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Abstracts

for

13th Scientific Session of Undergraduate, Masters and PhD Students, Iasi, Romania

October, 28, 2022

TABLE OF CONTENT

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C1. Synthesis of new fused heterocycles as potential anticancer agents

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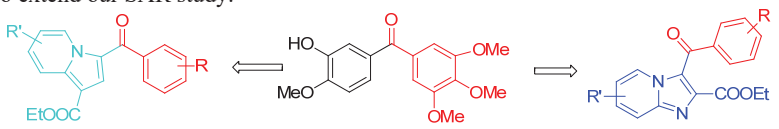
The fusion of two or more heterocycle rings results in different classes of compound, and fused heterocycles containing a pyridine ring are showing a broad range of properties including biological activity [1]. Among fused pyridine-heterocycles, the unique indolizine scaffold became an important system for the development of potent new drug candidates in medicinal chemistry [1]. Imidazopyridine heterocyclic system also acts as a key pharmacophore motif for the identification and optimization of lead structures to increase medicinal chemistry toolbox [2].

Recently, several indolizines have been reported to possess excellent anticancer activity and good tubulin polymerization inhibitory potency. Inspired by these results, the goal of this study was to synthesize several new 6, 7 and 8-substituted indolizine derivatives to have deeper insights regarding their anticancer activity. Therefore, our study started with 3-bromopyridine and ethyl isonicotinate in order to obtain new indolizines to be tested for their anticancer activity.

On the other hand, we also investigated the possibility to obtain several substituted imidazo[1,2-*a*]pyridine using ethyl cyanoformate as dipolarophile in [3+2] cycloaddition reactions, in order to extend our SAR study.



The structures of the new compounds (monoquaternary salts and fused pyridines) were proved using spectral methods. All new derivatives will be evaluated for their antiproliferative properties.

Keywords: dipolar cycloaddition, indolizines, anticancer.

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References:

[1] Amariucai-Mantu, D., Antoci, V., Sardaru, M.C., Al Matarneh, C.M., Mangalagiu, I.I., Danac, R., *Phys. Sci. Rev*. (2022), in press; https://doi.org/10.1515/psr-2021-0030.

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C2. Peculiarities in the chemical behavior of 1,3-bis(2-aminoethylaminomethyl)tetramethyldisiloxane

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The siloxane bond confers unique physico-chemical characteristics to the compounds based on it due to its double covalent - ionic dual character. The siloxane angle and the high bond length values give the structure conformational flexibility, while the methyl groups, which are highly nonpolar and attached to the silicon atoms at a great distance (1.87 Å), have freedom of rotation around the siloxane skeleton, giving the compound high hydrophobicity, low surface energy, and viscosity. The siloxane bond can be split by an ionic mechanism, in acidic or basic environment, and functions from the organic groups attached to the silicon atoms can also be affected. The instance of 1,3-bis(2-aminoethylaminomethyl)-tetramethyldisiloxane (SFA), a possible precursor for the creation of novel Schiff bases with siloxane spacers acting as ligands for metal ions, is discussed here [1]. The formation of a large variety of compounds was revealed to be possible depending on the reaction conditions (Figure 1).

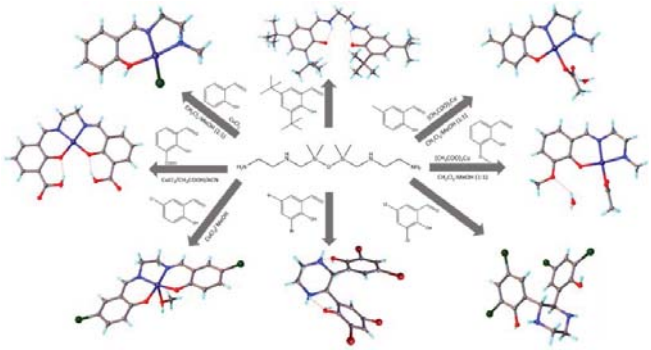

Figure 1. *SFA fragmentation products in systems involving different aldehydes and metal salts.*

The resulting compounds were isolated and thoroughly described, and theoretical quantum mechanics simulations were used to examine the electronic effects that appeared in the siloxane bond and caused some bonds in the molecule to break depending on the reaction media. These chemicals' production processes have been put forth.

Keywords: siloxane, amine, aldehyde.

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C3. The correlation between the number of police series with the desirability of participation in an optional of introduction in forensics of some students from Arad

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There is a large consensus across the literature regarding the crucial role played by the television in forming the youngsters' beliefs, attitudes and values. Adolescents usually turn to television for entertainment but they also get a considerable amount of information from what they watch. It was proven that television is an important source of information for adolescents and has the potential of introducing them to careers that they wouldn't have considered earlier. There were proposed two theories regarding the mechanism television exerts on youngsters about the way they develop values and aspirations related to labour market: cultivation theory and wishful identification. [1]

Curriculum at the school's decision (C.S.D.) is characterized by educational freedom and curricular flexibility [2]. Thus, it was verified the desire of a group of 113 students from Arad to participate in an optional course entitled "Introduction to Forensics" and if it will be included in the students' timetable. The students gave marks from 1 to 5, where 1 means that they do not want to participate and 5 that they would participate regardless of the number of hours in their timetable (Table 1) [3].

