76.7% and 41.8% in case of isopropyl lactate in direct esterification. At the same reactants ratio, the yield of isopropyl lactate was 64.9 % for the transesterification of methyl lactate with isopropanol.

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PD5. **PERFORMANCE OF Co-Mo-Ni CATALYSTS ON POLYCYCLIC AROMATIC HYDROCARBONS TRANSFORMATION IN HYDROCRACKING PROCESS**

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The goal of this study is to evaluate transformation of polycylic aromatic hydrocarbons in hydrocracking process over trismetallic γAl_2O_3 and HMS - γAl_2O_3 supported catalysts. Hydrocracking tests are realized using Co-Mo-Ni catalysts with different composition and support: 8.6%Mo-2%Co-2%Ni/γAl_2O_3, 11.5%Mo-2%Co-0.8%Ni/γAl_2O_3, and 11.5%Mo-2%Co-0.8%Ni/HMS-γAl_2O_3. The experiments are realized using different temperatures reaction: 370 ^oC, 400 ^oC, 420 ^oC, and different pressures: 50, 60 and 70 bar. The liquid hourly space velocity (LHSV) has been maintained at 1 h^{-1} and the raw materials used for experiments was delayed coking gas oil and atmospheric gas oil. The raw material and the hydrocraked gas oil obtained in experiments were analyzed in order to evaluate composition of aromatic hydrocarbons composition such as mono- , di- and polyaromatics. The distribution of aromatic hydrocarbons is correlated with physical-chemical properties: density and structural group analysis.

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[4]. ASTM D3238 Standard test method for calculation of carbon distribution and structural group analysis of petroleum oils by the n-d-m method.
[5]. ASTM D2502 Standard test method for estimation of mean relative molecular mass of petroleum oils from viscosity measurements.

PD6. **ADDITIVATED LUBRICATING GREASES MADE OF AGRICULTURAL RESOURCES**

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Lubricating greases are highly structured suspensions consisting of fatty acid soaps of lithium, calcium, sodium, aluminum or barium, most commonly used as thickeners, dispersed in mineral or synthetic oil [1, 2]. Comparing with mineral oils, vegetable oils have many advantages, such as low toxicity, low volatility, good lubricity and ability for adhering to metal surfaces, and small viscosity–temperature dependence [3].

Consequently, the aim of this study was to evaluate the effect that cellulose and lignin exert on the mechanical and rheological properties of traditionally calcium lubricating greases based on palm oil and corn oil. In this sense, new calcium lubricating greases were prepared based on palm oil and corn oil with calcium stearate in different concentrations (15%, 20% and 25% wt), at different manufacture temperature (90^{o}C, 100^{o}C and 110^{o}C). In order to improve rheological properties, consistency and mechanical stability, additives like crystalline cellulose or Kraft lignin (5%, 10% or 20% w/w) were added during manufacture process.

Finally, from all analyzed samples, we found that greases additivated with 20% (w/w) cellulose or 20% (w/w) lignin present the best rheological properties, consistency and mechanical stability. As a result, these formulations could be suitable for valves and fittings, gearboxes, rolling bearing, in applications for incidental contact with materials in food processing or paper mills.

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SECTION E: FOOD CHEMISTRY AND ENGINEERING

PE1. **SUMMER PROFILE OF LIPOPHILIC TOXINS IN SHELLFISH FROM BULGARIA**

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The presence of phytoplankton responsible for the production of marine biotoxins (phycotoxins) is well recognised globally. The frequency and intensity of harmful algal blooms (HABs) appear to be on the rise globally. There is also evidence of the geographic spreading of toxic strains of these algae. Phycotoxins accumulate in filter feeding bivalves and through the food chain find their way to humans. In certain quantities they can cause severe illness. According to the symptoms they cause marine biotoxins are classified as paralytic (e.g. saxitoxin), amnesic (e.g. domoic acid), which are hydrophilic and diarretic (e.g. okadaic acid) toxins etc. which have lipophilic nature.

Synergistic interaction among toxins may play an important role in the toxicity of shellfish and consequently in human intoxications. To date, the national monitoring program of phycotoxins in Bulgaria has limited the quantitation of hydrophilic toxins in cultivated mussel samples.

The aim of this study was to assess the presence of lipophilic toxins in both cultivated and wild mussel samples, harvested in summer 2017 from south coast of the Black Sea, Bulgaria. Determination was performed by liquid chromatograph coupled to tandem mass spectrometry.

Despite of the evidence published recently for the presence of variety of potentially toxigenic producers in the investigated area, this work reports the detection of only yessotoxins. YTX concentration increases up to 5-fold two times in the investigated period whereas in cultivated mussels the mean concentration is 5832.86 pg YTX/g hepatopancreas and in wild - 920.42 pg YTX/g hepatopancreas. Additionally, calculated concentrations per whole shellfish meat do not exceed the legislative limit. These results indicate that the risk through consumption of studied shellfish is low.

PE2. **HUMAN HEALTH RISK OF ORGANOCHLORINE COMPOUNDS IN FISH FROM THE DANUBE RIVER, BULGARIA**

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The present study evaluated the residual concentrations of selected organochlorine contaminants in fish and estimated the potential health risks associated with the exposure to these pollutants. Concentrations of organochlorine compounds (polychlorinated biphenyls (PCBs), DDT and its metabolites, hexachlorobenzene and hexachlorobutadiene) were determined in muscle tissue of six fish species: common carp *(Cyprinus carpio),* catfish *(Silurus glanis),* pike-perch *(Sander lucioperca),* common nase *(Chondrostoma nasus),* beluga *(Vimba vimba)* and bream *(Abramis brama).* Fish samples were collected in 2010 and 2015 from the Danube River, near Silistra, Bulgaria.

