

ICNTC CONFERENCE

INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

**10TH INTERNATIONAL CONFERENCE ON
NEW TRENDS IN CHEMISTRY
APRIL 19-21, 2024**

10th ICNTC BOOK OF ABSTRACTS

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10th ICNTC BOOK OF ABSTRACTS

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10th ICNTC Conference 2024

10th International Conference on New Trends in Chemistry

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Prof. Dr. Dolunay ŞAKAR

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Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of “10th International Conference on New Trends in Chemistry”, to be held in Budapest, Hungary on the dates between April 19 – 21 , 2024

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

- Polymer Chemistry and Applications
- Pharmaceutical Chemistry
- 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 19 – 21 April 2024,

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

Prof. Dr. Dolunay SAKAR
10th ICNTC 2024 | Conference Chair
Yıldız Technical University – Istanbul / Turkey
Chemistry Department

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10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

10th ICNTC 2024 PROGRAM

19 APRIL 2024 FRIDAY

09:00 – 16:00

Registration

09:45 – 10:15

Opening Ceremony

COFFEE BREAK 10:15 – 10:25

10:25 – 10:30

Welcome Speech

: Prof. Dr. Dolunay SAKAR/ Conference Chair
Yıldız Technical University, Turkey

10:30 – 11:00

Keynote Speech

Speech Title

: Flavio Massignan, Eötvös Lorand University
: Effective nanoparticulate-type encapsulation delivery system for hydrophilic proteins and peptides

SESSION A

SESSION CHAIR	ASSOC. PROF. DR. Emel AKYOL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:00 – 11:20	The Discovery of Hydrogen Electrode Reference $E^{\circ}_{H} = -0.2965$ Volts in Absolute Potential Scale Synchronizes the Sciences with Absolute Free Energy Scale.	<u>Aris KAKSIS</u>
11:20 – 11:40	Boron Fuels and Hydrogen Production in Renewable Energy Systems	Berfin Ekin ULGEN, <u>Aysel KANTURK FIGEN</u>
11:40 – 12:00	The Effect of Chemical Pretreatments on the Drying Behavior of Blueberries	Busra GOK, <u>Ekin KIPCAK</u>
12:00 – 12:20	Investigation of In Vitro Digestive Process in Optimization of Ultrasound-Assisted Extraction with Citric Acid Anhydride for Antioxidant Production from Red Beet, Swiss Chard, and Dragon Fruit	<u>Gulin Selda POZAN SOYLU</u> , Elif GUNGOR REIS
12:20 – 12:40	Carvacrol Derivatives: DFT Computations and Drug-likeness Studies	Goncagul SERDAROGLU

10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

12:40 – 13:40 LUNCH BREAK

Lunch is included into Full Package Registration.

Participants who registered as Light Package and/or want to purchase extra ticket should contact to conference registration desk

SESSION B

SESSION CHAIR	PROF. DR. Aysel KANTURK FIGEN	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
13:40 – 14:00	Improving Energy Conversion Efficiency in Dye-Sensitized Solar Cells Through TiO ₂ Photoanode Modification with Gold-Silver Nanoparticles and Cobalt-Imidazolate Frameworks	Zainab B. Al-Ruqeishi, Osama Abou-ZIED
14:00 – 14:20	The Effect of Pigment on the Final Properties of Black Glass Automotive Enamel	Selime OZTURK , İlknur KUCUK
14:20 – 14:40	Investigation of the Effects Of Cherry Stem Extract On Calcium Oxalate Monohydrate Growth In In-Vitro	Merve DANISMAN, Emel AKYOL
14:40 – 15:00	Continuous Flow Chromium(VI) Adsorption Onto Peach Stone And Acrylonitrile-Divinylbenzene Copolymer Based Activated Carbons	Dilek DURANOGLU, Ilknur KUCUK , Ulker BEKER
15:00 – 15:20	Determination of Lignocellulosic Fraction of Airplane Lavatory Wastewaters for Recovery Purposes	Cigdem KALKAN AKTAN, Zeynep YUCESoy , Neslihan SEMERCI

COFFEE BREAK 15:20 – 15:30

10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

SESSION C

SESSION CHAIR	ASSOC. PROF. DR. Nilufer BAYRAK	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
15:30 – 15:50	Multi-parameter Optimization of Layered hBN/PMMA Nanocomposite Under Mechanical Loading	Tatyana PETROVA , Elisaveta KIRILOVA, Rayka VLADOVA, Apostol APOSTOLOV, Boyan BOYADJIEV
15:50 – 16:10	Effect of TiO ₂ Synthesis Methods on Photocatalytic Hydrogen Production Via Water Splitting	Vatfa GUZEY, Esra BALKANLI UNLU, Halit Eren FIGEN
16:10 – 16:30	Drying Kinetics, Mathematical Modelling and Color Analysis of Solen Marginatus: A Comparative Study of Oven, Infrared, and Microwave	Azmi Seyhun KIPCAK , Zehra Ozden OZYALCIN
16:30 – 16:50	Development of Transdermal Patches for Alzheimer's Treatment and Improvement of Penetration Characteristics	Hatice MUTLU , Emel AKYOL
16:50 - 17:10	DFT Computations, FMO, NBO, Lipophilicity, and Water Solubility of Dihydromyricetin Derivatives	Goncagul SERDAROGLU , Nihat KARAKUS
17:10 - 17:30	Theoretical Study of Possible Reaction Pathways With the OH Radical of the Apranax (AP) Molecule, Whose Active Ingredient is Naproxen Sodium (NS)	Bahar EREN , Yelda YALCIN GURKAN

SESSION D – POSTER SESSION 1

SESSION CHAIR	ASSOC. PROF. DR. Goncagul SERDAROGLU PROF. DR. Dolunay SAKAR	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
17:30	Individual Detection of Phenolic and Polyaromatic Components in Tar Analysis From Biomass Gasification Process	Sergejs OSIPOVS , Aleksandrs PUCKINS
	Impact Of Temperature On Methane Production From Bog Sludge And Crushed Reed Biomass	Aleksandrs PUCKINS Sergejs Osipovs
18:30	Synthesis and Characterization of Novel Symmetric Phthalocyanines Containing Bromonaphthalene Groups	Gölnur KESER KARAOGLAN , Gülsah GUMRUKCU KOSE
	The Synthesis and Characterization of A3B Type A Novel Unsymmetrical Zincphthalocyanine	Gölsah GUMRUKCU KOSE , Gülnur KESER KARAOGLAN
	Synthesis and Evaluation of New Quinone-Based Heterocycles Against Tumor Cell Lines	Nilufer BAYRAK , Amaç Fatih TUYUN
	Identification of Aminobenzoquinones as Egfr Inhibitors	Amaç Fatih TUYUN , Nilufer BAYRAK

10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

Dinner & Live Music at Vadaspark - Budapest

Courtyard Marriott Hotel Departure: 19:00

Dinner is included into Full Package Registration. Participants who registered as Light Package and/or want to purchase extra ticket should contact to conference registration desk.

20 APRIL 2023 SATURDAY

SESSION E

SESSION CHAIR	PROF. DR. Dolunay SAKAR	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
10:00 – 10:20	Improved Packaging Performance of Olive-Tree Based Biochar Loaded Poly(Lactic Acid) Films	Zeynep Irem OZYORU, Serhat BALCI, <u>Filiz UGUR NIGIZ</u>
10:20 – 10:40	Dehydration of Industrial Isopropanol Wastewater by Pervaporation Using Carboxy Methyl Cellulose and Graphene Oxide Hybrid Membranes	<u>Derya UNLU</u>
10:40 – 11:00	Experimental and Modeling Investigation of Mass Transfer During Infrared Drying of Ahlat Pear	Osama T. A. ALSHAMHAZI, <u>Ilknur KUCUK</u> , İbrahim DOYMAZ
11:00 – 11:20	Synthesis, Characterization and Effects to Cholesteric Lyotropic Liquid Crystal Media of -ONNO- Type Schiff Bases and Metal Complexes	<u>Seher MERAL</u> , Aysen ALAMAN AGAR
11:20 – 11:40	Preparation of Boron Nitride / Titanium Dioxide Hybrid Nanofluids and Investigation Of Stability	İlgen CETİN, <u>Emel AKYOL</u>
11:40 – 12:00	Modelling of Continuous Flow Phenol Adsorption Onto Acrylonitrile-Divinylbenzene Copolymer	<u>Elsada NEZIRI</u> , Dilek DURANOGLU

10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

12:00 – 13:00 LUNCH BREAK

Lunch is included into Full Package Registration.

Participants who registered as Light Package and/or want to purchase extra ticket should contact to conference registration desk

SESSION F

SESSION CHAIR	PROF. DR. Azmi Seyhun KIPCAK	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
13:00 – 13:20	Composite Thin Films of Upconverting Nanoparticles: Characterization of Emission and Energy Transfer Properties	<u>Balázs BORBÁS</u> , Borbála TEGZE, Dóra HESSZ, Miklós KUBINYI, János MADARÁSZ, Zoltán HÓRVÖLGYI
13:20 – 13:40	Computational Modeling of N=1 Ruddlesden-Popper Type La ₂ NiO ₄ for Fluoride Ion Batteries	<u>Pinar BULUT</u>
13:40 – 13:50	Preparation and Characterization of Bionanocomposite Packaging Films Reinforced with Metal Organic Frameworks Based Additives	<u>Oznur YOLACAN</u> , Sennur DENİZ
13:50 – 14:00	Effects of Additives on Mechanical and Barrier Properties of Polyhydroxyalkanoate Derived Biocomposite Films by Solution Casting	<u>Oznur YOLACAN</u> , Sennur DENİZ
14:00 – 14:10	Methyl Viologen as Photochromic Cation in Ca(II) and Mg(II) Complexes	<u>Aishwarya CHAUHAN</u> , Ravi Shankar
14:10 – 14:20	Design and Synthesis of N ₃ O ₂ , N ₂ O ₃ , N ₂ (S/Se)O ₂ and N ₅ O ₂ type Donor Bases and their Interactive Behavior with UO ₂ ²⁺ Ion	<u>Rahul RADAV</u> , Renu Kumari, Jagriti Singh and Jai Deo Singh

10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

SESSION G – POSTER SESSION 2

SESSION CHAIR	PROF. DR. Yelda YALCIN GURKAN	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
14:30	Fabrication of Electrospun Polyvinylidene Fluoride Filter Material For Deep Purification of Multiple Impurities from Water	Seniyecan KAHRAMAN, Ayşenur KATIRCI, <u>Filiz UGUR NIGİZ</u>
	The Mechanism of Antimicrobial Activity of Naturally Originated Preservative Hinokitiol	<u>Beata WYŻGA</u> , Magdalena SKÓRA, Katarzyna HĄC-WYDRO
15:30	The Effect of Natural Additives on Preventing Breakage by Increasing Paper Strength Value	Sedanur POLAT, <u>İknur KUCUK</u>
	Cisplatin Analog With Photoswitchable Biological Activity	<u>Marta STOLAREK</u> Mateusz BRELA, Kamil KAMIŃSKI, Marta KACZOR-KAMIŃSKA, Piotr BONAREK, Maria NOWAKOWSKA, Krzysztof SZCZUBIAŁKA
	Optimization of Ozonation in the Removal of Basic Blue 41 In Aqueous Solution	<u>Kadir TURHAN</u>
	Photophysical Study of Novel Isothiocyanate Derivative as Fluorescent Label For Amino Acids	<u>Jelena KIRILOVA</u> , Armands MALECKIS, Romans FRIDMANS
	Synthesis of Substituted 4-Methylphenyl-2-Iminothiazolidinone Compounds via One-Pot Method	<u>F. Tulay TUGCU</u>
	The Effect of Ultrasonic Pretreatment Duration on the Drying Kinetics of Red Berries	Sena SURER, <u>Ekin KIPCAK</u>

COFFEE BREAK 15:30 – 15:50

10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

SESSION H – POSTER SESSION 3

SESSION CHAIR	ASSOC. PROF. DR. İlknur KUCUK	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
15:50	Optimization and Determination of The Factors, Influencing on the Delamination in Graphene/Mos2/PET Nanocomposite Under Mechanical Loading	Boyan BOYADJIEV Tatyana PETROVA, Rayka VLADOVA , Elisaveta KIRILOVA, Apostol APOSTOLOV
	Tailor-Made Synthesis of Chitosan-G-Poly (Dimethylamino) Propylmethacrylamide	Ceyda SIMSEK , Ayse Enda ZAVALSIZ, Candan ERBİL, Argun Talat GOKCEOREN
16:30	Synthesis and Electrochemical Properties of Soluble Cobalt(II) and Copper(II) Phthalocyanines	Gamze KOÇ, Altug Mert SEVİM, Argun Talat GOKCEOREN
	Kinetic and Thermodynamic Investigation of Methyl Violet Dye Adsorption On Agar-Agar Impregnated Activated Carbon	Burak HAZAR, Dolunay SAKAR
	Determination of Macro and Micro Element Contents in Thyme Oil and Rosemary Oil by ICP-OES	Nazan TOKATLI DEMİROK, Ayca KARASAKAL
	Methyl Violet Dye Adsorption Study On Submicron Particle Size Rubber Powder Obtained From Scrap Tyre and Functionalized with Agar-Agar	Zehra KADIOGLU, Dolunay SAKAR
	Determination of Trace and Major Elements in Commercial Propolis Samples by ICP-OES After Microwave Digestion	Gorkem ARDA, Ayca KARASAKAL
	Removal Of Penicillin Group Azlocillin, Cloxacillin, Methicillin Antibiotics from Waste Water by Dft Method	Nurdan GUVEN, Burak GURKAN, Yelda YALCIN GURKAN

16:30 – 17:00	CLOSING CEREMONY
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10th ICNTC APRIL 19 – 21, 2024, Budapest, Hungary

21 APRIL 2024 SUNDAY

FREE DAY

Budapest - Vienna Transfer with Bus

Hotel Departure 08:00

This service is only for the participants who are willing to travel to Vienna to enjoy city. Bus will drop guests at Vienna city center and no return arrangement will be done. For registration and information please contact conference welcome desk

Effective nanoparticulate-type encapsulation delivery system for hydrophilic proteins and peptides

Flavio Massignan¹, Éva Kiss²

1 Laboratory of Interfaces and Nanostructures, Institute of Chemistry, Eötvös Loránd University, Pázmány Péter sétány 1/A, 1117-Budapest, Hungary flavio.massignan@gmail.com

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Recent developments of nanotechnology find its way into pharmaceutical, cosmeceutical and food production fields. Nanoencapsulated bioactive components such as vitamins, antibacterial agents, proteins, and peptides can contribute to improve the way medicines are administered or the production of enriched food stuffs with the required appearance, flavour, taste, and texture. Nanomaterials can protect the sensitive compounds from environmental attack, release them in a programmed way, and provide favourable improvement in the bioavailability of nutraceuticals.

