11th ICNTC CONFERENCE
INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

11th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY
25 – 27 APRIL 2025

11th ICNTC BOOK OF ABSTRACTS

25 – 27 APRIL 2025 BOLOGNA – ITALY

International Conference on New Trends in Chemistry

11th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY
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http://www.icntcconference.com/

ICNTC Conference 2025

11th International Conference on New Trends in Chemistry

Published by the ICNTC Secretariat
Editor:
Prof. Dr. Dolunay ŞAKAR

ICNTC Secretariat
Büyükdere Cad. Ecza sok. Pol Center 4/1 Levent-İstanbul
E-mail: icntcconference@gmail.com
http://www.icntcconference.com

Conference organised in collaboration with Monre Academy

ISBN:978-605-73406-5-8

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Conference Chair

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Chemistry Department

Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of " **11th International Conference on New Trends in Chemistry**", to be held in Bologna, ITALY on the dates between April 25- 27 , 2025

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

- Analytical Chemistry
- Bio Chemistry
- Computational Chemistry
- Chemistry Education
- Environmental Chemistry
- Food Chemistry
- Forensic chemistry
- Inorganic Chemistry
- Material Chemistry
- Organic Chemistry
- Physical Chemistry
- Polymer Chemistry and Applications
- Pharmaceutical Chemsitry

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 25-27 April 2025,

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
11th ICNTC 2023 | Conference Chair
Yıldız Technical University – Istanbul / Türkiye
Chemistry Department

25 APRIL 2025 FRIDAY

MADRID MEETING ROOM

Welcome Speech / 09:00 – 09:10

Prof. Dr. Dolunay ŞAKAR / Conference Chair
Yıldız Technical University - Istanbul , Turkiye

Keynote Speech / 09:10 – 09:40

Prof. Dr. Julia LU
Toronto Metropolitan University, Canada

Speech Title: Artificial Intelligence (AI) in Chemistry in Higher Education

SESSION A (09:40 – 10:40)

SESSION CHAIR: Prof. Dr. Sevil YÜCEL

MADRID MEETING ROOM

09:40 – 10:00
PAPER TITLE : Catalytic Cycloaddition of Carbon Dioxide and Epoxides by Chloro-Iron and Cobalt Complexes with Functionalized Quadridentate Ligands: Structural Effect and DFT Calculation
AUTHOR(S) : **Adnan S. Abu-SURRAH**, Haitham H. Al-SA'DONI, Hamzeh M. ABDEL-HALIM, Khaleel I. ASSAF

10:00 – 10:20
PAPER TITLE : Determining the Tracer Performance of $ZnFe_2O$**4** Modified with Different Costing Agents for Magnetic Particle Imaging
AUTHOR(S) : Gülsüm ÇALIŞKAN, Muhammad IRFAN, **Nurcan DOGAN**

10:20 – 10:40
PAPER TITLE : Rational Protacs Design by Modelling the Ternary Complex Formation
AUTHOR(S) : **Tommaso D'ANGELI**, Massimo BARONI, Tommaso PALOMBA, Gabriele CRUCIANI

TEA & COFFEE BREAK 10:40 – 11:00

25 APRIL 2025 FRIDAY

SESSION B (11:00 – 12:40)

SESSION CHAIR: Prof. Dr. Nurcan DOĞAN

MADRID MEETING ROOM

11:00 – 11:20
PAPER TITLE : Production of 48S Bioactive Glasses Enriched with Various Metal Ions and Evaluation of Their Bioactivity Properties
AUTHOR(S) : **Sevil YÜCEL**, Gözde KELEŞ, Ali Can ÖZARSLAN, Cem ÖZEL, İlkay Turhan KARA, Mine KUCAK

11:20 – 11:40
PAPER TITLE : The Efficiency of Cadmium Extraction from Various Soil Types and Model Systems with the Selected Environmental Friendly Chelators
AUTHOR(S) : **Pawel MISKOWIEC**, Anna STREKALOVSKAYA

11:40 – 12:00
PAPER TITLE : Enhanced Ultrafiltration Membranes: Fabrication of Polysulfone Membranes with Functionalized TiO_2 Nanotubes for Superior Permeability and Fouling Resistance
AUTHOR(S) **: Ibrahim Hotan ALSOHAIMI**

12:00 – 12:20
PAPER TITLE : Development of the Injectable Bone Grafts
AUTHOR(S) : **Cem ÖZEL**, Ali Can ÖZARSLAN, Sevil YÜCEL

12:20 – 12:40
PAPER TITLE : Encapsulating Bergamot and Ginger Essential Oils in Binary Blends of Zein and Casein Polymers
AUTHOR(S) : Cansu NAYIR, **Yasar Andelib AYDIN**

LUNCH BREAK 12:40 – 13:20

13:30 Departure from Conference Venue for Florence Tour and Conference Dinner

23:30 Back to Hotel After Conference Dinner & Tour

26 APRIL 2025 SATURDAY

SESSION C (09:00 – 10:40)

SESSION CHAIR: Assoc. Prof. Dr. İlknur KÜÇÜK

MADRID MEETING ROOM

Session C & D are parallel sessions!

09:00 – 09:20
PAPER TITLE : Computational Evaluation of Cymenes: Substituent Group Effect, Pharmacokinetics and Drug-likeness
AUTHOR(S) : **Goncagül SERDAROĞLU**

09:20 – 09:40
PAPER TITLE : Theoretical Examination of Paroxetine Hcl, the Active Ingredient of the Drug Marketed As Paxil, Used in Antidepressant Treatment, Using the Dft Method
AUTHOR(S) : **Bahar EREN**, Yelda YALCIN GURKAN

09:40 – 10:00
PAPER TITLE : Synthesis and Characterization of Copper (II) Complex and Its Catalytic Activity on C(sp^3)-H Oxidation Reactions
AUTHOR(S) : **Yalçın KILIÇ**, İbrahim KANİ

10:00 – 10:20
PAPER TITLE : Investigation of the Degradation Reaction Kinetics of Cefalexin by Hydroxyl Radical
AUTHOR(S) : **Seyda AYDOGDU**, Arzu HATIPOGLU

10:20 – 10:40
PAPER TITLE : Pesticides in Albanian Vegetable Farming: Challenges and Strategies for Sustainable Agriculture
AUTHOR(S) : **Matilda LIKAJ**, Elda MARKU, Ridvana MEDIU, Jonida TAHIRAJ, Sonila SHEHU

TEA & COFFEE BREAK 10:40 – 11:00

26 APRIL 2025 SATURDAY

SESSION D (09:00 – 10:40)

SESSION CHAIR: Prof. Dr. Azmi Seyhun KIPÇAK

OSLO MEETING ROOM

Session C & D are parallel sessions!

09:00 – 09:20
PAPER TITLE : Challenges in Icp-ms Analysis of Elemental Impurities in Pharmaceutical Products: Methodological and Analytical Considerations
AUTHOR(S) :**Biljana BALABANOVA**

09:20 – 09:40
PAPER TITLE : Development of a High-performance Liquid Chromatography (hplc) Method for Coumarin Quantification in Medicinal Plants Via Soxhlet Extraction
AUTHOR(S) : Sinan ŞİMŞEK, **Emel AKYOL**, İlknur KÜÇÜK

09:40 – 10:00
PAPER TITLE : Hydrogen Production from Sodium Borohydride in Continuous Hydrolysis Systems: the Effect of Recirculation
AUTHOR(S) : Emine ÇİFTÇİ, Ayça TÜKENMEZ, Esra BALKANLI ÜNLÜ, **Halit Eren FİGEN**

10:00 – 10:20
PAPER TITLE : Valorisation of Polycationic Metals from Acid Mine Drainage for Sustainable Wastewater Treatment: a Circular Economy Approach
AUTHOR(S) : Khathutshelo Lilith MUEDI, Job Tatenda TENDENEDZAI, Vhahangwele MASINDI, Nils Hendrik HANEKLAUS, **Hendrik Gideon BRINK**

10:20 – 10:40
PAPER TITLE : Assessment of the Effects of Iron (III) Oxide Nanoparticles and Iron (III) Chloride on Glutathione Reductase Activities
AUTHOR(S) **: Hasan KARADAĞ**, Özge FIRAT

TEA & COFFEE BREAK 10:40 – 11:00

26 APRIL 2025 SATURDAY

SESSION E (11:00 – 12:40)

SESSION CHAIR: Prof. Dr. Aysel KANTÜRK FİGEN

MADRID MEETING ROOM

Session E & F are parallel sessions!

11:00 – 11:20
PAPER TITLE : Utilization of Inductively Coupled Plasma (ICP) in Monitoring and Analysis of Some Heavy Metals in Jordanian Dams
AUTHOR(S) : **Ayman A. ISSA**, Mohammad H. ZAHLAN

11:20 – 11:40
PAPER TITLE : Effect of Different Drying Technics on Drying Characteristics of Celeriac
AUTHOR(S) : Cansın KURT, **İlknur KÜÇÜK**, İbrahim DOYMAZ

11:40 – 12:00
PAPER TITLE : Life Cycle Assessment of Magnetic Carbon Based Adsorbant Synthesis
AUTHOR(S) : **Berfin Ekin ÜLGEN**, Zeynep TAŞ, Muhammed İberia AYDIN, Bilge COŞKUNER FİLİZ, Aysel KANTÜRK FİGEN

12:00 – 12:20
PAPER TITLE : Application of Gas Foaming Technique for Improving Porous Properties of Chitosan-polyvinyl Alcohol (cs-pva) Nanofiber Based Biodegradable Scaffolds
AUTHOR(S) : **Gizem ÖZDEMİR**, Demetnur ERKOYUNCU, Aysel KANTÜRK FİGEN

12:20 – 12:40
PAPER TITLE : Improved Biobutanol Recovery Through Mixed-matrix Pvdf Membrane with Hydrophobic Maf-6 As Filler
AUTHOR(S) : Rüveyda ÖZDEMİR, **Derya ÜNLÜ**

LUNCH BREAK 12:40 – 13:20

26 APRIL 2025 SATURDAY

SESSION F (11:00 – 12:40)

SESSION CHAIR: Prof. Dr. Goncagül SERDAROĞLU

OSLO MEETING ROOM

Session E & F are parallel sessions!

11:00 – 11:20
PAPER TITLE : Blanching and Osmotic Dehydration Effects on Lyophilised Shrimp
AUTHOR(S) : Zehra Özden ÖZYALÇIN, **Azmi Seyhun KIPÇAK**

11:20 – 11:40
PAPER TITLE : Nanomaterial-modified Carbon Paste Electrode-based Biosensor for the Investigation of Apigenin in Real Samples
AUTHOR(S) : Said Nur KAYRAN, **Hasret SUBAK**

11:40 – 12:00
PAPER TITLE : Eucalyptol-based Liquid-liquid Microextraction Coupled with Gas Chromatography for the Determination of Phthalates in Bottled Water Samples
AUTHOR(S) : **Natalia JATKOWSKA**

12:00 – 12:20
PAPER TITLE : Synthesis, Characterization, and Usage of Graphitic Carbon Nitride (g-C_3N_4) Species in pH-Controlled Drug Delivery
AUTHOR(S) : **Ümran GÜNTER,** Esra Maltas ÇAĞIL,Talha KURU, Emre ASLAN, Imren HATAY PATIR

12:20 – 12:40
PAPER TITLE : A Novel Perspective on Lateral Flow Assays: Fluorescence Protein-peptide Aptamers
AUTHOR(S) : Canan ÖZYURT, Serap EVRAN, Burhan BORA, İnci ULUDAĞ ANIL, **Mustafa Kemal SEZGİNTÜRK**

LUNCH BREAK 12:40 – 13:20

26 APRIL 2025 SATURDAY

SESSION G (13:20 – 15:00)

SESSION CHAIR: Prof. Dr. Emel AKYOL

MADRID MEETING ROOM

Session G & H are parallel sessions!

13:20 – 13:40
PAPER TITLE : Evaluation of Smart Packaging Functions of Black Carrot Extract with Polysaccharide-based Films
AUTHOR(S) : **Özde İPSALALI**, Filiz UĞUR NİGİZ

13:40 – 14:00
PAPER TITLE : In Silico Insight on Hyaluronic Acid and Boron-hyaluronate
AUTHOR(S) : **Goncagül SERDAROĞLU**, Melda BOLAT, Dursun Ali KÖSE, Zekeriya ÖZTEMÜR, Nihat KARAKUŞ

14:00 – 14:20
PAPER TITLE : Infrared Drying of Aronia Berries: the Effect of Sustainable Pretreatments on Drying Behavior
AUTHOR(S) : Berfin SALIK, Ata TAN, **Ekin KIPÇAK**

14:20 – 14:40
PAPER TITLE :The Impact of Metal Industry Waste on the Agricultural Development and Yield Increase of Tea Plants
AUTHOR(S) : Burcu Didem ÇORBACIOĞLU, **İlknur KÜÇÜK**

14:40 – 15:00
PAPER TITLE :Synthesis, Characterization and Photocatalytic Performance Of Modified $Cd_{0.7}Zn_{0.3}S$
AUTHOR(S) : İbrahim KABA, **Özge KERKEZ KUYUMCU**

TEA & COFFEE BREAK 15:00 – 15:30

26 APRIL 2025 SATURDAY

SESSION H (13:20 – 15:00)

SESSION CHAIR: Assoc. Prof. Dr. Halit Eren FİGEN

OSLO MEETING ROOM

Session G & H are parallel sessions!

13:20 – 13:40
PAPER TITLE : Evaluation of Different Fillers on Glass Fiber Reinforced Polymer Composites for the Automotive Industry
AUTHOR(S) : **Miray ÖZBAKIŞ**, Pınar TERZİOĞLU

13:40 – 14:00
PAPER TITLE : Mechanical Performance of Glass Fiber / Polyester Composites Containing Biofiller for the Automotive Applications
AUTHOR(S) : Miray ÖZBAKIŞ, **Pınar TERZİOĞLU**

14:00 – 14:20
PAPER TITLE : Obtaining Valuable Components from Various Citrus Product Wastes by Different Extraction Methods
AUTHOR(S) : **Deniz UYGUNÖZ**, Gamzenur ÇİFÇİ, Özgür Ozan DEMİRCİ, Emek MÖRÖYDOR DERUN

14:20 – 14:40
PAPER TITLE : Fabrication and Filtration of Arabic Gum Doped Electrospun Pla Membrane for Rejection of Gray Water Pollutants
AUTHOR(S) : **Seniyecan KAHRAMAN**, Ayşenur KATIRCI, Filiz UĞUR NİGİZ

14:40 – 15:00
PAPER TITLE : Green Tea-boron Nitrite Incorporated Pumpkin Pectin-alginate Food Packaging Film Preparation and Characterization
AUTHOR(S) : **Özde İPSALALI**, Filiz UĞUR NİGİZ

TEA & COFFEE BREAK 15:00 – 15:30

26 APRIL 2025 SATURDAY

SESSION I (15:30 – 17:10)

SESSION CHAIR: Assoc. Prof. Dr. Pınar TERZİOĞLU

MADRID MEETING ROOM

Session I & J are parallel sessions!

15:30 – 15:50

PAPER TITLE : The Effect of Modifiers on the Microstructure of Road Bitumen and Strength of Asphalt Concrete

AUTHOR(S) : **Yuliya BYZOVA,** Antonina Dyuryagina, Kirill Ostrovnoy, Tatyana Shirina

15:50 – 16:10

PAPER TITLE : Electrospun CuMOF/PLA Nanofibers as Biodegradable Antibacterial Membranes for Biomedical Applications

AUTHOR(S) : **Bilge Nur MEKTEPLİ**, Dilek DALGAKIRAN, Sennur DENİZ

16:10 – 16:30

PAPER TITLE : Development of L-asparaginase-enzyme Immobilized Cu(ii)-nanoparticles and Characterization of Binding Process Via Spr Sensor

AUTHOR(S) : **Monireh BAKHSHPOUR-YÜCEL**, Kübra KAYA, Samir Abbas Ali NOMA, Bilgen OSMAN

16:30 – 16:50

PAPER TITLE : Anticancer Drug Release from Graphene Oxide/bacterial Celluloses

AUTHOR(S) : **Melike KÜÇÜK**, Monireh BAKHSHPOUR-YÜCEL, Sine ÖZMEN TOĞAY, Emel T AMAHKAR IRMAK, Elif TÜMAY ÖZER, Bilgen OSMAN

16:50 – 17:10

PAPER TITLE : $NiCo_2O_4$/S,N-Codoped Graphene Oxide/Nafion/GCE Nanocomposite Electrode Material for Energy Storage Applications

AUTHOR(S) **: Nilüfer KOÇYİĞİT**, Melih Beşir ARVAS

TEA & COFFEE BREAK 17:10 – 17:45

26 APRIL 2025 SATURDAY

SESSION J (15:30 – 17:30)

SESSION CHAIR: Asst.Prof.Dr.Ekin KIPÇAK

PARIS MEETING ROOM

Session I & J are parallel sessions!

15:30 – 15:50
PAPER TITLE : Investigating the Properties of Recycled and Virgin Poly (ethylene terephthalate) Textured Yarns: Effect of Different Blending Ratios
AUTHOR(S) : **Simay ÖZBAKIŞ**, Ayça AYDIN, Pınar TERZİOĞLU

15:50 – 16:10
PAPER TITLE : Freeze Drying of Squid: A Study to Investigate the Effect of Different Pre-Treatments
AUTHOR(S) : **Zehra Özden ÖZYALÇIN**, Azmi Seyhun KIPÇAK

16:10 – 16:30
PAPER TITLE : Drug Analysis With Molecularly Imprinted Polymers From Ion Pair Complexes
AUTHOR(S) : **Ayşegül GÖLCÜ**

16:30 – 16:50
PAPER TITLE : Investigation of Metal Organic Framework Based Electrodes for Flow Capacitive Deionization Systems
AUTHOR(S) : Eren ÖZBAY, Ali Furkan ALBORA, Sadullah ÖZTÜRK, Arif KÖSEMEN, **Şahika Sena BAYAZIT**

16:50 – 17:10
PAPER TITLE : Development and Validation of HPLC Method Using Multivariate Optimization for the Simultaneous Determination of Niflumic Acid and Its Impurities
AUTHOR(S) : **Evridiki PİNGO**, Bürge AŞÇI

17:10 – 17:30
PAPER TITLE : Spectrophotometric Kinetic Assessment of Ruthenium (III) Catalyzed Oxidation of Aspirin by Hexacyanoferrate (III) in Alkaline Medium - A Mechanistic Pathway
AUTHOR(S) : Beena GUPTA, **Riya SAILANI**

TEA & COFFEE BREAK 17:30 – 17:45

26 APRIL 2025 SATURDAY

POSTER SESSION K (17:45 – 18:30)

SESSION CHAIRS: Prof. Dr. Julia LU, Prof. Dr. Sevil YÜCEL, Prof. Dr. Ayşegül GÖLCÜ

OSLO MEETING ROOM

Session K & L are parallel sessions!

PAPER TITLE : A New SPE Method Based on Polymeric Sorbent for the Determination of Organophosphorus Pesticides
AUTHOR(S) : **Gülfere ARSLAN**, Melike KÜÇÜK, Bilgen OSMAN, Elif TÜMAY ÖZER

PAPER TITLE : Development of Carbon Electrodes for Capacitive Deionization (cdi) Process
AUTHOR(S) : **Demet AÇIKGÜL**, Dilek DURANOĞLU DİNÇER

PAPER TITLE : New Environmentally Friendly Approach to Speciation Analysis of Selenium in Environmental Waters
AUTHOR(S) : **Malgorzata GRABARCZYK**, Cecylia WARDAK, Marzena FIALEK, Edyta WLAZLOWSKA

PAPER TITLE : Photocatalytic Degradation of Methylene Blue by Using Magnetic Photocatalyst
AUTHOR(S) : **Zeliha Betül KOL**, Dilek DURANOĞLU DİNÇER

PAPER TITLE : Removal of Oncology Group Epirubicin and Methotrexate Drugs from Wastewater by Dft Method
AUTHOR(S) : Mustafa Ernur BİLTEKİN, Burak GÜRKAN, **Yelda YALÇIN GÜRKAN**

PAPER TITLE : Synthesis of Hard Carbon from Different Biomass Sources As Electrode Material for Energy Storage Systems
AUTHOR(S) : **Derya ALTINTAŞ**, Yüksel BAYRAM, Murat ATEŞ, Ozan YÖRÜK

PAPER TITLE : Unlocking Soil Health: Carbon Determination in Agricultural Soils
AUTHOR(S) : **Biljana BALABANOVA**, V. ILIEVA, S. MITREV, K. PANEV, I. DONEV, A. PIPEREVSKI

PAPER TITLE: CO_2 As A Building Block İn The Synthesis Of Steroidal Oxazolidinones
AUTHOR(S) : **David ISPAN**, Aron KÜZDÖ, Reka GECSE, Rita SKODA-FÖLDES

PAPER TITLE : New Methoxy And Hydroxy Substituted Pyridyl Benzamides As Potential Ph Sensors
AUTHOR(S) : **Antonija MAMIC**, Robert VIANELLO, Kristina BUTKOVIC, Iva KULUSIC and Marijana HRANJEC

PAPER TITLE : The Effect of Alkali Pretreaments on the Drying Kinetics Of Blueberries
AUTHOR(S) : Beril GÜNORAL, Buse BEŞİKCİ, **Ekin KIPÇAK**

PAPER TITLE : Synthesis and Spectroscopic Investigation of Host-Guest Interactions in Ferrocenylpyrimidines
AUTHOR(S) : **Mark VARADI**, Matyas J. GAZSI, Rita SKODA-FÖLDES

PAPER TITLE: Preparation of 2-Oxazolidinone Derivatives Using Carbon Dioxide as C1 Building Block in Ionic Liquid Solvent
AUTHOR(S) : **Donat Adrian GACOV**, Rita SKODA-FOLDES

PAPER TITLE: Capillary Electrophoresis and Chemometrics
AUTHOR(S) : Andreas ZEMANN

PAPER TITLE Development and Validation of a RP-HPLC Method for Simultaneous Determination of Chlorhexidine Gluconate, Benzydamine Hydrochloride, and Cetylpyridinium Chloride
AUTHOR(S) : Gülşah ÇEBİ, **Evridiki PİNGO,** Bürge AŞÇI

PAPER TITLE:"Computational Study of Natural Substances in the Active Principles of Drugs: Reaction Between Berberine and Cisplatin – DFT and QSAR Investigations"
AUTHOR(S) : **BENSIRADJ Nour El Houda**, KARICHE Sihem, TIDJANI-RAHMOUNI Nabila

26 APRIL 2025 SATURDAY

POSTER SESSION L (17:45 – 18:30)

SESSION CHAIR: Prof.Dr. Adnan S. Abu-SURRAH, Prof.Dr.Emel AKYOL, Assoc.Prof.Dr.İlknur KÜÇÜK

MADRID MEETING ROOM

Session K & L are parallel sessions!