The sum of DDT and its metabolites was determined from 3.27 to 25.33 ng/g wet weight (in pike-perch and common nase, respectively). The sum of the six Indicator PCBs ranged from 2.51 to 10.67 ng/g wet weight in pike-perch and catfish, respectively, and did not exceed the European maximum limit.

The EDI of I-PCBs was calculated between 0.47 and 2.01 ng/kg bw day through consumption of fish. The mean EDI of DDTs in fish from Danube River was calculated between 0.62 and 4.79 ng/kg body weight/ day. The current dl-PCBs intake through fish consumption by a standard adult male of 70 kg body weight was 1.5% of the tolerable daily intake (TDI) for these compounds.

The human health risks were assessed using a risk quotient (RQ) and margin of exposure (MOE) of the fish consumption. The MOE is defined as the ratio of the no-observed-adverse-effect level (NOAEL) for the critical effect to the estimated exposure concentration. The calculated MOE > 100 and implies low risk of fish studied. All the RQ values were much lower than 1, suggesting that consumption of the fish species would not pose a non-cancer risk.

PE3. **COMPARISON OF FATTY ACIDS, CHOLESTEROL, FAT SOLUBLE VITAMINS AND CAROTENOIDS CONTENT OF SKIN AND EDIBLE TISSUE OF FARMED AFRICAN CATFISH (CLARIAS GARIEPINUS, BURCHELL, 1822)**

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Freshwater African catfish (*Clarias gariepinus*) is new species for the Bulgarian market and there is lack of information for the quality of its dietary lipids. This species is a valuable source of biologically active components that play an important role for healthier human diet. This study was focused on the assessment of lipid quality of skin and edible tissue of farmed African catfish (*Clarias gariepinus*) based on lipid content and detailed fatty acids, fat-soluble vitamins, cholesterol and carotenoids composition. Fish specimens were purchased from local fish markets in Varna.

Total lipids were extracted according to Bligh and Dyer method. Analysis of fatty acid methyl esters (FAME) was done by gas chromatography with mass spectrometer (GC/MS). Vitamins A, D_3 and E, beta-carotene, astaxanthin and cholesterol were analyzed simultaneously using high performance liquid chromatography (HPLC) with ultraviolet and fluorescence (for vitamin A and E) detectors.

Mean lipid content, cholesterol, astaxanthin amounts and the monounsaturated fatty acids (MUFA) were significantly higher in skin than in muscle tissue, whereas the proportion of vitamin A and E, and polyunsaturated fatty acids (PUFA) including were higher in the latter. Only vitamin D3 show similar amounts in both analysed tissues. The important indicator for nutritive quality of fish for human diet (content of eicosapentaenoic acid (C20:5 n-3) and docosahexaenoic acid (C22:6 n-3)) presented significantly high amounts of these omega-3 PUFAs. A 100 g filet without skin contains approximately 600 mg/100 g.

The potential nutritional and medicinal value of fatty acid composition, cholesterol, vitamins and carotenoids content for consumers were evaluated. Presented results confirmed the high lipid quality of African catfish meat, and we can conclude that both – with or without the skin fish fillet can be valuable and preferable source of analyzed biologically active lipids.

PE4. **LIPID COMPOSITION OF RAW AND COOKED *RAPANA VENOSA* FROM THE BLACK SEA**

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Vained rapa whelk (*Rapana venosa*) is a predatory marine snail, once an invasive species in the Black Sea, now has become a valuable seafood with nutritional and economic importance. There is still limited information available on their lipid composition. The aim of the present study is to provide new information on the lipid content, lipid classes, fatty acid profiles, fat soluble vitamins and cholesterol content of raw and boiled *Rapana venosa*.

Lipids were extracted by the method of Bligh and Dyer and subsequently separated into neutral lipids and phospholipids. Fatty acids of lipid classes were analyzed by gas chromatography–mass spectrometry. The non-saponifiable lipids were identified by high pressure liquid chromatography coupled with UV/Vis and fluorescence detectors.

Lipid content showed significant changes after cooking process. The distribution of lipid classes remained unchanged, but there were considerable differences in their fatty acid composition. The analyses of raw samples showed that saturated fatty acids (SFA) content is significantly higher than monounsaturated fatty acids (MUFA) and polyunsaturated fatty acids (PUFA) (SFA≥PUFA>MUFA), while cooked rapana showed the opposite trend (PUFA>SFA>MUFA). Fatty acid distribution of phospholipids remained unaffected by temperature treatment (PUFA>SFA>MUFA). In contrast, neutral lipids in raw samples (PUFA≥SFA>MUFA) presented significant variations after cooking process (SFA>PUFA>MUFA). In all samples the amount of omega-3 PUFAs was higher than omega-6 PUFAs. The ratio omega-6/omega-3 was below 1 and PUFA/SFA ratio was greater than 1, which falls within the FAO/WHO recommendations. *Rapana venosa* was characterized by significant amounts of fat-soluble vitamins. The results of the present study showed that cooking process alters significantly the concentrations of vitamin A, b-carotene and astaxanthin and to a less extent – vitamin E. Cholesterol and vitamin D_3 were affected by the thermal stress.

The study revealed that *Rapana venosa* meat could be a good natural source of high quality nutritional lipids, which are well preserved even after culinary treatment. Cooked rapana could be recommended as a part of a proper or preventive diet.

