OVIDIUS UNIVERSITY of CONSTANTA
Faculty of Applied Sciences and Engineering

Romanian Chemistry Society, Constanta Branch

INTERNATIONAL CONFERENCE "CHIMIA"

BOOK OF ABSTRACTS

Volume 2, 2016

26 – 28 May 2016
Constanta, Romania

OVIDIUS UNIVERSITY PRESS, CONSTANȚA 2016
ISSN 2360-3941

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INTERNATIONAL SCIENTIFIC COMMITTEE

Editor:
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PLENARY LECTURES

PL1. NEW CHEMOMETRIC APPROACH BASED ON LINEAR REGRESSION FOR HOLISTIC COMPARISON OF ANALYTICAL DATA

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Analytical data such as chromatograms or (+/-)ESI/MS spectra may be successfully compared in a holistic way through "classic" chemometric approaches as PCA or CA, to evaluate (dis)similarity between samples representing complex mixtures of compounds, more often of natural origins. When strictly comparing shapes, it is important to acquire raw data with an increased resolution (high acquisition/spectral resolution). However, softwares dedicated to PCA or CA barely accept data series with more than 1000 values. A new approach, based on linear regression analysis (LRA) is proposed, having the advantage to exhibit no limitations about the length of the data series being compared. A comparison between a set of five green teas, more precisely RPLC/UV chromatograms and (+/-)ESI/MS spectra of infused extracts, served as an application basis for the holistic evaluation through PCA, CA and LRA. The influence of sample preparation, as well as intra and inter day instrumental variability were assessed with respect to the discrimination power. Data pre-processing methods, such as normalization, peak alignment and background subtraction were also considered as factors affecting the holistic chemometric assisted evaluation. It was demonstrated that the proposed LRA approach was not affected by the data pre-processing algorithms and offered an increased capacity of discrimination. The inter-day instrumental variability, especially for (+/-)ESI/MS data, had a significant influence on the discrimination ability of all chemometric approaches being used. (+/-)ESI/MS spectra of infused mixtures (un-separated extracts) contained all the necessary information needed to produce differentiation between the considered samples.

PL2. MODIFIED ELECTRODES BASED ON AZULENE DERIVATIVES FOR HEAVY METAL IONS DETECTION

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Azulene derivatives have rarely been applied to the metal ions electroanalysis using chemically modified electrodes (CMEs). However, some examples can be found in literature [1], illustrating azulene peculiar advantage among the monomers used to functionalize electrodes, to make possible a spontaneous internal electron transfer. The seven-membered ring of the molecule may act as electron acceptor, while the five-membered ring – as electron donor. This makes it a very interesting building block for the synthesis of advanced materials.

Azulene derivatives form a versatile family of ligands, appropriate for forming complexes with metal ions. The coordination chemistry of its derivatives could be much more varied than that of simple compounds. This feature could be stressed when using CMEs. Our study concerns the synthesis and electrochemical characterization of new azulene-thiourea-like monomers.

Poly**L** films modified electrodes have been obtained by electropolymerization of an azulene based monomer (**L**). Different complexing structures known to complex heavy metal (Pb, Cd Hg, Cu) ions have been tested. The ligands have been characterized by electrochemical methods and the films have been examined by scanning electron microscopy. The complexing properties of **L** and poly**L** have been investigated by preconcentration – anodic stripping technique [2]. The best results have been discussed in connection with the initial structure of the ligand.

Acknowledgments. The authors are grateful for the financial support from: Executive Unit for Financing Education Higher, Research Development and Innovation (UEFISCDI) project ID PN-II-RU-TE-2014-4-0594 contract no. 10/2014, PN-II-ID-PCE-2011-3-1067 contract no. 15/2011, and PN-II-PT-PCCA-2013-4-2151 contract no. 236/2014.

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PL3. BIOMEDICAL APPLICATIONS OF NMR SPECTROSCOPY

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The paper describes several NMR applications in biomedical research and medical diagnosis.

Examples cover both a review of the state-of-the-art in the field and original results from our laboratory.

Original results range from advanced research on animals studying neurological metabolism based on cerebrospinal analysis to medical diagnosis on humans on diseases like Diabetes and Inborn Errors of Metabolism based on urine analysis.

In order to ensure reproducibility, apart from the NMR parameters and pulse sequences, several additional technical problems have to be solved. Some technical aspects are also discussed in the paper.

Acknowledgments. The authors acknowledge the financial support of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project numbers PNII-ID-PCCE-2011-2-0045 and PN-II-ID-PCCE-2011-2-0028.

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PL4. MASSIVE OPEN ON-LINE COURSES IN OPEN EDUCATIONAL RESOURCES AND E-LEARNING FOR TOXICOLOGY COURSES

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Remarkably, owing to the lack of European Massive Open On-line Courses (MOOCs) [1] in the field of the Toxicology and major differences in the teaching and learning of this important subject at various European biologically oriented faculties, we will present our TOX-OER European project which develops a scientific and pedagogical joint between research in the field of toxicology and MOOC pedagogical design [2]. This will consist in a guideline to support partners during: a) the creation of accessible Open Educational Resources (OER); b) course & module management; c) the implementation, monitoring and evaluation of individual and social learning activities. This procedure will contribute to the promotion of using the learning outcomes in the design and delivery of educational programs and activities in favor of pupils, students, young people, trainees, adult learners. Furthermore, the TOX-OER project could create the conditions for the RECOGNITION and CERTIFICATION (ECTS credits) of learning achievements, at least between partners. Finally, throughout the duration of the project, the partners involved in the educational tasks will manage a virtual space (server) within which the MOOC platform will be installed, and where all the Open Educational Resources will be available. TOX-OER project is coordinated by Universidad de Salamanca and partners are: Università di Bologna, Italy; Transilvania University of Brasov, Romania; Univerzita Karlova V Praze, Czech Republic; Universidade do Porto, Portugal; Space Research and Technology Institute, Bulgaria; Kymenlaakson Ammattikorkeakoululu Oy, Finland.

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PL5. FROM WHERE TO WHERE IN CHEMICAL ENGINEERING

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The paper presents aspects concerning the past,the present and the future of Chemical Engineering Science. In the paper opening it shows the bible roots of this science and give some date respect the this science importance for development of the ancient world. Looking back on the chemical engineering road will find their strong roots in medieval alchemy.The basic three alchemists dreams (Diderot Encyclopedia) which sought to obtain i) the creation of the fabled philosopher's stone, ii) the ability to transmute base metals into noble metals (gold or silver), iii) the development of an elixir of life for youth and longevity, can be today three major directions in which chemical engineering can go on. The processes Leblanc and Solvay for industrial sodium carbonate production and the processes (distillation and others) characterizing the beginings of petroleum industry are considered as roots of modern chemical engineering science. Now at the finish of 19^{th} and starting of 20^{th} century did time for chemical engineering to gather the results, to establish their theoretically explanation and to generalize them. Such have been created the conditions for her enrolling by specialists training in the triangle education-research-production. It is known that the name of chemical engineer began to be used since 1880 as it is known that the chemical engineer of this time was in fact a mechanical engineer by training with a very a good practical knowledge of applied chemistry (chemical engineering). George Davis, an inspector in the production of alkaline England hold in 1887 a total of 12 lectures with chemical engineering specifics and titles at the Technical School in Manchester. Recognizing the paradigm as a philosophical and theoretical framework of a scientific school or discipline within which theories, laws, and generalizations and the experiments performed in support of them are formulated, and looking with eyes to the passed time, we find for chemical engineering discipline three paradigms: the first paradigm called Unit Operations paradigm (1923-1960); a second paradigm called paradigm of Transfer Phenomena (1960 -2005), and that the third paradigm accepted as paradigm of Process Engineering as innovation, design and manufacture of high technology products (after 2005). In a different time period the chemical engineer training was done after one or other of these paradigms.

Therefore a succinct characterization of these paradigms is of interest. An important attention is given to the Amundson report (1984) because it recommend an alliance of industry, academia and government to invest in the future of chemical engineering, which promises to serve society by: 1) Starting of New Technologies that would improve the quality of life with new products through: a) biotechnology and biomedicine; b) electronic, photonic, and recording materials and devices; c) microstructured materials; 2) Maintaining Leadership in Established Technologies and particularly in: a) in-situ processing of energy and mineral resources; b) liquid fuels for the future; 3) Protecting and Improving the Environment and Health by: a) responsible management of hazardous substances; b) protection from sudden plant disasters; 4) Developing Systematic Knowledge and Generic Tools that would be used in all three previous areas, and particularly in: a) advanced computation methods and process control; b) surface and interfacial engineering. The Amundson report keeps today their actuality. This paper shows this by presenting and commenting on some basic directions in which will be the future development of chemical engineering.

SECTION A: NATURAL AND SYNTHETIC COMPOUNDS

OA1. CHARACTERIZATION OF BIOACTIVE COMPOUNDS FROM ROMANIAN *CETRARIA ISLANDICA* SPP.

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Lichens, belonging to the *Lichenophyta phylum*, which is the least exploited subdivision of fungus, are composite plants used as medicine for various diseases (tuberculosis, acute respiratory diseases, stomach and duodenal ulcers) due to the presence of several bioactive compounds in their structure [1]. Each species of lichen has its own set of lichen acids, such as atranorin, usnic acid, lecanoric acid, salazinic acid, lobar acid and other acids, with various biopharmaceutical applications as antimicrobial, antioxidant and cytotoxic agents [2]. The main goal of this study was to extract and to characterize the bioactive compounds (usnic acid) with antioxidant and antimicrobial potential from Romanian *Cetraria islandica* spp., (*Parmeliaceae* family). The evaluation of usnic acid from acetone extract was performed using IR spectroscopy and HPTLC technique. The extracts showed a superior antioxidant activity compared to other standard compounds used to evaluate the antioxidant activity. The assessment of the antimicrobial activity of *Cetraria islandica* extracts highlighted that both extracts and pure usnic acid have activity against certain Gram positive and Gram negative bacteria and fungi. So, the analyzed bioactive compounds responsible for antioxidant and antimicrobial actions of this vegetable can be used as the basis of some pharmaceutical formulations to treat various respiratory and digestive diseases and to improve bronchial disorders.

Acknowledgements. This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-ID-PCE-2011-3-0226

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OA2. IMPROVEMENT OF LAVENDER OIL CHARACTERISTICS BY HYDROGENATION

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Hydrogenation is a process highly used for improving the characteristics of the components used in the fragrance industry. In this context, the hydrogenation of unsaturated compounds from lavender oil could improve its stability to oxidation [1, 2].

The hydrogenation of lavender oil was performed over a heterogeneous catalyst in a continuous system and fixed bed reactor. The catalysts used in process are based on noble metals such as Pd and Pt. The process was studied at the following parameter values: pressure 0.2-0.4 MPa and temperature 120-200 ºC. The chemical composition was investigated using the Gas Chromatography coupled with Mass Spectrometer (GC-MS). The increase of the temperature and pressure favors the hydrogenation process of double bonds.

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OA3. SEPARATION, IDENTIFICATION AND CUANTIFICATION OF SOME COSMETIC EMULSION INGREDIENTS

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In the last few years, people have paid more attention to organic cosmetic products with natural preservatives and no chemicals added. This type of products, strictly made from pure and natural plant extracts, presents a very interesting perspective since it became a natural alternative for healing dermatological diseases [3].

The aim of this study was to continue the physical-chemical characterization started in 2014 [1] of one Romanian cosmetic emulsion [2]. The study followed the separation, identification and quantification of each compound from the plant extracts used by the manufacturer: *Abies sp., Crataegus monogyna, Hypericum perforatum, Lavandula angustifolia, Lavandula officinalis, Lilium sp., Melissa officinalis, Mentha silvestris, Mentha piperita, Origanum vulgare Pinus silvestris buds, Populus nigra buds and Thymus serpillum*. Plant extracts were analyzed by high performance liquid chromatography (HPLC). The analysis results have led to high levels of polyphenolic compounds with antioxidant properties. These results were confirmed by clinical tests that have shown positive effects on the skin.

