8th
2022
ICNTC CONFERENCE
INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

8th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY
16 – 18 MAY 2022

8th ICNTC BOOK OF ABSTRACTS

8th 2022 ICNTC CONFERENCE
INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

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16 – 18 MAY 2022

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Chemistry Department

Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of "8th International Conference on New Trends in Chemistry", to be held in Famagusta, North Cyprus on the dates between May 16 – 18 , 2022

Limited number of Papers and Posters with the below mentioned topics will be accepted for our conference:

Polymer Chemistry and Applications
Pharmaceutical Chemsitry
Computational Chemistry
Bio Chemistry
Physical Chemistry
Analytical Chemistry
Inorganic Chemistry
Organic Chemistry
Material Chemistry
Environmental Chemistry
Food Chemistry

The selected papers which are presented as oral in the conference will be published in an international peer-reviewed journal which is indexed by SCOPUS as Q4. Each manuscript will have doi Numbers.

We kindly wait for your attendance to our conference to be held on 16 – 18 May 2022,

All informations are available in conference web site. For more information please do not hesitate to contact us. info@icntcconference.com

Respectfully Yours,
On Behalf of the Organization Committee of ICNTC Conference
Assoc. Prof. Dr. Dolunay SAKAR DASDAN
8th ICNTC 2022 | Conference Chair
Yıldız Technical University – Istanbul / Turkey
Chemistry Department

16 May 2022 Monday

MORNING COFFEE BREAK 10:30 – 11:00

Welcome Speech 11:00 – 11:10	:Assoc. Prof. Dr. Dolunay SAKAR DASDAN, Yıldız Technical University Conference Chair

SESSION A (11:10 – 13:20)
SESSION CHAIR: Assoc. Prof. Dr. Dolunay SAKAR DASDAN

Invited Speech (11:10 – 12:00)
Prof. Dr. Huriye İCİL

Keynote Title : *TWO NOVEL TRIAZINE-BASED PERYLENE DYE MOLECULES*

12:00 – 12:20
PAPER TITLE : *POLLUTION CHARACTERISTICS OF LIFETIME LUNG CANCER RISK ON PM2.5-ASSOCIATED PAHS*
AUTHOR(S) : **Amgalan NATSAGDORJ**, Bulgankhangai.TUGSBAYAN, Soyol-Erdene.TsEREN-OCHIR, JiYi LEE, Yong Pyo KIM

12:20 – 12:40
PAPER TITLE :*THE INVESTIGATION OF CHARACTERIZATION OF THE ACTIVATED CARBON PRODUCED FROM PISTACHIO SHELL ON DIFFERENT TEMPERATURES*
AUTHOR(S) : **Hacer DOLAS**

12:40 – 13:00
PAPER TITLE : *GASEOUS OXIDIZED MERCURY CALIBRATION SOURCES: A REVIEW*
AUTHOR(S) : Matthew Davis, **Julia LU**

13:00 – 13:20
PAPER TITLE : *PREPARATION OF MODIFIED POLYETHERSULFONE MEMBRANES FOR HEMODIALYSIS*
AUTHOR(S) : **Özgür Şevval KAHRAMAN**, May Thazin PHOO, İlknur KÜÇÜK, Ayça HASANOĞLU

LUNCH BREAK 13:20 – 14:30

Information for regular participation; Lunch is included into Salamis Hotel Accommodation

SESSION B (14:30 – 16:20)
SESSION CHAIR: Prof. Dr. Huriye İCİL

E - Keynote Speaker (14:30 – 15:20)
Dr. Hatem AMIN

Keynote Title: *Biosynthesis of stabilized silver nanoparticles and their application as sensing probes and as antibacterial and antioxidant agents*

15:20 – 15:40
PAPER TITLE : *SYNTHESIS OF ZINC OXIDE NANOPARTICLES USING FICUS THONNINGII AQUEOUS EXTRACT AND EVALUATION OF ITS ANTIOXIDANT AND ANTIMICROBIAL ACTIVITIES*
AUTHOR(S) : **Huzaifa UMAR**, Doga Kavaz, Amina Lawan Abubakar, Maryam Rabiu Aliyu, Nahit Rizaner

15:40 – 16:00
PAPER TITLE : *SYNTHESIS AND CHARACTERIZATION OF POLY(ISOBUTYLENE-ALT-MALEIC ANHYDRIDE)-PREGABALIN COPOLYMER-DRUG DELIVERY SYSTEM in CATALYST MEDIA*
AUTHOR(S) : Rabia Nur Can, **Dolunay ŞAKAR DASDAN**

16:00 – 16:20
PAPER TITLE : *DEVELOPMENT OF A CARBON TUNGSTATE COMPOSITE FROM OLIVE MILL WASTEWATER FOR ADSORPTION AND SEPARATION OF CONTAMINANTS in AQUEOUS ENVIRONMENTS*
AUTHOR(S) : **Issam MECHNOU**, Imane Mourtah, Laurent Lebrun, Miloudi Hlaibi

COFFEE BREAK 16:20 – 16:40

Gala Dinner at Kybele Restaurant / Bellapais

Salamis Hotel Departure: 18:30

Gala Dinner invitation is valid only for Full Registration Package holders.
For Extra Gala Dinner Ticket please contact conference registration desk.

17 May 2022 Tuesday

SESSION C (10:00 – 11:40)
SESSION CHAIR: Prof.Dr. Julia LU

Invited Speaker (10:00 – 10:40)
Assoc.Prof.Dr. Akeem Adeyemi OLADIPO

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10:40 – 11:00
PAPER TITLE : *HEMOCOMPATIBILITY STUDIES OF LAYER-BY-LAYER POLYELECTROLYTE COMPLEXES FOR BIOBASED POLYMERS*
AUTHOR(S) **: Mthabisi Talent George MOYO**, Oğuz Han EDEBAL, Ece BAYIR, Aylin ŞENDEMIR, Terin ADALI

11:00 – 11:20
PAPER TITLE : *SYNTHESIS OF POLYFUNCTIONALIZED STEROIDAL HETEROCYCLIC DERIVATIVES AS POTENTIAL ANTIMICROBIAL DRUG*
AUTHOR(S) : Ahmad Q Daraosheh; **Khaled Q SHAWAKFEH**

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AUTHOR(S) : **Simal KURUMOGLU**, Yelda YALCIN GURKAN

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SESSION D (12:00 – 13:20)
SESSION CHAIR: Assoc. Prof. Dr. Akeem Adeyemi OLADIPO

12:00 – 12:20
PAPER TITLE : *SILICA XEROJEL SYNTHESIS WITH DRYING CONTROL CHEMICAL ADDITIVE*
AUTHOR(S) : Filiz AKTI, **Suna BALCI**

12:20 – 12:40
PAPER TITLE : *POSSIBLE REACTION PATHWAYS OF THE SELECTED ORGANOPHOSPHORUS AND CARBAMATE PESTICIDES ACCORDING TO THE DFT CALCULATION METHOD*
AUTHOR(S) : **Bahar EREN**, Yelda YALCIN GURKAN

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PAPER TITLE : *NON-TOXIC AND HEMOCOMPATIBILITY NANOCARRIER DERIVED FROM POLYGALACTURONIC ACID FOR SUSTAINABLE DRUG DELIVERY*
AUTHOR(S) : **Selin S SUNER**

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PAPER TITLE : *RESERVOIR CHARACTERISTICS OF THE KUSURİ FORMATION SANDSTONES IN THE ZONGULDAK SUB-BASIN OF WEST BLACK SEA, TURKEY*
AUTHOR(S) : **Aylin GEÇER**, Aynur BÜYÜKUTKU

LUNCH BREAK 13:20 – 14:30

POSTER SESSION (14:30 – 15:30)

SESSION CHAIR: Prof.Dr.Julia LU, Prof.Dr.Huriye İCİL, Prof.Dr.Suna BALCI, Assoc.Prof.Dr.Akeem Adeyemi OLADIPO

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PAPER TITLE : *SYNTHESIS AND BIOLOGICAL EVALUATION OF NOVEL N-SUBSTITUTED BENZIMIDAZOLE DERIVED SCHIFF BASES*
AUTHOR(S) : **Anja BEČ**, Maja CINDRIĆ, Emina MEHIĆ, Leentje PERSOONS, Dirk DAELEMANS, Marijana HRANJEC

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AUTHOR(S) : **Anja RAKAS**, Silvana RAIĆ-MALIĆ , Tatjana GAZIVODA KRALJEVIĆ

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AUTHOR(S) : **Arwa ABOU RAJAB**, Sermet KOYUNCU, Huriye İCİL

PAPER TITLE : *A WATER-SOLUBLE NDI DERIVATIVE AS A CHEMOSENSOR FOR THE DETECTION of HEAVY METAL CATIONS*
AUTHOR(S) : **Arwa ABOU RAJAB**, Sermet KOYUNCU, Huriye İCİL

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AUTHOR(S) : **Bahadır KESKİN,** Ecem Nur DEMİREL

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AUTHOR(S) : **Elif DOĞRU**, Bülent KIZILDUMAN, Huriye İCİL

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AUTHOR(S) : **Elif DOĞRU**, Bülent KIZILDUMAN, Huriye İCİL

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AUTHOR(S) : **Meltem BALÇIK**, Bahadır KESKİN

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AUTHOR(S) : **Meltem DİNLEYİCİ**, Huriye İCİL

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AUTHOR(S) : **Meltem DİNLEYİCİ**, Huriye İCİL

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PAPER TITLE :*THE SYNTHESIS AND CHARACTERIZATION OF NEW AMINO-SUBSTITUTED AZANAPHTOQUINONE COMPOUNDS WITH ANTIMICROBIAL ACTIVITY*
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PAPER TITLE :*THE SYNTHESIS, PHOTOPHYSICAL AND ELECTROCHEMICAL PROPERTIES OF PERYLENEMONOIMIDE AND ASYMMETRIC PERYLENE DIIMIDE*
AUTHOR(S) : **Nur PAŞAOĞULLARI AYDINLIK**, Devrim Ozdal, J. Babu Bodapati, Huriye Icil

PAPER TITLE : *SELF-ASSEMBLY, OPTICAL, THERMAL AND ELECTROCHEMICAL PROPERTIES OF N, N'-BIS-(BENZYL)-3,4,9,10-PERYLENEBIS(DICARBOXIMIDE)*
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AUTHOR(S) : **Raluca-Anamaria ŞEPTELEAN**, Iulia-Andreea AGHION, Gabriela-Nicoleta NEMEȘ

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AUTHOR(S) : **Sergejs OSIPOVS**, Aleksandrs PUČKINS

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AUTHOR(S) : **Vilma LOVRINČEVIĆ**, Dragana VUK, Ines DESPOTOVIĆ

PAPER TITLE : *DEGRADATION REACTIONS of COVID-19 ACTIVE INGREDIENTS BY MOLECULAR MODELING METHOD*
AUTHOR(S) : **Yelda YALCIN GURKAN**, Begum PANDIR

COFFEE BREAK and CLOSING CEREMONY OF CONFERENCE : 15:30 – 16:00

18 May 2022 Wednesday

FULL DAY (8 Hours) NORTH CYPRUS CITY TOUR

Salamis Hotel Departure: 10:30

Tour does not included into Registration Fee

Contents

TWO NOVEL TRIAZINE-BASED PERYLENE DYE MOLECULES

Huriye İCİL

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Abstract

The dramatic effect of the triazine core in enhancing the photovoltaic (PV) performance of non-fullerene organic solar cells (OSCs) is exciting. Interestingly, a novel perylene diimide trimer

based on an electron-deficient core (1,3,5- triazine) has shown one of the best power conversion efficiency (PCE, 9.54%) values reported in the literature [1]. Importantly, perylene bisimide-based donor-acceptor materials (D–A) have been extensively investigated due to their attractive features, such as outstanding absorption, emission, photochemical, electrochemical properties, and thermal, chemical and photochemical stabilities [2]. These characteristics of perylene compounds are the fundamental properties that lead to considerable research development regarding their uses in fluorescent dyes, NIR dyes, organic solar cells, sensors, optical switches, organic solar cells and photoconduction materials.

This study designed, synthesised, and characterised the novel 2,4-diamino-6-phenyl-1,3,5-triazine containing perylene diimide and oligomer. The absorption, electrochemical, spectroelectrochemical, and morphological characteristics have been investigated. It is noteworthy that the density functional theory (DFT) computational studies confirmed the compounds' structural and electrochemical features. The weight-average molecular mass (*Mw*) of 3500 g/mol was obtained for the helical oligomer from the gel permeation chromatography (GPC) measurements, indicating the heptamer structure formation for the oligomer. The diimide` and oligomer` HOMO/LUMO energy levels were −5.83/− 3.93 and −6.10/− 4.01 eV, respectively. The diimide based dye-sensitised solar cells (DSSC) photovoltaic parameters V_{oc}, I_{sc}, FF and η_{cell} are 0.316 V, 0.432 mA/cm^2, 0.08 and 0.011%, respectively. Those parameters for the oligomer dye are 0.318 V, 0.455 mA/cm^2, 0.15 and 0.0211%, respectively.

It is important to note that many metal complexes offer advanced properties as industrial catalysts. The novel diimide and oligomer synthesised in this study are potent compounds for the production of metal-based supramolecular architectures.

Key Words: Oligomer; Electrochemistry; Spectroelectrochemistry; DFT; DSSC

References

[1]X. Chang, S. Lin, G. Wang, C. Shang, Z. Wang, K. Liu, Y. Fang, P.J. Stang, Self-assembled Perylene Bisimide-cored trigonal prism as an electron-deficient host for C60 and C70 driven by "Like Dissolves Like", J. Am. Chem. Soc. 142 (37) (2020) 15950–15960, https://doi.org/10.1021/jacs.0c06623.

[2] P. P¨osch, M. Thelakkat, H.-W. Schmidt, Perylenediimides with electron transport moieties for electroluminescent devices, Synth. Met. 102 (1-3) (1999) 1110–1112, https://doi.org/10.1016/S0379-6779(98)01391-5

POLLUTION CHARACTERISTICS OF LIFETIME LUNG CANCER RISK ON PM2.5-ASSOCIATED PAHS

Amgalan.NATSAGDORJ[1]*, Bulgankhangai.TUGSBAYAN[1], Soyol-Erdene.TsEREN-OCHIR[2], JiYi LEE[3], Yong Pyo KIM[4]

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[2]Department of Environmental and Forest Engineering, School of Engineering and Applied Sciences, National University of Mongolia, Ulaanbaatar 210646, Mongolia
[3]Department of Environmental Science and Engineering, Ewha Womans University, Seoul 03760, Republic of Korea
[4]Department of Chemical Engineering and Materials Science, Ewha Womans University, Seoul 03760, Republic of Korea

Abstract

Polycyclic aromatic hydrocarbons (PAHs) are one species of air pollutant that formed during incomplete combustion of organic material and maybe one of the causes of lung cancer. In this study, we aim to risk assessments in each PAH species on both environment and human health. Sixteen polycyclic aromatic hydrocarbons were measured by methods developed by (Kang *et al.*, 2020)-s developed methods using the Agilent 7890B Gas chromatography-mass spectrometry instrument, in total $PM_{2.5}$ samples collected from heating periods in 2018 and 2021. Total polycyclic aromatic hydrocarbons concentrations were 255.1 ng/m^3 in 2018, 561.4 ng/m^3 in 2021 which is 2.2 times higher than 2018 heating period. For each PAH species concentration, all species except perylene (which is twice decreased) increased from 1.7 – 25.2 times than the 2018 heating period. PAH ratio profiles show that the main source of PAHs was coal burning, and the main source was unchanged in 2018 and 2021. The equivalent concentrations (Σ_8B[a]P-TEQ) were 24.2 ng/m^{-3} in 2018, 126.3 ng/m^{-3} in 2021, which is 5.1 times higher than in 2018, respectively. For estimating lifetime lung cancer risk Σ_8B[a]P-TEQ concentrations were used, and results were $6*10^{-3}$ in 2018 and $11*10^{-3}$ in 2021 which is increased 1.85 times from 2018. Based on results, $PM_{2.5}$ associated PAHs concentrations, lung cancer risk was significantly increased.