Proteins and peptides are increasingly recognized as valuable therapeutic agents [1] as well as protein/peptide-based drug delivery systems [2]. They can function as hormones, enzyme substrates, and inhibitors, antibiotics, biological regulators [3]. Their capability to participate in specific biochemical interactions enables the targeted delivery of drug molecules or carrier particles to pathological tissues while minimizing the side effects in other parts of the body.

A recent review on protein delivery systems in nanomedicine and tissue engineering emphasized that encapsulation of bioactive molecules needs special attention due to their structural and hence functional sensitivity [4]. Proteins/peptides suffer from metabolic instability, including unfolding, enzymatic degradation, short half-life, and poor bioavailability. To overcome such drawbacks effective protein delivery systems are required to carry and release the therapeutic proteins in a sufficient dose without altering their bioactivity. The appropriate carrier construction protects the load from the effects of harsh environments, such as gastrointestinal tracts in the case of most frequently used oral administration. The size in the nanometer range facilitates their cellular internalization and direct transport of the bioactive substances to the intracellular environment.

Polymeric nanoparticles are of special interest since they are more stable than other colloidal carriers, such as liposomes or emulsions, and offer satisfactory protection [5]. The elaboration of potent delivery systems for peptides/proteins is still a challenge but is increasingly needed in advanced therapy. In the present research, we have developed a nanoencapsulation system for peptides/proteins, which is suitable for the delivery of hydrophilic bioactive compounds. The preparation method combines the advantageous properties of reverse nanoemulsion and nanoprecipitation, resulting in the formation of nanoparticles in the size range of 350–500 nm. The polymeric coating composed of polycaprolactone allows chemical functionalization and protection while the inner microenvironment (containing 1-decanoyl-rac-glycerol and N,N-dimethyldodecylamine N-oxide surfactants) provides aqueous surrounding for the active with structural fidelity. Hen egg white lysozyme and β -lactoglobulin were successfully encapsulated, achieving protein contents of 10–60 $\mu\text{g}/\text{mg}$ and encapsulation efficiencies ranging from 5–50% depending on the protein type and loading concentration. In vitro release measurement showed a biphasic sustained release profile of both proteins in the time range of one month. In vitro cytotoxicity investigation of protein-loaded nanoparticles exhibited good cell viability (above 95% at the highest treatment concentration of 0.3 mg/ml). The encapsulated membrane-active peptides have shown improved bioactivity.

Keywords: *drug delivery system, polymeric nanoparticles, proteins, cell-penetrating peptides, sustained release*

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The discovery of Hydrogen electrode reference $E^\circ_{\text{H}} = -0.2965$ Volts in **absolute potential scale** synchronizes the sciences with **absolute free energy scale**.

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Abstract. Alberty-based **Absolute** free energy content $G_{\text{H}_2\text{gas}} = 85.6$ kJ/mol for gas, $G_{\text{H}_2\text{aqua}} = 103$ kJ/mol for water and $G_{\text{H(Pt)}} = 51$ kJ/mol for metallic hydrogen at zero reference $G_{\text{H}_2\text{O}} = G_{\text{CO}_2\text{gas}} = 0$ kJ/mol background energy for water and carbon dioxide for **CO₂gas** gas. [1,2] Metal hydrogen zero classic standard potential reference is used in its hydroxonium cations $\{\text{H}_3\text{O}^+\} = 1.01$ M solution of sulfuric acid concentration $[\text{H}_2\text{SO}_4] = 1$ M with 1.061 g/mL density. Since Nernst Nobel Prize in Chemistry 1920th all electrochemistry series reductant oxidation half reactions standard potentials are determined relative to hydrogen metal half reaction classic standard potential E°_{H} zero. [3,4]

Quantitative studies of the functional activity of oxygen, carbon dioxide and water protolysis reveal generated diverse Life-Organization Attractors: water concentration $[\text{H}_2\text{O}] = 55.3$ mol/Liter, pH=7.36, reactivity of the enzyme carbonic anhydrase (CA), air oxygen level 20.95 % , osmolar concentration 0.305 M, ionic strength 0.25 M, temperature 310.15 K degrees, etc. . [2,3] High rate protolysis in water make oxygen fire safe , CA functionally activates carbon dioxide by reacting with two water molecules to produce **H₃O⁺+HCO₃⁻** concentration gradients on either side of the membrane for osmosis against concentration gradients but for the transport of protons and bicarbonate ions down through protons and bicarbonate ions channels.

Former publications reveal indispensable accounting the water and hydroxonium in Thermodynamic expressions of equilibrium reactions including protolysis and electrochemistry Nernst's half reactions. [1,2] Studies reach a reference value of 0.10166 Volts for the thermodynamic standard potential of metallic hydrogen. Behalf of Alberty given data about free energy of Hydrogen $G_{\text{H}_2\text{gas}} = 85.6$ kJ/mol , $G_{\text{H}_2\text{aqua}} = 103$ kJ/mol have detected the $E^\circ_{\text{H}} = -0.2965$ Volts **Absolute standard Potential** as Thermodynamic reference value of electrode with **Absolute** Free Energy change value $\Delta G_{\text{eq}} = -28.6$ kJ/mol.

Key Words: *Physical Chemistry; Electrochemistry; Thermodynamics; Attractors; Biochemistry.*

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Boron Fuels and Hydrogen Production in Renewable Energy Systems

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Abstract

Power-to-X technology intends to enhance areas such consumption, transportation, and storage through extracting power from renewable energy sources and converting it into an alternative energy source (fuels, chemicals, etc.) [1,2]. In this manner, it is aimed to eliminate the effects of fossil fuels, which have been utilized ever since as the primary energy source from the past into the present, and the substantial amounts of greenhouse gases released as a result of their consumption, on climate change, and to increase interest in renewable energy sources such as solar, geothermal, wave and tidal energy and also find a solution to the storage problem that occurs when the amount of power produced exceeds the amount of power required [1,3].

Hydrogen, which has the potential to be a low-cost, clean raw material and carrier, attracts attention in relevant fields [2,4]. Boron fuels such as boron hydrides and boranes are promising for Power-to-X technology due to their high hydrogen content [2]. As a result, more research and study are required to integrate boron fuels into Power-to-X technology. This study reports the review and evaluation of relevant literature.

Key Words: *Boron Fuel; Hydrogen; Greenhouse Gases; Power-to-X Technology; Renewable Energy*

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THE EFFECT OF CHEMICAL PRETREATMENTS ON THE DRYING BEHAVIOR OF BLUEBERRIES

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Abstract

Blueberries (*Vaccinium corymbosum*) are small, perishable fruits with blue color, which are cultivated mostly in North and South America. They contain a lot of healthy nutrients, polyphenols, organic acids and minerals. Moreover, blueberries are very good antioxidant sources, having the potential to reduce the adverse impacts of some diseases like memory loss and cancer. However, they are seasonal fruits with very short shelf lives. Hence drying can be used as a way of preserving this important fruit. Drying processes are often accompanied by physical or chemical pretreatments, in which it is aimed to shorten the drying duration and to enhance the properties of the dried fruit. In the literature, although there are numerous articles focusing on the antioxidant capacities and nutritional contents of blueberries, studies investigating their drying kinetics and the effects of various pretreatments on the process are still scarce. For this reason, in this study, the effect of chemical pretreatments on the infrared drying and vacuum oven drying of blueberries is investigated. During the experiments, the drying temperatures were selected as 70°C and 80°C. Considering the chemical pretreatments, 500 ml K₂CO₃ solutions were prepared by adding 25 g of K₂CO₃, 2.5 g olive oil and distilled water to the desired solution volume. Blueberry samples were subjected to these solutions at 30°C and 60°C prior to drying. At each pretreatment temperature, the blueberries were contacted with the K₂CO₃ solutions for 1 minute and 3 minutes, respectively. At the end of the chemical pretreatments, the infrared drying and vacuum oven drying of the samples were carried out. The results of the aforementioned pretreatments on the drying behaviour of the blueberries were compared with those of untreated dried sample data. The kinetic parameters of effective moisture diffusivities (D_{eff}) and activation energy (E_a) values were calculated. Moreover, the drying curves were modelled with the most known mathematical modelling equations given in the literature. As a result, it was observed that the use of K₂CO₃ solutions decreased the drying time of blueberries. The pretreatment temperature and duration were observed to have a positive effect on the drying behaviour as well.

Key Words: Blueberry; infrared drying; vacuum oven drying; K₂CO₃; chemical pretreatment

Investigation of In Vitro Digestive Process in Optimization of Ultrasound-Assisted Extraction with Citric Acid Anhydride for Antioxidant Production from Red Beet, Swiss Chard, and Dragon Fruit

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ABSTRACT

In this study, extracts were obtained from Red Beet, Passion Fruit and Swiss Chard plants by using different parameters using citric acid anhydrate with the Box-Behnken experimental design method. Optimum extraction were determined by analyzing total antioxidant capacity, total phenolic substance amount during the digestion stages. In the studies conducted with Red Beet, Passion Fruit and Swedish Chard, as a result of the optimization made with the Box Behnken method using ultrasound extraction, 52.59 °C, 48.66 min, 1:5 substance-solvent ratio, 2.11% citric acid anhydrate ratio were determined as the most optimum conditions. Extraction studies were carried out from Passion Fruit and Swedish Chard plants at 52.59 °C, 48.66 min, 1:5 substance-solvent ratio and 2.11% citric acid anhydrate ratio. As a result of this prepared experimental model, response optimization was carried out according to the total antioxidant capacity and total phenolic component amount. For the Red Beet sample, the value of 865.03±6.18 mg TE/100 g dw for DPPH, 421.28±3.45 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 170.03±6.18 (mg GAE/100g) in the undigested stage, the value of 770.61±0.64 mg TE/100 g dw for DPPH, 215.58±0.87 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 121.61±0.64 (mg GAE/100g) in the stomach digestion stage; the value of 732.51±3.40 mg TE/100 g dw for DPPH, 153.09±5.33 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 96.51±3.65 (mg GAE/100g) in the intestine digestion stage were obtained. For the Passion Fruit sample, the value of 590.22±5.44 mg TE/100 g dw for DPPH, 100.87±3.00 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 191.13±2.99 (mg GAE/100g) in the undigested stage; the value of 546.21±3.61mg TE/100 g dw for DPPH, 92.85±2.22 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 112.44±3.23 (mg GAE/100g) in the stomach digestion stage, the value of 472.67±1.21 mg TE/100 g dw for DPPH, 80.54±2.42 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 92.29±4.82 (mg GAE/100g) in the stomach intestine stage were obtained. For the Swiss Chard sample, the value of 524.62±1.11 mg TE/100 g for DPPH, 114.16±4.20 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 122.23±3.42 (mg GAE/100g) in the undigested stage; the value of 454.85±2.69 TE/100 g dw for DPPH, 106.39±3.63 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 98.18±1.87 (mg GAE/100g) in the stomach digestion stage, the value of 372.85±3.32 mg TE/100 g dw for DPPH, 91.21±4.21 mg TE/100 g dw for ABTS, and the total phenolic substance amount: 68.61±2.71 (mg GAE/100g) in the stomach intestine stage were obtained.

Keywords: Antioxidant, phenolic component, optimization

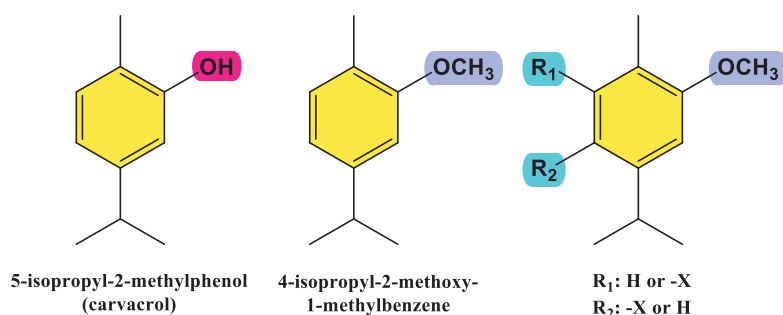
Carvacrol Derivatives: DFT Computations and Drug-likeness Studies

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Abstract

Carvacrol is a monoterpenoid phenolic compound that natural component in essential oils sourced from different phytochemicals. Herein, the halogenated carvacrol derivatives were designed to evaluate the possible drug-likeness properties in addition to the electronic and physicochemical properties. Computational tools have been currently applied to different organic, inorganic, or complex systems for the elucidation of the physicochemical, electronic, and spectroscopic characteristics, etc. In this regard, the thermochemical properties provide useful information and/or insight related to the chemical stability (-thermodynamic or kinetic). On the other hand, the global reactivity indexes of the systems have also been usefully used to estimate the possible electronic features, which can be calculated via the energies of the frontier molecular orbitals (HOMO and LUMO) [1]. Recently, drug-likeness and bioavailability scores have been also widely applied to estimate the possibility of a specific system in usage the pharmaceutical purposes [2]. All quantum chemical computations of these compounds have been conducted by the G09W [3] package at B3LYP/6-311G** [4,5] level to predict the thermochemical and physical properties. Also, HOMO& LUMO, and MEP diagrams are used to show the possible nucleophilic and electrophilic attack sites for specific reactions. Last, the drug-likeness and bioavailability of the designed compounds were computed and evaluated by using the SwissADME [6].



Scheme 1. The chemical structures of the carvacrol derivatives

Key Words: Carvacrol, DFT, FMO& MEP, Drug likeness

Acknowledgments

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Improving Energy Conversion Efficiency in Dye-Sensitized Solar Cells through TiO₂ Photoanode Modification with Gold-Silver Nanoparticles and Cobalt-Imidazolate Frameworks

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Abstract: This work reports a significant improvement in solar-to-electrical energy conversion efficiency of dye-sensitized solar cells (DSSCs) by modifying the TiO₂ photoanode with gold-silver nanomixtures and coating it with cobalt-imidazolate frameworks (ZIF-67). By incorporating nanospheres of Au–Ag into the TiO₂ photoanode there was a remarkable increase in solar-to-electrical energy conversion efficiency, reaching 7.33% which is ~230% higher compared to the unmodified TiO₂ photoanode (2.22%). Additionally, the incorporation of ZIF-67 with Au nanorods (AuNRs) resulted in a significant overall efficiency improvement to 8.38% under full sunlight illumination (100 mW cm⁻², AM 1.5G). The remarkable enhancement in solar energy conversion efficiency primarily stemmed from the synergistic interaction between Au and Ag, and their surface plasmon resonance effect. This interaction improved the optical absorption and interfacial charge transfer by minimizing charge recombination due to the formation of a Schottky barrier at the interface between TiO₂ and Au/Ag. Incorporating ZIF-67 into the TiO₂/AuNRs nanocomposite effectively augmented porosity and surface area, enhancing the adsorption of the sensitizing dye (N719) onto the photoanode's surface. The substantial leap in solar energy conversion efficiency using this modified photoanode underscores its promising potential for practical application in high-efficiency DSSCs.