Table 1. Marks given by the students.

Mark	Students' number	Students' percentage (%)
1	8	7
2	6	5
3	8	7
4	13	12
5	78	69

Keywords: optional, television, forensics

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C4. Binding of transition metal ions to an amyloid-like short peptide

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Peptide and protein aggregation is a common manifestation of several diseases, primarily neurodegenerative disorders. Short-model peptides are extensively researched with the goal of understanding fundamental and widespread mechanisms governing peptide self-assembly. Furthermore, a substantial amount of data points to the involvement of transition metal ions, such as Cu(II), in the occurrence of neurodegenerative disorders through a variety of processes including the disruption of the aggregation mechanism [1,2].

Herein, a solid-phase peptide synthesis strategy was employed to obtain the amidated form of the FESNF (where F-phenylalanyl, E-glutamyl, S-seryl, N-asparaginyl) pentapeptide. Reversed-phase high-performance liquid chromatography (RP-HPLC) was successfully used to isolate and purify the peptide. The molecular weight of this peptide was confirmed using Matrix-Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry (MALDI ToF MS), whereas its primary sequence was established by tandem mass spectrometry (MS/MS).

The peptide behavior after incubation at several pH values (5.5, 7.4, and 8.2) was investigated using atomic force microscopy (AFM). It was found that both buffer systems used, tris(hydroxymethyl)aminomethane and ammonium acetate solutions, with pH values of 5.5 and 8.2, respectively, create a suitable environment for peptide self-assembly into long, homogenous, and distinct fibrils.

In the presence of a PIPES (1,4-piperazinediethanesulfonic acid) 30 mM buffer solution at pH 6.5, the peptide forms a complex with Cu^{2+} ions characterized by an absorption maximum, at 225 nm. Moreover, in presence of sodium acetate 50 mM at pH = 7, the interaction with Cu^{2+} ions at different concentrations ranging from 25 to 1540 μM was emphasized by fluorescence quenching at the emission wavelength of 282 nm.

Thus, AFM images reveal a strong fibrillation tendency of the peptide, and UV-Vis and fluorescence studies confirm the peptide's ability to interact with Cu^{2+}.

Keywords: peptide, self-assembly, AFM, fluorescence.

Acknowledgments: The authors acknowledge support from the Romanian Government through UEFISCDI, funding reference number PN-III-P2-2.1-PED2019-2484 ("Bioinspired Peptide-based Scaffolds Assemblies", Bio-PASCAL).

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C5. OH-tracer versus OH-scavenger use in the gas-phase kinetic study of the methyl-butenols ozone-initiated reactions

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Significant amounts of OH radicals are generated during the ozonolysis of unsaturated volatile organic compounds via unimolecular decomposition of the zwitterionic carbonyl oxide intermediates known also as Criegee intermediates [1]. Use of an OH-scavenger diminishes the uncertainties due to secondary reactions which might occur during such investigations in the gas-phase. Often, the performance of the analytical instrumentation can be dramatically affected at the level of the OH-scavenger concentration which is at least three orders of magnitude higher than that of the reactant and/or reference compounds.

Within the present work, the gas-phase ozonolysis rate constants of three methyl-butenols were measured at 298 K and 1 bar total pressure of synthetic air using the ESC-Q-UAIC reaction chamber facilities. To limit and correct for secondary reactions initiated by OH radicals during the kinetic investigations two different approaches were involved during the experiments: (i) use of carbon monoxide (CO) and 1,3,5-trimethylbenzene (TMB) as OH-scavenges at concentrations level of 10^{15}-10^{16} molecule×cm^{-3} and (ii) use of TMB as an OH-tracer at concentrations level of 10^{13} molecule×cm^{-3} to assess the contributions of the OH-initiated secondary reaction for further kinetic-driven corrections. The efficiency of the corrections and advantages of the use of OH-tracer are discussed.

Keywords: methyl-butenols, ozone, gas-phase rate coefficients, scavenger, tracer.

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C6. Organic materials for layered hybrid perovskite photovoltaics

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Layered hybrid perovskites are based on organic spacers separating hybrid perovskite slabs [1]. To address the challenge of moisture stability of LHPs (layered hybrid perovskites), hydrophobic organic spacers with anthracene, benzothiadiazole and perfluoroarene based compounds (Figure 1) were investigated.

Specifically, this involved studying n = 1 systems as they form well-defined 2D phases, unlike higher n > 1 compositions that form mixed 2D phases. The spacers studied were the iodides and bromides of anthracene-9-ylmethanaminium (**ANTI** and **ANTBr**), anthracene-9,10-dimethanaminium (**DANTI$_2$** and **DANTBr$_2$**), benzo[*c*][1,2,5]thiadiazol-4-ylmethanaminium (**BTDZI** and **BTDZBr**), (perfluorophenyl) methanaminium (**PFMAI** and **PFMABr**) and (perfluoro-1,4-phenylene) dimethanaminium (**PFDMAI$_2$** and **PFDMABr$_2$**). The monofunctional compounds were expected to form Ruddlesden-Popper phases, while the bifunctional compounds should form Dion-Jacobson phases.