Keywords: Risk assessment, Fine particulate matter, $PM_{2.5}$, PAH, lung cancer.

Kang, M. *et al.* (2020) “Recent Occurrence of PAHs and n-Alkanes in PM2.5 in Seoul, Korea and Characteristics of Their Sources and Toxicity,” *International Journal of Environmental Research and Public Health*, 17(4), p. 1397. doi: 10.3390/ijerph17041397.

The investigation of characterization of the activated carbon produced from pistachio shell on different temperatures

Hacer DOLAS

Harran University, Hilvan Vocational School, Program of Occupational Health and Safety, Sanliurfa 63900, Turkey
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Abstract

While the developments in sectors such as industry and textile are taking place on the one hand, the wastes that the factories give to the air and water disrupt the order of nature, which is necessary for the continuity of life [1]. Adsorption is a process in which ions or molecules are adsorbed by active surfaces. Activated carbons (ACs), which are used as active surfaces in the adsorption process, cause the adsorption process to be successful due to their high surface area and high volume in terms of micropores. It is widely used to obtain adsorbent with high carbon content, which can achieve a porous structure thanks to the carboxyl and hydroxyl groups in the agricultural waste structure and thanks to its high quality fibrous structure. The characteristics of the method used in AC production help the AC to improve its porosity structure and to have a high surface area [2].

In this study, it was investigated how different temperatures and H_2SO_4 affect the surface area and porosity structure in obtaining AC from pistachio shells. For this purpose, the collected pistachio shells were kept in 10% NaCl and 10% H_2SO_4 solution for 24 h. At the end of the period, it was carbonized for 45 min using 3 different temperatures (500, 700 and 800 ^{o}C). The obtained ACs were characterized by using The surface area and pore size analyser, Fourier Transform- Infrared (FT-IR) and Scanning Electron Microscopy (SEM). According to the results obtained, it was understood that the AC-800 has the highest surface area compared to the other obtained AC. So, it had a BET surface area of 2093,063 m^2/g, and its micropore volume was 1,053 cc/g. All functional groups in the structure of raw pistachio shells are destroyed for pore formation and the resulting porosity is supported by FT-IR and SEM images. With this new method, ACs with a high surface area were obtained and it was understood that the surface area and micropore volume would increase with the increase in temperature.

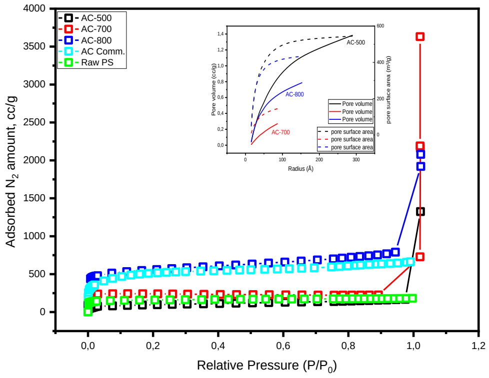

Figure 1. The comparison of the adsorption isotherms of obtained ACs from Pistachio Shell (inset: the comparison of pore volume and pore surface area of the ACs).

Key words: *Agricultural Waste, Carbonization, Activated Carbon, Surface Area, Micropore Volume.*

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Gaseous oxidized mercury calibration sources: a review

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Abstract

Gaseous oxidized mercury (GOM) is a significant species for understanding the transport and fate of mercury in the atmosphere. However, significant uncertainty is associated with the current speciation methods for GOM and no commercially available calibration method is available. While there has been extensive research in this field in the past years, to the best of our knowledge, no review exists on GOM calibration research. This paper examines the custom-made calibration sources that researchers have used in the development of GOM speciation methods, evaluates the factors influencing the source performance, and synthesizes recommendations for the design of GOM calibration sources in the future.

Keywords: gaseous oxidized mercury; calibration source; permeation tube; diffusion cell;

Submit to “the 8th International Conference on New Trends in Chemistry”, Famagusta, North Cyprus on the dates between May 16 – 18, 2022 for topics analytical and environmental chemistry

PREPARATION OF MODIFIED POLYETHERSULFONE MEMBRANES FOR HEMODIALYSIS

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Abstract

Hemodialysis is an important membrane separation technology which is used to remove toxic biological substances such as urea and creatinine from end-stage renal patients. It is estimated that 10% of adults worldwide have kidney disease, and more than two million people still live on dialysis and kidney transplant treatments worldwide [1]. In hemodialysis the membranes serve as artificial kidneys. The most important requirement in hemodialysis membranes is the ability to remove toxic substances as well as its biocompatibility. Therefore, the choice of membrane material is a very important parameter in hemodialysis. In hemodialysis, since one side of the membrane is in contact with blood, the membrane material must be compatible with blood and tissue. If high levels of blood proteins adsorb onto the membrane surface, blood clotting can occur, which can be fatal for the patient. Therefore, materials with high separation and blood and tissue compatibility should be developed. Polyethersulfone (PES) is one of the common materials used in hemodialysis. It is a chemically and mechanically resistant material and today, 22% of dialysis membrane materials contain PES [2]. PES is seen as the hemodialysis material of the future because it is a bisphenol-free polymer. Although PES has potential as a hemodialysis membrane, its use is limited since its contact with blood can cause various interactions between the membrane and blood cells including adsorption and transformation of plasma proteins, activation of blood cells, adhesion of platelets, and reactions of platelets with PES. All these phenomena can be fatal for the patients. Therefore, PES should be modified to reduce these reactions before its use in hemodialysis applications.

In this study, tissue and blood compatible PES based dialysis membranes were prepared by phase inversion method. To improve the biocompatibility and hemo-compatibility of the membrane, the PES polymer was blended with two polymers; polyvinylpyrrolidone (PVP) and polyethyleneglycol (PEG). 15% (wt) of PES polymer in n-methylpyrrolidon (NMP) was used to prepare the pristine PES membranes while a polymer blend of 5% (wt) PVP or PEG additives and 10% (wt) of PES in the same solvent was used to prepare the modified PES membranes. Biocompatibility and hemocompatibility of the prepared membranes were defined by water sorption, BSA protein and creatinine adsorption values. The sorption and BSA adsorption experiments indicated that the addition of PVP and PEG in the membrane matrix increased the hydrophilicity of the membrane and decreased the protein adsorption rate. In the light of these results, it was seen that the biocompatibility of the membranes can be increased using PVP and PEG additives in PES membrane by reducing the amount of protein adsorption, and the modified membranes can prevent complications from contact with blood.

Key Words: *Hemodialysis, Biocompatible membranes, phase inversion, polyether sulfone, polyvinlypyrrolidone, polyethylene glycol,*

Acknowledgement

This work has been supported by Yıldız Technical University Scientific Research Projects Coordination Unit under the project number YÜLAP 2019-3711.

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Biosynthesis of stabilized silver nanoparticles and their application as sensing probes and as antibacterial and antioxidant agents

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Abstract

Green synthesis of nanomaterials is of utmost interest as it offers an eco-friendly approach over chemical synthetic routes. Among others, silver nanoparticles AgNPs are rapidly being utilized in a variety of applications, including chemical and electrochemical sensing, catalysis, molecular imaging, drug delivery, nanomedicine, agriculture, cosmetics, food industry and antioxidant [1, 2]. Pathogens, heavy metals and free radicals are serious problems for environmental and health concerns. Therefore, the facile and green production of modified AgNPs with enhanced antibacterial as well as antioxidant activities is of utmost benefit in providing defense against several infections [3].

In this presentation, the synthesis of plant extract-mediated AgNPs and their application in heavy metals detection, antibacterial activity and antioxidant activity will be discussed. The synthesized particles are characterized using various techniques including SEM, EDX, DLS and cyclic voltammetry. The particles revealed excellent colloidal stability thanks to the unique capping agent. Plant-extract stabilized AgNPs exhibited potent antioxidant scavenging potential against H2O2 at most, followed by DPPH, O2– and OH– free radicals, and also showed the highest antibacterial activity against *E. Coli*. The capped AgNPs revealed selective sensing towards Ni ions. The stability and considerable antibacterial and antioxidant activities of plant extract-capped AgNPs render this simple and ecofriendly approach attractive for upscaling and application in biomedical and nutraceutical developments.

Keywords: Ag NPs; Sensing; Antibacterial activity; Antioxidant activity; Heavy metals

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Synthesis of Zinc Oxide Nanoparticles Using *Ficus thonningii* Aqueous Extract and Evaluation of its Antioxidant and Antimicrobial Activities

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Abstract

Zinc oxide nanoparticles (ZnO-NPs-AE) were synthesized using *Ficus thonningii* aqueous extract as an efficient stabilizing agent. Antimicrobial and antioxidant activity of the synthesized ZnO-NPs-AE were carried out using disc diffusion and DPPH (2,2-diphenyl-1-picryl-hydrazyl-hydrate) free radical method respectively. Characterizations of the synthesized ZnO-NPs-AE were achieved using UV-vis spectroscopy (UV-Vis), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), Scanning electron microscope (SEM), and energy-dispersive X-ray spectroscopy (EDX). Absorption peak in the range of 370 nm was observed using UV–vis following colour change from yellow to brown, both UV–Vis and FTIR spectra conformed the formation of ZnO-NPs-AE and SEM analysis result revealed spherical morphology with an average size of 18 nm. Antimicrobial analysis result of the Biosynthesized ZnO-NPs-AE showed significant activity against *Escherichia coli* and *B. cereus with lower concentrations. Moreover, A*ntioxidant activities result carried out using DPPH free radical scavenging activity of the ZnO-NPs-AE revealed IC_{50} values of 35 μg/mL. Biosynthesized ZnO-NPs-AE revealed antioxidant activity and antimicrobial potential against both gram negative and gram positive bacteria.

Key Words: Zinc oxide nanoparticles; Characterizations; Antimicrobial; Antioxidant; Ficus thonningii.

SYNTHESIS AND CHARACTERIZATION OF POLY(ISOBUTYLENE-ALT-MALEIC ANHYDRIDE)-PREGABALIN COPOLYMER-DRUG DELIVERY SYSTEM in CATALYST MEDIA

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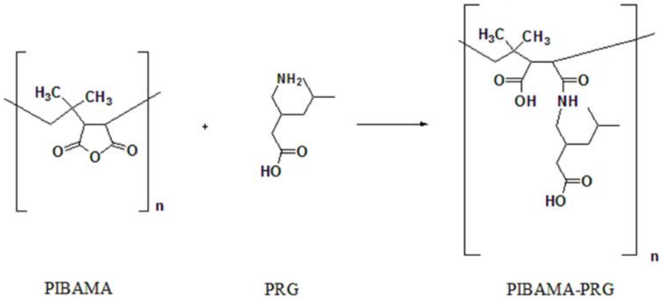
Abstract

In last years, several researches are running on for the development of new drug delivery system. In conventional therapy, drug is released immediately after medication. For the controlled drug delivery, polymers are used as drug carriers. They can be easily synthesized at low cost, and to be freely water-soluble, non-toxic and nonimmunogenic.[1,2] In the present study, it is aimed to be controlled delivery and prolong the half-life time of pregabalin (PRG) in body, we synthesized poly(isobutylene-alt-maleic anhydride)-PRG copolymer-drug delivery system with different PRG ratios in catalyst media (Scheme 1). The synthesized PIBAMA-PRG systems were characterized via ^{1}H NMR and FTIR/ATR. The stability and activity of PIBAMA-PRG copolymer-drug delivery systems were investigated at different pHs and various artificial body fluid mediums based on the time effect by zetasizer measurements and UV/VIS measurements at 37 ^{o}C, respectively.



Scheme 1 Synthesis of Poly(isobutylene-alt-maleic anhydride)-PRG copolymer-drug delivery system

Key Words: *Poly(isobutylene-alt-maleic anhydride); pregabalin drug; stability; activity*

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Development of a carbon tungstate composite from Olive mill wastewater for adsorption and separation of contaminants in aqueous environments

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Abstract

The increase in olive oil production is accompanied by the production of large quantities of liquid waste (Olive mill wastewater), is a very toxic liquid discharge, difficult to treat, has a phyto-toxic character and rich in non-biodegradable organic matter [1]. The analyses carried out indicate that this effluent presents a COD of 176 $g(O_2).L^{-1}$, translating an organic matter content of approximately 46.15% and consequently an organic carbon content of approximately 27.17%. The richness of the OMWW in organic carbon and its aqueous state were the main criteria to realize a mixture with tungstate and then carbonize it at high temperature (800 °C) according to an original process (pyrolysis with thermal shock), fast (2 minutes) and clean (without by-products), in order to obtain a high quality carbonaceous adsorbent, highly demanded and non-toxic. The influence of the amount of tungstate added was studied in the range of 1 to 5%. Scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and differential thermal analysis (DTA) were used to determine the composition, morphology, and porosity of the resulting carbon composites. The specific surface area and microporosity were measured by the (BET) method. The optimally prepared carbonaceous adsorbent, is thermally stable, richer in carbon, and highly porous, has a large specific surface area, and is rich in anionic active sites suitable for the adsorption of cationic species. The capacity and selectivity of the carbonaceous adsorbent were judged by adsorption tests performed using two contaminants from the textile industry with different loadings. The isotherm and kinetics were studied using the nonlinear modeling method, of which 5 isotherm and two kinetic models were verified. The results show that the adsorption on the prepared adsorbent behaves according to the mechanism described by Langmuir, where the adsorption is homogeneous and monolayer. The prepared adsorbent has an adsorption capacity 398.21 $mg.g^{-1}$ for methylene blue, while its adsorption capacity for indigo carmine does not exceed 79.96$mg.g^{-1}$. It is characterized by a kinetic of order 2 whatever the adsorbate studied, and the initial adsorption rate is of the order of 43.51$mg.g^{-1}.min^{-1}$ for methylene blue and 13.87$mg.g^{-1}.min^{-1}$ for indigo carmine. The thermodynamics was studied and the results show that whatever the adsorbate, the adsorption is spontaneous, endothermic, and the interactions established are physical. The prepared adsorbent thus shows significant stability after regeneration, losing only 26.5% of its capacity after 5 cycles of use. The selectivity was studied by performing simultaneous adsorption of the adsorbates, it was found that at pH=9, a complete separation is performed, from which the prepared adsorbent was able to adsorb up to 254.15 $mg.g^{-1}$ of methylene blue, while its capacity towards indigo carmine is zero. It was found that it is possible to find solutions to the environmental problems caused by toxic effluent discharges, according to the principles of green and sustainable chemistry, regardless of their origins, compositions and natures, and the method of elaboration of carbon composites from a liquid discharge constitutes a new approach to valorization.

