University of Bucharest **Faculty of Chemistry** **ASC-UB**

Students' Scientific Communications Session

– The 20th Edition –

Book of Abstracts

May 23rd - 24th, 2025

Bucharest, Romania

Scientific Committee

President, Conf. dr. Emilia Elena Iorgulescu
Vice-President, Conf. dr. habil. Iulia Gabriela David
Vice-President, Lect. dr. Delia-Laura Popescu

Evaluation Committee Members
Bachelor Level

Conf. dr. habil. David Iulia Gabriela
Lect. dr. Mitran Gheorghița
Lect. dr. Gheorghe Ruxandra
Lect. dr. Pincu Elena
Lect. dr. Popescu Codruța

Evaluation Committee Members
Master Level & PhD Level

Prof. dr. Bala Camelia
Prof. dr. habil. Marcu Ioan-Cezar
Prof. dr. Medvedovici Andrei
Conf. dr. habil. Matache Mihaela
Conf. dr. Cimpoeșu Marilena
Conf. dr. Jurca Bogdan

The Chemistry Students Association of the University of Bucharest (ASC-UB)

Dobrilă Victor, Project coordinator, ASC-UB
Albu Andrei, Graphic coordinator ASC-UB
Flangea Flavia Andreea, Assistant P.C., ASC-UB
Ghița-Oncete Andrada, Assistant P.C., ASC-UB
Pavel Radu Florin, Assistant P.C., ASC-UB
Popa Bianca Ioana, Assistant P.C., ASC-UB
Lect. Dr. Delia-Laura Popescu, Faculty of Chemistry

www.asc-ub.ro
ascub.contact@gmail.com

The Chemistry Students Association of the University of Bucharest (ASC-UB) acknowledges for their support:

MINISTERUL EDUCAȚIEI ȘI CERCETĂRII

UNIVERSITATEA DIN
BUCUREȘTI
VIRTUTE ET SAPIENTIA

FACULTATEA DE CHIMIE

ACS
Chemistry for Life®

NOVACHIM
TRADING

APA NOVA
o companie VEOLIA

BIOFARM®

Section 1

Bachelor Level

Valorization of Plastic Waste – PET as Spacer for the Enzyme Entrapment Model

Anghel Andreea-Ramona, **Iunia Podolean, Mădălina Săndulescu**

Department of Inorganic, organic Chemistry, Biochemistry and Catalysis,
Faculty of Chemistry, University of Bucharest

Polyethylene terephthalate (PET) is a synthetic polymer widely used in the plastic industry. It is obtained through the esterification reaction of terephthalic acid (TPA) with ethylene glycol (EG)[1]. High stability and persistence of PET in the environment generated a real issue of environmental pollution. So that, PET valorization is one of the most important challenges today for limiting the negative effect.

We propose to use micro-PET beads for construction of encapsulated enzyme composites

Microencapsulation is a method by which the enzyme is enclosed in a gel or a solid material formed around it, without being altered, maintaining its activity, and allowing the passage of the substrate to the enzyme catalytic site.[2]

For our experiments, the enzyme used, lipase from Aspergillus niger, was encapsulated with PET beads (obtained from a plastic bottle) in sodium alginate. PET surface was modified by grafing -NH2 groups using diethylenetriamine as reagent, under acidic conditions (pH=4). Entrapped lipase biocomposites developed with modified/original-PET were evaluated in term of enzyme activity. Characterization of the developed biocomposites demonstrated the promising perspective of PET applicability as spacer for entrapment model.

[1] Ed Ivan M. Bardoquillo, Jake Matthew B. Firman, D.B. Montecastro et al., Chemical recycling of waste polyethylene terephthalate (PET) bottles via recovery and polymerization of terephthalic acid (TPA) and ethylene glycol (EG), Materials Today

[2] Imam, H. T., Marr, P. C., Marr, A. C., *Enzyme entrapment: Biocatalyst immobilization without covalent attachment*, Green Chemistry, vol. 23, nr. 13, pp. 4980–5005, 2021.

Study of Luminescent Properties of Eu^{3+}– Doped Mixed Metal Phosphates

Andrei-Ștefan Buzatu, Viorel Cîrcu

Faculty of Chemistry, University of Bucharest, 4-12 Regina Elisabeta Boulevard, Sector 3, Bucharest

The luminescent properties of the Eu^{3+} ion can be exploited to produce light-emitting compounds from mixed metal phosphates that would otherwise lack intrinsic luminescence. In this study, this effect was achieved by doping a mixed phosphate compound comprising Na, K, Ca, Mg, and Zn with a small amount of Eu^{3+} (~0.1%). The synthesis was performed via a solid-state reaction at elevated temperatures.

The precursor materials included sodium phosphate and potassium phosphate, which were mixed in proportions to ensure that the combined molar percentage of Na^+ and K^+ constituted 60% of the total metal content, with each individually contributing 30%.

The ratios of Na^+:K^+ and Zn^{2+}:Eu^{3+} were kept constant, while the Ca^{2+}:Mg^{2+} ratio was systematically varied among different samples. The photoluminescent properties were analyzed using a time-resolved spectrofluorometer, including lifetime and absolute quantum yields of the prepared samples with the help of an integrating sphere.

The variations in emission intensity observed were assigned to structural changes within the phosphate matrix, likely influenced by the ionic radii differences between Ca^{2+} and Mg^{2+}. These structural modifications affect the local environment of the Eu^{3+} ions, thereby altering their luminescent efficiency. Consequently, an optimal Ca^{2+}:Mg^{2+} ratio can be determined to maximize luminescence for a given Eu^{3+} concentration.

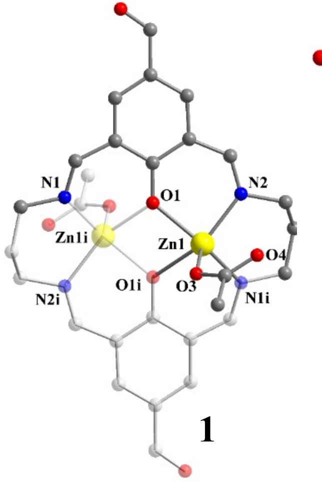
Strategically Functionalized Macrocyclic Dinuclear Zn(II) Complexes for Molecular Engineering of Metal-Organic Cages

Adelina Casandroiu,[1,2] **Adrian E. Ion,**[2] **Andreea Dogaru,**[2] **Cătălin Maxim,**[*1]
Marius Andruh[1,2] **and Simona Nica**[*2]

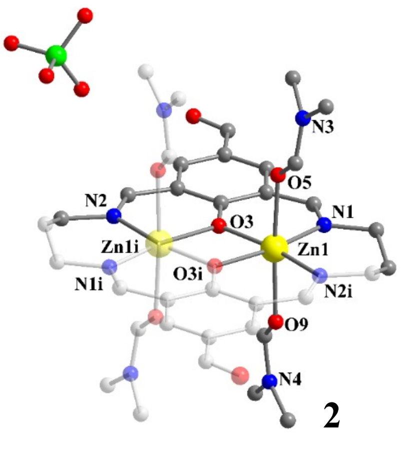
[1]*Faculty of Chemistry, University of Bucharest, Romania*
[2]*"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry, Splaiul Independenței, 060023 Bucharest, Romania*

The development of new polytopic organic ligands for constructing coordination-based materials is of high interest owing to their applications in gas storage, separations, sensing, catalysis, etc.[1] By carefully selecting ligand symmetry, rigidity, donor type, and functionality, structures ranging from discrete molecular cages to extended porous frameworks can be designed.

In this work, we report two new binuclear Zn(II) complexes with a macrocyclic ligand formed by *in situ* condensation reaction of 2-hydroxybenzene-1,3,5-tricarbaldehyde with 1,3-diaminopropane. Using $Zn(OAc)_2\cdot 2H_2O$, a neutral dinuclear macrocyclic complex, **1**, was obtained, whereas with $Zn(ClO_4)2\cdot 6H_2O$, a cationic dinuclear complex, **2**, was isolated. Single crystal X-ray diffraction shows the zinc ions placed inside the salen-like N_2O_2 cavities, bridged by the phenolic oxygens of the macrocycle. In complex **1**, the Zn(II) ions are five-coordinated with monodentate acetate ligands at the apical positions, whereas in complex **2**, the Zn(II) ions are six-coordinated with two DMF molecules in *trans* positions. The two complexes are powerful building blocks for the development of metal-organic molecular cages.



1



2

---

[1] G. Montà-González, F. Sancenón, R. Martínez-Máñez, V. Martí-Centelles, *Chem. Rev.* 2022, *122*, 13636

Lignin-Bitumen Biocomposite as New Materials with Different Properties

Chiriță Laura-Alexandra, **Iunia Podolean, Mădălina Săndulescu**

Faculty of Chemistry – Univeristy of Bucharest - Şoseaua Panduri nr. 90-92, sector 5, Bucharest

Currently, lignin is one of the main residues resulting from the extraction of cellulose from plant materials, with quantities ranging between 50 and 70 million tons per year [1]. Luo and Abu-Omar's research group estimates 225 million tons residual lignin per year until 2030[1]. Beside all these aspects, there is a strong desire to find an industrial-scale use for lignin to reduce waste quantities. On the other side, asphalt contains bituminous materials that are largely petroleum-based and, when characterized by several criteria, are both expensive and polluting, or at the very least, unsustainable[2]. Therefore, there is a serious interest for developing friendly environmental method for bitumen preparation with improved resistance as more sustainable and reliable alternatives.

