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Letter/Extended Abstract

COMPLEX [$Zn^{II}Ln^{III}$] COMBINATIONS ATTACHED ON GRAPHENE SUPPORT

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1. INTRODUCTION

Graphene is an intensely studied material due to its special abilities, such as electrical, high mechanical resistance and optical properties. Recent attempts have been made to functionalize the graphene surface with diverse complex combinations. To achieve this functionalization, the most used methods include the formation of covalent bonds between the support and the complex, the encapsulation or the use of noncovalent interactions, which contain hydrogen bonds and "π- π stacking" interactions [1].

Heterometallic [$Zn^{II}Ln^{III}$] complexes containing Schiff-derived from o-vanillin as ligand have been studied in the past due to their luminous properties, which will then allow them to act as antennae for lanthanide [2].

2. METHOD/MODEL

Using the appropriate lanthanide precursor, a complex containing a carboxylate bridge between the two metal ions was obtained [3]. Subsequently, it is possible to replace this bridge with the one derived from another acid, having different functional groups, thus obtaining a molecule with properties completely different from those of the precursor.

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3. RESULTS

In this work, the carboxylate group from 1-pyrenbutyric acid was added to the $[Zn^{II}Ln^{III}]$ type structure, resulting in complex combinations containing a pyrene moiety (where Ln = Nd, Eu, Gd, Tb, Sm, Dy, Tm , Yb). The molecules thus obtained have luminescent, magnetic properties, and an arrangement that creates channels in the extended structure. In these channels, with ~ 2 nm in size, the introduction of small molecules (e.g. halogens, naphthalene) was attempted.

Subsequently, having available the pyrene moiety, which interacts well with graphene, the obtained complex combinations were attached to the graphene support, in the form of nanoparticles. After attachment, the discussed materials retained their luminescent properties. In addition, new electrical properties specific for capacitors have emerged.

All compounds were characterized in solid state using FTIR and UV-Vis spectroscopy, luminescence measurements, X-ray diffraction on powder and single crystal. To demonstrate the attachment of the chosen complex to graphene, the functionalized material was characterized using SEM / EDX, Raman and luminescence measurements.

4. CONCLUSIONS

The introduction of new properties and the attachment to the graphene surface was succesfully achieved by replacing one particular fragment of the complex combination, thus obtaining a composite material with luminescent and electrical properties with a multiple applications.

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Letter/Extended Abstract

SINGLE WALLED CARBON NANOTUBES - EFFICIENT CARRIERS OF CISPLATIN IN TRIPLE-NEGATIVE BREAST CANCER THERAPY

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1. INTRODUCTION

Negative triple breast cancer (NTBC) is a subtype of breast cancer characterized by the absence of estrogen and progesterone receptors and overexpression of the epidermal growth factor HER2. Thus, the only available therapies are chemotherapy and surgery [1]. Because these treatment methods have low efficacy, targeted therapy using carbon nanotubes (CNTs) is the main treatment alternative in NTBC [2].

In this context, the purpose of this study is to evaluate the anti-tumor potential of cisplatin-conjugated single-walled CNT (SWCNT) (CDDP) in MDA-MB-231 breast adenocarcinoma cells.

2. METHOD/MODEL

SWCNT-COOH-CDDP nanocomposites were obtained by covalent functionalization with carboxyl groups and conjugation with CDDP. MDA-MB-231 cells were exposed to various doses of SWCNT (0.01 - 2 μg / mL) and CDDP (0.00632 - 1.26 μg / mL) for 24 and 48 h. The cell morphology was analyzed by optical microscopy techniques, and the cytotoxic character of the nanocomposites was evaluated by determining the cell viability using the

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MTT test and the fluorescence marking of the cells using the LIVE / DEAD kit. Membrane integrity was assessed by quantifying the activity of lactate dehydrogenase (LDH) released into the culture medium. The level of reactive oxygen species (ROS) and changes in mitochondrial membrane potential (MMP) were also evaluated. Some markers which were part of the signaling pathways in proliferation and cell death (PI3K, caspase 3, caspase 8) were evaluated by Western blot technique.

3. RESULTS

Cell viability decreased in a time-dependent manner and the dose applied in the presence of SWCNT-COOH-CDDP compared to control and free components, did not induce significant changes in cell viability. At the same time, in the presence of nanocomposites, fluorescence images and LDH level determinations indicated a low cell density and an alteration of membrane integrity at doses greater than 1 μg / mL. Also, an increased level of ROS was recorded in a dose-dependent manner of the applied nanocomposite. After 24 and 48 h of treatment, the MMP level decreased by 25.87% and 49.15%, respectively 49.42% and 78.41% in the presence of 0.5 and 1 μg / mL SWCNT-COOH-CDDP doses, in comparison to the control sample. PI3K expression was inhibited after 48 h of treatment with 0.5 and 1 μg / mL SWCNT-COOH-CDDP. At the same time, activation of caspases 3 and 8 was observed after the treatment of cells with 1 μg / mL SWCNT-COOH-CDDP for 24 and 48 h.

4. DISCUSSIONS AND CONCLUSIONS

The cytotoxicity of nanocomposites and their efficiency in CDDP transport to the breast adenocarcinoma cells was confirmed by the low level of cell viability and PI3K inhibition, implicated in the proliferation and survival of tumor cells. Since caspase 3 has been activated, it can be considered that apoptosis could be the main mechanism of cell death. At the same time, activation of caspase 8 protein, the high level of generated ROS, together with decreased MMP, may indicate a correlated activation of the extrinsic and intrinsic pathways of apoptosis.

The results of this study may indicate that in the mammary adenocarcinoma cells the SWCNT-COOH-CDDP nanocomposites determine the activation of the apoptotic mechanism by inhibiting the PI3K signaling pathway.

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Letter/Extended Abstract

3D AND 4F COMPLEXES WITH MANNICH BASE LIGANDS AND NITRONYL-NITROXIDE RADICALS

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1. INTRODUCTION

In coordination chemistry, Schiff base reactions, together with Mannich reactions, are an easy synthesis pathway for achieving rich data base of organic molecules with various coordinating abilities [1].

2. METHOD/MODEL

Symmetric ligands are typically used to obtain homo-oligonuclear complexes with 3d and 4f metal ions. Asymmetric organic molecules with multiple coordination sites present greater interest due to the possibility of synthesizing heterometallic complexes. While examples of complexes 3d-3d 'and 3d-4f are numerous, being synthesized for their optical and magnetic properties, examples with two different lanthanides are still rare [2]. The small difference between their properties, between ionic radii, makes the synthesis of heterodinuclear compounds f-f 'a difficult task to perform [3].

Furthermore, grafting of paramagnetic species such as nitronyl nitroxide radicals on the organic ligand can lead to the formation of heterodispin (2p-3d, 2p-4d, 2p-4f) or heterotrispin (2p-3d-4f) complexes [4-5].

3. RESULTS AND DISCUSSIONS

Thus, a series of symmetrical ligands from 2 ', 7'-dichlorofluorescein were used to form mononuclear species with 3d and 4f ions. The formed complexes were crystallized by slow evaporation of the solvent and then characterized by X-ray diffraction on single crystal and powder. The luminescent properties of the compounds were investigated in solution. Another serie of mono and dinuclear complex combinations with 3d or 4f metal ions was synthesized

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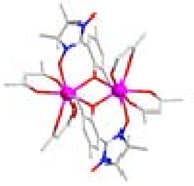
♣ Correspondent author: mihai.raduca@chimie.unibuc.ro by bicompartmental bonds derived from salicylaldehyde that exist in their nitronyl-nitroxide radical structure. The compounds were characterized from a structural point of view (Fig. 1), followed by an investigation referring their magnetic properties.

Figure 1: *Example of homodinuclear complex with bicompartmental ligand. The H and F atoms were omitted for better clarity of the image*



4. CONCLUSIONS

Using Mannich base ligand and paramagnetic, nitronyl-nitroxide radical ligand, several mono and dinuclear compounds with 3d and 4f metal ions were synthesized and structurally characterized.

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Letter/Extended Abstract

SYNTHESIS OF A NEW [2] ROTAXAN BY A METAL ACTIVE REACTION TEMPLATE CUAAC

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1. INTRODUCTION

[2]Rotaxanes are mechanically interconnected molecules, composed of an axis passing through a macrocycle. The axis is provided with 2 bulky groups at its ends that prevent the macrocycle from leaving the resulting supramolecular structure (Fig. 1) [1]. Due to the different possible structures of axes and macrocycles, and especially due to their interactions, [2]rotaxanes have found numerous applications in catalysis [2] and molecular devices, such as molecular motors that can convert solar energy into mechanical energy [3].

The synthesis of rotaxanes proceeds generally with modest yields, and the assembly of the structure is performed by non-covalent, weak interactions. Copper (I) catalyzed alkyne - azide cycloadditon (CuAAC) reaction is one of the most known click reactions and has high yields and mild conditions [1], ideal characteristics, given the limitations imposed by the synthesis of these supramolecular structures [4].