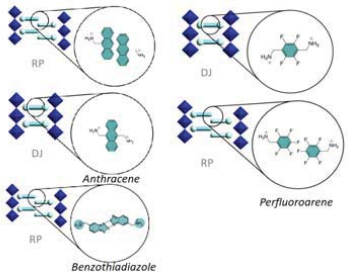

Figure 1. *Organic spacer molecules employed in this study.*

Moreover, their behaviour was probed in humid environments to reveal nanoscale segregation of layered perovskite species based on PDMA and F-PDMA components, along with enhanced stabilities of perfluoroarene systems, which is relevant to their application (perovskites solar cells) [1].

Keywords: LHP, organic spacers, stability.

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C7. A new series of pyridine derivatives as anticancer agents: design, synthesis and biological evaluation

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Cancer is one of the most important health problems worldwide because it is deemed to be the second major cause of mortality throughout the world after heart disease [1]. Therefore, there is a continuous demand for developing an effective anticancer drug.

Azaheterocycles are compounds of great importance in the pharmaceutical and health industries. Pyridine derivatives belong to the family of azaheterocycles and are known to have multiple biological activities such as antibacterial, anti-inflammatory, antifungal and anticancer properties [2-4]. In an attempt to develop new anticancer agents, we synthesized a new series of 2-amino-3-cyanopyridines, which have been tested for their anticancer activity against a panel of 60 human cancer cell lines at National Cancer Institute, Germantown, MD, USA. The newly synthesized compounds proved to be effective inhibitors of cancer cell growth.

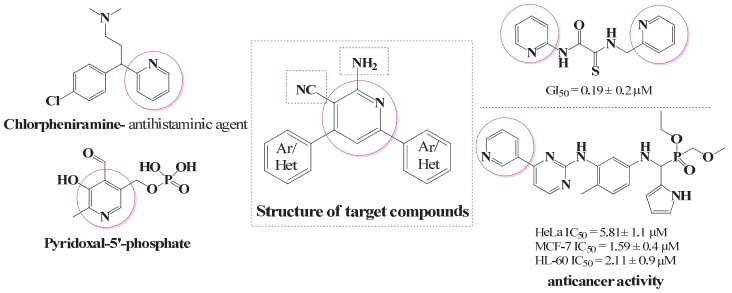

Figure 1. Biologically active pyridine derivatives and general structures for the newly synthesized compounds

Keywords: azaheterocycles, pyridines, anticancer agents.

Acknowledgments: The authors also thank the CERNESIM Center within the Interdisciplinary Research Institute at "Alexandru Ioan Cuza" University of Iasi, Romania for the infrastructure used in recording NMR experiments.

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C8. New indolizin-1-yl-chalcone hybrids as antifungal and anti-inflammatory agents: synthesis and biological evaluation

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The seeking for new compound capable of fighting pathologies related to microorganisms has always been one of the foundations of medical research. *Candida albicans* is an opportunistic unicellular yeast which develops over time resistance to conventional antifungal therapies, thanks to the emergence of new resistant strains. *Candida albicans* is responsible for most hospitalizations due to fungal infections [1]. Thus, the development of new therapeutic approaches is a major research challenge.

Compounds from the chalcone family have been used, over time, due to their biological activities they possess: anticancer, antiviral, antimalarial, antimicrobial, anti-inflammatory [2]. On the other hand, 3-acetylindolizine derivatives are of interest due to their versatility as key intermediates in organic synthesis [3] and as the first dual inhibitors of tubulin polymerization and farnesyltransferase [4]. Also, 3-aroylindolizines are important compounds in our research group, due to their applicability in medicinal chemistry. We are mainly interested in obtaining new compounds with multiple biological activities: anticancer or antifungal and anti-inflammatory.

Therefore, the objective of this study was to develop new indolizine-chalcone hybrids (with the units described above) as antifungal and anti-inflammatory agents and increase their bioavailability for the use of compounds in the field of pharmaceuticals. This family of compounds has been biologically evaluated against *Candida Albicans* (*in vitro* and *in vivo*) and for their anti-inflammatory effect caused by infection.

Keywords: *Candida albicans*, chalcone, indolizine, antifungal, anti-inflammatory.

Acknowledgments: The authors thank the CERNESIM Center within the Interdisciplinary Research Institute at „Alexandru Ioan Cuza" University of Iasi, Romania for the infrastructure used in recording NMR experiments.

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C9. Novel benzo[*f*]quinoline derivatives with antimicrobial properties

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Benzo[*f*]quinoline represents an azapolynuclear heterocycle, being a blue fluorescent emitter due to extended π-π conjugation [1]. Benzo[*f*]quinoline derivatives are described in the literature as potent biomolecules, with various biological properties, especially antimicrobial and anticancer activity [2]. Some of the analogs of this heterocycle could be used as organic light emitting devices (OLED) [3].

Having in view the above mentioned, our main objective was to synthesize novel benzo[*f*]quinoline derivatives adopting a general and straightforward strategy involving two steps only: quaternization and [3+2] cycloaddition reactions. The structures of benzo[*f*]quinoline derivatives were proved using NMR experiments (^{1}H, ^{13}C, 2D-correlations). The NMR apparatus is equipped with a 5 mm Broad-band Observe (BBO) detection probe, operating at 500.1 MHz for ^{1}H and respectively 125.7 MHz for ^{13}C nuclei. In the ^{1}H and ^{13}C spectra, chemical shifts are reported in δ units (ppm) relative to the residual peak of solvent (ref: DMSO-d_6/$CDCl_3$, ^{1}H: 2.50/7.26 ppm; ^{13}C: 39.52/77.16 ppm for salts/cycloadducts).