In this context, we proposed the use of lignin as additive for bitumen. Different types of lignin were involved in this study. Additionally, derivation of lignin was performed based on enzymatic catalysis with laccase enzyme. Bitumen composition was modified adding natural/derivatized lignin (bitumen-lignin composite). The properties of the bituminous material were evaluated performing Fourier-transform infrared spectroscopy (FTIR) analysis, more precisely, Attenuated Total Reflectance (ATR). Interpretation of the main spectral peaks allowed to identify any structural modifications of bitumen after lignin addition.

[1] Haq, I., Mazumder, P., Kalamdhad, A.S., Recent advances in removal of lignin from paper industry wastewater and its industrial applications-A review, Bioresource Technology (2020), doi: https:// doi.org/10.1016/j.biortech.2020.123636

[2] Norgbey E, Huang J, Hirsch V, Liu WJ, Wang M, Ripke O, Li Y, Annan GET, Ewusi-Mensah D, Wang X, Treib G, Rink A, Nwankwegu AS, Opoku PA, Nkrumah PN. Unravelling the efficient use of waste lignin as a bitumen modifier for sustainable roads, Construction and Building Materials, (230) 2020, https://doi.org/10.1016/j.conbuildmat.2019.116957

Synthesis and Electrochemical Characterization of Organic Compounds with Chromophoric Properties

Laurențiu Cotoc, **Irina Zarafu, Daniela Bala**

University of Bucharest, Faculty of Chemistry, Department of Analytical
Chemistry and Physical Chemistry, 4-12 Regina Elisabeta Blvd.,
030018 Bucharest, Romania

Azo dyes are an important group of synthetic colorants extensively used in industries such as textiles, cosmetics, and pharmaceuticals[1]. Their versatility and wide applicability make them essential components in many manufacturing processes. Nowadays, azo dyes incorporating heterocyclic moieties exhibit enhanced coloring properties, thermal stability, and more positive solvatochromic behavior than the dyes derived from a simple aromatic amine[2]. This study focuses on the synthesis and electrochemical analysis of two organic compounds containing the azo group (-N=N-). The compounds were synthesized through the diazotization of aromatic amines in water, followed by coupling with β-naphthol, a phenolic compound commonly used in industry. Structural confirmation was carried out using 1H-NMR spectroscopy, while the electrochemical properties of the synthesized azo dyes were examined using cyclic voltammetry and differential pulse voltammetry.

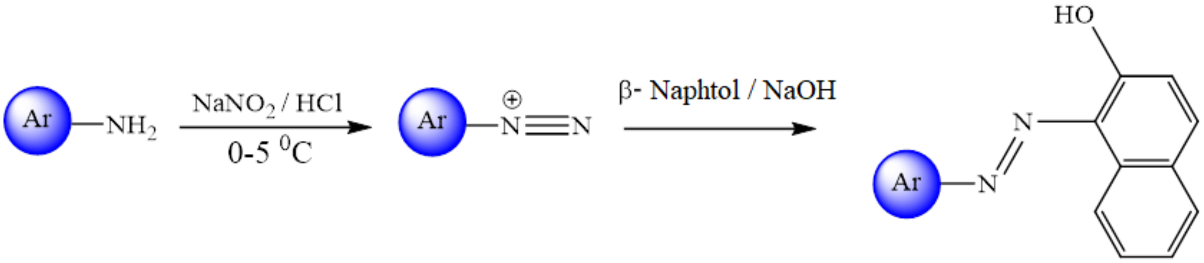


Figure 1. Synthesis of azo dyes

[1] Basutkar, M.R., Review – A History and Introduction of synthetic dye and their usage. International Journal of Life Sciences Research, vol. 7, 2 (2019), 396:406.
[2] Mezgebe, K., Mulugeta, E., Synthesis and pharmacological activities of azo dyes derivatives incorporating heterocyclic scaffolds: a review. RSC Advances, 12 (2022), 25932:25946.

Flavored Tofu Obtaining Process

Mihai-Constantin Covaci[1], **Adrian-Mihai Militaru**[1], **Ana-Maria Brezoiu**[2]

National University of Science and Technology POLITEHNICA Bucharest
[1]Faculty of Biotechnical Systems Engineering, Spl. Independentei 313, District 6, Bucharest, Romania
[2]Faculty of Chemical Engineering and Biotechnologies, Department of Chemical and Biochemical Engineering, 1-7 Gh. Polizu Street, District 1, Bucharest, Romania.

Plant based products represent a great option for people that have lactose or gluten intolerances and they can be good protein substitutes in a plant-based diet, due to their high amounts of nutrients (proteins, vitamins or mineral)[1].

Nowadays, there are several vegan products options compared to a decade ago, but in the flavored tofu domain not many options are commercially available. Therefore, the purpose of this study was to prepare tofu and further to improve its sensorial properties through the addition of different dried vegetables or plant, flavors that are not commercially available.

As flavors enhancers were used fresh vegetables that were dried at a constant temperature (45 °C and 60 °C respectively) until dry mass. Then the vegetables were grinded into a fine powder to be easier to use in the flavored tofu.

To obtain the tofu, the soybeans were soaked in water overnight, then were drained and blended with water (solid-liquid ratio=2.25 g/mL). To alleviate the bean-like smell characteristic to soy-products, the mixture was boiled for set time. Afterwards, the mixture was cooled and filtered to obtain soy-beverage as the milk substitute and Okhara. The tofu was prepared from soy-beverage after adding a coagulant. In this direction several magnesium and calcium salts were tested, and one was chosen based on the tofu taste.

For flavored tofu preparation, were tried different vegetables, in different amounts in order to cover the tofu characteristic taste that original has a bitter note and the final results showed the market potential of these products having improved texture color, smell and taste.

[1] Qin, P., Wang, T., Luo, W. A review on plant-based proteins from soybean: Health benefits and soy product development, J. Agric. Food Res. 2022, 7, 100265.

Electrochemical Determination of Sodium Diclofenac in Pharmaceutical Preparations

Ioana-Sorana Dibluș, Daniela Bala

University of Bucharest, Faculty of Chemistry, Department of Analytical Chemistry and Physical Chemistry, 4-12 Regina Elisabeta Blvd., 030018 Bucharest, Romania

Sodium diclofenac (DS) is a nonsteroidal anti-inflammatory drug widely used to treat mild to moderate pain. It is effective in relieving symptoms associated with arthritis—such as osteoarthritis and rheumatoid arthritis—including inflammation, swelling, stiffness, and joint pain[1]. Over time, various techniques have been employed for the determination of diclofenac, including potentiometry, capillary zone electrophoresis, high-performance liquid chromatography (HPLC and HPLC–MS), gas chromatography, and spectroscopic methods[2].

The electrochemical oxidation and determination of diclofenac sodium (DS) at glassy carbon electrode was evaluated for an alternative of quantitative determination of this compound in aqueous solutions. For this purpose, cyclic and differential pulse voltammetry were used to characterize the redox behaviour of sodium diclofenac in solution. Therefore, 1 mM DS was dissolved in Britton-Robinson buffer solutions with different pH values ranging from 3.0 to 11.0. The highest oxidation peak was observed at pH 7.00, making it the optimal condition for further electrochemical experiments. Hence, all subsequent analyses for determining DS in standard solutions and various pharmaceutical formulations were conducted at this pH.

[1] Altman R., Bosch B., Brune K., Patrignani P., Young C. Advances in NSAID development: evolution of diclofenac products using pharmaceutical technology. Drugs. 2015 May;75(8):859-77.

[2] Bilal Yilmazn, Ulvihan Ciltas, Determination of diclofenac in pharmaceutical preparations by voltammetry and gas chromatography methods. Journal of Pharmaceutical Analysis 2015;5(3):153-160

Inulin Extraction from *Jerusalem Artichoke*

Sabrina Duda, Roxana Oancea, Ana-Maria Brezoiu

National University of Science and Technology POLITEHNICA Bucharest, Faculty of Chemical Engineering and Biotechnologies, Department of Chemical and Biochemical Engineering, 1-7 Gh. Polizu Street, District 1, Bucharest, Romania.

There is currently an increasing interest in obtaining inulin for its multiple applications in various areas, such as biofuel production (bioethanol and hydrogen), emulsion gels development or its use as a food ingredient due to its prebiotic properties. Inulin is a water-soluble polysaccharide connected by β-(2,1) linkages of D-fructose bonds and terminated with a glucose residue through a sucrose-type linkage at a reducing end[1].

The purpose of this study is to determine the influence of different extraction parameters – particle size, extraction time, and raw material physical form (fresh or dried) - on obtaining higher yields of inulin from *Jerusalem artichoke* tubers using a conventional method (hot water extraction).