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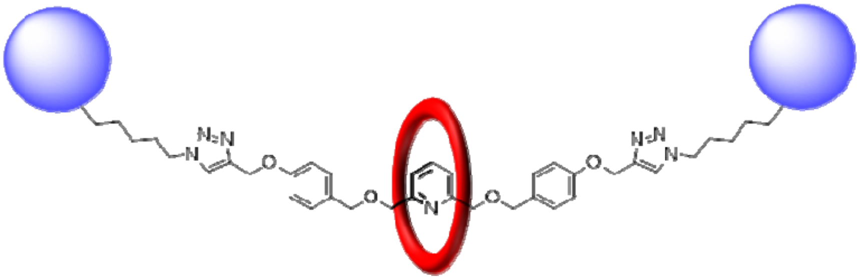
Figure 1: *Structure of the targeted [2]rotaxane*



2. MATERIALS AND METHODS

The compounds were characterized by nuclear magnetic resonance spectroscopy (^{1}H and ^{13}C) and high resolution mass spectrometry (HRMS).

3. RESULTS

In this paper we have realized the design and synthesis of a new [2]rotaxane through an active metal template CuAAC reaction. In the first phase we obtained the axis with the large groups attached at the end, the last stage of its synthesis strategy being a CuAAC reaction. For the synthesis of rotaxane we obtained the catalyst, consisting of an axis and a copper precatalyst, in situ. This allowed the formation of the macrocycle consisting of two components, a diazide and a dialchine, around the axis, through an active type metal template effect.

4. CONCLUSIONS

In conclusion, we synthesized a new [2]rotaxane through an active metal template CuAAC reaction. For the future, we propose the functionalization of triazoles from the axis in order to obtain a molecular shuttle and test its catalytic properties.

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MARCURY DETERMINATION ON FOOD AND ENVIRONMENTAL PROBES USING AN ATOMIC EMISSION MICROSPECTROMETER IN CAPACITATED MICROPLASM AND ELECTROTHERMAL VAPORIZATION (ETV- MICROCCP-OES)

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1. INTRODUCTION

Exposure to mercury can occur both from anthropogenic sources [1] and from food, especially from fish consumption [2,3]. The forms of mercury present in nature can be in the form of metal, vapors, salts or organic compounds, the greatest risk of exposure being the consumption of fish, dental fillings based on amalgam and exposure in the workplace [4]. Exposure to high levels of mercury can lead to the development of Minamata disease, and the effects of long-term exposure may include kidney disease and decreased intelligence [5].

2. METHOD/MODEL

The mercury determination was performed with a capacitive coupled plasma atomic emission microspectrometer and electrothermal vaporization. The vaporization device is made up of a piston at the top of which was attached a rhodium filament and a 'T' shaped tube which also acts as a vaporizing chamber. The plasma is supported by an argon flux, the argon flux will pass through the vaporization chamber on the path to the plasma and thus the analyte on the surface of the filament will be drawn to the plasma where it will emit radiation that

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will be detected by the microspectrometer. The principle of the method has been explained more detailed in a previously published paper [6].

The method is based on the total mercury extraction from the sample with a solution of 47% HBr, while the methylmercury was further extracted by successive extraction, first in toluene and then in a solution of L-cysteine 1%; the total mercury was determined from the 47% HBr solution, and methylmercury was determined from the 1% L-cysteine solution at 253.652 nm using a low resolution microspectrometer (Maya2000 Pro, Ocean Optics).

3. RESULTS

The accuracy of the method was determined by analyzing certified reference materials with a recovery degree between 96% and 104% for total mercury quantity, respectively between 95% and 104% for methylmercury, with an accuracy below ± 10%.

4. CONCLUSIONS

The study showed that the mercury speciation from fish and environmental samples can be achieved by this method (ETV- μCCP-OES), which is simple and relatively cheap due to the low consumption of reagents and energy, due to the low power of the micro-torque and the low Ar consumption, considering this approach as an alternative to the classical methods of mercury determination and speciation.

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Eco-Scale Specification of Hg^{2+} and CH_3Hg^+ by Optical Emission Spectrometry in Capacitated Coupled Microplasm and Generation of Cold Vapors by UV / Vis Photoinduced Derivatization (UV-Vis-PVG-microCCP-OES)

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1. Introduction

Mercury is a metal that is highly toxic for the human body, especially in its organomercuric forms, such as CH_3Hg^+, to which humans can be easily exposed through the consumption of fish meat [1]. Most laboratories consider the determination of CH_3Hg^+ unattainable due to the complicated method of sample processing, respectively due to the need for sophisticated instrumentation [2]. Thus, the objective of the present study was to develop a simple method for the speciation of Hg on CH_3Hg^+ and Hg^{2+} found in fish meat, which would satisfy at the same time as many of the principles of Green Analytical Chemistry (GAC).

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2. METHOD/MODEL

The method is based on the extraction of Hg species from 0.2 g sample in 10 mL solution 98-100% HCOOH by ultrasound, determination of total Hg (CH_3Hg^+ and Hg^{2+}) by UV radiation photoreduction obtained from a high power lamp, Hg^{2+} with Vis radiation (lamp off), and respectively the calculation of the CH_3Hg^+ concentration. UV-Vis-PVG-μCCP-OES determinations were performed on samples at an average of 0.6 mol L-1 HCOOH by external calibration with Hg^{2+} standards and detection at 253.652 nm using a low resolution microspectrometer (Maya2000 Pro, Ocean Optics).

3. RESULTS

The study of the performance parameters indicated a detection / determination limit (LOD / LOQ) of 9/27 μg kg^{-1} Hg total and 4.8 / 14.4 μg kg^{-1} Hg^{2+}, respectively between 2.0 - 14, 5% for total Hg, Hg^{2+} and CH_3Hg^+. The accuracy of the method, verified by the analysis of certified reference materials, indicated recovery levels of 99 ± 6% for total Hg, 99 ± 9% for Hg^{2+} and 99 ± 10% for CH_3Hg^+. The method satisfies the requirements of the European Commission and the Association of Official Analyst Chemists (AOAC) regarding the analytical performance of a method used to determine Hg from marine foods. Comparison of the results obtained from certified materials and test samples using UV-Vis-PVG-μCCP-OES and Atomic Absorption Spectrometry with Thermal Desorption (TD-AAS) ended in statistically similar values (Student- and F- test).

4. CONCLUSIONS

The study showed that Hg speciation in marine foods such as CH_3Hg^+ and Hg^{2+} can be achieved by a simple, relatively inexpensive method with a high degree of eco-scale using a single reagent for both sample extraction and photoinduced cold vapor derivatization of Hg. To the green profile of the method contributed the miniaturized instrumentation with a low power micro torch and low consumption of Ar. The method can be considered an alternative to the classical methods of determining / speciation of Hg.

ACKNOWLEDGEMENT(S)

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Letter/Extended Abstract

IMMOBILIZATION OF LIPASE B FROM *CANDIDA ANTARTICA* IN SOL-GEL FOR INDUSTRIAL APPLICATIONS

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1. INTRODUCTION

Lipases are one of the most widely used classes of enzymes because of their ability to catalyze a wide variety of reactions, such as: polymerizations, esterifications, transesterifications, aminolyses, etc. Other advantage of using lipases, besides their versatility, is the fact that they work independently in the presence of an external cofactor, with a high selectivity. Lipase B from *Candida antarctica* is a commonly used biocatalyst, being able to catalyze reactions to the production of biodiesel, flavors, fragrances and enantiopure drugs. The immobilization of lipases in sol-gel increases their tolerance to certain solvents, thermostability and mechanical resistance.

Soil-gel formation occurs in two stages: hydrolysis of tetraalkoxysilanes [$Si\ (OR)_4$], and their polycondensation which will lead to encapsulation of the enzyme in a silane polymer matrix [1].

2. METHOD/MODEL

All reagents, solvents and materials involved in enzyme immobilization were purchased from Merck (Germany), Sigma-Aldrich (Germany) and VWR Chemicals (USA). Lipase B from Candida Antarctica (CaL-B) was purchased from Novozym (Denmark). Enzyme reactions were perfected in Labtech thermostatic orbital shaker. The separation of racemic 1-phenylethanol, as well as of the corresponding acetates, was performed by gas chromatography using a chiral Chiraldex β-DM column.

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3. RESULTS

Lipase B from *Candida antarctica* (CaL-B) was successfully immobilized in sol-gel employing different silane precursors, using an liquid ionic (OmimBF4 - 1-methyl-3-octylimidazole tetrafluoroborate) additive to the silane matrix formation reaction. The obtained preparations were tested in batch mode for the enzymatic kinetic resolution (EKR) of racemic 1-phenylethanol transesterified with vinyl acetate. The interpretation of the results led to the choice for an optimal ternary mixture of used silanes.

For the transposition of the process on an industrial scale, it must be economically feasible. In this sense, it was desired to replace the ionic liquid used as an additive for sol gel formation with another type of cheaper additive, which can be obtained from renewable sources. The thus obtained enzymatic products were tested in batch mode for EKR of racemic 1-phenylethanol transesterified with vinyl acetate.