Keywords: *carbon composite; adsorption; treatment of contaminants; olive mill wastewater; olive oil by-products.*

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BIO-BASED DYES AND BIOWASTES FOR SOLAR ENERGY HARVESTING AND STORAGE SYSTEMS

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Abstract

Global energy consumption is becoming a big challenge for human society as the global population grows and the urbanization trend continues. According to a recent report from the International Energy Agency, worldwide energy demand will rise by 50% by 2030. As a result, to meet rapidly rising energy demand, numerous renewable energy sources must be created. One of the hottest study areas in recent years has been harvesting energy from the sun using photovoltaic technology and storing it in supercapacitor or battery technology. Since the 1990s, dye-sensitized solar cells (DSSCs) have gotten a lot of interest as a sort of photovoltaic technology. The DSSC technology is particularly promising because it is made up of low-cost materials that do not require significant processing technologies, making it inexpensive and simple to manufacture. The dye is essential for solar energy collection and conversion into electrical energy via a semiconductor photoanode. Ruthenium complexes are synthetic dyes and one of the best DSSC sensitizers, but they have several drawbacks. Synthesizing effective synthetic dyes takes a long time and requires the use of expensive and complex dye components. Natural or bio-based dyes are thus regarded as a suitable alternative. Bio-based dyes have many advantages as photosensitizers in DSSC, including low cost, non-toxic alternatives, easy extraction procedures, high relative abundance, and long-term sustainability. Higher plants (stems, leaves, flowers, and fruits) and microbes are abundant sources of bio-based dyes. To further develop and integrate DSSC technology into large energy infrastructures, innovations that improve the storage of solar captured energy are critical. Researchers are focusing on biowastes as part of their ongoing efforts to develop sustainable energy storage systems and to address the problem of continuous greenhouse gas emissions. Because of their high abundance, renewable nature, low cost, and eco-friendly qualities, biowastes can serve as the primary source of biobased carbon nanomaterials for electrochemical energy storage technologies such as batteries and supercapacitors. Bio-based/natural dyes for solar energy harvesting via DSSC and biowastes-based carbon materials for energy storage devices will be the focus of this scientific conference.

HEMOCOMPATIBILITY STUDIES OF LAYER-BY-LAYER POLYELECTROLYTE COMPLEXES FOR BIOBASED POLYMERS

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Abstract

Thrombogenesis is an important point of issue that causes blood-contacting biomedical device failure. This study focuses on hemocompatibility studies of novel blood-contacting polyelectrolyte complexes (PECs) for biomedical application designs. PEC films were fabricated from biobased polymers silk fibroin (SF), chitosan (CH), sodium alginate (AL) through the solvent casting method and Layer-by-Layer (LbL) technique. Characterization has been carried out by Fourier-transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Atomic force microscopy (AFM), and Differential scanning calorimetry (DSC) analyses. FTIR spectra displayed characteristic peaks of SF, CH, and Al in all layers. AFM images indicated that the addition of AL as an outer layer increased surface roughness. DSC analysis suggested that the best thermal stability has been observed with the CH outer layer of PECs. SEM micrographs analysis indicated that the morphologies of PECs have been affected by the inclusion of the drug. Hemocompatibility properties were investigated by complete blood count (CBC), prothrombin time (PT), international normalized ratio (INR), activated partial thromboplastin time (APTT), platelet adhesion, erythrocyte morphology analysis, *in vitro* cholesterol and albumin level tests. These hemocompatibility analyses demonstrated that the PEC surfaces provide favourable principles to design and develop antihemolytic and non-thrombogenic PECs for blood-contacting biomedical applications.

Keywords: Polyelectrolyte; Chitosan; Silk fibroin; Alginate; Hemocompatibility

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Synthesis of Polyfunctionalized Steroidal Heterocyclic Derivatives as Potential Antimicrobial Drug

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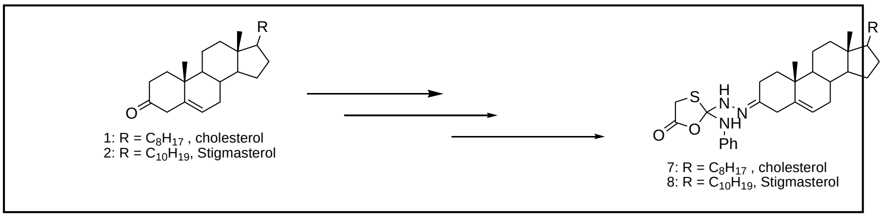

Abstract

A series of cholestane and stigmastane lactone derivatives were synthesized through a convenient and productive method. Cholest-5-ene-3-one **1** and stigamsta-5, 22-diene-3-one **2** is reacted with hydrazine hydrate to produce the hydrazone derivatives **3** and **4**. The latter derivatives are allowed to react with phenyl isothiocyanate to produce acyclic structures **5** and **6** (cholest- and stigmasta-N-phenylhydrazine-1-carbothioamide). These acylic dereivatives reacted with chloroacetic acid in boiling toluene affording the lactone adducts which cyclized to the desired products **7** and **8** (cholest- and stigmasta-hydrazinyl-2-(phenylamino)-1, 3-oxathiolan-5-one). In addition, we are reporting here the incorporation of sulfur heteroatom into the steroid moiety (Diosgenin) in order to prepare aminothiazol-diosgenin derivative **12**, by condensation of □-brom-ketone from diosgenin with thiourea in ethanolic sodium ethoxide solution. The new polyfunctionalized steroidal heterocyclic derivatives have been characterized by FT-IR, ^{1}H- and ^{13}C-NMR, mass spectroscopy and elemental analysis.

Keywords: Polyfunctionalization; steroidal; hydrazine; cyclization; lactone.

COMPUTATIONAL EXAMINATION OF DEGRADATION REACTIONS OF BUPROFEZIN

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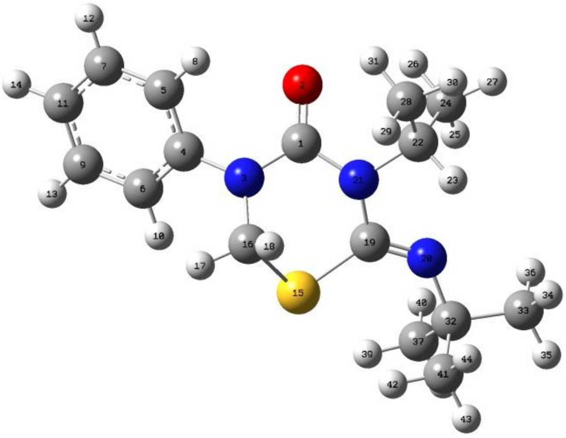
Abstract

Degradation reactions of molecules to be investigated will be examined by molecular modeling methods and theoretical approaches will be proposed for reaction pathways. For this purpose, possible reactions were calculated using Gaussian09 package program. DFT method was used in the theoratical study. In this study, possible reaction paths in the reaction between pesticide substances and OH radical were determined. Fragmentation reaction requires energy. OH radicals are used to degrade pesticide substances. The lowest energy molecule has the most stable structure. According to this, when we list the pesticide substances and fragments from the most stable to most unstable, they are Buprofezin, F1, F2, F3, F4. These results will guide experimental workers and determine the mechanism of fragmentation. [1]



The geometric shapes of molecule obtained because of optimization

Key Words: *Gaussian09, DFT, Pesticide, Buprofezin*

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SILICA XEROJEL SYNTHESIS WITH DRYING CONTROL CHEMICAL ADDITIVE

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Abstract

Silica xerogels are porous materials having low density with high surface area, adjustable pore sizes and high thermal resistance. The silica xerogels attract attention as micro-mesoporous structures in many application areas due to the adjustable surface chemistry with the sol-gel technique and the economic advantages of synthesis ease. In the synthesis of silica xerogel, pore shrinkage and structure collapses can occur with drying under atmospheric conditions due to the solvent surface tension and capillary effect at the solid-liquid-vapor interface in the pores of the gels. The limitation of these disadvantages is widely dependent on the preparation and drying parameters [1, 2].

In the present study, silica xerogels were synthesized using the sol-gel method. In the synthesis, firstly silica source (TEOS; tetraethylortosilicate) was dissolved in ethyl alcohol-water mixture and HCl acid was added until the pH of the solution was 2.0, and the mixture was stirred at 37 ^{o}C for 1 hour. Then 0.6 M ammonia solution was added to the mixture, the mixture was immediately taken into a Teflon-coated autoclave and kept in an oven at 80 °C for 2 days. The resulting solid gel was dried at room temperature, afterward the xerogels were calcined at 500 ^{o}C for 4 hours. In order to prevent pore collapse/shrinkage, glycerol and oxalic acid were selected as drying control chemical additives (DCCA). DCCAs were added after adding of ammonia and the other steps were applied in the same way. The xerogels characterized using TGA (thermogravimetric analysis), XRD (X-ray diffraction) and nitrogen adsorption/desorption isotherms. The thermal stability of the synthesized xerogels was determined by TGA analysis and the calcination temperature was decided. TGA analysis results showed that the water in the structure of xerogels using DCCA was removed later than the xerogel without DCCA. This behavior showed that the moisture was removed in a controlled manner and thus it was thought that pore collapse was prevented. In xerogels using DCCA, it was determined that the mass loss was fixed and the stable structure continued after 550 ^{o}C. All xerogels exhibited a broad peak showing the amorphous silica structure at the Bragg angle value of $2\theta = 23^{o}$. From the nitrogen adsorption/desorption isotherms, the BET (Brunauer–Emmett–Teller) surface area value and the total pore volume values of the xerogel synthesized without using DCCA were determined as 823 m^2/g ~0.60 cm^3/g, respectively. The use of DCCA caused to decrease of the surface area value from 823 m^2/g to 492 m^2/g and the total pore volume from 0.59 cm^3/g to 0.29 cm^3/g, while the micropore volume value increased from 0.150 cm^3/g to 0.392 cm^3/g. Micropore size increased slightly from 1.00 nm to 1.17 nm with the use of glycerol. It was concluded that the structure collapse prevented with the gradual removal of water from the structure due to the high micropore volume of the xerogel synthesized by using glycerol.

Key Words: *Silica xerogel; synthesis; characterization; drying control chemical additive*

Acknowledgment: This study was supported by Gazi University Scientific Research Projects Department (Project number: BAP 06/2019-09)

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Possible Reaction Pathways of the Selected Organophosphorus and Carbamate Pesticides according to the DFT Calculation Method

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Abstract

This research was carried out in order to analyse the reactions of three organophosphorous (OP) and three carbamate (CB) pesticides with the hydroxyl radical (.OH), and their degradation paths. The studied organophosphorous pesticides are Azamethiphos, Coumaphos, Temephos, and carbamate pesticides are Methiocarb, Carbofuran, Pirimicarb compounds respectively. Initially, in the reactions, the initial geometries of the reactants were determined. Geometric optimisations were determined using the DFT/B3LYP/6-31G (d) basic set of Quantum Mechanical Density Functional Theory (DFT). For each molecule, degradation reaction mechanisms were tried to be clarified using the calculated energy values. Since the reactions of pesticides with .OH are essential in terms of both water treatment and atmospheric chemistry, energy values were calculated both at gaseous phase and aqueous phase by modelling the solvent effect. For each molecule, fragments were found out by analysing the bond lengths, bond angles, and energy values, and as a result, degradation paths were determined.

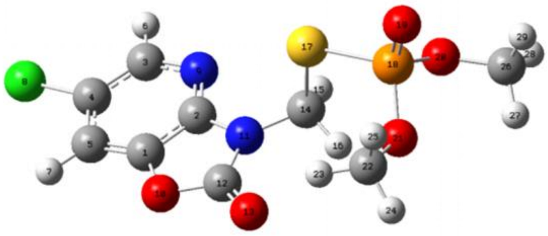

Figure 1. Optimized state of the same CA molecule. (Grey, C; white, H; blue, N; red, O; green, C; yellow, S; orange, P).

Key Words: *Organophosphorous Pesticides, Carbamate Pesticides, DFT.*

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Non-toxic and hemocompatibility nanocarrier derived from polygalacturonic acid for sustainable drug delivery

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Abstract

Polygalactronic acid (PGA) is a natural biopolymer consisting of branched saccharides which can be obtained from the cell wall of some plants. PGA known as pectic acid is generally utilized in pharmacological products because of its inherent non-toxic, biocompatible, biodegradable, non-immunogenic nature [1]. In this study, polymeric nanoparticles of PGA were synthesized in a single step by using trimethylolpropane triglycidyl ether (TMPGDE) as a degradable crosslinker. Vancomycin (VAN) is an antibiotic and amphotericin B (AMB) is an antifungal agent was separately encapsulated into PGA nanoparticles during the crosslinking reaction to prepare the drug-loaded forms of PGA nanocarriers as PGA@VAN and PGA@AMB, respectively. The drug release from PGA@VAN and PGA@AMB nanocarriers were carried out under physiological conditions, e.g., at pH 7.4 phosphate buffer solution (PBS), at 37 °C. Moreover, the antibacterial activity of PGA@VAN nanoparticles against *Staphylococcus aureus* ATCC 6538 as a gram-positive bacterium and the antifungal activity of PGA@AMB nanoparticles against *Candida albicans* ATCC 10231 as a fungus were investigated by using disc diffusion and microtiter assays. Furthermore, the blood and biocompatibility of these carriers were also determined by hemocompatibility tests, hemolysis, and blood clotting assays, and by cytotoxicity analysis on L929 fibroblast cells using MTT assay.

Key Words: *Polygalactronic acid; polymeric nanocarriers; sustainable drug delivery; antibacterial/antifungal; biocompatible*

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RESERVOIR CHARACTERISTICS OF THE KUSURİ FORMATION SANDSTONES IN THE ZONGULDAK SUB-BASIN OF WEST BLACK SEA, TURKEY

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Abstract

The West Black Sea Basin is one of Turkey's important natural gas-producing areas. Natural gas was first discovered in the West Black Sea Basin in 2007. In this study, samples taken from the B1 well opened in 2007 in Zonguldak sub-basin were studied. The objectives of this research are to reveal the presence of organic matter, analyse the petrophysical parameters (porosity, permeability), detecting clay minerals and their effects on the reservoir, determine the reservoir quality of the sandstones of the Zonguldak sub-basin. The Kusuri Formation sandstones were divided into three groups based on their grain size using petrographic analyses. Group 1 is composed of 0.4-0.6 mm grains, group 2 contains 0.3 mm grains and group 3 consists of very fine grains (0.1-0.2 mm). Illite, kaolinite, and mixed layer illite-smectite authigenic clay minerals were detected, and they negatively affected the reservoir characteristics of Kusuri Formation. Reservoir quality was interpreted according to porosity and permeability values using well logs. In group 1; the porosity varied between 35 % and 50%, while permeability values varied between 400 mD and 660 mD. In group 2; the porosity varied between 20 % and 35%, while permeability values varied between 100 mD and 400 mD. In group 3; the porosity and permeability values are very small. These data revealed that group 1 and 2 are medium-good quality reservoir rocks. Contrastingly, group 3 does not exhibit reservoir features. Samples with greater permeability displayed lower hydrocarbon peaks than those with less permeability in the Fourier-transform infrared spectra. Aromatic C-H peaks, and $CH=CH_2$ peaks of alkenes indicate the presence of unsaturated hydrocarbons. It has been determined that the Kusuri Formation sandstones of the Zonguldak Sub-Basin are a medium-good quality reservoir rock.