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OA4. PREPARATION OF HYBRID COATINGS WITH CONTROLLED WETTABILITY: PROCESS PARAMETER STUDY

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The aim of this paper is to investigate the effect of the variables that influence the wetting angle and the coating morphology on promising hybrid films with structured roughness for water repellent applications. Magnetic-chitosan *g*-styrene composite particles (Mag-CS*g*-ST), chitosan and pre-hydrolysed alkoxysilanes were used in various formulations to yield thin films. Magnetite (Fe_3O_4) nanoparticles obtained by co-precipitation [1] were embedded in matrices synthesized by radical graft co-polymerization of styrene (ST) with ethylene glycol di-methacrylate (EGDMA) onto previously modified chitosan bearing surface vinyl groups. Hybrid thin films containing composite particles, chitosan as a polymeric binder and pre-hydrolysed hexadecyltrimethoxysilane (HDTS) or/and tetraethyl orthosilicate (TEOS) [2] as a coupling/crosslinking agent were deposited by spraying. The films were cured by heating and subsequently characterized regarding their morphology (scanning electron microscopy), contact angle with water and adhesion to substrate (scratch test). The effects of the following process parameters upon coating morphology and wetting angle were studied: the coupling agent composition and hydrolysis extent, the solvent used to prepare the particle dispersion and the thermal regime for drying the base layer of the coating. The process was optimized to yield coatings with high wetting angle and good adherence to the substrate in a reproducible manner.

Acknowledgement. This work was supported by a grant of the Romanian Ministry of National Education, CNCS-UEFISCDI, project number PN-II-ID-PCE-2012-4-0433.

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PA1. STUDIES ON POLY-3-HYDROXYOCTANOATE BIOSYNTHESIS BY A CONSORTIUM OF MICROORGANISMS

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Polyhydroxyalcanoates (PHAs) are specifically produced by a wide variety of bacteria, as an intracellular energy reserve in the form of homo- and copolymers of [R]-*β*-hydroxyalkanoic acids, depending on the C source used for microorganism growth, when the cells are grown under stressing conditions [1-3].

In this paper we present microbiological accumulation of poly-3-hydroxyoctanoate (PHO) by using a consortium of bacterial strains, *Pseudomonas putida* and *Bacilius subtilis*, in a rate of 3:1, grown on a fermentation medium based on sodium octanoate as the sole carbon source.

The experiments performed in the above mentioned conditions led to the following results: from 18.70 g sodium octanoate (7.72 g/L in the fermentation medium) used up during the bioprocess, 3.93-3.96 g/L dry bacterial biomass and 1.834 - 1.884 g/L PHA, containing 85.83 - 86.8% PHO, were obtained.

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PA2. ENZYMATIC ACTIVITY OF SOME PLANT EXTRACTS BIOCATALYSTS USED IN CLICK CHEMISTRY REACTIONS

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The search of catalysts for chemical reactions is an old challenge in chemistry. Typically the catalysts used for the conversion of chemical compounds are organometallics or enzymes [1]. Enzymes are interesting biocatalysts providing an advantage over organometallic compounds because they are active in aqueous solutions instead of organic solvents, thereby minimizing waste and pollutants. Enzymes are used on large scales in numerous processes to make for example detergents, paper, pharmaceuticals, other fine chemicals, drugs or food [2]. The biocatalysis, which generally satisfy the principles of green chemistry, gain increasing importance in organic synthesis from their unique selectivity advantages over traditional methods [3]. Among the various biocatalytic reactions comprising hydrolytic, reductive and oxidative reactions, the selective oxidations with C-C bonds formation catalyzed by enzymes are particularly attractive and our current efforts was to expand the biocatalysis in click chemistry reactions [4] by investigating the plant biocatalysts *(Amoracia rusticana, Cucurbitacee, Apiacee, Alliacee)* which display oxidant high catalytic activity. The results obtained from this study can contribute to developing a biocatalyst that can be applied in diverse fields in the future.

Acknowledgements. This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-ID-PCE-2011-3-0226

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PA3.SYNTHESIS, STRUCTURE AND BIOLOGICAL ACTIVITY OF SOME AZINE AND AZOLS DERIVATIVES

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The five and six member ring azaheterocyclic derivatives are considered privileged structure in medicinal chemistry having many biological activities, these including anticancer, antimicrobials (antitubercular including), anti-inflammatory and antinociceptive, antihypertensive, diuretics, antithrombics, anticoagulants, antidepressant, anxiolytics, anticonvulsant, analgesic, and so on.

As part of our ongoing research in the field of nitrogen heterocycles with anticancer and antitubercular activity, we present here the synthesize, structure and in vitro anticancer and antitubercular activity of some imidazole and azine derivatives. The synthesis is straight and efficient, using either conventional thermal heating either energy of microwave and/or ultrasounds. Some of the compounds were tested for *in vitro* for anticancer activity against a panel of 60 human cancer cell lines (by the National Cancer Institute, (NCI, USA), under the Developmental Therapeutics Program (DTP), at a single high dose (10-5 M) cell assay) and/or for *in vitro* antimycobacterial activity against *Mycobacterium tuberculosis H37Rv* (as a part of the TAACF TB screening program under direction of the US National Institute of Health, the NIAID division). Some azaheterocyclic derivatives exhibit a very good antitumor activity against Renal Cancer, Breast Cancer, Leukemia, Non-Small Cell Lung Cancer, CNS Cancer and Melanoma. The data from cycle-1 (IC_{50}, IC_{90}, MIC) and cycle-2 [MIC, MBC, LORA, intracellular (macrophage)] antitubercular screening, indicate the intracellular drug effectiveness against *Mtb* of these compounds, the lack of toxicity, a significant activity against both replicating and non-replicating *Mtb* and, a bacteriostatic or bactericidal mechanism of action.

Acknowledgements. The authors are thankful to CNCSIS Bucuresti, grant PN-II-DE-PCE-2011-3-0038, no. 268/05.10.2011, for financial support, and also to the POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010 Project, CERNESIM, for the NMR and X-ray spectra.

PA4. EFFECT OF TWO SYNTHETIC ANTIOXIDANTS ON THE STABILITY OF ANTHOCYANINS IN SOME BERRIES EXTRACTS DURING STORAGE

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Anthocyanins, the broadest group of water-soluble pigments in plants, presents 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 beneficial effects on health, especially due to their antioxidant effects. A limiting factor for anthocyanins incorporation in food is low stability of these pigments under the influence of various factors, one of the most important being temperature [1].

In this study, the stability of ethanolic anthocyanin extracts from wild bilberry, blackberry and black mulberry with and without added ascorbic acid and butylated hydroxyanisole was investigated. The variations in anthocyanins content and antioxidant activity during storage for 2 weeks at 60°C and 4 months at room temperature were determined. Total monomeric anthocyanins content was quantified by using a pH differential method [2] and antioxidant activity evaluation was performed by using FRAP (ferric reducing/antioxidant capacity) assay [3]. The obtained results indicate that the anthocyanins degradation followed first-order reaction kinetics. A very fast degradation occurred at high temperature. During storage at room temperature, anthocyanins showed a better stability. The untreated extracts present a good stability. Generally, the extracts treated with ascorbic acid present a faster degradation.

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PA5. THE STUDY OF SOME ACTIVE COMPOUNDS IN THE ESSENTIAL OIL OF LAVANDULA ANGUSTIFOLIA

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The pharmaceutical products based on volatile essential oils also combine the special odorant and antiseptic properties of the volatile oils, and especially of lavender oil. The aim of this work is the qualitative and semi quantitative study of some bioactive compounds present in *Lavandula angusifolia* and the antioxidant and antimicrobial potential over a strain of *Staphylococcus aureus.* As a pharmaceutical application, we prepared an "eau de toilette" and an inhalant solution, turning to profit the lavender oil's properties. The following methods were used: the extraction of volatile oils through water vapors and supercritical fluid extraction; chromatography on thin layer; spectrophotometry; determination of RSC (radical scavenging capacity) by DPPH method and by hydrogen peroxide; Kirby-Bauer diffusion test. The extraction rates of lavender essential oil [1] with water vapors was of 39.4% and of 58.6% by supercritical fluids extraction [2]. The qualitative analysis by chromatography on thin layer of the terpene compounds of lavender volatile oil has highlighted the presence of compounds such linalool, limonene, α-pinene and geraniol. The determination of the antioxidant activity through DPPH method has been evaluated by measuring the activity of the samples of volatile oil on the 2,2-diphenyl-1-picrylhydrazyl (DPHH) radical. We have investigated the ability of the volatile oil samples of acting as donors of hydrogen atoms or electrons by reduction of the violet DPPH radical to its colorless form, DPPH-H. The determination of the antioxidant activity with hydrogen peroxide using the test of inhibiting the H2O2 radical. Following the determination of the antioxidant activity by employing the two methods, we have observed that the highest antioxidant activity is present at the lavender volatile oil obtained in our laboratory through supercritical fluids extraction. The analysis of the antimicrobial activity of the lavender volatile oil on *Staphylococcus aureus* was made by comparing it with the lavender oil extracted by Boots Company.

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PA6. SYNTHESIS AND CHARACTERIZATION OF SOME NOVEL N-(2-BROMO-PHENYL)-2-HYDROXY-BENZAMIDE DERIVATIVES

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Developing chemical compounds with the desired biological properties is time-consuming and expensive. Increasing interest is being directed towards technologies that allow more rapid synthesis and screening of chemical substances to identify compounds with functional qualities. So, microwave-assisted organic chemistry becomes an exciting field for research and development due to improved conditions obtained in comparison with classical methods. Salicylanilide derivatives exhibited antifungal, antibacterial, antimycobacterial, analgesic and antiinflammatory properties, being used in various pharmaceutical and biochemical domains [1-3].

In order to increase the biological activity, some novel molecules, esters, hydrazides, hydrazones of N-(2-bromo-phenyl)-2-hydroxy-benzamide, were obtained under microwave irradiation. Working at 150 °C, 500 W, 7-11 min, good yields (86-93%) were obtained. All new synthesized compounds were characterized using modern physico-chemical methods (FTIR, ^{1}H-NMR, ^{13}C-NMR).

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PA7. ANTIFUNGAL ACTIVITY OF SOME N-(2-BROMO-PHENYL)-2-HYDROXY-BENZAMIDE DERIVATIVES

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Eight dilutions in dimethyl sulfoxide (DMSO) of the six novel salicylanilide derivatives, esters, hydrazides and hydrazones, were tested against two phyto-pathogenic fungi, *Fusarium oxysporum*, *Sclerotinia sclerotiorum*, and one common yeast, *Saccharomyces cerevisiae*, in order to evaluate their biological activity. The antifungal activity was assessed using disc diffusion method, both negative, pure DMSO, and positive control, nystatin, were used [1-3]. *S. cerevisiae* was slightly more sensitive than filamentous fungi, the strongest inhibition, MIC=0.3125 g/L, was observed for N-(2-bromo-phenyl)-2-hydroxy-benzamide and N-(2-bromo-phenyl) - 2 - (4 - dimethylamino-benzylidene-hydrazinocarbonylmethoxy)-benzamide. The most active compounds against *F. oxysporum* and *S. sclerotiorum* were N-(2-bromo-phenyl)-2-hydroxy-benzamide (MIC= 0.625 g/L), N-(2-bromo-phenyl)-2-hydrazinocarbonylmethoxy-benzamide (MIC=1.25 g/L) and N-(2-bromo-phenyl)-2-(4-dimethylamino-benzylidene-hydrazinocarbonyl-metho-xy)-benzamide (MIC=0.625g/L), N-(2-bromo-phenyl)-2-hydrazinocarbonyl-methoxy-benzamide (MIC=1.25 g/L), respectively. The antifungal activity of the tested compounds was not as strong as for nystatin, but the inhibition was positive.

