12th ICNTC CONFERENCE
INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

12th INTERNATIONAL CONFERENCE ON
NEW TRENDS IN CHEMISTRY
10-12 APRIL 2026

12th ICNTC BOOK OF ABSTRACTS

10-12 APRIL 2025 BARCELONA – SPAIN

International Conference on New Trends in Chemistry

12th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY
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ICNTC Conference 2026

12th International Conference on New Trends in Chemistry

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Prof. Dr. Dolunay ŞAKAR

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Conference organised in collaboration with Monre Academy

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Yıldız Technical University – Turkey
Conference Chair

Prof. Dr. Yelda Yalcin Gurkan
Tekirdag Namik Kemal University – Turkey
Conference Co Chair
Chemistry Department

Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of " **12th International Conference on New Trends in Chemistry**", to be held in Barcelona, Spain on the dates between April 10-12, 2026

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 10-12 April 2026 in Barcelona, SPAIN

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
12th ICNTC 2026 | Conference Chair
Yıldız Technical University – Istanbul / Türkiye
Chemistry Department

Prof. Dr. Yelda YALCIN GURKAN
12th ICNTC 2026 | Conference Co Chair
Tekirdağ Namik Kemal University – Tekirdağ / Türkiye
Chemistry Department

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CONFERENCE VENUE

TEMBO HOTEL BARCELONA

10 APRIL 2026 FRIDAY

Welcome Speech (08:50 - 09:00)

Prof. Dr. Dolunay SAKAR, Yıldız Technical University
Conference Co Chair

SESSION A (09:00 – 10:40)

SESSION CHAIR: Prof. Dr. Sevil YÜCEL

09:00 – 09:20
PAPER TITLE : CARBON DIOXIDE-BASED FUNCTIONAL CYCLIC CARBONATES: AMINO ACID-BASED IRON(III) AND COBALT(III) COMPLEXES CATALYSED COUPLING OF CO2 AND EPOXIDES
AUTHOR(S) : **Adnan S. ABU-SURRAH**, Jumana N. AYYAD

09:20 – 09:40
PAPER TITLE : BIOMASS ENERGY PRODUCTION FROM SUNFLOWER PLANT
AUTHOR(S) **: Emek MOROYDOR DERUN**, Shalala HABIBZADE, Deniz UYGUNÖZ

09:40 – 10:00
PAPER TITLE : SYNTHESIS AND CHARACTERIZATION OF ECO-FRIENDLY EDIBLE FILMS BASED ON PISTACHIO SHELL AND PEANUT OIL
AUTHOR(S) : Kerem AKDEMIR, Hilal GÖNÜLTAİ, Burge KÖSE IŞIK, **Nurcan TUGRUL**

10:00 – 10:20
PAPER TITLE : UTILIZATION OF SUGAR BEET PULP AS AN AGRICULTURAL BY-PRODUCT IN VEGAN LEATHER PRODUCTION
AUTHOR(S) : Alize MENEKSE**, Burge KÖSE IŞIK**, Nurcan TUGRUL

10:20 – 10:40
PAPER TITLE : NATURAL PIGMENTS DOPED POLYMER FILMS SYNTHESIS BY SOLUTION CASTING METHOD AND CHARACTERIZATION
AUTHOR(S) : **Deniz UYGUNÖZ**, Ibrahim ŞENGÖR, Emek MOROYDOR DERUN

TEA & COFFEE BREAK 10:40 – 11:00

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SESSION B (11:00 – 13:00)

SESSION CHAIR: Prof. Dr. Emek MOROYDOR DERUN

11:00 – 11-:20

PAPER TITLE : A NEW APPROACH TO THE SYNTHESIS OF A SELENIUM-DOPED BIOACTIVE GLASS SYSTEM: IMPLICATIONS FOR BIOACTIVITY AND DEGRADATION BEHAVIOR

AUTHOR(S) : **Sevil YÜCEL**, Yeşim AYIK, Şeref YILDIRIM, Sinem ARSLAN, Doğa Berşan GÜNEŞ, Esra Nur TURAL, Alperen ARICI, Cem ÖZEL, Deniz SAKARYA, Ali Can ÖZARSLAN

11:20 – 11:40

PAPER TITLE : SYNERGISTIC THERMAL–UV STRESS ACCELERATES HBCD RELEASE FROM BACK-COATED TEXTILES: VOLATILE AND NANOSCALE PARTICULATE PATHWAYS

AUTHOR(S) : **Raed GHANEM**

11:40 – 12:00

PAPER TITLE : EFFECTS OF STRONTIUM AND SELENIUM-DOPED BIOACTIVE GLASSES ON SOFT TISSUE APPLICATIONS: AN IN VITRO EVALUATION

AUTHOR(S) : **Cem ÖZEL**, Semanur ERCAN, Yeşim AYIK, Şeref YILDIRIM, Sinem ARSLAN, Doğa Berşan GÜNEŞ, Esra Nur TURAL, Deniz SAKARYA, Ali Can ÖZARSLAN, Merve ERGİNER HASKÖYLÜ, Sevil YÜCEL

12:00 – 12:20

PAPER TITLE : EFFECT OF TANNIC ACID CONCENTRATION ON MECHANICAL AND STRUCTURAL PROPERTIES OF POLYVINYL ALCOHOL/CHITOSAN/POMEGRANATE PEEL POWDER BASED BIOCOMPOSITE FILMS

AUTHOR(S) : Neşe İŞMAN, **Pınar TERZİOĞLU**

12:20 – 12:40

PAPER TITLE : THE EFFECTS OF H_2O:TEOS RATIO ON THE COMPOSITION AND MORPHOLOGY OF BIOACTIVE GLASSES SYNTHESIZED BY THE STÖBER METHOD

AUTHOR(S) : **Yeşim AYIK**, Doğa Berşan GÜNEŞ, Sinem ARSLAN, Şeref YILDIRIM, Esra Nur TURAL, Alperen ARICI, Cem ÖZEL, Deniz SAKARYA, Ali Can ÖZARSLAN, Sevil YÜCEL

12:40 - 13:00

PAPER TITLE : ACTIVATED CARBON FROM GYPSOPHILA ROOTS: A SUSTAINABLE ADSORBENT FOR DYE REMOVAL

AUTHOR(S) : **Sena Nur KARABEKİROĞLU**, Meral KOCAOĞLU

LUNCH BREAK 13:00 – 14:00

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SESSION C (14:00 – 16:00)

SESSION CHAIR: Prof. Dr. Adnan S. ABU-SURRAH

14:00 – 14:20

PAPER TITLE : THE EFFECTS OF HELICHRYSUM ARENARIUM EXTRACT ON CALCIUM OXALATE CRYSTALLIZATION AS NATURAL INHIBITOR

AUTHOR(S) : Sinan ŞİMŞEK, Osman Yahya USOĞLU, **Emel AKYOL**

14:20 – 14:40

PAPER TITLE : SYNTHETIC METHODS FOR THE PREPARATION OF CYANO SUBSTITUTED OXAZOLO[4,5-b]PYRIDINES

AUTHOR(S) : **Jurja VUKOVİNSKİ**, Marijana Hranjec

14:40 – 15:00

PAPER TITLE : RAPID AND HIGH-ACCURACY CARBON DETERMINATION METHODS FOR SUSTAINABLE CARBON FARMING: IMPLICATIONS FOR NORTH MACEDONIA'S AGROECOSYSTEMS

AUTHOR(S) **: Biljana BALABANOVA**, Verica ILIEVA, Sasa MITREV

15:00 – 15:20

PAPER TITLE : SUPRAMOLECULAR INTERACTION OF GABAPENTIN AND LACTAM WITH CUCURBIT[N]URIL HOST MOLECULES

AUTHOR(S) : **Lubna ALRAWASHDEH**, Bayan F. KULAIB, Khaleel I. ASSAF , Musa I. EL-BARGHOUTHI,
Khaled BODOOR , Osama M. ABUHASAN , Ahmad A. ABDOH

15:20 – 15:40

PAPER TITLE : ENZYME-ASSISTED SOXHLET EXTRACTION OF HELICHRYSUM ARENARIUM AND INVESTIGATION OF THE EFFECT OF ENZYMES (CELLULASE, PECTINASE, XYLANASE) ON TOTAL FLAVONOID CONTENT

AUTHOR(S) : **Sinan ŞİMŞEK**, Emel AKYOL, İlknur KUCUK

15:40 – 16:00

PAPER TITLE : INVESTIGATION OF TORREFACTION PROCESS CONDITIONS FOR BIOCHAR PRODUCTION AS AN ALTERNATIVE RENEWABLE ENERGY SOURCE

AUTHOR(S) : Sakine MIZRAK, Merve ŞANALAN, **Hediye İrem ÖZGÜNDÜZ**

TEA & COFFEE BREAK 16:00 – 16:20

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POSTER SESSION A (16:20 – 17:20)

SESSION CHAIRS: Prof. Dr. Sevil YÜCEL, Prof. Dr. Adnan S. ABU-SURRAH, Prof. Dr. Dolunay ŞAKAR

PAPER TITLE : SYNTHESIS AND APPLICATION OF PENTAAMMINEACETATOCOBALT(III) NITRATE AS A LOW-TEMPERATURE BLEACHING CATALYST IN DISHWASHING DETERGENTS
AUTHOR(S) : **Abdullah AVŞAR** , Bilgehan GÜZEL

PAPER TITLE : SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION AND TITRATIONS WITH METAL CATIONS OF PYRIDINE HYDRAZONES
AUTHOR(S) : **Antonija MAMIĆ**, Marijana HRANJEC

PAPER TITLE : SYNTHESIS AND SUBSTITUENT-DEPENDENT TAUTOMERISM OF BENZOTHIAZOLYL AZO DYES DERIVED FROM 2-NAPHTHOL
AUTHOR(S) : **Anja BEČ**, Robert VIANELLO, Helena CERIĆ, Livio RACANÉ