4. CONCLUSIONS

Following the interpretation of the results it was found that the use of sorbitol as an additive to the immobilization process led to comparable results with those obtained when using an commercially available enzymatic product (Novozym 435).

An active and selective biocatalyst was prepared by sol-gel encapsulation of CaL-B which was effective in EKR of 1-phenylethanol.

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Letter/Extended Abstract

ω-TRANSAMINATES IN SYNTHESIS OF (R)- AND (S)-ENANTIOPURE AMINES

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1. INTRODUCTION

Chiral amines are valuable building blocks for obtaining pharmaceuticals, agrochemicals, etc. [1] ω -Transaminases (ω-TA) are the only enzymes that can catalyze the synthesis of enantiopure chiral amines directly by the asymmetric amination of prochiral ketones [2]. Despite their enormous potential, their widespread application as biocatalysts is disadvantaged by the emergence of byproducts that act as inhibitors and by the unfavorable displacement of the reaction balance [3].

2. METHOD/MODEL

The activity of the enzyme, an (R) -selective enzyme, was investigated in kinetic resolution processes of chiral ethylamines, substituted with aromatic and heteroaromatic residues. The reaction mixture in PBS buffer (50 mM, pH 7.5) contains racemic amine (5 mM), DMSO cosolvent (5%, vol.), Pyruvic acid (20 mM), PLP cofactor (0.1 mM) and the tested purified enzyme (50 g / mL). The reaction was monitored by HPLC (chiral column CROWNPAK CR-I (+) and eluent mixture $HClO_4$ pH 1.5-acetonitrile, 80:20 (v / v)), at 15°C.

3. RESULTS

The study presents the enzymatic kinetic resolution mediated by ω-transaminase for the synthesis of (R) -amines with high enantiopurities and the determination of kinetic

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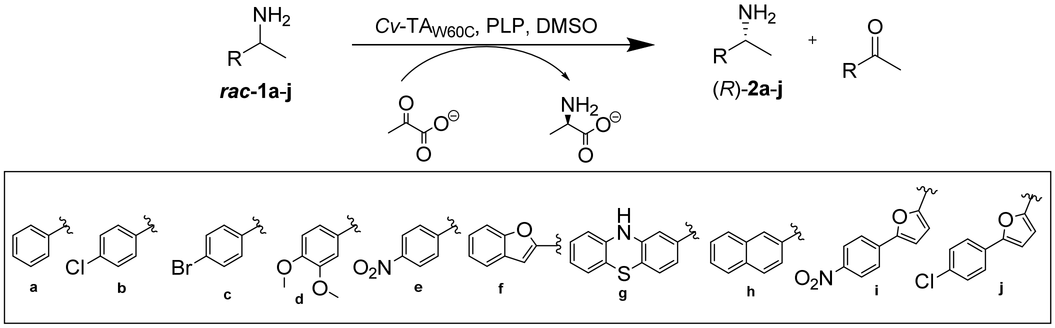
Figure 1: *The enantiomeric conversions and excesses of the products*



4. CONCLUSIONS

The synthesis of (R) -amines with high EKR enantiopurity of racemic amines, mediated by a high selectivity ω-transaminase with the ability to accept a wide range of aromatic (hetero) racemic substrates, was succeasfully achieved.

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Letter/Extended Abstract

DEVELOPMENT OF HIGH THROUGHPUT METHOD FOR DETERMINING THE PHENYLALANINE AMMONIA LYASES ACTIVITY

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1. INTRODUCTION

Phenylalanine ammonia lyase (PAL) catalyzes the non-oxidative deamination of L-phenylalanine with the formation of trans-cinnamic acid, and in the presence of high concentrations of ammonia and the reverse reaction, it can catalyze the addition of ammonia to the cinnamic derivative. PAL enzymes are intensively studied [1,2], but their application in the industrial synthesis of amino acids is limited by their stability, respectively their low promiscuity [3]. The use of directed / semi-rational evolution techniques [4,5] to improve the stability, activity and selectivity of PAL enzymes, is limited due to the lack of a high-efficiency ("high-throughput" method") For testing PAL activity, which would allow for the rapid identification of improved PAL variants from large mutant data bases (> 1000) generated by the mentioned techniques.

The developed high-throughput fluorescence (HTP) method uses ferulic acid decarboxylase (FDC1), an enzyme that catalyzes the decarboxylation of trans-cinnamic acid, the product of PAL-catalyzed reaction to styrene. The styrene thus obtained reacts with a fluorogenic diaryl-tetrazolone and forms a product with a pyrazolinic structure, which exhibits fluorescence.

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2. METHOD/MODEL

The reagents, solvents and materials used were purchased from Sigma Aldrich and Alfa-Aesar. IPTG was purchased from Thermo Fisher Scientific (Waltham, MA, USA) and LB medium from Liofilchem (Roseto, Italy). The enzymatic reactions were performed in 1.5 mL polypropylene tubes, respectively, in 96-well microplates.

The UV-mediated reaction between styrene and the fluorogenic reagent was performed at 302 nm for 1 minute, and the pyrazolinic product was analyzed by excitation at 368 nm, followed by emission detection at 460 nm using the TECAN Spark 10M microplate reader. The validation of the new developed method, to determine the PAL activity, was performed by comparing the results with those obtained previously with HPLC-based methods.

3. RESULTS

In order to determine the optimum excitation and emission, 3D excitation-emission tests were performed. The reaction between tetrazolone and styrene was investigated in various organic solvents (n-hexane, methanol and / or acetonitrile, 1,4-dioxane) miscible with water or having the ability to extract styrene from water. n-Hexane was found to be the optimal solvent, while n-octane was used as a co-solvent due to the low solubility of the tetrazolone derivative. For the deamination reactions, the native enzyme and mutants of PcPAL were used as both isolated and recombinant whole cells of E. coli. Decarboxylation reactions were performed with whole E. coli cells containing the FDC1 gene in Saccharomyces cerevisiae. The relative activity order of PcPAL enzymes was determined using the reaction of 4-methoxy-DL-phenylalanine deamination catalyzed by the native enzyme and different mutants of PcPAL: 1) by the newly developed fluorescence assay, 2) by HPLC, 3) by which purified PAL enzymes were used.

4. CONCLUSIONS

A new "high-throughput" method has been developed for the rapid determination of phenylalanine-ammonia-lyase activity in whole cells. This method allows the application of directed or semi-rational evolution techniques for the protein engineering of PAL enzymes.

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Letter/Extended Abstract

SYNTHESIS OF NEW, ACTIVE, UNI-COMPONENT, NONFULLERENIC MATERIALS, TOWARD MANUFACTURING ORGANIC SOLAR CELLS

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1. INTRODUCTION

An important step towards the efficiency of organic solar cells is the development of the concept of single-component materials containing donor units (D) and acceptor units (A) of electrons separated by a binding unit (L). The advantages of these materials consist in simplifying the procedure for the manufacture of solar cells, stabilizing the morphology of the active layer and reducing the time of excitation and diffusion of the load [1,2].

2. METHOD/MODEL

The final compound described in this paper was obtained by a multi-step synthesis strategy. The synthesized intermediates were purified in each step, either on silica gel chromatographic column using different elution systems, or by precipitation, and their structure was confirmed by different methods (HR-MS, ^{1}H and ^{13}C NMR).

3. RESULTS

The compound shown in Scheme 1 is a D-L-A-L-D type molecule used as a single component material in organic solar cells. The acceptor unit is a fluorine derivate, and the

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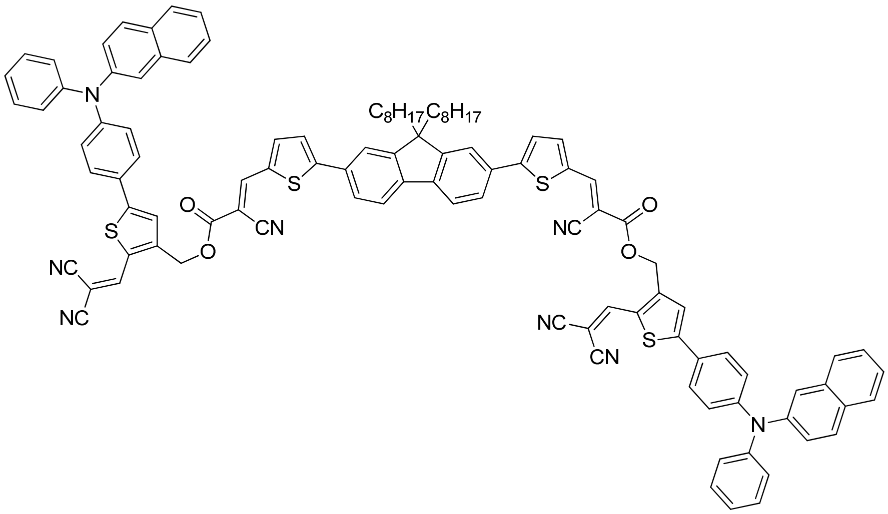
electron-donor unit is a triphenylamine derivate in which a phenyl group has been replaced by a β-naphthyl group in order to improve the mobility of the carriers [3,4].