PE5. **LEVELS OF SELECTED ESSENTIAL AND TOXIC ELEMENTS IN THE WHITE CABBAGES (*BRASSICA OLERACEA L. VAR. CAPITATA ALBA*) AND RED CABBAGES (*BRASSICA OLERACEA VAR. CAPITATA F. RUBRA*)**

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The aim of the present study was to evaluate total content of macroelement, microelement and heavy metal from cabbage leaves. In addition the ascorbic acid content, anthocyanins of *Brassica oleracea var. capitata f. rubra,* the total phenolics and colorimetric analyses (lightness-L^*, redness-a^*, yellowness-b^*, chroma - C^* and hue angle H^*) was investigated. Total macroelement, microelement, and heavy metal content were determined by atomic absorption spectrometry. Total phenolic content (TPC) in methanol cabbage' extracts was measured using Folin-Ciocalteu reagent. Ascorbic acid (AA) was separated, identified and dosed in a HPLC SHMADZU system coupled with UV–VIS detector (DAD).

The highest mean contribution of elemental interactions regarding total macroelements in white cabbage leaves from inside (14-16 leaf), was observed for calcium (Ca) and selenium (Se) with 750 and 415 mg/kg dry matter (dm), respectively, whereas the lowest was found for heavy metals, nickel (Ni), cadmium (Cd), and cobalt (Co) with 4.35, 0.143, 1.25, and 0.185 mg/kg head dm, respectively. The total contents of calcium (Ca) and selenium (Se) in red cabbage leaves from inside (14-16 leaf) were 1350 and 360 mg/kg dry matter. It was observed a possible correlation between color parameters and total macroelement.

PE6. **SOME QUALITY PARAMETERS OF MUSTARDS FROM THE ROMANIAN MARKET**

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Five commercial mustards, made by different manufacturers, were studied to examine their physico-chemical properties and to establish relationships between those properties. Physico-chemical analysis revealed distinct differences between the mustards in the dry matter and extract contents and smaller differences in the protein, fat and ash levels. Two of the investigated mustards did not satisfy the requirements of the relevant Romanian standard regarding dry matter content.

Statistical analysis of the results showed significant linear correlations between the dry matter, fat, protein and ash contents of mustards and some parameters of rheological model [1].

[1]. http://www.wseas.us/e-library/conferences/2013/Brasov/ACMOS/ACMOS-40.pdf

PE7. **STUDY OF THE METABOLIC ACTIVITY OF YEASTS USED IN BREWING INDUSTRY AND BIOETHANOL PRODUCTION**

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Determination of the percent of actively fermenting yeasts, during the production, can be used for optimization of the fermentation process in brewing industry and bioethanol production. The metabolic activity of brewing yeasts and yeasts used in bioethanol production was investigated using carboxyfluorescein diacetate (cFDA). cFDA penetrates the cell membrane, then active esterase enzymes inside the cell cleave acetate residues, and the released fluorescein stains the cell in green. The stained cells were counted by new fluorescent image cytometry EasyCounter YC from Milkotronic. EasyCounter YC is based on a fluorescence microscopic cell counting technique. Due to the fluorescent dye, LED optics, and CCD capture technologies, cell analysis is accurate, reliable, and fast. Optimal concentrations of the cFDA reagent for both types of yeast were determined. The cFDA optimal concentration for metabolic activity determination of the brewing yeast was found to be 50 μg/mL, and for yeasts in bioethanol production was found to be 200 μg/mL. The metabolic activity of cell suspensions with different concentrations of dead and live cells was determined. It was found that the assay provides very valuable information when the percentage of dead cells in the sample is significant, because there are a large number of cells with weak enzymatic activity in the suspension at that stage. The same samples were simultaneously tested for determination of total cell count, dead cell count and the percentage of viability. Great correlation between the individual parameters was established.

PE8. **MAGNETIC NANOPARTICLE BASED IMMUNOFLUORESCENCE ASSAY OF STAPHYLOCOCCAL ENTEROTOXIN A IN MILK**

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Staphylococcal Enterotoxins are one of the most frequent toxins involved in food poisoning outbreaks, especially in dairy products. The most common and toxic serotype is Staphylococcal Enterotoxin A (SEA). There are a number of methods for SEA detection but most of them are not sensitive and specific enough. In this work, fluorescent conjugate of SEA and ATTO620 was prepared and proved. Absorbance and emission characteristics of the obtained SEA-ATTO conjugate and fluorescent dye ATTO620 were analyzed. Monoclonal anti-SEA antibody was immobilized onto magnetic nanoparticles (MNP). Immunofluorescence (IF) assay was developed for SEA determination in buffer solutions and in raw cow milk. ATTO620 labeled SEA was used for a competitive IF assay. The concentrations of the conjugate and immobilized antibody were optimized. Milk samples were spiked with variety concentrations of the enterotoxin. SEA in samples bound to anti-SEA antibody linked to the MNP, and competitive binding of SEA-ATTO620 conjugate was performed. Magnetic separator was used for bounded components removal and the fluorescence intensity of the unbound tracer was measured. The assay has linear range 0.25 – 10 ng/mL SEA in buffer and 0.25 – 5 ng/mL SEA in milk. The developed assay has great sensitivity 0.2 ng/mL SEA. Furthermore, it takes less than 2 hours to complete the analysis and allows simultaneous analyzes of several samples. The developed assay offers fast and sensitive analysis of SEA in milk and can be included in dairy industry.

PE9. **OPTIMIZATION OF GLUTEN FREE BREAD PREPARATION USING ENZYMES**

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Gluten-free diet is now important not only for coeliac disease patients, but also for people who should avoid gluten-based for other reasons. The market of gluten-free products is increasing every year and a lot of efforts are done with the aim to improve the products quality. Different mixtures of alternative flours, starch, hydrocolloids, non-gluten proteins, enzymes, lipids, pseudocereals and other ingredients were used as substitute for gluten [1].

The aim of this work is to present the structure of gluten-free bread obtained using rice flour, guar gum and different enzymes like Neutrase® for its preparation. Neutrase® is an endoprotease which can be used in many applications where proteins have to be broken down to polypeptides or peptides. The enzyme is a bacterial protease produced from a selected strain of *Bacillus amyloliquefaciens*.