PAPER TITLE : REMOVAL OF ACETAMIPRID FROM WATER BY ADVANCED TREATMENT PROCESSES: EFFICIENCY AND ECOTOXICOLOGICAL ASPECTS
AUTHOR(S) : **Bruna BABIĆ VISKOVIĆ**, Danijela AŠPERGER, Anica PAVLINOVIĆ, Davor DOLAR

PAPER TITLE : INVESTIGATION OF THE CORRELATION BETWEEN SKIN PERMEATION AND GLOBAL REACTIVITY DESCRIPTORS IN PHENOLIC ANTIOXIDANTS: A COMPARATIVE DFT AND ADMET STUDY
AUTHOR(S) : **Beyza KEMANCI**, Şimal KURUMOĞLU, Burak GÜRKAN

PAPER TITLE : BRAIN PENETRATION IN CNS AND NON-CNS DRUGS USING MOLECULAR ELECTRONIC PARAMETERS
AUTHOR(S) : **Ceren ERGÜL**, Şimal KURUMOĞLU, Yelda Yalçın GÜRKAN

PAPER TITLE : REMOVAL OF FLUTAMIDE FROM AQUEOUS SOLUTIONS USING ACTIVATED CARBON DERIVED FROM LAVENDER: AN ADSORPTION STUDY
AUTHOR(S) : **Derya ALTINTAŞ**, Esra KULAKSIZ ALAYONT, Ozan YÖRÜK, Yüksel BAYRAK

PAPER TITLE : FORENSIC IDENTIFICATION OF PEN INK PIGMENTS USING DUAL-WAVELENGTH RAMAN SPECTROSCOPY COMBINED WITH CHEMOMETRICS
AUTHOR(S) : **Dilek SALKIM İŞLEK**, Eda KİRİŞ, Ayşegül Şen YILMAZ, Erdoğan KÖSE

PAPER TITLE : SUSTAINABLE HEAVY METAL ION DETECTION OF WASTE-BASED CARBON QUANTUM DOTS
AUTHOR(S) : Nour alhuda SALEHA, **Emel AKYOL**

PAPER TITLE : PERFORMANCE ASSESSMENT OF FAUJASITE VARIANTS FOR MULTI-METAL ADSORPTION: IMPACT OF MINERAL TYPE AND COMPETITIVE HEAVY METAL INTERACTIONS

AUTHOR(S) : **Enas N. MAHMOUD**, Sawsan JAAFREH, Khalil M IBRAHIM, Maram Na'es, Rawan Abu SARHAN

PAPER TITLE : MODIFICATION OF BITUMEN BY ADDING REACTIVE TERPOLYMER, POLYOLEFIN ELASTOMER, AND THERMOPLASTIC
AUTHOR(S) : **Hediye İrem ÖZGÜNDÜZ**, Burcu Didem ÇORBACIOĞLU, Seyfullah KEYF

PAPER TITLE : REMOVAL OF SELECTED POLLUTANTS FROM TEXTILE WASTEWATER USING A HYBRID MBR–NF SYSTEM
AUTHOR(S) : **Iva ĆURIĆ**, Anica PAVLINOVIĆ, Davor DOLAR

PAPER TITLE : SYNTHESIS OF A NOVEL SYMMETRICAL SILICON PHTHALOCYANINE PHOTOSENSITIZERS CONTAINING CARBOXYLIC ACID BASED AXIAL ANCHORING GROUPS
AUTHOR(S) : **Gülnur KESER KARAOĞLAN**, Gülşah GÜMRÜKÇÜ KÖSE

PAPER TITLE : SYNTHESIS AND CHARACTERIZATION OF A NOVEL SILICON PHTHALOCYANINE CONTAINING CARBOXYLIC ACID GROUPS
AUTHOR(S) : **Gülşah GÜMRÜKÇÜ KÖSE**, Gülnur KESER KARAOĞLAN

PAPER TITLE :PHOTOINDUCIBLE DECARBOXYLATION IN REACTIONS WITH ALKYNES: REGIOSELECTIVE ADDITION OF ALKYL RADICALS TO THE TRIPLE BOND
AUTHOR(S) : **Kinga PİOTROWSKA**, Sebastian BAŚ

PAPER TITLE : DOUBLE-SIDED CONTROL OF PRODUCT TYPE PREFERENCE IN THE VISIBLE-LIGHT INITIATED REACTION OF 1,3-DICARBONYL COMPOUNDS WITH ALKENES
AUTHOR(S) : **Małgorzata PAŁYGA**, Jan RZEPIELA, Sebastian BAŚ

PAPER TITLE : CHEMICAL CHARACTERIZATION OF PM2.5 IN THE URBAN AIR OF TIRANA: SOURCES, CHEMICAL MARKERS AND ATMOSPHERIC SECONDARY PROCESSES
AUTHOR(S) : **Megi CAUSHAJ**, Florian MANDIJA, Dhurata PREMTI, Spiro DUSHKU

PAPER TITLE : THE INFLUENCE OF THE EXPANSION OF THIOPHENE SUBSTITUENTS ON THE PHYSICOCHEMICAL PROPERTIES AND APPLICATION POSSIBILITIES OF FLUORENE DERIVATIVES
AUTHOR(S) : **Paweł KALARUS**, Agata SZLAPA-KULA, Michał FILAPEK, Sławomir KULA

PAPER TITLE : ANTIOXIDANT ACTIVITY OF BLACK CABBAGE *(Brassica oleracea L. var. sabellica)* FLOWERS
AUTHOR(S) : **Yeşim YEŞİLOĞLU**, Bircan ENGİN

PAPER TITLE : COMPUTATIONAL TOXICOLOGY of FLUFENAUXIRIM and AMINOCYCLOPYRACHLOR: A DFT REACTIVITY and ECOTOXICITY COMPARISON
AUTHOR(S) : Goncagül TUMTUM, Kaan DEMİR, Şimal KURUMOĞLU, **Yelda YALCIN GURKAN**

PAPER TITLE : DETERMINATION OF THE CHEMICAL COMPOSITION OF THE ESSENTIAL OIL OF THE RUBIA TINCTORUM PLANT
AUTHOR(S) : **Temine SABUDAK**, Bahar EREN, Cansu ÖZÇELİK

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PAPER TITLE : SYNTHESIS OF N-METHYL-GLUCAMINE VIA REDUCTIVE AMINATION OF GLUCOSE USING CARBON NANOTUBE-SUPPORTED PALLADIUM CATALYST

AUTHOR(S) : **Tuğba BAYCAN**, Abdullah AVŞAR, Halil KAVRAMA, Bilgehan GÜZEL

SOCIAL PROGRAM

HOTEL DEPARTURE 19:45

Will be organised as part of conference dinner program
Please have your ticket with you

Venue : Tablao de Carmen / Poble Espanyol
Dress Code Smart Casual

Dinner Starting Time : 20:30 / Flamenco Show Starting Time :21:00

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11 APRIL 2026 SATURDAY

SESSION D (08:20 – 11:00)

SESSION CHAIR: Prof. Dr. Emel AKYOL

08:20 – 08:40
PAPER TITLE : STABILITY AND ACTIVITY OF BETA-GALACTOSIDASE IMMOBILIZED ON POLYVINYL ALCOHOL-SODIUM ALGINATE HYDROGELS
AUTHOR(S) : **Doruk AKDOĞAN**, Ayşegül PEKSEL

08:40 – 09:00
PAPER TITLE : EFFECT OF HEMP FILLER ON THE MECHANICAL AND PHYSICAL PROPERTIES OF PLA/PBAT COMPOSITE FILMS
AUTHOR(S) : İlknur KÜÇÜK, **Oğuzhan TAVLIBIYIK**

09:00 – 09:20
PAPER TITLE : SYNTHESIS, STRUCTURAL CHARACTERIZATION AND BIOLOGICAL EVALUATION OF AMINO SUBSTITUTED BENZOXAZOLE DERIVATIVES
AUTHOR(S) : **Marina GALIĆ**, Viktoria RAVLIĆ, Leentje PERSONS, Dirk DAELEMANS, Mihailo BANJANAC, Marijana HRANJEC

09:20 – 09:40
PAPER TITLE : DEVELOPMENT OF A DEP-IMPRINTED GQD@PHEMA-PPIM NANOPARTICLE-BASED SURFACE PLASMON RESONANCE SENSOR FOR DIETHYL PHTHALATE (DEP) DETECTION
AUTHOR(S) : **Monireh BAKHSHPOUR-YUCEL**, Bilgen OSMAN, Cevher Gündoğdu HIZLIATEŞ, Elif TÜMAY ÖZER

09:40 – 10:00
PAPER TITLE : OPTIMIZED FABRICATION OF BIOPOLYMER-DERIVED HYBRID AEROGELS AS SMART DRUG CARRIERS
AUTHOR(S) : Didem AYCAN, Yaşar Andelib AYDIN, **Müge SENNAROĞLU BOSTAN**

10:00 – 10:20
PAPER TITLE : DEGRADATION MECHANISMS of SELECTED AMINOPOLYCARBOXYLIC ACID MOLECULES by DFT METHOD
AUTHOR(S) **: Bahar EREN,** Ayşe Handan DÖKMECİ

10:20 – 10:40
PAPER TITLE : SYNTHESIS AND BILOGICAL ACTIVITY OF 1,2,3-TRIAZOLE COUMARIN HYBRIDS
AUTHOR(S) : **Petra KOVAČEC**, Leentje PERSOONS, Dirk DAELEMANS, Tatjana GAZIVODA KRALJEVIĆ

10:40 – 11:00
PAPER TITLE : NICKEL SULFIDE QUANTUM DOTS ANCHORED ON ZIF-67 AS AN EFFICIENT ELECTROCATALYST FOR HYDROGEN EVOLUTION REACTION
AUTHOR(S) : **Yaren ERDAG MADEN**, Özge KERKEZ KUYUMCU