Keywords: Dye-sensitized solar cells, gold and silver nanoparticles, ZIF-67, light-harvesting, TiO₂ nanoparticles.

THE EFFECT OF PIGMENT ON THE FINAL PROPERTIES OF BLACK GLASS AUTOMOTIVE ENAMEL

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Abstract

The main processes used in the production of automotive glasses are lamination, tempering, sag bending, and press bending. Laminated glasses can be produced by sag bending or press bending [1]. The windshield glasses, produced through the sag bending process and referred to as front-side glasses, must ensure low tempering temperature, high chemical and physical properties, and low UV transmittance, indicating high optical density [2]. The automotive glass enamels [3] that comply with these specifications comprise three primary components: a high-opacity, low-melting bismuth-based frit [4], CuCr2O4 black spinel pigment, and an organic medium [5].

The composition of the enamel as well as process factors such as frit production method, frit grinding types, frit particle size distribution, pigment particle size, media contents and final process steps like 3 roll mill processing also affect the final glass enamel paint aspects.

The present study focused on investigating the effect of different types of black CuCr2O4 pigments, obtained from three different companies, used in glass enamel paint on physical properties such as colour, gloss, and optical density. The findings have revealed that variations in commercial product characteristics, such as particle size, optical density, and chemical resistance, also influence the physical properties of the glass enamel paint.

Key Words: *Automotive, black enamel, glass-ceramics, pigment*

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INVESTIGATION OF THE EFFECTS OF CHERRY STEM EXTRACT ON CALCIUM OXALATE MONOHYDRATE GROWTH IN IN-VITRO

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Abstract

Urethritis is one of the oldest known diseases of urinary stone formation. Urinary system stone disease ranks third among urinary diseases after urinary infection and prostate diseases. Depending on the geographical region, 1-20% of people in the world suffer from stone disease [1,2]. Calcium oxalate monohydrate (COM) crystals are known to be the main cause of urinary tract and kidney stones. Preventing the collapse and growth of COM crystals or converting COM nuclei into calcium oxalate dihydrate (COD) crystals, a less stable structure, prevents the development of kidney stones [3]. In addition to the fact that surgical methods and drug treatments used in the treatment of kidney stones are painful and costly, the fact that traditionally used herbs are thought to be natural and harmless has led to an increased interest in herbal medicines in recent years. [4]. Dried cherry stems have diuretic properties and can be used in the treatment of kidney stones reported in Iranian Traditional Medicine documents. When infused in hot water, it can be used as an herbal remedy in the treatment of high blood pressure and kidney stone disease [5]. In the light of this information, in this study, the effects of cherry stem extracts as a natural additive on the growth of calcium oxalate monohydrate (COM) crystals, which is of great importance in investigating the crystallization mechanism in terms of biomineralization, was investigated in vitro. Structural characterizations of CaOx crystals were investigated by XRD and FT-IR analyses, and morphological characterization and morphological changes were investigated by SEM images. As a result of the experiments, it was determined that the formation of COM crystals decreased and COD crystals were formed due to the increase in the concentration of cherry stem extract and the formation of COM crystals was completely inhibited at high concentrations.

Key Words: kidney stone; calcium oxalate; crystallization; inhibition; cherry stem

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CONTINUOUS FLOW CHROMIUM(VI) ADSORPTION ONTO PEACH STONE AND ACRYLONITRILE-DIVINYLBENZENE COPOLYMER BASED ACTIVATED CARBONS

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Abstract

Chromium compounds are widely used in many industries including leather, textile, metal plating, battery and pigment production. They exist in two primary oxidation states: Cr(III) and Cr(VI). Cr(III) is relatively benign and serves as an essential trace element for living organisms. However, due to its toxicity and carcinogenic properties, Cr(VI) compounds must be removed before discharge into the environment. Although activated carbons have great attention for chromium removal from wastewater, their application in this domain remains limited due to limited adsorption capacity and high cost of commercial activated carbons.

Peach stone based (PS-AC) and acrylonitrile divinyl benzene copolymer based activated carbon (ANDVB-AC), which were prepared in our previous study [1,2], have been evaluated in fixed bed continuous flow Cr(VI) adsorption studies. The results were compared with the commercial activated carbon (CPG-LF). Peach stone was converted into activated carbon by using one-step steam activation at 1073K [1]. ANDVB-AC was obtained with three successive steps; the partial oxidation of ANDVB at 573, carbonization at 673K for 4h and at 1123 for 1h. Continuous flow adsorption studies were carried out in a fixed bed column with 13mm diameter. Different concentrations of Cr(VI) solution prepared at pH 2 was fed into the fixed-bed polyethylene column using a peristaltic pump until all adsorbent was saturated. Additionally, the effect of flow rate on breakthrough capacity was investigated. The outlet solution from the column was collected into separate tubes using a time-controlled fractional sample collector, then Cr(VI) concentrations were measured. Breakthrough curves were obtained by plotting relative concentration (C/C_0) values against the amount of passed solution (as bed volume).

Although total adsorption capacities were obtained as 122, 58, and 103mg/g for PS-AC, ANDVB-AC and CPG-LF, respectively, the breakthrough capacities were determined to be 25.0, 35.2, and 30.0 mg/g. When polymer based AC was used, 61% of the capacity was effectively utilized, while with peach stone based AC, only 21% of the capacity was effectively utilized. This difference can be attributed to the shorter contact time of the solution in the column and the slower adsorption kinetics of the PS-AC. As a conclusion, peach stone and polymer based activated carbons can be effectively utilized in a fixed column under continuous flow with high Cr(VI) adsorption capacities.

Key Words: Chromium; activated carbon; continuous flow adsorption, peach stone; acrylonitrile divinyl benzene

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Determination of Lignocellulosic Fraction of Airplane Lavatory Wastewaters for recovery purposes

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Abstract

It is becoming more crucial to find alternative sources for reuse purposes to reduce the use of fossil sources for material production. The recovery of raw materials from wastewater sources is a substantial resource-valorization approach, such as cellulose. The primary sludge of the domestic wastewater comprises around 25-30 % of the lignocellulosic content, primarily derived from lavatory tissue[1]. The high lignocellulosic content of airplane lavatory waste makes it a viable substitute source for the recovery of cellulose. Although few studies have investigated the recycling potential for aircraft lavatory wastewater[2,3], no earlier reports have examined the potential use of recovered cellulose for bioethanol production in aircraft wastewater. One of the usage alternatives for recovered cellulose is bioethanol production. Cellulose and hemicellulose are composed of sugars. Nonetheless, lignocellulose makes up the widely held of cellulose found in the natural world. The main components in lignocellulosic biomass are cellulose, hemicelluloses, and lignin combined to form lignin-carbohydrates complexes. These complexes are resistant to degradation because of their structural characteristic and lignin encapsulation. However, the cellulose and hemicellulose content of biomass determines its usefulness for bioethanol production. Thus, to convert cellulosic biomass into biofuel, it is essential to apply the pre-treatment process to separate the cellulose component from hemicelluloses and lignin. Subsequently, enzymatic hydrolysis can be performed to liberate glucose for ethanol fermentation. Three distinct techniques were applied as pre-treatment methods in the literature. These techniques involve physicochemical, biological, and chemical pre-treatment methods using acids and alkali solutions. In this study, the lignocellulosic component of the waste sludge was investigated to determine whether waste sludge captured from coarse screens of the aircraft lavatory wastewater is acceptable for recovery as bioethanol. Four different trials were conducted on the sample using two different chemical alkali pre-treatment techniques [4,5] in an effort to determine the ratio of the cellulose-hemicellulose-lignin composition of the waste sludge. The average values of ash content, oil content, hemicellulose, lignin, and cellulose ratio were found to be 4% (± 0.2), 5% (± 0.6), 26% (± 0.2), 51% (± 3.6), and 14% (± 1.1), respectively.

Key Words: Cellulose; waste recovery; bioethanol; lignocellulosic fractionation; airplane wastewater

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Multi-parameter optimization of layered hBN/PMMA nanocomposite under mechanical loading

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Abstract

In the current study, the influence of the geometry and the magnitude of axially applied mechanical load on the delamination in hBN/PMMA nanocomposite, is investigated theoretically. First, the analytical solutions for the interface shear stress (ISS) in the middle layer of the structure are obtained, based on the application of 2D stress-function method and minimization of the strain energy [1]. Second, the theoretical criterion for delamination in the interface layer (non-linear equation in respect to debond length), based on the model ISS is formulated, including the geometry and loading of the structure as parameters. Then, the multi-parameter optimization problem including this criterion is defined and solved. By varying simultaneously all parameters, their safety intervals (without delamination) in the considered nanocomposite structure, are obtained. It was found, that the magnitude of applied load influences on the magnitude of ISS mainly. The thicknesses of the layers influenced mostly on the type of solution for ISS, especially the substrate thickness. The layers' length influence on ISS is weaker than that of layers' thicknesses, at fixed load. The obtained results could be used for fast prediction of delamination and appropriate design in similar nanostructured devices to assure their safety work.

Acknowledgements

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Key Words: *Multi-parameter optimization; hBN/PMMA nanocomposite; interface shear stress; delamination;*

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EFFECT OF TiO₂ SYNTHESIS METHODS ON PHOTOCATALYTIC HYDROGEN PRODUCTION VIA WATER SPLITTING

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Abstract

Energy consumption is rising significantly all around the world these days. Renewable energy sources are expected to be able to supply the world's growing energy demands. Hydrogen plays an essential role among renewable energy sources. Hydrogen may be produced using fossil fuels, water, and biomass. Fossil resources are finite, and because of the detrimental impacts of fossil resources on the environment, hydrogen, which can be produced using solar energy and water, may be utilized as a fuel to supply inexpensive, ecologically friendly, and infinite clean energy. Hydrogen energy is utilized to address the energy demands of transportation, industry, and households. In addition, hydrogen-based goods have a significant presence in the automobile sector.

It is well known that TiO₂ is a semiconductor material with a large band gap that will absorb visible light. For many years, researchers have looked at the potential of titanium dioxide as a photocatalyst for producing hydrogen using solar energy.

In this study, sol-gel, hydrothermal and wet techniques were used to synthesize TiO₂ photocatalysts that are sensitive to the UV wavelengths of the sun spectrum. The characterization of these photocatalysts was carried out by X-ray diffraction and SEM analysis. These photocatalysts were also investigated in terms of hydrogen production activity from water splitting reaction using a solar simulator system.

Key Words: photocatalyst, water splitting, hydrogen production, sol-gel, hydrothermal

DRYING KINETICS, MATHEMATICAL MODELLING AND COLOR ANALYSIS OF *SOLEN MARGINATUS*: A COMPARATIVE STUDY OF OVEN, INFRARED, AND MICROWAVE DRYING METHODS

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Abstract

This study investigates the drying kinetics and mathematical modeling of *Solen marginatus*, commonly known as the grooved razor shell. *Solen marginatus* is dried using three different methods: oven drying (OD), infrared drying (IRD), and microwave drying (MWD), each at various temperatures and power levels. The effects of drying equipment, temperatures, and power levels on drying time, drying rate, effective moisture diffusivity, and activation energy are analyzed, with color analysis performed for each method. 14 well-known mathematical models are applied, and the three models with the highest coefficient of determination ($R^2 > 0.999$) are selected. Results indicate that drying time decreases with increasing temperature or power of the equipment. The effective moisture diffusivities range from 2.00×10^{-10} - 3.53×10^{-10} m²/s in OD, 2.53×10^{-10} - 6.02×10^{-10} m²/s in IRD, and 4.08×10^{-9} - 9.34×10^{-9} m²/s in MWD. The activation energies for OD, IRD, and MWD are calculated as 27.83 kJ/mol, 42.35 kJ/mol, and 40.98 kJ/kg, respectively. In terms of color retention, IRD was found to be the most effective method followed by OD and then MWD.

Key Words: color change; grooved razor shell; drying kinetics; mathematical modeling; seafood

DEVELOPMENT OF TRANSDERMAL PATCHES FOR ALZHEIMER'S TREATMENT AND IMPROVEMENT OF PENETRATION CHARACTERISTICS

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Abstract

Transdermal patches are drug delivery systems that deliver the drug contained in the body through the skin and provide a controlled release [1]. The present study aims to develop transdermal patches to be used in Alzheimer's treatment and to improve the penetration characteristics of transdermal patches.

Donepezil hydrochloride drug active substance selected in this study is commonly used to treat Alzheimer's disease [2]. HEC (hydroxyethyl cellulose) and CHI (Chitosan) were used as polymer based matrix and natural additives as penetration enhancers for the transdermal patches. The effectiveness of the patches prepared using different plasticizer materials was investigated. Synthesized films under in vitro conditions were characterized by using UV spectrophotometer, SEM, FTIR and Zetasizer. The drug release kinetics were determined using the zero order, first order, Higuchi and Korsmeyer-Peppas kinetic models by analyzing samples taken at certain time intervals using a UV spectrophotometer [3].

The results in this study confirm the synthesized films can be the potential materials for developing treatments for Alzheimer's disease. This project aims to contribute to the healthcare sector by developing unique patch formulations with high stability in order to provide solutions to the problems encountered in the oral treatment of Alzheimer's disease, reducing the negative effects of existing commercial patches and improving their features.