PAPER TITLE : Farma-bant: Obtaining a Wound Covering Membrane from Calendula Officinalis, Centella Asiatica and Carthamus Tinctorius Plant Extract Mixtures
AUTHOR(S) : **Merve Duru EVCİMEN**, Öznur YAŞA ŞAHİN

PAPER TITLE : An Overview on Chemical Profile of Salvia Officinalis Population from Llogara Mountain Area, South Albania
AUTHOR(S) : **Jonida SALIHILA**, Edvina ÇIPI, Aida DAMA, Kleva SHPATI, Aurora NAPUCE, Aurel NURO

PAPER TITLE :Calculation of Electronic Properties of Adrenaline, Dopamine, Melatonin, and Serotonin Using Dft
AUTHOR(S) :Barış KOÇANA, Şeyda AYDOĞDU, **Arzu HATİPOĞLU**

PAPER TITLE :Cucurbit[10]uril Binding of Heteroleptic Iridium(iii) Complexes : Synthesis and Photophysical Characterization
AUTHOR(S) :**Lubna ALRAWASHDEH**, Khaleel I. ASSAF, Shoruq MARABEH, Lynne WALLACE, Anthony DAY

PAPER TITLE :Determination of Fatty Acid Composition of Some Plant Oils and Solid Soap Production with These Oils
AUTHOR'S :**Temine SABUDAK**, Elif OZCAN

PAPER TITLE : Modification of Some Bioorganic Products with Organosilicon Compounds for Use in Industrial Production
AUTHOR'S : **Lali TABATADZE**, Darejan IREMASHVILI, Qetevan EBRALIDZE, Irine BOTCHORISHVILI, Natia SHENGELIA

PAPER TITLE :New Trends in Design of Potentiometric Sensors
AUTHOR(S) : **Cecylia WARDAK,** K. MORAWSKA, M. GRABARCZYK

PAPER TITLE :The Inhibitory Effect of Hicaz Pomegranate Peel Extract on Enzymatic Browning in Potatoes: a Natural Solution
AUTHOR(S) : **Hatice PALÜZAR,** Şebnem MUTLU, Aysen SUEKİNCİ YILMAZ, Şebnem SELEN İŞBİLİR

PAPER TITLE : Ring Opening Copolymerization of Exoxides with CO2 and Organic Anhydrides Promoted by Dinuclear [OSSO]-type Metal Complexes
AUTHOR(S) : **Fatemeh NIKNAM**

PAPER TITLE : Synthesis and Biological Activity of New Benzoxazole Iminocoumarines As pH Sensors
AUTHOR(S) : **Marina GALIC,** Robert VIANELLO, Leentje PERSONS, Dirk DAELEMANS, Mihailo BANJANAC, Tea BRUKETA, Ela GASPARIC and Marijana HRANJEC

PAPER TITLE: Synthetic Flavonoid BrCl-flav-an Alternative Solution to Combat ESKAPE Pathogens
AUTHOR(S) : **Laura Gabriella SARBU**

PAPER TITLE : Dibenzofuran and Dihydrobenzodioxin-Based Hosts for Improved Stability Blue TADF OLEDs
AUTHOR(S) : **Eigirdas SKUODIS**, Goda GRYBAUSKAITE, Kristupas BAGDONAS, Domantas BERENIS, Dovydas BANEVICIUS, Gediminas KREIZA, Karolis KAZLAUSKAS

PAPER TITLE : Design of an Electrochemical Biosensing Platform Based on Metal-Doped Carbon Quantum Dots for Detecting Gastric Cancer-Related Genes
AUTHORS : **Dilek ÖZTÜRK**, Mahmut DURMUŞ

PAPER TITLE : The Cytotoxic Properties of Some Tricyclic 1,3-Dithiolium Flavonoids
AUTHORS : **Mihail Lucian BIRSA**

PAPER TITLE **:** Adsorption Investigation of Disperse Orange 30 Dye on H_2SO_4 Functionalized Activated Carbon
AUTHOR(S) : Kübra TOPAÇ, Hüsnü Kemal GÜRAKIN, **Dolunay ŞAKAR**

PAPER TITLE **:** Kinetic Studies of Disperse Orange 30 Dye Removal via H_2SO_4-Activated Scrap Tyre Particles
AUTHOR(S) : Sinem KARAGÖZ, Hüsnü Kemal GÜRAKIN**, Dolunay ŞAKAR**

27 APRIL 2025 SUNDAY

SOCIAL PROGRAM

Contents

Artificial intelligence (AI) in Chemistry in higher education

Julia Lu (julialu@Torontomu.ca)

Department of Chemistry and Biology, Toronto Metropolitan University, Toronto Canada

Abstract:

This presentation summarises the literature search results on Artificial Intelligence (AI) in chemistry in higher education. Results from different databases show that AI is a rapidly growing field. The search using Web of Sconce shows that AI in higher education accounts for only a few percent of the results returned. In higher education, majority of the reports are in computer related fields. Reports on AI in Chemistry started in 2000. The number of reports, although it accounts for only a few percent of the returned references in higher education, has increased steadily and rapidly since 2018 and this number accounts for only 5% of the search results of AI in chemistry. Test results of AI applied to course teaching will be discussed.

Catalytic Cycloaddition of Carbon Dioxide and Epoxides by Chloro-Iron and Cobalt Complexes with Functionalized Quadridentate Ligands: Structural Effect and DFT Calculation

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Abstract

Transition metal complexes with tetradentate salen ligands showed to be highly efficient as catalyst precursor toward the synthesis of cyclic carbonate via the coupling reaction of carbon dioxide and epoxides. Herein, new series of penta-coordinated complexes of iron(III) and cobalt(III) bearing quadridentate Schif base salicylideneimine based ligands were prepared and characterized by spectroscopic methods of analysis. The new complexes contain either chloro or methyl groups on the phenyl back bone and chloro or diethylamine on the terminal phenyl groups. The structural parameters and charge distribution as well as the influence of the electron withdrawing (EWG)/ electron releasing (ERG) substituents were evaluated via density functional theory (DFT). Furthermore, the complexes were evaluated as catalysts for the coupling reaction of carbon dioxide with styrene oxide in the presence of Bu_4NBr under solvent-free conditions.

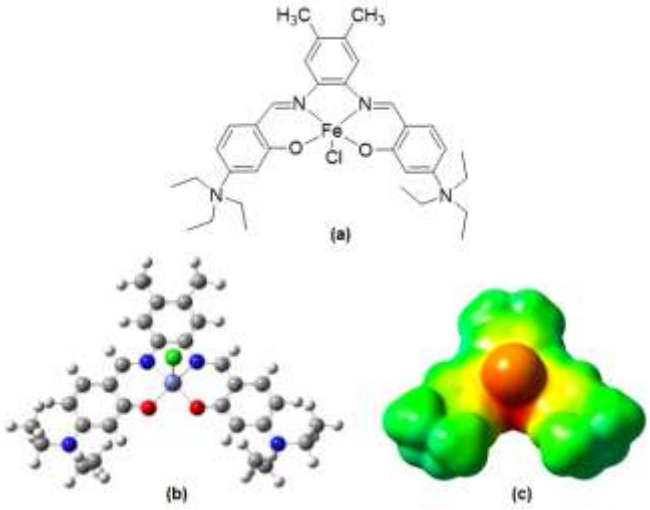

Figure 1: Complex **9**: a) Structure of the *penta*-coordinated iron(III) complex, b) DFT-optimized structure, c) Molecular electrostatic potential map (MESP).

Determining the Tracer Performance of $ZnFe_2O_4$ Modified with Different Coating Agents for Magnetic Particle Imaging

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Abstract: Magnetic nanoparticles (MNPs) have attracted significant attention for applications in clinical settings, including magnetic particle imaging (MPI), magnetic resonance imaging (MRI), hyperthermia, and drug delivery. In this study, $ZnFe_2O_4$ nanoparticles were synthesized by co-precipitating zinc (Zn^{2+}) and iron (Fe^{3+}) salts with ammonium hydroxide, followed by a reaction under nitrogen gas. These core nanoparticles were coated with citric acid (CA), L-ascorbic acid (AA), and L (+) tartaric acid (TA) to enhance colloidal stability and surface properties. Structural and magnetic properties were analyzed using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), dynamic light scattering (DLS), thermogravimetric analysis (TGA), and physical property measurement systems (PPMS). XRD confirmed the crystal structure of ZnFe2O4, with average crystallite sizes of 14–19 nm. Hydrodynamic diameters ranged from 112 to 218 nm, and zeta potential values were between -29.7 to -60.3 mV. SEM revealed spherical morphology, and all samples exhibited superparamagnetic behavior. The main goal was to evaluate ZnFe2O4 nanoparticles, coated with CA, AA, and TA, as contrast agents for MPI and MRI. The samples were tested using magnetic particle spectroscopy (MPS) and compared to commercial tracers (Perimag® and VivoTrax). Results showed that $ZnFe_2O_4$ nanoparticles, especially those coated with citric acid, performed best with the shortest relaxation time (2.09 μs for $ZnFe_2O_4$ @CA) and excellent spatial resolution (FWHM 5.89 mT). These findings suggest that surface-modified ZnFe2O4 nanoparticles hold great promise as molecular contrast agents for MPI and MRI, with potential for future biomedical applications

KEYWORDS: Magnetic nanoparticles, Magnetic particle imaging, $ZnFe_2O_4$ nanoparticles, Capping agents, Biomedical applications.
ACKNOWLEDGMENT: This study is supported by the Scientific and Technological Research Council of Türkiye (TUBITAK Grant No: 115E776 & 115E777).

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Rational PROTACs Design by Modelling the Ternary Complex Formation

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Abstract

PROTACs are a novel and promising therapeutical technology, that base their mechanism of action on the targeted protein degradation, offering numerous advantages over traditional small-molecule drugs.[1] Among all of the aspects that demand consideration for an effective PROTAC design, the stability of the ternary complex (Protein of Interest – PROTAC - E3 ligase), and the efficiency of ubiquitin transfer, are proving to be among the most impactful ones.[2] In recent years, several approaches have been developed with the ultimate goal of modelling ternary complex structures (TCs) and predicting their stabilities.[3] Unfortunately, none of these methods has established itself as a standard yet. In this scenario, the main intent of this work regards the development of a resource efficient and reliable approach based on GRID Molecular Interaction Fields (MIFs)[4], [5], to sample favourable protein-protein interactions mediated by the molecule. The goal is to generate reliable models of ternary complex structures, that could provide a robust foundation for understanding and optimizing PROTAC degradation efficiency. The software's capacity to accurately reproduce crystallographic poses was evaluated using a selection of ternary complexes downloaded from the Protein Data Bank. While in a second phase, a filtering and an RMSD-based hierarchical clustering approach was developed and tested on a subset of selected models. This method aimed at the identification of near-crystallographic ternary complex models in a blind way without relying on a prior knowledge of the crystallographic pose, while also refining the output of the algorithm to a smaller set of representative structures. The developed strategy successfully identified near-crystallographic orientations within the most populated clusters, for a portion of the tested cases. The program is currently being implemented to start from the coordinates of unbound structures (which don't belong to the ternary complex crystallographic data), through the use of local refinement strategies. As previously stated, this study introduces a novel methodology for the construction of ternary complexes and could offer valuable insights into the rationalization of their stabilities and of lysine exposure.

Key Words: *PROTAC, Ternary complex, MIF, Crystallographic structure, Clustering*

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Production of 48S Bioactive Glasses Enriched with Various Metal Ions and Evaluation of Their Bioactivity Properties

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Abstract

Hard tissue can be damaged due to various external factors and aging, and bioactive glasses play an effective role in the treatment of these damaged areas. Bioactive glass promotes bone formation and provides antibacterial properties by releasing ions, thereby creating an alkaline environment; thus, it is a potential candidate for bone applications. In hard tissue repair treatments, the biological activity of metal ions released from bioactive glasses can also be utilized. Therefore, bioactive glasses may offer additional advantages depending on the incorporation of different metallic ions into their structure. In this study, various metallic ions were incorporated into the 48S bioactive glass structure in different combinations using the sol-gel method. XRF analyses were performed to confirm whether the obtained BCs had the desired compositions. To observe the effects of metallic ions on bone tissue, the BCs were subsequently incubated in simulated body fluid (SBF) for specific durations. After SBF incubation, FTIR and SEM-EDS analyses were conducted to determine the potential formation of a Ca-P layer on the surface of the BCs and to examine changes in their morphology. The results before and after SBF exposure indicated that the metal-doped BCs with unique compositions exhibited bioactivity. As a result, the metal-doped BCs produced in this study can potentially be used as graft materials in bone tissue engineering applications.

This study was supported by the Scientific Research Projects Coordination Unit of Yıldız Technical University. Project Number: FYL-2024-6169.

Keywords – Bioactive Glass, Bioactivity, Bone Tissue Engineering, Metal Additives, Sol-Gel Method

The efficiency of cadmium extraction from various soil types and model systems with the selected environmental friendly chelators

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Abstract

One of the most sustainable approaches to addressing soil contamination with heavy metals is phytoremediation. While effective, this process requires time, which is sometimes a limiting factor. On the other hand, rapid interventions, such as removing the contaminated soil layer, are costly and have significant environmental impacts, making them applicable only in exceptional situations where human safety overrides environmental and financial concerns. However, there are numerous intermediate cases where time is a critical factor, but minimal environmental impact remains equally important. In certain instances, small and localized contaminated areas could benefit from support for phytoremediation to accelerate the process without causing significant harm to nature.

This research focuses on natural low-molecular-weight organic acids (LMWOA) that can bind heavy metals while being environmentally friendly. The study examines the efficiency of cadmium extraction using chelators such as citric acid, ascorbic acid, tartaric acid, and gallic acid from soils and model systems contaminated to varying degrees with heavy metals. The extraction was performed over time intervals ranging from 15 minutes to 4 hours. Additionally, the study evaluated the impact of extraction on cadmium bioavailability.

Heavy metal content measurements were conducted using flame atomic absorption spectrometry (FAAS). The bioavailability analysis utilized the BCR sequential extraction method.

The presented results clearly indicate that in soils with elevated cadmium levels, the use of chelators such as citric acid, tartaric acid, and ascorbic acid reduces the content of this element, especially in its active form, by as much as 30% to 40%. The extraction time was not a primary factor, as extending it did not significantly affect the amount of chelated cadmium.

The research results suggest that even short-term flushing with some of the described chelators can be an effective and environmentally safe method for rapid, ad-hoc remediation.

Key Words: *remediation, cadmium, sequential extraction, FAAS*

Enhanced Ultrafiltration Membranes: Fabrication of Polysulfone Membranes with Functionalized TiO_2 Nanotubes for Superior Permeability and Fouling Resistance

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Abstract

Recently, ultrafiltration (UF) approaches have worldwide applications in various areas, due to its performance in the reduction and treatment of food, medicinal, and products of paper in industrial separation procedures. In the pharmaceutical, food, contaminate water treatment, and biological sectors, ultrafiltration (UF) membranes are extensively employed for treatment and separation. The majority of the polymeric membranes demonstrated remarkable physicochemical characteristics, as well as chemical and mechanical durability. Furthermore, the miscibility of polymer blends is of tremendous interest in both industry and research due to Surface modifications after membrane fabrication equip the membrane with additional properties [1-4].

In this work, polysulfone blend ultrafiltration membranes with superior permeability and antifouling properties were successfully fabricated using TiO_2 nanotube functionalized aldimine Aminopropyltriethoxysilane vanillin composite (PSM-TNT@VOH) as a nanofiller. The membranes were fabricated using a combination of polysulfone (PSf) with TNT@VOH filler via the non-solvent induced phase separation (NIPS) method. The TNT@VOH nanocomposite was first prepared in three steps in order to successfully functionalized TiO_2 nanotube (TNT) with aldamie Aminopropyltriethoxysilane vanillin composite. Firstly, TNT was synthesized. Then, Aminopropyltriethoxysilane was added to TNT to produce aminated TNT. After that, aminated TNT, vanillin and thionyl chloride was heated in oil bath to produce as aldimine Aminopropyltriethoxysilane vanillin composite (PSM-TNT@VOH). Then, 1, 3, 5 and 7 wt.% of the composite was incorporated into the matrix of PSf for the fabrication of the nanocomposite membranes. The resulting membranes were characterized

using contact angle goniometer, atomic force spectroscopy (AFM), scanning electron microscope (SEM), X-ray diffraction (XRD), Thermogravimetry (TGA), and Fourier transform infrared spectroscopy (FT-IR). The porosity, charge density and surface morphology were altered and the nanocomposite membranes became more hydrophilic after the incorporation of the nanocomposite. The pure water flux of the nanocomposite membranes systematically increased with the loading amount of the nanocomposite. The pure water flux of the nanocomposite membrane containing 7 wt.% TNT@VOH nanocomposite at 1 bar feed pressure was 235 L m^{-2} h^{-1}, about 3-fold higher than that of pristine membrane (75 L m^{-2} h^{-1}). The fouling resistance of the nanocomposite membranes was evaluated and confirmed using humic acid (HA). The fabricated membranes were capable of removing more than 99.20%, improved from 80% without a nanocomposite of their rejection rate.

Keywords

Ultrafiltration membrane, polysulfone, vanillin, hydrophilicity, rejection rate

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Development of the injectable bone grafts

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Abstract

Bioactive glasses (BG) are inorganic bone grafts that bind to bone, with 45S5, S53P4 being the most recognized types (Özarslan et al. 2024). However, BG powders or granules may not adequately fill bone cavities, necessitating injectable grafts (Özel et al. 2023). FDA-approved polyethylene glycol (PEG) is suitable for injectable bone defect applications (Tuominen et al. 2010).

In this study, injectable bone grafts composed of PEGs, glycerol, and BGs were developed for bone defect applications. BGs were synthesized via melt-quenching, ground, and sieved. The grafts were then formulated by mixing PEG polymers with glycerol and glass in different ratios. *In vitro* bioactivity behavior of these grafts in simulated body fluid (SBF) for up to 28 days was analyzed using FTIR, SEM, and XRD. Ion releases of the injectable bone grafts were investigated by ICP-OES.

The SBF incubation results revealed Calcium-Phosphate (Ca-P) layer deposition and crystalline HA/HCA formation on BG surfaces from day 7 in SBF incubation, confirming the *in vitro* bioactivity of all injectable grafts. ICP-OES analysis showed an initial increase in Si and Ca ion release within the first 7 days, followed by a decline in Si and P levels up to 28 days. Additionally, grafts with high BGSs content exhibited greater bioactivity by high crystalline apatite on the glass surface. These findings suggest that grafts with a high amounts BG are highly bioactive. As a result, a high amount of BG containing injectable bone graft produced in this study can potentially be used as injectable graft materials in bone tissue engineering applications.

This work has been supported by Yildiz Technical University Scientific Research Projects Coordination Unit under project number FBA-2023-5377

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ENCAPSULATING BERGAMOT AND GINGER ESSENTIAL OILS IN BINARY BLENDS OF ZEIN AND CASEIN POLYMERS

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Abstract

Essential oils constitute a mixture of many organic compounds such as esters, ethers, aldehydes, monoterpenes, sesquiterpenes, diterpenes, and phenylpropanoids that are obtained either from the stems, leaves, fruits or roots of herbs and spices, by distillation or mechanical processing techniques [1]. Due to their unique composition, essential oils exhibit antioxidant, antiseptic, anti-inflammatory, anticancer and antimicrobial activity which endavours applications in the pharmaceutical, nutraceutical and cosmetic field [2]. Yet, the limitation of easy degradation under the effect of high temperature, oxygen and/or light should be eliminated. Nanotechnology and encapsulation applications are among the methods that ensure protection from external factors. Encapsulation technology refers to the process of enclosing or trapping active substances, within a protective shell or coating. The coating material must be biodegradable and compatible with the components to be protected. Carbohydrates, proteins, polysaccharides and synthetic polymers are used as coating materials in encapsulation systems [3].

In this research investigation, the anti-solvent precipitation method was employed to synthesize particles loaded with bergamot and ginger essential oils using zein and zein/casein blends. Surfactant type and ratio, polymer to oil ratio, pH, mixing speed, and casein to zein ratio were systematically explored as process parameters. The release behavior of particles loaded with bergamot and ginger essential oil were monitored over a week and storage stability was investigated at -20°C . The obtained particles underwent detailed characterization using SEM, SEM-EDX and FTIR analysis techniques. The composition of essential oils was confirmed by GC-MS analysis.

According to the data, as a result of the encapsulation of bergamot essential oil with zein, 58.68±0.02% efficiency, 77.46% solid yield and 55.11% oil retention capacity were obtained, while the efficiency increased significantly to 92.0±0.01% after casein was introduced as the second biopolymer. The diffusion of essential oils from the system spread over a period of 5 days, and at the end of this period, 50.44% release was achieved. When zein was solely used for ginger essential oil encapsulation protocol, 20.20±0.017% efficiency, 65.95% solid yield and 17.54% oil holding capacity were obtained. The inclusion of casein in the biopolymer mixture led to an enhanced efficiency of 51.28±0.010%, solid yield of 71.44% and oil holding capacity of 42.18%. The cumulative release of ginger essential oil was recorded as 88.73% within a 7-day period. According to morphological evaluation, it was observed that the encapsulated structures were spherical, nanoparticle sized and regular, and the structure enlarged with the addition of casein. In SEM-EDX analysis, it was determined that bergamot and ginger essential oil contents were included in the particle structure. In FTIR analysis, it was stated that the active components were present in the particle structure in preserved state. Thus, the synthesized carrier system can be facilitated in many different areas such as food, cosmetics, perfumery and medical after additional testing for toxicity and biocompatibility.

Key Words: *Encapsulation; zein; casein; essential oil; nanoparticle.*

Acknowledgements: This research was supported by Marmara University Scientific Research Coordination Unit with the grant number FYL-2023-10857.

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Computational evaluation of cymenes: Substituent group effect, Pharmacokinetics, and Drug-likeness

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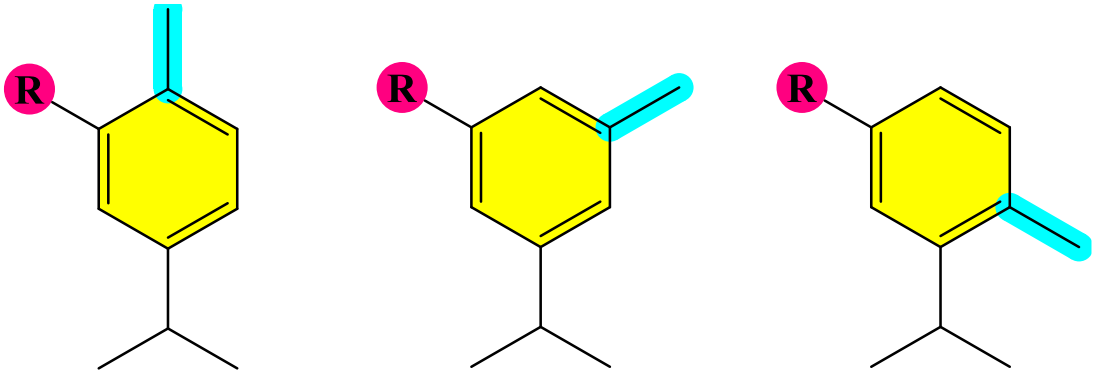
Abstract

Cymene is known as the type of monoterpene with the chemical formula of $CH_3C_6H_4CH(CH_3)_2$ and is found in essential oils of various plants including *Thymus*, *Protium heptaphyllum*, *Eucalyptus*, *Protium*, etc [1]. Until now, they have been under the spotlight due to their neurodegenerative potential in CNS diseases such as anxiety, Alzheimer's disease, oxidative stress, etc. Moreover, they have been considered natural protective agents with capabilities of antioxidant, antimicrobial, anticancer, etc due to the lipophilic character allowing them to interact with cell membranes. In addition to the bio-medicinal superiorities, p-cymene is used as a precursor in the organic synthesis of bio-based solvents, green chemicals, and agrochemicals. As known well, the optimized physicochemical properties like water solubility and hydrophobicity should be in balance with each other in designing the smart agents for biomedicinal applications, which are crucial in early-level drug-design. Herein, the functionalized ortho-, para-, and meta-cymene isomers have been investigated using computational tools to evaluate the relationship between the structure and pharmacokinetic characteristics. In this regard, the quantum mechanics simulations are employed to determine the optimized and confirmed structures, and then elucidate the thermochemical and physical properties. Also, in silico ADMET properties of the data set are predicted by using the SwissADME [6] tools and evaluated for the potencies in designing the drug agents.