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TEA & COFFEE BREAK 11:00 – 11:20

SESSION E (11:20 – 13:00)

SESSION CHAIR: Dr. Bahar EREN

11:20 – 11:40
PAPER TITLE : PRODUCTION AND CHARACTERIZATION OF A DOUBLE-LAYERED WOUND DRESSING CONTAINING ELECTROSPUN POLYLACTIC ACID AND HYPERICUM-INFUSED ALGINATE HYDROGEL
AUTHOR(S) : **Seniyecan KAHRAMAN,** Seniye UZUN, Emine ÖZBEY, Filiz UĞUR NİGİZ

11:40 – 12:00
PAPER TITLE : FABRICATION OF ACID-MODIFIED CLINOPTILOLITE DOPED PVDF NANOFIBER MEMBRANES AND OPTIMIZATION OF NITRATE ADSORPTION USING RSM
AUTHOR(S) : **Ayşenur KATIRCI**, Filiz UĞUR NİGİZ

12:00 – 12:20
PAPER TITLE : SYNTHESIS AND IN VITRO CHARACTERIZATION OF QUERCETIN-LOADED ALGINATE-KERATIN COMPOSITE HYDROGELS FOR ENHANCED WOUND HEALING APPLICATIONS
AUTHOR(S) : **Sezer YİĞİT**, Tijen Ennil BEKTAŞ, Seniyecan KAHRAMAN, Filiz UĞUR NİGİZ

12:20 – 12:40
PAPER TITLE : FROM ORANGE PEEL TO SUSTAINABLE BIOCOMPOSITE: PRODUCTION AND CHARACTERISATION OF PECTIN/CMC FILMS WITH MATCHA TEA EXTRACT
AUTHOR(S) : Buse Okyay, **Özde İPSALALI**, Filiz Uğur Nigiz

12:40 – 13:00
PAPER TITLE : PREPARATION AND CHARACTERIZATION OF ELECTROSPUN ZR-BASED UIO-66/SULFONATED PPSU PROTON EXCHANGE MEMBRANES FOR VANADIUM REDOX FLOW BATTERIES
AUTHOR(S) : **Elif ÇOLAK**, Buse ÇETİN, Derya ÜNLÜ, Filiz UĞUR NİGİZ

LUNCH BREAK 13:00 – 14:00

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SESSION F (14:00 – 15:20)

SESSION CHAIR: Prof. Dr. Dolunay ŞAKAR

14:00 – 14:20

PAPER TITLE : PHENYLBORONIC ACID-ENHANCED BENZOXAZINE RESINS AS PROMISING MATRICES FOR THERMAL PROTECTION COMPOSITES

AUTHOR(S) : **Ruveyda ÖZDEMİR**, Derya UNLÜ

14:20 – 14:40

PAPER TITLE : SESAMOL-FUNCTIONALIZED CYCLOPHOSPHAZENES: SYNTHESIS, STRUCTURAL CHARACTERIZATION, AND BIOLOGICAL EVALUATION

AUTHOR(S) : **Şule ŞAHİN ÜN ,** Hanife İBİŞOĞLU ,Yunus ZORLU , Devrim ATİLLA , Gülşah TOLLU, Ersin KILINÇ , Sadin ÖZDEMİR

14:40 – 15:00

PAPER TITLE : SUSTAINABLE AND BIOACTIVE CHITOSAN/PVA HYDROGELS INCORPORATING ALLANTOIN FOR WOUND HEALING APPLICATIONS

AUTHOR(S) : **Miray ÖZBAKIŞ**, Dea ISMAILI, Yusuf SICAK, Pınar TERZİOĞLU

15:00 – 15:20

PAPER TITLE : COMPARATIVE EVALUATION OF INFRARED AND MICROWAVE DRYING OF BERRIES: KINETICS, DIFFUSIVITY, AND MODELING APPROACHES

AUTHOR(S) : **Ekin KIPÇAK**

TEA & COFFEE BREAK 15:20 – 15:40

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POSTER SESSION B (15:40 – 16:40)

SESSION CHAIRS: Prof. Dr. Emel AKYOL, Prof. Dr. Temine ŞABUDAK, Prof. Dr. Yelda YALÇIN GÜRKAN

PAPER TITLE : EFFECT OF AROMATIC RING NUMBER AND SUBSTITUENT ARRANGEMENT ON THE PROPERTIES OF PHENANTHRO[9,10-D]IMIDAZOLE DERIVATIVES FOR OLEDS
AUTHOR(S) : **Agnieszka KRAWIEC**, Jaijanarthanan Lingagouder, Agata Szlapa-Kula, Michał Filapek, Karol Erfurt, Przemyslaw Data, Slawomir Kula

PAPER TITLE : PRODUCTION OF DESALINATION MEMBRANES FROM RECYCLED PVDF POLYMERS
AUTHOR(S) : **Ayşenur KATIRCI**, Filiz UĞUR NİGİZ

PAPER TITLE : CHEMICAL CHARACTERISATION OF MADDER (Rubia tinctorum L.), DETERMINATION OF ANTIOXIDANT ACTIVITY AND DFT STUDIES ON SELECTED COMPOUNDS
AUTHOR(S) : **Bahar EREN,** Temine ŞABUDAK, Hülya ORAK, Cansu ÖZÇELİK

PAPER TITLE : SYNTHESIS OF BIO-POLYOLS FROM AGRICULTURAL WASTE FOR SUSTAINABLE INSULATION PANEL APPLICATIONS
AUTHOR(S) : **Bilgehan GÜZEL**, Sinem TÜMÜK, Erdem DELİL

PAPER TITLE : SYNTHESIS AND CHARACTERIZATION OF N-METHYL-D-GLUCAMINE USING PD/C-SUPPORTED RANEY NICKEL CATALYST
AUTHOR(S) : Tuğba BAYCAN, Burak AY, Abdullah AVŞAR, **Bilgehan GÜZEL**

PAPER TITLE : INFLUENCE OF EXTRACTION TECHNIQUE ON THE POLYPHENOLIC COMPOSITION OF SOLIDAGO CANADENSIS L. AERIAL PARTS
AUTHOR(S) : **Cornelia FURSENCO**, Violeta Alexandra ION, Oana-Crina BUJOR, Simona MARCU, Tatiana CALALB, Alina ORȚAN, Liliana BĂDULESCU, Livia UNCU

PAPER TITLE : REMOVAL OF BISPHENOL A FROM WATER
AUTHOR(S) : **Demet AÇIKGÜL**, Nuran KINACIOĞLU, Dilek DURANOĞLU

PAPER TITLE : PREPARATION AND ANALYSIS OF A HERBAL EXTRACT SOLUTION HAVING RESTORATIVE EFFECTS POTENTIAL AGAINST RADIATION DERMATITIS
AUTHOR(S) : Ayşe Beril DEMİR, Duru BAHÇECİ, Sinem ÖZER, Öznur YAŞA ŞAHİN, **Dolunay ŞAKAR**

PAPER TITLE : REMOVING DISPERSE ORANGE 30 DYE FROM SIMULATED WASTEWATER WITH QUINCE LEAVES BIOADSORBENT
AUTHOR(S) : Zeynep Berra BAĞ, Hüsnü Kemal GÜRAKIN, **Dolunay ŞAKAR**

PAPER TITLE : INVESTIGATION OF THE EFFECT OF ULTRASONIC PRETREATMENTS ON THE OVEN DRYING OF ARONIA BERRIES
AUTHOR(S) : Esra Eylem ŞİMŞEK, **Ekin KIPÇAK**

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PAPER TITLE : FLUOROCARBON FREE WATER REPELLENT ADDITIVES FOR OUTDOOR POLYPROPYLENE YARNS: DEVELOPMENT AND PERFORMANCE EVALUATION
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AUTHOR(S) : **Özge Serra Çetin**, Esra Okay

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SYNTHETIC METHODS FOR THE PREPARATION OF CYANO SUBSTITUTED OXAZOLO[4,5-b]PYRIDINES

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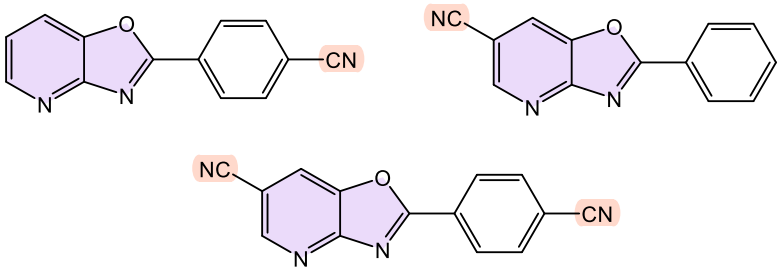
Abstract

Fused heterocyclic scaffolds continue to attract significant interest in modern organic and medicinal chemistry due to their structural diversity and pharmacological relevance. Among them, oxazolo[4,5-*b*]pyridines as nitrogen heterocycles, represent an important scaffold since their derivatives have been associated with a broad range of biological activities, including antitumor, antibacterial, antifungal, anti-inflammatory, antipyretic and analgesic effects [1,2]. The introduction of a cyano group further enhances the relevance of these compounds, as this strongly electron-withdrawing substituent modulates the electronic properties of the molecule and serves as a useful functional group for further chemical transformations important to improve the biological activities [3].

This work focuses on the synthesis and structural characterization of cyano-substituted oxazolo[4,5-*b*]pyridine derivatives. Targeted compounds obtained through a multistep synthetic approach and several optimized synthetic methods involving the construction of the oxazolo[4,5-*b*]pyridine core followed by selective functionalization of the aromatic system. The structures of the synthesized compounds were confirmed using standard techniques, particularly NMR spectroscopy and MS spectrometry. The results contribute to a better understanding of structure–property relationships within oxazolo[4,5-*b*]pyridine systems and underline the potential of cyano-substituted derivatives as valuable intermediates and target molecules for further chemical and biological investigation.