Digital image analysis was used for the quantitative evaluation of pore structure such as determining gas cell sizes and distribution. Response surface methodology was applied for bread composition optimization, taking into consideration the influence of several factors at many levels and could facilitate the obtaining of the corresponding interactions among these factors using a small number of experiments [2, 3]. The obtained results are promising and can represent a good start for a gluten-free bread recipe.

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PE10. **NITRITES IN PROCESSED VENISON MEAT**

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The polyatomic ion with molecular formula NO_2^- is a preservative used and controlled in meat industries [1, 2]. Nitrites are used as antimicrobial agents in meat to inhibit the growth of bacterial spoilage and it can react with meat myoglobin which gives the red color [3]. The bacteria clostridium botulinum can be prevented in meat by adding nitrites [4]. On the other hand, high intakes of nitrites in meat it's dangerous to human health [3].

The purpose of this study is to validate a method for the analysis of nitrites in some processed venison meat: deer salami, bear salami, wild boar marinated fillet, deer pastrami, wild boar sausages and venison mince burger. The nitrites content was measured using UV-VIS spectrometric method with Griess reagent. It was observed a good linearity of the method response in the 0.04-0.8 mg/L concentration range with $R^2 = 0.9995$. The LOD and LOQ was 0.0121 mg/L, respectively 0.0406 mg/L. The nitrites content varied from 0.0339 to 1.2396 mg/100 g and these values are lower than those encountered in the literature.

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PE11. **DETERMINATION OF THE POLYPHENOLIC COMPOUNDS IN SOME RED GRAPES AND DERIVATIVE PRODUCTS BY HPLC/DAD**

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Polyphenols are considered the most antioxidant ingredients in grapes and derivative products (juices and wines) and are related to human health because of their free radical scavenging activities. Five variety of commercial red grapes (*Cardinal*, *Muscat Hamburg* and *Alphonse Lavallée* - *Vitis vinifera L.*, *Isabella Vitis labrusca L.* and *Moldova* - hybrid variety) were analyzed and significant concentration of E-resveratrol, chlorogenic acid, gallic acid and ellagic acid were found in the peels and seeds of grapes, marc and macerate extracts, respectively.

The maximum contents of polyphenolic compounds were identified in peels and seeds of fresh grapes, like *Moldova* peels - 1020.73mg/100g sample and *Muscat Hamburg* seeds – 2721.15 mg/100g sample, in the dried marcs (*Isabella* – 120.65 mg/100g sample) and its juices (*Alphonse Lavallee* 391.15 mg/100g sample) after five days. The concentrations of these compounds seem to vary considerably, depending on diverse factors such as climate, cultivar and time or applied technique of maceration.

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WORKSHOP:

NEW MATERIALS FOR THE ELECTROCHEMICAL RECOGNITION OF MINERAL AND BIOLOGIC SPECIES

KN1. **AZULENE BASED MATERIALS FOR HEAVY METAL IONS DETECTION**

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Azulene derivatives have been seldom used to the metal ions electroanalysis. Our study concerns the synthesis and electrochemical characterization of several classes of azulene based monomers. Each monomer (**L**) has been used to obtain modified electrodes by electrochemical polymerization. Poly**L** films modified electrodes have been obtained and characterized by cyclic voltammetry, differential pulse-voltammetry, electrochemical impedance spectroscopy, and scanning electron microscopy, atomic force microscopy. The complexing properties of poly**L** based functional materials have been investigated towards heavy metals (Pb, Cd Hg, Cu) by preconcentration – anodic stripping technique in order to analyze their content from water samples. Derivatives such as from (5-[(azulen-1-yl) methylene]-2-thioxothiazolidin-4-one were found to be good ligands for heavy metals in homogeneous solutions and in heterogeneous systems based on chemically modified electrodes. Quantum mechanical calculations on azulene compounds have been performed in order to test their ability to coordinate heavy metals.

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KN2. A NEW EXAMPLE OF MOLECULAR METAMORPHISM: A MOLECULAR ASSEMBLY INVOLVING HINGES BASED ON INORGANIC Pd (II) COMPLEXES WITH π-DIMERIZABLE LIGANDS

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The strategy of pre-organizing subunits responding to electron transfer activation to promote an intramolecular π-dimerization process has been exploited essentially by considering purely organic hinges. There are some examples of organic structures composed of two dimerizable pyridinyl or TTF subunits, for which the presence of metal ions (Pd^{2+}, Mn^{2+}, Pb^{2+}, Mg^{2+} ...) allows the closure of the hinge, due to the formation of π- intramolecular dimers. The only π-dimerizable structures based on inorganic hinges were built around ferrocene, used as a pivot, the cyclopentadienyls being functionalized by π-dimerizable groups such as naphthalenediimide, verdazyl and viologen subunits.

We present here a new example of systems involving hinges based on inorganic complexes whose ligands carry π-dimerizable groups. It is constructed from a new viologen derivative substituted by an imidazole unit used as an anchor for a Pd (II) metal center. The reversible nature of the association between palladium and imidazole ligands allows an easy reorganization of the ligands around the metal center under the action of an external stimulus. The reorganization process involves assembling and disassembling equilibria accompanying the construction of dynamic systems. On the other hand, the plane-square geometry of the Pd (II) complexes is a favorable factor since the distances imposed by the coordination of two ligands in the adjacent (cis) or opposite (trans) position with respect to the metal center are adapted to the development of intramolecular π-dimer interactions involving the two ligands of the same complex. The π-dimerization properties of the electrogenerated viologen radicals at the palladium complex arms, and the geometry adopted by this complex according to the redox state of the viologen units, will be discussed on the basis of (spectro-) electrochemical, spectroscopic and theoretical calculations.