Scheme 1. The chemical structures of cymenes

Key Words: *cymene, substituent effect, DFT, drug-likeness*

Acknowledgments

All calculations have been carried out at TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). The author thanks the Scientific Research Projects Department of Cumhuriyet University (Project No: EĞT-2023-098).

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THEORETICAL EXAMINATION of PAROXETINE HCl, THE ACTIVE INGREDIENT of THE DRUG MARKETED as PAXIL, USED in ANTIDEPRESSANT TREATMENT, USING THE DFT METHOD

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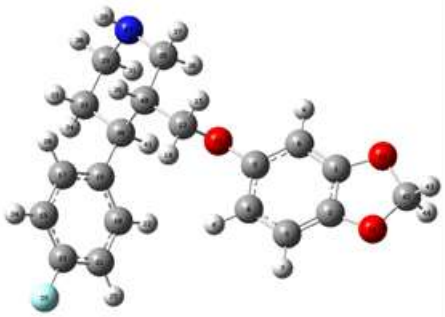
Abstract

Paroxetine HCl (PA) is a non-steroidal anti-inflammatory drug active ingredient, marketed as Paxil, a selective serotonin reuptake inhibitor antidepressant. In this study, PA was theoretically examined according to this pharmaceutical effect, that is, treatment group and site of action. Selected molecule is used for therapeutic purposes, but their fate in nature is not taken seriously when it is eliminated from the body or become waste when it is not used. The aim of this study is to theoretically elucidate the fate of both the main molecule and its hydroxylated fragments in nature as they enter the natural cycle because of mixing with wastewater.

Geometric optimizations of the fragments were made on the DFT/B3LYP/6-31G(d) basic set of DFT to theoretically determine all possible reaction pathways of the selected molecule with the OH radical. The Mulliken charges of the fragments were examined, the electronegative atoms in the molecule and the arrangement of the atoms around them, stable double bonds, weak bonds at the end of the molecule, calculated energies, bond lengths and bond angles between atoms helped us to select all the fragments that will determine the degradation mechanism. As a result of examining the molecules in terms of their reaction with OH radicals in air or water, the degradation reactions of each molecule were written, starting from the low-energy fragments, and their fate in nature were determined.



PA

Figure 1. Geometric structure of PA molecule optimized by DFT method (C atom is represented in grey, O is red, N is dark blue, F is blue and H atom is represented in white)

Key Words: Paroxetine HCl, Paxil, DFT, antidepressant, drug.

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SYNTHESIS AND CHARACTERIZATION OF COPPER (II) COMPLEX AND ITS CATALYTIC ACTIVITY ON C(SP3)-H OXIDATION REACTIONS

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In recent years, interest in the synthesis of coordination compounds has greatly increased due to various application areas (such as catalysis, gas storage, luminescence) [1]. Dicarboxylic acids are often used in the synthesis of metal complexes. Bis-thiosalicylate derivative ligands contribute to the synthesis of structures of crystal engineering interest, as they can have both rigid and flexible properties [2]. In addition, these ligands have great potential in terms of catalytic applications with the sulfur and oxygen donor atoms in their structures.

In this study, we synthesized a new Cu(II) complex $[Cu(tsaxyl)(phen)_2]\cdot CH_3OH$ (where tsaxyl = 2,2'-(1,2-phylenebis(methylene))bis(sulfanedyl)dibenzoate, phen = 1,10-phenantroline) and characterized through X-ray crystallography. The catalytic activities of Cu(II) complex on oxidation of ethylbenzene, cyclohexane, diphenylmethane, p-xylene and n-hexane were performed in acetonitrile with *t*-BuOOH as the source of oxygen.

Key Words: Complex, Crystallography, Catalysis, Oxidation.

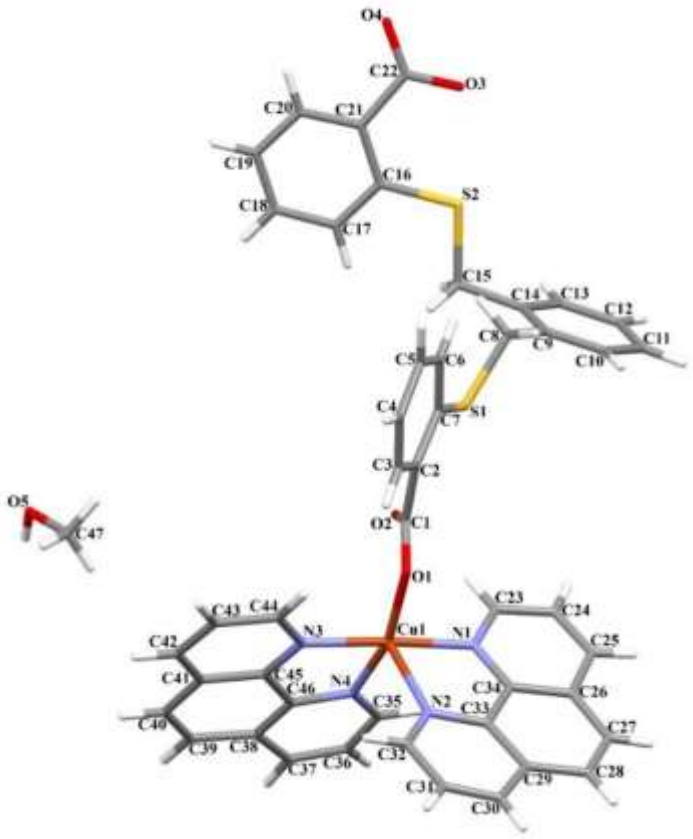

Figure 1. The molecular structure of Cu(II) complex

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INVESTIGATION OF THE DEGRADATION REACTION KINETICS OF CEFALEXIN BY HYDROXYL RADICAL

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Abstract

Cephalexin (CFL) is a beta-lactam antibiotic class that is consumed in large quantities all over the world [1]. It is used in the treatment of bacterial infections [2]. However, in recent years, due to the use of high amounts of CFL, its accumulation in aquatic environments has caused adverse health consequences. This has caused public concern [3]. For this reason, many studies have been carried out to remove these substances from aqueous medium. However, the fact that they are highly stable compounds with low degradability makes this difficult [4]. More detailed information is needed about the degradation reaction of CFL with hydroxyl radicals in aqueous environments.

In this study, the degradation reaction of CFL with hydroxyl radical at B3LYP/6-31G(d,p) level was investigated using Density Functional Theory. Hydroxyl radical reacts with CFL in the form of hydrogen abstraction and addition. The mechanism and kinetics of all reaction paths were investigated in detail. The thermodynamic parameters of all reaction paths and the contribution of each reaction path to the reaction mechanism were determined. The rate constant of the reactions was calculated using Transition State Theory. According to the results, the beta-lactam ring opening path was found to be the most probable reaction path.

Key Words: *Antibiotic, Density Functional Theory, hydroxyl radical, rate constant, aqueous medium.*

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PESTICIDES IN ALBANIAN VEGETABLE FARMING: CHALLENGES AND STRATEGIES FOR SUSTAINABLE AGRICULTURE

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Abstract

Objectives:
The widespread use of pesticides in vegetable farming raises concerns about food safety, environmental contamination, and human health risks. This study aims to assess pesticide use practices among Albanian farmers, evaluate their knowledge of pesticide application and safety measures, and identify key challenges to promoting sustainable agriculture.

Methodology:
A structured survey was conducted with vegetable farmers across various regions of Albania to collect data on pesticide selection, application practices, adherence to safety measures, and awareness of associated health risks. Face-to-face interviews were used to gather responses, and statistical analyses were performed to identify trends and correlations between farmer knowledge, risk perception, and pesticide use behavior.

Results:
Findings indicate that while many farmers recognize the risks associated with pesticide use, knowledge gaps persist due to limited training and access to information. A significant portion of respondents were unaware of restrictions on certain pesticides and had not received formal training on their proper application. Although farmers acknowledged the negative effects of pesticides on food safety, health, and the environment, adherence to protective measures, particularly the use of personal protective equipment (PPE), remained insufficient. The study also highlights challenges such as weak regulatory enforcement, economic constraints, and the need for improved farmer education programs.

Conclusion:
Addressing pesticide-related risks in Albanian vegetable farming requires a multifaceted approach, including continuous training for farmers, increased access to safer alternatives, and stronger regulatory enforcement. Enhancing farmers' knowledge and providing adequate resources are essential steps toward ensuring food safety, protecting public health, and promoting sustainable agricultural practices in Albania.

Key Words: *Pesticide residues, Food safety, Sustainable agriculture, Vegetable farming, Risk perception*

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Challenges in ICP-MS analysis of elemental impurities in pharmaceutical products: methodological and analytical considerations

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Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is a highly sensitive technique widely used for the detection of elemental impurities in pharmaceutical products. However, its application in this field presents several challenges that span methodological, analytical, and regulatory aspects.

One of the primary methodological challenges lies in the complex nature of pharmaceutical matrices, such as tablets, capsules, and injectable formulations. These products often contain excipients, buffers, and other organic compounds that can interfere with the ionization process in ICP-MS, leading to matrix effects that impact sensitivity and accuracy. To address this, matrix-matched calibration or the use of internal standards is often employed, but these solutions can add complexity to the analysis.

From an analytical perspective, ICP-MS faces the issue of isobaric interferences, where different elements share the same mass-to-charge ratio, leading to overlapping signals that can distort results. For example, calcium and potassium both have the same m/z of 40, which could result in false positives. High-resolution ICP-MS and the use of collision/reaction cells can mitigate these interferences, but these solutions may require more sophisticated instrumentation and longer analysis times.

Furthermore, contamination is an ever-present risk in pharmaceutical analysis. Even minute levels of contaminants introduced through laboratory equipment, reagents, or the environment can lead to erroneous results. Implementing rigorous cleanliness protocols, using high-purity reagents, and adopting contamination control measures are crucial to obtaining accurate measurements.

While ICP-MS remains a powerful tool for elemental impurity analysis in pharmaceuticals, overcoming the challenges related to matrix effects, interferences, low detection limits, contamination, and regulatory compliance requires a well-rounded approach. Method development, instrument optimization, and strict adherence to regulatory standards are essential to ensure accurate, reliable, and compliant results in the determination of elemental impurities in pharmaceutical products.

Keywords: Elemental impurities, ICP-MS, Pharmaceutical products, analytical challenges.

Development of a High-Performance Liquid Chromatography (HPLC) Method for Coumarin Quantification in Medicinal Plants Extracted via Soxhlet

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Abstract

Various analytical methods such as spectrofluorimetry, high performance liquid chromatography (HPLC), high performance thin layer chromatography (HPTLC) and gas chromatography (GC) are known for the determination of coumarins [1]. In this study, it was aimed to develop a new high performance liquid chromatography (HPLC) method for the efficient extraction and quantification of coumarin compound from *Helichrysum arenarium* (Golden Tuft), *Thymus vulgaris* (Thyme) and *Achillea millefolium* (Yarrow) plants by Soxhlet extraction method. Pure water, methanol, ethanol, acetone, acetone, n-hexane and toluene were used as solvents in Soxhlet extraction and the most suitable solvent was determined by comparing the extraction efficiency of the solvents. Experimental results revealed that there were significant differences in coumarin extraction efficiency depending on the solvent type and chemical structure of the plant. Methanol and ethanol provided the highest extraction efficiency in general, while the highest coumarin concentration (0.0339 mg/mL) was obtained for *Helichrysum arenarium* (Golden Tuft) when methanol was used. Acetone provided moderate yields, while n-hexane and toluene were the solvents with the lowest extraction capacity. In *Thymus vulgaris* (Thyme) samples, high coumarin content was obtained with acetone and n-hexane, but no extraction was achieved with ethanol. *Achillea millefolium* (Yarrow) was found to have the lowest overall coumarin content.

These results show that herbal extraction efficiency is not only dependent on the choice of solvent, but also the cellular structure specific to the plant species, the phytochemical distribution pattern of coumarin in the plant structure and Soxhlet extraction conditions directly affect the process. The HPLC method developed within the scope of the study provided high sensitivity, accuracy and reproducibility for coumarin quantification and its usability as a reliable analytical tool in pharmaceutical and phytochemical research has been confirmed in the literature [2]. The findings indicate that the choice of solvent for the analysis of coumarin-containing herbal extracts should not be based solely on polarity, but should be evaluated together with the matrix properties of the plant.

Key Words: *Coumarin Extraction, Soxhlet Extraction, High Performance Liquid Chromatography (HPLC), Solvent Selection*

Acknowladge

This work was supported by Research Fund of the Yildiz Technical University. Project Number FDK-2023-5966.

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HYDROGEN PRODUCTION FROM SODIUM BOROHYDRIDE IN CONTINUOUS HYDROLYSIS SYSTEMS: THE EFFECT OF RECIRCULATION

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Abstract

Hydrogen is a promising energy carrier due to its renewability and low environmental impact. Among various hydrogen storage methods, sodium borohydride ($NaBH_4$) stands out with its 7.8% hydrogen content and ability to enhance hydrogen release through hydrolysis. Given Türkiye's rich boron reserves, $NaBH_4$ offers a strategic advantage as a hydrogen storage material, enabling controlled hydrogen release with high yields via catalytic hydrolysis.

This study focuses on integrating $NaBH_4$ hydrolysis into a continuous hydrogen production system and optimizing the process through a recycling loop to maintain high efficiency at ambient temperatures. The use of ceramic-supported foam catalysts, known for their durability in liquid-phase continuous systems, was investigated. Various parameters, including catalyst type, temperature, flow rate, and concentration, were analyzed to assess their effects on hydrogen production.

Two supported catalysts (BaCoCu and NiCoCu), two temperatures (25°C and 55°C), two $NaBH_4$ concentrations (0.1 M and 0.2 M), and three flow rates (1 ml/min, 2 ml/min, and 3 ml/min) were tested. The experiments were conducted in a continuous system without recycling and then with two different recycling strategies: (i) integrating the recycling stream with the feed solution and (ii) collecting the recycling stream separately and feeding it back into the system after the initial solution was depleted.

Results indicated that increasing $NaBH_4$ concentration and temperature significantly enhanced hydrogen yield, while higher flow rates reduced hydrogen production due to decreased catalyst contact time. BaCoCu exhibited superior catalytic activity compared to NiCoCu. Moreover, both recycling strategies contributed a considerable amount of hydrogen to the system, highlighting the effectiveness of the looped design. This study demonstrates that optimizing recycling in continuous $NaBH_4$ hydrolysis can improve efficiency and minimize waste, advancing sustainable hydrogen production.

Key Words: *Sodium Borohydride, hydrolysis, hydrogen Production, Continuous System*

Valorisation of Polycationic Metals from Acid Mine Drainage for Sustainable Wastewater Treatment: A Circular Economy Approach

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Abstract

Acid mine drainage (AMD) is a significant environmental issue, characterized by high acidity and elevated concentrations of dissolved heavy metals such as iron (Fe^{3+}) and aluminium (Al^{3+}), which threaten water quality and aquatic ecosystems [1]. Simultaneously, municipal wastewater contains excessive nutrients, such as phosphate (PO_4^{3-}), ammonium (NH_4^+), nitrate (NO_3^-), and sulphate (SO_4^{2-}), which contribute to eutrophication and disrupt ecological balance [2]. Addressing these challenges requires sustainable remediation strategies that integrate waste valorisation within the framework of a circular economy [3].

This study explores the recovery and valorisation of polycationic metals (Fe^{3+} and Al^{3+}) from AMD as functional adsorbents for municipal wastewater treatment. The recovered materials exhibited high adsorption capacities, achieving removal efficiencies of >95% for phosphate and ammonium, 90% for nitrate, and 80% for sulphate under optimised conditions (2 g dosage, 90 min contact time, 35°C) [4]. Adsorption kinetics followed pseudo-first-order models for sulphate, phosphate, and nitrate, indicating physisorption, while ammonium adsorption conformed to pseudo-second-order kinetics, suggesting a chemisorption-driven mechanism [5]. Isotherm analysis revealed that nitrate and sulphate followed the Langmuir model, indicative of monolayer adsorption, whereas phosphate and ammonium exhibited multilayer adsorption behaviour, best described by the Freundlich and Two-Surface Langmuir models [6].

Fourier-transform infrared spectroscopy (FTIR), X-ray fluorescence (XRF), and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX) confirmed the presence of Fe–O, Al–O, and hydroxyl functional groups, which facilitated adsorption through electrostatic interactions, ion exchange, and surface complexation [4]. The recovered polycationic metals provide a low-cost and scalable alternative to conventional adsorbents, reducing the environmental footprint associated with AMD pollution while offering an effective solution for wastewater remediation [3].

The integration of AMD-derived materials into municipal wastewater treatment aligns with circular economy principles by transforming mining waste into high-value functional materials. This dual-purpose approach reduces reliance on costly adsorbents and provides an economically viable and environmentally sustainable solution for water treatment [1,3]. The potential for large-scale application is significant, particularly in regions impacted by mining activities and industrial wastewater contamination [2].

This study contributes to green chemistry and sustainable remediation by demonstrating a waste-to-resource strategy that advances both environmental and economic sustainability. Future research should focus on pilot-scale implementation, long-term material performance assessment, and potential applications beyond wastewater treatment, such as industrial effluent purification and soil remediation [5]. These findings highlight the role of interdisciplinary collaboration in developing innovative technologies for sustainable environmental management.

By bridging the gap between waste valorisation and water purification, this research promotes a resilient and resource-efficient approach to environmental sustainability and industrial waste management.

Key Words: *Acid mine drainage; wastewater treatment; adsorption; polycationic metals; environmental remediation.*

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Assessment of the Effects of Iron (III) Oxide Nanoparticles and Iron (III) Chloride on Glutathione Reductase Activities

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Abstract

Iron (III) oxide nanoparticles (Fe_2O_3 NPs) are used in magnetic resonance imaging, magnetic hyperthermia as a cancer treatment method, drug delivery as carriers, tissue engineering, cell separation, enzyme immobilization, protein purification and biosensing [1,2]. Iron (III) chloride ($FeCl_3$) is used in the drinking water production, the treatment of municipal and industrial wastewater and the processing of sludge as a coagulant and flocculant. Because of its reactive properties, iron(III) chloride is also used in the electronic industry as an etching agent [3].
Glutathione reductase (GR) (EC 1.8.1.7) is an antioxidant enzyme. Oxidized glutathione (GSSG) is converted to reduced glutathione (GSH) in the presence of NADPH (β-nicotinamide adenine dinucleotide 2'-phosphate reduced) by GR enzyme [4].

In this study, GR from baker's yeast (Saccharomyces cerevisiae) exposed to 0, 25, 50, 100, 250 and 500 ppm (mg/L) of Fe_2O_3 NPs and $FeCl_3$. When the concentration of Fe_2O_3 NPs increased, there were slight statistically significant decreases in the GR activities at high concentrations (100, 250, 500 mg/L) according to the control ($N=3$, $P<0.05$). When the $FeCl_3$ concentration increased, a statistically significant decrease was determined in GR activity only at 500 mg/L $FeCl_3$ concentration according to the control ($N=3$, $P<0.05$).

At conclusion, we observed statistically significant decreases related to effects of Fe_2O_3 NPs and $FeCl_3$ on GR activities. $FeCl_3$ inhibited the GR enzyme more than Fe_2O_3 NPs *in vitro*.

Key Words: *Nanoparticles; Iron(III) Oxide Nanoparticles; Iron (III) Chloride; Glutathione Reductase; Enzyme.*

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Utilization of Inductively Coupled Plasma (ICP) in Monitoring and Analysis of Some Heavy Metals in Jordanian Dams

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Abstract

During the summer in 2022 and winter in 2023, samples were taken from some Jordanian dams, which are: Kafrain Dam, King Talal Dam, Shuaib Dam, and Mujib Dam. The locations of these dams in Jordan are illustrated in Figure 1.

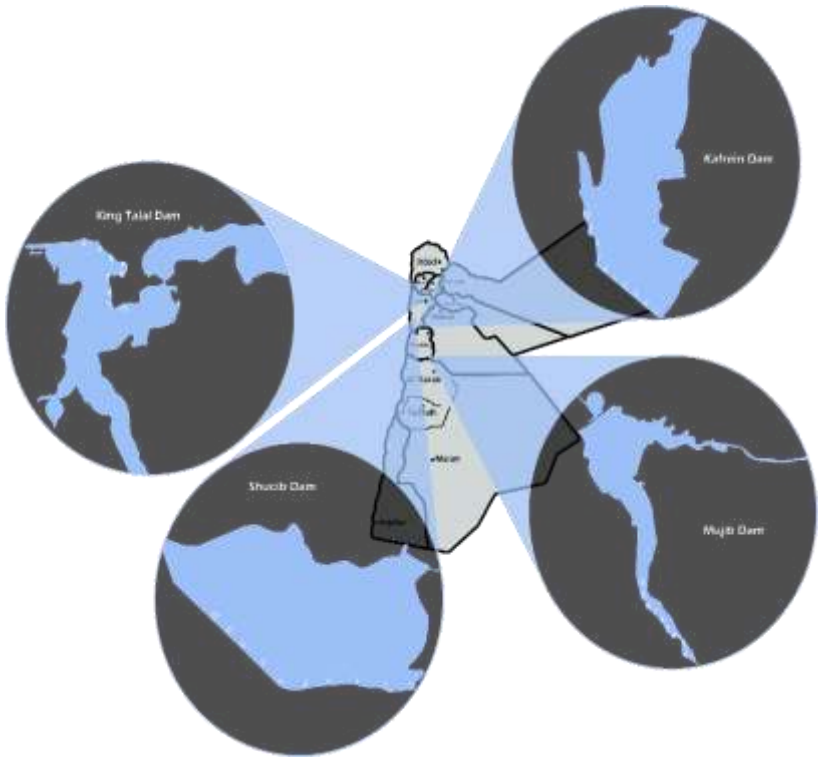

Figure 1: Map showing the distribution of the studied dams.

The samples were split into two categories: water samples and sediment samples. An ICP-OES device was used to measure the concentration level of metal ions in the samples, which include Cd, Co, Hg, Fe, Ni, Zn, and Pb.

Kafrain Dam was designated as the dam with the highest concentrations of metal ions in sediment samples during summer. The results showed that, according to the WHO, all the studied metal ions, excluding Zn, were above their normal limit. In Mujib dam, Pb and Fe ions were found to have concentrations in sediment samples that are higher than the permissible limit, and the dam was classified as the least dam containing high metal concentrations. Even so, Mujib Dam topped the list in metal ions concentrations in water samples taken during the summer season; where the concentrations of Fe, Co, and Cd ions were higher than the WHO and JSMO allowable limit. On the other hand, Shuaib dam was found to have only Cd, and Co, while and Kafrain dam was found to have only Fe and Cd ions above the allowed WHO limit in water samples.

During the winter season, no concentration (not detected) of metal ions was found in any of the water samples taken from the studied dams. For sediment samples, Mujib dam was

the dam with the highest concentrations of metal ions. It was found that Pb, Co, Cd, Ni, and Fe ions have concentrations that were higher than the permissible recommended percentage levels given by the WHO and JSMO. Moreover, each of Shuaib Dam, King Talal Dam, and Kafrain Dam contained four metal ions concentrations that were above allowable limits, (*viz*. Pb, Co, Cd, and Fe).