Key Words: *oxazolo[4,5-b]pyridines, cyano group, optimization, organic synthesis*

Acknowledgement: **The Croatian Science Foundation funded this work within the project *BenzHetPot IP-2024-05-7208.***

References

[1] Monier M, Abdel-Latif D, El-Mekabaty A, Elattar KM (2019) Synthetic Communications 50: 1-32.
[2] Sireesha R, Tej MB, Poojith N, Sreenivasulu R, Musuluri M, Subbarao M (2023) Polycyclic Aromatic Compounds 43: 915–931.
[3] Mac M, Baran W, Uchacz T, Baran B, Suder M, Leśniewski S (2007) Journal of Photochemistry and Photobiology A: Chemistry 192: 188-196.

Carbon Dioxide-Based Functional Cyclic Carbonates: Amino Acid-based Iron(III) and Cobalt(III) Complexes Catalysed Coupling of CO_2 and Epoxides

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Abstract

Paving the way for sustainability through carbon dioxide (CO_2) fixation, the utilization of CO_2 to produce value-added chemicals via catalytic systems for the incorporation of CO_2 and epoxides to form cyclic carbonates has garnered significant attention. To date, the most widely studied catalysts for the coupling reactions of CO_2 are those derived from *salen* cobalt complexes. The first generation of these catalysts consists of a binary system comprising a (salen)Co(III)X complex (X = Cl^- or 2,4-dinitrophenolate, etc.) and an exogenous onium salt as a co-catalyst, typically a quaternary ammonium (nBu_4NX) or phosphonium salt (PPNX).
Herein, a new type of mixed-ligand iron(III)- and cobalt(III)- complexes bearing amino acids and heterocyclic diimine ligands, with the general formula $[M(AA)_2(N–N)]Cl$, where M = Fe or Co; AA = L-leucine (Leu) or D-asparagine (Asn); and N–N = 2,2'-bipyridine or 1,10-phenanthroline, were utilized as catalysts for the coupling reaction of CO_2 with various epoxides, such as styrene oxide, epichlorohydrin, and butylene oxide, in the presence of Bu_4NBr under solvent-free conditions. In general, differences in the metal center, ligand substituents, and type of epoxide influence the catalytic activity. The catalytic system exhibited high selectivity toward the formation of cyclic carbonates and high conversion yields.

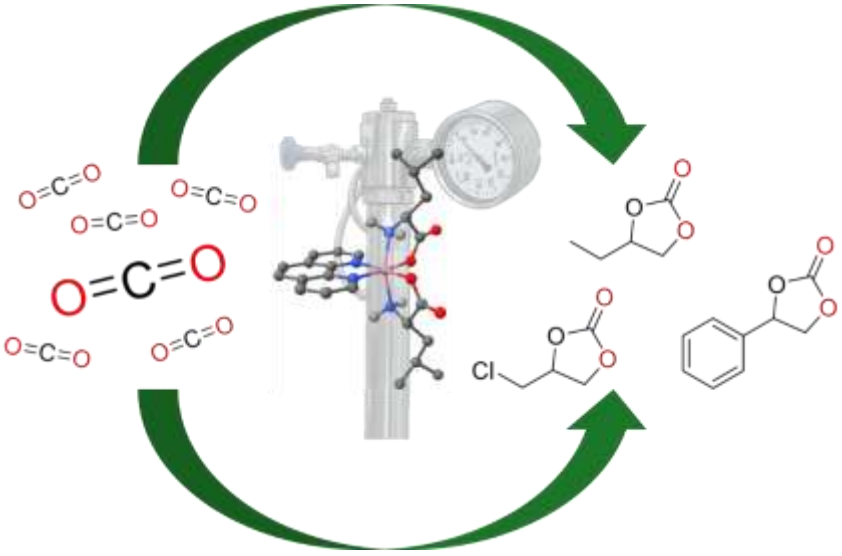

Figure: Catalytic pathway of the coupling reaction of CO2 and epoxides.

Fabrication of Acid-Modified Clinoptilolite Doped PVDF Nanofiber Membranes and Optimization of Nitrate Adsorption Using RSM

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Abstract

Nitrate pollution in water sources remains a critical environmental issue due to its adverse effects on human health and ecosystems. In this study, acid-modified clinoptilolite (Clp)-doped PVDF nanofiber membranes were produced to offer an efficient and sustainable solution for nitrate removal from aqueous solutions. Modification of the surface properties of natural zeolites is critical in nanocomposite membrane technologies developed for the removal of specific pollutants. In this study, an acidic activation process using a 0.3 M HCl solution was performed to improve the surface reactivity and pore structure of Clp. Studies in the literature have observed varying degrees of aluminum removal in modifications made with HCl solutions at different concentrations. The removal of framework aluminum atoms may alter the pore structure and increase micropore volume [1,2]. In this study, the physicochemical and morphological changes in the modified Clp were characterized using Fourier Transform Infrared Spectroscopy (FTIR), Zeta Potential, and particle size analyses. Zeta potential measurements revealed that the surface charge, which was -18.0 mV in the pure sample, increased to -16.1 mV (less negative) after modification. This charge change may reduce electrostatic repulsion between the negatively charged surface and anionic species, facilitating their approach to the adsorbent surface [3]. In addition, particle size analysis showed that the average particle size increased from 2139 nm to 4217 nm after modification, which may be attributed to aggregation effects.

The modified Clp obtained was integrated into PVDF polymer matrix and nanofiber membranes were produced using the electrospinning method. The nitrate adsorption performance of the membranes was optimized using the Response Surface Methodology (RSM). Within the scope of RSM, the effects of parameters such as initial nitrate concentration, Clp content, and adsorbent dose on adsorption and the interactions between these parameters were statistically modeled. Nitrate concentration and Clp addition ratio were determined to be the most effective factors on the adsorption process. According to the experimental design and optimization results, a nitrate concentration of 15 ppm, an adsorbent amount of 0.01 g, and a 4% addition ratio were determined as the optimal parameters. This study aims to contribute to the development of highly efficient and optimized nanocomposite adsorbents for water treatment applications by combining acid modification and statistical experimental design.

Key Words: *Acid Modification; Clinoptilolite; Nitrate Adsorption;Optimization; Response Surface Methodology (RSM)*

Acknowledgement: This study was supported by Çanakkale Onsekiz Mart University Scientific Research Projects Coordination Unit with Project Number of FDK-2026-5515.

References

[1] Allen, S. J., Ivanova, E., & Koumanova, B. (2009). Adsorption of sulfur dioxide on chemically modified natural clinoptilolite. Acid modification. *Chemical Engineering Journal*, *152*(2-3), 389-395.

[2] Akyalcin, S., Akyalcin, L., & Ertugrul, E. (2024). Modification of natural clinoptilolite zeolite to enhance its hydrogen adsorption capacity. *Research on Chemical Intermediates*, *50*(3), 1455-1473.

[3] Hunter, R. J. (2013). *Zeta potential in colloid science: principles and applications* (Vol. 2). Academic press.

DEGRADATION MECHANISMS of SELECTED AMINOPOLYCARBOXYLIC ACID MOLECULES by DFT METHOD

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Abstract

In this study, three molecules named Pentetic acid or diethylenetriaminepentaacetic acid (DTPA), Ethylene Diamine Tetra Acetic acid (EDTA) and Hydroxy Ethylene Diamine Tetra Acetic acid (HEDTA) were investigated, selected from the group of aminopolycarboxylic acids (APCA), which are chemical compounds in which one or more nitrogen atoms are bonded to two or more carboxyl groups via carbon atoms and used in various chemical, medical, and environmental applications. The toxicological properties of these compounds are important for both human health and the environment. Aminopolycarboxylic acids, such as EDTA and DTPA, are compounds that can persist in the environment and are difficult to biodegrade. Therefore, the risk of EDTA becoming a "persistent organic pollutant," is being discussed. Environmental degradation generally occurs through sunlight, and this process is slow. This increases the risk of accumulation in wastewater and natural environments. Their ability to bind metal ions can reduce the bioavailability of some metals in aquatic environments and lead to imbalances in ecosystems. This and similar factors have led to the investigation of the degradation pathways of these molecules in nature.

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 as a result of mixing with wastewater. Geometric optimizations of the fragments were performed using the DFT/B3LYP/6-31G(d) basis set of Quantum Mechanical Density Functional Theory (DFT) to theoretically determine all possible reaction pathways of the selected molecules with the OH radical. Since the reactions of molecules with the OH radical are important for both water treatment and atmospheric chemistry, calculations were performed in both the gas phase and the water phase using the COSMO (conductor-like screening solvation model) solvent model, using CPCM. The Mulliken charges of molecules, the electronegative atoms in the molecule and the arrangement of the atoms surrounding them, stable double bonds, weak bonds at the ends of the molecule, calculated energies, bond lengths, and bond angles between atoms were examined, and these data helped select all the fragments that would determine the degradation mechanism. By examining the molecules for their reactions with OH radicals in air or water, the degradation reaction of each molecule was documented, starting with the lower-energy fragments, and their fate in nature was determined.

Keywords: DFT, aminopolycarboxylic acids (APCA), DTPA, EDTA, HEPTA

References

[1] Eren, B., Yalcin Gurkan, Y. (2022). Possible reaction pathways of selected organophosphorus and carbamate pesticides according to the DFT calculation method, Bulgarian Chemical Communications, 54, 224-234.

[2] Eren, B., Yalcin Gurkan, Y. (2023), Theoretical study of the Azinphos-methyl, Monocrotophos and Omethoate compounds in two phases: Mechanism and DFT study. Innovative Research in Engineering, Duvar Publishing, İzmir Turkey,4,49-71.

