SECTION A: NATURAL AND SYNTHETIC COMPOUNDS

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

Elvan ÜSTÜN

Ordu University, Turkey
elvanustun@odu.edu.tr

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

[1]. R. Motterlini, L. E. Otterbein, Nat. Rev. Drug Discov. 9 (2010) 728–743.
[2]. C. G. Hartinger, P. J. Dyson, Chem. Soc. Rev. 38 (2009) 391–401.
[3]. E. Üstün, A. Özgür, K. A. Coşkun, S. Demir Düşünceli, İ. Özdemir, Y. Tutar, Transit. Met. Chem. 42 (2017) 331-337.
[4]. M. A. Gonzales, P. K. Mascharak, J. Inorg. Biochem. 133 (2014) 127–135.
[5]. S. Pai, M. Hafftlang, G. Atongo, C. Nagel, J. Niesel, S. Botov, H.-G. Schmalz, B. Yard, U. Schatzschneider, Dalt. Trans. 43 (2014) 8664-8678.

PA1. EVALUATING THE BIOLOGICAL POTENTIAL OF SOME NEW COBALT (II) COMPLEXES WITH 3,5-DIMETHYLPIRAZOLE AS LIGAND

Ecaterina-Daniela BĂJENARU,[1] Rodica OLAR,[1] Gina VASILE SCĂEȚEANU,[2] and Mihaela BADEA[1]

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania*
[2]*University of Agronomical Sciences and Veterinary Medicine, 59 Mărăşti Str., 011464 Bucharest, Romania*

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

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

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

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

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

PA2. SYNTHESIS, PHYSICO-CHEMICAL CHARACTERIZATION, CRYSTAL STRUCTURE AND BIOLOGICAL ACTIVITY OF NEW COPPER (II) COMPLEXES WITH NICOTINAMIDE

Ioana SOARE,[1] Rodica OLAR,[1] Gina VASILE SCĂEȚEANU,[2] and Mihaela BADEA[1]

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania*
[2]*University of Agronomical Sciences and Veterinary Medicine, 59 Mărăşti Str., 011464 Bucharest, Romania*

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

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

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

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

PA3. SYNTHESIS, SPECTRAL AND BIOLOGICAL CHARACTERIZATION OF NEW COPPER (II) COMPLEXES WITH PYRAZOLE TYPE LIGANDS

Iarina-Ana-Bianca STOICA,[1] Rodica OLAR,[1] Gina VASILE SCĂEȚEANU,[2] and Mihaela BADEA[1]

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania*
[2]*University of Agronomical Sciences and Veterinary Medicine, 59 Mărăşti Str., 011464 Bucharest, Romania*

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

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

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

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

PA4. COBALT (II) COMPLEXES AS ANTIBACTERIAL AGENTS

Ana-Maria HOLTEA,[1] Rodica OLAR,[1] Gina VASILE SCĂEȚEANU,[2] and Mihaela BADEA[1]

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania*
[2]*University of Agronomical Sciences and Veterinary Medicine, 59 Mărăşti Str., 011464 Bucharest, Romania*

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

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

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

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

PA5. PHYSICO-CHEMICAL AND BIOLOGICAL CHARACTERISATION OF SOME COBALT(II) COMPLEXES WITH MIXED LIGANDS

Ana Maria CHIREA, Mihaela BADEA, and Rodica OLAR

University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Sector 5, Bucharest, Romania

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

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

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

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

PA6. INSIGHT ON PHYSICO-CHEMICAL AND BIOLOGICAL PROPERTIES OF SOME COPPER(II) COMPLEXES WITH MIXED LIGANDS

Adriana CIURARU, Mihaela BADEA, and Rodica OLAR

University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania

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

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

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

[1]. H.M. Ashour, O.G. Shaaban, O.H. Rizk, I.M. El-Ashmawy, European Journal of Medicinal Chemistry 62 (2013) 341–351.

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

PA7. VANADIUM (V) COMPLEXES WITH BIGUANIDE DERIVATIVES DEVELOPED AS BIOLOGICALLY ACTIVE SPECIES

Andreea Gabriela DUMITRESCU, Mihaela BADEA, and Rodica OLAR

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania*

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

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

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

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

PA8. RUTHENIUM (III) COMPLEXES WITH A PURINE ANALOG DEVELOPED AS ANTITUMOR SPECIES

George GIOCAS, Mihaela BADEA, and Rodica OLAR

University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania

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

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

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

PA9. PHYSICO-CHEMICAL AND BIOLOGICAL CHARACTERISATION OF SOME COPPER(II) COMPLEXES WITH MIXED LIGANDS

Laura Ioana DOBRE,[1] Mihaela BADEA,[1] Anca DUMBRAVA,[2] and Rodica OLAR[1]