Key Words: Drug Delivery; Transdermal Patch; Donepezil Hydrochloride; Penetration; Alzheimer

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DFT Computations, FMO, NBO, Lipophilicity, and Water Solubility of Dihydromyricetin Derivatives

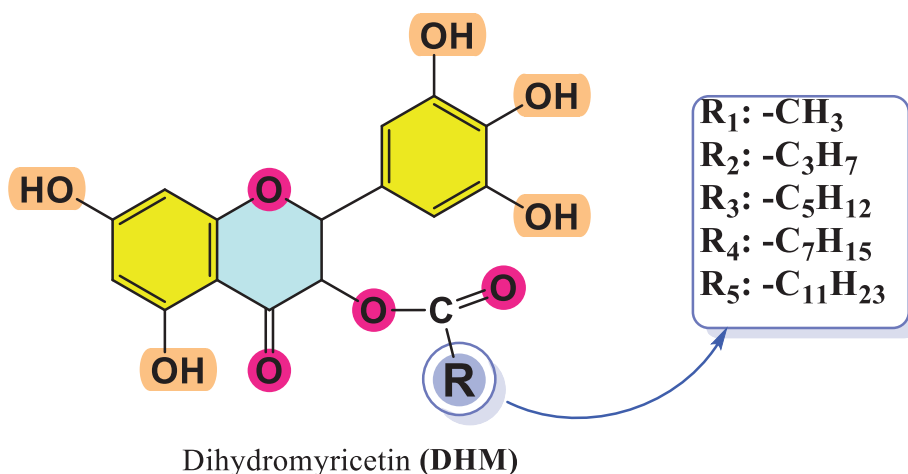
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Abstract

Dihydromyricetin (DHM) is known well as one of the essential phytochemicals and has a broad range of bioactive features in medicinal/pharmacological sciences (Scheme 1). Although it has a good water-soluble capability because of the abundance of the -OH groups, the lipophilic features also play an important role in developing the proper drug agent [1]. In this regard, we focus on the alkyl group substituted DHM derivatives to explore the lipophilicity of the main DHM molecule by using quantum chemical computations. For this purpose, the geometry optimizations and structural confirmations of the studied DHMs have been investigated by DFT computations, at the B3LYP/6-311++G** level [2,3]. Then, the FMO analyses [4] have been performed to evaluate the possible reactivity behaviors and predict the reactive sites of the compounds. Moreover, the second-order perturbation energy analyses of the compound have been calculated to elucidate the possible intra-molecular interactions [5]. Last, the lipophilicity and water-soluble characteristics of the compounds have been calculated and evaluated in terms of their relation with antioxidant activity [6]. The estimated results of this work are hoped to provide deep insight into developing future antioxidant compounds.



Scheme 1. The chemical structures of the dihydromyricetin derivatives

Key Words: Dihydromyricetin, antioxidant activity, DFT computations, lipophilicity

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THEORETICAL STUDY OF POSSIBLE REACTION PATHWAYS WITH THE OH RADICAL OF THE APRANAX (AP) MOLECULE, WHOSE ACTIVE INGREDIENT IS NAPROXEN SODIUM (NS)

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ABSTRACT

In this study, Apranax (AP), the active ingredient of which is Naproxen Sodium (NS), was examined. In the research, geometric optimizations of the fragments were made on the DFT/B3LYP/6-31G(d) basic set of Quantum Mechanical Density Functional Theory (DFT) in order to determine all possible reaction paths of AP with the OH radical theoretically. Since the reaction of the molecule with the OH radical is important for both water purification and atmospheric chemistry, calculations were performed both in the gas phase and in the water phase, modeled with CPCM in the COSMO (conductor-like screening solvation model) solvent model. The degradation mechanism was clarified by examining the energy values for all fragments, the bond lengths of the atoms in the fragments, the bond angles, and the mulliken charges.

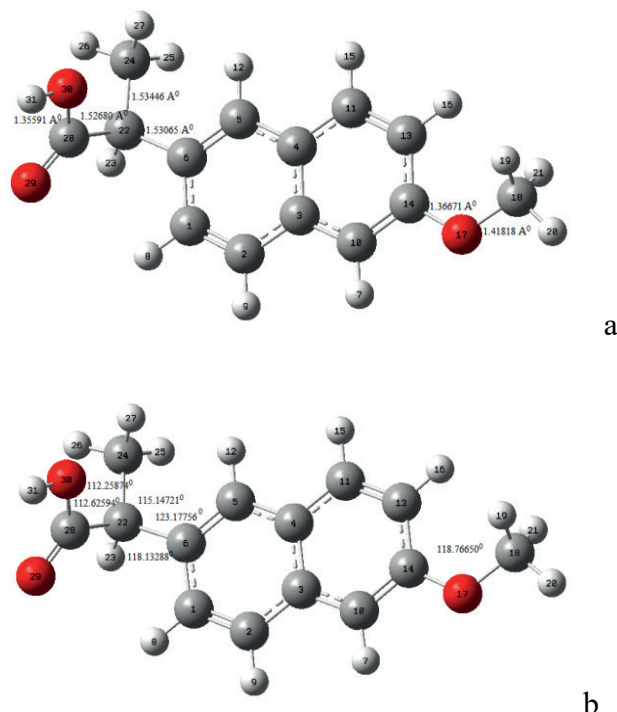


Figure 1. Bond lengths (a) and bond angles (b) between the atoms connected to the closed ring in the AP molecule (C atom is represented in grey, O atom in red and H atom in white.)

INDIVIDUAL DETECTION OF PHENOLIC AND POLYAROMATIC COMPONENTS IN TAR ANALYSIS FROM BIOMASS GASIFICATION PROCESS

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Abstract

Converting biomass into synthesis gas and hydrogen offers significant environmental advantages, including the generation of eco-friendly liquid fuels and the promotion of hydrogen as an efficient energy vector [1]. Gasification emerges as a notably promising technique for the energy conversion of biomass. Conventional gasification processes employ non-catalytic reactions with air (for partial oxidation) or steam at elevated temperatures to produce synthesis gas and hydrogen from biomass [2]. Gasification represents a strategic approach to biomass utilization, yielding a raw gas mixture that contains tar [3]. This study focuses on employing a solid-phase adsorption (SPA) technique for quantifying tar and its components. It was found that a dual-sorbent system, consisting of a sorbent with amino groups and activated coconut charcoal, is optimal for sampling tar and its volatile organic components. Furthermore, this research investigates the separate identification of aromatic and phenolic compounds by desorption from the amino-group-containing sorbent using dichloromethane, acetonitrile, or their mixture. Moreover, optimal conditions for the derivatization of phenols with bis(trimethylsilyl)trifluoroacetamide (BSTFA) were established. The evaluation of desorption efficiency revealed that aromatic compounds are effectively desorbed with dichloromethane, whereas phenolic compounds are not, and conversely, desorption of phenolic compounds with acetonitrile is nearly complete, but that of aromatic compounds is considerably lower. If the separate identification of aromatic and phenolic compounds is not required, a 4:1 mixture of dichloromethane to acetonitrile is determined to be optimal for the simultaneous desorption of both types of compounds from the sorbent containing amino groups.

Key Words: *biomass; gasification; tar; phenolic compounds; polyaromatic compounds*

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IMPACT OF TEMPERATURE ON METHANE PRODUCTION FROM BOG SLUDGE AND CRUSHED REED BIOMASS

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Abstract

This study delves into the biochemical processes involved in biogas production, emphasizing the significant influence of temperature on biogas yield, specifically methane output, from biomass sources such as marshy sludge and dried crushed reed biomass [1]. Recognizing temperature as a critical parameter, the research investigates the production of methane and biogas from bog sludge and crushed reeds, highlighting the correlation between temperature adjustments and the resultant biogas yield [2]. Employing a laboratory-scale bioreactor, the experiment yielded 4.48 liters of biogas with an average methane concentration of 38.7% at optimal conditions. The study confirms that a higher organic composition in the biomass enhances biogas output, advocating for the utilization of a mixed raw material approach for improved biogas production efficiency. The findings suggest that the optimal temperature for maximizing biogas yield, particularly methane, is 40°C, with variations in temperature impacting both the volume of biogas generated and the methane concentration within the biogas. The experiment demonstrates that temperature not only influences the rate of biogas production but also affects the optimal retention time and the mixture's overall fermentation efficiency. This research contributes to the optimization of biogas production processes, offering insights into the effective management of biomass resources for renewable energy generation.

Key Words: *anaerobic fermentation, biogas, methane production, biomass gasification, temperature influence.*

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SYNTHESIS AND CHARACTERIZATION OF NOVEL SYMMETRIC PHTHALOCYANINES CONTAINING BROMONAPHTHALENE GROUPS

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Abstract

Phthalocyanines which is a class of macrosyclic compounds [1] on account of their technological and scientific significance in various fields, have attracted considerable attention over many decades. They have been employed in several ‘hi-tech’ applications such as photo conducting material in laser printers [2], optical limiting devices [3], solar cells [4]. Due to the fact that diamagnetic central metal ions such as Zn enhance the photo toxicity of the phthalocyanines, the substituted phthalocyanine derivatives can also be used for photodynamic cancer therapy and other processes driven by visible light [5].

The main aim of the present work was the synthesis of a new mono substituted phthalonitrile derivative, 4-((6-bromonaphthalen-2-yl)oxy)phthalonitrile, was prepared by a nucleophilic displacement reaction of 4-nitrophthalonitrile with 6-bromonaphthanol. Novel metallophthalocyanine (M = Zn) and metal free phthalocyanine with four peripheral 4-((6-bromonaphthalen-2-yl)oxy)phenoxy groups were synthesized by cyclotetramerisation of the phthalonitrile and characterized by elemental analyses, FTIR, ¹H-NMR, UV–Vis and MALDI-TOF MS spectral data.

Key Words: *Synthesis, symmetric, phthalocyanine, bromonaphthanol, spectroscopy*

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THE SYNTHESIS AND CHARACTERIZATION OF A₃B TYPE A NOVEL UNSYMMETRICAL ZINCPHTHALOCYANINE

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Abstract

During the last century numerous studies have been reported phthalocyanine macrocycles. Tetrapyrrole compounds including phthalocyanines (Pcs) have many interesting properties such as optical, spectroscopic, and electronic. These properties provide that studied for a wide range of technical and medical applications [1,2]. Popularity of these macromolecules which arises from their unique physical and chemical properties, encourages many researchers to work on design and synthesis of novel Pcs to improve the physicochemical properties and organization capabilities for intended application [3,4]. Specificity in the applications of phthalocyanines can be introduced by modification of the phthalocyanine ring or by changes in the central metal or ligands [5]. In this work, we report on the synthesis and characterisation of a new unsymmetric metallophthalocyanines (ZnPc) which carry 6-bromonaphthoxy substituents on each of three of the benzenoid groups while the fourth one carries 4-carboxyethylphenoxy group. Despite the variety of synthetic routes developed to prepare symmetrically substituted phthalocyanines, relatively few methods can be applied for preparing unsymmetrical ones. The simplest approach to the preparation of phthalocyanines bearing different substituents is a mixed cyclization of two precursors with different substituents. This method was preferred in this work. The characterized of the synthesized complexes were employed by elemental analyses, FT-IR, ¹H-NMR, UV-Vis and MALDI-TOF MS spectral data.

Key Words: *Synthesis, phthalocyanines, unsymmetric, spectroscopy*

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SYNTHESIS AND EVALUATION OF NEW QUINONE-BASED HETEROCYCLES AGAINST TUMOR CELL LINES

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Heterocyclic quinones, which contain at least one carbon in the ring as well as one or more heteroatoms, especially nitrogen, are of interest to synthetic chemists and an extraordinarily important class of compounds because they exhibit broad-spectrum biological activities such as anticancer, antibacterial, anticancer, anticancer, anticancer, and antibacterial activities [1,2]. Isoquinolinequinone moiety represents a class of nitrogen containing bicyclic heterocyclic compounds with significant importance and is present as a crucial core in a wide variety of drugs, many natural products, and pharmaceutically active compounds [3].

In this study; the isoquinolinequinone compounds obtained in situ from the reaction of iodobenzene bis(trifluoroacetate) (PIFA) and isoquinolin-5-ol was then reacted with substituted aromatic amines. Among the synthesized compounds, NCI selected some compounds and anticancer activity of those was evaluated according to the protocol of the drug evaluation branch of the National Cancer Institute (NCI), Bethesda, USA, for anticancer activity. The results for each tested compound are reported as the percentage of growth inhibition of the treated cells when compared to the untreated control cells. The compounds were tested against a panel of 60 cancer cell lines, derived from different tumors, including leukemia, melanoma, lung, colon, central nervous system (CNS), ovarian, renal, prostate, and breast cancer.

Acknowledgements. This work was financially supported by the Scientific Research Projects Coordination Unit of Istanbul University (Project numbers: FBA-2022-39333) for supplying the equipment and materials.

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IDENTIFICATION OF AMINO BENZOQUINONES AS EGFR INHIBITORS

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A number of different types of human cancer have been linked to anomalies in the epidermal growth factor receptor (EGFR). The EGFR is a widely used and successful therapeutic target for non-small-cell lung cancer (NSCLC) and breast cancer, and in recent years, targeted EGFR treatment using EGFR-tyrosine kinase inhibitors (EGFR-TKIs) has produced excellent clinical results.¹

We have previously investigated the synthesis and potential application of variously substituted aminoquinones as anticancer agents against K562 and MCF-7 cell lines in addition to the antimicrobial agents. From those molecules synthesized, Plastoquinone analogs displayed the lowest micromolar GI₅₀ values in various cancer cell lines.²⁻⁴

Herein, we present synthesis, characterization, and further investigation of quinones based on amino-1,4-benzoquinones as EGFR inhibitors. Following the bioisosteric replacement strategy pyridinyl or dimethyl motifs were replaced with acetoamido moiety. Firstly, some of our molecules have been submitted and selected by NCI, USA; then they were screened for anticancer screening at a 10⁻⁵ M dose in the full panel of 60 human cell lines derived from nine human cancer cell types (leukemia, melanoma, non-small-cell lung, colon, central nervous system, ovarian, renal, prostate, and breast cancer) at the NIH, Bethesda, Maryland, USA. Also, the effect on biological activity was investigated with variously substituted amino moiety. The strongest antiproliferative activities in the panel of selected cancer cell lines displaying compound was chosen for further evaluation of its biological effects *in vitro*.

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Improved packaging performance of olive-tree based biochar loaded poly(lactic acid) films

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Abstract

Petroleum-containing packaging materials have created serious ecological problems for the environment due to their resistance to biological degradation. In this context, the use of biodegradable films as an alternative to packaging materials are gaining importance. Among various biopolymers, poly(lactide) (PLA) has found to be effective, durable, and antimicrobial materials [1]. However, the mechanical strength of PLA polymer is low. In addition, their vapor permeability is high, which limits the use of this material. Biochar is an additive that can be produced from many wastes and acts as a fertilizer in the soil. By adding it to the PLA material, it makes the packaging film completely compostable and improves its properties.

In this study, biochar was synthesised from olive pruning waste by the slow pyrolysis method. Biochar was added to the PLA films in different proportions (5, 10, 15, 20 wt.%). The packaging properties of the films were investigated. Specific surface area analysis (BET), biochar yield and ash determination were performed for biochar. Tensile strength, swelling, water vapor permeability, contact angle, opacity, and antimicrobial activity tests were performed for the films. Due to the high lignin rate and low volatile matter in the olive branch, biochar was produced with a yield of 29.75%. The ash content of biochar was found to be 3.37%. According to the swelling test results, it was observed that the swelling ratio increased as the BC concentration increased. When the BC concentrations of the films increased, the water vapor permeability capacity gradually decreased from 4.43% to 1.36%. The maximum tensile strength value was obtained as 14.91 MPa for 5 wt.% biochar loaded PLA films. According to the results of the antimicrobial activity test, no visible bacterial growth was observed after the bacteria planted on the produced packaging films.