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PA8. MODIFIED LIGNIN DISPERSANT FOR STABILIZING AQUEOUS SLURRY OF DOLOMITE

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Manufacture of oxygenated compounds with dispersant characteristics requires an appropriate chemical modification of lignin in order to increase its efficiency. Phenolic structure, specific to lignin, is the premise for the synthesis of cheaper dispersants for stabilization of suspensions. The main role of dispersants is to improve the stability of dolomite suspension used in the preparation of composites for treating cracks from the surface of pavement [1-4].

The experiments were directed toward modifying kraft lignin by applying processes of depolymerization and alkylation to obtain oxygenated compounds with dispersant characteristics for dolomite suspension. Lignin modification processes were carried out in two stages, first depolymerization and then alkylation. Depolymerization was carried out in heterogeneous catalysis by hydrogenolysis. The hydrocracking of lignin was carried in continuous system and catalytic fixed bed in a tubular reactor on a W-Mo / γ-Al_2O_3. The alkylation was carried out in batch system under acid catalysis. The catalysts used were based on heteropoly-acids (*e.g.* phosphotungstic acid) on powdered mesoporous supports. Modified lignin was added to aqueous suspension at concentrations up to 3%. The dispersants characteristics of dolomite aqueous suspension were determined with a Turbiscan Lab. The use of modified lignin as a dispersant is timely given by the high availability due to the fact that it is bio-renewable. Water-dolomite dispersion stability is improved as a result of the addition of depolymerized-alkylated lignin; using of the appropriate alkylating agent contribute to improving the stability of water-dolomite suspension.

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PA9. COMPARATIVE ANTIOXIDANT ACTIVITIES OF SOME DERMO-COSMETIC FORMULATIONS BASED ON FLUID INDIGENOUS MEDICINAL PLANT EXTRACTS

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Particularly interest on herbs and plant extracts is due to their content of active principles with remarkable pharmacological properties. Different medicinal plants species contain some vital bioactive compounds required for the good human body functioning, such as natural antioxidants, flavonoids, phenolic acids, cumarins, tannins, saponins, minerals, used for their dermatological disinfecting, anti-inflammatory and healing activity, justified by their action on free radicals. The purpose of this paper is to obtain selected dermo-cosmetic formulations type gels with an increased antioxidant activity based on mixtures of some fluid extracts from three indigenous medicinal plant species, sage *(Salvia officinalis* L.), common fennel (*Foeniculum vulgare* Mill.) and tarragon (*Artemisia dracunculus* L.), in popular tradition known for their antiinflamatory and antimicrobial activities. Fluid extracts were obtained using extraction method through cold maceration in ethylic alcohol 50% and 70% concentration of dry vegetal product, herba, leaves and fruits. The obtained fluid extracts were mixed in different ratio and analysed for their physico-chemical properties, total polyphenols content and total antioxidative capacity by photochemiluminescence method (ACL procedure, Analytik Jena AG, Germany). The selected mixed fluid extracts with an increased content of polyphenols and total antioxidant capacity, were used to obtain dermato-cosmetic preparations for external use type gels. The new formulations were analyzed for their physical-chemical properties, appearance, *p*H, penetration, spreadability and total antioxidative capacity. Preliminary results emphasize that proposed dermo-cosmetic forms type gels present a higher antioxidant activity compared with the one of fluid medicinal plant extracts, correlated with a good stability and increased polyphenols content and would represent a possible new efficacy dermatological anti-inflammatory preparations with antiradicals action.

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PA10. RESPONSE SURFACE METHODOLOGY FOR OPTIMIZATION OF MELOXICAM ORODISPERSIBLE TABLETS (ODTs)

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The aim of this study is to optimize meloxicam 7.5 mg orodispersible tablets. For this we used a Box–Behnken experimental design with four factors and four levels to establish the relation between independent variables, such as, Pharmaburst™ 500 (X_1), Mannitol (X_2), Lactose DCL (X_3), and Compression force (X_4) on dependent variables: hardness (Y_1), friability (Y_2), disintegration time (Y_3) and wetting time (Y_4) in order to obtain the optimal formula of the technological process using Response Surface Methodology (RSM).

To calculate the coefficients for the response equation we used Design Expert Trial version 7.0.0 software (Stat - Ease Inc. Minneapolis). ANOVA test was performed to estimate the significance of the model. At 5% level of significance, a model is considered significant if the p – value is less than 0.05. The estimation error values prove the validity of the mathematical method used.

After generating the polynomial equations that relate the dependent and independent variables, the process was optimized for all four responses. Optimum formulation was selected based on the constraints set on independent variables: Y_1 (46- 76N), Y_2 (0 – 1%), Y_3 (0 - 180s), Y_4 (28-204). Optimum formulation for meloxicam 7.5 mg ODTs was: 61 mg (X_1), 5 mg (X_2), 26 mg (X_3) at 5 kN (X_4) compression force, providing good tablet properties (hardness, friability, disintegration time and wetting time).

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PA11. ANTIMICROBIAL BACTERIAL CELLULOSE COMPOSITES

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Superabsorbent polymers are materials with three dimensional network structures that can absorb and retain large quantities of water, up to thousands times their own weight. Superabsorbent polymers could also be used as controlled release systems for antimicrobial agents [1]. Until now, most of these materials are synthetic polymers based on acrylic acid or acrylamide, which are not biodegradable and are producing environmental pollution. A new interest has growing to obtain superabsorbent biodegradable materials [2].

The aim of this study is to obtain antimicrobial superabsorbent materials starting from bacterial cellulose (BC) and carboxymethylcellulose (CMC) and using different antimicrobial agents.

Bacterial cellulose membranes were obtained in static culture in Mass Transfer Laboratory (UPB). A casting BC-CMC dispersion was made by dissolving CMC in water at 70^0C and then adding BC fibrils. The composites were dried at the room temperature and were characterized by means of scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). Swelling degree was also measured. The antimicrobial properties were tested against *E. coli* K12-MG1655. The results obtained are encouraging because the new composites display good swelling and antimicrobial properties.

In conclusion, superabsorbent materials with antimicrobial properties were obtained starting from bacterial cellulose and CMC. Enhanced antimicrobial properties were observed when plant extracts have also been included in the composite materials.

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PA12. NEW PYRROLOBENZIMIDAZOLE AND PYRROLOQUINOXALINE DERIVATIVES

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A one-pot, three-components reaction involving a 1-benzylbenzimidazole, a 2-substituted α-bromocarbonyl derivative and an activated acetylenic derivative may be tuned to lead either a pyrrolo[1,2-*a*]bezimidazole or a dihydropyrrolo[1,2-*a*]quinoxaline, depending on reaction conditions.

The pyrrolobenzimidazole derivatives exhibit activity against a variety of cancer cell lines and were found to be useful in treating central nervous system disorders.

Pyrrolo[1,2-*a*]quinoxaline skeleton is a constituent of several bioactive compounds that demonstrated anti-HIV and anticancer activities. These properties lead to a constant interest in developing more efficient ways for the synthesis of these heterocyclic systems.

We report here several new pyrrolo[1,2-*a*]quinoxaline and benzimidazole derivatives. The structures of newly synthesized derivatives were assigned by NMR spectroscopy using several 1D and 2D experiments.

Acknowledgments. The authors acknowledge the financial support of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-ID-PCCE-2011-2-0028.

PA13. INSIGHT ON PHYSICO-CHEMICAL AND BIOLOGIC PROPERTIES OF SOME COMPLEXES BEARING TRIAZOLE DERIVATIVES AS LIGANDS

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Triazole derivatives exhibit a large spectrum of biologic activity such as anti-inflammatory, antimicrobial, and antitumor [1]. As result, several complexes with this kind of ligands were synthesized and some evidenced antitumor, anti-inflammatory, or antimicrobial activity in most cases enhanced in comparison with ligand [2, 3].

Having in view these aspects, we extended this field in synthesis of new complexes of Co(II), Ni(II), Cu(II) and Zn(II) with 1,2,4-triazole polifunctional derivatives. The features of complexes have been assigned from elemental analyses, IR, UV-Vis, EPR and NMR spectra, magnetic susceptibility at room temperature as well as thermogravimetric analysis. The ligands behave as multidentate species resulting in a distorted octahedral stereochemistry in all cases.

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 ligand was enhanced upon coordination, the most active being Cu(II) and Zn(II) species.

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PA14. NEW BIOLOGIC ACTIVE COMPLEXES WITH IMIDAZOLE DERIVATIVES

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Imidazole moiety is a constituent of many bioactive heterocyclic compounds of biological interest. This heterocyclic group acts as ligand toward transition metal ions in a variety of biologically important systems like iron-heme systems, vitamin B_{12} and its derivatives, and other several metalloproteins.

A lot of coordinative compounds containing imidazole derivatives as ligands have been studied due their potential applications in material science, such as molecular-based magnet, luminescence, biomimetic catalysts, zeolite-like porous materials, and structural models for superoxide dismutase as well as their antimicrobial properties [1-3].

Taking into account all these, we report here the synthesis and characterization of three new complexes with the general formula: $[Co(L)_2(Macr)_2]$ (L: imidazole, 2-methylimidazole and 2-ethylimidazole; Macr: metacrylate anion). These complexes have been formulated on the basis of analytical, thermal and spectral data. The molecular structures have been elucidated using single crystal X-ray diffraction method.

All complexes were tested in order to establish their specific anti-infective properties. The results revealed a large antimicrobial spectrum, with low values for minimum inhibitory concentration, and the inhibition of the microbial ability to colonize the inert surfaces.

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SECTION B: ANALYTICAL AND ENVIRONMENTAL CHEMISTRY

OB1. DEVELOPMENT OF A FAST CHEMILUMINESCENT METHOD FOR TESTING AIR POLLUTION

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Several epidemiological studies have evidenced the harmful effect of atmospheric particulate matter [1, 2]. The presence of certain substances, such as metals, WSOC (Water Soluble Organic Carbon), sulfur dioxide (SO_2), nitrogen dioxide (NO_2) and their highly oxidizing radicals SOx and NOx is strongly related to this toxicity [3].

In order to measure the concentration of oxidizing radicals in the air particulate, a chemiluminescent method is being tested. To capture the air pollution particulate samples, various air filtering devices equipped with PTFE (Teflon) filters were allocated in different cities in Italy and left there for few days, then samples were collected and stored. Afterwards these filters were cut in halves and weighted, to find out the amount of particulate captured. To perform the assay, the filters were perforated with a paper puncher, creating small circles, which were distributed in the wells of a luminometer microplate and then the reagents' mixture (100 µL) of hydrogen peroxide and luminol was added. The oxidizing free radicals present in the particulate react with the mixture triggering a light emission, recorded by the luminometer, which intensity should be proportional to the radicals' amount.

Evidences of a significant correlation between samples' light signal and their toxicity are still under investigation. Preliminary results are very encouraging, suggesting that this luminescent assay can be a rapid method to estimate the toxicity of air particulates.

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OB2. ATMOSPHERIC BEHAVIOR AND SIZE DISTRIBUTION OF WATER SOLUBLE ACETATE, FORMATE AND OXALATE IONS IN URBAN AEROSOLS FROM IASI, ROMANIA

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Carboxylic acids, as ubiquitous components of atmospheric particulate matter, have gained an increased attention since they can affect the global radiation balance of the Earth [1]. While carboxylic acids, such as formic and acetic acids, are mainly prevailing in the gas phase [2], oxalic acid is mostly abundant in the particulate phase [3]. The atmospheric behavior and size distribution of particulate acetate, formate and oxalate, are investigated in the present work in urban aerosols collected in Iasi, north-eastern Romania. Size distribution of the interest species in the 0.0276-9.94 µm size range is appropriately investigated by using 13 specific fractions collected with a cascade Dekati Low-Pressure Impactor (DLPI). Ionic chemical constituents of the collected particles have been investigated by ion chromatography. Formate and oxalate ions showed significant statistical correlation with ammonium (Pearson coefficient, *r*, higher than 0.83) and potassium ions (r~0.68). A more atypical behavior has been observed for acetate ion since it didn't showed significant correlations with any of the identified species. The correlation between formate and oxalate ions could suggest common sources. However, while oxalate showed a monomodal distribution with maxima at 381 nm, formate showed clear multimodal distributions both in the fine and coarse modes. Acetate ion didn't show a clear size distribution.