Key Words: *Hydrocarbon; FTIR; Permeability; Porosity; West Black Sea*

synthesis and biological evaluation of novel *N*-substituted benzimidazole derived Schiff bases

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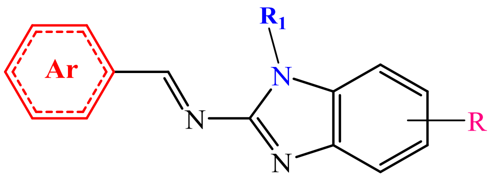
Abstract

Nowadays, there is a growing interest in the synthesis of benzimidazole derived Schiff bases, primarily due to the significant biological activities but also due to the fact that they can easily complexes with different types of metals giving the complexes with interesting electronic and biological properties. [1] They are frequently described as optical chemical sensors or chemodosimeters due to their desirable optical properties, where benzimidazole is often incorporated as a functional or electron-accepting unit. The special interest of scientists has been focused to evaluate the Schiff bases as ligands for transition metals since suchlike complexes possess different biological activities including anticancer, antimicrobial, antifungal etc. [2]

Target compounds were prepared by conventional reactions of organic synthesis as well as by microwave assisted reactions. Benzimidazole derived Schiff bases were prepared in the reaction of *N*-substituted 2-aminobenzimidazoles with 4-*N*,*N*-dimethylamino-, 2-hydroxy-4-*N*,*N*-dimethylamino- and 4-nitrobenzaldehyde. The structures of all newly prepared benzimidazole derived Schiff bases were confirmed by the means of ^{1}H and ^{13}C NMR spectra and elemental analysis. All Schiff bases were tested for their antiproliferative activity *in vitro* on a panel of human cancer cells as well as for antiviral activity on several chosen viruses.

Key Words: *antiproliferative activity, antiviral activity, benzimidazoles, cytotoxicity, Schiff bases*



Ar = 4-N,N-dimethylaminophenyl
4-N,N-diethylamino-2-hydroxyphenyl
4-nitrophenyl
R = H, CN
R$_1$ = isobutyl, methyl, phenyl, hexyl

Figure 1. Benzimidazole derived Schiff bases

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Acknowledgments: This work was funded by the Croatian Science Foundation (project IP-2018-01-4379).

AN ECO-FRIENDLY SYNTHESIS OF NOVEL 2-ARYL BENZOXAZOLE DERIVATIVES

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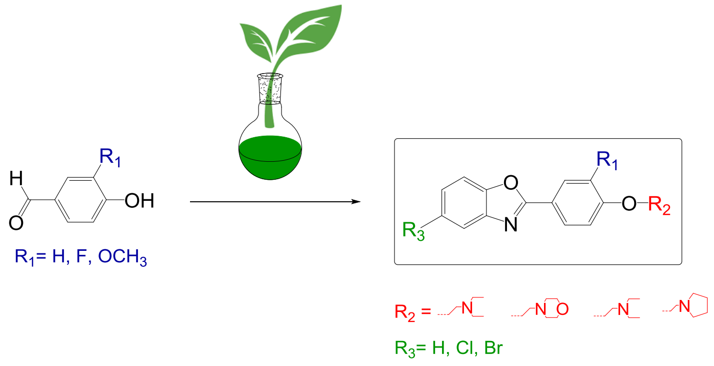
Abstract

The benzoxazole heterocycle is often found in ligands targeting a plethora of receptors and enzymes. Furthermore, bioavailability, metabolism and the use of benzoxazole as bioisostere are discussed. The development of new reaction media plays a key-role within the green chemistry framework [1]. The goal of obtaining novel media with low environmental impact represents, in fact, a challenge in modern chemistry, considering the toxicity and the high vapour pressure of traditional organic solvents [2]. Deep eutectic solvents (DES) have important physico-chemical advantages in terms of “greenness” compared to typical organic solvents. Moreover, DESs made of urea, glycerol, water or choline chloride are particularly promising in synthesis from green chemistry point of view because of their low cost and environment-friendliness [3]. The main aim of research is synthesis of novel 2-arylbenzoxazole derivatives by using modern synthetic green approach including mechanochemical and microwave reactions as well as application of different DES. The key precursors of 4-O-alkylated benzaldehyde for the synthesis of target benzoxazole derivatives were prepared in DES (ChCl/glycerol) with K_2CO_3 as a base. Schiff bases were performed by mechanochemical reactions of 4-O-alkylated benzaldehyde with 2-aminophenole in a ball mills. 2-arylbenzoxazole derivatives were synthesized by microwave assisted cyclization reaction of Schiff bases with NaCN in ethanol.



Key Words: *benzoxazoles, green chemistry, deep eutectic solvent, mechanochemical sycnthesis, solvent-free synthesis*

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A water-soluble NDI derivative as a chemosensor for the detection of heavy metal cations

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Abstract

This project investigates the selectivity and detection of a naphthalene diimide (NDI) derivative (SNDI) towards heavy metal cations. It is noteworthy that the role of ions is of great importance in both life and technological processes. A metal ion detector should have good water solubility, easy synthesis and cheap raw materials [1− 4]. Previously, NDI derivatives have been reported as sensors for detecting various heavy metal ions [5].

For our project, we have used a previously synthesized NDI derivative, SNDI, and various metal cations Ag^+, Hg^{2+}, Mg^{2+}, Cu^{2+}, Fe^{3+}, Ca^{2+}, Ni^{2+}, Co^{2+}, Zn^{2+}, Pb^{2+} and Cd^{2+}. All measurements were taken in HEPES, sodium salt, pH 7.2. The recognition properties of the SNDI towards the metal cations were primarily studied by UV-vis absorption and emission spectroscopy. The results have indicated that SNDI has a selectivity towards Cu^{2+}. Emission spectroscopy results have also shown that the emission intensity of SNDI at λ_{exc} = 225 nm has increased upon the addition of an increasing concentration of Cu^{2+}. Electrochemical measurements of SNDI and Cu^{2+} complex have also shown an interaction. This investigation shows that, upon the addition of increasing concentrations of Cu^{2+}, there is a shifting in the peak reaching to −1.18 V upon 10 equiv of Cu^{2+} is added.

Furthermore, the interaction of SNDI with Cu^{2+} was investigated via FTIR spectroscopy. The FTIR spectra of SNDI and Cu^{2+} in HEPES, has shown that the possible binding mechanism is from the sulfo group of SNDI. Upon the addition of Cu^{2+}, the emergence of a novel peak and shifting in peaks have shown a possible interaction between SNDI and Cu^{2+} via the sulfo group of SNDI.

All the results of this study, including UV-vis absorption and emission spectroscopy investigations, electrochemical measurements and FTIR studies, were in good agreement. This study concludes that SNDI has the highest selectivity towards Cu^{2+}.

Key Words: *water-soluble; NDI derivative; chemosensor; selectivity; interaction*

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Perylene Diimide Based Interlayer for Application in Perovskite Solar Cells

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Abstract

Perylene derivatives have shown outstanding physicochemical properties and been widely used in different electronic devices. N-annulated perylene based molecules have electron-rich properties, and the π-π interactions of molecular packing are favourable to having reasonable charge-transporting features [1].

In recent years, the organic-inorganic hybrid perovskite solar cells (PSCs) have revealed a powerful competitor in the photovoltaic community and generated broad research interests in the fields of both photovoltaic technology and material development [2].

Synthetic approaches for attaining sufficient access to bay-monobrominated PDIs are essential for this kind of study. Practical synthetic routes for different N-annulated PDI monobromides are of great interest since they are also significant intermediates for developing novel materials based on PDI molecules [3].

The aim of our study is to synthesize two perylene diimide (PDI) derivatives for application as an interlayer in perovskite solar cells (PSCs). Bay-monobrominated perylene diimide molecules were used to synthesize two novel compounds, **1** and **2**. The progress of the reactions was monitored using thin-layer chromatography (TLC) and FTIR spectroscopy. The FTIR spectra of the two molecules have shown that the peaks are consistent with the assigned structures of the molecules.

Key Words: *Electron transporting material; PSCs; PDI derivatives; bay-monobrominated; power conversion efficiency*

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Non-peripheral Cobalt Phthalocyanine bearing Phthalimide unit: Facile synthesis via click reaction, spectroscopic and DNA Binding Study

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Abstract

Phthalocyanines (Pc) and their metal complexes (MPc) have attracted considerable interest and have been found to be highly promising candidates for a variety of uses, such as optics, photodynamic therapy, liquid crystals, gas sensors, catalysts, photosensitizers and dye-sensitized solar cells [1]. Finding new suitable photosensitizers for photodynamic therapy is a focus of this study, it is aimed to investigate the photochemical and physical properties for the photosensitizer properties of the synthesized phthalocyanine compound.

The best known click reaction is the copper-catalyzed between azides and terminal alkynes and refers to biological syntheses that assemble small units together with high yields and very simple processes [2]. The aim of the present work will be to synthesize non-peripheral Co(II) phthalocyanine derivatives which contain tetra-substituted 1,2,3 triazole and electrochemical active phthalimide units on each benzo group. CoPcs structures were characterized by FT-IR, UV-Vis and MALDI-TOFF spectroscopy techniques. DNA binding behaviors of this CoPcs were also investigated by spectroscopic techniques [3] (Fig.1).

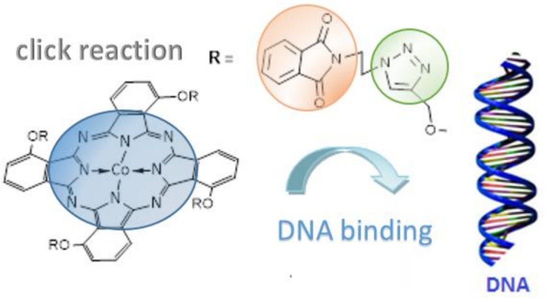

Figure 1: Schematic illustration of phthalocyanine structure and DNA molecule

Key Words: *phthalocyanine; DNA binding; cobalt; click reaction, phthalimide*

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MICROWAVE ASSISTED SYNTHESIS OF SOME 2(3H)-BENZOXAZOLONE DERIVATIVES

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Abstract

Microwave assisted organic synthesis has gained interest as it could be an alternative technique to traditional heating methods which could lead to clean, simple, efficient, fast and economically desirable synthesis of organic compounds [1].

2(3H)-Benzoxazolones are known to have versatile reactivity as a result it is possible to synthesize diverse derivatives which makes this molecule a desirable scaffold in medicinal and pharmaceutical research in efforts to develop a drug candidate. Such 2(3H)-Benzoxazolone derivatives have been reported to exhibit many different biological activities including analgesic, anti-inflammatory, anti-cancer and antibacterial [2-5].

In this present work, we have developed a facile and efficient approach for the synthesis of these 2(3H)-Benzoxazolone compounds under microwave condition. The reactions were also carried out by reflux so to compare between these two different synthesis methods. Six different Mannich bases of 2(3H)-benzoxazolone derivatives having a piperazine or piperidine group at the third position of the ring were synthesized by using a classic Mannich reaction. Shorter reaction times and improved yields were observed under microwave synthesis condition indicating use of less energy compared to that using reflux method. The reactions were monitored by TLC and melting point determination, whereas the chemical structures of the compounds were elucidated by using FT-IR and ^{1}H-NMR spectroscopic methods.

Key Words: *2(3H)-Benzoxazolone; Mannich reaction; microwave Synthesis; piperazine; piperidine*

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SYNTHESIS, CHARACTERIZATION AND ACTIVITY STUDIES ON PIPERAZINE SUBSTITUTED IMIDAZOLES

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Abstract

There are many drugs containing imidazole ring owing to its wide range of biological activity especially as antifungals, antibacterials, anti-HIV and anticancer agents [1-5]. In addition, in some biologically important natural compounds such as histidine there is an imidazole nucleus. As a result, imidazole is an attractive and important choice of pharmacophore in drug discovery efforts. In the light of the studies available in the literature, novel N1-substituted imidazole derivatives were synthesized through Mannich reaction. The imidazole core structure was reacted with three different piperazine derivatives (phenylpiperazine, 2-fluorophenylpiperazine, 4-fluorophenylpiperazine under reflux conditions to yield to the target molecules.

The piperazine substituted imidazole derivatives were characterized by Proton Nuclear Magnetic Resonance Spectroscopy (^{1}H-NMR), Fourier Transform Infra-Red (FT-IR) and Electrospray Mass Spectrometry (ESI-MS). Thin layer chromatography and melting point were done for checking the purity. The FT-IR spectra of the compound show the absence of N-H stretch, which indicating that the reaction has indeed taken place at the position N1 of the imidazole core structure. Disk diffusion technique was utilized to study antimicrobial activity toward several gram positive and gram-negative microorganisms including: *E. coli*, *Pseudomonas spp.* and *Staphylococcus spp.*

Key Words: *imidazole; Mannich reaction; antimicrobial; heterocycles; phenylpiperazine*

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STABILITY INVESTIGATION OF PAA-BSA BIOCONJUGATE AND PAA-CU^{+2}-BSA TERNARY BIOCOMPLEX IN DIFFERENT pHs and COMPARISION with in DIFFERENT SALT CONCENTRATIONS

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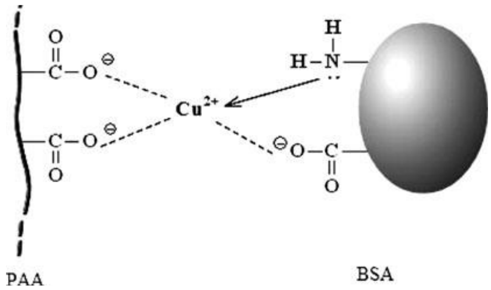
Abstract

The solubility, composition, and stability of polycomplexes depend on pH, metal/PE, and protein/PE ratios. Some of these polycomplexes reveal strong immunogenecity and provide a high level of immunological protection. Zetasizer parameters such as particle size, polydispersity, mobility and zeta potential are used to control the stabiliy of solutions. These parameters are also very important for polyelectrolyte–protein binary conjugate and polyelectrolyte–metal-protein ternary complexes because of bioavailability, dissolution and immune toxicity of these complexes.[1,2] In the present work, it was synthesized and investigated stability of PAA-BSA bioconjugate and PAA-Cu^{+2}-BSA ternary biocomplex (Scheme 1) in different pHs. The pH and salt concentration effect on the stability of PAA-BSA bioconjugate and PAA-Cu^{+2}-BSA ternary biocomplex were evaluated and compared with each other[3].



Scheme 1 The hypothetical structure of ternary water soluble complex of PAA-Cu^{2+}-BSA

Key Words: *PAA-BSA bioconjugate and PAA-Cu^{+2}-BSA ternary biocomplex; stability; zetasizer measurements*

Acknowledgement: This work was supported by the Scientific Research Project Coordination Center of Yıldız Technical University, Turkey (Project No: 2012-01-02-GEP04).