Key Words: *Poly(lactic acid) films; biochar; packaging*

Acknowledgements: This work has been supported by Çanakkale On Sekiz Mart Universty Scientific Research Projects Coordination Unit (FBA-2023-4345).

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DEHYDRATION OF INDUSTRIAL ISOPROPANOL WASTEWATER BY PERVAPORATION USING CARBOXY METHYL CELLULOSE AND GRAPHENE OXIDE HYBRID MEMBRANES

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Abstract

Isopropanol (IPA) is widely used as an industrial solvent, cleaning agent, and in producing chemicals, fuels and medical products. Many applications require anhydrous IPA without water. IPA-containing wastewaters are generated from its production and uses. Dewatering and recycling IPA from these waste streams is important for both economic and environmental reasons. It allows reuse of this valuable solvent while reducing waste. The ability to recover IPA in anhydrous form is important due to the need for water-free IPA in downstream applications.

IPA and water form an azeotropic mixture, making conventional dehydration methods like distillation and extraction challenging. Membrane-based processes such as pervaporation offer advantages over these processes, as it can break azeotropes while requiring lower energy and having a smaller footprint [1].

Indeed, pervaporation is a highly effective membrane-based separation technique developed for liquid feed solutions. In this process, the selective component present in the feed solutions dissolves into the membrane on the feed side, diffuses through the membrane and subsequently evaporates at reduced pressure on the permeated side of the membrane. Liquid-liquid separation of organic solvent mixtures and dehydration of aqueous solutions of organic solvents have been the main applications of this membrane-based pervaporation process. Permeation flux and selectivity could be the key factors in determining the separation performance of pervaporation [2].

The membrane is critical in pervaporation applications. Polymeric, inorganic and hybrid membranes have been widely used for pervaporative separation. However, polymer applications were limited by several issues, including low mechanical and biostability and low reject rates. Inorganic membranes have been limited by the high cost of manufacturing. The inclusion of inorganic components into polymer membranes is expected to enhance the membranes' separation properties. The synergistic effects of combining polymers with inorganic fillers/particles is hypothesized to result in higher performing membranes for the separation. The key requirements of these hybrid membranes are that the polymer component confers chemical/thermal stability, ease of processing and high hydrophilicity [3].

In this study, hybrid membrane was used to dehydration of industrial isopropanol wastewater by pervaporation. The hybrid membranes for pervaporation dehydration were prepared by dispersing graphene oxide into carboxy methyl cellulose matrix. Notably, the dehydration separation performance of the hybrid membranes was improved by the incorporation of graphene oxide. Also, the effects of graphene oxide concentration, operation temperature and feed IPA concentration on hydrophilicity, swelling, and dehydration properties were systematically characterized and evaluated. Optimum process conditions have been determined and under these conditions, water flux 4.7 kg/m² h and separation factor value of 128 were obtained.

These findings pave the way for future development of CMC based hybrid membranes employing at the pervaporative dehydration process.

Key Words: *Dehydration; Isopropanol; Membrane; Pervaporation; Wastewater*

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EXPERIMENTAL AND MODELING INVESTIGATION OF MASS TRANSFER DURING INFRARED DRYING OF AHLAT PEAR

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Abstract

Drying, a crucial energy-intensive process in food preservation, involves combined heat and mass transfer mechanisms aimed at removing moisture from food products to extend their shelf life [1]. The Ahlat pear (*Pyrus elaeagnifolia* L), naturally grown in Turkey, can be consumed dried or fresh and is commonly used in Turkish folk medicine for treating ailments such as diarrhea and snake bites, owing to its rich vitamins and nutritional values [2,3].

This study focuses on examining the infrared (IR) dryer efficacy under different infrared powers (38, 50, 62, 74 and 88 W) in the drying process of Ahlat pears. The initial moisture content of Ahlat pears' samples was successfully minimized from 68.75% to 20% (wet basis), and a thorough analysis was conducted to assess their drying characteristics and kinetics. The results clearly demonstrate the impact of the IR dryer on drying time. The drying curves illustrated a falling-rate period throughout the process, with no observable constant-rate period.

Using Fick's second law, the study determined the effective moisture diffusivity, which ranged from 1.07×10^{-8} to 2.03×10^{-8} m²/s across the experimental conditions. Additionally, the activation energy was calculated using a modified Arrhenius-type equation, resulting in 1.6382 kW/kg. Six mathematical models (Alibas, Aghbashlo, Logarithmic, Logistic, Page, and Henderson & Pabis) were evaluated for moisture ratios through nonlinear regression analysis. The results of the regression analysis identified the Alibas model as the most suitable for describing the drying behavior, exhibiting the lowest X² and RMSE values and the highest R² values.

Key Words : Ahlat pear, infrared drying, effective diffusivity, mathematical modelling,

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Synthesis, Characterization and Effects to Cholesteric Lyotropic Liquid Crystal Media of -ONNO- Type Schiff Bases and Metal Complexes

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Abstract

Cholesteric lyotropic liquid crystals having one-dimensional helical orientation are crucial in electro-optic devices and panels. A helical orientation allows for controlled properties based on temperature, pressure, and compound quantity. In this respect, a chiral dopant or a chiral amphiphilic molecule may prefer to depend on the desired solvent environment. The self-organization of micellar units or molecules in liquid crystal results in a selective reflection due to ordered structure and light interaction [1]. Julolidine is a type of heteroaromatic organic molecule that possesses strong electronic withdrawing and donating abilities, as well as high conjugation ability. [2]. We aimed to synthesize symmetric tetradentate Schiff bases and copper complexes using a julolidine derivative (8-hydroxy-1,1,7,7-tetramethyl-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline-9-carbaldehyde) and diamines with four and six carbons. The Schiff bases were characterized using various spectroscopic techniques including FT-IR, ¹³C and ¹H-NMR, and UV-vis. Spectroscopy. The synthesized compounds, which have the potential drug-active substances, were examined in a lyotropic liquid crystal medium which draws attention to similarity to cell membrane by polarized optical microscope. In this scope, the cholesteric phase was obtained from Decylammonium chloride (DACl) and an optically active molecule L-alanine decyl ester (L-ADE). In the prepared cholesteric phase, helical pitch, which is an important quantity for the cholesteric phase, and the effect of the synthesized Schiff bases and metal complexes on this quantity were examined.

Key Words: *Lyotropic liquid crystal; helical pitch; dopant molecule; metal complex; Schiff base*

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PREPARATION OF BORON NITRIDE/TITANIUM DIOXIDE HYBRID NANOFLUIDS AND INVESTIGATION OF STABILITY

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Abstract

Nanomaterials and nanofluid's importance increasing day by day with respect to new developments and the superior characteristics [1]. In that point of view, several industries began to use nanomaterials in their daily processes and the application areas of nanofluids increasing too [2]. Titanium dioxide one of the most preferred and known material to produce nanofluids and its superior qualifications demonstrated from researchers [3]. Titanium dioxide (TiO₂) has wide range of application areas such as food, textile, paint, and cosmetics. Also, boron nitride has some important qualifications for both different applications and industries. Boron nitride was not used as a nanomaterial previously for nanofluid systems[4].

In this study, it is aimed to prepare boron nitride/titanium dioxide hybrid nanofluid under different conditions. Several parameters examined for making a better understanding of the parameters which affect the stability of the nanofluid such as surfactant concentration, sonication time. Three types of nanofluids such as titanium dioxide nanofluid, boron nitride nanofluid and titanium dioxide/boron nitride hybrid nanofluid has been prepared and compared which other. Sodium dodecyl sulphate has been used as a surfactant and the concentration of the surfactant has been examined and analyzed the affects of it.

The findings reveal that augmenting the quantity of Sodium dodecyl sulfate and extending sonication duration enhance stability. Additionally, titanium dioxide emerges as the most efficacious nanofluid among the tested variants.

Key Words: *Nanomaterials, nanofluid systems, titanium dioxide, boron nitride, Sodium dodecyl sulphate.*

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MODELLING OF CONTINUOUS FLOW PHENOL ADSORPTION ONTO ACRYLONITRILE-DIVINYLBENZENE COPOLYMER

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Abstract

Phenol, a highly toxic organic compound, is commonly found in industrial effluents of pharmaceuticals, paper, plastics, and petrochemicals production processes. Due to the fact that phenol contamination in water sources causes significant environmental hazards, effective treatment methods should be improved to address these adverse effects. Continuous adsorption process can be an effective choice for the treatment of phenol contaminated water sources. In order to remove phenol from aqueous solutions, the usage of many adsorbents has been studied including activated carbon, clays etc. However, polymeric structures emerge as promising alternatives due to their advantageous properties, including high mechanical strength, surface area, ease of regeneration, and cost-effectiveness. In this study, continuous flow phenol adsorption onto Acrylonitrile-Divinylbenzene (AN-DVB) copolymer was investigated. Phenol adsorption was modelled in order to characterize the adsorption process, and the predictive accuracy of the models under continuous flow conditions was evaluated. Aqueous solution of phenol was passed through a fixed column packed with AN-DVB copolymer beads. The changes of the breakthrough curve with the adsorbent amount and flow rate were examined at room temperature. Increasing adsorbent amount in the column resulted in longer breakthrough and exhaustion times, on the other hand, increasing flow rate without changing the adsorbent amount resulted in shorter breakthrough and exhaustion time as well as lower adsorption capacity. The experimental breakthrough curves were modelled by using Adams & Bohart, Thomas, Yoon & Nelson, Clark and modified dose-response column models via non-linear regression analysis. The modified dose-response model fitted well with the experimental data for all studied conditions. Isopropanol was successfully examined to regenerate polymer beads through adsorption-desorption cycles.

Key Words: Adsorption; Modelling; phenol; Acrylonitrile-Divinylbenzene copolymer; continuous process.

Composite Thin Films of Upconverting Nanoparticles: Characterization of Emission and Energy Transfer Properties

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Abstract

Upconverting nanoparticles (UCNPs) are able to emit photons of higher energy - i.e. shorter wavelength – when excited by photons of lower energy (anti-Stokes effect)[1].

The aim of our research was the development of UCNP-containing functional composite thin films using silica, titanium dioxide and chitosan biopolymer as matrix materials. The main objective was to maximise the intensity of anti-Stokes emissions of the upconverting nanoparticles in the thin film systems. We aimed to control the composition of the matrix material, and the parameters of the coating formation process to maximise the upconversion emission intensity. The highest emission intensities were achieved using chitosan biopolymer as matrix material. Moreover, in case of chitosan matrix material no heat treatment was necessary during the coating process.

The energy transfer interactions between UCNPs and Rhodamine 6G fluorescent model dye molecules were also investigated. Energy transfer was measured both in suspensions and chitosan matrix composite coatings. The results of the radiative interactions in the developed composite thin film systems can later be utilised, among others, in the field of photodynamic cancer therapy[2] or efficiency enhancement of photovoltaic devices[3].

Key Words: *upconversion, upconverting nanoparticles, composite coatings, chitosan, energy transfer*

Acknowledgement

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COMPUTATIONAL MODELING OF n=1 RUDDLESSEN-POPPER TYPE LA₂NiO₄ FOR FLUORIDE ION BATTERIES

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Abstract

In today's world, it is imperative to promote the use of renewable energy sources whilst adopting more responsible production paradigms and lifestyles in order to meet the increasing global demand for energy and to mitigate the impact of global warming. Lithium-ion batteries, which are among the most widely used, and efficient energy storage systems in the modern world, are rapidly reaching their limits. Fluoride-ion batteries are a promising alternative technology to Lithium-ion batteries, but they have not been sufficiently researched yet. Fluoride-ion batteries have higher theoretical energy densities than lithium-ion batteries, and the abundance of fluorides and typical elements used to make these batteries offer an attractive alternative in terms of cost- effectiveness and scalability. In this study, using density functional theory within generalized gradient approximation(GGA) and plane-wave pseudopotential method, we have calculated the structural and electronic properties of high energy and high voltage n=1 Ruddlesden-Popper type La₂NiO₄ intercalation-based cathode material, which is one of the most promising materials that can be used in Fluoride-ion batteries. In addition, structural and electronic property calculations were also performed depending on the concentration of Fluorine ions (number of F⁻ atoms per unit formula) to further investigate different anion ordering scenarios and compared to available experimental measurements. From our study, it was found that the amount of Fluoride-ion concentration has a significant effect on the structural and electronic properties by changing the crystal order of the La₂NiO₄ structure in question. It is thought that the effect of these properties changing with different Fluoride-ion concentration on battery performance is important.

Key Words: *Flor-ion batteries; cathode materials; density functional theory; energy storage; structure-properties relationship*

Effects of Additives on Mechanical and Barrier Properties of Polyhydroxyalkanoate Derived Biocomposite Films by Solution Casting

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Polyhydroxyalkanoates (PHAs) are naturally occurring, non-toxic aliphatic polyesters. Nano/composite fabrication is an effective and cost-efficient approach to modulate polymer properties. This study explores the fabrication of amorphous P3HB4HB biopolymer-based biocomposites and bionanocomposites with its crystalline copolymer, PHB, and various fillers.

Solution casting was employed to prepare pure and plasticized (Joncryl[®] ADR4468) bioblends of P3HB4HB and PHB. The optimum composition of P3HB4HB was determined as 80%. Fillers used included bentonite, sepiolite, high-purity sepiolite (1, 2, 3 wt%) and copper-based metal-organic framework (Cu-MOF) nanocrystals, graphene-copper-based metal-organic framework hybrid nanocrystals (0.1, 0.5, 1 wt%).

The effects of fillers on biofilm structure, thermal behavior, mechanical and optical properties, and barrier performance were investigated. The results demonstrate the potential of these biocomposites and bionanocomposites for various applications, such as packaging, biomedical devices, and environmental remediation.