KN3. **ELECTROCHEMICAL SYNTHESIS OF NOVEL ANTIBACTERIAL SILVER DOPED POLY(VINYL ALCOHOL)/CHITOSAN/GRAPHENE HYDROGELS**

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The synthesis of silver nanoparticles (AgNPs) became very interesting for potential applications in biomedicine, since nanocrystalline silver is proved to be the most efficient antimicrobial agent with a wide inhibiting spectrum towards different types of microorganisms. AgNPs embedded in hydrogel matrices are attractive for biomedical applications due to possibility for their controlled release resulting in antimicrobial activity. Thus, combination of AgNPs with biocompatible hydrogels, like poly(vinyl alcohol) (PVA), and chitosan (CHI) provides potential for design of improved medical treatments and devices (antimicrobial wound dressings, soft tissue implants). Graphene (Gr) has exceptional mechanical properties and has therefore been applied in tissue implants and wound dressings, as well as adequate reinforcing component for composite materials.

Incorporation of AgNPs nanoparticles into PVA/Gr matrices was achieved by *in situ* electrochemical reduction of Ag ions at constant voltage in PVA/CHI/Gr hydrogels produced previously by freezing–thawing method and swollen in $AgNO_3$ precursor solution. Synthesized nanocomposites were characterized by UV-Vis, CV, FE-SEM, Raman, XRD, AAS, FT-IR, as well as by MTT cytotoxicity tests and test of antibacterial activity against pathogenic bacteria strain *Staphylococcus aureus* and *Escherichia coli*. The results indicated that both Ag/PVA/CHI/Gr and Ag/PVA/CHI are excellent candidates for soft tissue implants and wound dressings [1, 2].

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KN4. **DESIGN OF SUPRAMOLECULAR BIOASSEMBLIES BASED ON NANO-OBJECTS AND ORGANIC BINDERS FOR BIOSENSING OR ELECTROCATALYSIS APPLICATIONS**

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For four decades, the development of biointerfaces has been the subject of increasing research efforts in the field of analytical chemistry and energy conversion. In particular, the functionalization of electrodes by biomaterials based on electrogenerated polymers and / or carbon nanotubes or graphene is widely used for the design of biosensors and biofuel cells. These nano-objects were successfully functionalized by electropolymerization of pyrrolic monomers or via π−π stacking interactions with pyrene derivatives exhibiting both affinity or covalent binding interactions towards biomolecules. Various biomolecule immobilization strategies have been explored involving photografting process, affinity and host-guest interactions, or supramolecular coordination complex phenomena. Some new approaches for developing nanostructured biomaterials based on supramolecular assemblies will be illustrated. In particular, recent examples of electrochemical labeless immunosensors and aptasensors for bisphenol A, cocaine, dengue antibody or cholera toxin antibody will be presented [1-3]. For instance, carbon nanotube deposits with different controlled thicknesses were functionalized by electropolymerized films of polypyrrole-nitrilotriacetic acid and successfully employed for the design of impedimetric immunosensor for cholera toxin antibody [4].

The need for clean methods of producing electricity has stimulated the emergence of biofuel cells that convert chemical energy into electrical energy by electro-enzymatic reactions. A vast majority of biofuel cells generates electrical energy from the enzymatic degradation of glucose and oxygen, two substrates present in physiological fluids. Thus, in parallel to the powering of portable electronic devices (mobile phone, digital music player, laptop, GPS, etc), a fascinating application concerns the implantation of biofuel cells in the human body as an autonomous source of theoretically unlimited energy[5]. Recent advances in the design of bioelectrodes based on electrically wired enzymes onto carbon nanotube coatings will be reported. In particular, a new generation of enzyme electrodes based on flexible buckypaper was developed by using linear polynorbornene polymers containing multiple pyrene groups

as crosslinker. Furthermore, buckypapers based on bilirubin oxidase and FAD-dependent glucose dehydrogenase, were successfully applied to the elaboration of O_2/glucose biofuel cells providing 24.07 mW cm^{-3} [6].

Finally, an innovative approach based on the electrical wiring of enzymes in solution by redox glyconanoparticles resulting from the self-assembly of bio-sourced block copolymers will be presented. We demonstrate the self-assembly, characterization and bioelectrocatalysis of redox-active cyclodextrin-coated nanoparticles. These nanoparticles were used as electron shuttles between electrode and bilirubin oxidase providing enhanced current densities for enzymatic O_2 reduction [7].

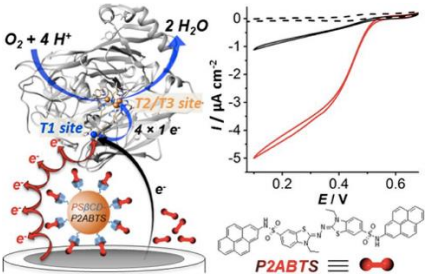

Fig. 1: Schematic representation of the electrical wiring of a bilirubin oxidase by redox nanoparticles (organic nanoparticle modified by ABTS), both in solution.

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OW1. **COLORIMETRIC AND VOLTAMMETRIC DETECTION OF MERCURY IONS USING AZULENE-EDTA**

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Given the advantages of both colorimetric and electrochemical sensors, it is desirable to find new molecules that lead to the obtaining of both types of sensors. It is not a very easy task, since the molecules must contain a metal ion complexing unit and a moiety with optical properties, being capable to electropolymerize as well. Moreover, it is desirable to obtain new sensors with high selectivity towards a specific analyte. Such demands could be fulfilled by specially designed azulene derivatives, because azulene moiety is a well-known chromophore with optical [1] and redox [2] properties. Here, we report the synthesis of a new monomer, 2,2'-(ethane-1,2-diylbis((2-(azulen-2-ylamino)-2-oxoethyl)azanediyl)) diacetic acid (**L**). It contains two active parts: azulene - which can serve as chromophore and polymerizable unit, and a metal ion complexing agent, derived from ethylenediamine tetra-acetic acid (EDTA). The sensing properties of **L** monomer towards metal ions were tested in homogeneous media. The monomer shows a color changing only in the presence of mercury ions. Moreover, the monomer was successfully deposited on glassy carbon electrodes through direct electropolymerization, modified electrodes being subsequently obtained. These new electrode materials are able to complex metal ions from aqueous solution [3].