RAPID AND HIGH-ACCURACY CARBON DETERMINATION METHODS FOR SUSTAINABLE CARBON FARMING: IMPLICATIONS FOR NORTH MACEDONIA'S AGROECOSYSTEMS

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Precise quantification of soil organic carbon (SOC) is a foundational requirement for contemporary carbon-farming frameworks, where measurement accuracy directly determines carbon-credit eligibility, agroecosystem modelling, and long-term soil-health assessment. In North Macedonia, the accelerating shift toward climate-smart agriculture highlights an urgent need for fast, reliable, and scalable analytical methodologies capable of supporting farmers, policymakers, and research institutions. This study critically evaluates the analytical performance, operational robustness, and practical applicability of several rapid SOC determination techniques, including dry combustion (elemental analysis), UV–Vis spectrometry, loss-on-ignition (LOI), and next-generation portable in-field sensors, benchmarking them against ISO 17025-aligned laboratory reference methods.

Comparative assessments reveal that elemental analysis remains the gold standard for SOC determination, delivering superior accuracy (±0.2%) and traceability. UV–Vis spectrometry, applied through chromogenic oxidation assays and calibrated against total carbon reference measurements, demonstrates very good predictive capability ($R^2 > 0.85$–0.90), especially when supported by multivariate chemometric models. Its high throughput, low cost, and minimal sample-preparation requirements underscore its value for routine SOC screening in regional laboratories. Although LOI provides a cost-efficient alternative, its sensitivity to mineralogical variability necessitates harmonized correction protocols tailored to local soil types. Portable sensors show promise for rapid field-level decision-support but require continuous calibration against standardized laboratory measurements to ensure data reliability.

Application of these methods across major cropping systems in North Macedonia, including barley, chickpea, sunflower, and corn, demonstrates their capacity to enable spatially explicit SOC mapping, improved sequestration estimates, and more precise evaluation of agroecological interventions. The results emphasize the need for strengthened cross-institutional analytical capacity, harmonized QA/QC procedures, and farmer-oriented monitoring strategies to support broad adoption of carbon-farming practices in the Western Balkans. Overall, the integration of high-accuracy and rapid SOC determination tools, particularly the complementary use of elemental analysis and UV–Vis spectrometry, provides a transformative pathway for advancing carbon-credit schemes, enhancing sustainable land management, and increasing the climate resilience of North Macedonia's agroecosystems.

Keywords: carbon determination, UV–Vis spectrometry, SOC, elemental analysis, analytical challenges.

UTILIZATION OF SUGAR BEET PULP AS AN AGRICULTURAL BY-PRODUCT IN VEGAN LEATHER PRODUCTION

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Abstract

The ecological degradation caused by traditional chromium-based tanning processes and the persistence issues of petroleum-derived synthetic leathers have established the development of biodegradable alternatives as a critical imperative within the frameworks of polymer science and sustainable development paradigms [1-4]. This study focuses on the strategic valorization of sugar beet pulp (SBP) an abundant and underutilized agro-industrial by-product of the Turkish sugar industry as a lignocellulosic matrix component for the production of high-performance bio-composite leather-like materials [5]. The methodology involves the molecular integration of SBP fibers into a complex polymeric network based on starch and sodium alginate, followed by their transformation into flexible, leather-like membranes via a controlled solution-casting technique. The fabricated leather-like materials were characterized using Fourier-transform infrared spectroscopy (FTIR), tensile strength testing, water vapor permeability (WVP), and water solubility analyses.

Experimental findings demonstrated that plasticizer selection and formulation parameters play a decisive role in matrix morphology, structural integrity, and barrier properties. FTIR analyses confirmed the presence of characteristic hydroxyl and polysaccharide-derived functional groups, empirically proving the molecular compatibility and stable cross-linking mechanisms among the composite constituents. The sorbitol-modified SPB4-So (So:Sorbitol) sample exhibited a superior mechanical performance with a tensile strength of 22.26 MPa and a Young's Modulus of 1374.22 MPa, making it competitive with traditional leather and superior to many synthetic and alternative vegan leathers [6]. Conversely, the glycerol-containing SPB6-G (G:Glycerol) and SPB6-SoG samples provided a more flexible structure with elongation percentages of 53.8% and 23.4%, respectively, depending on the thickness increase (1.1-1.2 mm). Regarding barrier properties, the SBP4-AG (A:Alginate) sample optimized the "breathability" and moisture management capacity critical for advanced textile applications by providing a minimized water vapor permeability of 1.15 g/m².h. Furthermore, the minimum water solubility rate of 31% (SBP6-G) achieved with high SBP concentration proved the structural stability of the material in aqueous environments.

In conclusion, this study reveals that sugar beet pulp can be effectively engineered as a mechanically durable, eco-friendly, functional, and competitive leather alternative. The developed bio-material offers a promising and scalable innovation model for the transformation of agricultural waste into high-value-added products, fully aligned with circular economy principles.

Key Words: *Vegan leather; sugar beet pulp; bio-based composite; biodegradable material; sustainable production*

References

[1] China, C. R., Maguta, M. M., Nyandoro, S. S., Hilonga, A., Kanth, S. V., & Njau, K. N. (2020). Alternative tanning technologies and their suitability in curbing environmental pollution from the leather industry: A comprehensive review. In Chemosphere (Vol. 254). Elsevier Ltd. https://doi.org/10.1016/j.chemosphere.2020.126804

[2] Muthu, S. S., & Ramchandani, M. (2024). Vegan alternatives for leather. Springer. https://doi.org/10.1007/978-3-031-65365-0

[3] Liu, X., Zhang, X., Wang, X., Yue, O., & Jiang, H. (2025). Engineered, environmentally friendly leather-like bio-based materials. Trends in Biotechnology, 43(5), 1104–1113. https://doi.org/10.1016/j.tibtech.2024.11.006

[4] Venturelli, G., Guida, L., Fasani, M. G. T., Mantero, S., Petrini, P., & Levi, M. (2025). 3D-printable circular composites as sustainable leather alternative for the valorization of tanneries' solid waste. Applied Materials Today, 44, 102776. https://doi.org/10.1016/j.apmt.2025.102776

[5] Crouse, J., Sellers, S., Wawrousek, K., & Sabino, R. M. (2025). Biopolymers from sugar beet molasses: Isolation, characterization, and bioactive properties. ACS Omega, 10(11), 12002–12013. https://doi.org/10.1021/acsomega.4c09633

[6] Meyer, M., Dietrich, S., Schulz, H., & Mondschein, A. (2021). Comparison of the technical performance of leather, artificial leather, and trendy alternatives. Coatings, 11(2), 226. https://doi. org/10.3390/coatings11020226

Effects of Strontium and Selenium-Doped Bioactive Glasses on Soft Tissue Applications: An *In Vitro* Evaluation

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Abstract

While bioactive glasses are extensively utilized in hard tissue engineering [1], their application in soft tissue regeneration has gained significant traction in recent years [2]. The dissolution of ions (e.g., silica, calcium, phosphate) from the glass network into physiological fluids accelerates angiogenesis, stimulates epithelial migration and fibroblast proliferation, and even enhances collagen deposition. Furthermore, ceratin elements such as selenium (Se) and strontium (Sr) are known to exhibit antioxidant, antibacterial, and anti-inflammatory properties, while also promoting angiogenesis, macrophage and fibroblast migration via collagen promoting [3,4]. This study aimed to synthesize a SiO_2–P_2O_5–CaO based bioactive glass system doped with Se and Sr, and to evaluate its *in vitro* biocompatibility and soft tissue applications potential, specifically focusing on collagen synthesis.

Undoped, Se-doped, and Sr-doped bioactive glasses were synthesized using a modified Stöber method and subsequently calcined in a muffle furnace at 600°C. The structural and morphological properties of the synthesized glasses were characterized using XRF, FTIR, XRD, and SEM-EDS. To assess *in vitro* biocompatibility, MTT assays were performed using Human Osteoblast (HOB) and Human Fibroblast (PCS) cell lines at 24, 48, and 72-hour intervals. Additionally, the effect of the bioactive glasses on total collagen and non-collagenous protein production was quantified in the PCS cell line using a Sirius Red/Fast Green staining kit.
Morphological characterization revealed that both doped and undoped glasses possessed monodisperse, spherical structures with the targeted oxide compositions. *In vitro* cytotoxicity assays demonstrated that cell viability remained above 70% for both cell lines in all time points, Furthermore, the Sirius Red/Fast Green assay indicated that Sr-doped glasses induced a higher increase in collagen production compared to the undoped and Se-doped glasses. The doping of Sr into the SiO_2–P_2O_5–CaO glass network significantly enhances fibroblast-mediated collagen synthesis while maintaining high cellular viability. These findings suggest that the developed Sr- and Se-doped bioactive glasses possess strong potential for integration into targeted carrier systems for enhanced soft tissue repair applications.

***Key Words**: Bioactive Glass; collagen; Se-doped, Sr-doped; Sol-Gel*
***Acknowledgement:** This work has been supported by The Scientific and Technological Research Council of Türkiye (TÜBİTAK) under project number 224M333*

References

[1] Özel, C., Özarslan, A. C., & Yücel, S. (2025). Ceramics International 51 (27) 53914-53933
[2] Temel-Soylu, T. M., Kececiler-Emir, C., Rababah, T., Ozel, C., Altug, M. E. (2024) ACS omega, 9(19), 21187-21203.
[3] Chen D, Liang Z, Su Z, Huang J, Pi Y, Ouyang Y, Guo L (2023) ACS Applied Materials & Interfaces, 15:34378-34396.
[4] El-Kady AM, Ali AA, El-Fiqi A (2020) Journal of Non-Crystalline Solids, 534:119889.