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N-CQD functionalized folic acid nanocapsules containing paclitaxel for increased in vivo and in vitro drug delivery and imaging of cancer cells in the MCF-7 and MTT breast cancer cell lines

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Abstract

A wide variety of drug delivery carriers for nanoscale, nanocapsules can be one that have been developed at the intersection of nanotechnology base and biomedicine. Furthermore, several new and innovative developments in recent scientific nanomedicine field, particularly utilized materials in the range of nanoscale to function as medical technologies or delivery carriers for pharmaceutical agents to targeted the specific areas. Treatment of different illnesses using nanomedicine has lately seen a number of notable applications (chemotherapeutic agents, biological agents, immunotherapeutic). Nanomedicine. As a vital example in this case, researchers are exploring new ways of administering drugs in order to ensure that they target specific regions, minimizing their toxicity and enhancing the bioavailability of these drugs [1]. Since the 1990s, the FDA has approved several nanotechnology-based products and clinical trials, including liposome, synthetic polymer particles, formulations, and also micellar nanoparticles, as well as proteins and nanocrystals. It is currently possible to diagnose diseases and even combine diagnostic with treatment through the use of nanomedicine. therefore, the fact that regulatory mechanisms for nanomedicines and toxicity assessments will be the subject of more study in the future. Biodegradability and biocompatibility of the chosen polymers in this study have been used to create nanocapsules containing paclitaxel to target breast cancer cells via positive folate receptor simultaneously with imaging and therapy. Nanocapsules containing nitrogen-rich carbon quantum dots nano emulsions is utilized to detect and interface to breast cancer cells (MCF-7, MTT) for the detection of surface antigens and also cytotoxicity test that the mean IC50 values on the MCF-7 cell line is measured [2]. FTIR, XRD, and PL spectroscopy, as well as FESEM and TEM, were all used to examine the produced nanocapsules for their unique properties and characteristics. paclitaxel-coating-encapsulated nanocapsules exhibit better biocompatibility and solubility in physiological fluids than the free paclitaxel, which has limited solubility. Another study indicated that the nanocapsules were capable of being taken up by cells and monitored in vitro, as demonstrated by cell imaging experiments. This study's findings demonstrate the efficiency, specificity, and controlled release of paclitaxel provided by the manufactured nanocapsules. Recent breakthroughs in nanomedicines, including technological advances in medication administration and new diagnostic methods, are discussed herein. Drug solubility and absorption, bioavailability and controlled-release were the primary goals of nanotechnology in the beginning. As opposed to some 50 years ago, when discovering pharmacologically active natural compounds was a preferred option, the discovery of nanodrugs deals with high levels of uncertainty. It is currently normal practice to use nanotechnology to enhance the effectiveness of recognized natural bioactive substances. Novel natural biomaterials are in high demand because of their biodegradability, biocompatibility, availability, renewable nature, and low toxicity. There have also been several introductions of lipid polymeric hybrid nanoparticles, and nanospheres made by the

solvent evaporation, polymerization emulsion to improve the stability of these biopolymers in industrial processing environments and biological matrixes [3].

Keywords: Nanocapsule, Drug release, Paclitaxel, MCF-7, cell imaging

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CMC/PEG BLENDED HYDROGELS FOR TISSUE ENGINEERING AND REGENERATIVE MEDICINE

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Abstract

Over the course of human life, wound healing and repair is an intricate and complicated biological process that occurs after an injury. Skin repair is an active process that reconstructs tissue after an injury by incorporating various interactions between cells, extracellular matrix (ECM), and growth hormones within the human body [1]. Accidental skin injuries including laceration, burns, contusion, chronic lesion, trauma, and infections can all create serious healthcare issues if not properly addressed.

Hydrogels are hydrophilic polymer networks that hold a considerable quantity of water or other biological fluids. They can mimic natural gel functions in biological agents, such as swelling [2,3]. The skeleton and crosslinking density of a hydrogel's network determine its capacity to swell. In terms of demonstrating stimuli responsiveness and reversibility, thermogelling systems have numerous benefits and strengths over the more prevalent use of cross-linked hydrogels. In addition, the in-situ phase transition at varied temperatures provides functional and manufacturing flexibility in terms of formulation, injectability, and performance management [4].

Novel hydrogels were created by crosslinking carboxymethyl cellulose (CMC) sodium salt with poly (ethylene glycol) 400 (PEG400) in this study. They were synthesised entirely at ambient temperature with the aid of a simple one-pot ecologically friendly liquefied technique. The degree of crosslinking and the action of PEG as a network modifier were proven to adjust the mechanical and physio-chemical properties, as well as morphological aspects, in order to mirror the characteristics of real and genuine skin tissue characteristics. An exceptional design methodology for the fabrication of CMC/PEG hydrogels was examined. Numerous instrumental procedures were employed in the characterisation of the CMC/PEG hydrogels. The hydrogels performed exceptionally in terms of moisture absorption and retention and have therefore proven to be compatible in regards to biomedical implementations including wound dressings.

***Key Words: hydrogel, natural biomaterial, carboxymethylcellulose, PEG, mechanical properties**,*

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SELF-ASSEMBLY AND PHOTOPHYSICAL PROPERTIES OF PERYLENE DIIMIDES WITH ELECTRON-WITHDRAWING SUBSTITUENTS

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Abstract

Self-assembled π-conjugated systems have attracted attention due to their potential application as conductive nanowires in organic electronics via the effective π-orbital interactions facilitating charge carriers' hopping [1]. Perylene diimides have been intensively investigated due to their outstanding chemical, thermal and photochemical stabilities, intense luminescence, light fastness, and n-type semiconductor properties [2-4]. Perylene diimides` aggregation in a solution due to the stacking of their planar π-systems was reported [2,5]. Thus, these dyes and their assemblies find functional application units in artificial light-harvesting and photoinduced electron transfer systems and organic electronic devices [2,6].

This work has studied the self-assembled π-π stack of perylene diimides at various concentrations and temperatures both in solution and solid-state using UV-vis and fluorescence spectroscopies. The stacking properties of perylene diimides have been extensively investigated and reported. This study has explicitly selected electron-withdrawing moieties to investigate the self-assembly of these perylene diimides. The optical properties of the π-π stacks and their appropriate application areas were investigated.

Besides the theoretical calculations, we have studied the concentration and temperature-dependent UV-vis and fluorescence spectra in detail. Conclusively, this study showed that the electron-withdrawing moieties increased the π-π stacking.

Key Words: *Perylene diimides; self-assembly; π-π stacking; electron-withdrawing groups, substituent effects*

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NAPHTHALENE DIIMIDES WITH ELECTRON ACCEPTOR SUBSTITUENTS: SYNTHESIS, CHARACTERISATION, PHOTOPHYSICAL AND SOLID-STATE ELECTROCHEMICAL PROPERTIES AND DFT STUDIES

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Abstract

Naphthalenediimides are used as industrial colourants in the form of dyes and pigments due to their fluorescence quantum yield and favourable photophysical and electrochemical properties. They are also effectively used as optical brighteners, laser dyes, electrophotography, conducting materials, metallomacrocycles, intercalators for DNA, models for the photosynthetic reaction center, and chemical sensors, optoelectronic devices such as organic solar cells, light-emitting diodes and field-effect transistors and rechargeable batteries [1-2].

Naphthalene diimide derivatives can be synthesised through N-imidization, allowing varying absorption and fluorescence properties. In general, electron-donating and electron-withdrawing moieties are used to change the electrochemical properties through core substitutions.

This work has successfully synthesised electron acceptor substituted naphthalene diimides under special conditions in high yields. The synthesised compounds' optical, thermal, and electrochemical properties were investigated in detail. In contrast to the absorption spectra, the emission spectra strongly depended on the solvent polarity. The excimer-like emission and low fluorescence rate constant suggest the formation of the ground state complex in DMF. The voltammetry of immobilised microparticles has investigated the electrochemical properties due to poor solubility. This technique is a simple and powerful tool to characterise the thermodynamics of electroactive compounds with poor water solubility and also elucidate their redox mechanisms [3]. Notably, the Density Functional Theory (DFT) calculations were performed to elucidate the electronic properties of the synthesized products.

Key Words: *Naphthalene diimides; solid-state electrochemistry; electron-acceptor substituent, voltammetry of immobilised microparticles; DFT*

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Characterisation of High-Tin Bronze Alloys in Archaeological Soil of Cyprus

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Abstract

Cyprus has particular importance in the Eastern Mediterranean with its harbour and copper ores, and the Karpas Peninsula location has always attracted attention with its advantageous reach to overseas cultures [1]. The Kral Tepesi site, next to Kaleburnu/Galinoporni on the Karpas peninsula of Cyprus, was discovered by Eastern Mediterranean University academicians during their hiking trip in June 2004 [2]. A pithos containing 26 metal objects were unearthed, including 16 vessels, three offering stands, five sickles, a shovel and a saw. All 26 objects were analysed using X-Ray-Fluorescence method by taking 1 mm sample with drilling [3]. As a result of the analysis, it was determined that the artifacts were bronze (copper-tin alloy). References on bronze artifacts are usually observed to be either low-tin bronze (up to 14% tin) [4] or high-tin bronze (15%-27%) [5-6]. Differences in the chemical compositions of artifacts directly affect the corrosion types on the artifacts. Because each artifact is unique, it is necessary to examine each corrosion type separately to understand and prevent the cause of this destructive process.

In this study, six bronze bowls with the same typology in the hoard are examined, and four of them are selected according to high-tin bronze classification. This study aims to characterise the corrosion products of 4 bronze bowls from Late Bronze Age, which were found in 2004, using Cyclic Voltammetry (CV) and Fourier Infrared Spectroscopy (FT-IR) for identifying corrosion products. This study is used to develop an approach for conservation studies to stop the corrosion-related destruction of artifacts.

Key Words: *Bronze; corrosion; conservation; infrared spectroscopy; cyclic voltammetry;*

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Electrochemical Approach to the Low-Tin Bronze Alloys in Archaeological Soil of Cyprus

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Abstract

Even though archaeological bronze artifacts have similar chemical composition and microstructure, the situation of each archaeological work is more complex than the other because they all have a unique individual story and interaction with the soil [1]. Given the variation of environmental elements and the diversity of alloy metals, it is not possible to make a generalization on the protection/degradation behaviour of archaeological bronze artifacts. Therefore, it is essential to determine a descriptive method for dealing with the corrosion stratigraphy of the works [2].

Characterization of corrosion products has been carried out for a long time to develop the conservation strategies and restoration procedures of archaeological copper alloys [3]. The analysis of archaeological bronze artifacts to identify corrosion products and evaluate possible causes of these products is carried out by a combination of different disciplines.

In June 2004, the hoard was discovered [4] included a pithos filled with 26 metal objects in Kral Tepesi site near Kaleburnu/Galinoporni on the Karpas peninsula of Cyprus. X-Ray-Fluorescence analysis result concluded that the artifacts were made from bronze (cooper-tin alloy) [5].

In this study, six bronze bowls with the same typology in the hoard were inspected, and two were selected according to low-tin bronze classification. This study aims to characterize the corrosion products of two bronze bowls from Late Bronze Age, unearthed in 2004, using electrochemical and spectroscopic techniques. Cyclic Voltammetry (CV) and Fourier Infrared Spectroscopy (FT-IR) are used for spectroscopic surface examination for identifying corrosion products.

Key Words: *Bronze; corrosion; conservation; infrared spectroscopy; cyclic voltammetry;*

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SYNTHESIS, AND ANTIMICROBIAL EVALUATION OF ARYLAMINO QUINOLINEQUINONES

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Abstract

Heterocyclic quinones with at least one heteroatom such as nitrogen [1] are an exceptionally important class of compounds [2]. Quinolinequinone (azanapthoquinone) is a class of nitrogen-containing bicyclic heterocyclic compounds that are of great importance and form the crucial core in a variety of drugs, many natural products, and pharmaceutically active compounds including anticancer, antibacterial, antimalarial, anti-HIV, antiviral, antichagasic, and antifungal agents [3].

Despite significant progress in research on heterocyclic quinone chemistry, considerable efforts continue to be made to identify new quinolinequinone compounds with strong bioactivity. A preliminary assessment of the structure-activity relationship (SAR) from our previous studies suggests that the replacement of the phenyl ring by the methyl groups (to form plastoquinone analogues) is essential for the biological activities [4]. In this study, the relationship between the bioactivity of quinones and the number and position of heteroatoms in heterocyclic quinones has been extensively studied.

Key Words: *Arylamino-substituted quinolinequinone, structure-activity relationship, antibacterial, antifungal*

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NOVEL IMINOCOUMARINE DERIVED IMIDAZO[4,5-*b*]PYRIDNES AS POTENTIAL ANTIOXIDANTS

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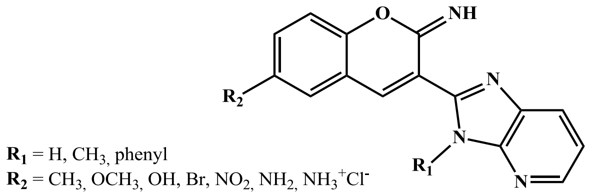
Abstract

Antioxidants are small organic molecules which have important role of maintaining healthy balance between reactive oxygen species and antioxidants by scavenging free radicals. It is well known that overproduction of ROS is linked to oxidative stress which is important factor in the development of many diseases and disorders. Many of naturally occurring and synthetic coumarines were vastly studied for their biological activities including antioxidant capacity.[1] On the other hand, the biological activity of imidazo[4,5-*b*]pyridine is still unexplored. As acrylonitrile derivatives of imidazo[4,5-*b*]pyridine showed promising antioxidative potential, series of iminocoumarine derivatives was logical next step in development of compounds with more pronounced antioxidative activity.[2]

This work presents the synthesis, structural characterization and antioxidative activity of 6-substituted iminocoumarin derivatives of imidazo[4,5-*b*]pyridine. For the synthesis of novel targeted compounds, classical reactions as well as microwave assisted synthesis were used. Main precursors were prepared by the uncatalyzed microwave amination starting from halogeno-substituted precursors followed by the reduction of nitro moiety to amino. 2-cyanomethlyimidazo[4,5-*b*]pyridines obtained in the cyclocondensation reaction with ethyl cyanoacetate, while targeted iminocoumarins were prepared in condensation reaction with 5-substituted salicylaldehydes. Additionally, amino-substituted derivatives were prepared by the reduction with $SnCl_2 \times 2H_2O$ which were further protonated to obtain their hydrochloride salts. The structures of newly prepared compounds were confirmed by means of ^1H and ^{13}C NMR spectroscopy as well as MS spectrometry. Newly prepared compounds were tested for their antioxidative activity *in vitro* by using several spectroscopic methods such as ABTS, DPPH and FRAP. Measured antioxidative capacities will be rationalized by computational analysis.



R_1 = H, CH_3, phenyl
R_2 = CH_3, OCH_3, OH, Br, NO_2, NH_2, $NH_3^+Cl^-$

Figure 1. The structures of newly prepared derivatives

Key Words: *imidazo[4,5-b]pyridine; iminocoumarines; antioxidants*

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Novel 1,3-diphosphapropenes and their use as ligands towards transition metal fragments

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Abstract

In the last few years, the chemistry of low coordinated phosphorus compounds, containing a phosphaalkenyl unit, gain interest due to their possible applications in catalysis [1]. Our group focused on studying compounds bearing a phosphaalkenyl unit in a P=C-P moiety as they can be further used as building blocks for new organometallic and coordinative compounds [2, 3].

The stabilization of such compounds can be achieved by using a bulky organic substituent on the phosphorus atom such as Mes*, Tip (Mes*= 2,4,6-tri-tert-butylphenyl, Tip= 2,4,6-tri-isopropylphenyl) and can be additionally stabilized by coordination to transition metals. Our group recently described the synthesis and complete characterization of a stable 1,3-diphosphapropene Mes*P=C(Cl)-P(S)(Cl)Tip [4].

We present here preliminary results regarding the use of Mes*P=C(Cl)-P(E)(Cl)Tip (where E=O,S) as ligands to transition metal fragments. Novel complexes with $Au(SMe_2)Cl$, $Cu(AcO)_2$ and $Pd(COD)Cl_2$ were obtained and characterized in solution through usual spectroscopic methods (NMR, MS). The multiple coordination sites of such 1,3-diphosphapropenes have been exploited, obtaining, as suggested by the physicochemical analyses, chelate ligands in the case of copper and palladium fragments.

This work was supported by a grant of the Romanian Ministry of Education and Research, CNCS-UEFSCDI, project PN-III-P1.1-TE-2019-2085 within PNCDI III.