Scheme 1: *Chemical structure of the targeted compound*



4. CONCLUSIONS

Following the studies of the electrochemical and absorption properties it was determined that the given compound can be used as an active material in the manufacture of single-component organic solar cells.

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Letter/Extended Abstract

IMPROVEMENT OF THE CATALYTIC PROPERTIES OF PAL (PHENYLALANINE AMMONIA LYASES) FROM *PETROSELINUM CRISPUM* BY PROTEIN ENGINEERING TECHNIQUES

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1. INTRODUCTION

Among the enzymes containing the MIO prosthetic group, phenylalanine ammonia lysases (PAL: EC 4.3.1.24) are of particular interest, as they accept a relatively wide range of substrates, being valuable tools in the preparation of enantioptic amino acids [1]. Furthermore, industrial processes based on PAL enzymes have been developed, such as the production of (S) -2,3-dihydro-1H-indole-2-carboxylic acid by DSM (Netherlands) [2]. The synthesis of phenylalanines or their analogues in enantiopure form through PAL enzymes therefore has an interest in the chemical industry, enantiopure products being valuable building blocks in the pharmaceutical industry, frequently incorporated into the structure of therapeutic peptides or proteins [3-5]. In our research we focused on mapping the hydrophobic binding pocket of phenylalanine ammonia ligase from *Petroselinum crispum* (PcPAL), in order to improve its catalytic properties.

2. METHOD/MODEL

PAL mutant genes were obtained by site-directed mutagenesis using wt-pcpal with the vector pET-19b as a template. The substrates were synthesized within the Center for Biocatalysis Research and Biotransformation. Enzymatic reactions were performed using E. coli Rosetta (DE3) pLysS whole cells carrying native or mutant pcPal gene, in 96-well

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microplates, in 1.5 mL polypropylene tubes (for analytical reactions) and 500 mL Erlenmeyer containers (for preparative scale reactions). Purification of recombined enzymes was performed by a previously developed method 5, using Ni-NTA affinity chromatography. Enzyme reactions of ammonia addition and elimination were monitored by HPLC method, and in the case of elimination reactions the UV spectrophotometric method was used to determine the initial velocities.

3. RESULTS

Modification of the hydrophobic binding pocket of phenylalanine ammonia lyase in *Petroselinum crispum* (PcPAL) was successfully performed by targeted mutagenesis. The catalytic properties of the different mutant variants of PcPAL were monitored in both addition and ammonia removal reactions. The protein engineering strategy allowed the identification of some amino acid residues in the hydrophobic area of the enzyme, which changed with smaller hydrophobic amino acids (alanine or valine), depending on the spatial orientation of the aromatic substituents of the substrate, caused an increase in the catalytic activity and selectivity of PAL enzyme. The results of the mutational strategy were also confirmed by the crystallographic analysis of the p-MeO-cinnamic acid binding mode in the active site of the PcPAL I460V mutant. The biocatalytic utility of PcPAL mutants was demonstrated by the efficient preparative synthesis of some D- and L-phenylalanine analogues, following the optimization of the addition and removal reactions of ammonia.

4. CONCLUSIONS

Mapping of the hydrophobic binding site of PAL enzyme from *Petroselinum crispum* and testing the activity of the obtained mutants was successfully performed following a mutational strategy. These results allowed the rational design of some changes in the active site of the enzyme to extend the substrate domain to phenylalanine analogues and mono-substituted cinnamic acids not transformed by the native enzyme. Thus, non-natural substrates of high synthetic importance could be transformed by the optimum mutant, specifically chosen according to the spatial orientation of the substituent on the aromatic ring of the substrate.

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Letter/Extended Abstract

INVESTIGATION OF ORGANIC MOLECULAR MARKERS IN THE URBAN ATMOSPHERE BY HPLC-ESI-TOF-MS. METHOD DEVELOPMENT

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1. INTRODUCTION

The identification and quantification of the organic molecular markers in the particulate matter environment plays an important role in attributing the sources and investigating the mechanisms of formation and evolution of the organic aerosols [1].

2. METHOD/MODEL

In this study, a method was developed to quantify the markers of secondary biogenic organic aerosols (oxidation products of α- and β-pinene: cis-pinonic acid, cis-pinic acid, terebic acid, terpenyl acid, etc.) and anthropogens (benzoic acid, phenolic derivatives: 4-nitrophenol, 2,6-dinitrophenol, 4-nitrocatechol, 4-methylcatechol, etc.) by high-performance liquid chromatography coupled with time-lapse mass spectrometry and electrospray ionization (HPLC-ESI- TOF-MS) in negative mode.

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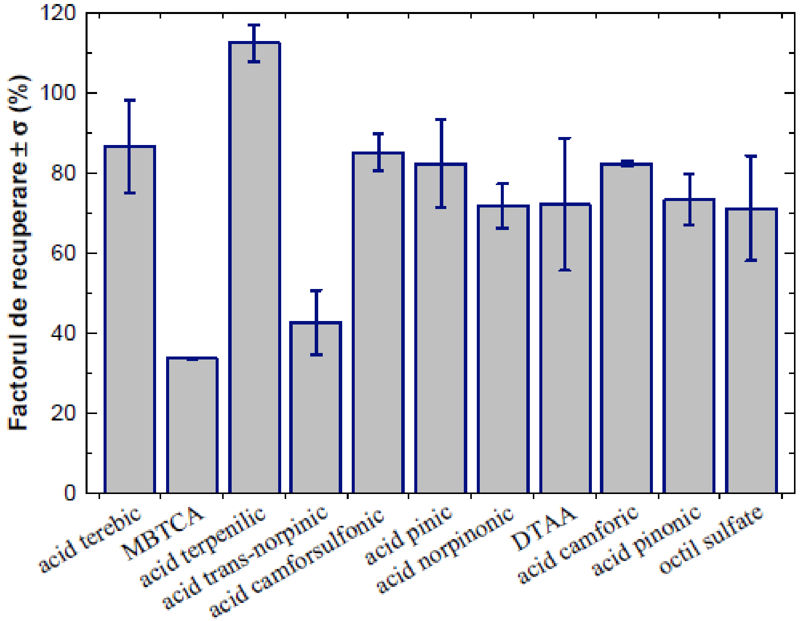
3. RESULTS AND DISCUSSIONS

For the separation of the species of interest, three analytical columns were tested: Zorbax Extend C18 (2.1 × 50 mm, 1.8 µm), HILIC Month (4.6 × 150 mm, 5 µm) and Poroshell 120 EC-C18 (4,6 × 50 mm, 2.7 µm) together with different elution methods. For the improvement of the sensitivity, the ionization source parameters were optimized. Also, performance parameters of the optimized method were determined.

Optimal separation was obtained using the Poroshell column and gradient elution with 0.1% aqueous acetic acid and acetonitrile at a flow rate of 0.8 mL min^{-1}. The reproducibility for the retention times, under the optimized conditions was 0.02 -0.29% RSD. The limits of quantification were in the range 0.88 -25.57 µg L^{-1} (0.004 -0.107 ng m-3, relative to a collecting volume of 120 m3). The elution method with acetonitrile, compared to the use of methanol, offers a higher analytical sensitivity for the species of interest, with a factor between 1.14 and 2.02. The accuracy of the molecular mass determinations, estimated for the compounds of interest, was in the range 2.92-8.84 ppm. The tests performed to determine the recovery factors, in the case of the extraction with acetonitrile: water (95: 5, v / v) of 11 compounds from aerosol samples collected on aluminum filters, led to an average value of (74.0 ± 21,3)%, lower values being for 3-methyl-1,2,3-butantricarboxylic acid and *trans*-norpinic acid (Fig. 1).

Figure 1: *Recovery factor values of acetonitrile: water (95:5) for extraction method (Legends are in Romanian)*



4. CONCLUSIONS

The developed method has the potential for determining target compounds in atmospheric aerosol samples. Other extraction methods will be tested to improve the recovery factors.

ACKNOWLEDGEMENT(S)

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DESIGN, SYNTHESIS AND ANTIMICROBIAL PROPERTIES OF SOME NEW 8-AMINOCHINOLINE DERIVATES

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1. INTRODUCTION

Currently, heterocyclic compounds occupy an important place in the development of new classes of structural entities with high medical significance. The quinolinic nucleus is present in a wide range of compounds possessing different biological activities, being present also in drugs that are used as antibiotics against a variety of bacteria that have acquired resistance to common antibiotics [1].

2. METHOD/MODEL

Taking into account the existing data in the literature on the antimicrobial activity of quinoline and imidazole derivatives [2,3], in this study, the design, synthesis and evaluation of the antibacterial and antifungal properties of new quinoline-imidazole hybrid derivatives was obtained. The synthesis of the target compounds was performed using two types of reactions, N-acylation and N-alkylation. The structure of the newly synthesized compounds was demonstrated by IR spectrometry, ^{1}H-NMR, ^{13}C-NMR and two-dimensional correlations.