The experimental procedure consisted of an initial phase of cleaning and grating the tubers, from which a part was kept pristine, and another was subjected to drying experiments at set temperature to investigate the drying kinetics. Further, eight experiments were performed for inulin hot water extraction as considered through the experimental design. After the extraction time, the solids were filtered off, and the extract was characterized through rheological measurements and an analysis of total solids content. Afterwards, the extracts were dried until constant mass in an oven for inulin yield determination and then redissolved in water and isolated through alcohol precipitation.

The obtained results proved that *Jerusalem artichoke* is an alternative and valuable source of inulin for the food industry as well as for other areas of interest, using cheap raw materials and simple isolation techniques as well as offering high extraction yields.

[1] X. Zhang, X. Zhu, X. Shi, Y. Hou, and Y. Yi, "Extraction and Purification of Inulin from Jerusalem Artichoke with Response Surface Method and Ion Exchange Resins," *ACS Omega*, vol. 7, no. 14, pp. 12048–12055, Apr. 2022, doi: 10.1021/acsomega.2c00302.

Determination of Collagen Secondary Structure Using Infrared Molecular Absorption Spectroscopy

Daria Hălean, **Ioana Stănculescu**

Faculty of Chemistry, University of Bucharest, 4-12 Regina Elisabeta Bd, Bucharest, 030018 Romania

Collagen is one of the most studied proteins due to its widespread use in numerous fields, such as medical, cosmetic and food. This protein plays an essential role in maintaining the structural integrity of connective tissues and is involved in complex physiological processes such as skin regeneration, wound healing, maintaining the elasticity and strength of bones, tendons and ligaments.

In this work, the secondary structure of collagen from different industrial and food gelatin samples was determined by using Fourier Transform Infrared spectroscopy (FTIR). Collagen can exhibit one or more secondary structures along its polypeptide chain, which directly influence the functional properties of the protein. The main collagen secondary structures are: α-helix, β-sheet, β-turns and random coil.

FTIR spectroscopy allows the analysis of the chemical and structural composition of proteins by identifying the characteristic vibrational bands like Amide I, II and III. The secondary structure of collagen gelatin samples was obtained by Amide III band deconvolution. The variation of collagen secondary structure pourcentages was correlated with the gelatin type.

The Effect of Asplenium Ceterach Extracts on Saccharomyces Cerevisiae Cells

Marin Ovidiu-Cristian

University of Bucharest, Faculty of Chemistry, Bulevardul Regina Elisabeta 4-12, Bucharest, 030018, Romania

Every living organism is, in some way, exposed to environmental factors that can affect it, either positively or negatively. To minimize the negative impact, every species alive today has found a way to adapt to factors that would otherwise have adverse effects.

Asplenium ceterach is a plant used as a medicinal herb. Also known as the rustyback fern, it has been used traditionally to treat many different problems, such as hemorrhoids, kidney stones, hypertension, and spleen issues.

In eukaryotic cells, the fern extract is believed to mitigate the harmful effects of highly reactive oxidative species produced during cell death, likely due to its high content of antioxidant compounds such as caffeic acid, chlorogenic acid, and other phenolic substances.

Saccharomyces cerevisiae serves as an essential model organism in certain domains, such as genetics, cellular, and molecular biology, owing to several key features: its rapid growth rate, the easy-to-manage and well-characterized genome, and minimal growth requirements. In this study, we utilized extracts of the *Asplenium ceterach* herb prepared in various solvents to investigate their antioxidant potential. The *Saccharomyces cerevisiae* cells were treated with extracts and then subjected to oxidative stress by adding hydrogen peroxide to the growth medium. The following tests were conducted to determine the maximum concentrations of the solvents used in the extracts that could be present in the liquid medium without adversely affecting cell growth, thereby ruling out any potential cytotoxic effects of the solvents during the experiments.

The Folin–Ciocalteu reagent was used to assess whether the *Saccharomyces cerevisiae* cells absorbed components of the *Asplenium ceterach* extract, with a specific focus on detecting the presence of caffeic and chlorogenic acids.

Synthesis of Tricarboxylated Compounds Using Suzuki-Miyaura Coupling

Silvia Mato, Diandra Gheorghe, Nicoleta Sandu, Codruța Popescu, Mihaela Matache

University of Bucharest, Faculty of Chemistry, 90 Panduri Street, RO-050663 Bucharest, Romania.

Cross-coupling reactions represent an important method used in organic synthesis that generally involve combination of an organometallic reagent with an organic electrophile in presence of transitional metal catalysts to form new C-C bonds.[1]

The Suzuki-Miyaura coupling – a palladium-catalyzed reaction between organoboron compounds and organic halides or triflates – is such an example of great importance for new C-C bond formation due to a number of advantages, for instance the reagents' availability, mild reaction conditions, non-toxic inorganic by-product and much more.[2,3]

In this context we present synthesis of tricarboxylated compounds starting from commercial phenols via three steps: Duff formylation, oxidation and Suzuki-Miyaura coupling.

[1] Nolan, S.P., Navarro, O., C-C Bond Formation by Cross-Coupling. Comprehensive Organometallic Chemistry III, 11 (2007) 1:37.

[2] Campeau, L.C., Hazari, N., Cross-Coupling and Related Reactions: Connecting Past Success to the Development of New Reactions for the Future. Organometallics, 38 (2019) 3:35.

[3] Bogdan, E., Hădade, N.D., Socaci, C., Terec, A., Coupling Reactions in Organic Chemistry – From Theory to Applications, Presa Universitară Clujeană, 2013, Chapter 2. Suzuki-Miyaura Coupling Reaction, pgs. 13-67

Curcumin: UV-Vis Profile – pH Influence and Quantitative Assay

Alexandra Minea, **Iulia-Gabriela David**

University of Bucharest, Faculty of Chemistry, Department of Analytical Chemistry and Physical Chemistry, 90-92 Panduri Av., Bucharest, Romania

Curcumin, the main bioactive compund in the rhizomes of turmeric, also named Curcuma Longa, exhibits remarkable physicochemical and biological properties, making it a subject of significant interest for pharmaceutical and therapeutic applications[1].

In this study, curcumin spectrophotometric profile was investigated at different pH values, and applying the optimum analysis conditions, its content from a commercial dietary supplement (Curcumin 95) was quantitatively determined. The UV-Vis absorption spectra revealed a proeminent maximum in the range 425 nm – 475 nm with shifts in intensity depending on pH values. Curcumin spectra family recorded in Britton-Robinson buffer solutions with different pH values and in media with various NaOH concentrations, respectively, presented an isosbestic point, which enabled the calculation of $pKa = 10.95 \pm 0.6$.[1] This value is in accordance with those reported in the literature for the deprotonation of the phenolic -OH groups. The influence of NaOH concentration on curcumin stability and aborbance was also evaluated. Absorption was highest in 0.05 M NaOH solution, indicating these as optimal conditions for maintaining a stable form and a reliable detection of curcumin. At higher concentrations, a decrease in absorbance suggested partial degradation of curcumin. The absorbance of curcumin solutions in 0.05 M NaOH medium varied linearly with the analyte concentration in the range 1×10^{-6} - 2×10^{-5} M. Recovery tests, using standard addition method on ethanolic extracts of Curcumin 95 capsules, yielded a good percentage recovery (98,60%), highlighting the method's reliability and effectiveness for quantifying curcumin in complex matrices.

[1] David, I.G.; Iorgulescu, E.E.; Popa, D.E.; Buleandra, M.; Cheregi, M.C.; Noor, H. Antioxidants 2023, 12, 1908.

Quince Wine Production Process. From Laboratory-Scale Production to the Industrial Manufacturing Potential

Adrian-Marian Mitrică, Florin-Cristian Tănase, Ana-Maria Brezoiu

National University of Science and Technology POLITEHNICA Bucharest,
Faculty of Chemical Engineering and Biotechnologies, 1-7 Gh. Polizu Street,
District 1, Bucharest, Romania.

Lately an increased interest in producing fruit wines was shown probably due to the different sensory attributes, properties and a various scale of taste, alcohol content as well as appearance[1]. However, quince wine is not so well explored in scientific literature, only a few research papers focus either on the production of this type of fruit wine, different analysis on the few comercial available quince wines or utilizing the quince residue as biocatalysts.

The purpose of this study is to prepare quince wines from two different variety (a commercial one from Turkey, and a bio- variety from Romania) using both fresh fruit and frozen quince as raw materials. The wines were further analyzed regarding their alcohol content, total soluble solids, as well as sensory analysis.

The experimental procedure consisted of an initial phase of cleaning, peeling and grating the fruits, from which a part was used directly in the vinification process, and another part was kept at -20 °C until use. The quince wine must was prepared using the juice resulted after boiling fresh or frozen quince materials in water, sugar and wine yeast (*S. cerevisiae var. bayan*). Quince wines were subjected to a primary fermentation (10 days) followed by a secondary fermentation period of about 6 weeks. During this process, CO_2 release was monitored and from this sugar consumption as well as ethanol production were determined. To compare the obtained results, a wine without added sugar, from the comercial quince fruits was also prepared.

After the fruit wine maturation, a sensory analysis was carried out, followed by a survey to gather the tasters' opinions about the prepared wines and their commercial potential.