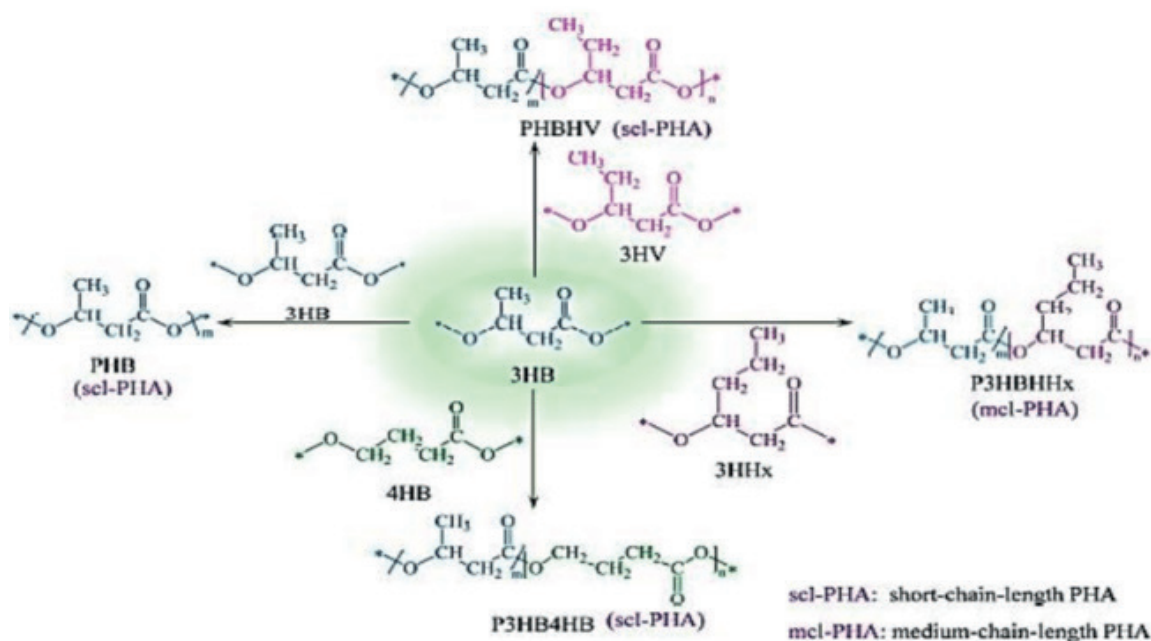


Figure 1. General structure of PHA derived copolymers [3]

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Preparation and Characterization of Bionanocomposite Packaging Films Reinforced with Metal Organic Frameworks Based Additives

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In the context of emerging green chemistry and sustainable manufacturing technologies, the development of packaging films from renewable resources has gained significant momentum as an alternative solution for the packaging industry [1,2]. In this study, copper-based metal-organic framework (Cu-MOF) nanocrystals and with graphene oxide (GO), Cu-MOF@GO hybrid nanocrystals were fabricated [3]. The structural and morphological characterizations of the synthesized nanocrystals were performed. The nanocrystals were incorporated into PHA/PBS and PHA/PHBV biodegradable polymer blends at 0.1, 0.5, and 1 wt% ratios, and bionanocomposite films were prepared by solution casting. The mechanical, optical and barrier properties of the bionanocomposite films were investigated to assess the effect of metal-organic framework-based additives and their potential for packaging applications. The results obtained from the characterization tests revealed that the films containing Cu-MOF nanocrystals exhibited superior mechanical strength and barrier properties compared to the Cu-MOF@GO hybrid nanocrystals. Considering the mechanical properties of the 1 wt% Cu-MOF containing PHA/PBS and PHA/PHBV bionanocomposites, the tensile strength, elongation at break, and Young's modulus values of the PHBV-based bionanocomposite were found to be comparable to those of the reference polyethylene.

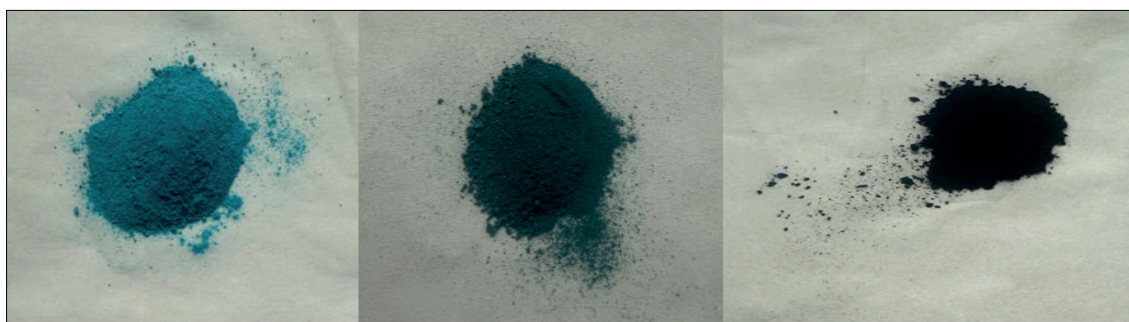


Figure 1. Images of Cu-MOF, Cu-MOF@GO and GO nanocrystals

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Acknowledgement

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Methyl Viologen as Photochromic Cation in Ca(II) and Mg(II) Complexes

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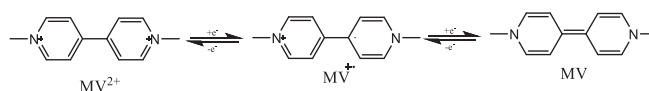
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Abstract

Coordination frameworks comprising photochromic components are widely studied for their application in diverse fields such as sensing, optoelectronic devices, medical engineering, and energy storage.[1] In this context, 1,1'-disubstituted 4,4'-bipyridine, also termed as viologen has featured prominently as photo responsive cations due to their intrinsic redox properties upon photoinduced electron transfer process from the counter anions. The first reduction step is accompanied by distinct color change both in solid state and in solution due to the different absorption domains of RV^{2+} (UV) and $RV^{\cdot+}$ (visible).



We report herein the synthesis and structural features of $[Me_2-4,4'Bipy][Ca_2(OSO_3Me)_6(H_2O)_4](1)$ and $[Me_2-4,4'Bipy][Mg_2(OSO_3Me)_6(H_2O)_4](2)$ along with a detailed study on their photophysical properties using electron spin resonance and UV vis spectroscopy in the solid state. Slow diffusion of hydrazine into the solutions of **1** or **2** in water, DMSO or MeOH results the formation of $MV^{\cdot+}$ as the reduced species of MV^{2+} and is visually evident by an intense blue color. Keeping the solution under ambient conditions for several days led to the isolation of crystalline solid in each case and identified as $M(NH_2NHCOO)_2(H_2O)_n$ [$M = Ca(3), n=1$; $Mg(4), n=2$]. Considering extensive body of work dedicated to CO_2 capture from air under ultra-low concentration, the results represents the first example of CO_2 capture using **1** and **2** as molecular scaffolds, which take advantage of lability of metal-sulfonate bonds.

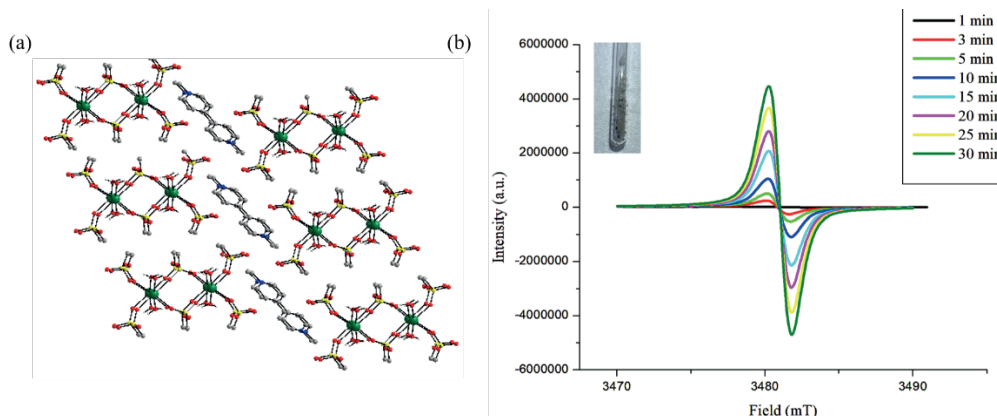


Figure 1. Crystal Structure and EPR spectra of **1** in solid state under UV light.

Key Words: Coordination framework, photochromic, electrochemistry, viologen, radical cation.

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Design and Synthesis of N₃O₂, N₂O₃, N₂(S/Se)O₂ and N₅O₂ type Donor Bases and their Interactive Behavior with UO₂²⁺ Ion

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The uranyl (UO₂²⁺) cation, the much-recognized and foremost functional species in the chemistry of uranium and is classified as a *hard* cationic species and preferably binds to *hard* oxygen donor atoms of a donor species on complexation. An increasing interest, in developing their chemistry with the organic donors to bear oxygen or nitrogen or as in their mixed (O,N) combinations has been prime target of researchers for selective and effective binding of the uranyl ion (UO₂²⁺) besides to their diverse practical applications. This include from mining, purification and processing, as nuclear fuel, extraction from seawater, nuclear fuel cycle reprocessing, chelation therapy against poisoning and finally ecological impacts and remediation due to recognized uranyl species. Categorically, these studies have contributed new fundamental understanding associated with the coordination chemistry of the uranyl ion that may play an important role in controlling the nuclear waste management. Indeed, stable U(III), U(IV) and unstable U(V) oxidation states only may come into existence when UO₂²⁺ (in the (VI) oxidation state) contributes in chemical, biological and environmental processes or under the influence of external stimuli in natural environment. For example, role of external influences in UO₂²⁺ ion chemistry have also raised obvious reasons for new experimental understanding, as change in pH, light, colloidal formation, redox processes, hydrolysis, radiolysis, solubility, dissolution/precipitation, complexation, and bonding with other metal ions are critical issues. The role of external influences in uranyl ion interaction chemistry is complicated and needs to be addressed as they may provide new fundamental basis for different unforeseen coordination nuclearities. Genuinely, this generates more experimental basis in thoughtful way by inorganic and analytical chemists in finding practical solutions relevant to extraction processes and nuclear waste management. Therefore, the design and synthesis of new chelating ligands that bind to the uranyl ion with high affinity and selectivity are of prime importance. In our previous studies, we have found the hypersensitivity of uranyl cations under non-aqueous reaction conditions and such a reaction scenario also contributed to find the experimental basis to explore new uranyl compounds with different nuclearities and unforeseen coordination modes. Herein we report synthetic and structural studies of complexes of uranyl(VI) ions with N₃O₂, N₂O₃, N₂(S/Se)O₂ and N₅O₂ type Schiff base donors offering different steric and electronic properties. We specifically focus on the changes in the geometric and electronic structure, bonding characterization, and ligand charge transfer as these properties may be related to changes in ligand extraction behavior. The distinctive chemistry of uranyl compounds can be attributed to the unique geometrical and electronic structures of the uranyl ion.

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Fabrication of electrospun polyvinylidene fluoride filter material for deep purification of multiple impurities from water

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Abstract

Water is one of the most valuable natural resources on earth. Rapid population growth, urbanization, and industrialization create problems for natural resources [1]. Therefore, keeping existing water resources clean is important both in terms of resources and cleaning costs. There are many pollutants in domestic greywater, including dyestuffs, nitrates, phosphates, oils, and microplastics. On-site cleaning these pollutants greatly reduces the load on wastewater facilities. The design of new generation zero waste houses and the development of domestic filtration systems are promising in this context. Domestic filtration is an on-site separation method in which domestic contaminants are cleaned before being discharged. Similar to drinking water, in this system the water is cleaned before being discharged. Especially in the last 5 years, this process has been carried out with polyester, polyamide and metal filters.

In this study, electrospun filters with polyvinylidene fluoride (PVDF) polymer were produced, characterized, and tested for the separation of oil, microplastics, dyestuffs, and detergents in simulated domestic water. Electrospinning is a very fast fiber film production technology. In this way, fast and practical filters can be produced without the need for solvent evaporation. The diameter of the films produced within the scope of the study was 1 micron and their porosity was more than 80%. The filter removed 100% of microplastic (polyester), 99.9% of dyestuff (methylene blue), 82% of anionic detergent surfactant (Linear Alkyl Benzene Sulfonic Acid), and 99% of oil (soya oil) from the wastewater. It was observed that the mechanical strength of the films was more than 8MPa. As a result, filters with high commercialization potential were obtained. The SEM image of the nanofiber film is seen in Figure 1.

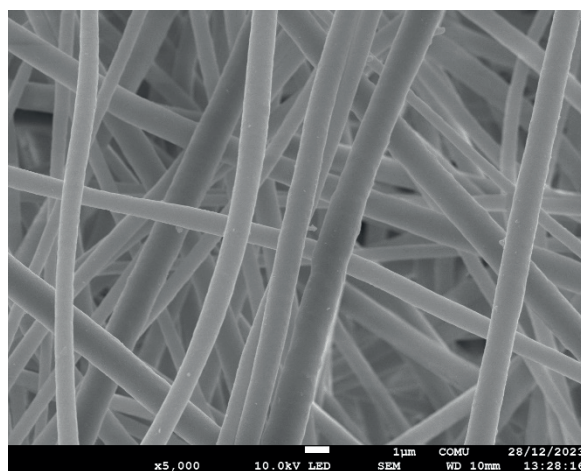


Figure 1. PVDF fiber filter

Key Words: *polyvinylidene fluoride; electrospun filter; greywater separation*

Acknowledgements: This work has been supported by TUBİTAK (123Y119).

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THE MECHANISM OF ANTIMICROBIAL ACTIVITY OF NATURALLY ORIGINATED PRESERVATIVE HINOKITOL

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Abstract

The European Union cosmetic market is controlled by the European Parliament and Council Regulation on cosmetic products. The regulation strictly distinguishes between prohibited and permitted compounds for the use in the industry [1]. However, although many cosmetic preservatives are claimed to be safe and are permitted to be used (annex V of Regulation [1]) they often have negative reputations and are controversial among consumers [2]. Preservatives might be responsible not only for allergic reactions but also some of them, such as parabens, can increase the occurrence of serious health problems, due to their similarity to oestrogen [2,3]. However, it is undeniable that preservatives play a crucial role in protecting against microbial contamination, and therefore they cannot be eliminated [2]. A way to address these problems is to introduce more natural ingredients, including antimicrobial ones, into cosmetics. The antimicrobial potential of many plant derivatives is commonly known and some of them (e.g. essential oils) are successfully used in the cosmetic industry [4].

The mechanism of antimicrobial compounds' activity on cells is very complex. However, the influence on the cell membrane is a highly important aspect of their activity and selectivity [4]. There is a lack of information in the literature on the mechanism of action of hinokitiol (one of the naturally originated preservatives) on bacterial cell membranes, therefore the experiments conducted aimed to investigate the influence (also to establish the mechanism) of hinokitiol on bacterial model membranes (*E.coli* and *S.aureus*). The obtained results were compared to the antimicrobial tests on bacterial strains. The experiments involved the Langmuir monolayers study (surface pressure-area, penetration measurements and Brewster angle microscopy studies of model membrane and single lipid components), liposomes experiments (change in fluorescence anisotropy of DPH probe and liposome sizes) and antibacterial tests on bacterial strains. The obtained results suggest that the presence of hinokitiol causes fluidization of mono- and bilayers and influences the lipids' order in monolayers. Moreover, the impact of preservatives on membrane components varies depending on the type of phospholipids and their head charge. The hinokitiols' capacity to integrate into monolayer lipids was moderately effective.