Acknowledgements. The authors acknowledge the financial support provided by UEFISCDI within the PN-II-PCE-2011-3-0471 Project (EVOLUTION-AIR). CERNESIM Center is also gratefully acknowledged for the infrastructure used in this work.

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OB3. METHOXY PHENOLS AND OTHER STRUCTURAL CONSTITUENTS IN *DATURA INOXIA* SEEDS. MECHANISTIC APPROACHES

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Higher plants produce a wide array of secondary metabolites among which alkaloids, terpenoids, and phenolic compounds are the most important [1]. Methoxy phenols, as potential biomarkers of biomass smoke exposure, often have been identified also in atmospheric samples [2]. Moreover, plants have evolved strategies to combat individual pathogen strains (*e.g*., through specific biosynthesized aminoacids) [3] or to defense against animals and microorganisms (*e.g*., through phenylpropenes such as isoeugenol) [4]. In the present work assay of the most important chemical class existent in *Datura inoxia* has been performed by analyzing various plants extracts on a gas-chromatography-mass spectrometry Agilent system. Although with a relatively small contribution to the total chemical composition a large array of methoxy phenols have been identified in the present work (*i.e.*, *o*-guaiacol, *p*-vinylguaiacol, syringol, 3-methoxycatechol, vanillin, *cis*-isoeugenol, vanillic acid methyl ester, guaiacylacetone, 3,4,5-trimetoxyphenol, coniferol, ferrulic acid methyl ester). It has been observed that in *Datura inoxia's* chemical fingerprint significant contributions were brought by alkaloids, sterols, squalene and fatty acids. The data obtained for methoxy phenols allow us to trace the discussion toward a mechanistic approach.

Acknowledgements. The authors acknowledge the financial support provided by UEFISCDI within the PN-II-PCE-2011-3-0471 Project. CERNESIM Center is also gratefully acknowledged.

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OB4. GRAPHENE QUANTUM DOTS: ANALYTICAL CHARACTERISATION AND APPLICATIONS

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Recent research on graphene quantum dots (GQDs) properties aimed to emphasize their emerging potential as active layer in optoelectronic devices and in electrochemical sensors or biosensors. Compared to other carbonaceous nanomaterials, GQDs are characterized by distinctive advantages including charge carriers quantum confinement, tunable band gap, strong luminescence and enhanced electronic conductivity. Structural properties together with appropriate surface functional groups enables the control of optical properties like optical bandgap, static and lifetime features of photoluminescence and quantum yield.

Few nanometers in size aqueous solution-processable GQDs with different surface groups were synthesized through a bottom-up approach starting from glucosamine and tris(hydroxymethyl)aminomethane [1, 2] or poly(ethyleneimine) as precursors. Silicon nanowires decorated with GQDs were achieved and investigated as photodetectors. The performance of GQDs attached on nanoporous titanium oxide in a typical Gratzel solar cell was investigated and electrochemical impedance spectra (EIS) were acquired for GQDs and GQDs and MoS_2 nanoassembly ascertaining the enhanced electronic conductivity [3]. A decrease in resistance to charge transfer (Rct) was achieved when MoS_2 and GQDs were mixed, the Rct change being more than two orders of magnitude, illustrating the synergistic interaction between GQDs and MoS_2 sheets.

Acknowledgements. This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CNCS – UEFISCDI, project number PN-II-RU-TE-2014-4-1095.

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OB5. NOVEL BLOOD AND URINE MICROSAMPLING STRATEGIES FOR THE MONITORING OF ALCOHOL CONSUMPTION MARKERS

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Ethyl glucuronide (EtG) and ethyl sulfate (EtS) are direct alcohol consumption markers, detectable in blood and urine even after consumption of trace amounts of ethanol. The detection window of these biomarkers is dose- and individual-dependent and ranges between 1 and 3 days after alcohol uptake, covering the time gap between short-term (e.g. ethanol) and long-term alcohol markers. Simultaneous determination of EtG and EtS could be, therefore, a suitable strategy for detection of recent alcohol consumption, with applicability in alcohol abstinence programs, workplace alcohol testing or as proof of alcohol uptake by court. However, the risk of bacteria presence in urine, that might hydrolyze or synthesize EtG and EtS and cause false identification of alcohol consumption, detracts from method reliability [1]. On the other hand, classic blood withdrawal *via* phlebotomy suffers from a number of inherent drawbacks: invasive sampling, conservation and transport requirements under controlled temperatures, the need to handle the samples immediately after collection (plasma separation) make this approach unappealing for application to large cohorts of subjects. The purpose of this study is the development of a new strategy for biosampling based on the use of dried matrix micro volumes: dried blood spots (DBS) and dried urine spots (DUS), followed by high-performance liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). The application of these original methods for the determination of alcohol consumption markers will lead to standardized sampling, pretreatment and analysis protocols for a simple, reliable and high-throughput application for workplace alcohol testing.

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PB1. NEW MODIFIED ELECTRODES BASED ON FUNCTIONALYSED AZULENES FOR HEAVY METAL IONS DETECTION

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The worldwide increasing demand for cleaner drinking water imposes a rigorous monitoring of surface waters regarding the presence of heavy metals, in accordance with European Water Framework Directive. The use of chemical modified electrodes has been widely recognized as powerful tool for trace metal analysis in natural waters. The most efficient approach towards chelating-modified electrodes is the direct electropolymerization of complexing monomers, producing in one step stable functionalized polymers films with controlled sizes and sites concentrations. Azulene is one of the most recommended monomer able to give conductive films, for the chemically modified electrodes. By electrochemical oxidation of azulene derivatives a deposit of an organic film on the electrode surface can be obtained. If the deposit is conductive, thick films can be grown [1].

The chelating azulene compound 2,6-bis((E)-2-(thiophen-3-yl)vinyl)-4-(4,6,8-trimethylazulen-1-yl)pyrylium (**L**) has been examined as a chelating ligand for heavy metal ions recognition. The electrochemical experiments were carried out by cyclic voltammetry (CV), differential pulse voltammetry (DPV), and rotating disk electrode voltammetry (RDE). The complexing properties of **L** and poly**L** have been investigated towards heavy metals by preconcentration – anodic stripping technique [2]. The stripping curves presented well defined peaks for each cation, which can be used as analytical signals. The best results have been obtained for Pb, Cu and Hg. A detection limit of 10^{-7} M has been obtained for Pb.

Acknowledgments. The authors are grateful for the financial support from: Executive Unit for Financing Education Higher, Research Development and Innovation (UEFISCDI) project ID PN-II-RU-TE-2014-4-0594 contract no. 10/2014, PN-II-ID-PCE-2011-3-1067 contract no. 15/2011, and PN-II-PT-PCCA-2013-4-2151 contract no. 236/2014.

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PB2. MODIFIED ELECTRODES BASED ON (Z)-5-((5-ISOPROPYL-3,8-DIMETHYLAZULEN-1-YL)METHYLENE)-2-THIOXOIMIDAZOLIDIN-4-ONE FOR HEAVY METAL IONS

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In order to avoid, prevent or reduce harmful effects on human health and the environment the monitoring heavy metal ion levels in surface waters is essential. The EU Water Framework Directive limits the maximum allowable concentrations of lead, cupper, cadmium and mercury in waters, and consequently, performant analytical methods are needed for their detection. Among the recommended methods for heavy metals ions detection, the electrochemical methods become more and more attractive due to their characteristics. Our approach regarding an easy detection of heavy metal ions is based on azulene chelating modified electrodes. By electrochemical oxidation of azulene derivatives a deposit of an organic film on the electrode surface can be obtained. If the deposit is conductive, thick films can be grown.

((Z)-5-((5-isopropyl-3,8-dimethylazulen-1-yl)methylene)-2-thioxoimidazolidin-4-one (L) has been investigated as a chelating ligand for heavy metal ions homogeneous and heterogeneous recognition. The electrochemical experiments were carried out by differential pulse voltammetry (DPV), cyclic voltammetry (CV), and rotating disk electrode voltammetry (RDE). The complexing properties of L and polyL have been investigated towards heavy metals by preconcentration – anodic stripping technique [1]. The stripping curves presented well defined peaks for each cation, which can be used as analytical signals. The best results have been obtained for Pb and Cd. A detection limit of 10^{-6} M has been obtained for Pb and Cd.

Acknowledgments. The authors are grateful for the financial support from: UEFISCDI project ID PN-II-RU-TE-2014-4-0594 contract no. 10/2014, PN-II-ID-PCE-2011-3-1067 contract no. 15/2011, and PN-II-PT-PCCA-2013-4-2151 contract no. 236/2014.

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PB3. VARIATION OF WATER QUALITY INDEX (WQI) AND PHYSIC-CHEMICAL PARAMETERS IN PRUT RIVER ALONG GALATI COUNTY

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The main objective of the study realised was assesing water quality status for Prut River (Lower Area) in terms of physico-chemical parameters and by calculation of water quality index (WQI). The following physico-chemical parameters were determined: pH, suspensions, CCOCr, CBO5, OD, fixed residue, $N\text{-}NO_3$, $N\text{-}NO_2$, $N\text{-}NH_4$, HCO_3^-, Ca^{2+}, Mg^{2+}, Cl^-, SO_4^{2-}, K^+, Na^+, O_2 saturation, burnt residue. Water samples were collected from 5 sampling points during of 2012 - 2015 years. Monitoring water quality dynamics in this perriod and areas could lead to conclusions about antropic influence on water quality. Water quality asessment was realised by processing the measurements results, calculation of water quality index (WQI), PCA analysis and ANOVA technique to higligt correlation between the indices obtained for different stations and physico-chemicale parameters in different time periods.

PB4. PHYSICAL-CHEMICAL STUDY ON DRINKING WATER FROM GALATI, BRAILA, BUZAU, FOCSANI AND CORRELATION WITH THE POPULATION HEALTH

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The aim of the work is the study of drinking water quality indicators in Galati, Braila, Buzau, and Focsani. Water samples were taken from sources frequently used by the population. They were subjected to chemical and physico-chemical analysis in order to determine the physical, chemical parameters of quality that can affect the health of residents.

The results show that the samples analyzed show in most cases pH within the limits recommended by the national standard. Oxidability varies from area to area and mineralization is increased. In some areas it was found concentrations of Al(III) which exceeds the allowed limit of 0.05 mg/L.

The results will be correlated with the health of the population.

PB5. A GC-MS METHOD FOR MONITORING OF SOME PESTICIDES RESIDUES IN MAIZE AND WHEAT CULTIVATED IN BANAT COUNTY

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There are more than one thousand pesticides in the world used in different combinations and at different stages of plants for cereals protection, but pollution due to uncontrolled use of these compounds triggered an alarm signal for health [1, 2]. Nowadays, the chain: soil-plants-pesticides-environment-human and animals health is very strictly controlled [3]. The aim of research was to develop a high sensitive modern analytical method in order to monitoring some pesticides. The pesticides residues from maize and wheat cultivated in Banat County were extracted by ultrasound technique, at 59 kHz and 30^{o}C, during 30 min., using acetonitrile and methanol as solvents. The analyses were made on an Agilent Technologies GC 7890A coupled with MSD 5975C.