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OW2. **ADHESIVE PROPERTIES STUDIES OF F-SWCNTS BASED NANOCOMPOSITE THIN FILMS**

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The P3OT polymer and SWCNTs conjugates show promise in optoelectronic applications, such as organic photovoltaic cells, organic light emitting diodes and chemical/optical sensors. The purpose of the current work is to study the adhesive properties of the nanocomposite thin films prepared by spin coating technique using different mass concentration of f-SWCNTs. The influence of CNTs addition into the P3OT polymer matrix on the morphological, compositional and mechanical surface properties was evaluated by Micro-Raman, ATR-FTIR and AFM measurements. The successfully incorporation of the carbon nanotubes into the host is confirmed by the Raman spectra. The arrangement of carbon nanotube bundles into the polymer matrix was revealed by the AFM topography images. The surface roughness of the prepared nanocomposites increases with the increase of the amount of added filler, while force adhesion values are decreasing, but their distribution over the analysed surfaces becomes more uniform.

OW3. **NEW MODIFIED ELECTRODES FOR HEAVY METAL SENSING**

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The azulene is a particular monomer used to function electrodes because of its high polarizability as it allows spontaneous transfer of electrons from the 5-atom cycle (negative polarized) to the 7-atom cycle (positive polarized). Our study relates the electrochemical characterization by cyclic voltammetry, pulse-differential voltammetry and rotating disk electrode voltammetry of a new 4'-(E-zulen-1-ylvinyl)-6-crown-2-ether azulene monomer.

L-monomer has been used to obtain complexing modified electrodes by electrochemical polymerization. The study led to the finding of the best conditions for this azulene polymerization. Poly**L** modified electrodes were characterized by cyclic voltammetry in ferrocene solutions. The complexing properties of this polyfunctional material for the recognition of heavy metals (Pb, Cd, Hg, Cu) were investigated by anodic pre-concentration technique. The best non-optimized response was obtained for Pb.

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OW4. **SYNTHESIS OF Cu NANOWIRES USING AQUEOUS AND IONIC LIQUID ELECTROLYTES FOR ELECTROCHEMICAL DETECTION**

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The use of 1D metallic nanoarchitectures (i.e. nanowires, nanotubes, nanorods) are of great interest in the building of electrochemical sensors and biosensors thanks to their efficient electron transfer along 1D direction and good mechanical strength. Moreover, they allow the fabrication of high-density nanoscale devices [1, 2].

Cu based nanowires are particularly attractive due to their catalytic ability and availability representing suitable materials for electrochemical detection of several analytes, including glucose and hydrogen peroxide [2, 3].

Herein, Cu nanowires using template-assisted method are developed, involving both aqueous solutions and ionic liquids based on eutectic mixtures of choline chloride with ethylene glycol or urea (the so-called “deep eutectic solvents” - DES). The electrochemically synthesized nanowires have been characterized using SEM and XRD investigations. Cyclic voltammetry has been selected as electrochemical technique in order to evidence processes of deposition of copper nanowires and the influence of the main operation parameters, mainly the applied current density/ deposition potential and the temperature. The electrodeposited films have been characterized using SEM and XRD investigations. A comparative analysis of the structural features of the obtained Cu nanowires against the electrolyte type is presented.

Preliminary results related to their electrochemical sensing performance for glucose and hydrogen peroxide are also discussed.

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OW5. **ELECTROCHEMICAL DISSOLUTION OF PLATINUM GROUP METALS FROM A MULTI COMPONENT MATRIX**

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Platinum is a well-known catalyst used in the automotive industry, petrochemical industry and in the pharmaceutical industry [1]. The 2017 PGM Market Report by Johnson Matthey® shows that there is an increasing demand of platinum especially in the European automotive market while the supply was flat [2]. It is foreseeable in the near future for the platinum demand to exceed the supply. As a result, the EU has placed platinum on its critical raw materials list. Platinum has a high resistance to corrosion which makes *aqua regia* the only leaching medium. New techniques are needed to achieve an environmentally friendly platinum recycling strategy.

Herein, we present our most recent results on the electrochemical dissolution of platinum in different electrolytes at acidic pH. The efficiency of the process is measured by a state-of-the-art inductively coupled plasma – optical emission spectrometer. Our findings indicate that the reaction is accelerated at transient conditions in the presence reducing/oxidizing species.

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OW6. **THREE CARBON NANOMATERIALS SYNTHESIZED BY KRF LASER ABLATION IN AN INNOVATIVE REACTOR**

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We successfully synthesized single wall carbon nanotubes (SWCNTs), carbon nanoonions (CNOs) and graphene by KrF excimer laser ablation in an innovative home build reactor. Ablation target for CNOs and graphene were made from commercial graphite powder pressed at 15 tones for 15 minutes at room temperature. For SWCNTs we use a unique recipe, along with reactor design being patent pending. All carbon nanomaterials were characterized by: SEM-STEM (Scanning Electron Microscopy - Scanning Transmission Electron Microscopy), Micro Raman Spectroscopy and TGA (Thermo Gravimetric Analysis). Atomic resolution images will be presented. The images of SWCNTs and graphene sheets in: SEM, Z-Contrast, STEM modes ***at the same sample location*** will be revealed. Electron nano-diffraction was also used to prove graphene presence in the ablation product. All experiments confirm the high quality of carbon nanomaterials synthesized in our laboratory.