Also, a process flow and a technological scheme were designed to show the possibility of a scale up production from laboratory to industrial level.

[1] He, L.; Yan, Y.; Wu, M.; Ke, L. Advances in the Quality Improvement of Fruit Wines: A Review. Horticulturae 2024, 10, 93. https://doi.org/10.3390/horticulturae10010093.

Experimental Determination of Excess Volumes for the Binary Mixtures of DMF-Chloroform and DMF-Carbon Tetrachloride

Andreea-Denisa Nagodă, **Elena Pincu**

University of Bucharest, Faculty of Chemistry, Bulevardul Regina Elisabeta 4-12, Bucharest, 030018, Romania

Binary mixtures represent the combination of two different compounds, resulting in a new homogeneous solution. The study of non-ideal behavior in binary liquid mixtures is essential towards understanding the interactions between molecules and even developing chemical applications. In this work, it is determined the excess molar volumes for the binary mixtures of dimethylformamide (DMF) and chloroform, and also, DMF and carbon tetrachloride.

These specific solvents were chosen based on how commonly they are used in the chemical field, as DMF is considered to be a high polar compound, also known as a "super solvent" and chloroform, carbon tetrachloride are predominantly non-polar solvents.

The data were obtained using a high-precision 10 mL pycnometer, which was utilized to obtain the density of solutions with different compositions. The experimental data were used to calculate the excess molar volumes and for developing the graphical dependence between the molar fraction specific to DMF and the excess volume. Furthermore, the partial molar volumes were obtained.

As a result, comparing the two systems, considering that chloroform and carbon tetrachloride have few structural differences between them, it is observed that both of these systems obtained negative excess molar volumes, which suggests that the forces of attractions between the molecules are stronger than the pure components. The graph for the DMF-carbon tetrachloride system shows an exponential decrease until it reaches a minimum point, where $x_{DMF}=0.5402$, after which it increases until $x_{DMF}=1$, therefore implying that the strongest forces of attraction between the two substances appeared when there was the smallest difference between their quantities. On the other hand, the graph for the DMF-chloroform system presents almost instantly a minimum point at $x_{DMF}=0.7107$, followed by a slowly increase until $x_{DMF}=1$, which suggests that a significantly small amount of DMF combined with almost triple the amount of chloroform exhibits the strongest attractive forces.

Synthesis of Hydrazides and Aldehydes „Building Blocks” for Covalent Organic Frameworks Adsorbent Materials Used in Quality Air Control

Bianca-Andreea Paltin, Codruța Popescu, Mihaela Florea,
Mihaela Matache

University of Bucharest, Faculty of Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, RO-050663 Bucharest, Romania;

Clean air is essential for clearing and ventilating interior spaces, but the operations involved in processing it consume a large amount of energy. Thus, there is an urgent need to develop energy-saving air conditioning technologies that manage fresh air more efficiently[1]. Covalent organic frameworks are porous adsorbent materials with large specific surface areas, high thermal stability, well defined and ordered structures. They show great potential for the photocatalytic removal of VOCs (volatile organic compounds), which are pollutants with very high vapor pressures[2].

Herein we present the syntheses of a functionalized dihydrazide, trihydrazide and aldehyde as precursors (Figure 1) in obtaining *COFs*. Synthesis of the target compound began with formylation of p-hydroxybenzoic acid. The resulted aldehyde was subjected to oxidation and the carboxylic acid was subsequently esterified. Lastly, the ester was reacted with hydrazine hydrate in different amounts to obtain the hydrazides of interest. All compounds were obtained in good yields, without requiring additional purification processes and were characterized by physical (melting point, solubility, retention factor) and spectral (^{1}H- NMR, ^{13}C-NMR) analysis.

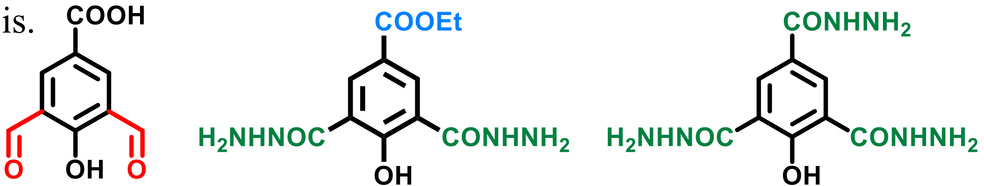


Figure1.Target compounds

[1] Yang, F., Ma, J., Chen, L. Study of the CO2 Adsorption Performance of a Metal Organic Frameworks: Applications in Air Conditioning, ChemistrySelect 2023, 8 (20), e202203314.

[2] Deng, M., Sun, J., Van Der Voort, P., Chakraborty, J., Zhou, M. From Design to Applications: A Comprehensive Review on Porous Frameworks for Photocatalytic Volatile Organic Compounds (VOCs) Removal, ChemCatChem 2024, 16, e202300783

Synthesis and Stabilization of Magnetite Nanoparticles via Co-precipitation Method

Rodeanu Dragoș[1], **Laura Mădălina Cursaru**[2], **Anca Monica Tencaliec**[1]

[1]Faculty of chemistry, University of Bucharest, Bulevardul Regina Elisabeta, București 030018,
[2]National Institute for Research and Development for Non-Ferrous and Rare Metals - I M N R, B-dul Biruinței 178-184 Pantelimon, jud ILFOV, 077145, Romania.

Magnetite (Fe_3O_4) nanoparticles were synthesized via a co-precipitation method using iron(II) chloride ($FeCl_2$) and iron(III) chloride ($FeCl_3$) as precursors. The reaction was performed at 25°C under vigorous stirring, with ammonia used as the precipitating agent. A 1.7:1 molar ratio of Fe^{3+} to Fe^{2+} was maintained to favor the formation of pure magnetite. The pH was controlled throughout to ensure proper nucleation and growth.

To stabilize the nanoparticles and prevent agglomeration, oleic acid was added post-synthesis, acting as a surfactant. The resulting black powder displayed strong magnetic response and good dispersion stability in nonpolar solvents.

Preliminary results suggest that this synthesis route offers higher purity than some commercial alternatives. From the obtained powders, a ferrofluid will be prepared using kerosene. Additionally, a hydrothermal synthesis will be explored before the final the presentation to improve crystallinity and uniformity.

This study confirms the efficiency of co-precipitation as a simple and scalable route for magnetite nanoparticle production, with potential for further functionalization and applications.

Biocatalytic Method for Derivatization of Aspirin

Țîrdia Iosif – Ionatan, **Mădălina Săndulescu**

Universitatea din București, Facultatea de Chimie
B-dul Regina Elisabeta Nr. 4-12, Sector 3, București – 030018 România

Today, green chemistry is one of the important aspect of advanced chemistry looking specifically to eliminate the chemical pollution by reducing the reaction waste, the energy consumption and replacing potentially toxic reagents used in most syntheses. In this context, biocatalysis is a promissing alternative. Additionally, biocatalysis has made great progress in the medical and pharmaceutical fields by creating more efficient, sustainable and greener alternatives to the classical organic synthesis of drugs, , and opened up new opportunities to recycle unwanted by-products of reactions. The development of the biocatalysts design, especially enzyme biocatalysts, allowed to set up new sustainable processes, either in aqueous or organic environments, so that both water/oil-soluble compounds can be redesigned with high efficiency and selectivity.

We proposed a biocatalytic alternative for acetyl-salicylic acid, also known as aspirin, derivatization using both menthol and fatty acid esters in order to improve the modulate the therapeutic effect of aspirin.. Therefore, lipase enzyme was used as biocatalyst assisting the aspirin derivatization with both menthol and fatty acid esters based on esterification/transesterification reaction. The experiments were performed testing acetyl-salicylic acid (ASA) and salicylic acid (SA) as substrates, and methyl laurate (ML), methyl valerate (MV), methyl decanoate (MD), methyl palmitate (MP) as reagents. Novozym 435 (N435), a commercial immobilized enzyme of *Candida antarctica lipase B*, was the enzyme biocatalyst. The biocatalytic system was evaluated for different solvents , e.g. dimethylformamide (DMF), dimethyl sulfoxide (DMSO), tetrahydrofuran (THF) and 1,4-dioxane in order to set up optimum experimental conditions. The performance of the biocatalytic process was evaluated based on substrate conversion after HPLC analysis of the reacted mixture. The experimental results will be presented during the lecture.

Spectrophotometric Determination of Salivary Cortisol Levels

Vlad Ionut Vitelaru[1], **Radu Gabriel Hertzog**[2], **Ileana Cornelia Farcasanu**[1], **Claudia Valentina Popa**[1]

[1]Faculty of Chemistry, University of Bucharest, Sos. Panduri 90-92, 050657, Bucharest, Romania
[2]Micro Science SRL, Narciselor 1, Craiova, Dolj, Romania

Cortisol is a glucocorticoid hormone, secreted by the adrenal cortex. It is the major stress hormone in humans and an important biomarker for detection and monitoring of mental illnesses evolution.

The aim of the study is to determine the cortisol levels in saliva samples by two spectrophotometric methods, using as the colorimetric indicator dyes: Prussian blue and blue tetrazolium (BT), respectively.