Antibacterial and antifungal activity was determined using the Kirby-Bauer diffusimetric method

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3. RESULTS

The synthesis of the precursors was carried out starting from 8-aminoquinoline. In the first step, the N-acylation reaction of 8-aminoquinoline was performed, followed by the achievement of the N-alkylation reaction of imidazole with the acylated quinolinic derivative and the quinoline-imidazolic heterocyclic unit. Quaternization reactions were then carried out using various substituted phenacyl bromides when the imidazole salts of interest were obtained.

The compounds were tested on the following pathogenic strains: the bacteria Staphylococcus aureus ATCC® 25923 and Escherichia coli ATCC®28922, and the fungus Candida albicans ATCC®10231, respectively. Test data confirm the antimicrobial and antifungal activity of synthesized imidazole salts.

4. CONCLUSIONS

The synthesis method of quinoline-imidazole hybrid compounds is a direct and efficient method, consisting of three reaction steps. All compounds were obtained with good yields. The results of the antibacterial and antifungal activity tests showed that most of the compounds have very good biological activity.

The synthesis strategy of quinoline-imidazole hybrid compounds is direct and efficient. Preliminary results confirm the antimicrobial activity of quinoline-imidazolic hybrid compounds.

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Letter/Extended Abstract

STUDY ON THE FORMATION OF SECONDARY ORGANIC AEROSOLS FROM ATMOSPHERIC PHOTO-OXIDATION OF 1.2 DIHYDROXI (ALKYL) BENZENES INITIATED BY OH RADICALS IN NO_X CONTROLLED CONDITIONS

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1. INTRODUCTION

Atmospheric degradation of hydroxylated aromatic hydrocarbons is predominantly initiated by OH radicals and contributes both to increasing the oxidation capacity of the atmosphere and to the formation of secondary organic aerosols (SOA), especially in urban environments [1].

2. METHOD/MODEL

In this study, the ESC-Q-UAIC (Environmental Simulation Chamber made out of Quart from "Alexandru Ioan Cuza" University of Iași) photoreactor was used for the study of chemical reactions under simulated atmosphere conditions. The reactor consists of three quartz tubes with a total volume of 760 ± 2 L. Controlled quantities of 1,2-dihydroxy- (alkyl) benzene were transferred to the reactor. OH radicals were generated in situ by photolysis of methyl nitrite at 365 nm in the presence of NO. The concentration of the species in the gas phase was evaluated using IR spectrometry with an enlarged optical path (492 ± 0.1 m). The distribution of aerosol particles by number and size was recorded using a tandem consisting of a particle counter (TSI CPC 378700) and a particle mobility discriminator (TSI DMA3080100).

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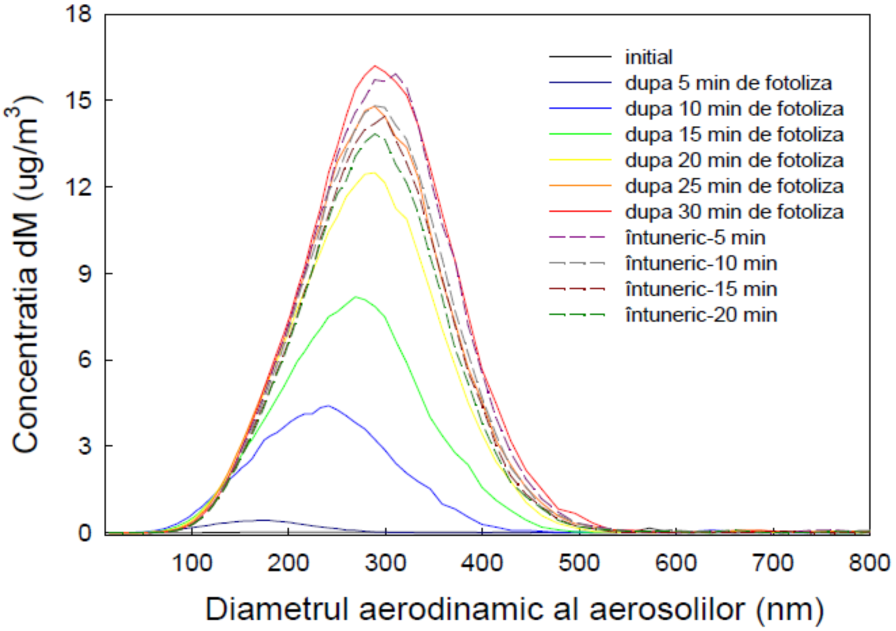
3. RESULTS

By evaluating the mass of secondary organic aerosols formed as a result of the oxidation reaction of 1,2-dihydroxy (alkyl) benzene initiated by the OH radicals and the ratio to the mass of the reacted organic compound, applying the wall loss corrections, the formation yields were determined. SOA for the three investigated compounds (1,2-dihydroxybenzene, 3-methyl-1,2-dihydroxybenzene and 4-methyl-1,2-dihydroxybenzene). Figure 1 shows a distribution of the aerosols formed in one experiment. Thus, SOA formation yields were estimated between 3 and 35%.

Figure 1: *Distribution of the mass concentration of aerosols by diameter (Legends are in Romanian)*



4. DISCUSSIONS AND CONCLUSIONS

In the case of 3-methyl-1,2-dihydroxybenzene, higher values of SOA formation yields were recorded compared to the other two investigated compounds. The increased reactivity of 3-methyl-1,2-dihydroxybenzene to its counterparts, relative to the OH radicals, can lead much faster to the formation of reaction products, products that act as precursors of SOA under the used experimental conditions.

The ESC-Q-UAIC reactor was used to study the formation of secondary organic aerosols from photo-oxidation of 1,2-dihydroxy- (alkyl) benzene initiated by OH radicals under simulated urban atmosphere conditions. The present study highlights a variation of the SOA formation efficiency as a function of emission concentration, the presence and position of the methyl group in the aromatic nucleus.

ACKNOWLEDGEMENT(S)

The financial support was provided by UEFISCDI in the research-development project PN-III-P4-ID-PCE-2016-0270 (OLFA-ROA) and by the research-innovation program of the European Union-Horizon 2020 through grant No. 730997 -EUROCHAMP 2020.

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Letter/Extended Abstract

SYNTHESIS AND CHARACTERIZATION OF ALGINATE-BASED MEMBRANES CONTAINING DIFFERENT ACTIVE COMPOUNDS FOR ORAL ADMINISTRATION

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1. INTRODUCTION

Oral administration of active compounds using different mucoadhesive polymers has been a subject of interest since the early 1980s and today has a promising strategy to prolong the drug effect and to improve the specific localization of drug delivery systems in different membranes [1]. The muco-adhesive polymers are synthetic or natural macromolecules, capable of attaching to the mucosal surfaces. Natural polymers, being biocompatible and biodegradable, are currently widely researched in the pharmaceutical industry for the development of new drug delivery systems. Of the natural polymers we used sodium alginate, which is a hydrophilic polymer, obtained from marine algae [2]. Among the drugs that present great potential, we mention methotrexate (MTX), which in low doses, presents an effective treatment, used as an immunosuppressant in inflammatory conditions: rheumatoid arthritis, psoriatic arthritis, juvenile idiopathic arthritis and in chemotherapy and treatment; and theobromine (Th) which is a bitter alkaloid from the methylxanthine family (3,7-dimethylxanthin), and is mainly found in cocoa green tea leaves, dark chocolate, with an important role in preventing tooth decay, for which reason it is added in toothpaste [3].

2. METHOD/MODEL

The TG, DSC and FT-IR studies were used to highlight the degree of incorporation of the active substances into the membrane and the possible interactions between the drug and the polymer.

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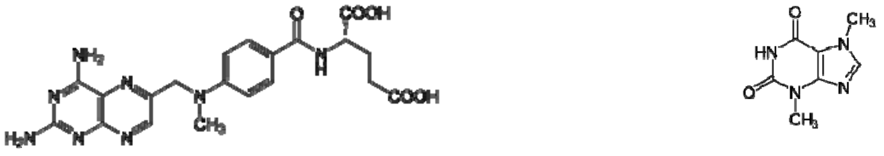
Figure 1: *Left: Methotrexate; Right: Theobromine.*



3. RESULTS

From the thermogravimetric analysis we can see that MTX is stabilized by its incorporation in the alginate membrane and in the case of Th. it can be said that it has a high thermal stability which leads us to the idea that this active substance can be used at higher temperatures, associated with different excipients, with the aim to obtain systems with oral mucoadhesive administration for the prevention of dental caries, especially in children [3].

The study will be complemented by other techniques that will lead us to the best choice.

4. CONCLUSIONS

The paper presents a study realized by spectroscopic and thermoanalytical techniques of the membranes in which different active substances have been incorporated, among them methotrexate and theobromine. The study reflects the synthesis and characterization of several types of membranes for choosing the best drug delivery system.