OW7. **OPTIMIZATION OF PMMA PROCESSING AS A PREREQUISITE FOR NANODEVICE BUILDING USING ELECTRON BEAM LITHOGRAPHY**

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Although poly(methyl methacrylate) (PMMA) is a common resist used for Electron Beam Lithography (EBL), there are many of its properties that influence the outcome of this technique. We studied the parameters for spin coating and the thermal treatment needed for the deposition of commercial PMMA 950K on SiO_2/Si substrates. After the deposition process, the doses that need to be applied in order to achieve good results for EBL exposures were studied along with the influence of the developer's temperature on the developing process and the influence of the deposition of PMMA on the lift-off process after metallization. All these efforts were prerequisites for building future micro- and nanodevices using EBL as a technique for device contacting. The results of the entire process were evaluated using Scanning Electron Microscopy, Energy Dispersive Spectroscopy and Atomic Force Microscopy.

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PW1. **ELECTROCHEMISTRY APPLIED ON SOME PLANT-SOURCE EXTRACTS**

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Medicinal plants have been used for centuries as remedies for human diseases because they contain components of therapeutic value [1]. Moreover, the increasing use of plant extracts in the food, cosmetic and pharmaceutical industries suggests that, in order to find active compounds, a systematic study of medicinal plants is very important [2]. Electrochemical methods used for the determination of antioxidant capacity have been still developing. These provide rapid, simple and sensitive alternative methods in the analysis of bioactive compounds associated with the scavenging of the radicals as well as the antioxidant capacity itself. They are low-cost and usually do not require time consuming sample preparation [3].

In the present paper, we aimed to summarize basic electrochemical techniques, differential pulse polarography (DPV) and cyclic voltammetry (CV), for the electrochemical analysis of some plant-source waters used as ingredients in organic dermato-cosmetics formulations, and obtained from: sea buckthorn (*Hippophae rhamnoides*) fruits, seeds and peel, and from birch (*Betula pendula*) sprouts.

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PW2. **COMPETITIVE SORPTION OF HYDROPHOBIC ENDOCRINE DISRUPTORS BY MULTI-WALLED CARBON NANOTUBES IN AQUEOUS SYSTEMS**

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This study proposes the use of multi-walled carbon nanotubes (MWCNTs) pristine and irradiated as nanosorbents for triclocarban (TCC), a hydrophobic organic contaminant. Solutions with different concentrations of humic acid (HA) have been used to perform the competitive sorption experiments between the TCC and the NOM at the active sites of the MWCNTs.

Adsorption of TCC was studied on two types of MWCNTs, pristine and irradiated in aqueous solutions with or without HA, at different concentrations, mimicking the natural environmental solutions. It was observed that the presence of HA inhibited TCC adsorption, based on competitive interactions and possible covering of the active sites on the available sorption surface of MWCNTs. HA adsorbed on the MWCNTs surfaces may alter the electrostatic and hydrophobic interactions [1] between TCC and MWCNTs pristine and irradiated, decreasing the adsorption of the studied hydrophobic contaminant [2].

In order to describe the equilibrium adsorption of TCC on MWCNTs aggregates in conditions mimicking the environmental ones [3], non-linear Langmuir and Freundlich isotherms were adopted. The values of the Freundlich and Langmuir adsorption parameters were calculated.

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PW3. **COMPETITIVE SORPTION OF ORGANIC CONTAMINANTS BY MULTI-WALLED CARBON NANOTUBES IN THE PRESENCE OF AQUATIC NATURAL ORGANIC MATTER**

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Natural Organic Matter (NOM) consisting of negatively charged macromolecules is an omnipresent component of all natural aquatic media [1] that is present as dissolved organic matter (DOM) in water, or in other natural systems, in the form of sediment or sewage sludge [2]. The composition of natural organic matter depends on environmental factors and may change considerably over time. The presence of natural organic matter in environmental systems influences the adsorption of organic contaminants on carbon-based nanomaterials [3], leading to a decrease in their sorption capacity. On the other hand, the presence of NOM influences the stability of the MWCNTs suspension and their aggregation.

This study proposes the use of multi-walled carbon nanotubes (MWCNTs) pristine and irradiated as nanosorbents for bisphenol A (BPA), as a moderate hydrophobic organic contaminant in saline solutions in the presence of sediments. Several types of sediment with different compositions from a saline lake have been used to perform the competitive sorption experiments between the BPA and the NOM at the active sites of the MWCNTs.

In order to describe the equilibrium adsorption of BPA on MWCNTs aggregates in environmental conditions, non-linear Langmuir and Freundlich isotherms were adopted. The values of the Freundlich and Langmuir adsorption parameters were calculated.

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PW4. **ELECTROCHEMICAL STUDY OF NEW AZULENE-ETHER CROWN COMPOUND**

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The azulene is a particular monomer recently used to functionalize electrodes [1] because of its high polarizability as it allows spontaneous transfer of electrons from the 5-atom cycle (negative polarized) to the 7-atom cycle (positive polarized). Our study relates the electrochemical characterization by electrochemical methods [2, 3] cyclic voltammetry, differential pulse voltammetry and rotating disk electrode voltammetry of a new 4'-(E-azulen-1-ilvinil)-12-crown-4-ether azulene monomer (**L**-monomer).

L-monomer has been used to obtain complexing modified electrodes by electrochemical polymerization. The study led to the finding of the best conditions for this azulene polymerization. Poly**L** modified electrodes were characterized by cyclic voltammetry in ferrocene solutions.

In this paper the electrochemical behavior of azulene-ether compound **L** was studied on a stationary electrode in acetonitrile containing tetra-butyl-ammonium perchlorate as supporting electrolyte.