LIFE CYCLE ASSESSMENT OF MAGNETIC CARBON BASED ADSORBANT SYNTHESIS

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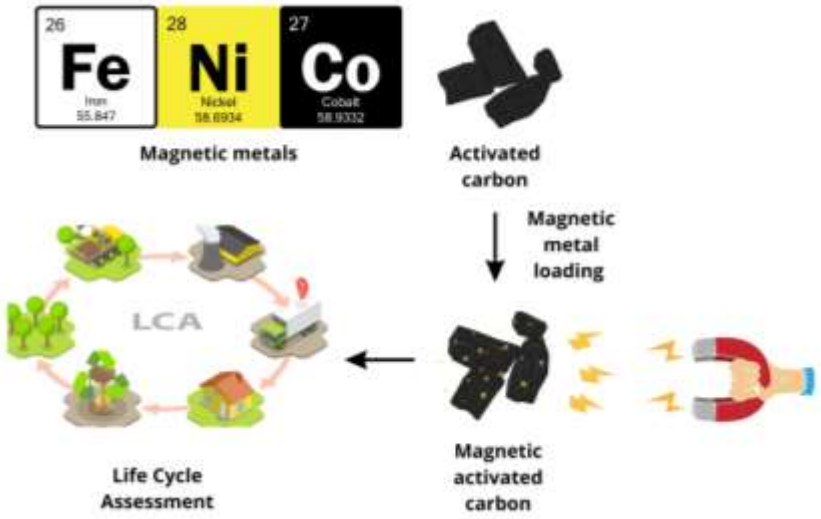
Abstract

Water supplies are being polluted continuously due to factors including population increase, climate change, and growing industrialization. Numerous chemical contaminants are continuously damaging aquatic ecosystems [1]. Due to the chemical pollution, they cause, wastewater is removed employing a variety of techniques. Among the methods explored in the literature, adsorption is one of the most widely used. This method increases the density of the material on the surface by attaching the dissolved solid material to an appropriate surface [2]. Adsorbents ensure that the substance remains on the surface where it is located. In addition to the use of polymeric materials and adsorbents like zeolites, activated carbons favoured for several reasons. It is effortless to produce, has an enormous surface area, developed pore structures, and is affordable [3]. The difference between magnetic activated carbon and activated carbon is in the method of removing the adsorbent from the solutions. This difference is based on the use of the magnetic property of the adsorbent. Magnetic activated carbon benefits from its magnetic properties, making the adsorption process faster and more efficient. It is critical that the adsorbent used for industrial applications has minimal environmental impact after production.



Scheme 1. Methodology of the research

Life Cycle Assessment (LCA) is a methodology defined by International Organization for Standardization standards and the International Reference Life Cycle Data System Handbook recommendations. The goal of LCA is to assess the potential environmental and resource impacts from the purchase of raw materials to their manufacture and consumption, as well as

waste management, over the lifespan. Furthermore, LCA is the most widely used method for assessing the environmental effects of systems controlled by humans. All system components improve ecological outcomes by utilizing resources, releasing molecules into the biosphere, and promoting other ecological exchanges. LCA investigates system interdependence and offers data regarding the impact on the environment. The findings of the LCA are used as indicators in a variety of environmental impact categories, including toxicological impacts, resource depletion, and global warming potential [4].

Within the scope of this study, it is aimed to investigation of LCA of magnetic activated carbon synthesis (Scheme 1). Research for studies on magnetic carbon-based adsorption systems, which are essential for the removal of pollutants from wastewater, can be implemented in areas where industrial adsorption will be acquired as part of this investigation. Moreover, since the environmental effects of the study to be carried out using LCA can be examined in advance, the damages of these effects can be predicted before they occur. This work was supported by the Yıldız Technical University Research Foundation (Project no: FBA -2024-6474).

Key Words: *Adsorption; Magnetic carbon-based adsorbent; Environmental pollution; Life cycle assessment*

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EFFECT OF DIFFERENT DRYING TECHNICS ON DRYING CHARACTERISTICS OF CELERIAC

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Abstract

The drying process is an essential method in food preservation, influencing both the quality and shelf-life of products. Celeriac (Apium graveolens var. rapaceum), a root vegetable with high nutritional value, is often subjected to drying to extend its usability. Different drying techniques, such as air drying, freeze drying, and microwave drying, can have significant impacts on the drying characteristics, including drying rate, moisture content, texture, and nutrient retention. Present study investigates the impact of various drying methods on the drying characteristics of celeriac, focusing on parameters like drying rate, moisture loss, and time efficiency. Understanding these kinetic aspects is essential for optimizing drying processes and improving the quality of the final product.

Celery samples were divided into two groups: one group was pretreated with a 1% citric acid solution, while the other remained untreated. Both groups were dried at 55, 65, and 75 ˚C in a cabinet dryer, and at 62, 74, 88, and 104 W power levels in an infrared dryer. The study also examined the effects of combined drying (infrared followed by cabinet drying) and pretreatment on drying kinetics and color change. In the combined system, samples were initially treated with 74 W infrared power for 30 minutes and then dried at 65°C in the cabinet dryer to reach the target moisture content.

The variation of moisture content during drying of celery samples was investigated by selecting eight mathematical models. The performances of the models were evaluated by using statistical analysis methods such as regression coefficient (R^2), mean square root errors (RMSE) and chi-square ($\chi 2$). Based on the findings of the studies, it was determined that the Midilli & Küçük model provided a better explanation of the drying behavior of the samples compared to the other models. The diffusion coefficient values of celery which were dried in the cabinet dryer, between 1.701×10^{-10} and 3.317×10^{-10} m^2/s for the control group samples, 1.753×10^{-10} and 3.797×10^{-10} m^2/s for the pretreatments with citric acid solution, activation energy values were calculated as 31.66 and 32.70 kJ / mol, respectively. The diffusion coefficient values of the celery dried in the infrared dryer varied between 2.746×10^{-10} and 4.987×10^{-10} m^2/s for the control group samples and the activation energy value was calculated as 2.99 kW/kg

Key Words : Celery, drying, effective diffusivity, mathematical modelling,

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APPLICATION OF GAS FOAMING TECHNIQUE FOR IMPROVING POROUS PROPERTIES OF CHITOSAN-POLYVINYL ALCOHOL (CS-PVA) NANOFİBER BASED BIODEGRADABLE SCAFFOLDS

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Abstract

The human body consists of systems, systems are organs, organs are cells and extracellular matrix. The extracellular matrix has an important role in the human body with the task of connecting cells to each other [1]. Due to various reasons, diseases in which the extracellular matrix is damaged have been witnessed from the past to the present. Tissue engineers are in research to improve and prevent this damage [2]. As a result of these researches, the production of tissue scaffolds has started. Tissue scaffolds are structures designed to mimic the extracellular matrix. These scaffolds can perform functions belonging to the extracellular matrix, such as providing mechanical strength, helping to establish communication with the surrounding tissue to respond to physiological and biological changes, as well as forming suitable adhesion surfaces for cells [3]. They may also contribute to the regeneration of the true extracellular matrix. Tissue scaffolds can be produced by many methods, one of which is the electrospinning technique [4]. In our study, tissue scaffolds produced by this method were used, and it was aimed to increase the porosity of these scaffolds by applying the gas foaming technique.
In the experiments, tissue scaffolds were obtained by electro-spinning method and NaBH4 - Methanol solution was used for gas foaming method. As a result, it was observed that the porosity properties of the tissue scaffolds inflated in 0.1 M solution were increased. These observations were determined and documented by the analysis results. This work was supported by the TUBITAK 2209-A- Research Project Support Programme for Undergraduate Students/2022-1.

Key Words: *Polymer chemistry; Biotechnology; Electro-spinning; Gas foaming; Nanofiber; Materials Science*

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IMPROVED BIOBUTANOL RECOVERY THROUGH MIXED-MATRIX PVDF MEMBRANE WITH HYDROPHOBIC MAF-6 AS FILLER

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Abstract

The global shift towards alternative renewable energy sources was accelerated in the late 1990s due to the escalating prices of petroleum products and raw materials, coupled with the depletion of fossil fuels [1-2]. These biofuels include densified solid agricultural residues, ethanol, butanol, hydrogen, and biodiesel produced through biochemical or thermochemical conversion processes involving various plant and organic wastes [3]. Butanol, a flammable alcohol, stands out as a viable biofuel option. Biobutanol offers several advantages over bioethanol, including non-hygroscopicity, higher heating value, improved compatibility with gasoline and diesel fuels, as well as reduced corrosion and flammability issues. Additionally, butanol is widely utilized as a solvent in industrial applications [2-3]. The production of biofuels through acetone, butanol, ethanol (ABE) fermentation dates back to 1861 and regained attention due to the ongoing quest for alternative fuels, especially with the resurgence of interest in butanol produced via ABE fermentation following the 1960s [4]. During the recovery of butanol from the fermentation medium, conventional methods such as distillation, adsorption, extraction, and gas stripping can be employed; however, each method comes with its own set of challenges. Pervaporation, a membrane-based process, presents an alternative to conventional methods and can mitigate some of these drawbacks. In a pervaporation process, the liquid feed is introduced to the upstream side of the membrane, and the product is obtained as vapor on the downstream side due to the application of a vacuum. The selectivity of the membrane is influenced by the relative solubility and diffusion characteristics of the components being separated within the membrane. Hence, the development of membranes exhibiting high affinity for the target component is crucial for efficient pervaporation systems [5].

In this study, enhancing the hydrophobicity of the membrane by using MAF-6 was considered an effective strategy to improve the performance of organophilic pervaporation (PV) membranes. This was achieved by incorporating superhydrophobic MAF-6 into polyvinylidene fluoride (PVDF) polymer to create mixed matrix membranes (MMMs). Various characterization techniques were employed to assess the morphologies, physical, and chemical properties of the MAF-6 nanocrystals and the membranes, including BET, SEM, FTIr, TGA and contact angle measurements. The pervaporation experiments involving butanol/water mixtures demonstrated that the MMMs exhibited enhanced flux and separation factor compared to the PVDF pristine membrane. The optimal flux achieved was 1.35 g/m² h, with a separation factor of 16.7. This enhancement in performance was attributed to the hydrophilicity and high porosity of MAF-6, which effectively overcame the trade-off effect usually observed in such membranes.

Key Words: *Biobutanol, MAF-6, Membrane, PVDF, Pervaporation*

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BLANCHING AND OSMOTIC DEHYDRATION EFFECTS ON LYOPHILISED SHRIMP

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Abstract

Shrimp is the most widely consumed seafood worldwide, both as an ingredient in various dishes and as a tasty snack. Like many food products with high moisture content, shrimp are subjected to various drying processes. Among these drying systems, lyophilisation is the method that preserves the nutritional values and the unique taste and texture of shrimp the most. In this study, the effects of blanching, blanching in saltwater and saltwater osmotic dehydration pretreatments on the lyophilisation processes of shrimp were investigated. The effective moisture diffusion coefficient was calculated with the data obtained from the drying process and their compatibility with mathematical models was tested. Drying processes were completed between 240 - 360 minutes. It was observed that drying times could be reduced by blanching and osmotic dehydration applied before lyophilisation. It was determined that the initial moisture content could be highly reduced by blanching. In the compatibility with mathematical models, control and blanched samples were fitted with Alibas model and osmotic dehydration samples were fitted with Midilli et al. model with R^2 values higher than 0.99999.

Key Words: *Blanching; Freeze-Drying; Osmotic dehydration; Saltwater; Shrimp*

Nanomaterial-Modified Carbon Paste Electrode-Based Biosensor for the Investigation of Apigenin in Real Samples

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Abstract

The Apigenin is a naturally occurring flavonoid that has gained significant attention due to its strong antioxidant, anti-inflammatory, and anticancer properties (Zhang et al., 2015). It is abundantly found in various plant-based foods, such as parsley, chamomile, and celery, and has been extensively studied for its therapeutic effects on human health. Studies indicate that apigenin plays a crucial role in modulating key biological pathways involved in immune response regulation, oxidative stress reduction, and inhibition of cancer cell proliferation (Kandemir et al., 2022). However, despite its promising pharmacological attributes, the accurate detection of apigenin in real-world samples remains a challenge due to its complex molecular structure and low concentration levels in biological matrices.

This study aims to develop an electrochemical biosensor based on a nanomaterial-modified carbon paste electrode (CPE) for the selective and sensitive detection of apigenin. The electrode surface was modified with [specific nanomaterial, e.g., graphene oxide, gold nanoparticles], enhancing its conductivity and providing a larger surface area, which led to improved electrochemical performance (Cammann et al., 1991). The detection mechanism was systematically evaluated using cyclic voltammetry (CV), differential pulse voltammetry (DPV), and square wave voltammetry (SWV) techniques (Wang, 2002).

Additionally, the interaction between apigenin and DNA was explored to better understand potential binding mechanisms, including intercalation, groove binding, and electrostatic interactions (Waihenya et al., 2021). The biosensor demonstrated high sensitivity, excellent selectivity, and a low detection limit, making it a reliable tool for real sample applications. To validate its efficiency, the sensor was applied to the analysis of [specific samples, e.g., herbal extracts, biological fluids], confirming its suitability for pharmaceutical and biomedical research.

Compared to conventional techniques such as spectrophotometry and chromatography, this biosensor provides a cost-effective, rapid, and environmentally friendly alternative for apigenin detection (Jordan, 2021). This research contributes to the field of electrochemical biosensing by introducing an innovative and efficient method for detecting bioactive compounds in complex sample matrices.

Key Words: Biosensor, Apigenin, DNA Interaction, Electrochemical Sensor, Carbon Paste Electrode, Voltammetry

Funding: This work was supported by the Scientific Research Projects Coordination Department of Van Yüzüncü Yıl University (Project no:11821)

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Eucalyptol-Based Liquid-Liquid Microextraction Coupled with Gas Chromatography for the Determination of Phthalates in Bottled Water Samples

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Phthalates, a subgroup of endocrine-disrupting compounds (EDCs), are among the most hazardous chemicals to human health. Their accurate determination and continuous monitoring in everyday products are crucial for public health protection, as phthalates are suspected of contributing to various diseases, including hormonal disorders, infertility, and hormone-dependent cancers. This necessitates the development of advanced analytical methods capable of detecting phthalates in complex sample matrices at low concentration levels. However, many existing procedures rely on toxic organic solvents for sample preparation, posing environmental and health concerns. To minimize their impact, it is essential to develop new analytical methods aligned with the principles of green analytical chemistry (GAC).

In response to this need, a novel analytical procedure involving eucalyptol-based liquid-liquid microextraction (LLME) coupled with gas chromatography-mass spectrometry (GC–MS) has been proposed for the determination of selected phthalate esters (PAEs) in bottled water samples. The effects of extraction assistance type and extraction time on extraction efficiency were evaluated. The method achieved limits of quantification (LOQs) ranging from 0.27 to 0.72 $\mu g \cdot mL^{-1}$. Additionally, relative recoveries ranged from 76% to 131%, with relative standard deviations below 6% for most of the analyzed compounds.

Synthesis, Characterization and Usage of Graphitic Carbon Nitride (g-C_3N_4) Species in pH-Controlled Drug Delivery

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ABSTRACT

Nanotechnological applications have a broad usage area in the development of drug delivery systems in both developed and developing countries, particularly in the diagnosis and treatment of chronic diseases (Ochekpe ve ark., 2009). In this study, the synthesis of g-C_3N_4 was carried out using thermal and chemical transformation methods under specific conditions (Papailias ve ark., 2018). The synthesized nanomaterials were characterized and compared using FT-IR, BET, Zeta potential, and SEM analyses. The FT-IR analysis identified the chemical structure and functional groups of g-C_3N_4 for determining the physicochemical properties of the nanomaterial. SEM analysis was used to examine the surface and morphological properties of the nanomaterials. Their specific surface area and pore volume were determined by the Brunauer-Emmett-Teller (BET) method. The g-C_3N_4 synthesized by the thermal method exhibited high adsorption capacity with a BET surface area of 7.4580 m^2/g and a Langmuir surface area of 9.4625 m^2/g, showing a large pore structures and mesopores. In contrast, the g-C_3N_4 synthesized by the chemical method had a lower capacity, with a BET surface area of 2.6809 m^2/g and a Langmuir surface area of 3.2511 m^2/g, displaying a macropore structure. These results indicated that the g-C_3N_4 synthesized by the thermal method had high adsorption capacity and small pores, while the g-C_3N_4 synthesized by the chemical method had a wider pore structure. Additionally, the zeta potential was measured to evaluate their surface charge and stability. It was concluded that the average size of the g-C_3N_4 synthesized by both methods were approximately 1600 nm, and there was no statistically significant difference between them.

A fluorescent drug, irinotecan was loaded onto g-C_3N_4 particles synthesized by thermal and chemical methods. The loading of the drug was confirmed by FT-IR analysis. The release amounts of irinotecan from the drug-loaded g-C_3N_4 were studied at various pH levels, including 2.2, 4.0, 6.0, 7.4, and 8.6, using buffer solutions. The drug release percentages were calculated using fluorescent spectroscopy (Cagil, 2020). According to the results, pH-controlled release amounts depend on the effect of the synthesis mechanism of the g-C_3N_4 such as thermal and chemical methods.

As a result, it was concluded that g-C_3N_4 could be effectively used in drug delivery systems, and particularly, the thermal method, with its high adsorption capacity, could enhance the drug delivery potential.

Keywords: Pharmaceutical, g-C_3N_4, Drug delivery, Irinotecan, Nanoparticle.

A NOVEL PERSPECTIVE ON LATERAL FLOW ASSAYS: FLUORESCENCE PROTEIN-PEPTIDE APTAMERS

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Abstract

Lateral flow assay (LFA) systems are simple-to-use, disposable diagnostic devices that can test biomarkers in samples such as saliva, blood, urine and food. LFAs have received significant attention in recent years, especially during the pandemic period, as it is a powerful tool in analyte determination and sample analysis. LFA systems are a promising pre-diagnostic alternative to costly, time-consuming and laboratory equipment that requires trained personnel [1, 2]. Within this research, a fluorescent protein labelled peptide aptamer-based lateral flow analysis system is designed for the analysis of CTX-M type enzymes, a group of a-class extended-spectrum β-lactamases (ESBLS) spreading rapidly among enterobacteriaceae worldwide. For this purpose first, peptide aptamers for the CTX-M enzyme was developed using the mRNA display method. The peptide aptamer, a unique recognition element for the CTX-M enzyme and was generated within the project for the first time. The design of the peptide aptamer library used for the *in vitro* selection of peptide aptamer sequences specific to the CTXM-1 enzyme was carried out and the primer sequences used in PCR amplification were determined. *In vitro* transcription conditions of the resulting peptide aptamer DNA library were optimized. The working conditions of the NEB PurExpres *in vitro* protein synthesis kit, which will be used throughout the mRNA display tours, have been optimized. Functionality of the *in vitro* protein synthesis kit was confirmed using the plasmid DNA encoding dihydrofolate reductase (DHFR) provided in the kit and the CTXM-1 cloned pET-28a vector.

Key Words: *Lateral Flow Assays; Conjugation; CTXM-1; Peptide Aptamer; Fluorescence Protein*

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Acknowledgements

The financial support from The Scientific and Technological Research Council of Türkiye (Grant number: 122Z354) is gratefully acknowledged.

Evaluation of smart packaging functions of black carrot extract with polysaccharide-based films

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Abstract

The expression "smart packaging" describes systems for enclosing food, medication, and several other products that have sensors inside. This technology, which generally has many positive outcomes, has the potential to increase product and customer safety, monitor freshness, provide quality information and extend shelf life. By the year 2024, the smart packaging industry has the potential to grow to a value of $26.7 billion globally [1]. Composite films based on biopolymers and active compounds derived from waste offer great opportunities to reduce the destructive overuse of plastic-based packaging. In this study, we aimed to evaluate the characteristic changes in polysaccharide-based films production from carrot waste with pectin (P) and development alginate (A) matrix with black carrot extract (BC). It has been reported that black carrot and carrot can be used in the development of biopigment-rich functional sustainable films [1,2]. To produce pectin from carrot waste to be used in the film matrix, the extraction process of pectin was treated by using acidific extraction conditions: pH 1.1; temperature 80 ^{o}C; heating time 90 minutes. Carrot pectin extraction yield under these conditions was determined to be geneally 17.71%. The casting method was employed for the preparation of A/P and A/P/BC films. Carrot pectin in different concentrations (0-1% w/w) with alginate solution (2% w/w) and black carrot extract (0.2; 0.4 and 0.6% v/v) were prepared in this study. The results showed that pectin concentration had a significant effect on increasing the opacity, swelling and moisture content values of the film samples and decreased the mechanical strength of the films. Furthermore, opacity and mechanical strength increased and moisture content decreased as the amount of black carrot extract added to the films increased. Overall the results, indicated that carrot and black carrot extract could be used in the development of smart packaging film**.** Making these composite films can be an innovative approach to deal with food waste that otherwise would have been thrown away and have an impact on the environment. Although, this idea has the potential to produce sustainable bio-based packaging as well as reducing waste output.

This research was financially supported by the Çanakkale Onsekiz Mart University Scientific Research Projects Coordination (Grant Number FYL-2024-4900).

Key Words: *Smart packaging; film; waste; sustainable*

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In silico insight on Hyaluronic acid and Boron-hyaluronate

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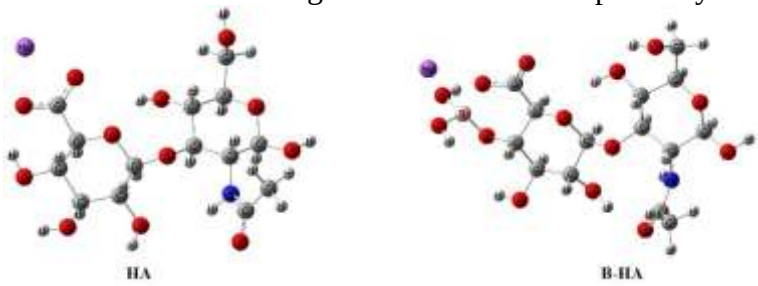
Abstract

Hyaluronic acid, a natural and unbranced polymer, is a member of heteropolysaccharides, and pioneering research on HA goes back to the 1880s. HA and related molecular systems are getting increasing attention due to including the hydroxyl, carboxyl, acetamido, and anomeric carbons, which gain them structural advantages [1]. The viscoelasticity and hyrophilicity nature of these kinds of compounds with biocompatible and degradable properties make them very useful in biomedicinal applications such as regenerative medicine and target-specific therapies. Nowadays, *in silico* investigations provide great advantages in early-stage drug design via saving the time- and source- consuming in the related processes. First, the quantum mechanic simulations of HA and B-HA systems are performed by G09W [2] package to predict the main structural, electronic, and possible reactivity characteristics, at DFT/B3LYP level [3,4]. In this regard, FMO and MEP analyses [5] are employed to provide an insight into the possible reactivity tendency and regions of the studied molecular systems. Last, the physicochemical properties and pharmacokinetics of the compounds are computed by SwissADME [6] tools to evaluate the drug-likeness and biocompatibility.



Scheme 1. The chemical structures of the HA and BHA salts

Key Words: *Hyaluronic acid, Bor-hyaluronate, DFT, bioavailability*

Acknowledgments

All calculations have been carried out at TUBITAK ULAKBIM, High Performance and Grid Computing Center (TR-Grid e-Infrastructure). The author thanks the Scientific Research Projects Department of Cumhuriyet University (Project No: EĞT-2024-099).