Key Words: *lipid monolayers, liposomes, preservatives, hinokitiol, bacteria*

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THE EFFECT OF NATURAL ADDITIVES ON PREVENTING BREAKAGE BY INCREASING PAPER STRENGTH VALUE

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Abstract

Corrugated cardboard boxes have become the predominant choice for packaging material in various transportation and material packaging applications. They are favoured for their versatility and eco-friendliness, as they are easily recyclable. These boxes are crafted from packaging papers with diverse fiber and tensile qualities. Starch plays an important role in both waste recycling and the manufacturing of paper.

Oxidized and enzymatically degraded starch enhances the water retention capacity, thereby increasing the paper's resistance to moisture [1]. When applied to the paper's surface, it enhances adhesion, thus improving the paper's strength and reducing the risk of tearing and breaking.

Alginate, PEG, and PVA, which are biobased additives derived from either biodegradable sources or biological origins, are applied onto the paper's surface to bolster its strength and flexibility. Their robust water absorption capacity, flexibility, durability, and water solubility contribute to the increased strength of the paper. These biopolymers, alongside corrugated cardboard packaging dispenser modules, enhance sustainability through their favourable properties, including mechanical strength, film-forming ability, compatibility with paper materials, and barrier durability [2,3].

In this study, the effect of applying surface coating materials obtained by mixing starch with natural additives such as alginate, PEG, and PVA in various ratios on the mechanical properties of paper has been investigated. The prepared solutions was applied onto the base paper surface using a rod, and mechanical properties such as SCT kN/m (compression strength), burst strength kPa, and tensile strength kN/m were tested.

The findings have revealed that the use of natural components in paper coating alongside starch has increased the SCNT value by 5%, burst strength by 4%, and tensile strength by 5%. Consequently, it enhances the paper's strength and flexibility, thus improving its resistance to breaking.

Key Words : *Coating bio-based additives, mechanical properties*

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CISPLATIN ANALOG WITH PHOTOSWITCHABLE BIOLOGICAL ACTIVITY

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Abstract

Cisplatin is one of the most frequently used oncological drug. It is estimated that every second patient with cancer disease is treated with cisplatin or its analog [1].

The cisplatin activity involves creation cross-links between adjacent and within the same DNA strands [2] thus inhibiting the transcription and translation, ultimately leading to cell death. Unfortunately, treatment with cisplatin is burdened with serious adverse side effects [3]. We have assumed that these sequelae could be avoided or at least limited if cisplatin cytotoxicity in cancer and normal cells could be more spatiotemporally selective.

Recently we have developed a new, photoswitchable analog of cisplatin (*cis*-PtCl₂(PS1)₂). The degree of cytotoxicity of the obtained compound can be controlled - increased or decreased - by selectively irradiating it in the tumor tissue using light with the appropriate wavelength. That new molecule was obtained by replacing two adjacent ammonia ligands in cisplatin with the photosensitive substituents, the so-called photoswitches (PS), which can undergo *trans-cis* and *cis-trans* photoisomerizations on irradiation with light from the visible spectral region of two different wavelengths.

The *in vitro* studies carried out using several types of cancer cells have shown that *cis*-PtCl₂(PS1)₂ containing a photoswitch in the *trans* configuration (i.e., *cis*-PtCl₂(*trans*-PS1)₂) is considerably more cytotoxic than the molecule in which PS1 is in the *cis* configuration (i.e., *cis*-PtCl₂(*cis*-PS1)₂). The results obtained indicated that it is possible to increase or decrease the cytotoxicity of the *cis*-PtCl₂(PS1)₂ complex by irradiating it with a green (530 nm) or blue (400 nm) light, respectively. These new platinum(II) complexes can be especially useful in treating skin malignancies where direct irradiation can be easily realized. One can also consider to apply it to treat the tumors located in such organs where the irradiation can be carried out endoscopically.

Acknowledgments

Authors gratefully acknowledge the financial support from National Science Centre (grant UMO-2021/41/B/NZ7/02484).

Key Words: cisplatin; arylazopyrazole; photoswitch; photopharmacology; anticancer

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OPTIMIZATION OF OZONATION IN THE REMOVAL OF BASIC BLUE 41 IN AQUEOUS SOLUTION

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Abstract

The textile industry is one of the most important industries contributing to national economic growth worldwide. Approximately 10,000 types of dyes and pigments, amounting to over 700,000 tonnes per year, are produced worldwide, of which approximately 20% are assumed to be discharged as industrial waste during textile dyeing processes. The dyeing process uses a lot of water, chemicals, materials, etc. is used. The risk of environmental pollution caused by the textile industry is inevitable due to the unique characteristics of a complex manufacturing industry in which wastewater from the textile industry is used. Many countries face such environmental problems. Textile wastewater is characterized by heavy colors resulting from dyes remaining in the water. In addition to the aesthetic problems caused by colored wastewater reaching natural water resources, dyes strongly absorb sunlight, disrupting the photosynthetic activity of aquatic plants and seriously threatening the entire ecosystem. Moreover, many of these dyes cause health problems such as allergic dermatitis. Some of these dyes are toxic and are suspected of having carcinogenic and mutagenic effects. Pollutants in wastewater can be eliminated by precipitation, advanced oxidation processes (AOPs), biological techniques, adsorption, etc. can be purified by methods. However, dyes do not break down easily and cannot be easily removed from wastewater by conventional wastewater treatment systems [1-4].

This study investigated the feasibility and optimization of ozone (O₃) application to reduce color content in wastewater caused by commercial basic dye (Basic Blue 41). In the laboratory-scale experiment, experimental parameters including pH, ozone dosage, and reaction time were evaluated in a 5 L reactor to obtain optimum operating conditions. The results show that ozone dosage and pH dominate the effectiveness of the decolorization process. The degree of decolorization was primarily proportional to the ozone dosage. The results obtained from this study provide insight into the characteristics and mechanisms of decolorization with the O₃ technique. The results will also help design a system for practical application [5].

Key Words: *Basic Blue 41; Ozonization; Decolorization; Optimization; Removal of textile dye*

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PHOTOPHYSICAL STUDY OF NOVEL ISOTHIOCYANATE DERIVATIVE AS FLUORESCENT LABEL FOR AMINO ACIDS

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Abstract

Biomolecules are often chemically modified by covalent conjugation to examine their structure, molecular interactions, and reaction kinetics to gain insight into their biological functions. Many labeling methods have been developed and are in use, including chemical modification of biomolecules through covalent or non-covalent binding. Isothiocyanates are amine-responsive fluorescent probes that label biomolecules by forming a covalent bond between their isothiocyanate group and the primary and secondary amine groups of the biomolecule. Reactions of isothiocyanates with amino acids are often used in bioanalytical practice. Some isothiocyanates have been used in protein chemistry as reagents for determining the primary structure of peptides and proteins, and in the analysis of amino acids by derivatization with isothiocyanates. Fluorescein isothiocyanate, one such probe, has long been widely used for labeling amino acids, proteins, and peptides due to its high quantum efficiency, conjugate stability and detection sensitivity. Today, conjugation continues to attract research efforts to develop new labels and new methodologies that meet the ever-increasing demands of modern applications for studying biomolecules.

Present work has focused on synthesis, properties and reactions of newly developed benzanthrone-based isothiocyanate with seven natural amino acids. Photophysical parameters of obtained conjugates with used amino have been investigated in details. Considering the fluorescence properties of prepared conjugates the synthesized isothiocyanate seems to be promising for fluorescent labelling purposes.

Key Words: *benzanthrone; isothiocyanate; synthesis; amino acids; fluorescence spectroscopy*

Synthesis of Substituted 4-Methylphenyl-2-Iminothiazolidinone Compounds via One-Pot Method

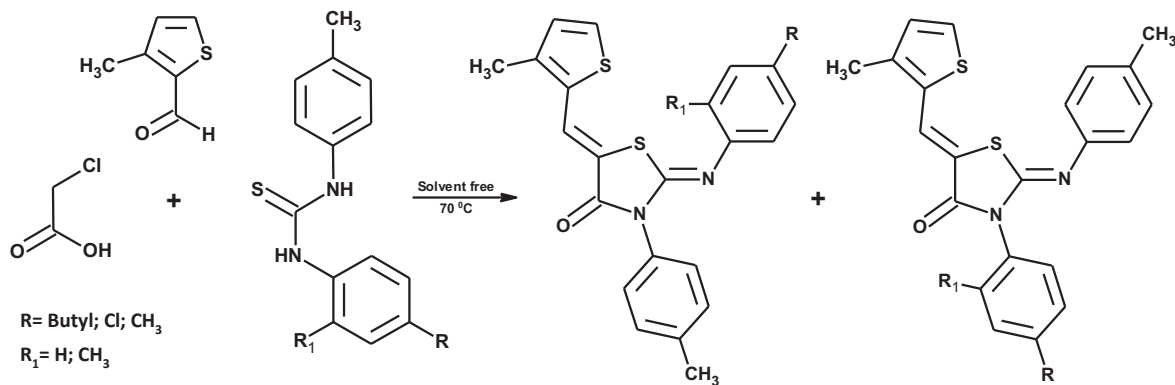
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Abstract

In recent years, iminothiazolidinone derivatives, a class of nitrogen-containing heterocycles, have garnered significant attention in chemical research due to their remarkable biological and pharmacological activities such as antimicrobial, anti-inflammatory, anticonvulsant, antioxidant, antidiabetic, antitumor, and sedative characteristics [1-3]. This study aims to contribute to the field by synthesizing new iminothiazolidinone derivatives with potential biological activity. The synthesis is conducted using a one-pot multicomponent reaction technique, allowing for efficient and cost-effective production of these compounds. The chosen methodology involves a single-step approach, wherein thiourea derivatives, hetaryl aldehydes, and chloroacetic acid are subjected to a one-pot reaction, progressing in a domino-process fashion. This method offers advantages over traditional multi-step organic reactions, ensuring ease of execution within a shorter timeframe and at reduced costs.

The targeted substituted 4-methylphenyl-2-iminothiazolidinone derivatives were obtained through a one-pot multicomponent method, utilizing 3-methyl-thiophene-2-carboxaldehyde, chloroacetic acid, and various aryl-thiourea compounds [4]. Characterization of the synthesized compounds is achieved through a comprehensive analysis utilizing infrared, nuclear magnetic resonance, mass spectral data, and elemental analysis results.



Key Words: Iminothiazolidinone, thiourea, one-pot reaction, multicomponent reaction, solvent free

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THE EFFECT OF ULTRASONIC PRETREATMENT DURATION ON THE DRYING KINETICS OF RED BERRIES

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Abstract

Drying of foods is an ancient preservation method used since the early ages. Since dried foods can be preserved for a long time, they can be used even when there is no production season. Moreover less labour, less equipment, and less costs are required for the storage and transportation of the dried products. In order to improve the product quality, some physical and chemical pretreatments can also be applied prior to the drying process. In this study, the effect of ultrasonic pretreatments is investigated on the drying kinetics of red berries. Red berries (*Ribes rubrum*) are small fruits that are cultivated mainly in Europe. Red berries have an important place in diets for a balanced nutrition, since they are rich in dietary fiber, vitamins and minerals. For instance, red berries have higher vitamin C contents than most of the citrus fruits. However, they are seasonal and perishable fruits with very short shelf lives. Therefore, drying can be used as a way of preserving this important fruit. According to the literature investigations, there is only small amount of study about the drying characteristic and modelling of red berries. The impact of the effects of pretreatments has not been fully covered. For this reason, in this study, the effect of ultrasonic pretreatments on the infrared drying and vacuum oven drying of red berries is investigated. During the experiments, the drying temperatures were selected as 70°C and 80°C. For both methods, experiments were conducted with 30 s - 20 min prior ultrasound pretreatments and the results were compared with the untreated dried sample data. The kinetic parameters of effective moisture diffusivities (D_{eff}) and activation energy (E_a) values were calculated. Moreover, the drying curves were modelled with the most known mathematical modelling equations given in the literature. The drying times were seen to be not greatly affected by the application of the ultrasound pretreatment.

Key Words: Red berry; infrared drying; vacuum oven drying; drying kinetics; ultrasonic pretreatment

Optimization and determination of the factors, influencing on the delamination in Graphene/MoS₂/PET nanocomposite under mechanical loading

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Abstract

The current theoretical study is devoted to the identification of the factors, influencing on the interface shear stress (ISS) and respectively, the possibility of delamination appearing in three-layer nanocomposite structure graphene/MoS₂/PET under mechanical loading. A model criterion for delamination in the structure is proposed and the model ISSs are calculated at different geometry and external loads [1]. Then, a multi-parametric optimization procedure is performed and shows the exact geometrical and external factors, influenced on the ISS value – the layer's thickness, load and length of the considered nanocomposite structure. The obtained results could be used to predict safe design and working conditions in similar nanocomposite devices or parts of them, as sensors, nano- and optical electronic devices, energy devices, etc.

Acknowledgemnets

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Key Words: *Multi-parameter optimization; graphene/MoS₂/PET nanocomposite; interface shear stress; delamination;*

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TAILOR-MADE SYNTHESIS OF CHITOSAN-g-POLY(DIMETHYLAMINO)PROPYLMETHACRYLAMIDE

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Abstract

Chitosan (Cs), which is a linear cationic polysaccharide constituted of β -1,4-D-glucosamine moieties, is frequently used in biomedical applications due to its biocompatibility, nontoxicity, biodegradability, and ease of modification through hydroxyl and primary amine groups [1]. The cationic charge of chitosan provides an effective means of attracting the therapeutics such as DNA and RNA to the target cells. However, as chitosan could only be dissolved in some dilute acid solutions its applications are restrained. In order to overcome the solubility problem and expand its application areas, the hybrid systems of chitosan with mostly cationic synthetic polymers are studied. To obtain well-defined chitosan derivatives, especially controlled polymerization methods such as (reversible addition fragmentation chain transfer) RAFT, atom transfer radical polymerization (ATRP) are used.

In the present work, chitosan chains are functionalized with poly[3-N-(dimethylamino) propylmethacrylamide] (PDMAA) to design a novel graft copolymer which is intended to be used for biomedical applications. PDMAA is a water soluble monomer, which contains pendant tertiary amino groups, and is considered as biocompatible due to hydrophilic amide functionality. PDMAA shows pH responsive behaviour ($pK_a \sim 8.8$) due to tertiary amine groups. Also, they lead to increasing solubility and swelling degrees. PDMAA hold promise for diverse biomedical applications such as targeted drug delivery and gene therapy due to cationic and biocompatible nature [2,3]. To improve the solubility and transfection efficiency of chitosan chains, PDMAA chains with various lengths named as macroCTAs were synthesized via RAFT polymerization (Figure 1a). Chitosan chains with different molecular weights were prepared by potassium persulfate (KPS) degradation. Then, chitosan-graft- poly[3-N-(dimethylamino) propylmethacrylamide] (Cs-g-PDMAA) graft copolymers were synthesized via 1-ethyl-3-(3-dimethyl aminopropyl) carbodiimide/N-hydroxysuccinimide (EDC/NHS) coupling method (Figure 1b). All the chitosans, macroCTAs and graft copolymers with various chain lengths were characterized by ¹H-NMR, FT-IR, UV-visible spectrophotometer, gel permeation chromatography and capillary viscometry methods. Hemolytic activity and buffer capacity tests will be performed to determine their usability for biological applications.