The *in vitro* antimicrobial activity of benzo[*f*]quinoline derivatives was determined by the disk diffusion Kirby-Bauer method, using nutrient agar medium (Mueller Hinton agar for antibacterial tests and Sabouraud agar for antifungal tests). The antibacterial activity was evaluated against two bacterial strains (Gram-positive/negative *Staphylococcus aureus ATCC 25923*/*Escherichia coli ATCC 25922*) and the antifungal activity against fungus *Candida albicans ATCC 10231*.

Keywords: benzo[*f*]quinoline derivatives, quaternization, [3+2] dipolar cycloaddition, antimicrobial properties.

Acknowledgments: Grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P4-ID-PCE-2020-0371, within PNCDI III. POC/448/1/1 Research infrastructure projects for public R&D institutions/Sections F 2018, through the Research Center with Integrated Techniques for Atmospheric Aerosol Investigation in Romania (RECENT AIR) project, under grant agreement MySMIS no. 127324. Authors are also gratefully to CERNESIM center, for NMR and IR experiments.

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C10. First insights into atmospheric bioaerosols from the Iasi urban area

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Materials and chemicals released in the atmosphere by various organisms (plants, animals, bacteria, fungi etc.) comprise the fraction known as primary biological aerosol particles or bioaerosols.[1]. Early and reliable detection of pathogenic microorganisms existent in atmospheric biological aerosol particles is of utmost importance especially in terms of the requirements derived from the need to identify their potential hazardous effects [2].

The present work represents the first attempt in revealing microbiological features of specific primary biological aerosol particles collected at the Air Quality Monitoring Station (AMOS) from the "Alexandru Ioan Cuza" University of Iasi, Romania. Sampling of aerosol particles was carried out using a cascade impactor operable at low pressure (DLPI Dekati) consisting of 13 stages collecting particles in the size range 0.0276 μm – 9.94 μm. Luria Bertani (LB) nutritionally rich medium was used for investigations performed either directly on the collected particles or on diluted samples. Gram staining technique was used to differentiate between Gram-positive and Gram-negative bacteria. Actinomycetes were stained by using the fuchsine dye, while the fungi by using Gentian Violet solution. Type S bacterial colonies (smooth and shine surface) were mainly identified on prepared nutritionally rich medium Petri dishes. In the investigated smears Gram-positive or Gram-negative bacteria, cocci or bacilli were often identified. Microscopic analysis of the smears indicated also the presence of fungal-like spores and hyphae. The present investigations bring evidences that atmospheric particles, through their surface, are carriers over long distances of substantial bacteria and other biological forms. Their potential role in various atmospheric processes or capacity to act as linkers between various geographically isolated microbial communities will be a subject of further investigations.

Keywords: bioaerosols, bacteria, fungi, urban area

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C11. Gas-phase ozonolysis of three *cis*-3-hexenyl esters under simulated atmospheric conditions

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Biogenic volatile organic compounds (BVOCs) represent about 90% of the total emission of volatile organic compounds into the atmosphere [1]. While in the atmosphere reactions with OH radicals may be the predominant degradation pathways for unsaturated esters, reactions with O_3, especially those occurring in polluted areas, can represent also a significant atmospheric sink process [2].

In this study, the rate constants for the gas-phase reactions of O_3 with three *cis*-3-hexenyl esters at (298 ± 2) K and (1000 ± 5) mbar pressure of synthetic air were evaluated using the relative kinetic technique and the 760 L ESC-Q-UAIC atmospheric simulation chamber. For the purpose of the present study three reference compounds have been used. The reference compounds and their rate coefficients (in cm^3 $molecule^{-1}$ s^{-1}) were: isoprene ($k = 1.28 \times 10^{-17}$), *E*-2-butene ($k = 2 \times 10^{-16}$) and propene ($k = 1.06 \times 10^{-17}$). The long path FT-IR technique was used to monitor the reactants and reference decay in the reactor during the kinetic investigations. Wall loss and photolysis rates for all three hexenyls were measured prior initiating the reactions with O_3 in order to correct the analytes decay.

The obtained gas-phase ozonolysis rate constants (in cm^3 $molecule^{-1}$ s^{-1}) were $(4.55 \pm 0.65) \times 10^{-17}$ for *cis*-3-hexenyl formate, $(5.56 \pm 0.81) \times 10^{-17}$ for *cis*-3-hexenyl acetate and $(8.00 \pm 1.18) \times 10^{-17}$ for *cis*-3-hexenyl isobutyrate, respectively. The results obtained in the present study are discussed to assess the impact of these reactions concerning photochemical species and SOA generation. Comparison with other relevant literature data and structure-activity related estimates is also provided [3].

Keywords: gas-phase kinetic, ozonolysis, *cis*-3-hexenyl esters.

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C12. Mass spectrometry-based molecular profile evaluation for new insights into the atmospheric aerosols

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Besides the targeted analysis methods, the large number of unknown compounds in the atmospheric aerosols requires a suitable approach to reveal relevant changes of the organic aerosol concentration and composition [1,2].