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INFRARED DRYING OF ARONIA BERRIES: THE EFFECT OF SUSTAINABLE PRETREATMENTS ON DRYING BEHAVIOR

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Abstract

Drying is a traditional and highly effective physical food preservation method widely used in the food industry for both direct product preparation and further processing [1]. This technique reduces packaging needs by decreasing the volume and lowers transportation, storage, and processing costs; while extending the shelf life and enhancing the product value [2]. This study investigates the drying of aronia berries by using infrared drying method and examines the effect of ultrasonic pretreatment on drying efficiency. Aronia berries are of great importance as functional foods, due to their high antioxidant contents. Nevertheless, maintaining their nutritional value while ensuring an efficient drying process is crucial. To address this issue, ultrasonic pretreatment was applied to evaluate its impact on the infrared drying process. The experimental study was conducted by selecting drying temperatures of 60°C, 70°C and 80°C. For each drying temperature, aronia berries underwent ultrasonic pretreatment for durations of 1, 3, 5, 10 and 15 minutes before being dried. The drying durations of pretreated samples were compared to those of untreated samples. During the experiments, parameters such as drying time and moisture loss rate were assessed, and the obtained data were analysed in terms of drying kinetics. The kinetic parameters, including effective moisture diffusivity (D_{eff}) and activation energy (E_a), were determined and drying curves were modelled. The results indicate that ultrasonic pretreatment significantly accelerated the drying process at 80°C. This finding suggests that the combination of ultrasonic pretreatment and infrared drying enhances the drying efficiency, while potentially preserving the nutritional properties of the fruit. The study contributes new insights into the use of infrared drying for delicate food products like aronia berries, and offers valuable information for advancements in food drying technologies.

Key Words: *Aronia berry; drying; drying kinetics; infrared drying; ultrasonic pretreatment*

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The Impact of Metal Industry Waste on the Agricultural Development and Yield Increase of Tea Plants

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Abstract

The use of chemical inorganic fertilizers in agriculture has become essential for meeting the nutritional needs of the growing human population. In addition to nitrogen, phosphorus, and potassium, the presence of trace elements also plays a significant role in enhancing agricultural yields and supporting plant development. Today, the utilization of industrial wastes as a source of trace elements within the framework of the circular economy presents a viable alternative. This approach is gaining attention both among chemical fertilizer producers and within regulatory frameworks governing fertilizer production.

In this study, the effects of a metal plating industrial waste—characterized for its trace element composition—on the growth of tea plants were investigated. The waste material was incorporated into the fertilizer production process, and its potential toxic effects on tea plants were evaluated. The toxicity threshold was determined, and process optimization was carried out. As a result, important statistical data were obtained regarding the extent to which metal industry wastes can be utilized in agricultural lands within the scope of the circular economy.

Key Words: *Circular economy, heavy metal, chemical fertilizer, agricultural yield, process optimization*

SYNTHESIS, CHARACTERIZATION AND PHOTOCATALYTIC PERFORMANCE OF MODIFIED $Cd_{0.7}Zn_{0.3}S$

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Abstract

$Cd_xZn_{1-x}S$ has gained significant attention due to its adjustable optical properties, making it a promising candidate for photocatalytic hydrogen production [1]. MoS_2 is utilized as an additive in semiconductor photocatalysts because of its large surface area, ability to prevent charge recombination, low cost, high reactivity in the H_2 evolution reaction, and enhanced sensitivity to visible light [2]. Transition metal carbides, such as Mo_2C, are excellent electrocatalysts for hydrogen production and also function as effective cocatalysts for various photocatalysts [3]. In this study, $Cd_{0.7}Zn_{0.3}S$ photocatalyst modified by MoS_2/MoC-Mo_2C was synthesized to achieve highly efficient photocatalytic H_2 production and improve the stability of the photocatalyst. Hydrogen production was observed at a rate of 37 mmol g^{-1} h^{-1} with bare $Cd_{0.7}Zn_{0.3}S$ nanorod. However, this rate increased 3.5-fold to 132 mmol g^{-1} h^{-1} for N-$Cd_{0.7}Zn_{0.3}S$/1% MoS_2 following the incorporation of MoS_2. Furthermore, the N-$Cd_{0.7}Zn_{0.3}S$/1%MoS_2/1%MoC-Mo_2C composite, which was consistent with photoelectrochemical measurements, demonstrated a 4.5-fold increase in hydrogen production, reaching 168 mmol g^{-1} h^{-1}.

Key Words: *Green Energy; Photocatalytic H_2 Production, $Cd_xZn_{1-x}S$, MoS_2, MoC-Mo_2C*

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EVALUATION of DIFFERENT FILLER MATERIALS on GLASS FIBER REINFORCED POLYMER COMPOSITES for the AUTOMOTIVE INDUSTRY

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Abstract

Composite materials were developed through intensive research in materials science as a result of the failure of pure materials to meet the performances demanded in sectors such as automotive, aerospace and defense over the years. In line with the developments in the composite industry, studies are implemented to improve performance with fillers and reinforcements. Considering both cost and accessibility, research on the reuse of waste materials is rapidly increasing and producing sustainable solutions. [1,2] Disposal of organic waste produces greenhouse gases that will affect climate conditions. Instead of a disposal process, it is possible to convert it into a carbon based product called Biochar which can be used as a filler in polymer composites. [3]

In this study, the effect of conventional and bio-based flame-retardant fillers on glass fiber reinforced polyester composites was investigated. Biocarbon was used as a bio-based and environmentally friendly additive, which can replace with aluminum trihydrate that is one of the conventionally preferred flame-retardant chemicals. Composite production in various compositions was carried out open mold lay-up method. Apart from the control sample, 2 different compositions were determined and glass fiber reinforced composite was produced. Synergistic effects were observed when conventional and bio-based additive materials were used together in the structure. Glass fiber discontinuous mat and plain-woven glass fiber were used as reinforcement materials. At the end of production, 3 composite plates were obtained. Tensile, three-point bending and impact tests were performed to investigate the mechanical properties of the produced samples. The flame retardant characteristics were evaluated by horizontal burning test (UL 94 HB) to compare the effects of filler materials. The results of the tests applied to composites containing aluminum trihydrate, biocarbon and hybrid structures were compared. Results showed that the biocarbon-added samples showed higher tensile, bending, impact resistance and flame-retardant properties than the unfilled composite. As a result, it was observed that biocarbon-added composites can compete with the functionality provided by conventional additive materials and show sufficient performance to be used in the automotive industry.

Key Words: *Aluminum Trihydrate, Biocarbon, Filler, Glass fiber, Polymer composites*

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Mechanical Performance of Glass Fiber/Polyester Composites Containing Biofiller for the Automotive Applications

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Abstract

Polymers reinforced with bio-based fillers are being used as substitutes for plastic components to enhance environmental sustainability. The present study aims to investigate the effect of adding biofiller in different particle sizes on the mechanical properties of glass fiber reinforced polyester composites produced by hand lay-up method. Glass fiber reinforced polyester composites developed with the eggshell powder additive, which is in the bio-structured filling material class. Commercially obtained eggshells were sieved with a graduated sieve (100-500 μm). Three different composites were fabricated using eggshell with two different particle sizes at 10 wt.% filler loading. Within the scope of the study, mechanical properties of the obtained composites were determined using three-point bending and impact tests according to ISO 14125 and ISO 179-1 standards, respectively. From the experimental investigation, it was revealed that, the particle size of the eggshell affected the final properties of composites. The mechanical characterization results showed that the impact strength of eggshell incorporated composites were slightly reduced in comparison to neat glass fiber reinforced polyester composites. The results of the study will provide added value to eggshell, which is abundant in the environment that will enable the production of more environmentally friendly composites.

Key Words: Eggshell; Glass Fiber; Particle-reinforced composites; Polymer composite; Sustainability.

Acknowledgements

This work has been supported by the Research Fund of Bursa Technical University (Project Number: 240Y019).

OBTAINING VALUABLE COMPONENTS FROM VARIOUS CITRUS PRODUCT WASTES BY DIFFERENT EXTRACTION METHODS

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Abstract

This study aimed to obtain valuable components from various citrus product waste using different extraction methods as conventional and ultrasonic-assisted extractions. Wastes obtained from orange, tangerine, and lemon fruits, the three most commonly grown citrus fruits in Türkiye and around the world, were used as raw material sources [1]. Ultrasonic-assisted extraction, one of the green extraction techniques, was used to obtain valuable components from orange, tangerine, and lemon citrus fruit wastes. Green extraction techniques stand out with features such as higher efficiency, less time requirement, and less cost when compared to traditional extraction techniques [2]. By comparing the above-mentioned extraction techniques, multifaceted comparisons were made between the citrus types used as raw materials and the properties of the valuable components to be obtained. The valuable components targeted to be extracted from citrus fruits were determined as pectin and hesperidin considering their industrial usage areas [3]. Ultrasonic-assisted extraction method was used to prevent the environmental damage caused by traditional extraction methods used in the disposal processes of citrus waste or in obtaining valuable components. Citrus fruit wastes were dried, and moisture content of each citrus species were determined then citrus species were extracted by using conventional and ultrasonic-assisted extraction methods. In the analysis of the obtained extracts, data close to optimized values were obtained by using Fourier Transform Infrared Spectrometry (FTIR) and Ultraviolet-Visible Spectrometry (UV-VIS) analyses. According to UV-Vis analysis; band, covering the range of 240–280 nm (max absorbance around 255–265 nm) attributed to the A–C benzoyl system confirming the flavonoid structure. All extracts showed similar peaks in FTIR analysis [4]. It is envisaged that the extracted valuable components will be used in various industrial areas. In the future, it is aimed to add the bioactive component data obtained as extracts to the literature.

Key Words: *Citrus waste; extraction; bioactive component; quantitative analysis*

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Acknowledgements

The work was financial supported by Yıldız Technical University Scientific Research Project Coordination Research Fund (Project Number: FHD-2024-6329).

Fabrication and Filtration of Arabic Gum Doped Electrospun PLA Membrane for Rejection of Gray Water Pollutants

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Abstract

Today, with increasing global warming and climate change, water scarcity is one of the most important environmental problems that urgently needs to be addressed [1]. Among the measures taken against water scarcity, water use reduction, rainwater harvesting and gray water treatment systems are promising. Gray water is wastewater from domestic activities such as bathrooms, washing machines, dishwashers and kitchens [2]. The properties of gray water vary according to its source. Gray water, especially water from washing machines, may contain pollutants such as organic matter, oil and grease, nitrate, suspended solids, phosphorus, surfactants and dyes [3]. The electrospun nanofibers produced have the potential to remove organic and inorganic pollutants from wastewater due to their tunable wettability, high length-to-diameter ratio and surface morphology. Gum arabic (AG) is a compatible, inexpensive and functional additive that will complement the deficiencies of polylactic acid (PLA) material and make it suitable for membrane material, simultaneously improving its hydrophilicity, mechanical strength, elasticity, antimicrobial properties, separation performance. In this study the nanofiber membrane of an AG doped PLA electroscope for gray water filtration was produced by an electro spinning technique. AG was added to the PLA membrane at different ratios (1-5 wt%). According to the results of FTIR and SEM analysis, PLA membranes were successfully produced. As a result of methylene blue filtration with PLA membrane, it is seen that there is over 93% rejection. With the addition of AG, methylene blue rejection increases by 99%. Emulsified oil rejection was 87% in the membrane with 2% AG additive. Approximately 50% rejection is observed in LAS filtration and 100% rejection is observed as a result of microplastic filtration. It was observed that the surface contact angles of PLA membranes without AG were 127º and decreased by about 10º to 118º as the additive ratio increased and increased hydrophilicity. The membrane prepared without the addition of AG has a tensile strength of about 7 MPa. The addition of AG increased the tensile strength to 11.8 MPa at 4 wt% and significantly increased the mechanical strength and elasticity.

This research was supported by the Çanakkale Onsekiz Mart University Scientific Research Projects Coordination Unit (BAP) and Grant Number FYL-2024-4825.

Keywords: *Electrospinning; filtration; grey water; multiple impurities; polylactic acid.*

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Green Tea-boron nitrite incorporated pumpkin pectin-alginate food packaging film preparation and characterization

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Abstract

Petroleum-based packaging poses a major environmental threat to life on Earth. This type of packaging does not degrade in nature for many years and causes environmental pollution as it is difficult/costly to recycle. Packaging is used in food storage to preserve food quality, ensure food safety and extend shelf life. With the increasing need for food in the world, the demand for packaging materials is also increasing. It is therefore difficult to strike a balance between the use and recycling of packaging. Efforts should be made to design food packaging according to the type of food, to produce it in an environmentally friendly way and to be applicable in food packaging systems [1,2]. Within the scope of this study, smart food packaging films that are biodegradable, increase the shelf life of food, antimicrobial, pH-sensitive and have sensor properties have been produced to utilize the agricultural residues left by the farmers after the harvest and bring them into the economy. In this study, pectin was obtained from pumpkins and mixed with alginate to make biodegradable packaging films. The aim of the study is to obtain a food-usable packaging with high strength, low water permeability, antimicrobial and biobased renewable resources. Within the scope of the study, green tea extract was added up to 1% as an antioxidant to increase water permeability and strength. Boron nitride nanoparticles (nBN) were added to the film up to 1% to increase antimicrobial properties. The degree of opacity, degradation/dissolution tests in water and simulated foods with different pH levels, mechanical analysis and antimicrobial activities of the films were measured. Both mechanical strength and antimicrobial properties of boron nitride added films increased. According to the soil degradability test, the degradation rate of green tea added films in 70% moist soil was higher than pure and boron nitride films and it was observed that all films were completely degraded in an average of 2-4 weeks.

This study was financially supported by the Çanakkale Onsekiz Mart University Scientific Research Project Coordination (Grant Number: FBA-2024-4847).

Keywords: *Pumpkin pectin films; boron nitride; green tea extract; food package*

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THE EFFECT OF MODIFIERS ON THE MICROSTRUCTURE OF ROAD BITUMEN AND STRENGTH OF ASPHALT CONCRETE

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Abstract

This work reports a significant improvement in the strength of asphalt concrete and a reduction in the size of bee-like structures of road bitumen by modifying with additives. This required studying the changes in distribution of microdispersions in binary and triple bitumen compositions from the concentration of additives, as well as determining the strength characteristics of modified asphalt concrete. The following chemicals have been used as additives: the original product AS-1 and used sealant AG-4I, a product based on polyisobutylene and petroleum oils. The Atomic Force Microscopy makes it possible to obtain a digital model of the topographic surface of bitumen in the form of an image [1-2] to establish the effect of the studied surfactant (AS-1) and polymer (AG-4I) additive on the microstructure of the bitumen. To assess the effect of bitumen dispersion on the physical and mechanical characteristics of modified asphalt concrete samples, the ip-100m-auto test press was applied to determine the compressive strength.

The results show that the determining factor for strength of asphalt concrete samples is the average size of the bee-like structures of bitumen. As a result of intermolecular interactions between additives and bee-like structures of bitumen, the size of microassociates, the density of their distribution in the dispersion medium of the binder, and, accordingly, the strength of asphalt concrete change.

It has been established that the condition for achieving the minimum size of bee-like structures is the introduction of 1.0 g/dm^3 AG-4I and 1.0 g/dm^3 AS-1 into the bitumen; the average size of dispersions is 1.66 μm. In these concentration regimes, as a result of simultaneous exposure to AG-4I and AS-1, fractions with a size of more than 4.0 μm were completely destroyed, and aggregates in the range 2.0–4.0 μm were destroyed two times; the content of fine fractions (≤2.0 μm) increased by 57.4% compared to virgin bitumen and amounted to 81.9%.

A close correlation was revealed in the nature of changes in the dispersed composition of modified bitumen and the strength indicators of asphalt concrete samples. In the asphalt mixture sample made on the basis of the ternary composition “bitumen-AG-4IAS-1” (C_{AG-4I} =1.0 g/dm^3; C_{AS-1}=1.0 g/dm^3), the maximum increase in compressive strength was achieved with the smallest size of bee-like structures of modified bitumen. This shows that the modifying role of additives is in the formation of dense, durable asphalt concrete, which is achieved due to the deep disaggregation of bitumen microdispersions and their uniform distribution over the entire volume of the binder.

Key Words: *microstructure of bitumen; strength of asphalt concrete; surfactant; polymer; bitumen modification*

Acknowledgements. This research was funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP19677707).

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Electrospun CuMOF/PLA Nanofibers as Biodegradable Antibacterial Membranes for Biomedical Applications

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Abstract

Bacterial spread and infections are remaining as a critical challenge in biomedical application with the rise of sustainability and biodegradability issues with in-use materials. An antibacterial fibrous membrane employing high antibacterial efficiency has great potential in healthcare applications**.** Electrospinning technique has excellent advantages such as tunable functionality, thin fibers with large surface areas, ease of processing and good physical properties and provides wide usage area with these advantages in biomedical applications. The study focuses on the development of antibacterial and biodegradable fibrous membranes composed of polylactic acid (PLA) integrated with copper-based metal organic frameworks **(**CuMOF**)**. The CuMOF/PLA membranes were designed to create environmentally friendly and anti-infection membranes to be used in biomedical applications primarily as wound dressing. The membrane production was carried out with electrospinning, a versatile and facile to scale method in production of nanofibers. Copper based MOFs were chosen and incorporated into PLA at concentrations ranging from %0.1 and %8 by weight to enhance antibacterial effect and membrane formation due to the high conductivity of copper. The solvent system was also studied and a binary system of dichloromethane (DCM) and dimethylformamide (DMF) found to be optimal with enhanced yield, reduced crystal sizing and improved coordination between metal and ligand particles [1]. SEM images showed that compared to PLA membranes the addition of the MOFs significantly reduced the bead formation and supported the uniformity of fiber structures. CuMOF/PLA integrated membranes show over 99.70% antibacterial effect against common wound-infecting bacteria [2]. The study confirms that incorporation of the CuMOF into PLA membranes via electrospinning is a facile and effective method of antibacterial material production. Copper based MOF included in electrospun mats provide antibacterial activity suitable to be used to prepare membranes for various biomedical applications.

Key Words: *CuMOF, Metal organic frameworks, Electrospun membranes, Antibacterial activity, Wound dressing*

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DEVELOPMENT OF L-ASPARAGINASE-ENZYME IMMOBILIZED CU(II)-NANOPARTICLES AND CHARACTERIZATION OF BINDING PROCESS VIA SPR SENSOR

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Abstract

L-asparaginase (L-ASNase) is a key chemotherapeutic agent used in the remission induction treatment of acute lymphoblastic leukemia (ALL). Despite its effectiveness, L-ASNase, derived from bacterial sources such as Escherichia coli and Erwinia chrysanthemi, has a notably short in vivo half-life. Furthermore, its therapeutic use is often associated with significant side effects. These limitations highlight the need for strategies to extend the enzyme's half-life and reduce its adverse effects. Recently, the half-life of L-ASNase has been extended, and some side effects have been mitigated through pegylation, where the enzyme is coated with polyethylene glycol (PEG). However, this approach has certain drawbacks, including reduced enzyme activity both in vitro and in vivo. As a result, achieving the same therapeutic effect requires larger doses of the PEG-coated enzyme, which is less than ideal. Consequently, there is a pressing need to develop alternative strategies to prolong the enzyme's half-life in the bloodstream while maintaining its activity with minimal dosage, ultimately leading to more effective treatment. Enzyme immobilization presents a promising solution to these challenges by enhancing enzyme activity, stability, and reusability. This technique involves attaching the enzyme to a solid support material, which prevents aggregation and denaturation while allowing for better control over its functional properties. For enzyme immobilization, it is crucial that the support materials are non-toxic, enable efficient mass transfer with minimal diffusion resistance, and are capable of preventing enzyme degradation. In this study, we developed nanoparticles composed of p(2-hydroxyethyl methacrylate-N-methacryloyl-(L)-histidine methyl ester) that were chelated with Cu(II) ions, referred to as poly(HEMAHCu(II)). We then investigated the immobilization of L-asparaginase (L-ASNase) onto these polymeric nanoparticles, using a surface plasmon resonance sensor (SPR) to monitor the process. This study aimed to enhance the thermal and storage stability of L-ASNase. We analyzed the immobilization process using L-ASNase concentrations ranging from 250 to 3000 UI, passing the enzyme through a surface plasmon resonance sensor (SPR) chip based on poly(HEMAHCu(II)) nanoparticles. Successful binding was confirmed by monitoring the percentage change in the refractive index recorded on the SPR sensor. Using SPR sensors to demonstrate the immobilization process is particularly effective, as they provide real-time analysis of the interactions.

Key Words: *L-asparaginase, Enzyme, Polymeric Nanoparticles, Immobilization, Sensor system*

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ANTICANCER DRUG RELEASE FROM GRAPHENE OXIDE/BACTERIAL CELLULOSES

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Abstract

Cancer is a disease in which growth control is lost in one or more cells. It can occur as a liquid or solid mass called a tumor [1, 2]. Since many people around the world die of this disease, powerful treatment methods are needed [3]. It can be treated with methods such as chemotherapy, radiotherapy, and surgery. Chemotherapy aims to selectively destroy tumor cells or limit their proliferation using classical anticancer drugs [1, 2]. Chemotherapeutic drugs are classified according to their mechanism of action and chemical structure: alkylating agents, topoisomerase I and II inhibitors, antibiotics, antimetabolites, mitosis inhibitors, platinum compounds, etc. [3]. Antimetabolites are the oldest class of anticancer drugs, acting through their interaction with essential biosynthetic pathways. Antimetabolite class anticancer drugs, such as widely using 5-Fluorouracil (5-Flu), are structural analogs of pyrimidine and purine, and these compounds inhibit the synthesis of nucleic acids by incorporating them into cellular components [1]. 5-Flu is widely used in the treatment of many types of cancer, including colorectal and breast cancers, as well as respiratory and digestive system cancers [4]. 5-Flu showed considerable toxicity when administered by intravenous injections or via the alimentary tract [5]. Controlled transport of 5-Flu is very important, and the development of new composite materials is necessary for this. This study developed a new material based on bacterial cellulose (BC) added with graphene oxide (GO). Bacterial celluloses were produced using the bacterium *Gluconobacter xylinus* (ATCC 10245). The material was characterized by Fourier Transform Infrared Spectrometry and Scanning Electron Microscopy. 5-Flu loaded with adsorption method into GO/BC composites. The release kinetics of 5-Flu from GO/BC into phosphate buffer simulating the body environment was studied. When cumulative release was examined, 72% of 1000 ppm 5-Flu was released four days in a controlled manner. Considering the adverse side effects of excessive intake of 5-Flu, controlled release of 5-Flu from GO/BC composite material seems promising for use in cancer treatments.