Key Words: *phosphaalkenyl unit; metal complexes; bulky substituents; palladium; cooper*

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INVESTIGATION OF POLY(METHYLVINYLETHER-ALT-MALEIC ANHYDRIDE) FUNCTIONALIZED WITH PREGABALIN DRUG (1:1) RATIO COPOLYMER-DRUG DELIVERY SYSTEM in CATALYST FREE MEDIA

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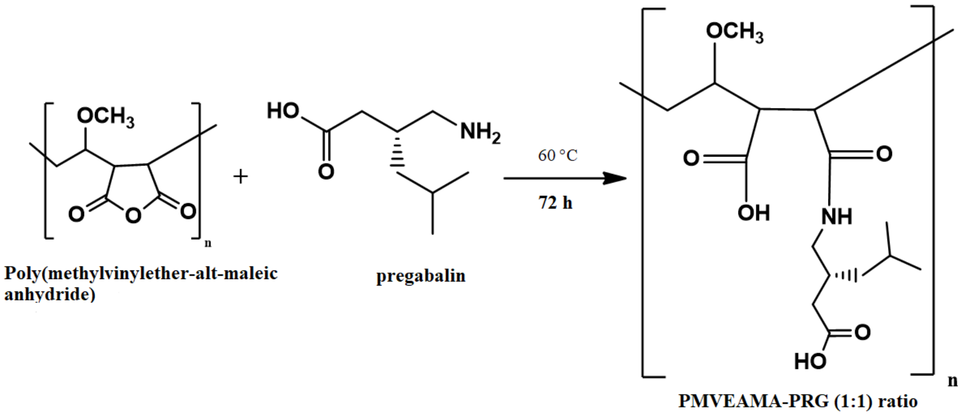
Abstract

Pregabalin is called as an anticonvulsant and an anti-epileptic drug, It is very important to control its delivery in body. In the current study, we aimed functionalized the poly(methylvinylether-alt-maleic anhydride) (PMVEAMA) with pregablin (PRG) drug active substance to obtain copolymer-drug delivery system and thus, controlling the delivery of pregabalin in the body fluid and different pHs. For this purpose, we synthesized poly(methylene-alt-maleic anhydride)-PRG copolymer-drug delivery system PRG with (1:1) ratio in catalyst free media (Scheme 1). The synthesized PMVEAMA-PRG system were characterized via ^{1}H NMR and FTIR/ATR. The zetasizer measurements of PMVEAMA-PRG copolymer-drug delivery system were investigated at in vitro conditions based on the time effect by zetasizer measurements and UV/VIS measurements, respectively.



Scheme 1 Synthesis of Poly(methylvinylether-alt-maleic anhydride)-PRG (1:1) ratio copolymer-drug delivery system in catalyst free media

Key Words: Poly(methylvinylether-alt-maleic anhydride); pregabalin drug;zetasizer measurements

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SPECTROSCOPIC INVESTIGATION OF NEW BENZANTHRONE LUMINESCENT DYES

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Abstract

Luminescent dyes have received a considerable attention for their potential applications in biochemical and medical assays. Benzanthrone dyes are a special class of environmentally sensitive, photostable, bright luminophores. Therefore, many benzanthrone derivatives have found application in a number of areas, including coloring materials, laser-active media, electroluminescent materials, and as fluorescent markers and sensors in biology.

In present work, a series of novel benzanthrone dyes with various nitrogen containing heterocyclic moieties at 2 and 3-positions of benzanthrone core were obtained and studied. During our investigation new preparation methods were developed for synthesis of emissive derivatives of benzanthrone. Synthesized derivatives have bright from green to red luminescence in various media. The structure of obtained compounds was confirmed by NMR and FT-IR spectroscopy and mass spectrometry.

To characterize the optical properties of newly obtained compounds, the absorption and luminescence spectra in several organic solvents with various polarities were recorded and analyzed. The studied luminophores are characterized by pronounced fluorescence solvatochromism. In present research, interesting results about substituents effects on reactivity and physical properties of prepared dyes are obtained and discussed.

Key Words: *Luminescent dyes; Benzanthrone derivatives; Synthesis; Fluorescence spectroscopy; Solvatochromism*

SYNTHESIS, ANTIPROLIFERATIVE EVALUATION AND DNA/RNA BINDING STUDY OF NOVEL AMIDINO-SUBSTITUTED PHENYLENE-BIS(BENZAZOLES)

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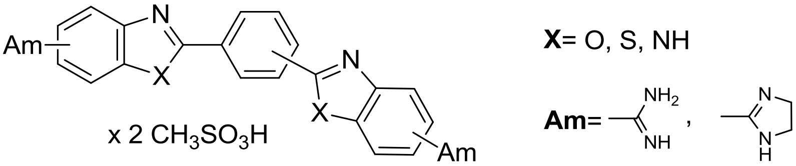
Abstract

In the field of drug discovery and development, biologically important heterocyclic molecules known as “privileged structures” play an important role as promising future drug candidates, because of their versatile binding properties for different biotargets. In continuation of our recent research in the synthesis and evaluation of antiproliferative activities of amidino-substituted 2-arylbenzazole derivatives [1,2], we present here a series of twelve novel amidino-substituted phenylene-bis(benzazoles), differing in heteroaromatic scaffolds as well as in type of amidine moiety.



The synthesis of 1,3- and 1,4-phenylene bis-benzothiazole, benzimidazole and benzoxazole functionalized with unsubstituted and 2-imidazolinyl amidine moiety were carried out by condensation reaction of amidino-substituted 2-aminothiophenols, 2-aminophenols or *o*-phenylenediamines with 1,3- and 1,4-phenylene dicarboxylic acids. Antiproliferative evaluations of compounds were performed *in vitro* on several human tumour cell lines (LN-229, Capan-1, HCT-116, NCI-H460, DND-41, HL-60, K-562, Z-138). It was observed that the antiproliferative activity strongly depends on heteroaromatic scaffolds, as well as on type of amidine moiety. The 2-imidazolinyl-substituted 1,3-phenylene-bisbezoxazole and bisbenzothizole exhibited the highest activity and inhibit tumour cell proliferation (IC_{50}) in submicromolar concentration on almost all tested cell lines. Several compounds have been further tested for their DNA/RNA binding ability using UV/Vis (thermal denaturation), fluorescence and circular dichroism (CD) spectroscopy with the aim of investigating possible mechanisms of action.

Key Words: *synthesis; amidines; benzazoles; antiproliferative activity; DNA/RNA binding*

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SYNTHESIS AND SPECTROSCOPIC CHARACTERIZATION OF BENZIMIDAZOLE DERIVATIVES AS POTENTIAL pH SENSORS

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Abstract

Heterocyclic molecular systems with pronounced and diverse spectral responses are among the most extensively studied classes of organic compounds. Design and development of small molecules for (chemo)sensing and optoelectronic applications is of great interest in organic chemistry and sensing technology [1]. Structural similarity of benzimidazole (BI) nuclei with naturally occurring purines enabled the applications of such molecules in molecular biology or medicinal chemistry. The BI moiety can serve as a multifunctional unit in molecular systems and an especially attractive building block in D-π-A systems for different applications in optoelectronics and as pH sensors [2]. The photophysical and chemical properties of push-pull systems are defined by the position, number and electron donating and accepting strengths of donor and acceptor groups and their chemical nature [1].

Herein we present multifunctional D-π-A molecular systems containing an *N,N*-diethylamino group as a pH sensitive donor group connected to the electron accepting substituents like cyano group and the pH sensitive benzimidazole moiety. We have prepared acrylonitrile, Schiff base and iminocoumarin derived benzimidazoles (Figure 1). The photophysical characterisation and computationally supported determination of species involved in prototrophic equilibria, including their respective p*K*a values, have been performed in order to better understand the effects of the D-π-A molecular structure on the UV–Vis spectral properties and pH sensing potential of these chromophores.

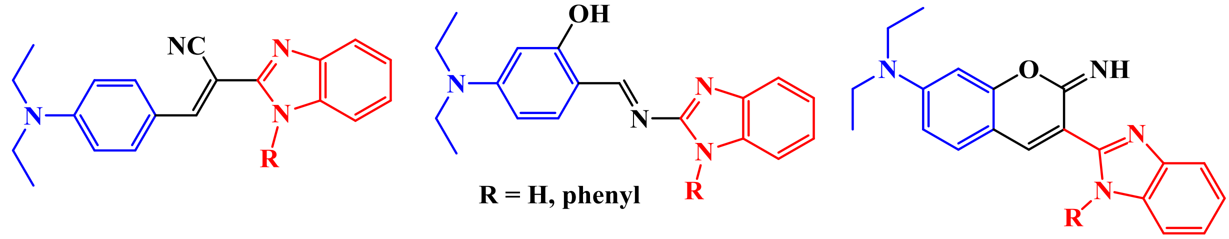

Figure 1. Structures of investigated benzimidazole derivatives

Key Words: *benzimidazoles, acrylonitriles, computational chemistry, iminocoumarins, Schiff bases, pH sensors*

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Acknowledgments: This work was funded by the Croatian Science Foundation (projects IP-2018-01-4379 and IP-2020-02-8090).

GREEN SYNTHESIS AND ANTITUMOR STUDIES OF NOVEL RACEMIC AND OPTICALLY PURE ARYL-SUBSTITUTED PURINE BIOISOSTERES

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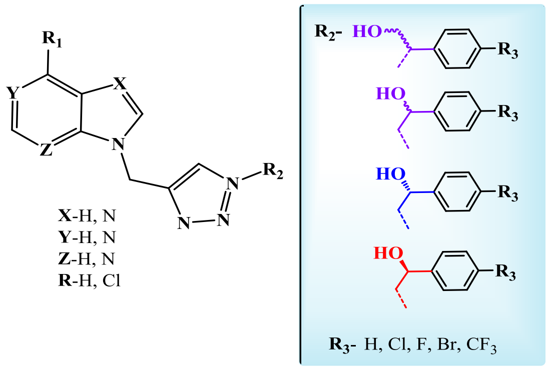
Abstract

Enzymes, receptors, and other binding molecules in biological processes can recognize enantiomers as different molecular entities, consequently, using a single pure enantiomer instead of a racemate can enhance the effectiveness and safety of the treatment [1]. The simplest method for the synthesis of enantiopure or highly enantio-enriched compounds is asymmetric organometallic catalysis, which has been recently replace by biocatalysis due to its toxicity. An important example of enzymatic biocatalysis is the nucleophilic opening of epoxy rings with sodium azide catalysed by halohydrin dehalogenase (HHDHs) [2]. Enantiomerically pure β-azido alcohols are very important building blocks in the synthesis of novel 1,2,3-triazole derivatives [3]. As part of our research on developing multi-target small molecule anticancer agents, we designed, synthesized, and biologically evaluated a series of 66 novel purine derivatives. A series of 50 racemic and 16 optical pure 1,4-disubstituted 1,2,3-triazoles were synthesized by the copper(I)-catalyzed Huisgen 1,3-dipolar cycloaddition of terminal alkynyl derivatives of purine isosteres and aryl substituted 1,2-azido alcohols under environmentally friendly ultrasound irradiation. The antitumor effects of all derivatives were evaluated.

Key Words: *purine, 1,2,3-triazole; azido alcohols; enantiomers; halohydrin dehalogenase*



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PRODUCTION OF HIGH ENERGY CAPACITY OF REDUCED GRAPHENE OXIDE-QUINOLINE ZINC PHTHALOCYANINE NANOHYBRID MATERIAL

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Abstract

Phthalocyanines (Pcs) are macroheterocyclic compounds consisting of four isoindole units bonded to each other by nitrogen atoms at meso positions and can be obtained by changing the central metal ion and peripheral substituents and are used as pigments and have many applications such as energy conversion, gas sensor and liquid crystal. Quinoline is a heterocyclic aromatic organic compound that has various pharmacologically active synthetic and natural compounds of its derivatives are common [1]. The graphene family includes reduced graphene oxide (rGO), graphene oxide (GO), graphene sheets, and several-layer graphene members. GO has unique physical and chemical properties [2]. In this project, graphene oxide were obtained first, starting from graphite. Then, new rGO-metallic quinoline-zinc substituted Pc nanohybrid materials (rGO-KZnPc) have been obtained as a result of the hydrothermal reduction reaction of GO with the zinc metal quinoline-substituted phthalocyanines (KZnPc) we have also synthesized [3]. After the necessary characterizations are made, new anode materials have been prepared and investigated energy density by electrochemical methods after these materials and other electrode additives were coated on Ni-foam (NiF) as a substrate (Fig. 1). This study was supported by Scientific Research Projects Unit of Yildiz Technical University (Proje No: FYL-2022-4873).

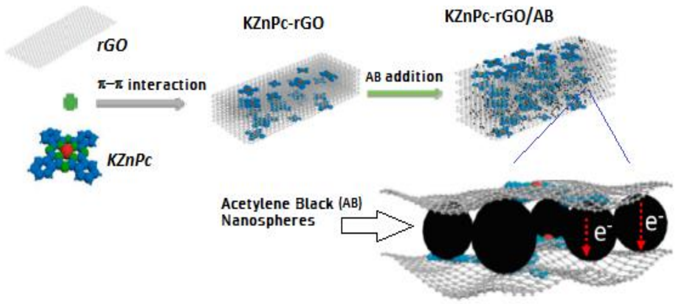

Figure 1: Schematic illustration of preparation for the KZnPc-rGO/AB electrode

Key Words: *phthalocyanine; graphene; electroactive material; nanomaterial, supercapacitor*

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PERYLENE–BASED METAL COMPLEXES: THEIR SYNTHESIS, PHOTOVOLTAIC PROPERTIES AND EFFICIENT DYE-SENSITIZED SOLAR CELLS

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Abstract

Perylene diimides (PDIs) are generally considered a class of excellent organic dyes with significant molar absorption coefficients at visible wavelengths of the electromagnetic spectrum, high fluorescence quantum yields near unity and long singlet excited state lifetimes [1]. PDIs present a model of an intrinsically potent and exceptionally adaptable class of organic materials that were used for a broad sequence of technological applications such as solar cells.

The solar cell is a technological device that converts solar light into electrical energy using the photoelectric phenomenon [2]. Photovoltaic technology is considered the most encouraging of all sustainable energy technologies. PDIs are performed in solar cells as photosensitizers because they can be modified through anhydride groups that serve as anchoring groups for binding to the working electrode, a semiconductor material.

In this study, chromogenic perylene diimide, N,N'–bis(3–amino–5–phenyl–2,4,6–triazinyl)perylene–3,4,9,10–tetracarboxylic diimide and its metal complex were designed and synthesized successfully. The chemical structures of products were confirmed by using general spectroscopic methods. Photochemical properties of the compounds were studied by using UV−vis absorption and spectroscopic emission methods. The photovoltaic parameters V_{oc}, I_{sc}, FF and η_{cell} of perylene diimide based DSSC are 0.316 V, 0.432 mA/cm^2, 0.08 and 0.011%, respectively. Those parameters for its metal complex are 0.190 V, 1.920 mA/cm^2, 0.19 and 0.069%, respectively.

Key Words: *Perylene; PDI; metal complex; solar cell; DSSC*

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SYNTHESIS AND CHARACTERIZATION OF NOVEL BAY SUBSTITUTED PERYLENE DYES

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Abstract

Perylene diimides (PDIs) have received substantial research attention due to their outstanding absorption and emission in the spectral region from visible to near-infrared (NIR), photochemical and electrochemical properties, and thermal, chemical and photochemical stabilities [1].