The following parameters have been optimized: concentration of reagents, temperature and reaction time, solvent nature. Absorbance calibration curves were obtained as a function of cortisol concentration with good correlation coefficients ($r^2 > 0.99$). Cortisol concentrations (expressed in µg/mL and nmol/L) were determined from saliva samples collected from human volunteers and comparisons between the results obtained by the two methods and values reported in the literature were made. The method with Prussian blue dye allows for cortisol determination within 0.5 – 10 µg/mL domains of cortisol, and with a relative standard deviation (RSD) = 9.1% (n= 10) when cortisol concentration is 10 µg/mL. The second method allows for hormone determination within 0.2 – 1 µg/mL of cortisol domain, and with a RSD = 0.75 % (n = 10) for 1 µg/mL cortisol concentration. The cortisol levels in the analyzed saliva samples ranged between 64.8 ± 6.5 and 200 ± 20 nmol/L by the first method and between 25.7 ± 2.6 and 46.1 ± 4.5 nmol/L by method with BT dye.

The method using BT pigment is more sensitive method than method with Prussian blue dye for the measurement of salivary cortisol.

From Biowastes to Fuel Components

<u>Marius Marciuca. Sofia Oleinic</u>, Marian Băjan, Cristina Dușescu-Vasile

Universitatea Petrol – Gaze din Ploiești, Bulevardul București 39, Ploiești

European fuel regulations mandate the inclusion of biocomponents in automotive fuels, requiring up to 7% in diesel and 5% in gasoline. Despite this, Romania relies heavily on biofuel imports, with approximately 40% of biodiesel and 70% of bioethanol sourced externally. This dependency underscores the need for innovative domestic biofuel production solutions.

Using Phragmites australis, a fast-growing perennial plant commonly found in wetlands, can significantly enhance renewable energy production. The plant's energy potential is boosted by its lignin content (15–25%), which provides a calorific value of approximately 15–17 MJ/kg—higher than that of many traditional biomass sources. Moreover, the absence of nitrogen and sulfur in this biomass helps prevent the formation of pollutant compounds during combustion or pyrolysis processes.

This paper evaluates the potential of utilizing the liquid fraction produced from the slow pyrolysis of this type of biomass as an ingredient in heating fuels. The raw material underwent mechanical conditioning processes and was characterized using specific methods. The study analyzes the relationship between the size of the raw material particles and the efficiency of the slow pyrolysis process, as well as the properties of the resulting bio-oils, particularly their compatibility with petroleum products. The experimental results obtained in the laboratory support the feasibility of blending these bio-oils with diesel and residual petroleum products.

The Synthesis of Cholesteryl Esters as Intermediates in the Transport and Storage of Cholesterol

Ciolan Tudor-Alexandru, Codruța Popescu

University of Bucharest, Faculty of Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, RO-050663 Bucharest, Romania;

Cholesterides are fatty acid esters and they play a major role in the transport and storage of cholesterol, as well as in lipid metabolism. The synthesis of such cholesterol derivates allows a controlled and detailed study of these compounds in the matter of cell-biology.

The aim of this study is to synthesize a certain type of cholesterol ester, using as an electrophile partner a double unsaturated fatty acid, such as linoleic acid. The choice of this acid was made based on studies that show metabolic activity of this ester in the receptor-dependent hydrolysis of cholesteryl esters contained in plasma low density lipoprotein (LDL).[1]

A first attempt was made to synthesize the ester starting from cholesterol and linoleoyl chloride, focusing on the purification methods of the linoleic acid, the acyl chloride formation and separation as well as the esterification reaction. The product obtained in this case (cholesteryl linoleate) has a higher hydrophobicity thus it is more soluble in cell-membrane. We then optimized the reaction conditions and purification methods so we can replicate the synthesis using 19-ethynylcholesterol[2] as a starting material. The product obtained (19-ethynylcholesterol linoleate) has the advantage of the triple bond found in the 19th position of the sterane ring, which allows the possibility of attaching a fluorophore via a Click Reaction to facilitate a better observation of cellular processes.[2]

Therefore, we want to emphasise that studying cholesteryl esters in cell-membrane and their metabolism requries a close attention of their laboratory synthesis, optimizing reaction conditions along with elaborating adequate purification methods.

---

[1] Brown, M.S., Dana S.E., Goldstein, J.L., Receptor-dependent hydrolysis of cholesteryl esters contained in plasma low density lipoprotein. Proc. Nat. Acad. Sci. USA. 72, 8 (1975) 2925:2929;

[2] Jao, C.Y., Nedelcu, D., Lopez, L.V., Samarakoon, T.N., Welti, R., Salic, A., Bioorthogonal Probes for Imaging Sterols in Cells, ChemBioChem, 16, 4, (2015), 611:617

Section 2

Master
Level

Display of Metallothionein and Metallothionein Cys-containing Peptides on the Surface of Yeast Cells

Andrei Bărboi[1],**Livia Ciobanu**[2]

[1]Department of Inorganic&Organic Chemistry, Biochemistry and Catalysis,
Faculty of Chemistry, University of Bucharest
[2]Interdisciplinary School of Doctoral Studies, University of Bucharest

Conventional chemical synthesis of large peptides can be both time-consuming and extremely expensive. A widely used and much more feasible alternative is employing biological systems (phages, bacteria, yeast cells, or other organisms) for the biosynthesis of a large variety of peptides.

In this study, we used yeast cell surface display (YSD) to induce the expression of metallothionein-derived chimeric peptides featuring redox-active cysteine residues on the surface of *Saccharomyces cerevisiae* cells.

The vector we used for the expression of the target peptides was pYD1, which utilizes the Aga1p-Aga2p system as a protein anchor for the cell wall display. Using recombinant DNA technology, we inserted the DNA sequence of the fungal metallothionein *CUP1* and several cysteine-rich subsections of this gene into the shuttle vector. To monitor the recombinant gene expression, we fused each peptide of interest with the green fluorescent protein (GFP) by incorporating its coding DNA sequence into the insert.

The primary function of the fungal metallothionein Cup1p is to mediate the cellular response to metal ion exposure, binding these ions through its cysteine-rich domains. By displaying these redox-active peptides, we aim to investigate their capacity for reducing selenite ions to elemental selenium and their impact on cellular resistance to selenite ions.

The Effect of ABC Transporters Deletion on Xenobiotic Accumulation

Alexandra Cârlan, **Antonio Lucian Miu**

Department of Inorganic&Organic Chemistry, Biochemistry and Catalysis,
Faculty of Chemistry, University of Bucharest, Sos. Panduri 90-92, Bucharest
050663, Romania

ABC (ATP-binding cassette) transporters are one of the largest protein superfamilies, present in all living organisms, with a highly conserved nucleotide binding domain that facilitates the active import and export of allocrites through the cellular membrane.

This study evaluates the effect of ABC efflux pump deletion on accumulation of various compounds in *Saccharomyces cerevisiae* cells.

S. cerevisiae BY4741 (wild type, WT) and isogenic strains with individual deletion of efflux pumps (*Δsnq2, Δpdr5, Δpdr15*) or of efflux pump regulators (*Δpdr, Δpdr8*) were cultured in liquid and solid media in the presence of various xenobiotics (rhodamine B, caffeine, colchicine, bleomycin, triazole and oxazole derivatives).

Accumulation of rhodamine B (a known substrate of ABC transporters) was impaired in all mutant strains compared to the wild type. Efflux of rhodamine B from the wild type was decreased in the presence of caffeine, another known allocrite of ABC transporters.

Colchicine presented little citotoxicity, with a slight increase in this effect in some mutant strains.

Bleomycin (a cytotoxic chemotherapeutic drug) showed increased citotoxicity in the *Δsnq2* and *Δpdr5* strains, its effect being potentiated by a series of triazole and oxazole derivatives.

Efflux of xenobiotics by ABC transporters is an important mechanism of drug resistance in fungi, bacteria, and malignant cells. The investigation of this process in a model organism is a step forward in developing better clinical alternatives.

Paramagnetic Ligands with Nitronyl-nitroxide Moieties Attached by Alkylation Reactions and Their Coordination Compounds

Ștefan Dimitriu,[1,2] **Mihai Răducă**[1,2], **Marius Andruh**[1,2]

[1]University of Bucharest, Faculty of Chemistry, Regina Elisabeta Blvd.
4-12, Bucharest, Romania
[2]"C. D. Nenitzescu" Institute of Organic and Supramolecular Chemistry,
Splaiul Independenței nr. 202B, Bucharest, Romania

Coordination compounds with nitronyl-nitroxides ligans have been intensively studied because of their interesting magnetic behaviors that arise from the interaction between different spin carriers. Despite the variety of such ligands reported in the literature, the wide majority of them have been obtained through the synthesis of the radical unit starting from formyl-bearing substrates. However, the radical unit can also be grafted onto a substrate through alkylation reactions involving 2-(chloromethyl)-nitronyl-nitroxide (Figure 1a). This approach brings advantages, including higher yields and simpler synthetic procedure, but it also allows the design of more flexible ligands. In this work, our first results concerning this promising research topic are presented. The study of the coordination chemistry of 2-(chloromethyl)-nitronyl-nitroxide and a ligand obtained through the alkylation of morpholine yielded a Ni(II) dinuclear complex (Figure 1b), and a Ni(II) mononuclear complex (Figure 1c), respectively. The structures of the coordination compounds, as well as the one for the alkylation agent, have been solved using single crystal X-ray diffraction. Several novel ligands have also been obtained through N-alkylation and C-alkylation and confirmed by mass spectrometry. The use of these new radicals as ligands and the characterization of the corresponding complexes is work in progress.