Key Words: *Drug delivery, anticancer, bacterial celluloses, graphene oxide*

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$NiCo_2O_4$/S,N-codoped Graphene Oxide/Nafion/GCE nanocomposite electrode material for energy storage applications

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Abstract

As a conventional energy storage system, supercapacitors have advantages such as low cost, fast charge/discharge, long cycle life, and low internal resistance. For high performance supercapacitors, the development of electrode materials is significant. Among the existing transition metal oxides, Nickel cobaltite ($NiCo_2O_4$) has a high theoretical capacitance, which has attracted much attention [1]. $NiCo_2O_4$ has been shown to exhibit excellent electrochemical performance, with a greater number of electroactive sites in comparison to both NiO and Co_3O_4. In addition, it has been demonstrated to possess a minimum of two orders of magnitude higher electrical conductivity [2]. Consequently, $NiCo_2O_4$ has emerged as a novel class of energy storage materials for electrochemical supercapacitors and it exhibits both high power density and high energy density [3]. However, $NiCo_2O_4$ electrode materials have disadvantages such as poor intrinsic conductivity, agglomeration, and thus significantly reduce the rate capacity and cycling stability of supercapacitors. Therefore, various carbonaceous materials (carbon nanotube, carbon fiber, graphene, activated carbon etc.) have been used as additives or supports to improve the electrical conductivity and dispersion of $NiCo_2O_4$ nanoparticles. Among them, graphene has been used to produce composite materials with $NiCo_2O_4$ recently due to its ultra-high electrical conductivity, large specific surface area, natural flexibility and great mechanical strength [4]. The performance of the system is considerably improved by the use of heteroatom-doped graphene-based materials as supercapacitor electrode materials. Graphene oxide (GO) shows higher capacitance than graphene due to an additional pseudo-capacitance effect of the attached oxygen-containing functional groups in its basal planes. Due to its higher capacitance, shorter processing time, and lower cost, graphene oxide may be a better choice than graphene as an electrode material for supercapacitor applications. It has been reported in the literature that heteroatom doping of graphene oxide improves the energy storage performance [5,6]. Doping GO with two different heteroatoms is a promising approach to further improve the catalytic performance. Sulfur- and nitrogen-doped graphene oxide (S,N-codoped GO) was prepared in a single step.

Considering the excellent properties of S,N-codoped GO and $NiCo_2O_4$, we report herein the $NiCo_2O_4$/S,N-GO/Nafion/GCE nanocomposite electrode was prepared. The structural and morphological properties of the hybrid nanocomposite electrode composed of $NiCo_2O_4$ nanostructures, S,N-codoped GO and Nafion were investigated by FTIR and SEM analyses. Cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and galvanostatic charge-discharge (GCD) measurements in 6 M KOH aqueous solution were utilized to evaluate the electrochemical performance of the hybrid nanocomposite electrode.

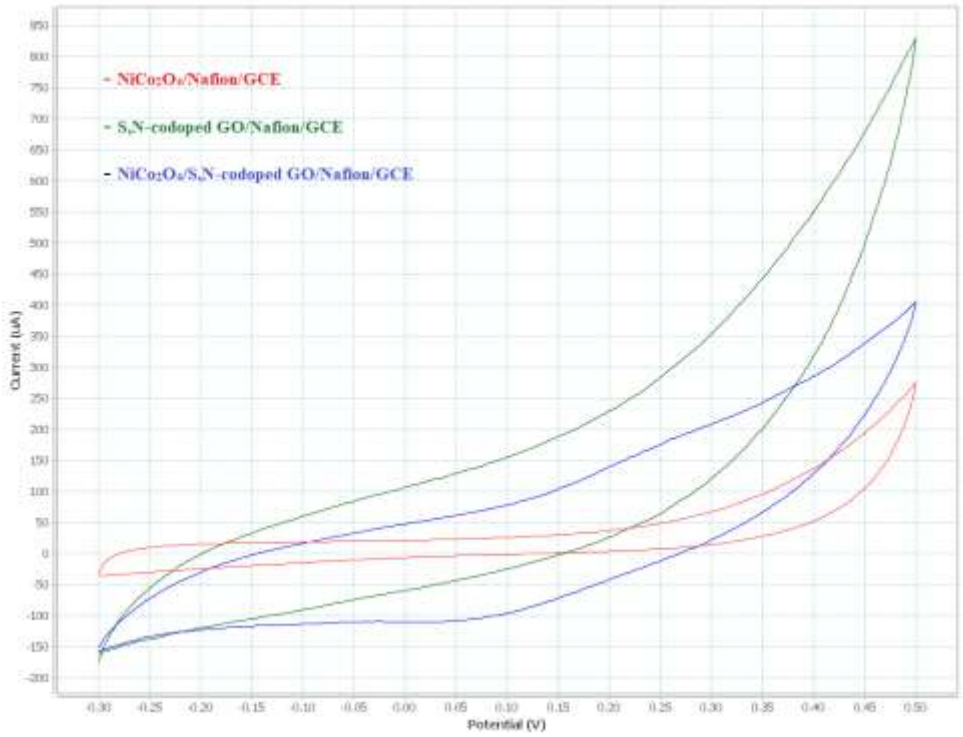

Fig. 1 Cyclic voltmmograms of $NiCo_2O_4$/Nafion/GCE, S,N-codoped GO/Nafion/GCE and $NiCo_2O_4$/S,N-codoped GO/Nafion/GCE nanocomposite electrodes

Key Words: *Nickel cobaltite; S,N-codoped graphenoxide; nafion; nanocomposite; supercapacitor*

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Investigating the Properties of Recycled and Virgin Poly (ethylene terephthalate) Textured Yarns: Effect of Different Blending Ratios

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Abstract

Nowadays, there is an increasing interest on the evaluation of recycled polyester in textile industry due to European Green Deal sustainable goals. The recycling and reuse of polyester from wastes is very desirable however it is still challenging. In this study, it is aimed to investigate the blending of recycled and virgin poly (ethylene terephthalate) to obtain textured yarns. The effect of recycled and virgin poly (ethylene terephthalate) yarns blending ratio (25:75, 50:50, 75:25 % w/w) on the mechanical, thermal and color properties of textured yarns were investigated. The results showed that blending ratio affect the thermal and mechanical properties of the yarns while have no significant effect on dyeability characteristic.

Key Words: *Recycled polyester, Recycling, Sustainable textiles, Textile waste*

FREEZE DRYING OF SQUID: A STUDY TO INVESTIGATE THE EFFECT OF DIFFERENT PRE-TREATMENTS

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Abstract

Among food preservation methods, freeze drying is the method that preserves nutritional and sensory qualities the most. This study investigated the freeze-drying kinetics of different pretreated squid samples and their compatibility with mathematical models. Fresh squid samples were sliced into strips, subjected to eight pretreatments including blanching, blanching with salt, and osmotic dehydration at different salt concentrations, and then freeze-dried. Drying times were between 420 - 600 minutes and pretreatments were found to be effective in decreasing drying time and final moisture content. Effective moisture diffusivity values were calculated between 4.74×10^{-10} - 2.41×10^{-10}. In the compatibility tests of the drying data with the mathematical models, the control samples had an R^2 value of 0.999997 with Two-Term, while all pretreated samples fit the Alibas model with R^2 values higher than 0.99999.

Key Words: *Blanching; Freeze-Drying; Mathematical Modeling; Squid Osmotic Dehydration*

DRUG ANALYSIS WITH MOLECULARLY IMPRINTED POLYMERS FROM ION PAIR COMPLEXES

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Abstract

Until the mid-nineteenth century, nature's remedies were available to alleviate human pain and suffering. Later, the first synthetic drug, “chloral hydrate”, which is still used in some countries, was discovered in 1869[1]. Then, the active ingredient in White Willow, salicylic acid (aspirin), entered the pharmacopeia from the barbiturate family of drugs at the beginning of the twentieth century by a simple chemical modification. In the 1980s, BP and USP recommended different determining methods for salicylic acid in aspirin. Since then, various techniques have been developed to quantify different drug substances in pharmaceutical preparations and biological fluids.

In this presentation, the parts of drug analysis in pharmaceutical forms performed by our research group with spectrophotometric methods based on ion pair complexes and metal-drug complexation reactions were discussed. At the same time, drug analysis studies ranging from pharmaceutical forms to biological liquids were examined voltammetrically. Finally, studies on molecularly imprinted polymers were mentioned. Spectrophotometric and voltammetric studies were compared at the limit of quantification level.

Key Words: *Drug analysis, voltammetry, spectrophotometry, molecularly imprinted polymers*

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Investigation of Metal Organic Framework Based Electrodes for Flow Capacitive Deionization Systems

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Abstract

The drought, caused by global warming and climate change and is becoming more severe and is making it impossible for people to access clean water resources. Billions of people already do not have access to clean water and Türkiye is one of the regions that will be most affected by drought. Therefore, it is very important to increase our water resources. As our country has easy access to seawater, turning salt water into usable or potable water is one of the most practical solutions. The CDI system is one of the most researched topics for desalination process. One of the most important goals is to improve the electrodes used in this system and to be able to selectively adsorb high levels of ions. One of the most important features of the CDI system is its low energy consumption requirement [1]. In this study, metal organic frameworks (MOF) were selected as electrode materials. The chosen MOF is UiO-66-F4. The fluorinated MOFs are known as efficient electrode materials for electrochemical processes. In this study, this material was tested for CDI systems. Graphene nanoplatelets were used as counter electrodes. The results obtained in the experiments conducted in a small volume CDI cell are promising. Figure 1 shows the pre-desalination efficiencies obtained because of 5 cycles, each cycle lasting 5 minutes. For this system, where the electrode surface area is 1 cm^2 and the total cell volume is 10 mL, the highest efficiency obtained is 18% and the salt adsorption capacity is 2 mg/g.

Acknowledgement: This research was supported by TÜBİTAK, project number:223M189

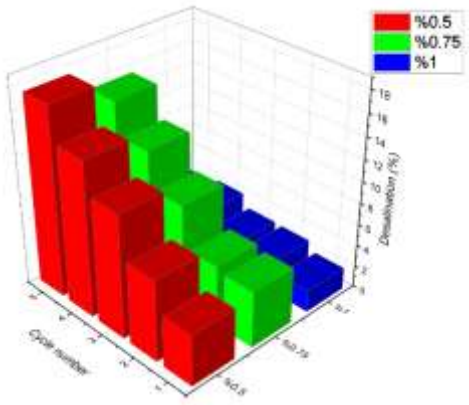

Figure 1: Desalination precentage of UiO-66-F4

Key Words: MOFs; FCDI; Desalination; Electrodes

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DEVELOPMENT and VALIDATION of HPLC METHOD USING MULTIVARIATE OPTIMIZATION for the SIMULTANEOUS DETERMINATION of NIFLUMIC ACID and ITS IMPURITIES

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Abstract

High-performance liquid chromatography (HPLC) is widely used in the analysis of multicomponent pharmaceutical formulations due to its advantages such as speed, ease of automation, specificity, precision, and accuracy in quality control laboratories. To develop and optimize HPLC methods, the effects of multiple variables must be carefully investigated through systematic and well-coordinated studies. Traditionally, HPLC optimization relied on a time-consuming trial-and-error approach, which provided limited insight into analyte separation and interactions among variables. In contrast, experimental design offers a more efficient and practical strategy. This approach enables the simultaneous evaluation of multiple factors and their interactions with a reduced number of experimental runs, making it superior to conventional optimization techniques. Recent studies have demonstrated that the application of experimental design significantly enhances the robustness and reliability of HPLC methods in pharmaceutical analysis [1, 2, 3]

Moreover, HPLC plays a crucial role in drug degradation studies, which are essential for understanding the stability, safety, and efficacy of pharmaceutical products. Identifying and quantifying degradation products under various stress conditions ensures regulatory compliance and supports the establishment of proper storage and handling conditions throughout the drug's shelf life. Furthermore, the validation of HPLC methods is critical to ensure the accuracy, precision, and reproducibility of the results, which are essential for regulatory approval and ongoing product quality control.

In this study, the development and optimization of a sensitive analytical method based on high-performance liquid chromatography with diode array detection (HPLC-DAD) for the simultaneous determination of Niflumic Acid is presented. Chromatographic separations were performed on an Inertsil C8 column (4.6 mm x 150 mm x 5 μm particle size) with a mobile phase consisting of a mixture of acetonitrile and water (with 1/100 acid). The effects of three factors—mobile phase composition, flow rate of the mobile phase and the amount of acid added to the water in the mobile phase—were evaluated. The optimum conditions of the developed HPLC method were determined through experimental design, using a five-level-three-factor design requiring 20 experiments. Forced degradation studies were conducted to detect the degradation products of both the active substance and excipients in the drug tablet, which may be formed by hydrolysis, oxidation, and photolysis. In acidic, basic, and oxidative degradation studies, the effects of each factor on degradation, both individually and as a result of their interactions, were examined with three factors. The factors studied included concentration (HCl, NaOH, and H_2O_2), temperature, and time. The developed method was validated in terms of linearity, precision, accuracy, limit of detection/quantitation, and solution stability, and it was successfully applied to the determination of Niflumic Acid and its impurities in the tablet form of the drug.

Key Words: Experimental design, HPLC determination, forced degradation, niflumic acid, active substances.

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Spectrophotometric Kinetic Assessment of Ruthenium (III) Catalyzed Oxidation of Aspirin by Hexacyanoferrate (III) in Alkaline Medium - A Mechanistic Pathway

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Abstract

The redox reaction between aspirin and hexacyanoferrate (III), catalyzed by ruthenium (III) in an alkaline medium, has been thoroughly investigated. The reaction kinetics in this case complex dependence of hydroxide ion and aspirin whereas the order with respect to oxidant and the catalyst respectively has been observed to be one based on the kinetic results, A plausible reaction mechanism has been suggested. The rate law derived from the mechanism accounts for all experimental observations. Kinetic parameters have also been evaluated under varied conditions. Utilizing the Arrhenius and Eyring equations, the activation and thermodynamic parameters of the reaction have been accurately estimated. Furthermore, the reaction's behaviour in various organic solvents has been extensively explored, with Taft's and Swain's multiparametric equations shedding light on the solvent effects. Interestingly, the rate constants show strong correlation with Kamlet-Taft's solvatochromic parameters (α, β, π*), indicating a significant influence of solvent properties on the reaction kinetics. Notably, solute-solvent interactions have not been found to impact the reaction constants significantly. Based on the kinetic findings, a compelling reaction mechanism has been proposed. This proposed mechanism gains further credibility from additional evidence obtained through Density Functional Theory (DFT) computations at the b3lyp/6-311*g (d,p) level. These computational results demonstrate a remarkable alignment between the activation energy barriers and the reactivity trends observed in the kinetics experiments. Therefore, these computational insights provide robust support for the proposed mechanism.

Key Words: *Aspirin; DFT; Hexacyanoferrate (III); Ruthenium (III); Oxidation Kinetics & Reaction Mechanism.*

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A NEW SPE METHOD BASED ON POLYMERIC SORBENT FOR THE DETERMINATION OF ORGANOPHOSPHORUS PESTICIDES

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Abstract

The world population increase rapidly to brings with it the need for food and necessitates the use of more pesticides in the agricultural industry to both increase production and obtain high-quality products [1]. Pesticides are defined by the World Health Organization (WHO) as mixtures of substances of biological or chemical origin that aim to prevent and reduce all kinds of pests, including insects, fungi, weeds, microorganisms such as bacteria and viruses [2]. A very small amount of applied pesticides reaches the target pest. The rest is carried to other environments through the water cycle, evaporation, winds, and some processes taking place in the soil, causing serious soil and water pollution. Pesticide use, one of the biggest environmental problems caused by agricultural practices, reaches the food chain and negatively affects human health and other living things [3]. Pesticides in various forms are basically classified according to their physical and chemical properties. Organophosphorus pesticides, which belong to the chemical class, stand out as a pesticide group that is widely used in agriculture and has many varieties. These pesticides are important because of their high solubility in water. In addition, many of them are in the carcinogenic category because they are rapidly metabolized into bioactive forms that increase toxicity in humans and animals [4]. The most important step before analysing pesticide residues in food and aquatic products is sample preparation. Most sample preparation techniques are based on the separation of the analyte from the matrix using sorbent material. Solid-phase extraction (SPE) is frequently preferred in pesticide analysis since adsorbents are prominent and highly selective analytical performances are obtained [5]. In recent years, polymeric materials with different structures and physicochemical properties have been developed in addition to commercial adsorbents. These polymeric adsorbents have an important place in pesticide analysis in terms of affinity, selectivity, mass transfer, low cost and reusability [6]. In this study, a new solid phase extraction material with hydrophilic and hydrophobic polymer structure was synthesized. Optimization of experimental parameters such as polymer ratios, total sorbent amounts, and pH was carried out using chemometric surface response system. As a result of optimization, response values were obtained using GC-MS. Optimum polymer ratio 70:30, sorbent amount 132,26 mg and pH 7.07 were obtained. As a result, data comparable to commercial cartridges were obtained and it is promising in the extraction of organophosphorus pesticides.

Key Words: *Pesticide; organophosphorus pesticides; solid phase extraction; polymers; chemometric application*

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DEVELOPMENT OF CARBON ELECTRODES FOR CAPACITIVE DEIONIZATION (CDI) PROCESS

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Abstract

Capacitive deionization (CDI) is a water treatment process that has recently gained significant attention for various applications, including water softening, removal of ionic pollutants such as fluoride, heavy metals like lead and cadmium, organic contaminants like humic acid and dyes, and salt removal [1]. In a CDI system, desalination occurs via ion electrosorption in a CDI cell consisting of a pair of porous electrodes. Water flows between or through these charged electrodes, where ions are attracted due to the formation of electric double layer (EDL) [2]. The electrodes can be regenerated by applying a reverse voltage or short-circuiting, allowing for repeated use.

In this study, activated carbon electrodes were fabricated using commercially available activated carbons and lab-produced activated carbons from various precursors. While polyvinylidene fluoride (PVDF) was used as a binder, organic solvent, N-Methyl-2-pyrrolidone (NMP) were utilized to dissolve PVDF and ensure uniform electrode formation. The produced electrodes were subjected to electrochemical and physical characterization to evaluate their suitability for CDI applications. Electrochemical measurements were performed using cyclic voltammetry (CV) in a three-electrode system, where the current response was recorded across different voltage ranges and scan rates to observe the electrode's charge storage behaviour. The capacitance values for each electrode were calculated and compared. Various capacitance values were obtained for different electrodes. This study provides a comparative analysis of different activated carbon sources and the effect of chemical additives on CDI electrode performance. The findings contribute to optimizing electrode material selection for more efficient CDI systems.

Key Words: *capacitive deionization, electrode, activated carbon, desalination, cyclic voltammetry*

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Acknowledgment

This study was supported by Yildiz Technical University Scientific Research Projects Coordinator with the projects numbered FBA-2023-5440 and FYL-2025-6842.

New environmentally friendly approach to speciation analysis of selenium in environmental waters

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ABSTRACT

Knowledge of the total concentration of an analyte in a sample has now become insufficient. Hence the rapid development of speciation analysis, which makes it possible to determine the various chemical and physical forms in which an element occurs in a sample. In our study, we focused on the speciation analysis of selenium in environmental waters. Inorganic selenium compounds have been shown to be more toxic than organic compounds (which are better absorbed by the body). In inorganic compounds, selenium occurs in the following oxidation levels: Se(0) - elemental selenium, Se(-2) - metal selenides, Se(+4) - selenines (IV) and Se(+6) - selenines (VI). Of which, in natural waters selenium occurs mainly as the inorganic compounds Se(IV) and Se(VI).

The most toxic, and most bioavailable, of the inorganic compounds is Se(IV) therefore our aim was to develop a simple and sensitive procedure for the determination of trace concentrations of Se(IV) in environmental waters. For this purpose, we applied the stripping voltammetry technique using a solid bismuth microelectrode, which allowed the determination of low Se(IV) concentrations. Solid bismuth microelectrode offers a number of advantages, such as spherical diffusion, so that measurements can be made from unmixed solutions, simplifying the measurement procedure and enabling field analysis, and they also have a more favourable signal-to-noise ratio. In addition, it is an environmentally friendly electrode in contrast to the mercury electrodes previously used for selenium speciation analysis. Parameters of the development analytical procedure under optimised measurement conditions: linearity: 2×10^{-9} - 3×10^{-6} M, repeatability: RSD = 4.2%, detection limit: 5×10^{-10} M. The developed procedure was successfully validated by analysing certified reference materials SPS SW-1 (waste water) and TM-25.5 (lake water) containing precisely defined amounts of selenium [1].

Keywords: speciation of selenium; stripping voltammetry; solid bismuth microelectrode; environmental water samples

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PHOTOCATALYTIC DEGRADATION OF METHYLENE BLUE BY USING MAGNETIC PHOTOCATALYST

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Abstract

Dyes present in different concentrations in water resources are considered potentially harmful pollutants for the environment and human health. These coloured chemical compounds are widely used in textiles, plastics, paper, food, medicine, and biological dyeing industries. Methylene blue (MB) is a basic dye commonly utilized in biological dyeing, chemical analysis, and medical applications. Advanced oxidation processes, which break down organic molecules in water into biodegradable substances and ultimately convert them into water and carbon dioxide through complete mineralization, have emerged as innovative water treatment methods for removing pollutants such as dyes. Nano-sized TiO_2 particles, exhibiting high thermal and chemical stability along with strong mechanical properties, serve as efficient photocatalyst in heterogeneous advanced oxidation techniques. However, separation of nano-sized TiO_2 particles from water after usage requires expensive nanofiltration steps.

In this study, development of photocatalyst on a magnetic core was investigated in order to overcome the separation problem of TiO_2 nanoparticles from water. Iron-based magnetic nanoparticles (Fe_xO_x) were prepared using the co-precipitation method then SiO_2 was developed around the magnetic core using the sol-gel method, followed by TiO_2. In addition, S-doped and N-doped photocatalysts were produced to investigate the effect of Nitrogen and Sulphur content on the methylene blue degradation capacity of prepared catalysts. Photocatalytic degradation of MB was investigated in a batch photoreactor equipped with the 90W (5x18W) lamb at 365 nm, and the photocatalytic degradation efficiencies were determined by the time. As a result, about 99% degradation efficiency was obtained with the prepared catalyst in 120 minutes. Photocatalytic degradation kinetics data fitted the Langmuir-Hinshelwood kinetic model. When the catalyst was reused, it was seen that the removal percentage decreased to 95% but it still maintained high removal capacity. Owing to the magnetic property of the developed photocatalyst, separation of photocatalyst nanoparticles from the system was achieved simply by applying a magnetic field after photocatalytic degradation experiments, without the need of nanofiltration step required with pure TiO_2 photocatalysts.

Key Words: *Methylene blue; magnetic photocatalyst; photocatalytic degradation; iron oxides; titanium dioxide.*

Acknowledgments:
This study was supported by Yildiz Technical University Scientific Research Projects Coordinator with the project number of FYL-2024-6192.

REMOVAL of ONCOLOGY GROUP EPIRUBICIN and METHOTREXATE DRUGS FROM WASTEWATER BY DFT METHOD

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Abstract

In the first 48 hours after treatment, a small amount of chemotherapy drugs are excreted from the body through urine, vomit and other body secretions. It is important to keep these chemicals away from yourself and other people. For this reason, wastewater containing drug residues must be purified. The possible reactions that occur when the oncology group drugs studied are removed from water were investigated and determined computationally by the DFT method, which is the Molecular Modeling Method. The oncology group molecules studied are Epirubicin and Methotrexate compounds. This method has not been used on the molecules studied before. Optimized geometries were drawn with Gauss View 5.0, and then geometric optimization was performed using the Functional Density Theory (DFT) method with the Gaussian 09W program. The geometric structure (bond angles and bond lengths) of two molecules selected at the B3LYP theory level and the possible fragmentation products of these molecules were calculated with the DFT among ab-initio methods in the 6-31G(d) basis set. Thus, the possible degradation mechanisms of these two molecules in water were determined. These results will guide experimental studies.