The present study investigates the composition of the organic fraction in urban atmospheric aerosols using targeted and non-targeted approaches of liquid chromatography coupled with time-of-flight mass spectrometry. Size-resolved aerosol samples were collected weekly, from July to December 2018 at the Air Quality Monitoring Station (AMOS) from the "Alexandru Ioan Cuza" University of Iasi, using a 13 stages cascade Dekati Low-Pressure Impactor (0.0276-9.94 μm size range). The MS data files of the aerosol samples were processed together in one experiment file using the open-source software MZmine and the automated data analysis pipeline for chromatogram deconvolution. The molecular formulas of the unknown compounds were estimated using the measured exact mass, isotopic signature and constrained elemental ratios. After workflow optimization, the exact mass, molecular formula, retention time, and peak area of the compounds in each sample were obtained. Finally, the molecular fingerprints of aerosol samples were evaluated after classification into the molecular formula groups (CHO, CHNO, CHOS, and CHNOS). The normalized abundance of the CHO molecular group presented a significant correlation with the target phthalic acid, suggesting that the anthropogenic and secondary processes influence the atmospheric aerosols from the investigated area. Additionally, a global unimodal size distribution was observed for CHO group, with maxima at 0.381 μm.

The presented approach of molecular non-targeted analysis provides a deeper insight into relative abundance variation of a large number of biogenic and anthropogenic origin compounds in the atmospheric aerosols.

Keywords: organic aerosols, mass spectrometry, MZmine.

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P1. Microemulsion-based controlled codelivery system of fluorouracil and ibuprofen

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A microemulsion is a mixture of oil, water, surfactant, and frequently a cosurfactant. Scientists are increasingly interested in microemulsions due to their potential to act as drug delivery systems since they are highly soluble, transparent, thermodynamically stable, simple to prepare, have a high diffusion and absorption rate compared to solvents without surfactants, and last but not least, can incorporate a wide range of drugs [1,2].

The purpose of this study was the coencapsulation of fluorouracil (FU), an anticancer drug, and ibuprofen (IBU), an anti-inflammatory drug, in a microemulsion (ME)-based nanosystem in order to potentiate the effect of FU based on a synergistic effect. By using the phase titration method, MEs were created using Maisine CC as the oil phase, Tween 20 as the surfactant, and ethanol as the cosurfactant. The total drug content was 2 % (weight ratio of 1:1, drug:oil).

Samples were characterized by DLS (size, polydispersity index, and Zeta potential). The results revealed average sizes between 146 and 250 nm (PDI of 0.1 – 0.35) and zeta potential of -15 – -19 mV, depending on composition. NMR spectroscopy was used to assess the microemulsion type: oil/water, bicontinuous or water/oil. Diffusion-Ordered NMR spectra were recorded and the self-diffusion coefficients were calculated for water and oil in each sample. According to literature data, if there is a difference of at least one order of magnitude between the self-diffusion coefficients of water and oil, small particles are suggested to exist, whereas if the self-diffusion coefficients of the components are similar, a bicontinuous structure exists. Even more, the O/W or W/O microemulsion type can be determined from the difference between the self-diffusion coefficients. Thus, if the self-diffusion coefficient of oil is much smaller than that of water, the microemulsion is O/W, the W/O microemulsion being the reverse case [3-5]. After analyzing the DOSY spectra and calculating the self-diffusion coefficients, we concluded that the type of microemulsions is oil in water. The controlled release of drugs was investigated by dialysis method for 24 h. The released amount was determined by UV-Vis and HPLC based on the absorption at 266 and 221 nm for FU and IBU, respectively.

Keywords: microemulsion, fluorouracil, ibuprofen.

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P2. Investigations on the gas-phase kinetics of the OH radical initiated oxidation of selected nitrotoluenes

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Nitroaromatic hydrocarbons represent one of the most important classes of gas-phase pollutants directly emitted or formed in the atmosphere. Their presence is a result of primary anthropogenic activities such as biomass burning, vehicle exhaust, coal combustion, etc., or secondary gas-phase products formation following the photooxidation of other aromatic hydrocarbons. Most of these compounds have toxic, carcinogenic, and mutagenic properties and can affect air quality and human health [1]. Direct photolysis of 2-nitrotoluene is thought to produce secondary organic aerosols and HONO through a mechanism similar to that proposed by Bejan et al. (2006) [2]. To our knowledge, there is only one kinetic study of the OH radical-initiated gas-phase reaction of 3-nitrotoluene [3].

The ESC-Q-UAIC simulation chamber was used to investigate kinetic rate coefficients of 2- and 4-nitrotoluene. It consists of three cylindrical quartz tube with a volume of 760 L and a total length of 4.2 m. Investigations were performed at 298 K and 1 atm of synthetic air using FTIR spectroscopy at a total optical path length of (492 ± 1) m. The spectra were collected at a resolution of 1 cm^{-1}. The OH radicals were generated through the photolysis (365 nm) of methyl and isopropyl nitrite. The wall loss and photolysis were investigated to asssess their influence on the gas-phase decay of nitrotoluenes. The rate coefficients for the gas-phase reactions of 2- and 4-nitrotoluene with OH radicals were measured using the relative method, for which dimethyl ether and cyclohexane were used as reference compounds.