NATURAL PIGMENTS DOPED POLYMER FILMS SYNTHESIS BY SOLUTION CASTING METHOD AND CHARACTERIZATION

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Abstract

Recently, research and development activities in both public and private sectors have gained significant momentum due to the use of polymeric and polymer composite films in various fields, including packaging, optics, electronics, coatings, and solar cells. However, the increasing consumption of synthetic polymers makes a rise in plastic waste, causing adverse environmental impacts. To eliminate these effects, the use of biodegradable polymers has become increasingly important. In this study, polyvinyl alcohol (PVA) was selected as a biodegradable polymer matrix, and dye-doped polymer films were fabricated by doping natural pigments—lutein and β-carotene—at concentrations ranging from 3% to 5%. The produced films were characterized using differential scanning calorimetry (DSC), Fourier transform infrared spectroscopy (FTIR), tensile testing, scanning electron microscopy (SEM), and X-ray diffractometry (XRD). Tensile test results revealed that β-carotene enhanced the tensile strength of pure PVA films, whereas lutein combination resulted in a reduction in mechanical strength. DSC analysis indicated that the addition of both β-carotene and lutein increased the melting temperature of the PVA matrix. Polyvinyl alcohol, has been proven to be one of the polymers suitable for packaging materials and many other sectors in terms of production conditions, usability and biodegradability. The produced pure and dye-added films can be preferred as packaging materials due to their smooth surface and good durability.

Key Words: *Polyvinyl alcohol; Biodegradable polymers; Natural pigments; Polymeric films; Packaging materials*

Acknowledgement: This study was supported by the Yildiz Technical University Scientific Research Projects Coordination Department, Project Number: FYL-2022-4877.

STABILITY AND ACTIVITY OF BETA-GALACTOSIDASE IMMOBILIZED ON POLYVINYL ALCOHOL-SODIUM ALGINATE HYDROGELS

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Abstract

β-Galactosidase (EC 3.2.1.23) is an enzyme with long-recognized significance in the food and health industries [1]. It catalyzes the hydrolysis of lactose, which is essential for the development of lactose-free dairy alternatives, and it further contributes to the formation of galacto-oligosaccharides, bioactive compounds linked to prebiotic effects and enhanced gut health [2,3]. This study investigates the immobilization of commercial β-galactosidase derived from *Aspergillus oryzae* within a hydrogel matrix composed of polyvinyl alcohol and sodium alginate, and compares its catalytic performance with that of the free enzyme, as well as with immobilization approaches previously reported in the literature. Immobilization allowed the enzyme to operate efficiently at higher temperatures and provided greater resistance to heat related activity loss. Although both free and immobilized enzymes showed their highest activity under mildly acidic conditions, the immobilized form remained more stable under near neutral and slightly alkaline conditions. Evaluation of kinetic parameters suggested that immobilization limited substrate diffusion while simultaneously enhancing the overall catalytic capacity of the enzyme. The immobilized enzyme also demonstrated improved stability during refrigerated storage over extended periods, whereas freezing conditions resulted in faster loss of activity. In addition, the enzyme maintained high catalytic efficiency over repeated uses. Lactose hydrolysis experiments confirmed that the immobilized system sustained effective catalytic performance over time. Overall, the PVA–SA hydrogel matrix emerges an effective immobilization material that enhances the operational stability of β-galactosidase under challenging processing conditions.

Key Words: *β-Galactosidase; Enzyme; Immobilization; Sodium Alginate, Polyvinyl Alcohol*

References

[1] Wei W, Zhou Z, Li T, Li H, Gong J, Jiang M, Xu Z, Shi J (2025) LWT 228:118024.
[2] Chengolova Z, Ivanova R, Gabrovska K (2024) Journal of the American Nutrition Association 43:213-220.
[3] Singh RV, Sambyal K (2023) Chemical Papers 77:11-31.

COMPARATIVE EVALUATION OF INFRARED AND MICROWAVE DRYING OF BERRIES: KINETICS, DIFFUSIVITY, AND MODELING APPROACHES

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Abstract

Berries are highly valued fruits, which are widely cultivated for their distinctive flavor, rich nutritional composition, and health-promoting properties. They are abundant in bioactive compounds, including anthocyanins, flavonoids, and phenolic acids, which contribute to their strong antioxidant, anti-inflammatory, and anticarcinogenic nature. However, despite their nutritional value and health benefits, berries have a perishable nature due to their high moisture content and delicate structures. Therefore, effective preservation methods are essential to extend their availability and reduce losses associated with microbial spoilage and seasonal production. Drying is a commonly employed preservation technique that prolongs the shelf life while helping to retain nutritional quality and bioactive components. Although numerous studies have investigated changes in antioxidant capacity and nutritional composition during drying, research focusing on drying kinetics and mathematical modelling remains relatively limited. Therefore, the present study examines the infrared and microwave drying behavior of two types of berries: blueberries and golden berries. Infrared drying experiments were conducted at temperatures of 60°C, 70°C, and 80°C, while microwave drying was performed at power levels of 140 W, 210 W, and 350 W. For all experimental conditions, key kinetic parameters, including effective moisture diffusivity (D_{eff}) and activation energy (E_a) were determined. In addition, drying curves were analysed using widely recognized mathematical models reported in the literature. The results demonstrated that both drying methods are effective for the thin-layer drying of blueberries and golden berries. The shortest drying times and the highest effective moisture diffusivity values were obtained at the highest infrared temperature and microwave power level.

Key Words: *Blueberry; golden berry; infrared drying; microwave drying; mathematical modelling*

Preparation and Characterization of Electrospun Zr-Based UiO-66/Sulfonated PPSU Proton Exchange Membranes for Vanadium Redox Flow Batteries

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Abstract

The increasing global energy demand and the integration of renewable energy sources at the grid scale have significantly heightened the need for safe and long-lasting energy storage systems [1]. In this context, vanadium redox flow batteries (VRFB) stand out among systems for large-scale energy storage applications due to their high cycle life, safe operating principle, and scalable structures [1, 2]. One of the most critical components determining the performance of VRFBs is the proton exchange membranes. These membranes need to provide high proton conductivity while limiting the passage of vanadium ions and demonstrating long-term chemical and mechanical stability in a strongly acidic environment [2]. However, the high cost of commercial perfluorinated membranes and their limited ion barrier performance necessitate the development of hydrocarbon-based alternative membranes [3].

In this study, the polyphenylsulfone (PPSU) polymer, known for its high thermal and chemical stability, was functionalized through a controlled chemical sulfonation method, introducing sulfonic acid groups into the matrix and thereby obtaining sulfonated PPSU (sPPSU) with enhanced proton conductivity [3]. The sulfonation degree was controlled to achieve an optimal balance between proton transport capability and mechanical integrity. sPPSU-based proton exchange membranes have been produced in fibrous morphology using the electrospinning method.

To improve the membrane performance, Zr-based UiO-66 series metal-organic frameworks (MOFs) were integrated into the sPPSU matrix at a weight ratio of 3%. In this context, pure UiO-66, amine-functionalized UiO-66-NH_2, and polydopamine-coated UiO-66 (UiO-66PDA) variants have been used. Thanks to the tunable pore structure and surface functionality of the MOFs, the aim was to support proton conduction pathways and limit the passage of multivalent vanadium ions [4]. In addition, amine- and PDA-modified MOF structures were employed to strengthen polymer–filler interfacial interactions and improve membrane stability [5].

The produced electrospun composite membranes were examined using FTIR for chemical structure verification and SEM for morphological analysis; their physicochemical properties were determined through ion exchange capacity (IEC), water retention capacity, dimensional swelling, contact angle measurements, and mechanical tests. Thermal stability was evaluated using TGA and DSC analyses. Proton conductivity was measured using electrochemical impedance spectroscopy (EIS); vanadium ion permeability was determined using a diffusion cell system and UV-Vis analyses [2,6]. Additionally, the chemical and oxidative stability of the membranes was examined through acidic environment tests.

The results show that the 3% UiO-66 series MOF addition significantly improved the balance between proton conductivity and vanadium ion barrier performance. In particular, it has been observed that in membranes containing PDA-modified UiO-66, structural integrity, mechanical strength, and chemical stability have significantly improved due to the increased interfacial compatibility. The combined effect of controlled sulfonation of PPSU and functionalized MOF incorporation enables the design of next-generation composite proton exchange membranes with optimized performance parameters for VRFB applications [1–6].

For the 3 wt% UiO-66 series membranes, the UiO-66-NH_2 sample showed the highest proton conductivity (27.95 μS/cm) and IEC (13.51 meq/g), together with increased porosity (77.27%) and water uptake (263.63%). In contrast, the PDA-modified membrane exhibited lower conductivity (16.64 μS/cm) but significantly improved mechanical strength (20.91 N/mm^2) compared to the pristine UiO-66-S membrane (5.06 N/mm^2). These results indicate that amine functionalization enhances ionic transport, while PDA modification mainly improves mechanical stability.

Key Words: *Vanadium redox flow battery, proton exchange membrane, sulfonated PPSU, UiO-66, electrospinning, ion selectivity*

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References

[1] Skyllas-Kazacos M, Chakrabarti MH, Hajimolana SA, Mjalli FS, Saleem M (2011) Progress in Energy and Combustion Science 37: 386–404.

[2] Weber AZ, Mench MM, Meyers JP, Ross PN, Gostick JT, Liu Q (2011) Journal of Applied Electrochemistry 41: 1137–1164.

[3] Kerres J (2001) Journal of Membrane Science 185: 3–27.

[4] Zhang H, Li X, Zhang H (2018) Energy Storage Materials 15: 324–350.

[5] Park JS, Park S, Shin DW (2021) Chemical Engineering Journal 420: 129743.

[6] Li X, Zhang H, Mai Z, Zhang H, Vankelecom IFJ (2019) Energy & Environmental Science 12: 1147–1160.

BIOMASS ENERGY PRODUCTION FROM SUNFLOWER PLANT

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Abstract

Growing interest in renewable fuels has increased the focus on biodiesel production and the development of efficient heterogeneous catalysts. In the present work, a nano-CaO catalyst was prepared from a calcium carbonate ($CaCO_3$) precursor to be used in transesterification-based biodiesel synthesis. The precursor was calcined at 900 °C for 3 h to obtain CaO.