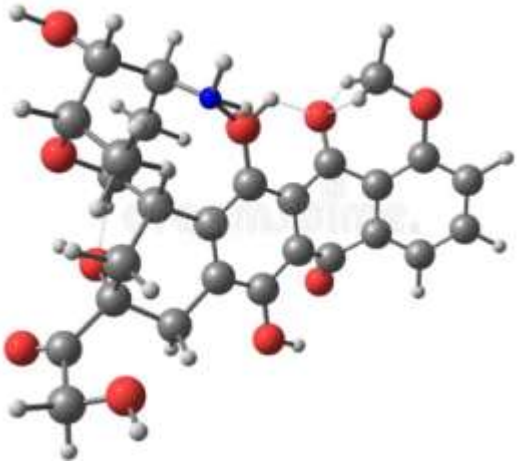

Figure 1. Optimized state of the same Epirubicin molecule (Grey, C; white, H; blue, N; red, O).

Key Words: *Oncology Drugs, DFT, Wastewater*

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SYNTHESIS OF HARD CARBON FROM DIFFERENT BIOMASS SOURCES AS ELECTRODE MATERIAL FOR ENERGY STORAGE SYSTEMS

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Abstract

The increasing energy consumption in the world in recent years brings with it the need for new generation energy storage systems. For this reason, in order to develop a new generation of energy storage systems, it is important to determine the materials that are different from the current studies in the literature, to characterize them and to investigate their electrochemical properties. The aim of this study is to synthesize new electroactive materials in accordance with the construction of energy storage systems and to characterize these materials. In our study, rice husk and sunflower seed husks were activated with the chemical $ZnCI_2$. Carbonization process was applied to the post-activation samples at a temperature of 1000 ^oC and hard carbons were synthesized. Characterization of hard carbons was carried out with Brunauer-Emmett and Teller (BET) surface area measurement device and thermogravimetric and differential thermal analysis (TGA-DTA) measurement device. In line with the obtained results, the surface area, pore volume, pore width and thermal behavior of hard carbons were comparatively investigated. As a result, it is thought that our study will contribute significantly to scientific research in energy storage.

Key Words: *Rice husk; sunflower seed; hard carbon; chemical activation; BET surface area.*

Unlocking Soil Health: Carbon Determination in Agricultural Soils

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By accurately measuring organic carbon, the method helps farmers and soil scientists understand soil health, fertility, and the carbon sequestration potential of the soil. It is an essential tool in developing sustainable agricultural practices, such as managing organic amendments and crop rotations, to improve soil quality and mitigate soil degradation.

The cost-effective **Black-Walkley method** is a widely used and effective technique for determining **organic carbon** in agricultural soils. While it mainly targets organic carbon, it provides critical insights into soil health, helping distinguish the biological contributions of carbon. When used in conjunction with other mineralogical techniques, it can help identify the role of lithogenic (inorganic) carbon sources and further enhance soil health assessments.

The method helps to isolate and focus on **organic carbon,** but when combined with **mineralogical** analyses (such as clay content or other geological markers), it can contribute to a clearer understanding of how much of the soil's carbon comes from biological processes and how much is influenced by the underlying lithogenic or mineral sources.

If the soil contains a significant amount of **lithogenic** minerals, such as carbonates from parent rock, these can impact the overall carbon content. However, the Black-Walkley method primarily targets the organic fraction, and the effect of lithogenic sources would need to be accounted for separately in some cases. This method helps quantify the **organic carbon** in the soil, which is a key indicator of **soil fertility** and microbial activity. Organic carbon is a critical component for improving soil structure, water retention, and nutrient availability, all of which affect soil health. The Black-Walkley method does not directly measure **lithogenic carbon** (inorganic carbon from parent rock), but it is useful for estimating the **organic fraction** of carbon in the soil, which is influenced by both biological processes and geological sources.

Soil samples were collected from the Ovce pole region, (eastern part of the territory of North Macedonia), including the landfill with the carbon farming practice (pilot site) as well. The method validation was improved with QA protocol in accordance with the ISO/IEC 17025:2017. Accuracy, precision, LOD, LOQ, reproductivity, reputability, measurement uncertainty and working range were included for the quality insurance of the method. The data normalization has been introduced using log-normal transformation, for excluding the outliers. Data matrix has been improved with bivariate statistics of correlation matrix and multivariate extraction of dominant variables.

Keywords: Soil carbon, soil health, geo-markers, lithogenic base, Black-Walkley method, quality assurance.

CO_2 as a building block in the synthesis of steroidal oxazolidinones

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Abstract

Fixation of carbon dioxide *via* chemisorption has drawn increasing attention in synthetic organic chemistry. Carbon dioxide is available in large quantities, is safe and is very attractive as a low-cost carbon source in various synthetic methods. [1] In this work the aim was to use CO_2 as a one-carbon building block to synthesize steroidal 2-oxazolidinones with biological activity. [2]

Carbon dioxide can be activated by organobases, by transition metal catalysts or ionic liquids. Furthermore, ionic liquids can increase the activity of transition metal compounds and they are suitable carriers for metal catalysts. [3-5] Therefore, by combining ionic liquids with transition metals, a catalytic system can be obtained that is suitable for the use of carbon dioxide in organic reactions. Our goal was to show that this methodology can be used not only for simple model compounds but even for the preparation of biologically valuable derivatives.

Reaction conditions were optimized using ethinylestradiol as a starting material together with benzylamine as an amine component to produce a 2-oxazolidinone in the presence of CO_2. Attempts were made to carry out the reaction at atmospheric conditions in the presence of different palladium and copper catalysts, but the conversion and selectivity were low. When a carbon dioxide pressure was applied, the conversion and selectivity increased significantly. During the reactions side products were observed to form, which were identified using GC-MS and NMR techniques.

Efficiencies of the catalysts were compared and the reaction conditions were optimized to produce 17-spiro-2'-oxazolidinone product. Then the recyclability of the catalyst was investigated. By using this method the target steroid was synthesized in good conversion through five cycles.

Key Words: *ionic liquid; carbon dioxide; steroid; oxazolidinone; metal catalysts*

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NEW METHOXY AND HYDROXY SUBSTITUTED PYRIDYL BENZAMIDES AS POTENTIAL pH SENSORS

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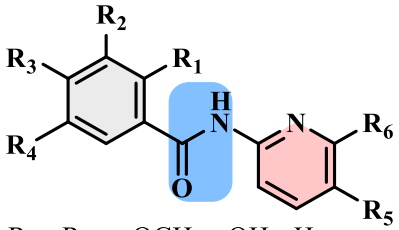
Abstract

Nitrogen containing heterocycles play a significant role in medicinal chemistry and pharmacology due to their wide range of biological activities. Among them, pyridine and its derivatives possess many properties including polarity, basicity, and hydrogen bond-forming capacity that make them a key component of the large number of medications [1]. On the other hand, amide bonds are privileged structural motifs which present essential linkages in organic chemistry. Thus, pyridyl benzamides are one of the most critical types of *N*-heterocyclic amides and play a crucial role in the composition of many important medicines [2]. Heterocyclic molecules are among the most extensively studied classes of organic compounds for their (chemo)sensing and optoelectronic applications as optical pH sensors in solutions, with monitoring the pH range being crucial for studying many biological processes in live cell organelles [3]. In this work we prepared methoxy and hydroxy substituted *N*-(pyridine-2-yl)benzamide in order to investigate their UV/Vis spectral properties in several organic solvents with different polarities and pH sensing potential. In the first step of synthesis, via amidation reaction from methoxy substituted benzoyl-chloride and corresponding 2-aminopyridines we prepared methoxy substituted pyridyl benzamides. In the next step, we performed demethylation to remove the protecting groups and obtain hydroxy derivatives. The structures of newly prepared compounds were confirmed by means of ^{1}H and ^{13}C NMR spectroscopy as well as MS spectrometry. pH spectroscopic titrations in buffered water solutions were performed in order to determine a possible application as pH sensors in solutions followed by determination of pK_a values experimentally.



R_1 - R_6 = -OCH_3, -OH, -H

Fig. 1. Structures of prepared pyridyl benzamides

Key Words: *pyridine; benzamide; pH sensors; UV/Vis spectroscopy*

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Acknowledgments: The Croatian Science Foundation funded this work (project BenzpHSens HRZZ-IP-2020-02-8090).

THE EFFECT OF ALKALI PRETREAMENTS ON THE DRYING KINETICS OF BLUEBERRIES

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Abstract

Drying is a widely used food preservation technique that extends the shelf lives of berry products, while retaining their nutritional contents and bioactive components. This process involves moisture removal through internal diffusion and surface evaporation, necessitating the development of appropriate models to analyze the drying behavior and transport phenomena. These models are essential for designing efficient drying systems, optimizing conditions, and predicting heat and mass transfer mechanisms [1]. Drying is often preceded by physical or chemical pretreatments to reduce drying time and enhance product quality. While extensive research has focused on the antioxidant capacity and nutritional composition of blueberries, studies on their drying kinetics and the effects of pretreatment methods remain limited. Therefore, this study investigates the impact of chemical pretreatments on the oven drying of blueberries. In the experimental procedure, drying temperatures were set at 60°C, 70°C and 80°C. For the chemical pretreatment, 500 mL NaOH solutions were prepared by dissolving 5 g of NaOH in distilled water, with the addition of 0.5 mL olive oil. Blueberry samples were immersed in these solutions at 30°C and 60°C prior to drying. At each pretreatment temperature, the blueberries were subjected to the NaOH solutions for 1 minute and 3 minutes. Following the chemical pretreatment, the samples were transferred to the drying oven under the specified drying temperature conditions. The effects of the aforementioned pretreatments on the drying behavior of blueberries were analyzed and compared with those of untreated samples. Kinetic parameters, including effective moisture diffusivity (D_{eff}) and activation energy (E_a) were calculated. Additionally, drying curves were fitted to widely recognized mathematical models from the literature. The results indicated that the application of NaOH solutions reduced the drying time of blueberries. Furthermore, both pretreatment temperature and duration had a positive impact on drying behavior. This study provides novel insights into the application of oven drying for delicate food products such as blueberries, and contributes valuable data for the advancement of food drying technologies.

Key Words: *Blueberry; drying; drying kinetics; NaOH pretreatment; oven drying*

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Synthesis and spectroscopic investigation of host-guest interactions in ferrocenylpyrimidines

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Abstract

Ferrocenylpyrimidine derivatives of different structure have been deployed in order to detect neutral molecules and ionic species by both electrochemical and spectroscopic means. The sensing of a neutral guest, 2,6-diaminopyridine (DAP), has been investigated previously in our research group by cyclic voltammetry and NMR spectroscopy by a conformationally flexible ureidopyrimidine host displaying a complementary hydrogen bonding array [1]. As an extension of this area, the introduction of some heterocycles to the pyrimidine ring was carried out, which led to different conformational preferences between the two rotameric forms of the intramolecularly H-bonded host molecules [2]. Low temperature NMR measurements and lineshape analysis have been applied to determine the activation parameters of the conformational change of the hosts. Low temperature NMR titrations of ferrocenyl-ureidopyrimidines with DAP were carried out to study the participation of the heterocyclic moiety in the complexation of the guest molecule. Association constants of the host-guest system have been computed from NMR measurements.
Electrochemical measurements conducted in solution concluded that the change of the redox potentials of the Fc/Fc^+ pair upon the addition of DAP shows the beneficial effect of the pyridin-2-yl moiety. Immobilization by sol-gel electrodeposition was employed to bind ureas onto an electrode surface in order to examine their response to DAP.
Quantum chemical calculations were applied to determine the energy difference between the host conformers and their adducts with DAP. Results of the conformer and adduct ratios as well as the energy barrier of the conformational change in the host were in good agreement with the experimentally gained values.
For the detection of metal ions, ferrocenylpyrimidine compounds have been developed in our research group that display a binding motif analogous to terpyridine ligands. The binding of transition metal ions was monitored by UV-Vis and NMR spectroscopic means, as well as by electrochemical means through the shift in the redox potential of the ligand. The binding constants of metal ions to the ligand were also determined from titration curves. The investigated metal ions, that formed either ML or ML_2 type complexes, were also subjected to extraction from aqueous solutions by the ligand into the organic phase, a phenomenon that gives way to the use of naked-eye sensing.

Key Words: *ferrocenylpyrimidine; 2,6-diaminopyridine; host-guest; NMR spectroscopy; electrochemistry*

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PREPARATION OF 2-OXAZOLIDINONE DERIVATIVES USING CARBON DIOXIDE AS C1 BUILDING BLOCK IN IONIC LIQUID SOLVENT

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Abstract

One of the most recent methods for the synthesis of 2-oxazolidinones is the carboxylative ring closure of propargylamine derivatives with carbon dioxide. Conditions reported in the literature include the application of expensive metal catalysts with complex structures and harsh conditions (high pressure, high temperature, long reaction times) [1]. Imidazolium-based ionic liquids can be used for carbon dioxide chemisorption in the presence of an organic base and can also serve as suitable supports for transition metal catalysts, increasing their activity and stability [2].
In our research, we investigated whether the incorporation of carbon dioxide into propargylamine derivatives is feasible in an ionic liquid solvent and what the synthetic advantages of doing so are. We have demonstrated that the synergistic effect of certain metal-catalyst-base pairs promotes the formation of 2-oxazolidinone derivatives. The catalytic system of the ionic liquid, base and metal complex was found effectively recyclable without significant loss of its catalytic activity. It has been determined that the loss of base and metal during processing is negligible.

Key Words: *2-oxazolidinone; ionic liquid; recyclability; carboxylative cyclization*

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Development and Validation of a RP-HPLC Method For Simultaneous Determination of Chlorhexidine Gluconate, Benzydamine Hydrochloride and Cetylpyridinium Chloride

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Abstract

This work was concerned with development, validation and application of reversed phase high performance liquid chromatography method for analysis of Chlorhexidine Gluconate, Benzydamine Hydrochloride and Cetylpyridinium Chloride in gargle.
Optimal chromatographic separation of three active substances was performed by using an analytical column of CN 4.6 mm x 150 mm, 5 µm. The active substances were eluted by a mobile phase consisted of 10% buffer solution (30 mM KH 2 PO 4 containing 2,5% tetra butyl ammonium hydroxide was adjusted to pH 5.0 with acetic acid), 90% methanol under isocratic conditions, at a flow rate of 2 mL/min and detection wavelength at 257 nm. The developed method was validated in terms of linearity, precision, accuracy, limit of detection/quantitation and solution stability and successfully applied to the determination of Chlorhexidine Gluconate, Benzydamine Hydrochloride and Cetylpyridinium Chloride.

Key Words: Chlorhexidine Gluconate, RP-HPLC determination, Benzydamine Hydrochloride, Cetylpyridinium Chloride, active subtances.

AN OVERVIEW ON chemical profile of *salvia officinalis* population from llogara mountain area, south albania

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ABSTRACT

In this study were analyzed essential oil of Salvia officinalis samples from Llogara Mountain, located in Vlora area, at South Albania. Wild population of Salvia officinalis are widespread almost in all Albanian territory, which is one of the main exporter countries in Europe for this plant. Sage plants have a long history of medicinal and culinary use, and as an ornamental garden plant. Arial parts of sage herbs are known to have disease preventing, and health promoting properties because they contain many chemical compounds (minerals, vitamins, terpenes, flavones, etc). Salvia herbs were collected in eight different stations of Llogara Mountain in the end of the June, for a five years period (2020-2024). The airdried plant samples were subjected to European Pharmacopoeia apparatus (Clevenger type) for 4 hours to obtain Salvia officinalis essential oil. The chemical composition of the essential oil was analyzed using GC/FID technique. VF-1ms capillary column were used for separation of compounds.

Alpha- and beta-Thujone were identified as main constituents in all analyzed Salvia officinalis samples from Llogara Mountain. Their total concentrations ranged between 31.3 and 37.2 %. The differences between stations and among the study period can be related with precipitation, sunny hours, air temperatures, changes in soil composition, etc. Even though it weren't observed significant changes in the chemical profile of sage plants for the analyzed samples, climate changes and human activity can impact directly on the physiological processes of plants as well as at their chemical profile. Sage samples from Llogara Mountain had similar profile with other population from Albania as well as from Balkan area.

Keywords: Llogara Mountain**,** *Salvia officinalis*, Essential oils, α-and β-Thujone, GC/FID

Farma-Bant: Obtaining a Wound Covering Membrane from Calendula Officinalis, Centella Asiatica and Carthamus Tinctorius Plant Extract Mixtures

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Research and applications related to wound dressings used for wound treatment worldwide hold significant importance. Various types of dressings are used globally for injuries, which cover the wound to protect the skin from external factors and aid healing. Among the first dressings we use for minor home accidents is the adhesive bandage, an essential component of first aid kits. The skin barrier is vulnerable to internal and external elements. However, certain plant extracts have promise for protecting the skin [1]. Recently, modern dressings have incorporated various functional plants to promote faster healing and protect against infections. Antimicrobial plants have been integrated into dressings to expedite healing. In this study, three high pharmacological plants Centella asiatica (Indian pennywort), Carthamus tinctorius (Safflower), and Calendula officinalis (Pot Marigold) have been highlighted. Research shows that Indian pennywort has significant wound healing properties [2], Safflower offers pain relief [3], and Marigold promotes skin healing [4].

This study aims to extract the essences of these plants and incorporate them into adhesive bandages for small wounds and cuts. The release of plant extracts from the bandages was analyzed using time-dependent UV-VIS spectrum measurements in a phosphate buffer saline (PBS) as artificial body fluid. Swelling test was used for the investigation of liquid absorption properties. Microscopy was also used to confirm the incorporation of plant extracts into the bandages.

Key Words: *Centella asiatica, Carthamus tinctorius, Calendula officinalis, wound dressing, antimicrobial.*

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CALCULATION OF ELECTRONIC PROPERTIES OF ADRENALINE, DOPAMINE, MELATONIN, AND SEROTONIN USING DFT

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Abstract

Hormones play a critical role in body physiology and metabolism. They are biological regulators that help cells communicate with one another. Consequently, they hold unresolved mysteries regarding the mechanisms of metabolic events in the body. Investigating the interactions between hormones and their receptors and the resulting reactions is essential for understanding how our bodies function [1,2].

In this study, the electronic and molecular properties of four hormones; Adrenaline, Dopamine, Serotonin, and Melatonin are calculated by using Density Functional Theory (DFT). In addition to that, potential energies, dipole moments, energies of HOMOLUMO orbitals, and partial charges are calculated using ORCA software. Also, HOMOLUMO orbitals and electrostatic potential surfaces are drawn. The energy calculations and geometry optimizations are done with B3LYP functional and 6-31G(d,p) basis set [3,4]. After the geometries are optimized, global and local reactivity indices are calculated, and nucleophilic, and electrophilic sites of the molecules are determined.

These results can be used for further research on how these hormones interact with their receptors in cell signaling and metabolism. In light of this information, new treatment methods that mimic the properties of these hormones can be designed or hormonal disorders can be better understood by further investigating their mechanisms.

Key Words: *hormones, FMO, ESP, global indices, local indices*

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Computaionnal study of natural substances in the active principles of drugs, Reaction between Berberine and Cisplatin: DFT and QSAR investigations

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Abstract

Berberine is a clinically important natural isoquinoline alkaloid derived from Huang Lian, berberis vulgaris, Tinospora cordifolia and many other medicinal herbs, it exhibits multiple beneficial effects including anti-diabetic and cardio-protective effects.According to several researches; it has an anti-tumor role in many types of cancer[1].
Chemotherapy has definitively proven that cancer drugs can cure cancer when combined with other treatment options. An important feature that differentiates anticancer drugs from other antimicrobial agents is the extent of side effects that often limit the use of the drugs. Side effects can be acute or chronic, self-limiting, permanent, mild, or life-threatening.
The main obstacles to the clinical effectiveness of chemotherapy are toxicity to normal body tissues. In addition, chronic and cumulative toxicities can also occur with anti-cancer drugs [2].
Experiments have proven that the use of natural materials in combination with anti-cancer drugs gives positive results and many benefits such as minimization of dose and reduction of drug resistance, increased efficacy of chemotherapeutic agent.
In this context we carried out a study on the reaction between berberine and cisplatin ,which is a drug in Chemotherapy using molecular modeling, which has seen significant advances and has become very useful in pharmaceutical chemistry.the Theoretical study of the berberine and cisplatin and the chemical reaction between them was carried out at the level of the density functional theory (DFT) implemented in the program Gaussian 09.
The code QSAR TOOLBOX was used to determine the relationship between the chemical compositions of the berberine either alone or in combination with cisplatin and its biological activity and toxicity.

KeyWords : *Berberine , Cisplatin, Reactivity descriptors, DFT, QSAR*

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Cucurbit[10]uril Binding of Heteroleptic Iridium(III) Complexes : Synthesis and Photophysical Characterization

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Abstract

Some of Iridium(III) complexes show weak luminescence properties in aqueous solution. This limits using them as a chemosensors for variety of analytes [1, 2]. This work outlines a strategy to enhance the photophysical properties of heteroleptic Iridium(III) complexes, after forming a supramolecular system in aqueous medium. Heteroleptic Ir(III) complexes that possess two phenylpyridine (ppy) ligands and a single R-bipyridine (bpy-R) ligand; $[Ir(ppy)_2(bpy\text{-}(CHO)_2]^+$(complex **1**), $[Ir(ppy)_2(bpy\text{-}(COOH)_2]^+$ (complex **2**), were encapsulated in cucurbit[10]uril (CB[10]) to form host-guest systems in aqueous solution. The photophysical properties of these complexes were altered after encapsulation process. A significant enhancement in the luminescence properties of both Ir(III) complexes (emission intensity, quantum yield and lifetime) was observed upon the addition of CB[10] in aqueous solution. This suggests that encapsulation process can cause a change in character of the emitting state. Binding study of these systems, showed the presence of 1:1 and 1:2 host-guest emitted species, this was also supported by lifetime study. The temperature and pH effect on the encapsulation process were discussed in this work. Density functional theory (DFT) calculations showed that introducing different substituent groups (CHO, and COOH) on the bpy ligand has no significant effect on the orientation and accommodation of these complexes within the CB[10] cavity.

The large enhancement in the luminescence properties of such large complexes after adding CB[10] in aqueous media, is a valuable result for variety of applications that depend on the luminescent properties of iridium(III) complexes.

Key Words: *Iridium(III)complexes; Cucurbit[10]uril; host-guest; Encapsulation; Photophysical properties.*

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DETERMINATION OF FATTY ACID COMPOSITION OF SOME PLANT OILS AND SOLID SOAP PRODUCTION WITH THESE OILS

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Abstract

From past to present, plants and plant extracts have been used in many scientific and commercial fields for various purposes. Today, there is a trend away from synthetic products and towards natural products. Chemical compounds produced by plants as a result of natural defense mechanisms are now used in cosmetics and pharmaceutical industry, paint industry and various industrial fields and have economic importance [1). The compounds mostly found in plants used in cosmetic products are fixed oil, tannin, essential oil, carbohydrate, phenolic acid, flavonoid, sterol, saponin, vitamin and minerals [2]. Soap is one of the oldest treatment and cleaning agents in the world. It has been used by humans since ancient times and its use continues to increase today. The most useful soap for human health consists of solid soaps made from natural vegetable oils without any chemicals [3].

The aim of this study is the production and analysis of soap by cold method using natural plant oils and characterization of the used oils by Gas Chromatography (GC). For this purpose, a cold method saponification reaction was carried out without heating, using olive oil as the main raw material. In addition, some plant oils (coconut oil, castor oil, cocoa butter, shea butter, menengic oil, etc.) were added to the reaction medium in order to increase the utilization of the soap on the skin. Free alkali determination and total fatty acid analysis of the produced soaps were carried out. In addition, the fatty acid contents of the vegetable oils used in soap production were determined by GC method and the soaps obtained were analyzed….According to the gas chromatography results, oleic acid, linoleic acid and palmitic acid were the most abundant fatty acids in all four oil types (olive oil, daphne oil, argan oil, menengic oil) used in the saponification reaction.