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Letter/Extended Abstract

ECO-TOXICOLOGICAL AND BIOCHEMICAL STUDIES ON THE EFFECTS OF CHITOSAN CONCERNIING *LEMNA SP.*

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1. INTRODUCTION

The Chitosan substance, a natural cationic polysaccharide, due to its chemical, physical and biological properties, is widely used in the medical, pharmaceutical and cosmetic industries [1]. This can lead to environmental pollution with chitosan, which makes it necessary to test the ecotoxicity of chitosan.

2. METHOD/MODEL

The growth inhibition test of duckweed (*Lemna sp.*) was performed according to the OECD standard [2], testing four chitosan samples, which had different molecular masses (MM) and degrees of deacetylation (DD): Chi 1 (MM) = 278 kDa; DD = 48%), Chi 2 (MM = 198.2 kDa; DD = 81%), Chi 3 (MM = 306.8 kDa; DD = 84%) and Chi 4 (MM = 604 kDa; DD = 83%), each at three concentrations (0.5%, 0.05% and 0.005%). The fronds at the end of the assay were analyzed biochemically, determining the chlorophyll content, the protein concentration and the enzymatic activity of catalase, acid phosphatase and enzymes that depolymerize starch. Protein analysis was also performed by polyacrylamide gel electrophoresis.

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3. RESULTS AND DISCUSSIONS

The highest concentrations tested by chitosan (0.5%) resulted in total chlorosis of the fronds. The most toxic chitosan was Chi 1, and the least toxic was Chi 4. In all samples, the concentration of chlorophyll a was higher than that of chlorophyll *b*, and the highest concentration of chlorophyll was observed in the samples treated with Chi 4. The samples treated with Chi 4 showed the highest concentration of proteins and the highest enzymatic activity of catalase and acid phosphatase. The highest enzymatic activity of the enzymes that depolymerize starch was observed in the samples treated with Chi 1. All the samples had protein bands with molecular masses of about 72 and 55 kDa, only the samples treated with Chi 2 having prominent bands and molecular mass about 170 kDa. Only in the cases whentreated with Chi 4, clear bands were observed and also in the case of 0.05% chitosan concentration. When treated with Chi 1 and Chi 2, wider and more diffuse bands were observed in comparison to the rest of the samples. The obtained results does not show a dependence on molecular mass or degree of deacetylation, which simultaneously contribute to the toxicity of the samples.

A possible explanation for the appearance of wider and more diffused bands in the electrophoresis gel may be the presence of glycosylated proteins. They thus appear due to the fact that the glycosylation of proteins is heterogeneous, the mass of the protein being able to change with several hundred Daltons. Both the molecular mass and the degree of deacetylation influence chitosan toxicity on duckweed, but there is no literature data to show the mechanism by which the two factors influence the tested parameters.

4. CONCLUSIONS

In the case of duckweed samples treated with Chi 4, the polymer with the highest molecular weight, exhibited lowest toxicity on the ducweed leaves, the highest concentration of chlorophylls and proteins, together with the highest enzymatic activity of catalase and acid phosphatase.

ACKNOWLEDGEMENT(S)

These activities were funded by the research project with the identification number: 14/2017 PN3-P3-285, title: Polymeric nanobiomaterials for drug delivery: developing and implementing a "safe-by-design" concept that will allow solutions safe medical care, acronym: GoNanoBioMat.

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Letter/Extended Abstract

TOXICITY OF ORGANIC ACIDS ON MICROORGANISMS

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1. INTRODUCTION

Organic acids have been used as antimicrobial agents, preservatives and food additives since ancient times [1]. The mechanism of antibacterial action differs depending on each acid, and in general, the main targets are the cell wall and the bacterial cytoplasmic membrane, together with the metabolic functions of the bacterial cell such as DNA replication and protein synthesis [2,3].

The purpose of this study is to highlight the effect of different organic acids on the growth of microorganisms, together with the subsequent identification of the most suitable solvent for the solubilization of chitosan, used as biomaterial in medical applications.

2. METHOD/MODEL

The toxicity of some organic acids (acetic acid, lactic acid, tartaric acid, malic acid, citric acid and ascorbic acid) was tested by microdilution method, using bacterial strains (*Escherichia coli* ATCC 25922, *Pseudomonas aeruginosa* ATCC 27853, *Acinetobacter baumannii* V19, *Staphylococci aureus* ATCC 29213, *Staphylococcus aureus* MRSA U50) and yeasts (*Candida albicans* ATCC 90028 and *Candida albicans* CCUG 39343), in order to identify a solvent that least affects the growth of microorganisms.

3. RESULTS AND DISCUSSIONS

Acetic acid is one of the most widely used solvents in the solubilization of chitosan, but the results obtained from this study indicate that this acetic acid is the solvent with the most pronounced inhibitory effect on the growth of microorganisms, followed by lactic, tartaric,

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citric, malic and ascorbic. The yeast strains were inhibited only when tested at very high concentrations of the aforementioned acids.

The final aim of the study is to show the results regarding the solubility of chitosan in organic acid that least inhibits the growth of microorganisms. The chitosan solution will be subsequently used to test the antimicrobial activity of chitosan, in order to develop a suitable biomaterial in the treatment of wounds, which will have both antimicrobial effect and also speed up wound healing. It is important to use a solvent in which chitosan is highly soluble but not toxic for the cells involved in the wound healing process.

4. CONCLUSIONS

The antimicrobial activity of acids depends on both the type of acid and the type of microorganisms. Thus, Gram-positive bacterial strains were more resistant to the inhibitory action of organic acids compared to Gram-negative strains. From the Gram-negative bacteria, E. coli was the most sensitive. The explanation may be due to the fact that this strain is more sensitive to variations in pH. The two species of *C. albicans*, were inhibited only by acetic and lactic acid, at high concentrations. Fungal species are much more resistant to pH variations and this may explain the low sensitivity.

ACKNOWLEDGEMENT(S)

This study was supported by the research project with the identification number: 4/2017 PNIII-P3-284, title: Implementation of biotechnological tools for new applications in the treatment of wounds using products obtained from the waste from the food industry of shellfish processing, acronym: CHITOWOUND

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Letter/Extended Abstract

THERMOSTABLE CHITINASES: BIOCATALYSTS FOR OBTAINING CHITO-OLIGOSACCHARIDES USED IN THE BIOFUEL INDUSTRY

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1. INTRODUCTION

The Chitin substance, the second most abundant polysaccharide on Earth after cellulose, with ~ 109 tons naturally produced each year, is a polymer consisting of β-linked (1,4) N-acetyl-D-glucosamine residues. Chitin is mainly found in the exoskeletons of marine crustaceans, large quantities of chitin waste being generated from the fish and seafood processing industry [1].

Recent concerns about global climate change have led to the shift from fossil fuels to renewable fuels, such as ethanol, produced from cellulose, used as biofuel [2]. In this context, the recovery of chitin and chitosan waste can be directed towards the production of bioethanol having as starting material chitooligosaccharides (COS) obtained by enzymatic degradation. The enzymes responsible for the hydrolysis of the β (1,4) glycosidic linkages in chitin are known as chitinases (CE 3.2.1.14) and are produced by many types of bacteria and fungi.

In this work, two objectives are pursued: the first one refers to the obtaining and biochemical characterization of a chitinase from an aquatic bacterium, of the genus Photobacterium; the second aims to identify the types of chitooligosaccharides obtained from the hydrolysis of chitin and chitosan. Also, the enzyme's ability to tolerate high temperatures was tested, a useful property for the industrial-scale preparation of COS with well-defined molecular weights for biotechnological applications.

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2. METHOD/MODEL

Techniques of molecular biology, protein engineering and biochemistry (cloning and gene expression, ion exchange chromatography, thin layer chromatography, fluorogenic and chromogenic methods for analyzing enzymatic activity) have been used to obtain and characterize a recombined chitinase, and also to analyze chito-oligosaccharides that are resulted from chitin conversion.

3. RESULTS AND DISCUSSIONS

The chitinase gene was expressed in *Pichia pastoris* KM71H and the corresponding protein was secreted into the culture medium as a recombined glycosylated enzyme. The optimal pH and temperature range for the proper enzyme activity were determined. Characterization of the recombinant enzyme on colloidal chitin substrate showed optimum pH at 5.0 and optimum temperature at 50 ° C, but the enzyme retained over 50% of its activity in a wide range of pH (3.0- 10.0) and temperature (28-70 ° C) values. Most importantly is the fact that the enzyme retained more than 50% of its initial activity after boiling at 100 ° C for up to 60 min. Kinetic analysis and nonlinear regression revealed KM and Vmax values of 14.2 mM and 0.2 mM min-1, respectively. Separation by thin layer chromatography of hydrolysis products indicated the formation of monomers and dimers of chitin and chitosan (N-acetylglucosamine, glucosamine, N, N-diacetylchitobiosis, chitobiosis).

4. CONCLUSIONS

The discussed chitinase, which is functionally expressed as a glycosylated recombinant enzyme in *P. pastoris* KM71H, is a hypertermostable endochitinase, retaining over 50% of activity over a wide range of pH and temperature. The properties of this enzyme make it an ideal candidate for the industrial production of COS from chitin biodiesel.