The determined rate coefficients for the gas-phase reaction of nitrotoluenes with OH radicals will be compared with the values estimated by Structure-Activity Relationship kinetic approach. The atmospheric implications would be also assessed and the potential impact on the regional scale discussed.

Keywords: nitroaromatics, gas-phase kinetic, OH radical, simulation chambers.

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P3. Investigations of the p-tolualdehyde gas-phase reaction rate coefficient with oh radicals

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The oxygenated aromatic hydrocarbons (OVOCs) are ubiquitous compounds present in the atmosphere. While their presence in urban environment is related with the anthropogenic activities, OVOCs are included also as constituents of biomass burning and wildfire emissions. Tolualdehydes reach the atmosphere both as primary pollutants, emitted by industrial processes and as secondary pollutants from reactions of aromatic hydrocarbons with tropospheric oxidants. The atmospheric degradation of *p*-tolualdehyde could lead to photooxidants formation and secondary organic aerosols (SOA). The daytime gas-phase removal processes of *p*-tolualdehyde are mainly represented by reactions with OH radicals and direct sunlight photodegradation [1].

In this study, the kinetic rate coefficient for the reactions of *p*-tolualdehyde with the OH radicals was determined under simulated atmospheric conditions. The ESC-Q-UAIC reaction chamber unit, a cillindrical quartz-made reactor with a total volume of 760 L connected to a long path FT-IR technique, has been used for present kinetic experiments. An external White type multiple reflection optical system helps to achieve a total pathlength of (492±1) m inside the ESC-Q-UAIC chamber. The OH radical was produced through the methyl nitrite photolysis at λ_{max}=365 nm. Propene and cyclohexene have been used as reference compounds in present investigations. The wall loss was measured to correct the *p*-toluadehyde decay. The photolysis was tested to evaluate the possible interferences.

For the reaction of *p*-tolualdehyde initiated by OH radicals, an average rate coefficient value of $(1.60\pm0.27)\times10^{-11}$ cm^3 $molecule^{-1}$ s^{-1} was obtained, with an associated atmospheric lifetime value of 15.3 hours.

Keywords: tolualdehyde, gas-phase kinetic, OH radical, simulation chamber.

Acknowledgement: The study was carried out with the financial support provided by the project PN-III-P2-2.1-PED-2019-4972 (PHONIC-HONO-SOA) and PN-III-P2-2.1-PED2021-4119 (SOA-REACTOR) from UEFISCDI. Also, recognition is given to the RECENT AIR project under the MySMIS grant agreement no. 127324

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P4. The synthesis and characterization of tricalcium phosphate doped with Ag and Zn used as a biomaterial

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In recent years, considerable attention has been paid to the introduction of bio-ceramics in medical applications due to their resistance to grinding, better compression and relatively low density and weight. To combat postoperative infections, silver has been proposed as an antimicrobial agent and as an additive to tricalcium phosphates, its presence favoring the process of tissue reconstruction and wound healing [1]. Silver has been intensively studied as an antimicrobial agent for a wide spectrum of bacteria due to its low toxicity. An antimicrobial effect was observed with *Staphylococcus aureus*, which is one of the most frequent infectious agents that appear after the implant is performer [2]. Zinc is important due to its stimulating effect on bone formation in vitro and in vivo, but it is also used as a drug transportation for its slow release, speeding up the patient's healing [3].

In the present study, undoped and Ag- and Zn-doped tricalcium phosphate (β-TCP) samples: $Ca_{3-x}Ag_{2x}(PO_4)_2$ and $Ca_{3-x}Zn_x(PO_4)_2$ (x =00.3) respectively were obtained by the co-precipitation method, using as precursors $(NH_4)_2HPO_4$, $Ca(NO_3)_2{\cdot}4H_2O$, $AgNO_3$ and $ZnCl_2$ synthesized at different temperatures of 700 and 900°C, respectively. The structure of the synthesized samples was investigated by X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR), the textural properties were analyzed by the BET (Brumauer-Emmett-Teller) technique, and the morphology of the samples by scanning electron microscopy (SEM). The FTIR spectra indicated the presence of specific bonds from tricalcium phosphate. From the XRD analysis of the undoped samples, a structure specific to β-TCP was obtained (hexagonal structure - G.S. R-3c), but in a smaller proportion a second phase is also observed specific to hydroxyapatite (hexagonal structure - G.S. P63/m). From the XRD analysis of the sample doped with Ag, the appearance of two majority phosphate phases, these being β-TCP and Ag_3PO_4 respectively, was observed, while Zn doping of tricalcium phosphate favors the formation β-TCP type monophasic structure. From the SEM analysis of the doped samples, it was observed that the silver-doped samples present acicular microcrystals, while in the case of the zinc-doped samples porous samples are obtained.

Keywords: doped tricalcium phosphate, coprecipitation, biomaterial.

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P5. Investigations on particle formation numbers resulted from electronic cigarettes using a newly developed device

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Tobacco use is of huge concern regarding the global human health. The tobacco smoke is a major cause of morbidity from cancer, cardiovascular and respiratory diseases. Electronic cigarettes have recently become very popular among the population, being considered less harmful than classic cigarettes. This aspect is maintained by the motivation to keep smoking and replacing the classic way of inhaling the smoke produced by burning tobacco, with the use of electronic cigarettes [1].