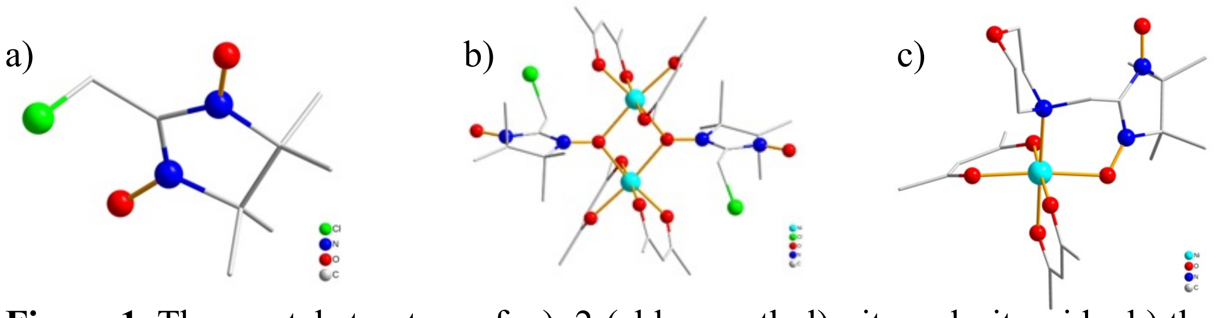


Figure 1. The crystal structure of: a) 2-(chloromethyl)-nitronyl-nitroxide; b) the Ni(II) complex of 2-(chloromethyl)-nitronyl-nitroxide; c) the Ni(II) complex of alkylated morpholine. The hydrogen and fluorine atoms have been omitted for clarity.

Polytriazole-Based Chelating Ligands for Accelerating Copper-Catalyzed ”Click” Reactions

Andrada Eremia[1,*], **Anamaria Hanganu**[1,2], **Codruța Popescu**[1],
Anca Păun[1], **Mihaela Matache**[1], **Adrian Șalic**[3,*]

[1]University of Bucharest, Faculty of Chemistry, Department of Inorganic, Organic Chemistry, Biochemistry and Catalysis, 90 Panduri Street, 050657 Bucharest, Romania;
[2]Institute of Organic and Supramolecular Chemistry “C. D. Nenitzescu” of the Romanian Academy, 202B Spl. Independenței, 060023 Bucharest, Romania;
[3]Harvard Medical School, Dept. of Cell Biology, LHRRB 401A, 240 Longwood Avenue, Boston MA, 02115, Boston, USA.

The copper(I)-catalyzed azide-alkyne cycloaddition (CuAAC), often called the “click” reaction, is a highly efficient method for covalently linking two molecules, resulting in the regioselective formation of a 1,4-disubstituted 1,2,3-triazole[1]. Azide and terminal alkyne groups can be easily introduced into various biologically relevant molecules, enabling bioorthogonal coupling reactions[2]. CuAAC is typically catalyzed by copper(I) complexed with a suitable chelating ligand like polytriazoles (e.g., TBTA, THPTA), which protect Cu(I) from oxidation and thus enhance the reaction kinetics[3,4]. Interestingly, copper(II) acetate can also facilitate CuAAC reactions in the absence of reducing agent[5].

Herein, we describe the synthesis of several intermediates and novel triazole-based polydentate ligands, including the target compound, tris(2-(4-(((3-azidopropyl)amino)methyl)-1H-1,2,3-triazol-1-yl)ethyl)amine, a chelating azide designed for “click”-based fluorescent probes to monitor cellular processes via fluorescence microscopy. A new synthetic methodology is presented, along with the challenges encountered during both synthesis and purification, and the strategies used to overcome them. Structures were confirmed by ^{1}H-NMR, ^{13}C-NMR, and HRMS.

AKNOLEDGEMNTS: This work was supported by grant from the Romanian Ministry of Research, Innovation and Digitisation, PNRR/2022/C9/MCID/I8, project number CF 760056/23.05.2023, code 235/29.11.2022

[1] V. V. Rostovtsev, L. G. Green, V. V. Fokin, K. B. Sharpless, Angew. Chem. Int. Ed. 2002, 41(14), 2596.

[2] C.Y. Jao, D. Nedelcu, L.V. Lopez, T.N. Samarakoon, R. Welti, A. Șalic, ChemBioChem. 2015, 16(4), 611.

[3] V. O. Rodionov, S. I. Presolski, S. Gardinier, Y. H. Lim, M. G. Finn, J. Am. Chem. Soc. 2007, 129(42), 12696.

[4] G.C. Kuang, H.A. Michaels, J.T. Simmons, R.J. Clark, L. Zhu, J. Org. Chem. 2010, 75 (19), 6540.

[5] H.A. Michaels, L. Zhu, Chem. Asian J. 2011, 6(10), 2825.

Copper Complexes with Schiff Bases as Biologically Active Species

Grezi Bianca - Andreea, Badea Mihaela

University of Bucharest, Faculty of Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, 90-92 Panduri Av., District 5, Bucharest, Romania

Copper is an essential trace element involved in key physiological processes such as mitochondrial respiration, antioxidant defense, and cell proliferation. While tightly regulated, both copper deficiency and excess can disrupt cellular homeostasis. Recent advances highlight cuproptosis, a unique copper-dependent cell death pathway, as a promising strategy in cancer therapy. Copper complexes also exhibit antitumor activity through redox-driven ROS generation, DNA damage, and apoptosis, positioning copper-based agents as emerging tools in oncology[1].

The present work consists in the synthesis and characterization of four new Cu(II) complex combinations, using the two previously obtained starting materials (copper acrylate , $Cu(acr)_2 \cdot H_2O$ and copper methacrylate, $Cu(Macr)_2 \cdot H_2O$) and Schiff bases obtained from salicylaldehyde and 2-(2-aminoethyl)pyridine, (Salamepy) and respectively 2-(2-aminomethyl)pyridine, (Salampy). The characterization of these compounds is based on elemental analysis, FTIR spectroscopy, UV-Vis-NIR spectroscopy, and X-ray diffraction. Only two compounds, $[Cu(Salamepy)_2]$ and $[Cu(Salamepy)(Macr)] \cdot H_2O$, were obtained in single-crystalline form, their structure being determined by X-ray diffraction. It has been observed in the obtained compounds only methacrylate ion is found, acting as a chelated ligand.

Therefore, the compounds obtained from copper acrylate have the general formula $[Cu(L)_2]$ and those obtained from copper methacrylate have the general formula [Cu(L)(Macr)] (L = Schiff base ligand).

The complexes will be tested for both antimicrobial and antitumor activities.

[1] Wang, C., Yang, X., Dong, C., Chai, K., Ruan, J., Shi, S., Cu-related agents for cancer therapies. Coord. Chem. Rev., 487 (2023), 215156.

Development and Electrochemical Evaluation of Sensors for L-DOPA Detection

Darius Mirea, **Emilia-Elena Iorgulescu**

University of Bucharest, Faculty of Chemistry, Department of Analytical and Physical Chemistry, 90-92 Panduri Street, Bucharest-5, Romania

L-DOPA (l-3,4-dihydroxyphenylalanine), commonly known as levodopa, is an amino acid and a precursor of dopamine widely used in the treatment of Parkinson's disease[1]. Due to its electroactive nature, it can be effectively analyzed using electrochemical techniques which have some advantages offered by portable instrumentation and sensitive methods suitable for drug and biological sample analysis. Recent advances in electrode modification allow enhanced sensitivity, selectivity, and reliable quantification of levodopa at nanomolar concentrations, offering a powerful approach for pharmaceutical and clinical applications[2].

This study describes the electrochemical behavior and the quantitative determination of L-DOPA by cyclic voltammetry and differential pulse voltammetry, respectively, using different electrodes. Firstly, a series of carbon paste electrodes were developed using various carbon materials, including standard carbon powder, glassy carbon powder, and a composite modified with electrochemically reduced graphene oxide. The modified electrodes demonstrated enhanced sensitivity, with linear ranges reaching as low as 0.5 μM. Subsequently, pencil graphite electrodes were explored; both unmodified and a molecularly imprinted polymer (MIP) modified version were evaluated. The MIP modified electrode showed improved selectivity toward L-DOPA, highlighting its potential for application in complex biological matrices.

[1] Poewe, W., Mahlknecht, P., Pharmacologic Treatment of Motor Symptoms Associated with Parkinson Disease, Neurologic Clinics, 38(2) (2020), 255-267.

[2] Beitollahi, H., Safaei , M.,, Tajik, S., Electrochemical deduction of levodopa by utilizing modified electrodes: A review, Microchemical Journal 152 (2020), 104287.