The synthesized catalyst was characterized by Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscopy (SEM) analyses. FTIR spectra indicated Ca–O bond formation, while additional O–H and CO_3^{2-} related bands suggested that partial hydration and carbonation occurred on the catalyst surface. XRD analysis confirmed CaO as the main crystalline phase; however, weak $CaCO_3$ peaks were also detected, which can be explained by recarbonation after exposure to ambient air. SEM micrographs showed a porous and irregular surface with noticeable particle agglomeration, which is frequently reported for CaO-based catalysts derived from carbonate sources.

Based on the obtained characterization results, the $CaCO_3$-derived nano-CaO catalyst appears suitable for heterogeneous base-catalyzed biodiesel production. The mixed $CaO/CaCO_3/Ca(OH)_2$ phase composition is consistent with the known reactivity of CaO towards CO_2 and moisture. The outcomes of this work provide an experimental foundation for upcoming biodiesel synthesis studies and reaction parameter optimization.

Key Words: *Biodiesel; Transesterification; Nano-CaO catalyst; $CaCO_3$ precursor; characterization*

Acknowledgement: This study was supported by Yildiz Technical University Scientific Research Projects Coordination Unit under project number FYL-2025-6639.

The Effects of *Helichrysum Arenarium* Extract on Calcium Oxalate Crystallization as Natural Inhibitor

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Abstract

Calcium oxalate, particularly in its monohydrate phase, is the main component of typical kidney Stones [1,2]. Kidney stone formation is one of the most significant clinical problems in the human body. Kidney stone disease reduces a person's healthy life expectancy and places a heavy financial burden on healthcare systems; both of these significantly lower an individual's quality of life [3,4]. Therefore, calcium oxalate crystallisation has become an important topic of interest to researchers in biomineralisation. Research indicates that traditional medicine, including herbal remedies, is used by individuals in various cultures and countries to treat kidney stones. *Helichrysum arenarium* possesses antibacterial, antiviral, antifungal, anti-inflammatory, antimicrobial, anti-allergic and antioxidant properties and is used in folk medicine for the treatment of liver and gallbladder disorders, stomach ache, asthma, cystitis and jaundice, skin infections, respiratory and digestive system disorders, kidney stone treatment and urogenital disorders [5,6].

In this study, the spontaneous precipitation of calcium oxalate monohydrate (COM) at 37 °C was investigated in the presence of Helichrysum arenarium extract as natural inhibitor on COM crystallisation, which is highly significant in terms of biomineralisation. The degree of inhibition is measured as the reduction in initial crystallization rate, determined by conductivity of the crystallizing solution. The inhibition increases with a Helichrysum arenarium extract content. The presence of Helichrysum arenarium inhibited the crystal growth of calcium oxalate possibly through adsorption onto the active growth sites for crystal growth.

Key Words: *Calcium oxalate monohydrate (COM), Kidney stone, Helichrysum arenarium extract, Natural inhibitor, Adsorption*

References

[1] Khan, S. R., Pearle, M. S., Robertson, W. G., Gambaro, G., Canales, B. K., Doizi, S., Traxer, O., & Tiselius, H. G. (2016). Kidney stones. Nature Reviews Disease Primers, 2, Article 16008. https://doi.org/10.1038/nrdp.2016.8

[2] Akyol, E., Danisman, M., & Oner, M. (2025). In vitro and in silico evaluation of the inhibitory effects of Persea americana leaf extract against calcium oxalate stones. Urolithiasis, 53(1). https://doi.org/10.1007/s00240-025-01791-4

[3] Suijker, C. A., van Mazijk, C., & Roemeling, S. (2025). Kidney stone disease: Phenomenological perspectives. Medicine, Health Care and Philosophy. https://doi.org/10.1007/s11019-025-10301-7

[4] Akram, M., & Somani, B. (2025). Epidemiology and management of kidney stone disease: Current insights. Research and Reports in Urology, 17, 449–459. https://doi.org/10.2147/RRU.S517758

[5] Klein-Junior, L. C., de Souza, M. R., Viaene, J., Bresolin, T. M. B., de Gasper, A. L., Henriques, A. T., & Van Heyden, Y. (2021). Quality control of herbal medicines: From traditional techniques to state-of-the-art approaches. Planta Medica, 87, 964–988. https://doi.org/10.1055/a-1529-8339

[6] Ivanović, M., Albreht, A., Krajnc, P., Vovk, I., & Razboršek, M. I. (2021). Sustainable ultrasound-assisted extraction of valuable phenolics from inflorescences of Helichrysum arenarium L. using natural deep eutectic solvents. Industrial Crops and Products, 160, 113102. https://doi.org/10.1016/j.indcrop.2020.113102

INVESTIGATION OF TORREFACTION PROCESS CONDITIONS FOR BIOCHAR PRODUCTION AS AN ALTERNATIVE RENEWABLE ENERGY SOURCE

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Abstract

In recent years, there has been increasing interest in using renewable biomass to reduce greenhouse gas emissions associated with the widespread use of fossil fuels [1]. Due to its natural structure, biomass exhibits high moisture, oxygen, ash, and volatile matter contents. Furthermore, its energy density and calorific value are relatively low for efficient energy production limit its direct utilization as an source. Torrefaction is a thermochemical pretreatment process applied under an inert atmosphere at 200-300 °C to improve the chemical structure and fuel quality of biomass [2]. This study aimed to evaluate sesame bran, from the tahini production, as a raw biomass in the production of biochar with improved fuel content. As a result of the torrefaction, the removal of moisture and volatile components from the biomass led to the production of biochar with increased calorific value, while a decrease in O and H and an increase in C content were observed [3]. The effects of temperature and duration time on the operation were also investigated to determine the optimum conditions. To produce torrefied sesame bran (TSB) with improved combustion performance, a torrefaction process was carried out under an N_2 atmosphere at a heating rate 10 °C/min and 220 °C, 250 °C and 280 °C, with 20, 30 and 40 minutes for each temperature. The samples were characterized by proximate and ultimate analysis, energy densification, thermal analysis and Higher Heating Value (HHV) [4]. The results revealed that temperature is more effective than residence time for production. Under optimum conditions determined as 280 °C-30 minutes, TSB with an energy density of 1.14 was obtained, showing an approximately 14% increase in HHV compared to the raw biomass.

Key Words: *Biomass; torrefaction; higher heating value; renewable energy; biochar.*

Acknowledgement:
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References:

[1] Thengane SK, Kung KS, Gomez-Barea A, Ghoniem AF (2022) Progress in Energy and Combustion Science 93:101040.
[2] Simonic M, Goricanec D, Urbancl D (2020) Science of the Total Environment 740:140086.
[3] Guo S, Deng X, Zhao D, Zhu S, Qu H, Li X, Zhao Y (2024) Molecules 29:1889.
[4] Xu N, Wang Z, Chen G, Li Z, Lei T, Gupta A (2026) Renewable Energy 262:125352.

SYNTHESIS, STRUCTURAL CHARACTERIZATION AND BIOLOGICAL EVALUATION OF AMINO SUBSTITUTED BENZOXAZOLE DERIVATIVES

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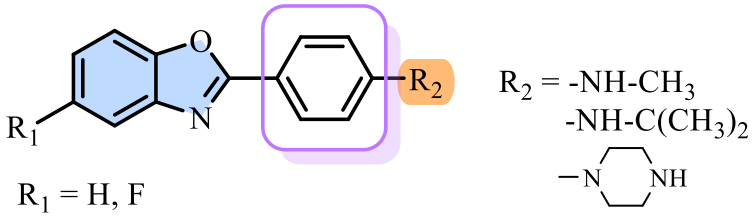
Abstract

Benzoxazole, as a structural bioisostere of the nucleobases adenine and guanine, is recognized in medicinal chemistry as a notable nitrogen-containing heterocycle. Its interactions with macromolecules such as DNA, RNA, and proteins are generally explained by bioisosteric similarity to naturally occurring nucleotides. The heteroatoms within the benzoxazole framework facilitate the formation of non-covalent interactions that are crucial for rational drug design [1, 2]. Benzoxazole derivatives exhibit versatile biological activities like antitumor, antimicrobial, antiviral, antiprotozoal, anti-inflammatory or antioxidative [2, 3].
In this work, we present the synthetic methods, structural characterization and biological evaluation of novel amino substituted 2-arylbenzoxazole derivatives. The targeted derivatives have been prepared by three synthetic methods. Halogeno substituted 2-arylbenzoxazoles have been used as precursors in thermal and microwave assisted amination reactions with various amines. The structures of newly prepared compounds were confirmed by means of ^{1}H and ^{13}C NMR spectroscopy and well as MS spectrometry. Antiproliferative activity *in vitro* was evaluated on the several human cancer cells, while the antiviral activity *in vitro* was evaluated on a panel of viruses. Antibacterial activity *in vitro* was tested on Gram-positive and Gram-negative bacterial strains.



Key Words: *benzoxazole; amination; Buchwald-Hartwig amination; biological activity;*

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References

[1] Kumar A., Singh A.K., Singh H., Vijayan V., Kumar D., Naik J., Thareja S., Yadav J.P., Pathak P., Grishina M. (2023) Pharmaceuticals 16:299.
[2] Di Martino S., De Rosa M. (2024) Topics in Current Chemistry; 382:33.
[3] Galić M., Rohtek T., Persoons L., Daelemans D., Banjanac M., Bruketa T., Radić Stojković M., Hranjec M. (2025) ChemMedChem; 20: e202500429.