[1] University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Sector 5, Bucharest, Romania
[2] Ovidius University of Constanta, Department of Chemistry and Chemical Engineering, 124 Mamaia Blvd., 900527 Constanta, Romania

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

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

Having in view these aspects, we extended this field in synthesis of new complexes of type [Cu(vntsc)(N-N)(X)] (Hvntsc: 2-hydroxy-3-methoxybenzaldehyd thiosemicarbazone, N-N: 2,2'-bipyridine (bipy) or 1,10-phenantroline (phen), X: ClO_4, NO_3) with vntsc as multifunctional ligand and N-N as auxiliary ligand. The features of complexes have been assigned from elemental analyses as well as IR and UV-Vis spectra. The thiosemicarbazone ligand behave as tridentate species while aromatic amine (dipy, phen) acts as chelate. The distorted octahedral stereochemistry is completed by perchlorate or nitrate anions acting as unidentate.

The thiosemicarbazone was obtained in [1+1] condensation of 2-hydroxy-3-methoxybenzaldehyde (o-vanillin) with thiosemicarbazide.

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

PA10. NEW BIOLOGICAL ACTIVE COPPER(II) COMPLEXES WITH MIXED LIGANDS

Adriana Camelia CEBUC,[1] Mihaela BADEA,[1] Rodica OLAR,[1] Gina VASILE SCĂEȚEANU,[2] and Anca DUMBRAVA[3]

[1]*University of Bucharest, Faculty of Chemistry, Department of Inorganic Chemistry, 90-92 Panduri Str., 050663 Bucharest, Romania*
[2]*University of Agronomical Sciences and Veterinary Medicine, 59 Mărăşti Str., 011464 Bucharest, Romania*
[3]*Ovidius University of Constanta, Department of Chemistry and Chemical Engineering, 124 Mamaia Blvd., 900527 Constanta, Romania*

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

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

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

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

PA11. GLUCOSINOLATES FROM SOME ROMANIAN SPECIES OF BRASSICACEAE FAMILY

Mariana Nela ŞTEFĂNUŢ*,[1] Adina CĂTA,[1] Cristian VASZILCSIN,[1] and Ioana Maria IENAŞCU[1,2]

[1]National Institute of Research and Development for Electrochemistry and Condensed Matter, Dr. A. P. Podeanu 144, 300569 Timişoara, Romania
[2]"Vasile Goldiş" Western University of Arad, Faculty of Pharmacy, 86 Liviu Rebreanu, 310045, Arad, Romania
** mariana.stefanut@gmail.com*

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

[1]. A.P. Vig, G. Rampal, T.S. Thind, S. Arora, Bio-protective effects of Glucosinolates-A review, LWT-Food Sci. Tech. 42 (2009) 1561-1972.
[2]. A. Aires, R. Carvalho, Rapid Separation of Indole Glucosinolates in Roots of Chinese Cabbage (Brassica rapa Subsp. Pekines) by High Performance Liquid Chromatography with Diode Array Detection, Int. J. Anal. Chim. 2017 (2017) 5125329. https.//doi.org/10.1155/2017/5125329.
[3]. M. N. Ştefănuţ, A. Căta, R. Pop, C. Tănasie, D. Boc, I. Ienaşcu, V. Ordodi, Anti-hyperglycemic effect of bilberry, blackberry and mulberry ultrasonic extracts on diabetic rats, Plant Food for Human Nutrition 68 (2013) 378-384.

PA12. SYNTHESIS AND CHARACTERIZATION OF SOME N-(2-CHLORO-PHENYL)-2-HYDROXY-BENZAMIDE DERIVATIVES

Ioana M. C. IENAŞCU*,[1,2] Adina CĂTA,[1] Cristina MOŞOARCĂ,[1] Iuliana M. POPESCU,[3] and Mariana N. ŞTEFĂNUŢ[1]

[1]*National Institute of Research and Development for Electrochemistry and Condensed Matter, 144 Dr. A. P. Podeanu, 300569, Timişoara, Romania*
[2]*"Vasile Goldiş" Western University of Arad, Faculty of Pharmacy, Department of Pharmaceutical Sciences, 86 Liviu Rebreanu, 310045, Arad, Romania*
[3]*Banat's Agricultural Science University, Faculty of Agriculture, Department of Chemistry and Biochemistry, 119 Calea Aradului, 300645, Timişoara, Romania*
**imcienascu@yahoo.com*