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PB6. CHEMICAL ANALYSIS AND MORPHOLOGICAL CHARACTERIZATION OF USED THREE-WAY CATALYSTS

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Nowadays, catalysis has become indispensable in environmental pollution control, with selective catalytic routes replacing stoichiometric processes that generate waste problems. Pollution removal in gasoline vehicles is successfully accomplished with a Three Way Catalyst (TWC) which catalyzes the reactions between oxidizing (O_2 and NO_x) and reducing (CO and HC) species in the exhaust [1]. TWC consist of a ceramic monolithic honeycomb where the different active phases are loaded. These active phases are mainly composed of noble metals, cerium-based oxides and alumina [2]. The monoliths are made from cordierite because this material has a very low thermal expansion coefficient, which is needed to prevent them from cracking when thermally stressed during use. The catalyst can be deactivated by chemical, mechanical or thermal phenomena after some time of operation, depending on the composition of the used fuel and lubricants, and of the vehicle adjustment.

We report here experimental studies performed on used TWC in order to study the deactivated level. Two catalytic monoliths contained in the cartridge of cars with more than 150 000 km were chosen to perform this study focused on the chemical, structural and morphological characterization by X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques, including energy dispersive X-ray (EDAX) analysis. Investigations made by several complementary analytical methods reveal the presence of some contaminants in the structure of TWC catalysts coming to the fuel (S) or from lubricating oils (P, Ca, Zn). The main contaminants detected by X-ray diffraction were $Zn_2P_2O_7$ and $CaZn_2(PO_4)_2$, some of the major contaminants that contribute to deactivation of TWC.

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PB7. ANALYTICAL CHARACTERISATION OF ORIGINAL EMULSION FOR COSMETIC USE

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Natural plant extracts have a lot of therapeutic benefits to maintain a healthy skin [1].

The aim of the paper is to characterize original emulsion [2] containing a mixture of plant macerate and essences. Next wild and/or garden plants have been processed to prepare the studied emulsion: *Abies sp*., *Crataegus monogyna*, *Hypericum perforatum*, *Lavandula angustifolia*, *Lavandula officinalis*, *Lilium sp.*, *Melissa officinalis*, *Mentha silvestris*, *Mentha piperita*, *Origanum vulgare*, *Pinus silvestris* buds, *Populus nigra* buds *Thymus serpillum.*

Some of the emulsion ingredients: single plant and plant mixture essential oils, lily macerate together with the final product have been analyzed. The measurements of physical and chemical properties (refractive index, density, pH, oxidation-reduction potential, acidity index, iodine index and peroxide index) show interesting results that could explain the curative effects on skin. The beneficial effects of new emulsion are due to the bioactive compounds that penetrate deep into the tissue and ensure regeneration. The obtained results confirm our previous conclusions concerning the effectiveness of cosmetic mixtures ORP measurement on the antioxidant activity description [3].

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PB8. POLYPHENOL CONTENT ANALYSIS OF SOME BIOLOGICAL SAMPLES

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An adapted Folin-Ciocalteu method for micro scale assay was used for the determination of phenols from biological samples. Total phenolics assay using Folin-Ciocalteu reagent measures the reducing capacity of a sample can be easily use to determine phenols from complex samples (vegetable extracts, wines, urine).

In this study two strains of *Saccharomices cerevisiae* (baker's yeast) were used: the "wild-type" (WT) parental strain By and *Δypl257w* (having the gene YPL257W deleted) [1, 2]. To obtain the samples, early log cell suspensions were treated with chlorogenic acid and cell extracts were obtained after 2 hours of cell exposure to the antioxidant. The extracts were deproteinized and solution of chlorogenic acid was added to get final concentration in sample of 0.20, 0.25 and 0.30 mg/mL respectively.

A calibration curve (absorbance *vs.* concentration) was drawn for chlorogenic acid in ethanol 30% (v/v) for a range of concentrations between 10-120 mg/mL [3]. The correlation coefficient obtained for calibration curve was r^2=0.9960.The wavelength used for measurements was determined by recording the spectra standard chlorogenic acid and Folin-Ciocalteu solution over a wavelength domain between 200-1000 nm. The maximum absorbance was observed at wavelength 757 nm and this was subsequently used for all determinations.

Preliminary data showed that concentrations of chlorogenic acid over 0.25 mg/mL may have toxic effect on cell growth.

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PB9. PILOT STUDY ON NMR DISCRIMINATION FOR DEPRESSION CONDITIONS IN CHILDREN AND ADOLESCENTS

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Depression is a widespread mood disorder that interferes with daily life and normal functioning, causing a persistent feeling of sadness and loss of interest. Currently, the depression diagnostic is based mainly on a psychological evaluation rather than on laboratory tests. This diagnostic modality can have considerable error rate, as clinical depression can manifest in many different ways.

The use of ^{1}H-NMR Spectroscopy in biomedical research has widely spread in the last three decades, different biological fluids being analyzed through this technique.

In this study we used the non-urea and non-water parts of the ^{1}H-NMR spectra for the classification of urine samples from depressed and non-depressed subjects. For the statistical analysis, the spectra were first segmented in equal bins and then analyzed using Partial Least Squares Discriminant Analysis (PLS-DA) method. The obtained PLS-DA plot shows good separations between the two groups

Acknowledgments. The authors acknowledge the financial support of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PNII-ID-PCCE-2011-2-0045.

PB10. NMR CHARACTERIZATION OF THE ARNICA MONTANA PLANT

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Arnica Montana L., is a medicinal species with traditional use in Europe. Phytopreparations based on Arnica extracts are used for the symptomatic treatment of muscular aches, sprains, hematoms, rheumatic pains, acnea, and post surgery recovery.

Although the use of Arnica extracts is very common on the Romanian pharmaceutical market, the chemical composition of the plants growing in Romania was not fully investigated.

The chemical composition of different vegetal matrices is important for life sciences such as food science and medicine.

One of the ways to characterize plants through high resolution NMR is to analyze the juice obtained by squeezing different plant components.

We present here a ^{1}H NMR study of *Arnica Montana L.* extracts from flowers, leaves and strains. The obtained spectra are very complex containing signals from tens of different metabolites.

Acknowledgements. The authors acknowledge the financial support of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-PT-PCCA-2013-4-0791.

PB11. HUMIDITY CHEMIRESISTIVE SENSOR BASED ON CALCONCARBOXYLIC ACID-DOPED PANI

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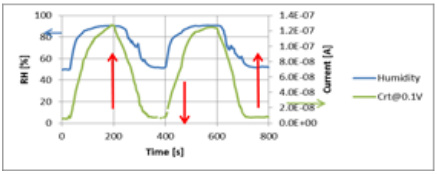
Relative humidity (RH) sensing is of paramount importance in fields such as control of living environment in buildings, food processing, pharmaceutical processing, automotive. Among the RH detecting structures, chemiresistive sensors are an attractive option due to their excellent linear response. This paper presents a novel RH chemiresistive sensor [1] employing calconcarboxylic acid-doped polyaniline as sensing layer. The synthesis was performed by doping PANI, as emeraldine free base, with calconcarboxylic acid [2]. Emeraldine and calconcarboxylic acid were mechanically blended with a pestle in an agate mortar for 15 min. The mixture was heated at various temperatures for obtaining efficient doping. The RH sensor was obtained on two interdigitated metal combs (Al) deposited on glass. The response of the sensor (resistance of the layer decreases, while RH increases, as depicted in figure) is fast, due to the high speed with which doped polyaniline absorbs water, altering its geometry and increasing charge transfer across the polymer chain.



[1] M.N. Mihaila *et al*., US Patent 8,710,354 B2, 2014;
[2] B. Serban *et al*., EP Patent Application 15187999.6.

PB12. OVERCOMING BIOSAMPLING ISSUES IN SPORT DRUG TESTING: ANABOLIC STEROIDS IN DRIED URINES

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Some crucial points are still under evaluation in the field of sampling and analysis for sport drug testing, including some limitations related to the biological fluid of choice: urine.

Dried matrix (DM) collection is a very promising tool for improving anti-doping analysis, addressing those issues related to frequent and impromptu sampling, detection of substance concentrations, enhanced compound stability and need for rapid and high-throughput protocols. Ongoing innovations have demonstrated DM reliability, which is now directly applicable with the coupling to a wealth of microsampling techniques. This research involves in particular the use of dried urine spots (DUS) and volumetric absorptive microsampling (VAMS) on urines, for the collection of accurate volumes, followed by the LC-MS analysis of the main classes of the substances included in the World Anti-Doping Agency (WADA) prohibited list [1], with particular focus on compounds belonging to the class of anabolic steroids (testosterone, epitestosterone, dihydrotestosterone, androstenedione, methandrostenolone, mesterolone, nandrolone, norethandrolone and danazol.

The goal of this project is to establish and validate simple but reliable protocols for the collection of urine microvolumes, unlikely to be tampered but transportable and, above all, storable with no precautions, to perform screening tests and targeted analysis according to the International Standard for Testing and Investigations (ISTI) and the International Standard for Laboratories (ISL), as part of the World Anti-Doping Code. These protocols would substantially reduce overall analysis costs, allowing their application not only to elite athletes, but also to amateurs in local laboratories.

[1] "The World Anti-Doping Code: the 2016 Prohibited List". World Anti-Doping Agency (WADA)

SECTION C: PHYSICAL CHEMISTRY

PC1. CHARACTERIZATION OF INTERACTIONS BETWEEN Pb(II) AND Cd(II) IONS AND CHEMICALLY MODIFIED ELECTRODES WITH POLYAZULENE-BASED COMPLEXING FILMS

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In order to understand the processes/interactions which occur between metal ions and modified electrodes (which are essential for metal detection sensors) with azulene based complexing polymeric films, access to thermodynamic characteristics is necessary. Thus, we report a thorough characterization of metal ions chemical preconcentration processes in azulene based complexing polymer films, which relies on the interactions/incorporation of charged metallic Pb(II) and Cd(II) species within electrogenerated poly(4-azulen-1-yl-2,6-bis(2-thienyl)pyridine) films (poly**L**). The results regarding the interactions between Pb(II) or Cd(II) ions and poly**L** films were analysed using three isotherm models: Langmuir, Freundlich, and Redlich–Peterson. The Langmuir and Redlich–Peterson isotherms were found to be the best-fitting models for Pb(II) and Cd(II) sorption within poly**L** film. The sorption capacity of poly**L** film for Pb(II) and Cd(II) was of about 42 and 17 mg g^{-1}, with small variations with temperature in the range of 293–308 K [1]. Also, the sorption thermodynamic parameters $\Delta G°$, $\Delta H°$, and $\Delta S°$ were calculated using the sorption equilibrium constant obtained from a linearized Langmuir isotherm which gave the best fitting with experimental data. Therefore, the combination of theoretical models with original data obtained for a series of anodic stripping experiments turned out to be an efficient method to achieve full characterization of these heterogeneous interactions.

Acknowledgments. The authors are grateful for the financial support from: Executive Unit for Financing Education Higher, Research Development and Innovation (UEFISCDI) project ID PN-II-RU-TE-2014-4-0594 contract no. 10/2014.