In this study the vaporization of *e*-liquid was found to produce particles. Using a system consisting of an Evolv DNA 250C controller connected to an atomizer the produced particles were analysed by using a 6-channel Kanomax particle counter. The heating coils material made by Ni200 (Ni>99%) and SS316L were used to compare the effect on particles formation. Although the particles were recorded for all 6 channels, the significant results were obtained for PM0.3; PM0.5; PM1 and PM3. In this investigation we compared the particle formation number for different ratio of vegetable glycerine and propylene glycol. The effect on the particle formation from the use of mentholated liquid, sweet liquid and tobacco liquid has been also investigated when different coil material and base aroma were used.

Preliminary results show the influence of coil material, temperature, composition of *e*-liquid and aroma on the number of particles formation.

Keywords: electronic cigarette, e-liquid, particle numbers, aerosol formation

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P6. Studies on the NO_2, O_3 and formaldehyde detection using newly developed sensor device

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The entire world is currently facing remarkable challenges in terms of air quality degradation. Air quality in urban and densely populated areas is of a serious concern due to high concentrations of pollutants and the health hazards they induce. People spend most of their free time indoors, which contributes significantly to the total human exposure to air pollutants. Indoor air pollution includes both pollutants entering from outside and indoor emission sources. Due to their harmful effects on health as well as the continuous degradation of the environment, there is an increased demand to have developed new devices to detect and monitor air pollutants. New devices requiring as less as possible interferences, robustness and accuracy, financial accessibility and easy to handle features must be developed nowadays. The well recognized advantages of high performance measuring devices (*e.g.*, PTR-TOF-MS, HPLC, GC, monitors) are surpassed by their very high costs and low mobility [1].

The present work highlights experimental features for a newly developed device containing three sensors for the measurement of O_3, NO_2 and HCHO with atmospheric interest in the urban and semi-urban atmosphere. The instrument prototype was built using individual off-the-shelf electronic components connected together on a perfboard. The "brain" of the device was an Arduino development board, on which a custom program was loaded, to "bring the device to life". The prototype of this device is available as a portable tool that is easy to use and robust as possible. Preliminary correction factors on sensors were measured against the FTIR technique employing the advanced ESC-Q-UAIC simulation chamber from the CERNESIM center. First measurements in urban and semi-urban environments are already available. The sensors have proven to be good alternatives for conventional measuring instruments, offering a number of advantages, the most important of which are portability and low costs.

Keywords: sensors, ozone, NO_2, formaldehyde, atmospheric pollution.

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P7. New glycosidic derivatives with heterocyclic skeleton

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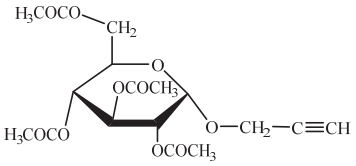
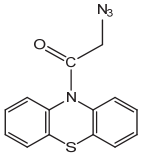
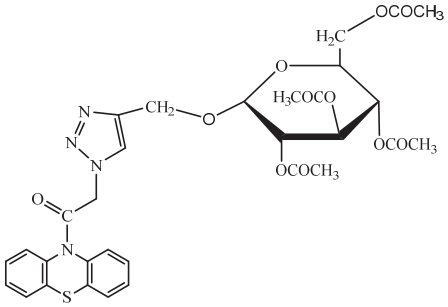
Glycosides are component parts of the structures of natural products with a role in biological processes, being recognized as chiral substances in the synthesis of glycosides. Glycosidic compounds containing in their structure *β*-aminoglycoside bonds are substances with various pharmacological activities, one is of antibiotic [1, 2]. Due to the high stability of the triazole rings against metabolic degradation and also due to their increased solubility in water, the glycosidic compounds containing a triazole rest have aroused the interest in the detailed study of their properties related to the inhibitory activity for neurodegenerative diseases, but also for their biodegrability[3, 4]. Given our interest in triazole derivatives, we have proposed the synthesis of glycosidic compound with *aza*hetherocyclic units (**III**), different synthesis strategies being approached in order to obtained it. The propargyl derivative **I**, was obtained from *β*-pentaacetylglucose in reaction with propargylic alcohol. Azidic derivative with phenothiazinic skeleton (**II**) was obtained by phase transfer catalysis from *N*-chloroacetylphenotiazine, sodium azide and catalytic amounts of tetrabutylammonium bromide. All synthesized compounds were purified and physically and spectrally characterized (IR, ^{1}H-NMR, ^{13}C-NMR, 2D, MS).



Propargylic derivative **I**



Azidic derivative **II**



Glycoside with *aza*heterocyclic unit **III**

Keywords: azide; 1,2,3-triazole; dipolar cycloaddition; glycosides.

Acknoledgements: The authors are grateful to the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra.