This study falls under the “Valuable Chemicals from Plant Sources” section within the framework of TUBITAK 2022-2023 Priority R&D and Innovation Topics and contributes to the development of more environmentally sensitive products and the production of valuable chemicals from plant sources [4]. In addition, it is envisaged to be a study that benefits the cosmetics industry, natural product industry and phytotherapy in Türkiye and the country's economy by utilizing plant parts that are effective in terms of phytotherapy.

Key Words: Plant oil, gas chromatography, fatty acid, natural solid soap, soap analysis

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Modification of some bioorganic products with organosilicon compounds for use in industrial production

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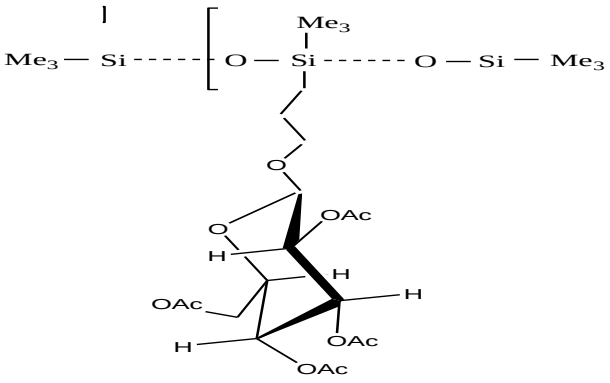
The widespread use of organosilicon polymers in many areas of technology has led to the development of organosilicon chemistry and a sharp expansion of applied research in this area. With the development of industry and technology, the need to create new, more advanced polymeric materials with improved performance properties has increased, which in itself has led to the development of methods for synthesizing high-molecular compounds of various compositions and structures [1-3]. Natural carbohydrate macromolecules undergo chemical modification or serve as building blocks in hybrid substances of biological or synthetic origin. The carbohydrate-containing polysiloxane - poly[methyl-3-(tetraacetylglucosidyl)propyl]siloxane - is synthesized by hydrosilylation of functionalized (allylated) and protected (acetylated) carbohydrate products.



Modified polysiloxanes with a low degree of substitution remain soluble in non-polar solvents, whereas with increasing carbohydrate content the polymers become increasingly soluble in polar solvents such as chloroform, isopropanol and methanol. Thus, by introducing carbohydrates into a non-polar polymer matrix, a polymer with amphiphilic properties and the ability to self-organize (coagulate) was obtained. The hydrophilic hydrocarbon component will enhance the interaction of the polymer with more hydrophilic solvents, which will allow the use of such polysiloxanes as surfactants and coatings. A structural and functional study of free and acetylated polysiloxanes modified with a monosaccharide was carried out.

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New trends in design of potentiometric sensors

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Ion-selective electrodes (ISEs) belongs to the electrochemical sensors and they are the largest and most popular sensors in this group. ISEs are widely used in many areas, such as clinical analytics, environmental protection, industrial analytical control and food quality control, among others []. At the end of the last century, a new type of ISEs was developed in which the internal electrolyte solution was removed. Such electrodes are called solid contact electrodes. The elimination of the internal solution enabled the miniaturisation of ISEs and made them easier to handle, transport and use. When constructing SCISEs, it is very important to select a suitable material that will act as an ion-electron transducer, ensuring that the electrodes function correctly. There are many materials used as a solid contact. The most common materials used as a solid contact are conductive polymers, carbon based nanomaterials, metal and metal oxide nanoparticles and ionic liquids. In recent years, mixed materials have begun to be used including composite and hybrid materials.

In this paper, we will present the results of our recent research on the use of composite and hybrid materials to develop solid contact ion-selective electrodes. The properties of the resulting sensors and thus the performance of the new materials used in their construction have been investigated using various electrochemical techniques such as potentiometry, chronopotentiometry and electrochemical impedance spectroscopy. It has been shown that composite materials often have better mechanical, thermal, electrical, optical and chemical properties than the original components [1]. With regard to their use in the design of ion-selective electrodes, it is particularly important to increase the capacitance and surface area of the material, which makes them more efficient in the charge transfer process between the polymer membrane and the substrate material. This allows for sensors with improved analytical and operational performance. To date, we have successfully developed electrodes sensitive to nitrate, chloride, potassium, lead and copper ions using various nanocomposites based on carbon nanomaterials and ionic liquid [2,3], polyaniline nanofibres [4] nickel-cobalt nanoparticles [5] and copper oxide nanoparticles [6,7]. The results of research on the impact of a composite material based on carbon nanotubes and other components on the most important parameters of selected ion-selective electrodes with solid contact, i.e. the slope of the characteristics, the limit of detection and the range of linearity, stability and reversibility of the potential. The electrodes we have developed can be analyzed in real samples such as natural water, food and pharmaceutical preparations. Examples of such applications will also be presented on the poster.

Keywords :*ion-selective electrode, potentiometry, solid contact, nanocomposite*

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The Inhibitory Effect of Hicaz Pomegranate Peel Extract on Enzymatic Browning in Potatoes: A Natural Solution

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Abstract

Enzymatic browning in fresh-cut vegetables is a significant issue that negatively affects the appearance and shelf life of products, leading to substantial losses in the food industry. The potential adverse health effects of traditionally used chemical inhibitors have increased interest in natural alternatives [1]. In this study, the inhibitory capacity of a phenolic extract obtained from the peel of the Hicaz variety pomegranate, which is widely cultivated in Türkiye, on polyphenol oxidase (PPO) enzyme in potatoes was investigated. The components of the phenolic extract obtained by ultrasonic extraction were analyzed using LC-MS/MS, and molecular docking studies were conducted on the seven most abundant phenolic compounds (Kaempferol, Myricetin, Luteolin, Gallic acid, Abscisic acid, Apigenin, Ethyl gallate). The inhibitory effect of Hicaz pomegranate peel extract on PPO enzyme, isolated from potatoes and partially purified by ammonium sulfate precipitation, was examined. The IC50 value for potato PPO was determined as 0.86 mg/mL. Analyses conducted to determine the inhibition mechanism revealed that the extract exhibited mixed-type inhibition on potato PPO. Molecular docking studies showed that the phenolic compounds in the extract had lower binding energy compared to the reference compound ascorbic acid and interacted with the PPO enzyme through multiple hydrogen bonds, Van der Waals forces, π interactions, and alkyl interactions. Additionally, the binding of phenolic compounds to different regions outside the active site supported the experimentally observed mixed-type inhibition.

The effect of Hicaz pomegranate peel extract on the quality properties of fresh-cut potatoes was evaluated. In this context, potato slices were treated with a 2 mg/mL concentration of the extract and stored at +4 °C. The texture, pH, total soluble solid content, color changes, and surface sulfhydryl group levels were analyzed on days 0, 3, and 7 of storage. The results showed that the potato slices treated with the extract demonstrated resistance to enzymatic browning, and the color change was successfully delayed for up to 7 days.

Key Words: Polyphenol oxidase; Enzymatic browning; Molecular docking; Phenolic compounds; Natural antioxidants

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Dinuclear [OSSO]-type metal complexes for coupling of CO2 with epoxides

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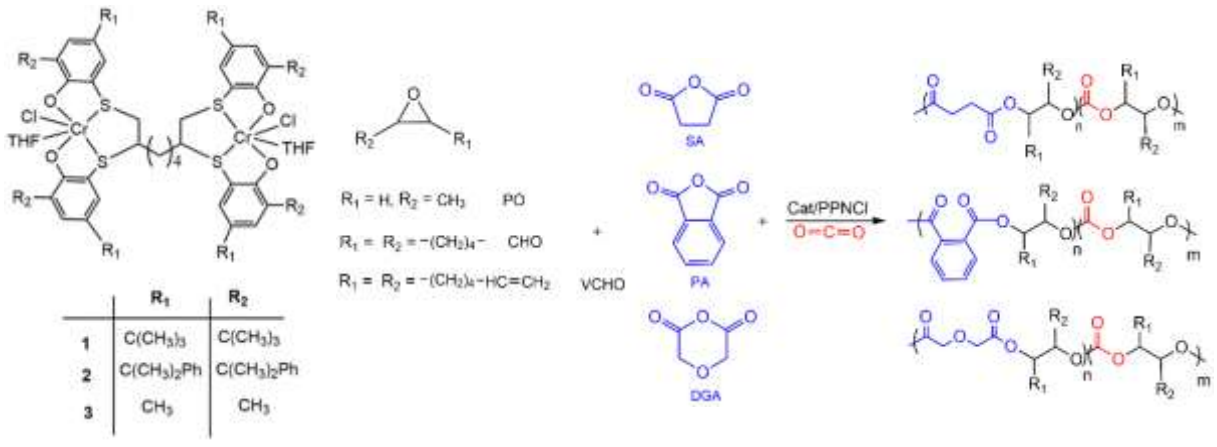
Abstract

Carbon dioxide (CO_2) has been utilized as a nontoxic, abundant, and cost-effective C1 feedstock for polymer synthesis since the pioneering work of Inoue et al. in 1969 on epoxide/CO_2 copolymerization [1]. This research is motivated by the need to mitigate the greenhouse effect, as CO_2 emissions significantly contribute to global warming. Additionally, converting CO_2 into valuable chemicals plays a crucial role in establishing a circular economy by integrating captured CO_2 into sustainable material cycles rather than releasing or storing it. In this context, ring-opening copolymerization (ROCOP) of epoxides with cyclic anhydrides or CO_2 enables precise control over polymer properties through strategic monomer selection. This approach yields copolymers containing ester and carbonate functionalities, which can potentially lead to hydrolyzable and environmentally friendly materials [2].

In this study, we introduce a novel family of inexpensive and highly selective dinuclear chromium complexes (**1-3**) featuring bis-thioether-diphenolate ligands. These complexes facilitate the binary copolymerization of carbon dioxide and epoxides, as well as the ternary copolymerization with phthalic anhydride (PA), succinic anhydride (SA), and diglycolic anhydride (DGA), using bis(triphenylphosphine)iminium chloride (PPNCl) as a co-catalyst (Scheme 1) [3].



A B

Scheme 1. The [OSSO]-type Cr (III) complexes **1-3** (A); CO_2/cyclic anhydride/epoxide terpolymerization (B)

Key Words: *OSSO-type homogeneous catalysts, Ring-opening copolymerization, Polycarbonates, polyesters, CO_2.*

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SYNTHESIS AND BIOLOGICAL ACTIVITY OF NEW BENZOXAZOLE IMINOCOUMARINES AS pH SENSORS

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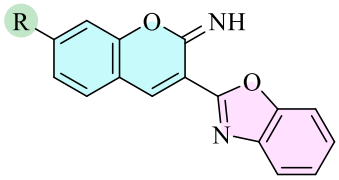
Abstract

Benzoxazole ring is well known attractive scaffold in medicinal chemistry due to the wide range of biological and pharmacological properties of its derivatives, among the most important are antitumor, antiviral or antimicrobial. In addition, it can be used as a starting building block for the synthesis of various biologically active molecules [1]. Iminocoumarine derivatives are known for their interesting spectroscopic properties as well as their application as fluorescent sensors [2, 3]. pH determination stands as a crucial bio-marker for evaluating the status of mitochondria in the cell micro-environment. Monitoring pH is vital for the survival of living organisms and cells, production, manufacturing, environmental protection, water and food safety, and air quality assurance [4]. This work presents the synthesis, biological evaluation and spectroscopic characterization of novel iminocoumarine derived benzoxazoles. Main precursor, 2-cyanomethylbenzoxazoles was prepared using microwave synthesis from *ortho*-aminophenol and 2-cynoacetamidate hydrochloride. Targeted iminocoumarines were prepared in condensation with differently substituted salicylbenzaldehydes. The structures of newly prepared compounds were confirmed by means of ^{1}H and ^{13}C NMR spectroscopy. Antiproliferative activity *in vitro* was evaluated on the several human cancer cells while the antibacterial activity *in vitro* was tested on Gram-positive and Gram-negative bacterial strains. Additionally, spectroscopic characterization and pH spectroscopic titrations were performed in order to determine possible application of chosen compounds as pH sensors in solutions followed by determination of p*K*a values.



R = H, -OH, -*N,N*-$(CH_2CH_3)_2$

Fig. 1. Structures of investigated benzoxazole derivatives

Key Words: *benzoxazole; iminocoumarines; biological activity; pH sensors*

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Acknowledgments: The Croatian Science Foundation funded this work (projects BenzpHSens HRZZ-IP-2020-02-8090 and BenzHetPot IP-2024-05-7208).

Synthetic flavonoid BrCl-flav – an alternative solution to combat ESKAPE pathogens

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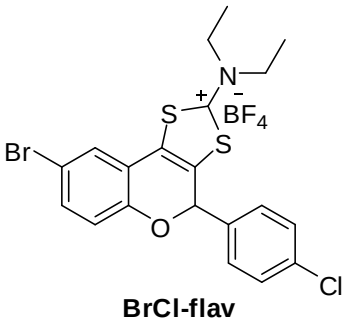
Abstract

ESKAPE pathogens are considered a global threat to human health. The discovery of new molecules for which these pathogens have not yet developed resistance it's a high medical priority. Synthetic flavonoids are good candidates for developing new antimicrobials. Therefore, we report here the potent *in vitro* antibacterial activity of BrCl-flav (Figure 1), a representative of a new class of synthetic sulfur containing tricyclic flavonoids.[1-3] Checkerboard assay was used to study the effect of the tested compound in combination with antibiotics. Our results showed that BrCl-flav possess an important inhibitory activity against all tested clinical isolates, with MICs ranging between 0.24 and 125 μg/mL. A total kill effect was recorded after only 1 h of exposing *Enterococcus faecium* cells to BrCl-flav. Also, BrCl-flav displayed an important biofilm disruption potential against *Acinetobacter baumannii*. Those effects are induced by membrane integrity damages. BrCl-flav expressed synergistic activity in combination with penicillin against a MRSA strain. Based on the potent antibacterial activity, low cytotoxicity and pro-inflammatory effect, BrCl-flav has a good potential to develop new effective drugs against pathogens from ESKAPE group.



BrCl-flav

Figure 1

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DIBENZOFURAN AND DIHYDROBENZODIOXIN-BASED HOSTS FOR IMPROVED STABILITY BLUE TADF OLEDs

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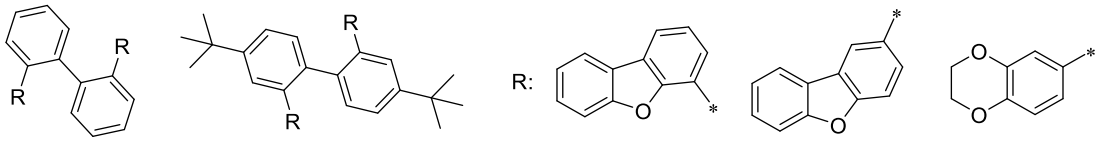
Abstract

A significant hurdle in advancing and commercializing TADF-OLED technology, especially for blue devices, is their short operational lifetime [1]. Blue TADF devices typically exhibit a half-life in the range of 1-100 hours when operated at a practical luminance of 500-1000 cd/m², and this value is rarely exceeded [2].
Typical hosts for blue OLEDs include N-aryl substituted chromophores such as carbazole, acridine, carboline, indole, di- or triphenylamine, and other structures containing C-N single bond [3]. Unfortunately, the C-N bond has a low bond dissociation energy, which adversely affects device stability [4]. Thus, it is essential to avoid amino-containing structural components in non-conjugated systems and, instead, investigate less-explored alternatives, such as dibenzofuran or benzodioxine (**Fig. 1**). This chromophore incorporates electron-donating segments based on oxygen, with the C-O bond offering superior stability (358 kJ/mol or 3.7 eV) compared to both the C-N single bond (305 kJ/mol or 3.04 eV) and the C-C bond (346 kJ/mol or 3.58 eV) [5].
In this work, we present the properties of six new biphenyl-based compounds containing dibenzofuranyl or dihydrobenzodioxinyl chromophores (**Scheme 1**), which serve as high-triplet-energy hosts of blue OLEDs. Additionally, we report the characteristics of OLEDs containing these synthesised host materials..



Scheme 1: Structures of derivatives

Key Words: *Dibenzofuran; Dihydrobenzodioxine; Biphenyl; Hosts; OLED*

Acknowledgement: *This work has received funding from the Research Council of Lithuania (LMTLT), agreement No S-PD-24-73.*

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DESIGN OF AN ELECTROCHEMICAL BIOSENSING PLATFORM BASED ON METAL-DOPED CARBON QUANTUM DOTS FOR DETECTING GASTRIC CANCER-RELATED GENES

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Abstract

Carbon quantum dots (CQDs) exhibit a large surface area, excellent electronic conductivity, and biocompatibility, making them highly suitable for biosensing applications. Heteroatom doping is a well-established strategy for modifying the electronic structure of CQDs, thereby enhancing their physicochemical properties [1]. Among these strategies, metal doping has been particularly effective, as metals act as efficient electron donors, form chelates with surface functional groups and improve the physical and chemical properties of CQDs by increasing electron mobility [2]. In this study, iron-doped carbon quantum dots (Fe-CQDs) were synthesized via a hydrothermal method using citric acid, ethylene diamine, and iron (III) chloride as precursors (Figure 1). The structural and optical properties of Fe-CQDs were characterized by UV-Vis spectroscopy, fluorescence spectroscopy, FT-IR, XRD, and TEM analysis. Chitosan and Fe-CQDs were combined to develop a novel electrochemical sensing platform, and immobilized onto a glassy carbon electrode (GCE). The modified electrode was further functionalized with glutaraldehyde and amine-modified single-stranded DNA (ssDNA) specific for bacteria associated with gastric cancer. Upon introducing the target complementary ssDNA (cDNA), hybridization occurred, and the event was monitored using differential pulse voltammetry (DPV) with methylene blue as an electrochemical indicator. The results indicate that Fe-CQDs can be utilized in electrochemical biosensors for the detection of bacterial DNA associated with gastric cancer, improving detection sensitivity by enhancing sensor performance.

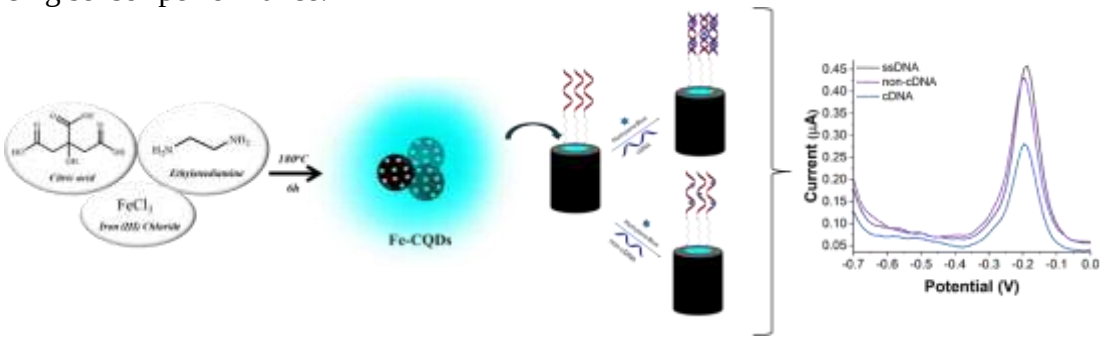

Figure 1. Synthesis of Fe doped CQDs and detection of strategy

Key Words: *Metal doped carbon quantum dots, DNA hybridization, electrochemical sensor, gastric cancer, bacterial DNA*

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The Cytotoxic Properties of Some Tricyclic 1,3-Dithiolium Flavonoids

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Abstract

Due to the emergence of multidrug resistant microorganisms, new classes of antibiotics are needed. We are presenting the cytotoxic effects of five tricyclic flavonoids, one of which was previously identified as a potent antimicrobial agent.[1-3]

All five derivatives were tested against human HOS and MCF7 cancer cell lines using a wound scratch assay. The cytotoxic properties of previously reported flavonoid **1** (Figure 1) were also evaluated using the standard MTS and live/dead assays, using NHDF, HOS and MCF7 cell lines.

All five derivatives were found to inhibit to some degree the proliferation of cancer cells. Compound **1** was also found to be less toxic towards regular versus cancerous human cells. Moreover, the minimum bactericidal concentration of **1** against *S. aureus* was found to be non-toxic for any of the tested human cell lines.

Derivative **1** has the potential of being used as a therapeutical agent against certain microorganisms.

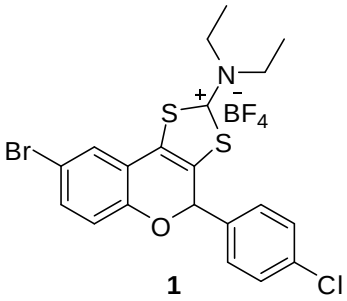

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Figure 1

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ADSORPTION INVESTIGATION OF DISPERSE ORANGE 30 DYE ON H_2SO_4 FUNCTIONALIZED ACTIVATED CARBON

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Abstract

In the physicochemical treatment process known as adsorption, dissolved molecules in contaminated water form a chemical and physical bond with the surface of the adsorbent. Due to its ease of use and effectiveness, the adsorption process is a highly recommended method for treating wastewater that contains dyes. Various synthetic and natural materials worked well as adsorbents to remove color from soiled textile effluents. Because it can remove a variety of contaminants from contaminated media, commercial activated carbon, also referred to as charcoal, is a type of industrial adsorbent that is frequently used. Dispers orange 30 dye (DO) is mono azo dye and used for used he coloring of polyesters, nylon, natural fibres, and acetate in the textile sector. [1-2]

In this current study, H_2SO_4 functionalized activated carbon was synthesized and used for the adsorption of DO from synthetic waste water. The effects of different reaction parameters such as the adsorbent dosage, initial DO concentrations, contact time and solution temperature on the adsorption of DO onto activated carbon and H_2SO_4 functionalized activated carbon were investigated. To determine the best adsorption equilibrium and adsorption kinetic data of DO adsorption on activated carbon and H_2SO_4 functionalized activated carbon were applied different models for equilibrium and for kinetic.

Key Words: *Disperse Orange 30 Dye; H_2SO_4 functionalized activated carbon; Dye Removal; Kinetic Study and Adsorption Isotherms*

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KINETIC STUDIES OF DISPERSE ORANGE 30 DYE REMOVAL VIA H_2SO_4-ACTIVATED SCRAP TYRE PARTICLES

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Abstract

One of the persistent pollutants that traditional treatment techniques have difficulty in removing from wastewater is dyes. Adsorption technique is a cheap and convenient method for removing dyes from wastewater.[1] To understand the adsorption process of dye removal from waste water via adsorbent can be investigated adsorption kinetics and isotherms. The rate of solute adsorption and the duration of adsorbate residence at the solid-liquid interface are both described by adsorption kinetics. Adsorption isotherms are crucial for figuring out how the adsorbent and adsorbate interact as well as the adsorbent's ideal adsorption capacity. [2]

In this study, disperse orange 30 dye (DO) was removed from a liquid solution using cheap adsorbents made from tire rubber waste and H_2SO_4 activated scrap tire particles. Adsorption isotherm and adsorption kinetics of DO dye removal from synthetic wastewater by adsorption technique were investigated by changing the adsorbent dosage, contact time, dye concentration and temperature.

Key Words: *H_2SO_4 Activated scrap tyre particles; Disperse Orange 30 Dye; Dye Removal; Adsorption Kinetic and Adsorption Isotherms*

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