These outstanding properties were vital characteristics leading to significant research development concerning their uses in fluorescent dyes, organic solar cells, sensors, optical switches, organic solar cells and photoconduction materials [1]. Modifying PDI derivatives at imide positions has been accomplished by altering the imide substituents, mainly increasing these materials' solubility and solid-state color. However, the imidization does not significantly affect either the optical or electronic properties of perylene dyes due to the nodes in the HOMO and LUMO orbitals at the imide nitrogens. Importantly, modification of the optical and electronic properties could be only possible with the bay-positions functionalization of the perylene core [2].

In this study, two novel bay substituted (1,7) symmetrical perylene diimides were designed and synthesized starting with dibromination of perylene-3,4,9,10-tetracarboxylic dianhydride to yield 1,7-dibromoperylene-3,4,9,10-tetracarboxylic dianhydride. Next, bromine atoms was replaced by alkoxy and alkynyl groups to produce bay–substituted perylene dianhydride. Finally, bay-substituted perylene diimides were produced through N, N‘–imidization.

We have investigated and compared the compounds' optical, thermal, and electrochemical properties. Further, their solid-state absorption, fluorescence and electrochemical characteristics were obtained and discussed.

Key Words: *dyes; bay substituted perylene diimides; thermal stability; intermolecular interactions*

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ANTIOXIDANT AND ANTIDIABETIC ACTIVITIES OF HEXANE EXTRACT OF *Genista januensis var. lydia*

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Abstract

The genus *Genista* L. (Fabaceae), with its cosmopolitan distribution, has been interested in human beings since ancient times. Some of the *Genista* genera have been used in folk medicine and mainly in the Mediterranean to treat respiratory diseases, rheumatic disorders, diabetes, and ulcers. Moreover, the genus is also well known for its yellow pigment [1] by the local people. Some *Genista* species have been used for many purposes, including antidiabetic properties. Since α-amylase and α-glucosidase are the chief enzymes of diabetes mellitus, this study aims to search α-amylase and α-glucosidase inhibitory potential of *Genista januensis* Viv. var. *lydia* (Boiss.) Kit Tan & Ziel. (Fabaceae), growing in the Trakya region. To the best of our knowledge, there has been no study on *G. januensis* var. *lydia* up to date. Therefore, α-amylase/α-glucosidase inhibitory activity and antioxidant activity hexane extract of *G. januensis* var. *lydia* were aimed to study by spectroscopic *in vitro* experiments to search the potential and relationships of both activities.

The plant was collected from Tekirdağ. After dried and sliced into small pieces, the plant was successively macerated using hexane, chloroform, ethyl acetate, and methanol. The solvents were evaporated using the rotary evaporator, and the crude extracts were obtained. Then, total phenolic/flavonoid content, antioxidant activity [2], and α-amylase /α-glucosidase inhibitory activities [3-4] of hexane extract of *Genista januensis* were determined spectrophotometrically.

***Key Words:** Genista januensis, antioxidant activity, α-amylase, α-glucosidase.*

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INHIBITORY EFFECTS AGAINST α-GLUCOSIDASE, α-AMYLASE AND ANTIOXIDANT ACTIVITY OF METHANOL EXTRACT OF *Genista januensis*

Cansel ÇAKIR[1], H. Hulya ORAK[2], Merve ARGON[3], Hilmican CALISKAN[3] Temine SABUDAK[3], Mehmet OZTURK[1], Necmettin GULER[4]

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Abstract

Diabetes mellitus has become a threat to human health and a growing public health issue [1]. The capability of a diet or drug to delay the production or absorption of glucose by inhibiting carbohydrate hydrolyzing enzymes, namely, *α*-amylase and *α*-glucosidase**,** is one of the therapeutic approaches for decreasing postprandial hyperglycemia [2]. Furthermore, the causal correlation between oxidative stress and type 2 diabetes has been explained through molecular mechanisms [3]. Therefore, the overproduction of reactive oxygen species related to hyperglycemia likely leads to an imbalance of the amount of antioxidants inside the body and, finally, may lead to oxidative stress. For that reason, providing antioxidants and α-amylase and α-glucosidase inhibitors due to nutriments is a potential and feasible method for managing type 2 diabetes. Therefore, to search for new natural inhibitors of *α*-amylase and *α*-glucosidase, we have studied *Genista januensis* since some of the species of the *Genista genus* have been used against diabetes mellitus. In addition, we also investigated the in vitro antioxidant and α-amylase/α-glucosidase inhibitory activities of crystals parts obtained during the methanol extraction.

Genista januensis Viv. var. *lydia* (Boiss.) Kit Tan & Ziel. (*Fabaceae*) plant collected from the Trakya region (Turkey). All dried and powdered aerial parts were cut into small pieces. The plant was then macerated using hexane, chloroform, ethyl acetate, and methanol successively. At the end of the maceration process, crystals formed during the evaporation of methanol. After the mixture was filtered, the formed crystals (7.748 g) were separated. Then, total phenolic/flavonoid content, antioxidant activity [4], and α-amylase/α-glucosidase inhibitory activities [5] of separated crystal parts of *Genista januensis* were studied.

Keywords: *Genista januensis, antioxidant activity, α-amylase, α-glucosidase.*

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THE SYNTHESIS AND CHARACTERIZATION OF NEW AMINO-SUBSTITUTED AZANAPHTOQUINONE COMPOUNDS WITH ANTIMICROBIAL ACTIVITY

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Abstract

Organic compounds with a quinone skeleton, which stands out as a new class of inhibitors against various microorganisms, including Gram-positive/negative bacteria as well as fungi, have become the focus of attention by synthetic chemists and pharmacologists [1]. Many quinone compounds synthesized in previous studies by our group also showed impressive activities against bacteria and fungi [2-4].

In this study, new amino-substituted azanaphtoquinone analogs were synthesized from the nucleophilic reaction of halogenated azanaphtoquinone with amines containing different substituents at various positions of the aromatic ring, and the structures of the new compounds obtained were characterized by appropriate spectroscopic methods. In addition, the activities of these compounds against some Gram-negative, Gram-positive and fungal species were investigated.

Key Words: *Azanaphtoquinone, Gram-negative bacteria, Gram-positive bacteria, antimicrobial*

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Self-assembly, optical, thermal and electrochemical properties of N, N'-bis-(benzyl)-3,4,9,10-perylenebis(dicarboximide) Top of Form

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Abstract

One of the main ways which address the environmental issues of sustainable energy production from renewable sources is harvesting energy directly from sunlight for photovoltaic applications, where the most successful devices are based on semiconducting materials such as silicon [1-3]. On the other hand, different organic dyes are synthesized to construct dye synthesized solar cells with uncomplicated production, high stability and low cost. O’Regan and Gratzel reported that DSSC’s attracted considerable attention in the past few years. Perylene molecules are attractive for photovoltaic applications owing to their strong absorption and fluorescence, electroactive and photoactive properties, and excellent thermal, chemical and photochemical stability [4, 5].

A new intelligent perylene molecule (*N, N'-bis-(benzyl)-3,4,9,10-perylenebis(dicarboximide)*) was synthesized as a potentially suitable material for optoelectronic devices such as organic solar cells (OSCs), light-emitting diodes (OLEDs), transistors, and lasers.

The compound is characterized using NMR, IR, MS, UV–vis, MS, DSC, TGA, elemental analysis and cyclic voltammetry. We detailed the new molecule’s optical, thermal, and electrochemical properties.

Key Words: Renewable energy; Perylene; Organic Dye; Solar Cell; Photovoltaic

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The Synthesis, PHOTOPHYSICAL AND ELECTROCHEMICAL PROPERTIES of Perylene monoımıde and Asymmetric PERYLENE Diimide

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Abstract

Perylene diimides are valuable organic chromophores that stand out for their outstanding optical and redox properties. Owing to these features, Perylene diimides have emerged as prominent dyes capable of acting as photocatalysts for numerous relevant organic transformations.

Researches on solar cells have consequently been focused on the development of new eco-friendly technologies, such as dye-sensitized solar cells (DSSC) and organic photovoltaics (OPV) [1-3].

A study on generating organic solar cells with high efficiency showed that optical, electrical, and structural properties have crucial role in the development of new materials presenting optimized thermal and photochemical stabilities. Perylene based dyes and polymers are demandable, because they have strong absorption and fluorescence, electro-active and photoactive properties, and accomplished thermal, chemical and photochemical stability [4-5].

The aim of this study is to synthesize N-(thiaminehydrochloride)-3,4,9,10- perylene tetracarboxylic-3,4-anhydride-9,10-imide **(THCl-PMI)** and N-(thiaminehydrochloride)-N'-(1-phenylethylamine)-3,4,9,10-perylenebis(dicarboximide) **(THPA-PDI)** for dye synthesized solar cells.

Synthesized compounds were purified and characterized by FTIR, UV-vis and Emission measurements. The electrochemical properties of the compounds were investigated by cyclic voltammetry (CV) in deoxygenated DMF solution containing 0.1 M of $NaBF_4$ as supporting electrolyte. The potential was externally calibrated by ferrocene/ferrocenium couple (Fc/Fc+). The thermal stability of the compounds was studied by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) at a heating rate of 10 $°C.min^{-1}$. For comparison, photophysical, electrochemical and thermal properties of all products were carried out in parallel.

Key Words: Asymmetric Perylene Diimide; Organic Dye; Solar Cell; Photovoltaic

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A NAPHTHALENE DIIMIDE-BASED POLYMER AS ELECTRON ACCEPTOR FOR ORGANIC SOLAR CELLS

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Abstract

Fullerene derivatives such as phenyl-C61-butyric acid methyl ester are the most commonly used electron acceptors in organic solar cells due to their attractive properties. However, their limitations, such as instability, weak light absorption and high costs, require the design of new acceptors to replace fullerenes.

In the past decade, research showed that n-type semiconducting polymers as acceptors have the potential to overcome the drawbacks of fullerene derivatives [1]. Compared to fullerene derivatives, semiconducting polymers have a broad and strong absorption in the visible region. Also, molecular design can adjust the lowest unoccupied molecular orbital (LUMO) energy levels of acceptor polymers, which can lead to higher power conversion efficiencies. Among n-type polymers, naphthalene diimide-based polymers are highly promising acceptors due to their high electron mobility, high electron affinity and broad light absorption [2]. The electron-deficient core of naphthalene diimides can be easily copolymerized with various electron-rich units to tune the optoelectronic properties of the polymers.

This study aims to synthesize a naphthalene diimide containing polymer conjugated along the backbone with an electron-donating unit. To this end, a naphthalene diimide molecule is polymerized with a bithiophene unit using the Stille-coupling polymerization reaction method.

The synthesized polymer has a solubility in most commonly used organic solvents such as chloroform and toluene.

Key Words: *n-type semiconducting polymer; conjugated polymer; naphthalene diimide; organic solar cells; electron acceptor*

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SYNTHESIS, CHARACTERIZATION AND INVESTIGATION OF ELECTROCHEMICAL PROPERTIES OF A BAY-SUBSTITUTED NAPHTHALENE DIANHYDRIDE AND A BAY-SUBSTITUTED NAPHTHALENE DIIMIDE

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Abstract

Naphthalene diimides are important compounds that belong to the more prominent family of rylene dyes with high electron affinity, good charge carrier mobility and exceptional chemical stability [1,2]. Due to these advantageous properties, naphthalene diimides have been widely applied in various research fields, including supramolecular chemistry, organic field-effect transistors (OFETs), photovoltaic cells and DNA intercalation [3]. Structural properties of naphthalene diimides can be modulated by functionalization at imide and bay positions. Substituents at the imide positions can be used to alter the solubility, aggregation and intermolecular packing in the solid-state. However, imide-substituents have an insignificant effect on the optoelectronic properties of these molecules. Notably, naphthalene diimides' optical and redox properties can only be adjusted by functionalizing bay-position at the naphthalene core [4].

This work aimed to synthesize a novel bay-substituted naphthalene dianhydride and a bay-substituted naphthalene diimide molecule to observe the photochemical and electrochemical properties of the resulting compounds, respectively. We report the synthesis of a N,N'-substituted 2,6-diphenoxy naphthalene diimide and a 2,6-diphenoxy naphthalene dianhydride. N,N'-substituted 2,6-diphenoxy naphthalene diimide is synthesized in three different steps. At the first step, naphthalene dianhydride is brominated using molecular bromine to yield 2,6-dibromo naphthalene dianhydride. Next, 2,6-dibromo naphthalene dianhydride is imidized with an amine to give N,N'-substituted 2,6-diphenoxy naphthalene diimide. Finally, bromines on the 2,6-dibromo naphthalene diimide is replaced by phenoxy groups to produce N,N'-substituted 2,6-diphenoxy naphthalene diimide.

In addition, 2,6-diphenoxy naphthalene dianhydride is synthesized from dibrominated naphthalene dianhydride and phenol group. Spectroscopic techniques characterize the two synthesized compounds. Optical, electrochemical and solubility characteristics are investigated. The properties of 2,6-diphenoxy naphthalene dianhydride and N,N'-substituted 2,6-diphenoxy naphthalene diimide are compared.

Key Words: *naphthalene diimide; bay-substitution, optical properties, electrochemistry, photochemistry*

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REACTIVITY OF 9-CHLORO-PHOSPHAALKENYLCHLORO-9-GERMAFLUORENE TOWARDS LITHIUM REAGENTS

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Abstract

The element-organic analogues of propenes containing a phosphaalkenyl unit bearing a P(III) phosphorus atom and a heavier element of group 14 or 15 are interesting compounds due to their possible use as molecular bricks in organometallic or coordinative chemistry.

We present here a reactivity study of a dichlorogermaphosphapropene having the P=C(Cl)-Ge(Cl) unit in which the germanium atom is stabilized by including it into a fluorenyl cycle [1] with different organolithium reagents (methyllithium, normal-, sec- and tert-butyllithium).

In the most cases described in the scientific literature, the reaction of such compounds undergoes with the formation of a lithiated species bearing the P=C(Li)-Ge(X) unit [2,3].

However, the reactions of 9-chloro-9-phosphaalkenylchloro-9-germafluorene [1] undergo through different pathways depending on the organolithium reagent. Unexpectedly, the reactions with MeLi and n-BuLi afforded the corresponding alkylated 3,1-germapropenes in almost quantitative yields and the products were completely characterized in solution and solid state by the usual physico-chemical methods (multinuclear NMR, HRMS, X-ray diffraction).

However, in the case of *sec*- and *tert*-butyllithium, the reaction underwent in both cases through the lithiation of the carbon atom followed by the formation of an unstable carbanion (through elimination of lithium chloride). The carbanion stabilized through three different dimerization reactions leading to two cyclic and an acyclic dimers. Two of the resulted compounds were separated and characterized through all the usual spectroscopic methods in liquid and solid state.

Part of this work was supported by a grant of the Romanian Ministry of Education and Research, CNCS-UEFSCDI, project PN-III-P1.1-TE-2019-2085 within PNCDI III.

Key Words: *3,1-germaphosphapropenes; organolithium reagents; X-ray diffraction; reactivity; p-block elements*

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In silico studies for developing an anticancer agent targeting G-quadruplex in DNA

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Abstract

Cancer is a heterogeneous disease and is regarded as a challenging disease to cure. Cancer is the leading cause of death worldwide, and only in 2020 cancer count for more than 10 million deaths, which is approximately one of six for all the deaths [1]. Research shows that **1** in **2** persons will develop cancer [2]. Therefore, there is an emerging need to develop new potent anticancer agents with less harmful side effects. One of the targets for cancer treatment that has increased the attention of scientists lately is G-4 as a target for anticancer drugs [3].