ACKNOWLEDGEMENT(S)

The authors acknowledge the project: Implementation of biotechnological tools for new applications in the treatment of wounds, using products obtained from the waste from the food industry of shellfish processing (ChitoWound) [PN3-P3-284]

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Letter/Extended Abstract

COMPUTATIONAL EFFECTS PREDICTION ON THE ENVIRONMENT OF OLIGOMERS RESULTED FROM THE DEGRADATION OF POLYHYDROXYALKANOATES AND POLYLACTIC ACID

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1. INTRODUCTION

Polyhydroxyalkanoates (PHA) and polylactic acid (PLA), due to their biodegradability in the natural environment, are biopolymers widely used in many fields as substitutes for non-degradable plastics derived from petroleum products.

In this study we used a computational approach to predict the effects of small PHA and PLA oligomers on small organisms and microorganisms.

2. METHOD/MODEL

Two computational tools available online were used, admmetSAR2.0 [1,2] and T.E.S.T. (Toxicity Estimation Software Tool) [3] with the purpose of predicting acute rat toxicity, skin sensitivity, AMES mutagenesis, carcinogenic effect, fish toxicity, *Tetrahymena pyriformis* species toxicity, bee toxicity and biodegradability.

3. RESULTS

Results show that the biodegradability of these compounds decrease as the increases of molecular mass. None of these oligomers can be considerate as posing toxicity against some referential organisms: fishes, crustacean, bee, ciliates (*Tetrahymena pyriformis*).

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In the last years, with the improvement of the accuracy of the predictions, the computational studies have been admitted as methods of testing the ecotoxicity of the various chemicals. It is necessary for the predictions obtained in this study to be verified experimentally, proposing that the obtained results can be used to guide the experimental studies.

4. CONCLUSION

The results show that the degradation products of polyhydroxyalkanoates and polylactic acid do not produce toxic effects on the environment.

ACKNOWLEDGEMENT(S)

This work was made within the project - PN3-3-285 / 2017 NanoBio Polymeric materials for drug delivery: developing and implementing the concept of safe-by-design that will enable safe healthcare solutions

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Short Letter for Sci-Events

NANOMOD (22-23 APRIL), TIMISOARA[†]

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With the second edition of the International Workshop dedicated to NanoModeling of Strategic Materials for Knowledge Economy (NANOMOD), conducted in logistical-administrative-scientific cooperation between West University of Timişoara, with the Faculties of Chemistry, Biology, Geography (FCBG) and Faculty of Economy and Business Administration (FEAA), as a higher academic institution - on the one hand, and the National Research Institute for Electrochemistry and Condensed Matter (INCEMC) Timişoara, as a research-development institution - on the other hand, has reached toward a comprehensive level of communication and activation of NANO phenomena between the essential disciplines for the present and future of global-local society and technology (Global-Locale, GLOCAL scale): Nano-Chemistry, Nano-Physics, Nano-Biology, and Nano-Economy. Thus, NANO meant, following the presentations and the debates, not only the phenomena on the sub-micron scale, but also the production of macro-scopic effects through intelligent action (i.e. strategic) at the nano level: atoms, interfaces and radiation in the Nano- Physics, chemical bond, topology and molecular symmetry in Nano-Chemistry, along doses with chronic/acute effects and membranes in Nano-Biology (with extension in Biochemistry, Medicine, Pharmaceutical, and Ecology), and even to the respective distinctive advantage of apparent peripheral economic (R&D based) units and coopetition (cooperation + competition) of these for Nano-Economics (as the tech approach for Knowledge Economy). These topics were presented at a high scientific level and in working sessions with a consistent audience of guests with exceptional international expertise, with cross-disciplinary, multi-cultural, and multi-generational impact, such as: Pablo D. Esquinazi (*Felix-Bloch-Institute for Solid State Physics, University of Leipzig, Leipzig, Germany*) with a challenging and far-reaching theme (probably challenging among

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[†] The work presented at 2nd NANOMOD: Nano-Modeling of Strategic Materials for Knowledge Economy, 22-23 April 2019 are included in *New Front Chem 28 (**2019**) 1-66*

♣ Correspondent author: Tel: ++40-(0)256-466184/-592638, Fax: ++40-(0)256-592620, E-mails: mv_putz@yahoo.com, mihai.putz@e-uvt.ro the future Nobel laureates in Physics or Chemistry) related to the role of graphene interfaces in superconducting graphite at 300K; Valentin Paul Nicu ("*Lucian Blaga*" *University of Sibiu, Romania*), one of the few young world-class Romanian researchers (co-author of the Amsterdam molecular calculation program with Density Functional Theory) who recently chose a "come back" from the West, in Romania, with a computational approach to modeling vibrational circular dichroism (very important in the spectral determination of the percentage of chirality of a substance, with consequences related to toxicity); Ottorino Ori (*Actinium Chemical Research Institute, Rome, Italy*), already a devoted friend and collaborator of West University of Timișoara, Faculty-CBG and of NANO- research and development in Timisoara, through continuous collaborations over the last 10 years, with a theme related to establishing the connection between the network topology (of Carbon) extended, with curvature, torsion and defects - and the macroscopic properties (energies) manifested; Fanica Cimpoesu (*Institute of Physical Chemistry, Bucharest, Romania*) with a topic not generally addressed but very promising through nano-technological applications (especially in the light and LED technology industry), related to the molecular properties resulting from electronic configurations *non-aufbau* in Lantanide; Mugurel Țolea (*National Institute of Materials Physics, Bucharest-Magurele, Romania*) with a physical approach (in terms of specific Hamiltonians), recently published in the Physical Review of the American Institute of Physics, of the famous Hund rules of stability for the electronic states in atoms and molecules through the intra- and inter-layer spin interactions.

They were joined by colleagues, students and researchers from the *Timisiensis,* academic and research area, all animated and chaired by the Organizing Directors of the NANOMOD 2019 event, Mihai V. Putz (university professor of Chemistry, Master and PhD student in Management, scientific researcher degree I) and Corina Duda-Seiman (university lecturer, pharmacist doctor, graduate student in legal sciences, contractor), from FCBG, who also had their own transdisciplinary presentations in applied chemistry-physics, economics-chemistry, nano-technology, and cognitive pharmaceuticals (i.e. prospecting of drugs and their treatments by comparative analysis and even the proper drafting and international translation of drugs prospectuses). Not least, the presence of FCBG students from all Bologna cycles, Bachelor's degree in Chemistry, Master's Degree in Clinical Chemistry and Sanitary Laboratory, and doctoral and post-doctoral students of the Doctoral School of Chemistry at West University of Timișoara, with poster presentations - in -a special session of the program, highly appreciated in terms of format and content by those present. The organizers (West University of Timișoara with FCBG, FEAA; INCEMC-Timișoara; and the NANOMOD Directors 2019) have undertaken all the logistical, administrative, and personal efforts for a success of this event - in the justified and already shared hope that NANO-MOD will soon become truly the supporter and the primary dissemination ramp of the studies of the first Master of Research in NANO Chemistry and Advanced Materials from Timisoara and Romania, with international participation and impact, trans-disciplinary and trans-institutional, in-and-out, from, and through Alma Mater UVT, as a veritable *Magnet University*.

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Short Letter for Sci-Events

NATIONAL CONFERENCE OF DOCTORAL SCHOOLS FROM THE UNIVERSITY CONSORTIUM - CHEMISTRY SECTION, WEST UNIVERSITY OF TIMISOARA, 11–14 NOVEMBER 2019‡

Mihai V. PUTZ **(♣)**
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After a regrettable absence of the Doctoral School of Chemistry from the UVT at the 1st Edition of the Doctoral Schools of the University Consortium (31 October - 3 November 2018, Alexandru I. Cuza University from Iaşi), the presence at the Second Edition organized at the West University of Timişoara (11 -14 November 2019) was consistent (relative to the "rule" of about 3 participations from the Doctoral School at the National Conference of Doctoral Students of the University Consortium), being mainly oriented to the researches in the field of Bio-Chemistry: 2 papers focused on the study and applications of chitosan/chitinases (Ecotoxicological-biochemical studies on the effects of chitosan on *Lemna sp.*; "thermostable" Chitinases), a bio-informatics study (related to the computational prediction of the environmental effects of the oligomers resulted from the degradation of polyhydroxyalkanoates and polylactic acid), a study of general toxicity on some microorganisms (with a very exciting discussion about precursors vs. bio-markers of the studied toxicity), and a paper presenting the analysis of alginate-based membranes containing different active compounds for oral administration. On the other hand, the Doctoral Schools form Babes-Bolyai in Cluj and the University of Bucharest had presentations focused on organic nano-chemistry, while the Doctoral School form Ioan Cuza University in Iaşi addressed chemistry-bio-physics topics. In general, one can observe a

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UNIVERSITATEA „ALEXANDRU IOAN CUZA" din IAŞI