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P8. New 1,4-disubstituted 1,2,3-triazole derivatives

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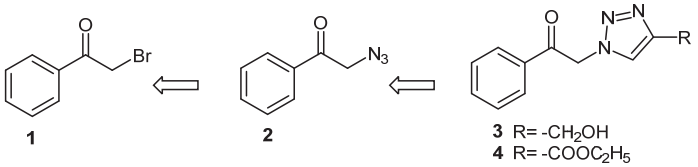
1,2,3-Triazole moieties are attractive connecting units because they are stable to metabolic degradation and capable of hydrogen bonding [1], which can be favourable in the binding of biomolecular targets and can improve their solubility [2]. The importance of triazolic compounds in medicinal chemistry is undeniable [3]. Contrary to other *aza*heterocycles, the 1,2,3-triazole ring is not protonated at physiological pH because of its poor basicity. Recently, a number of amphiphilic dextran esters obtained by functionalizing the polysaccharide with different acids have been identified. The compounds show antimicrobial activity on *Staphylococcus aureus* and *Candida albicans* [4]. With the aim of identifying new biologically active compounds, the reactions of *O*-alkylation and *C*-alkylation were performed for 1,2,3-triazoles (**3**) and (**4**), in the presence of sodium hydride and ethyl bromoacetate. The triazoles used in the study were synthesized in two stages from *ω*-bromoacetophenone, with a yield of 82-85% (Scheme 1).



***Scheme 1**: Synthesis of 1,2,3-triazoles from ω-bromoacetophenone.*

The research carried out has led to the conclusion that the methylene group fixed to the nitrogen atom in position 1 can be alkylated, and an appropriate reaction mechanism is proposed. Synthesized compounds were purified and physically and spectrally characterized (IR, ^{1}H-NMR, ^{13}C-NMR, 2D).

Keywords: 1,2,3-triazole; *C*-alkylation; ethyl bromoacetate.

Acknoledgements: The authors are grateful to the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra.

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P9. Behavior of maleamic acid in the presence of carbonyldiimidazole

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The condensing agent *N*,*N*-carbonyldiimidazole (CDI, Figure 1) is reactive to amines and alcohols, being frequently used in organic synthesis, especially in obtaining peptides [1]. Maleamic acid (acid (2*Z*)-3-carbamylpropenoic, MA) is an important monomer in the synthesis of hydrophilic polymers [2, 3], some derivatives being used to obtain anode material for Lithium-ion accumulators [4], respectively in the decontamination of heavy metal waters (Pb^{2+}, Cu^{2+}, Ni^{2+}, Cd^{2+}) [5]

In the last decade, propargylic esters have been reported as basic units in a large number of chemical transformations, of particular importance being their presence in cycloaddition reactions of the type: *click* [6], [4+2] catalyzed by the oxazaborolidinium chiral cation [7], [3+3] in the catalysis of Au(III) [8].

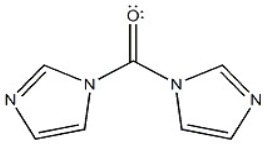

Figure 1. *Structure of CDI.*

The researches carried out aimed at transforming maleamic acid into the corresponding propargylic ester, using two experimental procedures, in both CDI having the role of activating agent of the carboxylic function. The only isolated, purified, physically and spectrally characterized compound was *N*-maleamilimidazole (Figure 2) and not the propargylic ester of interest.

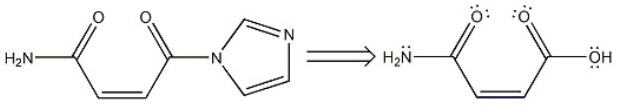

Figure 2. *Retrosynthesis of the N-maleamilimidazole derivative from maleamic acid.*

Keywords: maleamic acid, CDI, propargylic ester, *N*-maleamilimidazole.

Acknoledgements: The authors are grateful to the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra.

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P10. Dimethyl fumarate, precursor in the synthesis of pechmann γ-lactones

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Pechmann's lactones (dyes) are a class of organic pigments that possess conjugated γ-lactonic cycles, being discovered in 1882 [1] and characterized only in 1950 [2, 3]. The most important characteristics of these dyes are high planarity, high ability to accept electrons, absorption respectively fluorescence in the visible and near infrared, as well as a multiple range of redox properties. Pechmann's lactones can be thermally isomerized in protic solvents, or under basic conditions with a concomitant displacement of absorption maxima, the color changing from yellow to orange-red. In recent decades [4, 5], with the increasing progress in the field of organic electronic devices, interest in this class of organic compounds has also been amplified, with the development of new methods of their synthesis [6, 7]. In this communication we report a new method of synthesis of γ-Pechmann's lactones, using as a starting material the bromide of 4-dimethylamino-phenacylpyridinium and dimethyl fumarate, the alkenic dipolarophyle with *trans* stereochemistry. The synthesized compounds were purified and physically and spectrally characterized (IR, ^{1}H-RMN, ^{13}C-RMN, 2D, RX).

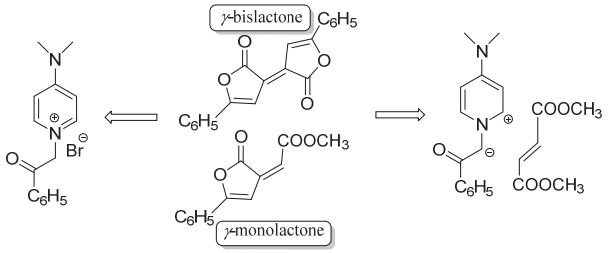

***Figure 1**. Mono- and bislactone retrosynthesis.*

Keywords: bislactones; *N*-ylides; dimethyl fumarate.

Acknoledgements: The authors are grateful to the project POSCCE-O 2.2.1, SMIS-CSNR 13984-901, No. 257/28.09.2010, CERNESIM for the NMR spectra.

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