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PC2. COMPUTATIONAL STUDY ON 3D STRUCTURE OF L-ASPARTIC ACID AND L-GLUTAMIC ACID: MOLECULAR DESCRIPTORS AND PROPERTIES

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The aim of this work is to provide a comprehensive and complex analysis of molecular descriptors and properties of two similar amino acids, L-aspartic acid and L-glutamic acid, using a software tool for calculations and properties predictions. As amino acids are model compounds for predicting the physico-chemical properties and behavior of biological, larger molecules as peptides, proteins or enzymes, researches were focused on providing accurate mechanical calculations using various methods: molecular mechanical methods, quantum mechanical models or a hybrid approach [1, 2]. Our study aims to initiate a linear scaling approach, by dividing a large system into small subsystems and performing the calculations for each, individually, then, embedding and correcting the information globally. The calculations were performed on the 3D structure of the studied amino acids that were first generated, as CPK model, and optimized by energy minimization. A comparative assay on their topological, molecular descriptors and properties vas conducted, in vacuum and in water at 298.15K, using the Hartree-Fock model for predicting structure, energy and property calculations, with Spartan'14 V.1.1.4 software on Intel(R) Core i5 at 3.2 GHz CPU PC. Values of properties such as area, volume, polar surface area, polarizability, ovality, log P, dipole moment, HOMO-LUMO gap, distances and angles between atoms, were obtained. The results have been interpreted in terms of electronic effects of side chain groups, molecular deformability, steric factors and reactivity. This approach can be extended to other amino acids in order to predicting protein-ligand interactions, important aspects in drug design studies and protein engineering.

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PC3. RHEOLOGICAL BEHAVIOR OF SUSPENSIONS MADE UP OF ALGAE FROM THE BLACK SEA

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Currently, scientific research is directed towards the development of the third generation of biofuels. Algal biomass from the Black Sea can be accounted for renewable energy as an answer to the depletion of fossil reserves.

Therefore, studying the rheological behavior of the algal suspensions is a step in improving biofuels manufacturing in mixing processes. The four algal species studied (*Ceramium rubrum*, *Cladophora vagabunda*, *Ulva lactuca* and *Cystoseira barbata*) [1] were harvested from the sea, washed with distilled water and cleaned of impurities, then sorted and dehydrated at 50 °C in an apparatus with horizontally circulating air flow. Subsequently, dry algae were finely ground.

Then, three algal suspensions in water of different concentration, *i.e.*, 5%, 10% and 15%, were made up of the seaweed powder of each species. Algal suspensions were vigorously stirred for about 2 hours at 25 °C and further analyzed using a rotational viscometer.

The correlation between the shear stress and the shear rate allowed for dynamic viscosity to be calculated [2]. The samples were analyzed at 25 °C at shear rate values ranging from 0.5 to 437 s^{-1}.

The more diluted suspensions (5%) were non-newtonian fluids obeying a power law, but the more concentrated ones were Herschel-Bulkley fluids and the corresponding rheological equations were developed in this work. The rheological behavior also explained the stability/ instability of suspensions.

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PC4. DISTILLATION CURVES OF GASOLINE+ALCOHOLS BLENDS

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The use of biofuels as additives or fossil fuels replacements is a common technique today. Bioethanol presents an increasing interest as fuel component for gasoline in order to reduce environment pollution and to preserve fossil fuels reserves. Being the possible renewable origin of n-butanol, and taking into account the tendency of biofuels diversification in the transport sector, gasoline+butanol blends could be of interest in the near future.

Gasoline+bioalcohol blends exhibit interesting behavior as a result of the complex nature of the fossil fuel and the molecule polarity of the alcohol. To be used as fuel for internal combustion engines, these blends must fulfill fuel standard requirements. The distillation curve is one of the most important characteristic of a gasoline, being testing criterion for such liquid transportation fuels in order to evaluate their quality [1-3].

The distillation curves of a reformate gasoline blended with ethanol and *n*-butanol were determined and analyzed. The presence of alcohol determines the depression of the distillation curve from that of the gasoline. The depression is the result of vapor-liquid equilibrium behavior of pure components and blends compositions. The initial boiling temperature increases with the increase of alcohol content, while the final boiling point remains almost unchanged, whatever the alcohol nature and content in the blends.

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PC5. STUDY OF DENSITY AND VISCOSITY VARIATION OF DIESEL FUEL BLENDS WITH *n*-BUTANOL

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The use of biofuels in the transport sector has significantly increased in the last years as a result of renewable fuels advantages: emissions reduced toxicity and renewable nature. n-Butanol could be a best choice when considering diesel fuel+alcohols blends as fuel for internal combustion engines since it exhibits some advantages over other bioalcohols with lower hydrocarbon chain (methanol and ethanol), when blended with diesel fuel: improved miscibility, lower volatility and physicochemical properties more similar to that of petrodiesel [1-3].

The most important properties affecting atomization and respectively ignition and combustion processes of a fuel in a diesel engine are viscosity and density. Experimental density and viscosity measurements for diesel fuel+*n*-butanol blends over the entire composition range were performed. The obtained data were used to evaluate the capacity of different models to accurately predict these properties. Density and viscosity of the blends were measured at atmospheric pressure using an Anton Paar SVM 3000 viscometer which is equipped with a density measurement cell based on the "U" vibrating tube method, and a rotational viscometer cell.

Adding n-butanol to diesel fuel lowered the viscosity and the density of the blends. Equations used to predict density and viscosity variation with composition and temperature for diesel fuel+biodiesel mixtures give moderate results for n-butanol blends, because of the polar nature of alcohol molecule. Deviation in viscosity was found to be negative for the studied diesel fuel+*n*-butanol blends.

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PC6. CORRELATIONS FOR REFRACTIVE INDEX OF DIESEL FUEL+*n*-BUTANOL MIXTURES

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The use of bioalcohols in transportation as additives or fossil fuels replacements registered a growing interest in the last years [1].

n-Butanol is a potential alternative fuel, competitive with methanol and ethanol to be blended with diesel fuel, due to its superior miscibility, lower hygroscopicity and corrosivity, higher flash point and higher energy content [2]. The knowledge of the physical and chemical properties of blends components is important for the formulation of a fuel with characteristics within the required specifications. Among other physicochemical properties, refractive index is an important property, easy to determine with a good accuracy and with no expansive equipments. Refractive index can be correlated with other fuel mixtures properties like density and viscosity, important for the processes of fuel atomization and combustion and influencing emissions toxicity.

The purpose of this study is to report experimental data on refractive index of diesel fuel+*n*-butanol mixtures on the whole composition range. The refractive index was determined with an Attago 3T refractometer coupled with a thermostatical bath. Refractive index values ranged between 1.3991 and 1.4626. Empirical equations were proposed to correlate the refractive index of the mixtures with density and viscosity. Absolute average deviations are low, demonstrating the suitability of these models to predict the density and viscosity of diesel fuel+*n*-butanol mixtures from refractive index measurements.

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PC7. THE GREAT SOLUBILITY OF BENZOIC ACID IN A PURE IONIC LIQUID AND THEIR BINARY AQUEOUS MIXTURES

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Successfully used in various fields of chemistry, ionic liquids at ambient temperature (RTILs) present an increasingly interest for the pharmaceutical research and industry [1] because their good thermal and chemical stability, a low vapor pressure and implicitly a low volatility, indicating they are 'environmentally friendly'. Thanks to the multiple solvation interactions, RTILs are used to dissolve a wide of range of both organic and inorganic compounds. In this work the solubility of benzoic acid (BAc) has been investigated in a pure protic ionic liquid, such as imidazolium formate carboxylate (ImForm)[2], constituted by an organic cation such as imidazolium and an carboxylate anion, such as formate, and their aqueous mixtures. The solubility of BAc in pure ImForm and their binary aqueous mixtures of [ImForm/water] were determined depending on the ImForm concentration, and by varying the temperature between 277 and 323 K. Results obtained for pure ionic liquid show that the BAc increase from 1073 g/L (at 293 K) up to 2200 g/L (at 323 K). The BAc solubility presents the greater solubility in pure ImForm, compared to some pure organic solvents, such as: cyclohexane<chloroform<ethanol<ImForm [3]. The BAc solubility in [ImForm/water] binary mixtures was compared with that determined in mixtures as [NaCl/water] [4]. At the same salt concentrations, ranging from 1.66 to 4.33 g/L, at a constant work temperature (323 K), the increasing concentration of NaCl lowers the solubility of BAc in [NaCl/water] mixtures. In the opposite case, the increasing of ImForm concentration determines a considerable increase in BAc solubility into the [ImForm/water] mixtures.

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PC8. FLUORESCENCE CHARACTERISTICS OF 3, 6-*di*HYDROXYFLAVONE ON PEG - COATED SILVER NANOPARTICLES

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Studies based on silver nanoparticles (SNPs) and polyethylene glycole (PEGs) are mainly in the field of the pharmaceutical and bio-medical, with PEG as good "vehicle" to transport protein - based drugs [1-3].

In this work, fluorescence characteristics of 3, 6-diHydroxyflavone (3, 6-diHF) when bound to Bovine Serum Albumin (BSA) on PEGs (Tween 20/40/60, L64 and Myrj 52) coated silver nanoparticles (SNPs) have been investigated by steady-state and time-resolved fluorescence spectroscopy. The mean particle size, polydispersity index as well as zeta potential, have been determined by DLS (Dynamic Light Scattering). Monitor changes in the excited states of 3, 6-diHF as well as the effect of temperature on the thermal stability of the BSA have been studied. 3, 6-diHF has an aggregation effect on the PEG-coated SNPs, especially in the case of Tween 20 and thermal stability of BSA improved by PEG. The results have relevance in drug delivery processes.

Acknowledgements. This work was supported by a grant of the Romanian National Authority for Scientific Research, CNCS – UEFISCDI, project number PN-II-RU-TE-2012-3-0055.

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PC9. KINETICS OF CATALASE INACTIVATION

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Catalase is an enzyme that catalyzes the decomposition of hydrogen peroxide to water and oxygen. Some studies have been reported that the rate of catalase inactivation increases rapidly with temperature [1, 2].

The aim of this research was to study the kinetics of inactivation of catalase obtained from fresh and frozen cherry juice and to observe the influence of the pH, temperature and substrate concentration on the catalase activity. The optimum pH for catalase activity was found to be pH 7. For fresh cherry juice, the enzyme lost its activity at a substrate concentration of 7%, while for frozen cherry juice the enzyme is inactive at a substrate concentration of 0.5%. Catalase inactivation temperature of fresh and frozen cherry juices was found to be 52^0C respectively 25^0C.

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PC10. LEAD REMOVAL FROM AQUEOUS MEDIA USING MICROPOROUS SODIUM TITANOSILICATE SYNTHESIZED BY SOL-GEL METHOD: KINETICS AND ISOTHERM STUDIES

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Microporous sodium titanosilicate was synthesized by modified sol-gel method from NaOH (5M), tetraethylorthosilicate $Si(OCH_2CH_3)_4$ (TEOS) and titanium tetraisopropoxide $Ti(O_3C_3H_7)_4$ in ideal cation stoichiometry for Na_2TiSiO_5. The synthesized product was characterized by structural (XRD), spectroscopic (FTIR), thermal analyses (TG) and electron microscopy (SEM and HRTEM).

Adsorption potential of the synthesized microporous sodium titanosilicate for lead removal from aqueous solution was investigated by varying experimental conditions such as shaking time, temperature and initial metal concentration [1]. The main parameters influencing the sorption process, were investigated. Three kinetic models including a PF-order, PS-order and intraparticle diffusion equation were selected to follow the sorption process of lead on microporous sodium titanosilicate nanopowder. The sorption data were also analyzed by the Langmuir, Freundlich, Halsey, Redlich-Paterson Temkin and Dubinin – Radushkevich models of adsorption [2]. The results obtained showed that the sorption of lead ions onto microporous sodium titanosilicate nanopowder was fitted well with the linear Freundlich and Langmuir models over the concentration range studied. Under the optimum experimental conditions employed, the removal of about 86% of lead ions was attained.