CONFERINŢA NAŢIONALĂ A
ŞCOLILOR DOCTORALE DIN
CONSORŢIUL UNIVERSITARIA

Biologie, Chimie, Geografie,
Geologie, Ştiinţa mediului

Timişoara
11-14 noiembrie, 2019

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‡ The works presented at National Conference of Doctoral Schools of Chemistry in "Universitaria" Consortium of Romania, 11-14 November 2019 are included in *New Front Chem 28 (**2019**) 67-107*

♣ Correspondent author: Tel: ++40-(0)256-466184/-592638, Fax: ++40-(0)256-592620, E-mails: mv_putz@yahoo.com, mihai.putz@e-uvt.ro reorientation of the advanced research in chemistry towards the transdisciplinary chemistry, with nano-sciences, nano- and bio-materials gaining a constant ground. The organization was of the “student” type, but with presentment in the West University of Timişoara headquarters, well promoted in the university space, with a select auditorium, even too select in certain work sessions;

Yet, the interaction of doctoral students from the doctoral schools of Biology and Chemistry of the University Consortium, grouped together also with alternative presentations, restored the atmosphere of multi- and cross-disciplinary debates, sustained with fervor by the present chairmen (Prof. univ. dr. habil. Carmen Mariana CHIFIRIUC, Prof. univ. dr. Ion GROSU, Prof. univ. dr. habil. Mihai PUTZ, Prof. univ. dr. m.c. from the Romanian Academy Cătălin TĂNASE, Prof. univ. dr. Otilia ZĂRNESCU) especially competent and close to the doctoral students and their work. Goodbye and see you in 2020!

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Short Letter for Sci-Events

”WEAPON OF MASS DESTRUCTION” (WMD) ISSUE: THE TIMISOARA CASE - NOVEMBER 2019[§]

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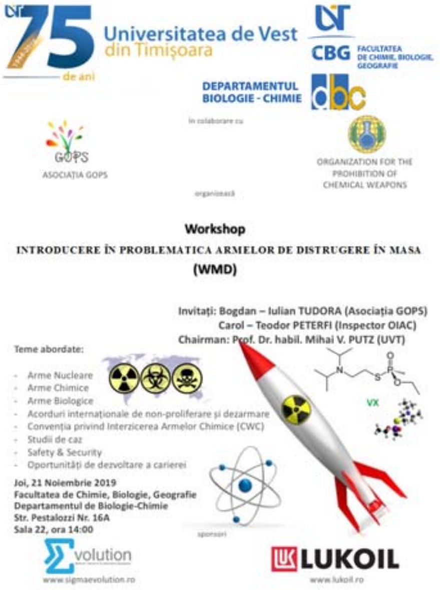
It was supposed to be a special event in the meaning of the presentation topic: weapons of mass destruction (chemical, biological, radiological, nuclear, and the newer – the cyber ones); and even so, the event’s organization, especially related to the choosing of the right title, in the economy of "politically correctness" for a presentation, even of the workshop’ type, at the academic level, has aroused a "creative tension": it is the topic so wide, current, interesting, impactful, and acknowledged to be assigned to a "field" of study? Or is it more appropriate to be introduced as an interrogative form (*quo vadis*?), or it may be seen as a refutation of the physical and life sciences in the sense of "unethical applications"? The internal pre-debate has turned in accepting the topic as "problematic" in the sciences! The guest lecturer, on the other hand, Chim. Tudora Bogdan-Iulian, graduate of Chemistry at the University of Bucharest, with a cross-disciplinary professional background, with a master's degree in applied psychology in national security issues (also at the University of Bucharest), with "on-going" educational projects under voluntary regime at GOPS –Romania (http://www.gops.ro/), but also as entrepreneur and general manager at Sigma Evolution SRL, and not least a contributor to OPCW (Organization for Prohibition of Chemical Weapon, https://www.opcw.org/), an organization already awarded with the Nobel Peace Prize in 2013 (https://www.nobelprize.org/prizes/peace/2013/press-release/), has pursued on a remarkable national effort to raise awareness of the university environment. In the WMD issue, especially


75 de ani
Universitatea de Vest din Timişoara
CBG Facultatea de Chimie, Biologie, Geografie
Departamentul Biologie - Chimie
în colaborare cu
GOPS Asociația GOPS
Organization for the Prohibition of Chemical Weapons
organizează

Workshop
INTRODUCERE ÎN PROBLEMATICA ARMELOR DE DISTRUGERE ÎN MASA
(WMD)

Invitați: Bogdan – Iulian TUDORA (Asociația GOPS)
Carol – Teodor PETERFI (Inspector OIAC)
Chairman: Prof. Dr. habil. Mihai V. PUTZ (UVT)

Teme abordate:
- Arme Nucleare
- Arme Chimice
- Arme Biologice
- Acorduri internaționale de non-proliferare și dezarmare
- Convenția privind Interzicerea Armelor Chimice (CWC)
- Studii de caz
- Safety & Security
- Oportunități de dezvoltare a carierei

Joi, 21 Noiembrie 2019
Facultatea de Chimie, Biologie, Geografie
Departamentul de Biologie-Chimie
Str. Pestalozzi Nr. 16A
Sala 22, ora 14:00

sponsori
Σvolution www.sigmaevolution.ro
LUKOIL www.lukoil.ro

[§] Presented at related Workshop CBG, Biology - Chemistry, Faculty of , 21 November 2019.

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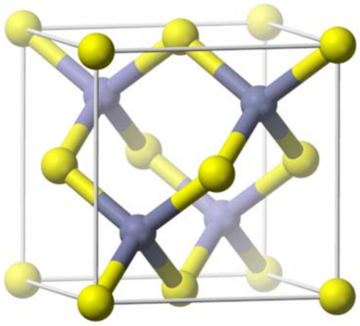
focused on the universities from the University Consortium (https://ro-ro.facebook.com/gops.ro/) - starting with the Western University of Timisoara (November 21, 2019), through the enchanting collaboration with Prof. dr. Mihai V. Putz.

The presentation was very dense, comprising practically 2 presentations; from Introduction to the History of WMD, Classification, Description of weapons of mass destruction (with 3 essential lists, distributed according to destination and accessibility: from military ones - List 1, to research ones - List 2, to those for industrial/economic use - List 3), the International Legislation in the field and the ratification phases (transposition into national laws), to case studies, and even to career development opportunities - the latter exposed in a true motivational discourse addressed to students (sincerely fascinated by presentations, especially from Biology specializations). But, beyond all that, what it supposed to be an interesting, fascinating, even courageous presentation for many, has become more than necessary, especially in the part of the discussed case studies, in the unhappy context of including Timisoara on the map of "national victims of chemical weapons with potential for mass destruction"! No more, no less, our guest stayed near the Faculty of Chemistry, Biology, Geography, in the Student Complex, just opposite the "death block", on Miorița Street. As a consequence, he changed the prepared case studies, in this case the Syria and the Skipal cases, with the new case study: "Timișoara, November 2019". The fatal aluminum phosphide, the central component of the Delicia-GASTOXIN product, (attention!) with marketing authorization in Romania (but only to authorized persons), is classified by ECHA (European Chemical Agency, https://echa.europa.eu/ro/home) as being fatal when swallowed, or when the released phosphine is inhaled, being nevertheless toxic to skin contact, very toxic to aquatic life, while, when in contact with water generating flammable gas that can ignite spontaneously. It must therefore be administered under strict authorization, with precise and mandatory information of those directly involved, along with many other procedures for the safety of administration and dosing (including by mixing with other substances in order to inhibit the released gases, considering the surface, time and type of exposure, etc.). But what is even more interesting, following the case study, appears especially in the management of managing such a crisis:



The National Toxicological Information Registry (ReTox) has just been established in the summer of 2019 (http://retox.registre-insp.ro/user), and it is intended to be a key element within the National Poison Monitoring and Toxicological Information System (SNMIIT) coordinated by the National Institute of Public Health (INSP), and which is related to "Toxicological Emergency Information" within a strict time interval (https://www.insp.gov.ro/index.php/biroul-rsi-si-informare-toxicologica) and which, un-inspirational, has been proven “not responding to emergencies”. In this management of national emergency calls, it is therefore desirable that in the chain of "112 connections" one should add with necessity also the service of emergency toxicological information, with specialized guidance and coordination of this type of crises, from the first phases of triggering. Otherwise, even substances which appear to be non-acute can become acutely dangerous at uncontrolled doses and time flowing. From here, and as a result of this unfortunate event, a new role of the academy emerges: *studying and/or introducing the issue of weapons of mass destruction as an area of a constant (pre)occupation now*, in the millennium in which Chemistry is more than ever part of The Circular Economy, which instead, as on any recycling, it can introduce new and new errors in the system, once each new "loop". It remains for West University of Timişoara and the Faculty of Chemistry, Biology, Geography to assume this role through future and periodic seminars, summer schools, courses and perhaps even trans-disciplinary specialties (chemistry-biology-physics) in order to control and reduce "to zero" as an ideal of circulation/use/recirculation of substances/compounds with toxic potential, as new organic, artificial and new nano-materials syntheses constantly emerge.