Acknowledgements. The authors are grateful for the financial support from: PCCDI program, INTELMAT project complement 5 and UEFISCDI project contract no. 236/2014.

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PW5. **ELECTROCHEMICAL STUDY OF CERTAIN TRIPHENYLALKYLARSONIUM DERIVATIVES**

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Organoarsenium compounds are less studied due to both arsonium relatively low abundance and their toxicity. However, in the last years it was proved that the organic arsonium compounds are much less toxic than their inorganic correspondents [1]. Therefore, new research efforts were made to determine the arsonium ions properties (especially those containing fluorine) in order to find new industrial and medical applications [2]. As a consequence, their electrochemical properties must lead to understanding of their chemistry and toxicity.

Our study relates the electrochemical characterization by cyclic voltammetry, pulse-differential voltammetry and rotating disk electrode voltammetry of new triphenylbenzylarsonium compounds. Their electrochemical study was performed in order to establish the main features for subsequent applications, such as: treatments for leukaemia and other cancers [3], triphenylarsonium-functionalised gold nanoparticles as potential nanocarriers for intracellular therapeutics [4] or XO_4^- (X = Ru, Tc, Re) ions extraction by arsonium ions [5].

Acknowledgements. The authors are grateful for the financial support from: PCCDI program, INTELMAT project complement 5 and UEFISCDI project contract no. 236/2014.

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PW6. **EVALUATION OF CHEMICALLY MODIFIED ELECTRODES PERFORMANCES FROM QUANTUM MECHANICAL CALCULATIONS**

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Derivatives of (5-[(azulen-1-yl) methylene]-2-thioxothiazolidin-4-one are reported as ligands for heavy metals in heterogeneous systems based on chemically modified electrodes [1]. Their ability to coordinate heavy metals has been tested and the detection limits for heavy metals complexation have been evaluated [2]. A computational study on the structure, using Density Functional Theory (DFT), was conducted in order to achieve a complex structural analysis by calculating and evaluating a series of molecular descriptors and properties [3], related to their reactivity and electrochemistry. Correlations of quantum parameters related to global chemical reactivity with the heavy metal detection limits of the modified electrodes based on studied ligands have been done in order to assess their complexing properties. Correlations between predicted and experimental chemical shifts from RMN data have been performed to check the accuracy of predicted structural data.

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PW7. **CHARACTERIZATION OF POLYAZULENE COMPLEXING FILMS**

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Azulene is a particular monomer used to functionalize the electrodes due to its spontaneous transfer of electrons from the negatively polarized cycle to the positively polarized cycle. Our study relates the ways of evaluation of the chemical species fixed on the electrode after the electrochemical deposition of an azulene monomer (**L**) in organic solvents [1-3].

L-monomer has been deposited onto glassy-carbon electrodes by electrochemical polymerization. The modified electrodes were examined and their spectra revealed the characteristics of the films obtained in different pathways and also the influence of heavy metals complexation on the surface properties. Morphological characterizations of the polymer films were performed using Scanning Electron Microscope (SEM) and Spectrofluorimetry.

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PW8. QUANTUM CHEMICAL CALCULATIONS FOR EVALUATION OF AZULENES AS COMPLEXING AGENTS FOR ELECROCHEMICAL APPLICATIONS

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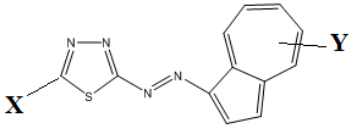
A computational study on several structures has been performed, using Density Functional Theory, for azulene derivatives as ligands for heavy metals in heterogeneous systems based on chemically modified electrodes, in order to achieve a complex structural analysis by calculating and evaluating a series of molecular descriptors and properties, related to their reactivity, by applying Koopmans' theorem [1]. The calculations were carried out using Spartan software (Wavefunction, Inc. Irvine CA USA [1], with the Becke's 3-term functional (Lee, Yang, Parr) exchange hybrid algorithm (B3LYP) [2]. The accuracy of the predictions has been verified by comparing predicted and experimental chemical shifts from RMN data. Attempts to correlate the quantum parameters to the heavy metal detection limits of the modified electrodes based on studied ligands have been done in order to assess their complexing properties and electrochemical behaviour.



X = t-butyl, phenyl, 1-naphtyl, 2-thienyl, 2-furyl, CH_3S, $CH_3S(O)$, $CH_3S(O_2)$, SH
Y = H, 4,6,8-trimethyl, 3,8-dimethyl-5-isopropyl

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PW9. **EXPERIMENTAL INVESTIGATIONS ON THE ANALYTICAL PERFORMANCES FOR LEAD ANALYSIS USING CHEMICALLY MODIFIED ELECTRODES BASED ON POLYAZULENE COMPOUND**

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Heavy metals are pollutants often found in waters, of which lead is one of the most dangerous. The main purpose of this study was to evaluate analytical performances for lead determination in water samples using chemically modified electrodes based on a new azulene compound, 2,6-bis((E)-2-(thiophen-2-yl)vinyl)-4-(4,6,8-trimethylazulen-1-yl)pyrylium perchlorate, synthesized according to the procedure established in our group [1, 2]. The electrochemical characterization of azulene compound was performed by two voltammetric methods: cyclic voltammetry (CV) and differential pulse voltammetry (DPV) using a three-electrode cell in which the working electrode was a glassy carbon disk modified with the new azulene compound. For investigations on the analytical performances for heavy metal analysis the working electrode was a glassy carbon disk modified with the new azulene compound, the reference electrode was Ag / AgCl and a platinum electrode served as an auxiliary electrode [3]. Best results for lead determination were obtained by DPV method and therefore the main analytical parameters for this technique were determined.

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