Curcumin and Inulin Release from LDH Matrixes

Adina Georgiana Mușat, **Rodica Zăvoianu**

University of Bucharest, Faculty of Chemistry, Department of Inorganic and Organic Chemistry, Biochemistry and Catalysis, Bd. Regina Elisabeta No. 4-12, S3, 030018, Bucharest, Romania

This work is aimed to investigate the possibility of incorporating two biologically active compounds, e.g. curcumin (CR) extracted from Curcuma longa and inulin (I) extracted from chicory into layered double hydroxides (LDH) having ternary or quaternary composition of the brucite-type layer (Mg/Fe/Al; Mg/Ca/Fe; Mg/Ca/Fe/Al) and the in vitro release of these compounds from the inorganic matrix at pH 1.2 (simulating gastric pH) and pH 6.8 (simulating intestinal pH). Three CR-containing samples (e.g. RM4AF-CR, RMCF-CR and RM9CF4A-CR, where R = reconstruction, M, A, F and C are the first letters of the elements and the numbers represent the atomic ratio between elements in the LDH) were prepared using the reconstruction of the LDH structure using a solution of CR in ethanol-water mixture. It was found that the CR-retention is different depending on the cationic composition of the LDH. Al presence leads to the increase of the amount of incorporated CR while Ca presence hinders its retention. This fact may be explained by the chelation of Al and Fe by CR. The CR-release from RM4AF-CR (having the highest concentration of CR e.g. 10 wt.%) was slower at pH 1.2 and faster at pH 6.8. Six inulin (I) containing samples (M10F4A-I-NH3, M9CF5-I-NH3, M9CF4A-I-NH3, M10F4A-I-TMAH, M9CF5-I-TMAH, M9CF4A-I-TMAH were synthesized by the mechanochemical method using either NH_3 (25 wt. %) or TMAH as pH-adujsting agents. Inulin was better retained by the Al-free-LDH (M9CF5) since it can form chelates with Fe, Ca and Mg. When TMAH was used, the yield of the syntheses increased but the concentrations of retained inulin were 5-up to 9% lower. The highest I-concentration (27 wt.%) was reached for M9CF5-I-NH3. This sample released 50% of the incorporated inulin after 2 h at pH 1.2 followed by 2 h at pH 6.8.

The obtained results showed that both curcumin and inulin could be retained by LDH matrixes and the retained concentration depended on the cationic composition of the LDH. Curcumin which has a poor water solubility could be retained in concentrations of maximum 10 wt.%, while inulin was retained in concentrations varying in the range of 15-27 wt.%. Both types of solids could be used for slow release of the biologically active compounds since only 50 % of the incorporated amount was released after 4 h.

MIP Modified Disposable Voltametric Sensor for Rifampicin Analysis

Daniela Partene, Iulia Gabriela David

University of Bucharest, Faculty of Chemistry, Department of Analytical Chemistry and Physical Chemistry, 90-92 Panduri Av., District 5, Bucharest, Romania.

Rifampicin (RIF) is a macrocylic antibiotic effective against *Mycobacterium tuberculosis*. It was the first drug used to treat tuberculosis and other bacterial infections like leprosy and some types of meningitis. Taking too much RIF can cause harmful side effects, including liver toxicity, dizziness, nausea, and rashes, and can lead to serious conditions like anorexia, seizures, and kidney failure. RIF works by blocking bacterial RNA polymerase, which is vital for bacteria to grow and survive. Therefore, it is important to develop sensitive methods to detect this drug's presence in various matrices[1].

This research aimed to investigate RIF electrochemistry by cyclic (CV) and differential pulse voltammetry (DPV) at a molecularly imprinted polymer pencil (MIP) modified graphite electrode (PGE). The polymerization medium, number of cycles, scanning rate, monomer and template concentration, extraction time were optimized. CV recordings emphasized a quasi-reversible redox process, mainly diffusion controlled. The influence of the solution pH on RIF DPV response showed that an equal number of protons and electrons were involved in RIF oxidation.

Under optimized conditions (0.1 mol/L HCl), DPV quantitative determinations of RIF presented a linear range from $1{,}00 \times 10^{-8}$ to $1{,}00 \times 10^{-7}$ M with detection and quantification limits of $2{,}00 \times 10^{-9}$ M RIF and $5{,}99 \times 10^{-9}$ M RIF, respectively. The repeatability of the RIF DPV response at MIP modified sensor, expressed as relative standard deviation (n=6) was assessed at two concentration levels situated within the linear range. The obtained values were within the accepted limits.

The applicability of the developed method was tested on pharmaceutical tablets. The mean recovery was 103.52 %

[1] Arumugam, J., Shanmugam, G., Venkatesan, M., Sreedhar, S., Synergistic activity of copper and molybdenum based organic frameworks for the exceptional electrochemical detection of rifampicin in commercial dairy products, *Microchem. J.*, 199 (2024), 110115.

Luminescent Molecular Materials Based on Chalcones

Valentin L. Virgil, **Augustin M. Mădălan**

Faculty of Chemistry, University of Bucharest

Chalcones are organic compounds classified as *α,β*-unsaturated ketones, characterized by a 1,3-diaryl-2-propen-1-one (chalconoid) moiety. They can exist as both *trans* and *cis* isomers, with the trans form being more thermodynamically stable. Over time, it has been proven that chalcones are notable for a variety of applications, including use as chemical intermediates, biologically active agents, and fluorescent materials. Their conjugated systems, when substituted with suitable electron-donating and electron-withdrawing groups on the aromatic rings, facilitate electron transfer, endowing them with fluorescent properties. Luminescent properties can also be enhanced by generating extended π conjugated systems. From this point of view, we synthesized chalcones by reacting 2-acetylpyridine with various aldehydes, including 9-anthracenecarboxaldehyde, 1-pyrenecarboxaldehyde and 2-naphthaldehyde. Using these ligands, we aim to obtain luminescent complex combinations targeting metal ions with emission properties in the VIS (Eu^{3+}, Tb^{3+}, Sm^{3+}) and NIR (Er^{3+}, Yb^{3+}, Nd^{3+}) regions (Fig. 1).

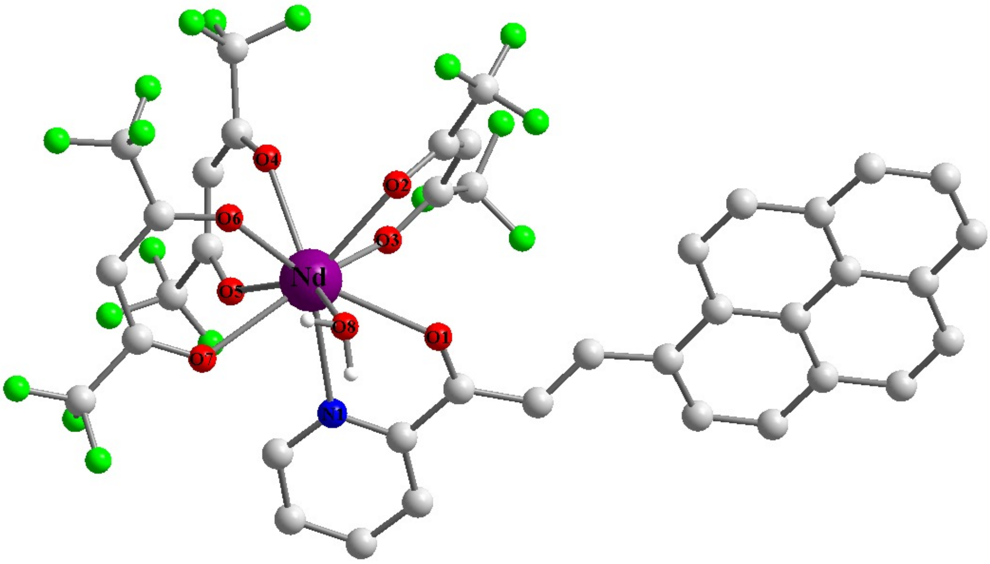


Fig. 1. Perspective view of the crystal structure of the complex $[Nd(L^2)(OH_2)(hfac)_3]$.
The hydrogen atoms were omitted for clarity.

[1] Zhuang, C.; Zhang, W.; Sheng, C.; Zhang, W.; Xing, C.; Miao, Z., Chem. Rev. 2017, 7762- 7810.

Section 3

PhD
Level

Mitigating Non-Specific Adsorption in the Development of Aptamer-based SERS Biosensors

Roberta Maria Banciu[a,b], **Alina Vasilescu**[b], **Monica Potara**[c],
Simion Astilean[c], **Camelia Bala**[a]

[a]*Department of Analytical and Physical Chemistry, University of Bucharest,*
4-12 Regina Elisabeta Blvd., Romania
[b]*International Centre of Biodynamics, Intrarea Portocalelor 1B, 060101,*
Bucharest, Romania
[c]*Nanobiophotonics and Laser Microspectroscopy Center, ICIBNS, Babeș-Bolyai*
University, T. Laurian Str. 42, 400271, Cluj-Napoca, Romania

Aptamers (APTs) are single-stranded DNA molecules capable of binding target analytes with high specificity. Coupling APTs with surface-enhanced Raman scattering (SERS) enhances detection sensitivity, but nonspecific adsorption (NSA) in complex samples like human serum remains a major challenge[1,2].