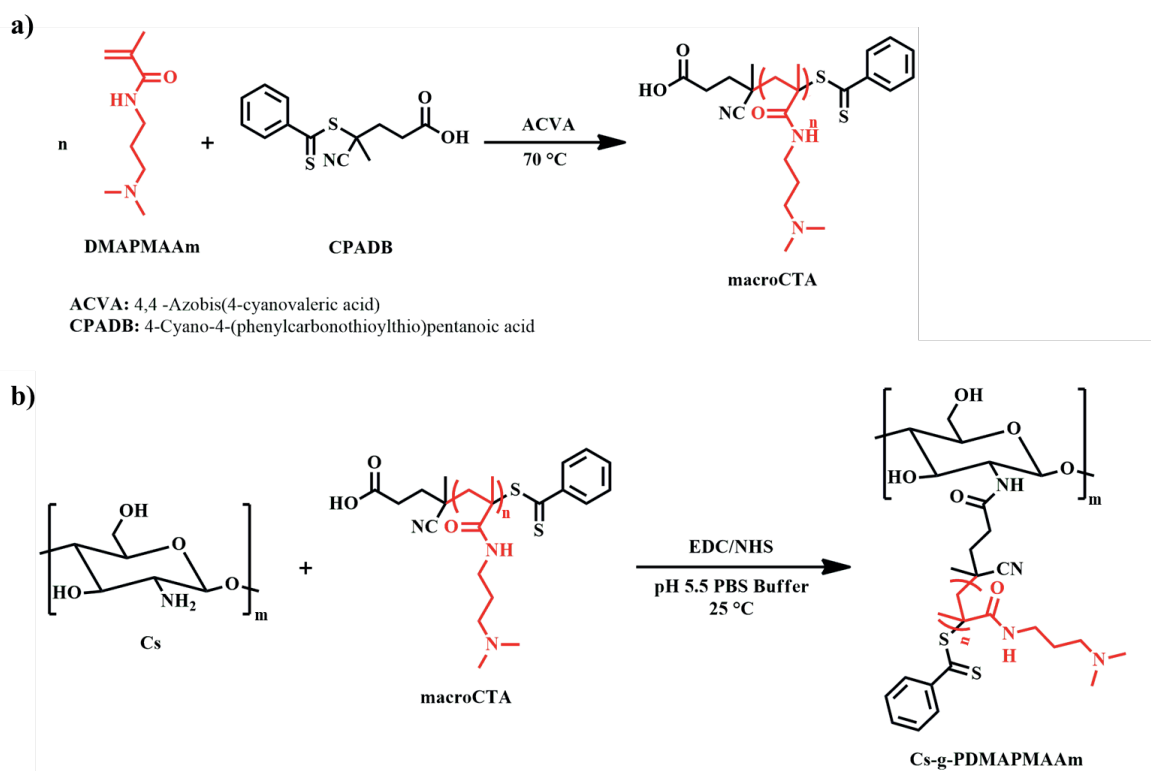


Figure 1: Synthesis of a) PDMPMAAm macroCTA via RAFT polymerization b) Cs-g-PDMPMAAm graft copolymer via EDC/NHS coupling reaction.

Key Words: Chitosan, poly[3-N-(dimethylamino) propylmethacrylamide], RAFT polymerization, CS-g-PDMPMAAm graft copolymers, EDC/NHS coupling reactions

Acknowledgements

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SYNTHESIS AND ELECTROCHEMICAL PROPERTIES OF SOLUBLE COBALT(II) AND COPPER(II) PHTHALOCYANINES

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Abstract

Due to their rich π -electron content, phthalocyanine (Pc) compounds give two characteristic absorption peaks, B and Q, corresponding to $\pi \rightarrow \pi^*$ electronic transitions in the UV and visible region [1]. The first broad peak in the 300-400 nm range is called the B band (Soret) and the sharp peak in the 600-700 nm range is called the Q band. As a result of successive redox reactions in the ring, the HOMO orbital can be oxidized to cationic species by giving multiple electrons, while the LUMO orbital can be reduced to anionic species by taking multiple electrons [2]. The most important problem encountered in phthalocyanines is the low solubility of these compounds. The addition of alkyl, alkoxy, alkylthio chains or bulky groups to the peripheral positions increases the solubility of phthalocyanines considerably. The addition of carboxylic acid or amino groups, as in this study, results in water-soluble phthalocyanines. The synthesis of soluble phthalocyanines gives these compounds new optical, electronic, redox and magnetic properties, increasing their potential use in biology, catalysis and materials [3,4]. In the electrochemical characterization of highly soluble symmetric cobalt(II) and copper(II) phthalocyanine structures which were synthesized for the first time in this study, the reduction and oxidation behaviors of Pc macrocycles were determined by cyclic voltammetry (CV) and square wave voltammetry (SWV) techniques. With the help of these electrochemical properties, the HOMO and LUMO energy levels of both metalphthalocyanines were determined.

Keywords: Phthalocyanine, Synthesis, Electrochemistry, Redox property, Voltammetry

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KINETIC and THERMODYNAMIC INVESTIGATION OF METHYL VIOLET DYE ADSORPTION ON AGAR-AGAR IMPREGNATED ACTIVATED CARBON

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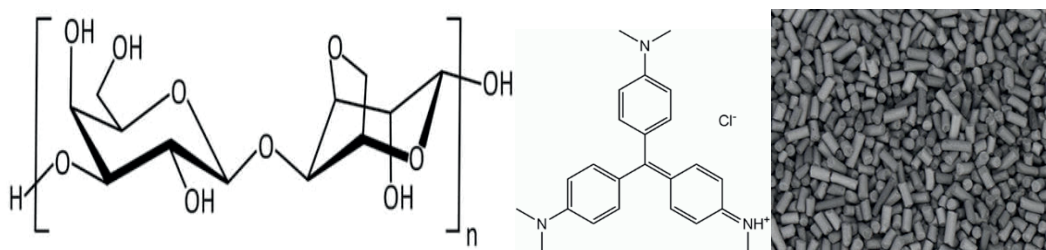
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Abstract

Activated carbons as granular or powdered form are the most widely used sorbents because of their excellent sorption capability for inorganic pollutants. Agar-agar is a porous galactose polymer. Agar-agar impregnated activated carbon (AAC) is biopolymer based adsorbent and has been used successfully to remove Pb^{+2} from water. AAC has also dye removal capacity from waste water [1].

In this current study, AAC was prepared, characterized via FTIR-ATR and used for the adsorption of methyl violet (MV) dye (Scheme 1) from synthetic waste water. The effects of different reaction parameters such as the initial MV concentration, contact time and solution temperature on the adsorption of MV onto AAC at constant adsorbent dose were investigated. To determine the best adsorption equilibrium and adsorption kinetic data of MV adsorption on AAC were applied such as Freundlich, Langmuir and Temkin models for equilibrium, the pseudo-first-order, the pseudo second order and Intraparticle diffusion models for kinetic. Then, some adsorption thermodynamic parameters of MV on AAC were also determined.



Scheme 1 The chemical structure of Agar-Agar, Methyl Violet Dye and image of Activated Carbon

Key Words: Methyl Violet Dye; Agar-Agar impregnated Activated Carbon; Dye removal; Kinetic and Thermodynamic parameters

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Determination of Macro and Micro Element Contents in Thyme Oil and Rosemary Oil by ICP-OES

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Abstract

Essential oils are defined as a complex mixture of natural compounds that contain unsaturated and saturated phenols, aldehydes, hydrocarbons, alcohols, and terpenes. Thyme oil, obtained by steam distillation from the perennial plant and its flowers known as *Thymus vulgaris*, has antioxidant, antiseptic, antibacterial, antifungal and calming properties. It has been used as a medicinal plant since ancient times. It is also used as a preservative in foods and cosmetics. Rosemary (*Rosmarinus officinalis* L.) is one of the most preferred natural sources for drug active substances. Rosemary oil is a natural oil obtained from the leaves and flowers of the rosemary plant. Rosemary oil has antibacterial and antioxidant properties. In addition, It is stated that rosemary oil is among the plants that the body supports in protecting against cancerous cell formation.

The content of elements (Cu, B, P, Fe, Na, Mg, K, Ca) in commercial thyme and rosemary oils was determined using inductively coupled plasma optical emission spectrometry (ICP-OES) after wet digestion. 0.5 gram sample was weighed and HNO₃-H₂O₂ (10 ml, 2:1, v/v) was added. The oil samples were heating of oil samples at 80 °C until clear solutions are achieved. Additionally, the method was validated with accuracy, precision, linearity, recovery, LOD (Limit of Detection) and LOQ (Limit of Quantification) parameters. The lowest metal content was found Fe (0.68 mg/kg) while the highest metal content was observed P (100.73 mg/kg) in thyme oil. For rosemary oil, the lowest metal content was found Mg (0.15 mg/kg) while the highest metal content was observed P (220.98 mg/kg).

Key Words: *Thyme oil; Rosemary oil; ICP-OES, Essential oil, Wet digestion*

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METHYL VIOLET DYE ADSORPTION STUDY ON SUBMICRON PARTICLE SIZE RUBBER POWDER OBTAINED FROM SCRAP TYRE AND FUNCTIONALIZED WITH AGAR-AGAR

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Abstract

Adsorption process is the process of separating chemical substances that cause pollution such as toxicity, color and odor, which are difficult to purify with classical purification, by adhering to the surface of an adsorbent solid material (adsorbent) with chemical and physical bonds. The adsorption process is affected by pH, temperature and the surface area of the adsorbent used. [1] Lots of adsorbents such as activated carbon, date seed, wood, zeolite, some waste sources such as scrap tyre, plant have been used to treat and to remove dye from wastewater.[2]

In this study, submicron particle size rubber powder adsorbent obtained from scrap tyre and functionalized with agar-agar (RP-AA) was prepared from waste tyre, functionalized with agar-agar to use removal of methyl violet (MV) dye from synthetic wastewater. The effects of different reaction parameters such as the initial MV concentration, contact time and solution temperature on the adsorption of MV onto RP-AA at constant adsorbent dose were investigated. To explain the adsorption character of MV adsorption on RP-AA were applied some kinetic models and calculated thermodynamic adsorption parameters.

Key Words: *Scrap tyre; Methyl Violet Dye; Agar-Agar; Adsorption Parameters*

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Determination of Trace and Major Element Contents in Commercial Propolis Samples by ICP-OES After Microwave Digestion

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Abstract

Propolis is a partially digested bee product obtained by honey bees (*Apis mellifera* L.) by adding salivary enzymes (β -glucosidase) to the resin they collect from shoots, leaves, buds and bark cracks in trees and plants and mixed with beeswax [1]. There are more than 300 compounds in the structure of propolis [1]. The structure of propolis includes phenolic compounds (flavonoids and phenolic acids), benzoic acid and its derivatives, cinnamic alcohol, cinnamic acid and its derivatives, monoterpenes, diterpenes, triterpenes and sesquiterpenes and their alcohol and benzaldehyde derivatives, alcohols, sugars, ketones, heteroaromatic compounds, aliphatic hydrocarbons, minerals, steroid hydrocarbons and amino acids [2]. Studies have reported that propolis has anti-inflammatory, antihepatotoxic, anticancer, antiviral and antibacterial activities [3].

This study aims to determine the concentrations of sodium (Na), magnesium (Mg), potassium (K), calcium (Ca), phosphorus (P), iron (Fe), copper (Cu), boron (B), manganese (Mn), zinc (Zn) and aluminum (Al) in commercial propolis drop products by using Inductively Coupled Plasma Optical Emission Spectrometer (ICP-OES). For microwave digestion method, 1 mL of propolis samples in reaction vessels directly, added to each flasks 9 mL concentrated HNO₃. The method was validated for accuracy, precision, linearity, recovery, LOD (Limit of Detection) and LOQ (Limit of Quantification) parameters. The recovery percentages are in the range from 69.67 to 104.05% in propolis samples.

Key Words: *Propolis; Microwave digestion; ICP-OES, Food supplement, Spectroscopy*

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REMOVAL of PENICILLIN GROUP AZLOCILLIN, CLOXACILLIN, METHICILLIN ANTIBIOTICS FROM WASTE WATER BY DFT METHOD

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Abstract

Antibiotics taken by living things are excreted in the living metabolism either unchanged or with little conversion. Discarded antibiotic residues may not be treated in conventional wastewater treatment plants and may enter the receiving environment directly. Low concentrations of antibiotic residues in the receiving environment may cause increased resistance of microorganisms, and high concentrations may cause toxic effects. For this reason, wastewater containing antibiotic residues must be treated. The possible reactions of the penicillin group antibiotic compounds to be studied will be investigated by the DFT method, which is the Molecular Modeling Method, and will be stated computationally. The penicillin group antibiotic molecules studied are Azlocillin, Cloxacillin and Methicillin compounds, respectively. No study has been done with this method before on the molecules studied. Optimized geometries were drawn with Gauss View 5.0, and then geometric optimization was carried out using the Gaussian 09W program using Functional Density Theory (DFT) and Hartree-Fock methods. The geometrical structure (bond angles and bond lengths) of all three molecules and their possible degradation products were calculated at the level of B3LYP theory within the Hartree-Fock (HF) method and density function theory (DFT) in the basic set of 6-31G(d). Thus, the possible degradation mechanisms of these three pesticide molecules in water were determined. These results will guide experimental studies.

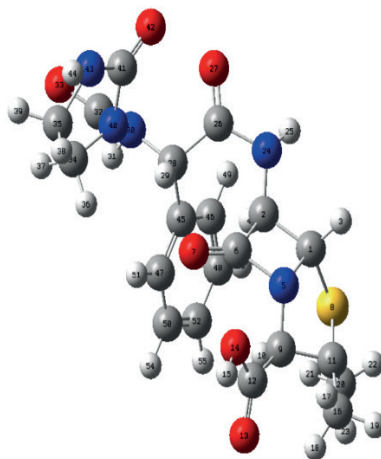


Figure 1. Optimized state of the same Azlocillin molecule (Grey, C; white, H; blue, N; red, O; yellow, S).

Key Words: Antibiotics, Azlocillin, Kloxacillin, Methicillin, Gaussian09, DFT

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