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SECTION D: PETROLEUM TECHNOLOGY AND MANAGEMENT

OD1. RHENIUM INFLUENCE ON THE PERFORMANCE OF HYDRODESULFURIZATION CATALYST

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Hydrodesulfurization process has been studied on synthetic mixtures containing aromatic sulfur compounds. Catalysts used in the study are granulated and were prepared by successively impregnation[1]. The distribution of the acid strength of the catalyst was determined by thermodesorbtion of diethyl-amine in the temperature range 150-600 °C. Experiments were carried out on a micropilot plant with a fixed catalytic bed and downflow of the reactants[2], at a pressure of 30-60 atm, with a volume hourly space velocities of the raw material of 1-4 h^{-3} and a volume ratio of hydrogen / raw material of 25 * 10^3 NL / L The temperature ranged from 175-250 °C[3]. The reaction products were identified by GC-MS [4]. The activity of the catalysts prepared was influenced both by the presence of Re promoter as well as by value of operating parameters.

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OD2. HYDROCRACKING OF HEAVY COKER GAS OIL OVER TRIMETALLIC γAl_2O_3 AND HMS- γAl_2O_3 SUPPORTED CATALYSTS

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Hydrocracking of heavy delayed coking gas oil was performed over two Co-Mo-Ni catalysts supported on γAl_2O_3 [1] and HMS - γAl_2O_3 materials [2]. The catalysts were characterized by X-ray diffraction, scanning electron microscopy (SEM). The distribution of the acid strength of prepared catalysts was determined by thermodesorption of diethylamine [3]. Hydrocracking tests were carried out in a laboratory equipment with fixed bed reactor using the following conditions: reaction temperatures of 370°C, 400°C, 420°C, a pressure of 50, 60 and 70 bar, at the liquid hourly space velocity (LHSV) of $1h^{-1}$. The raw material and the product obtained in hydrocracking experiments were analyzed in order to evaluate the main physical-chemical properties such as: density, boiling range, sulphur content, structural group analysis. Performance of the catalysts was evaluated by conversion, yields of products fractions and selectivity for diesel fraction.

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PD1. INFLUENCE OF DIESEL FUEL FLOW FROM THE ATMOSPHERIC DISTILLATION COLUMN ON DIESEL FUEL PROPERTIES

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Fossil fuels continue to remain the most utilized transportation fuels, even if in the last years the utilization of biofuels was encouraged as a result of their advantages like renewability of raw materials, biodegradability, reduced air pollution. Diesel fuel is one of the most important petroleum derivative utilized as fuel for compression ignition engines. In order to reduce environment pollution and to improve urban air quality, standard requirements for diesel fuel have frequently changed. The most important improvement in standard requirements refers to sulfur (max 50 mg/kg for Euro 4) and polycyclic aromatic hydrocarbons content reduction (max 11 % w/w for Euro 4). Diesel fuel is a complex mixture of a wide range of liquid hydrocarbons made from petroleum. Some of these hydrocarbons result from separating them from the oil by the means of distillation process, others result by physical and chemical transformation processes developed in complex plants from a refinery. It is known that density, distillation curve, sulfur content and freezing point, among other diesel fuel properties, affect engine operation [1, 2]. Variations in diesel fuel flow from the atmospheric distillation column of an industrial crude distillation unit affects diesel fuel properties. It was found that density, final boiling point and freezing point of diesel fuel stream increase with flow increasing; sulfur content increases too, but this variation is not significant.

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PD2. MULTI-OBJECTIV PLANNING OF THE PETROLEUM PRODUCT TRANSPORTATION IN A SINGLE PIPELINE SYSTEM

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Transportation of petroleum products by pipelines is an economic activity to supply large volumes over long distances.

In such a pipeline, oil products are pumped back to back without separation. The sequence and lengths of products pumped is a function of market demand and operational costs.

In this study, a mathematical nonlinear programming model is proposed for optimal planning and scheduling of oil multiple products by a single pipeline, from refinery to depots.

The objective of this work is to generalize the single linear programming by considering the economic pumping as a part of decision process, and production planning and scheduling not being a part of decision process, but its output [1].

To solve this problem, it is necessary to develop a mathematical model based of a multi objective function and a set of constraints.

All equations of the model are grouped into the following subsets (objective function, production planning, volume of products transferred from refinery to depots, control of quantity in refinery tanks, market demands and pumps station necessary) [2].

This work also reviewed the theory of scheduling of pumping operation of oil products for a single planning period [3].

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PD3. OPTIMISATION OF PIPELINE CRUDE OIL NETWORK WITH GENETIC ALGORITHM

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The security of oil pipelines requires additional costs in the price of crude oil transport. Therefore, the optimization of oil transport is discussed in this study together with the determination of the optimal spending for each section of pipe and the correct allocation of funds to ensure the security of pipelines and the protection of the environment [1].

The idea of the model is to transform the double goal by programming model into a single linear combination treatment.

This paper presents a genetic algorithm based on the following genetic model: the oil pipelines are presented as chromosomes and their security attacks are outlined as well as viruses.

Behavioral model of pipelines is presented in a multi-objective program [2].

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PD4. INFLUENCE OF AZEOTHOPY ON THE ETHERIFICATION IN SITU OF FCC GASOLINE

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The etherification in situ of olefins from Fluid Catalytic Cracking gasoline is arguable an application of the reactive distillation. The etherification between the iso-olefins and alcohols in the reaction zone of the distillation column would lead to the increase of octane number in gasoline. In practice, the increase is not always as high as expected, demonstrated in previous studies [1-6], and in our opinion this can be explained by losses of valuable compounds by multiple azeotropes forming during the distillation.

This work was aimed to find the effect of the azeotropy in the reactive distillation, in order to optimize the process. We combined the experiment with the simulation of the process. The experimental study consisted in observing the forming of azeotropes hydrocarbon-alcohols (methanol, ethanol, isopropanol and 1-butanol), taking into account the specific complexity of the hydrocarbon mixture. The conclusions of this study followed by simulations in ChemCad allowed us to find the optimal alcohol –to-feed ratio and the right position of reaction zone in the column, for each alcohol used in etherification.

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PD5. HYDROGENATION OF FURFURAL DERIVATES FOR GASOLINE OXIGENATES COMPONENTS

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Concerns about the total or partial replacement of fossil fuels has been directed in recent years on the conversion of biomass in such fuels. Ethanol is the most known green gasoline. Ethanol content in gasoline is limited due to its low heat of combustion and relatively high corrosivity. In this context, the valorization of furfural, the major product obtained by treating of natural polymeric carbohydrates, into value-added products, could correct these drawbacks. The objective of this research is to obtain furan derivatives by hydrogenation of furfural. Hydrogenation reaction was performed in the presence of a heterogeneous catalyst (Pt-Pd/ γ-Al_2O_3) in a fixed bed reactor and continuous operation. The synthetized compound was conditioned and added to gasoline Density of gasoline and the content in naphthenic hydrocarbons increase with content in furfural derivatives while content of olefins, aromatics and paraffin decreases with it.

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PD6. RESEARCH ON DETERMINING THE PARAMETERS OF THE COMBUSTION PROCESS TO A C.I.D.I. ENERGIE POWERED BY DIESEL FUEL BLEND WITH BIODIESEL AND ETHANOL

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The fuels used for internal combustion engines can influence the quality of life and health of people. In this paper, we present the performances regarding energy and environmental performance achieved by feeding a diesel engine with direct injection using alternative fuels obtained by mixing diesel fuel with ethanol and biodiesel. The engine tests were carried out on the Hatz 1B20 engine mounted on experimental module CT159 G.U.N.T. Base platform. In these tests on the bench, there were determined: the power, the effective work on the cycle, the chromatogram, fuel flow per cycle, the heat release, the effective yield and the energetic recovery ratio. Also, the emissions of CO_2, CO, HC and NOx were determined. The most important influences at mixing diesel with alcohols are on flammability limits, boiling points curve and combustion heat value, which led us to concentrations of up to 5% ethanol- biofuel.

PD7. GEOMETRY OPTIMISATION OF A THERMO-PHOTOVOLTAIC SYSTEM USING THE FINITE ELEMENT METHOD

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A thermophotovoltaic (TPV) system is able to convert the radiant energy of a combustion into electrical energy, and this conversion is realized by using photovoltaic cells. In the case of a combustion flame, thermophotovoltaics can be a technology for co-generation of heat and electricity without the need of any moving parts, commonly referred to as combined heat and power (CHP) generation unit.This new, smarter CHP technology is currently developed in order to substitute in the future the classical oil-fired boilers. The work of T.A. Butcher *et al.* [1] has demonstrated the feasibility of achieving a self powered oil-fired CHP heating system incorporating electric power generation using TPV technology. The present work uses the Heat Transfer with Surface-to-Surface Radiation interface from commercial Finite Element Method (FEM) package Comsol Multiphysics (version 5.0) in order to model a TPV system based on a TPV prototype system developed by B. Bitnar [2], where a selective Yb_2O_3 emitter, heated by a butane burner illuminates high efficiency Si solar cells; gold coated glass mirrors were included in this experimental system having a voltaic efficiency of 2.4% in order to focus the radiation onto photocells. The purpose of this paper is to optimize the length of the mirrors and of the photocells in terms of surface radiosity and irradiation by selecting a model having an optimal operating temperature low enough to ensure a reduced temperature gradient in the vicinity of the mirrors.

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SECTION E: FOOD CHEMISTRY AND ENGINEERING

OE1. DETERMINATION OF DIFFERENT ACTIVE PRINCIPLES FROM RED WINES, OILS, COFFEE AND TEA BY MEANS OF SENSORS/BIOSENSORS

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Nowadays, researchers are focusing their attention on the public health, especially on food as there is a direct relation between the two areas of research. Therefore, there is an increasing interest in developing simple analytical tools able to determine different compounds from food samples with low-cost, fast-response and good sensitivity.

In this work four such analytical tools were developed and applied for different active principles determination from different samples. Two laccase based biosensors were constructed by modifying carbon screen-printed electrodes with different nanoparticles for the determination of total polyphenols from tea infusions [1] and red wine samples [2].

A dual sensor array was also developed for the simultaneous determination of chlorogenic acid and caffeine from coffee samples. One of the carbon working electrodes was modified with platinum nanoparticles, reduced graphene oxide and laccase for chlorogenic acid determination and the second carbon working electrodes was modified with reduced graphene oxide and Nafion for caffeine determination [3].

Finally an electrochemical method based on the use of 2,2′-diphenyl-1-picrylhidrazyl free radical (DPPH) for the determination of the antiradical properties of several olive oils was developed and optimized [4].

Acknowledgments. This work was supported by a grant of the Romanian National Authority for Scientific Research, CNDI– UEFISCDI, project number PN-II-PT-PCCA-2011-3.1-1809.

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PE1. INTAKE AND BIOACCESSIBILITY OF LUTEIN AND β-CAROTENE FROM NETTLE ENRICHED FOODS

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It is well known that edible nettle leaves can contain several bioactive components with potential nutraceutical effects (*e.g.*, essential amino acids, antioxidants, fatty acids and mineral elements) [1, 2]. Dried leaves can be used as additive for foodstuffs, such as bread and pasta. The carotenoid content of common nettle (*Urtica dioica*) was evaluated by means of HPLC-UV-MS technique on different extracts obtained from various pasta samples (durum wheat and egg pasta) [3]. A dynamic *in vitro* gastrointestinal tract model was employed to study the intake of carotenoids from nettle enriched pasta and to address their bioaccessibility. Carotenoid profiles were firstly assayed in nettle dried powder matrix and then in processed foods to determine the maximum availability of active compound. Two major carotenoids were found: lutein and β-carotene. These two can be seen as representative target compounds with no need of focusing also on other low concentration carotenoids. Five different stages of digestive process were considered: stomach; duodenum; colon after 2 hours; colon after 24 hours; colon after 48 hours. Samples were taken out of the *in vitro* system and lutein and β-carotene were quantified. Results showed that the largest bioaccessibility of active compound during food digestion occurs for lutein in duodenum and colon stage (three to four times larger than that of β-carotene). On the contrary, it was null in the stomach step: this is a well known effect due to micellization process of carotenoid molecules that initiates in duodenum by bile salts. Maximum bioaccessibility of lutein and β-carotene occurs in correspondence of colon step after 2 h (about 36% for lutein and 10% for β-carotene) and it decreases after 24 h and 48 h.