We explored APT-based SERS biosensors to improve the specific-to-nonspecific signal ratio in the direct detection of lysozyme (LYS) and matrix metalloproteinase 9 (MMP9). Gold-based SERS substrates were evaluated following APT immobilization, with NSA reduced using various surface blocking agents. Immobilization was confirmed by characteristic SERS peaks of adenine and Cyanine 3 (Cy3). The outcomes indicated that backfilling with 11-mercaptoundecanol SAMs effectively diminished NSA, yet simultaneously led to a significant reduction in LYS. In the case of the MMP9 aptasensor, blocking with BSA reduced surface fouling. Chemometric analysis of SERS spectra enabled the identification of key features associated with specific binding.

In conclusion, strategic surface modifications, such as BSA blocking, and advanced spectral data analysis techniques can significantly enhance the performance of APT-based SERS biosensors in complex biological environments.

Acknowledgements:
This work was financially supported by the UEFISCDI projects PN-III-P4-ID-PCE-2020-2297 E-MAP, and PN-III-P2-2.1-PED-2021-1998.

[1] R. M. Banciu, N. Numan, A. Vasilescu, J. Mol. Struct. 1250 (2022) 131639.
[2] M. J. Russo, M. Han, P.E. Descroches, C.S. Manasa, J. Dennaoui, A. F. Quigley, R. M. I. Kapsa, S. E. Moulton, R. M. Guijt, G. W. Greene, S. Moraes Silva, ACS Sensors 6(4) (2021) 1482-1507.

Rational Design and Synthesis of Zn(II) Complexes with Polydentate Schiff Base Ligands

Robert I. Botea, **Augustin M. Mădălan**

Faculty of Chemistry, University of Bucharest, Regina Elisabeta Blvd. 4-12, Bucharest – 030018, Romania

The development of polydentate imino and amino ligands has significantly advanced the design of Zn(II) coordination complexes. These ligands, derived from N-(1-naphthyl)ethylenediamine and various phenol aldehydes, feature multiple coordination sites that facilitate diverse structural arrangements and tunable physicochemical properties[1].

In this study, a series of novel Schiff base ligands were synthesized, utilizing N-(1-naphthyl)ethylenediamine and various phenol aldehydes. These imino ligands and the amino derivatives obtained by reduction were used either alone or in combination with other chelating ligands to generate both mono- and multinuclear complexes. Single-crystal X-ray diffraction was employed to structurally characterize the ligands and complexes, revealing the versatility of these imino and amino derivatives and showing the coordination geometries and organization of the complexes. Figure 1 shows the schematic synthesis of a Zn(II) complex using the aforementioned type of ligands.

Furthermore, the study analyzed the optical properties of the synthesized ligands and complexes in the solid-state through various types of spectroscopies. The luminescence properties of these complexes were of particular interest due to the extended π-systems of the ligands, which are capable of enhanced fluorescence emission.

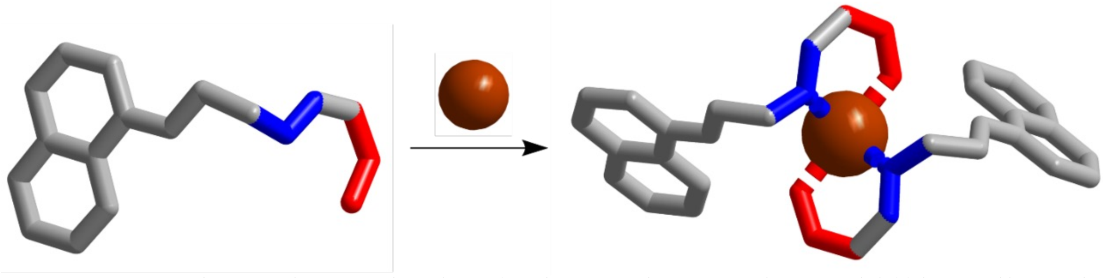


Figure 1. Schematic synthesis of 3d complexes using Schiff base ligands

Enzymatic Labeling of Aptamers Using a Novel Enzyme for Enhanced Bioassay and Biosensor Applications

Andreea Ftodiev[1], **Georgiana Necula Petrareanu**[3], **Cristina Purcarea**[3], **Alina Vasilescu**[2], **Camelia Bala**[1]

[1]Department of Analytical Chemistry and Physical Chemistry, University of Bucharest, 4-12 Regina Elisabeta Blvd, Bucharest, Romania
[2]International Centre of Biodynamics, Intrarea Portocalelor 1B, Bucharest, Romania
[3]Institute of Biology of the Romanian Academy, Splaiul Independentei, 296, Bucharest, Romania

Aptamer-based biosensors often employ catalytic labels such as enzymes, nanozymes, or DNAzymes to amplify detection signals [1]. In the search for novel enzyme tags with unique properties, we investigated a cold-active aldehyde dehydrogenase (F-ALDH) from the Antarctic bacterium Flavobacterium PL002 as a labeling agent for a lysozyme-specific DNA aptamer. The aim was to develop a sandwich-type biosensor on a microarray plate using a complex formed between histidine-tagged F-ALDH and a nickel–Nα, Nα-Bis(carboxymethyl)-L-lysine hydrate (Ni-NTA) surface. Lysozyme immobilized on the plate enabled specific binding of the aptamer–F–ALDH complex via target recognition. Successful conjugation was confirmed by UV absorbance at 260 and 280 nm. Enzymatic activity assays demonstrated effective binding of the complex to lysozyme, and control experiments confirmed that aptamer functionality was retained after labeling. These results support the use of cold-active F-ALDH as a novel enzymatic label in aptamer-based biosensors, particularly for applications requiring low-temperature conditions.

Acknowledgements:
This work was financially supported by the UEFISCDI project PN-III-P2-2.1-PED-2021-1998.

[1] A. Rhouati, J.-L. Marty, A. Vasilescu, Electrochimica Acta, 390, (2021) 138863.

[2] M. Mascini, in Aptamers in Bioanalysis, Wiley, Heidelberg (2009) 348 pages.

Synthesis of Novel Materials Based on N-acylhydrazone Motif

Nicoleta Sandu[a], **Mihaela Matache**[a]

[a] *University of Bucharest, Faculty of Chemistry, Research Centre of Applied Organic Chemistry, 90 Panduri Street, Bucharest, Romania*

N-acylhydrazones[1] are versatile and useful molecules which were reported as ligands for metal-ions[2], precursors in synthesis of heterocycles, such as 1,3,4-oxadiazoles[3], gelators[4] or switchable-light emissive molecules. The reversibility of hydrazone bond and dynamic covalent chemistry (DCC)[6] principles lead to a wide range of polyfunctionalized building blocks used for preparation of interesting materials such as dynamic polymers (dynamers)[7] , crystalline polymers (covalent organic frameworks - COFs)[8] or macrocycles used like hosts for various anions (F^-)/ metallic ions (Ca^{2+})/ small organic molecules (quinine)[9] .

In this context, we designed, synthesized and characterized novel N-acylhydrazone-based macrocycles using a pool of dialdehydes and dihydrazides, under thermodynamic control. Additionally, we investigated the hosting capacity towards various guests using NMR, HRMS, UV-visible and fluorescence spectroscopy.[10]

Acknowledgements: This work was supported by a grant from the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1003, within PNCDI III.

[1] Skene, W. G., Lehn, J. M. P., PANS, 2004, 101, 8270-8275.

[2] Anbu, S., Kamalraj, S., Jayabaskaran, C., Mukherjee, P.S., Inorg. Chem., 2013, 52, 8294–8296.

[3] Anghel, C.C., Mirea, A.G., Popescu, C.C., Mădălan, A.M., Hanganu, A., Bende, A., Hădade, N.D., Matache, M., Andruh, M., Dyes Pigm., 2023, 210, 111023.

[4] Maity, A., Ali, F., Agarwalla, H., Anothumakkool, B., Das, A., Chem. Commun., 2015, 51, 2130–2133.

[5] Coman, A.G., Paun, A., Popescu, C.C., Hădade, N.D., Hanganu, A., Chiritoiu, G., Farcasanu, I.C., Matache, M., Bioorg. Chem., 2019, 92, 103295.

[6] Huc, I., Lehn, J.-M., PNAS 1997, 94, 2106-2110.

[7] Zhang, Y., Barboiu, M., Chem. Rev., 2016, 116, 809–834.

[8] Uribe-Romo, F.J., Doonan, C.J., Furukawa, H., Oisaki, K., Yaghi, O.M., J. Am. Chem. Soc., 2011, 133, 11478–11481.

[9] Matache, M., Bogdan, E., Hădade, N. D., Chem. Eur. J., 2014, 20, 2106-2131.

[10] Sandu, N., Hanganu, A., Popescu, C., Demeter, A. M., Mirea, A. G., Kuncser, A., Tăblet, C., Hădade, N. D., Florea, M., Funeriu, D. P., Matache, M., J. Mater. Chem. A, 2025, 13, 10232-10242.