In addition, developing anticancer agents or any other class of drugs is expensive and time-consuming. Therefore, employing bioinformatics in drug discovery and development truncates the cost and increases the chances of hitting the lead. NDI derivatives show interesting electrochemical, photophysical and biological properties. Due to their conjugation and planer structure, they can form pi-pi stacking bonds with G-quadruplex.

Our research designed 50 NDIs derivatives and screened them with G-4 parallel and anti-parallel structures obtained from PBD (ID: 3SC8, 5HIX), respectively. The ADME studies were done using Swissadme to measure their drug-likeliness, solubility, and GI absorptions. The best two structures with the highest binding affinity (-11.1 Kcal/mol and -9.7 kcal/mol with 3SC8, and (-10.2 kcal/mol and -8.3 kcal/mol with 5HIX) were selected to study their molecular docking and molecular dynamic simulations in detail. Both the derivatives reached stability at 20 ns with the parallel G4, whereas found higher fluctuating and RMSD with anti-parallel G4 structure.

Key words: *Cancer; G-Quadruple; ND; molecular docking*

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Design, synthesis and characterization of novel bay substituted naphthalene diimide derivative and evaluate its antibiotic activity

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Abstract

Naphthalene diimide (NDIs) derivatives have exciting properties for organic electronic applications due to their high electron affinity, charge carrier mobility, and thermal and oxidative stability [1,2]. Nevertheless, naphthalene dianhydride (NDA) is the precursor of NDIs used in dyes and solar cells. Moreover, their planar surface and chemical accessibility made them favourable molecules for DNA and RNA intercalating agents [3]. However, not much study has been carried out investigating their antimicrobial activity. Bacterial and infectious pathogens resistance is an increasing worldwide issue, and much focus has been projected on developing agents to overcome drug-resistant infectious pathogens.

In our research, we designed various NDI derivatives and studied their antibacterial activities. The first line of defence in bacteria is the cell wall, which has various proteins and enzymes to protect the bacteria from the surroundings and maintain the osmotic pressure inside the bacterial cell. We have studied both *in silico* and *in vitro* investigation for our molecules. Due to the solubility and sizeable molecular structure, some compounds face solubility issues. However, molecule **4** showed high potency against *E. coli* and *S. aureus* bacteria.

We studied the molecular docking and molecular dynamic simulations for both species (Gram-negative and Gram-positive) bacteria, showing good binding affinity and stability. The *in-silico* studies confirmed the cell culture findings with higher binding affinity against gram-negative species (*E. coli).* The crystal structures of both bacterial cell walls were obtained from the PDB web server (www.pdb.org). Their ID (3VMA and 1MWS) are penicillin-binding proteins 'PBP' of cell walls and play a major role in beta lactamase resistance. The binding energies for compound 4 were found to be -7.49 kcal/mol with 3VMA and -6.1 kcal/mol with 1MWS.

Importantly, our findings suggest extensive studies to overcome the solubility issue of the compounds, which can be achieved by substituting imide positions with suitable amines [4].

Key words: *antibacterial; NDI; Docking; molecular dynamic simulation*

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The adsorption study of oleuropein using functionalized Halloysite Nanotubes as adsorbents

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Abstract

Halloysite nanotube (HNT), is a hydrophilic, biocompatible, environmentally friendly, and readily available natural clay, which contains positively charged Al_2O_3 in the inner part, and negatively charged Si-O-Si groups in the outer part. Because of the high surface area, thermal and mechanical stability, and modifiable surface, HNT is a promising material in separation and purification applications [1]. In this study, HNT was modified with different numbers of amine groups containing modifying agents such as ethylenediamine (EDA), triethylenetetramine (TETA), pentaethylenehexamine (PEHA), and branched polyethyleneimine (PEI) agents to prepare positively charged modified HNTs (m-HNTs). The mmorphological and physicochemical characterization of m-HNTs was done by Scanning electron microscopy (SEM), Thermogravimetric analyzer (TGA), Fourier transform infrared radiation spectroscopy (FT-IR), and zeta potential measurements. These HNT-based materials were tested for potential adsorbents in the recovery of oleuropein (OLRPN). OLRPN is the most important phenolic component of olive mill wastewater. The adsorption tendency of HNT and m-HNTs as adsorbents for OLRPN were determined via the batch method. Then, the most effective m-HNT was used as an adsorbent to study the adsorption kinetics of OLRPN and employed in the desorption studies.

Key Words: *Halloysite nanotube (HNT); Cationic adsorbents; Polyethyleneimine (PEI); Cryogel composite; Phenolic compound*

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DONOR-ACCEPTOR PERYLENE FLUOROPHORES: SYNTHESIS, CHARACTERIZATION AND PHOTOPHYSICAL PROPERTIES

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Abstract

Perylene dyes (PDIs) are essential compounds due to their stupendous absorption and emission in the spectral region from visible to near-infrared (NIR), photochemical and electrochemical properties, and thermal, chemical and photochemical stabilities. They are part of a versatile class of dyes with great potential in optoelectronic applications such as photovoltaic devices, organic field-effect transistors, light-emitting diodes, and organic solar cells [1-4].

Donor−acceptor perylene architectures have been extensively investigated as the most promising materials in energy transfer and light−harvesting systems for photovoltaic devices. More specifically, we were interested in investigating low molecular weight donor−acceptor−donor system material with low bandgap, high solubility and strong electron-donating/accepting ability with controllable conductivity. The band gap energy of such models can be reduced by raising the HOMO energy level selectively via influential electron donors [1–4].

The purpose of this study is to design and synthesize two novel donor-acceptor fluorophores, N,N'-(4-hydroxyphenyl)-perylene tetracarboxylic bisimide (**3**) and N,N'-(o-phosphoethanoylamine)-perylene tetracarboxylic bisimide (**5**). Products **3** and **5** were characterized by NMR, IR, UV–vis, DSC, TGA, elemental analysis, and cyclic voltammetry.

All products` absorption, electrochemical, spectroelectrochemical, and morphological characteristics have been investigated.

Both products showed excellent thermal stability and are particularly suited for high-temperature applications. In the polar aprotic and strongly electron-donating solvents such as DMF, DMAC and NMP, the compound has intense absorption in the visible spectrum in the wavelength range of 300–800 nm.

Conclusively, the overall results revealed that the donor-acceptor fluorophores are promising candidates for high-performance photonics, sensors and light-harvesting systems.

Key Words: *Perylene derivatives; donor/acceptor; thermal stability; conductivity; photovoltaic applications*

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ANTIBACTERIAL AND CYTOTOXICITY STUDIES ON PERYLENE FLUOROPHORES

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Abstract

Some of the harmful bacteria showed resistance to certain antibiotics. Therefore, it is vital to find out new drugs. Perylene diimide (PDIs) derivatives` antibacterial, antifungal, and anti-cancer properties are reported in the literature [1]. Moreover, PDIs can intercalate inside DNA, and it is possible to increase their binding property via conjugation to other binding species, nucleic acids [2.3].

Naturally obtained PDIs such as hypericin and its derivatives have shown inhibitory activity against bacteria. Even though PDI-based natural dyes are available as antimicrobial agents, few literature reports are available for synthetic PDI-based materials with antimicrobial activity. Notably, the multidirectional application of synthesised materials is a need for us. PDIs are important chromophores in biomedical applications due to their anti-cancer and antibacterial activities [1-3].

This study investigates the antibacterial activity and minimum inhibitory concentrations (MICs: the lowest concentrations of derivatives that inhibited the growth of bacteria) of two new perylene fluorophores **3** and **5**. The antibacterial activity against Gram-positive (Staphylococcus aureus) and Gram-negative (Klebsiella pneumoniae and Escherichia coli) bacteria were investigated. Two perylene compounds were tested with broth dilution assay. In addition, the effect of cell proliferation of two fluorophores on breast cancer cells was studied using an MTT assay.

The present work has shown that both compounds are good antibacterial agents against *Klebsiella pneumoniae* bacteria. Moreover, compounds **3** and **5** inhibit MCF-7 cancer cell lines at IC_{50} concentrations of 147.318 μM and 128.655 μM, respectively. The multidirectional applicability of the fluorophores is discussed.

Key Words: *Perylene derivatives; antibacterial activities; cytotoxicity; anti-cancer; fluorophore*

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IMPROVEMENT OF ANALYTICAL METHOD FOR DETERMINATION OF TAR IN PYROLYTIC GAS IN THE BIOMASS PYROLYSIS PROCESS

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Abstract

Pyrolysis is a one of promising technique for the production of energy from biomass. Pyrolysis dissolves biomass and also produces useful by-products. In this case, gas, liquid and solid phases are formed. Gas mixture containing tar, among other components. Traditional methods for tar sampling are based on cold solvent-trapping coupled with solvent absorption in impingers.

The present work focuses on a solid-phase adsorption method for determining the concentration of tar compounds. A sampling device consisting of 500 mg of amino-phase sorbent and 100 mg of activated coconut charcoal was chosen as optimal for sampling tar (including its volatile organic compounds) in gas produced in biomass pyrolysis [1-3]. For research in a real-life context, the double-layered fixed-bed reactor situated in eastern Latvia (Daugavpils) was used. Varying volumes of pyrolytic gas were drawn through the adsorbents, and the total amount of tar was then compared to the number of its individual component compounds.

Tar was sampled at the pyrolytic gas temperature of 200°C. It was drawn through the adsorbent cartridges at the flow rate of 100 – 200 mL min^{-1} for various periods of time, resulting in 200, 400, and 600 mL of the pyrolytic gas being drawn through the adsorbents respectively.

All heavy compounds of the tar are completely adsorbed on amino-phase adsorbent, and light compounds of the tar, such as benzene and toluene, are partially adsorbed on this adsorbent, and partially on activated coconut charcoal. The total amounts of each compound were calculated, as well as the tar on both sorbents. The dependence of the concentration of the total tar and some of its compounds on both sorbents on the volume of the pyrolytic gas passed through them has been investigated. It was concluded that the volume of pyrolytic gas had little or no effect on the total amount of tar found on both adsorbents.

Testing the device in real life conditions, along with varying volumes of the pyrolytic gas drawn through the adsorbents, gave results that were comparable in the total amounts of both tar and its individual component compounds. However, with an increase of the volume of pyrolytic gas drawn through the adsorbents, greater amounts of light compounds pass through the amino-phase adsorbent and are collected on the activated coconut charcoal. An increased volume of pyrolytic gas leads to a growing number of compounds detected and identified on the amino-phase adsorbent. It appears reasonable to take into account the concentration of tar in the pyrolytic gas while selecting the volume of gas for sampling, as well as whether it is necessary to detect those individual tar compounds whose concentration is very small.

Key Words: *biomass; tar; pyrolysis; solid-phase adsorption; GC-MS*

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EXPERIMENTAL AND COMPUTATION STUDY OF THERMAL TRANSFORMATIONS OF THIENYL AND FURYL *o*-DIVINYLBENZENES IN ACIDIC MEDIA

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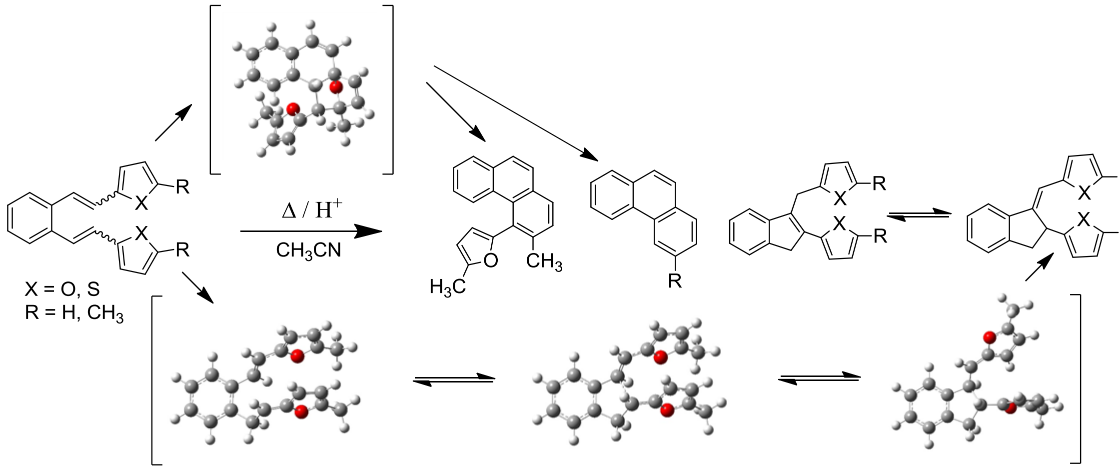
Abstract

Distyrylbenzenes are known for their interesting photophysical and chemical properties [1]. Due to the extended delocalization of π electrons in the excited state they can form new complex structures that cannot be prepared by classical synthesis [2]. In addition to well-known photochemical transformations of distyrylbenzenes, over the past years, their thermal transformations in neutral and acidic media were also studied. While thermal reaction in neutral medium did not indicate significant reactivity, acidic conditions can cause protonation of the double bond and the formation of new intramolecular products [3].

The aim of this study is to investigate in more detail the influence of the initial substrate on the mechanism of formation of the products of thermal protonated reactions. Therefore, the thermal reaction under acidic conditions of variously substituted furan derivatives of distyrylbenzene have been conducted and compared to their thiophene analogues thermal reactivity. The mechanism of the thermal reaction of furyl and thienyl *o*-divinylbenzenes under acidic conditions and the formation of products were explained in detail by quantum chemical calculations at the SMD/M06-2X/6-311+G(2df,2pd)//SMD/M06-2X/6-31G(d,p) level of theory and confirmed experimentally.

Key Words: *thermal transformations; distyrylbenzenes; reaction mechanism; DFT calculations; protonation*



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DEGRADATION REACTIONS of COVID-19 ACTIVE INGREDIENTS BY MOLECULAR MODELING METHOD

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Abstract

The coronavirus (Covid) is a large family of viruses known to cause a variety of illnesses, from the common cold to acute respiratory infections. The severity of the infection can be seen as pneumonia, acute respiratory syndrome and even death. This group of viruses was largely ignored until the SARS epidemic. However, since the SARS and MERS outbreaks, these viruses have been studied in more detail to advance vaccine research. On December 31, 2019, mysterious cases of pneumonia were detected in the city of Wuhan in China's Hubei Province. On January 7, 2020, the cause was identified as a novel coronavirus (2019-nCovid), and the disease was later named Covid-19 by WHO. In this study, possible reaction pathways of Afzelin, Delta Viniferin and Hesperidin molecules between OH radical were determined. Optimized geometries were plotted with Gauss View 5. Then, the lowest energy states were found by geometric optimization with the Gaussian 09 program. These results will guide experimental studies and determine the fragmentation mechanism.

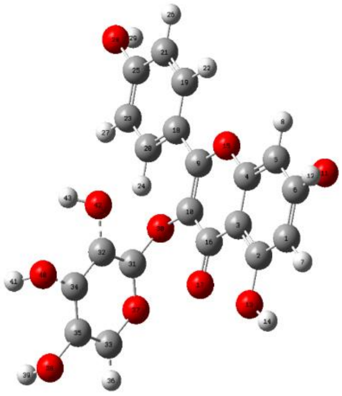

Figure 1. Optimized state of the same Afzelin molecule. (Grey, C; white, H; red, O)

Key Words: *DFT, Covid-19, Gaussian 09*

References

[1] Keni R, Alexander A, Nayak GP, Mudgal J, Nandakumar K (2020) Possible Treatments, and Global Burden. Front. Public Health, 8:216.