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PE2. ALKALINE WATER BETTER THAN PLAIN WATER? A CRITICAL REVIEW

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Water is the basic element of living beings. No other substance is more important for human body than water. In fact, in the reference man, 60% of body weight (BW) (about 45 L) is represented by total body water (TBW) [1]. Some people believe that alkaline water can help to drain toxins more efficiently than regular tap water, leading to better health and fitness. Alkaline water has a higher pH level than plain water. Proponents say that it can neutralize acid in bloodstream, boost the metabolism and help the body to absorb nutrients more effectively. Some even say that alkaline water can help prevent diseases and slow the aging process. An investigation in the scientific literature has been done to verify these claims. The main consideration that could be done is that the alkalinity in ionized water is due to the sodium hydroxide formed during electrolysis if salt is the electrolyte in the water. Most alkaline water representatives do not like to admit this, but when the sodium hydroxide enters the stomach, it is immediately neutralized by the strong stomach acidity back into water and salt ions. There is no reason to expect that the water formed when the alkaline hydroxide ion is neutralized will retain any special characteristics (even if it had some in the beginning) or that dissolved salt, which results from the neutralization process, will have any special properties when it is absorbed. The alkalinity level of the incoming water relative to the acidity of the stomach acid and to the pH the body's well-buffered blood is negligible. This means that there would be almost no resulting effect on pH of the body. The EFSA (European Food Safety Authority) does not authorize any health assertion about alkaline water because is not based on solid scientific data [2]. In conclusion, at this moment, there is no credible evidence in standard medical or scientific literature to support claims that alkaline water has any greater health effects or health benefits than drinking regular water.

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PE3. QUALITATIVE INVESTIGATION OF ALFALFA SPROUTS

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Alfalfa (*Medicago sativa L.*) sprouts contain high levels of nutrients with important impact on human health. During germination, the enzymes released nutrients from seed in order to grow a new plant [1]. The aim of this study is to observe the effect of spouting on phytochemical compounds.

The seed of alfalfa was germinated for 6 days. After sprouting the seeds were dried at 37˚C and powdered for further use. Ethanolic extracts of the sprouts were subject of qualitative determination [2]. The presences of carbohydrates, saponins, phenolic compounds, flavonoids were confirmed in alfalfa sprouts. A decrease in concentration of carbohydrates during spouting was observed due to a different coloration of sprouts extracts. The presences of bioactive compounds was confirmed by FTIR investigation of the extracts. Frequency bands belong to specific functional groups of organic compounds such as polyphenols, vitamins, carbohydrates and proteins.

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PE4. INVESTIGATION ABOUT THE PRESENCE OF ORGANOCHLORINE POLLUTANTS IN MUSSELS FROM BLACK SEA, BULGARIA

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The aim of this study was to investigate the presence of polychlorinated biphenyls, DDT and its metabolites in mussels from Bulgarian Black Sea coast. Mussels *(Mytilus galloprovincialis)* are aquatic organisms which are immobile so that the concentration of pollutants should primarily be considered as an indication of local levels of organochlorine compounds [1]. Samples were collected from three areas of Black Sea coast of Bulgaria in summer 2015.

The fifteen congeners of PCBs, DDT and its metabolites DDE and DDD were performed by gas chromatography system with mass spectrometry detection. The metabolites DDE and DDD were found in all analyzed mussel samples, but PCBs were not detected in any sample. DDE concentrations were found in mussels from 1.09 to 1.63 ng/g wet weight. In mussel total DDT concentrations (2.14 ng/g ww) were found comparable to those in mussels, sampled in 2013 and 2014 (1.87 ng/g ww).

The levels of DDTs and polychlorinated biphenyls in mussels from the Black Sea were found comparable to levels measured in the same molluscs from neighbor seas - Marmara Sea and Mediterranean Sea [2].

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PE5. NUTRITIONAL EVALUATION OF AQUACULTURE MUSSEL (*M. GALLOPROVINCIALIS*) FROM BLACK SEA, BULAGRIA

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In recent years black mussels are one of the most commercially important species from Bulgarian Black Sea. Many studies suggest that marine molluscs are valuable health food, low in calories and fats, and high in proteins. They are one of important dietary sources of fat soluble pigments - astaxanthin and carotenoids and polyunsaturated fatty acids (PUFA). To our knowledge information available on the nutrition quality based on chemical composition, fat soluble pigments, cholesterol and PUFA content of Black mussel from Bulgarian Black Sea waters is very limited. The aim of the present study is to determine and compare protein, lipid, carbohydrate, energy values, fat soluble pigments, cholesterol and fatty acid composition in farmed mussels (*Mytilus galloprovincialis*) from North and South parts of Black Sea. The mussel samples were analyzed for lipids (Bligh & Dyer method), crude proteins (Kjeldahl method), carbohydrates and moistures according to the AOAC (1990) methods. Fat soluble pigments and cholesterol were analyzed simultaneously by RP-HPLC system. Fatty acids were analyzed by GC-MS system.

Lipid and protein content were found to be higher in mussels from North region. In accordance with Commission Regulation (EC) No 116/2010 [1] all analyzed mussel samples can be classified as a high in protein and low in fats and carbohydrates. All black mussels' populations contain significantly low cholesterol amounts and significantly higher omega-3(n-3) than omega-6 PUFA. A portion of 100 g edible tissue provides over than 0.500 g of required amounts of eicosapentaenoic acid (20:5) and docosahexaenoic acid (22:6) n-3 PUFA according to EFSA (2012) [2]. It can be concluded that studied aquaculture Black Sea mussels are beneficial food for human health and it is advisable to be a part of a proper or preventive diet for Bulgarian consumers.

[1] Commission Regulation (EU) No 116/2010 of 9 February 2010 amending Regulation (EC) No 1924/2006 of the EU Parliament.
[2] EFSA 2012. *EFSA Journal 2012* 10(7), 2815. Available online: www.efsa.europa.eu

PE6. THE CORRELATION BETWEEN ANTIOXIDANTS AND MINERAL EXTRACTABILITY OF TEA PLANT INFUSIONS

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The aim of this study was to investigate the antioxidant activity and mineral extractability of six different types of tea infusion: mint, linden, chamomile, St. John's wort, green and black tea, which are provided from the same brand. More, the mint and linden from private manufacturer were analyzed also.

Total phenolic content was evaluated by Folin-Ciocalteu method, while antioxidant activity was tested using DPPH (2,2-diphenyl-1-picrylhydrazyl) radical scavenging method. It was studied also the content of iron and copper extractability in order to calculate Pearson correlation coefficients. The water extract, which is considered a quality indicator for tea plants, ranged from 5.25% to 29.25%; values lower than the maximum admissible limit of 32% [1].

Among the tested samples, the highest amounts of total phenolic compounds, respectively antioxidant activity were detected in green tea. The results showed that there are many correlations (positive, negative and weak) between antioxidants and mineral extractability of tea plants. The total phenolic content is closely correlated with iron content ($r = 0.4680$) and copper ($r = 0.8654$) for all samples of tea. A significant correlation was observed statistically between the total phenolic content and the concentration of copper ($p = 0.0054 < 0.05$). No significant correlation was observed in the case of iron ($r = -0.1850$). The most accurate correlation between the DPPH values and total phenolic content was observed for mint and linden from private manufacturer ($r = 0.9956$, respectively $r = 0.8111$). Water extract was weakly correlated with the copper concentration in tea ($r = 0.109$, $p = 0.7927$). Consequently, the correlations of water extract, total polyphenols and antioxidant activity with mineral extractability suggested the influence of antioxidant compounds on mineral bioavailability.

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PE7. CONTENTS OF POLYPHENOLS IN NATURAL COMMERCIAL FRUIT JUICE

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The aim of this work was to analyses qualitatively and quantitatively the level of the polyphenols in natural commercial fruit juices available in the Romanian market, and then selecting these with the highest contents of the studied compounds. Polyphenols are micronutrients and their roles are to prevent of degenerative diseases such as cardiovascular disease, degenerative disease and cancer. Sources of polyphenols are: fruits, tea, coffee, red wine, vegetables, cereals, chocolate and fruits juices.

The research material comprised six natural juices from different companies. The juice fruit includes: grape juices, cranberry juice, pomegranate juice, black currant juice, grape and raspberry juice and berries juice. The identified polyphenols were: gallic acid, 3 methyl gallic acid, chlorogenic acid, *p* coumaric acid, ferullic acid, cinnamic acid, caffeic acid, ellagic acid, E resveratrol. The polyphenols were determined by a HPLC-DAD method. The analysis was conducted on a Zorbax XDB-C18 column with gradient elution of acetonitrile-orhophosphoric acid.

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PE8. INFLUENCE OF FOOD EMULSIFIERS ON EMULSIONS STABILITY

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Food emulsions are the basis of many food products and their properties define the quality of food. Some studies have already highlighted the importance of food emulsifiers on emulsions stability [1-2].

The purpose of the paper was to study the long-term stability of oil in water emulsions in the presence of food emulsifiers. For emulsions were used six types of oils: sunflower oil, olive oil, rapeseed oil, corn oil, peanut oil and soybean oil and three types of emulsifiers: glycerin, lecithin, and polyethylene glycol 4000 (PG 4000). For a period of six months a series of characteristics have been analyzed such as density, dynamic viscosity, refractive index, conductivity, pH, type of emulsion and their microstructure. Comparative microscopic analyze shows a homogeneous structure in time for emulsions with lecithin as emulsifier, demonstrating their stability.

The statistical interpretation of results was carried out calculating the arithmetic mean, standard deviation and linear deviation of the results achieved on each stage.

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PE9. VARIATION OF PHYSICO-CHEMICAL PROPERTIES OF VEGETABLE OILS DURING STORAGE

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Vegetable oils and derived products have an important role in food industry. The role of lipids in the body is mainly that to store energy in the tissues, to protect against cold and also to dissolve fat-soluble vitamins, thus ensuring their introduction into the body through the gastrointestinal tract. Oils vegetable contain valuable vitamins such as A, D, E and K [1-3].

Depending on the composition, vegetable oils degrade slowly or stressed, suffering oxidation (rancidity). Oxidative potential thus depend on the nature and concentration of the fatty acid composition. When considering vegetable oils degradation during storage, some other factors depending on storage conditions: light, heat and moisture, should be taken into account [4-5].

The aim of this study was to determine the variation of some physico-chemical properties for different types of vegetable oils (sunflower, almond, corn and rapeseed) during storage. The samples were deposited at dark at room temperature over a long period of time. Some physicochemical characteristics like the density, refractive index, saponification value, acid value, peroxide value and iodine value were determined at fixed intervals of time. Only after about one year there were registered noticeable variations in the value of the physicochemical properties of the investigated vegetable oils.

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SECTION F: OPEN EDUCATIONAL RESOURCES AND E-LEARNING

PF1. UTILIZING E-LEARNING TO BUILD CAPACITY FOR HEALTHCARE PROFESSIONAL EDUCATION IN BULGARIA

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E-learning training has attached much attention in recent years as a potential way to build capacity in students in different European countries. By using the power of Internet technologies to share information via electronic platforms, E-learning helps to increase the access to training, education and high quality resources.

This paper provides a background to E-learning and discussions of its two-year implementation at Medical University-Varna, Bulgaria. Results from two online institutional surveys conducted in 2015 among students (n=115) and faculty (n=120) showed that on average E-learning is been used in all medical departments (about 33%). Students have used primarily the online electronic sources in their 1st, 2nd and 3rd year of education in pre-clinical fields, including Chemistry. Both, assistant and associate professors rated sharing materials, evaluation and communication tools to be the most useful in their practice. E-learning can effectively be adopted to enhance the accessibility to health care education while simultaneously enhance faculty effectiveness and efficiency.

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