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

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

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

[1]. M. Krátký, J. Vinšová, J. Stolaříková, Molecules 17 (2012) 12812–12820.
[2]. T.J.R. Cheng, Y.T. Wu, S.T. Yang, K.H. Lo, S.K. Chen, Y.H. Chen, W.I. Huang, C.H. Yuan, C.W. Guo, L.Y. Huang, et al., Bioorg. Med. Chem. 18 (2010) 8512–8529.
[3]. M. Krátký, J. Vinšová, Curr. Pharm. Des. 17 (2011) 3494–3505.
[4]. A. Fomovska, R.D. Wood, E. Mui, J.P. Dubey, L.R. Ferreira, M.R. Hickman, P.J. Lee, S.E. Leed, J.M. Auschwitz, W.J. Welsh, et al. J. Med. Chem. 55 (2012) 8375–8391.
[5]. M. Zuo, Y.W. Zheng, S.M. Lu, Y. Li, S.Q. Zhang, Bioorg. Med. Chem. 20 (2012) 4405–4412.

PA13. ANTHOCYANIN EXTRACTS FROM DIFFERENT PLANT MATRICES AS POTENTIAL NATURAL FOOD DYES

Adina CĂTA,[1] Ioana M. C. IENAŞCU,[1,2] and Mariana N. ŞTEFĂNUŢ[1]

[1]*National Institute of Research and Development for Electrochemistry and Condensed Matter, 144 Dr. A. P. Podeanu, 300569, Timişoara, Romania*
[2]*"Vasile Goldiş" Western University of Arad, Faculty of Pharmacy, Department of Pharmaceutical Sciences, 86 Liviu Rebreanu, 310045, Arad, Romania*

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

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

[1]. C. Spence, Flavour 4 (2015) 21.
[2]. N. Martins, C.L. Roriz, P. Morales, L. Barros, I.C.F.R. Ferreira, Trends in Food Science & Technology 52 (2016) 1-15.
[3]. P. Amchova, H. Kotolova, J. Ruda-Kucerova, Regulatory Toxicology and Pharmacology 73 (2015) 914-922.
[4]. J. He, M.M. Giusti, Annual Review of Food Science and Technology 1 (2010) 163-187.

PA14. CHEMICAL COMPOUNDS AND ANTIOXIDANT ACTIVITIES IN TWO FLAVONIC EXTRACTS FROM *HELICHRYSUM ARENARIUM* FLOWERS AND *ROBINIA PSEUDOACACCIA* FLOWERS

Mihaela Mirela BRATU,[1] Semaghiul BIRGHILA,[2] Antoanela POPESCU,[1] Lenuța ZGLIMBEA[3], and Larissa Mihaela STANCU[3]

[1] Department of Pharmaceutical Sciences II, Ovidius University of Constanta, University Avenue, Campus 1, Constanta, Romania
[2]Department of Chemistry and Chemical Engineering, Ovidius University of Constanta, 124 Mamaia, Constanta, Romania
[3] Biotehnos Institute - Otopeni, Gorunului 3-5, Avenue, Bucharest, Romania

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

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

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

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

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

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

PA15. CELLULOSE FIBER EXTRACTION FROM *ULVA LACTUCA* ALGAE BY CHEMICAL TREATMENT

Doinița-Roxana CIOROIU TIRPAN,[1,2] Claudia Irina KONCSAG,[1] and Tănase DOBRE[2]

[1]Ovidius University of Constanta, 124 Mamaia Blvd., Constanta, 900527, Romania
[2]University "Politehnica" of Bucharest, Chemical and Biochemical Engineering Department, 1-7 Gheorghe Polizu Str., Bucharest, 011061, Romania

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

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

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

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

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

Thus, a yield of 41.85% cellulose per d.m. was obtained proving that *Ulva Lactuca* specie is a viable alternative resource in cellulose production.

Acknowledgement. *The work has been funded by the Operational Programme Human Capital of the Ministry of European Funds through the Financial Agreement 51668/09.07.2019, SMIS code 124705.*

[1]. M.A. Jmel, N. Anders, G.B. Messaoud, M.N. Marzouki, A. Spiess, I. Smaali, Journal of Cleaner Production 234 (2019) 1421-1427.

PA16. NUMERICAL MODELING OF MIXED-MODE DELAMINATION FRACTURE IN UNIDIRECTIONAL AS4/PEEK COMPOSITES

Viorel IONESCU

Ovidius University of Constanta, Mamaia Bd. No 124, Constanta, 900527, Romania

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

[1]. E.L. Steinberg, E. Rath, A. Shlaifer, O. Chechik, E. Maman, M. Salai, J Mech Behav Biomed Mater. 17 (2013) 221-228.
[2]. C.S. Li, C. Vannabouathong, S. Sprague, M. Bhandari, Clin Med Insights Arthritis Musculoskelet Disord. 8 (2015) 33–45.
[3]. L. Gornet, H. Ijaz, Composites Part B: Engineering 42 (2011) 1173-1180.