ACTIVATED CARBON FROM GYPSOPHILA ROOTS: A SUSTAINABLE ADSORBENT FOR DYE REMOVAL

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Abstract

This study investigates the production and characterization of activated carbon derived from the roots of Gypsophila spp., an endemic genus of flowering plants belonging to the Caryophyllaceae family. Due to their high saponin content and abundant biomass in the Anatolian region of Türkiye, Gypsophila roots represent a sustainable precursor for carbon-based adsorbent materials. In this work, the effects of activating agent type and dosage on pore formation during the preparation of activated carbon from Gypsophila roots were examined. For this purpose, chemical activation was carried out using potassium hydroxide (KOH), phosphoric acid (H_3PO_4), sulfuric acid (H_2SO_4), and citric acid ($C_6H_8O_7$) at various concentrations. To achieve the desired porous structure, the process parameters activation temperature, activation time, and impregnation ratio were optimized using the Box–Behnken experimental design. The activated carbons produced under optimal conditions were characterized using Brunauer–Emmett–Teller (BET) surface area analysis and a series of complementary tests to evaluate their textural properties. The sample exhibiting the most developed porous structure was selected for further adsorption studies. In particular, the performance of the Gypsophila-derived activated carbon in removing cationic and anionic dyes from aqueous solutions will be investigated to assess its potential application in wastewater treatment.

Key Words: *Gypsophila spp., activated carbon, wastewater treatment, dye, environmental*

Development of Phosphazene Nanostructures Encapsulated with Natural Polymers as Drug Carriers for Colon Cancer

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Colon cancer is one of the leading causes of cancer-related mortality worldwide, necessitating the development of effective and targeted drug delivery systems. In this study, monodisperse spherical phosphazene particles were synthesized via a polycondensation reaction using hexachlorocyclotriphosphazene (HCCP) and 1,3-bis(aminomethyl)benzene. The synthesized particles were successfully loaded with the anticancer drug 5-fluorouracil (5-FU), and the resulting structure was encapsulated within a sodium alginate-based natural polymer containing quercetin.The morphological, structural, and thermal properties of the developed system were characterized using transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and zeta potential measurements. In vitro drug release studies were performed under simulated gastrointestinal conditions, where quercetin release was investigated in gastric and intestinal environments, while 5-FU release was evaluated under simulated colonic conditions. Drug release kinetics were calculated based on the data obtained from different gastrointestinal environments.Following the successful drug release studies, the cytotoxic effect of the developed system was evaluated on the HT-29 colon cancer cell line. The results demonstrated that the encapsulated phosphazene-based system effectively protected the drug throughout the gastrointestinal tract and enabled controlled drug release at colonic pH. The combined use of phosphazene nanoparticles with natural polymers presents a promising approach for targeted and effective colon cancer therapy.

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Supramolecular Interaction of Gabapentin and Lactam with Cucurbit[n]uril Host Molecules

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Abstract

Gabapentin (GAB) is a drug molecule used as an anticonvulsant medication [1] and in the treatment of epilepsy, bipolar disorder, neuropathic pain and other disorders [2]. GAB can undergo lactamization and turn into a toxic form called gabapentin-lactam (LAC), with reduced activity [3,4]. In this study, we introduced host-guest concept to encapsulate the GAB within cucurbituril (CBs) host molecules, to study the effect of the encapsulation on the undesirable lactamization process. Different members of CB were used for this purpose, CB6, CB7, and CB8. Spectroscopic and computational techniques have been used to study the complexation of GAB drug and its LAC with CBs. Experimental results showed that GAB drug and its LAC was successfully encapsulated within CB7 and CB8 host molecules, with different binding affinities. ^{1}H NMR spectra recorded over a period of two weeks revealed that the rate of GAB lactamization increased when it was encapsulated within the cavity of CB7. This is a direct result of the lower activation free energy of the lactamization process within the cavity of CB7, as computed by quantum-chemical calculations. Molecular Dynamic (MD) simulations were also used to study the structures and dynamics of the complexation between cucurbit[n]uril (CBn, n = 6–8) and Gabapentin forms (acidic: GLP, zwitterionic: GAB, and basic: GHP) as well as LAC. Results indicated that GLP has the highest binding free energy with the studied hosts.

Key Words: *Gabapentin; Lactam; cucurbituril; encapsulation; lactamization.*

References

[1] M. Herrmann, J. Menz, O. Olsson, K. Kümmerer, (2015). Water Res. (85) 11–21.

[2] L.T. Young, J.C. Robb, I. Patelis-Siotis, C. MacDonald, R.T. Joffe, (1997).Biol. Psychiatry, (42)851–853.

[3] M. Guo, X. Sun, S. Zhang, T. Cai,, (2022). Pharm. Res. (39) 2305–2314.

[4] J.V.P. Katuri, V.S. Ekkundi, K. Nagarajan, (2016) Org. Process Res. Dev. 20 1828–1832.

Sustainable and Bioactive Chitosan/PVA Hydrogels Incorporating Allantoin for Wound Healing Applications

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Abstract

Wound healing is a multifaceted and highly regulated biological process that progresses through four interconnected and overlapping stages: hemostasis, inflammation, proliferation, and remodeling. Each stage involves different cell types such as platelets, fibroblasts, and immune cells, requiring wound dressings that can support multiple healing mechanisms. In the early stages, rapid hemostasis and prevention of microbial infection are critical, while in later stages accelerating tissue regeneration and reducing scar formation become essential. Conventional wound care materials such as gauze and bandages mainly provide physical protection and often fail to create an optimal healing environment, which may delay recovery and increase scarring [1].

Currently available wound dressings exhibit several limitations, including low water vapor transmission rate, insufficient exudate absorption, and inability to maintain a moist environment. To address these challenges, biopolymer-based hydrogels have attracted considerable attention. Hydrogels are three-dimensional hydrophilic polymer networks with excellent water retention, biocompatibility, biodegradability, and exudate absorption capacity. Their ability to maintain a moist and breathable environment while acting as a barrier against microorganisms makes them promising candidates for advanced wound dressing applications [2].

In this study, a PVA/chitosan-based hydrogel wound dressing was developed as an alternative to conventional wound care materials. Polyvinyl alcohol (PVA), a biocompatible and hydrophilic synthetic polymer, and chitosan, a naturally derived biodegradable polymer with inherent hemostatic and antimicrobial properties, were selected as the polymer matrix. To enhance the biological activity of the hydrogel, allantoin (0.5-1.5%) was incorporated as a bioactive additive due to its anti-inflammatory, antioxidant, antimicrobial, and tissue-regenerative properties. The hydrogel films were prepared using the solution casting method [3]. The effect of allontoin concentration on the antioxidant activity, water absorption capacity, mechanical properties, and stability under physiological conditions of PVA/chitosan hydrogels were evaluated. The results indicate that the PVA/chitosan/allantoin hydrogels exhibits suitable mechanical strength, high water absorption capacity, and improved biological functionality.

Overall, the developed hydrogels demonstrated strong potential as effective, biocompatible, and sustainable wound dressing materials for biomedical and healthcare applications. Moreover, the hydrogels were suitable for bioactive cosmetic mask applications.

Keywords: *Wound healing, Hydrogel, Polyvinyl alcohol, Chitosan, Allantoin, Biopolymer composites*

References

[1] Min Peng, Lihong Fan, Huan Yang, Jing Yang, Jin Hu (2016);Preparation and characterization of chitosan/gelatin/PVA hydrogel for wound dressing; Carbohydrate Polymers

[2] Karen Zulema Meza Valle , Rosa A. Saucedo Acuña , Judith V. Ríos Arana , Naun Lobo, Carlos Rodriguez , Juan Carlos CuevasGonzalez , and Karla Lizette Tovar-Carrillo (2020) ; Natural Film Based on Pectin and Allantoin for Wound Healing: Obtaining, Characterization, and Rat Model ; Hindawi BioMed Research International

[3] Chenyu Wang, He Liu, Chen Li, Yanguo Qin, Zhonghan Wang, Fan Yang, Zuhao Li and Jincheng Wang (2018) ; A functional chitosan-based hydrogel as a wound dressing and drug delivery system in the treatment of wound healing; RSC Advances

Development of a DEP-Imprinted GQD@pHEMA-PPIM Nanoparticle-Based Surface Plasmon Resonance Sensor for Diethyl Phthalate (DEP) Detection

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This study aims to develop a surface plasmon resonance (SPR) sensor based on graphene quantum dot (GQD)-functionalized molecularly imprinted nanoparticles (MINPs) for the selective, sensitive, and rapid determination of diethyl phthalate (DEP), an endocrine-disrupting compound. Phthalate esters (PEs) are widely used in various industrial applications, particularly in the plastics industry, and can persist in the environment. The novelty of the proposed SPR sensor lies in the use of GQD@MINP structures on the recognition surface. GQDs are nanoscale graphene derivatives possessing superior mechanical, optical, and physicochemical properties. These features enable their application in a wide range of fields, including bioimaging, solar cells, drug delivery systems, and sensor technologies. Recent reports have shown that integrating GQDs into SPR sensor systems significantly enhances optical performance. Studies on the use of GQDs as a recognition layer in SPR sensors are relatively recent, and to the best of our knowledge, no SPR sensor combining GQDs with molecularly imprinted polymers (MIPs) has yet been reported. Within the scope of this study, highly selective MINPs for the DEP molecule were synthesized. Subsequently, GQDs were synthesized and characterized. The MINPs were functionalized with GQDs and immobilized onto the SPR chip surface to form the recognition layer. The developed SPR sensor system was evaluated for key analytical performance parameters, including selectivity, sensitivity, reusability, limit of detection, and stability. This comprehensive approach enabled the development of a low-cost, rapid-response, reusable, and portable platform suitable for on-site analysis.

Keywords: Graphene quantum dots, Surface plasmon resonance, Nanoparticle, Molecular imprinting, Diethyl phthalate,

OPTIMIZED FABRICATION OF BIOPOLYMER-DERIVED HYBRID AEROGELS AS SMART DRUG CARRIERS

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Abstract

Aerogels provide a highly adaptable material platform where porosity, surface chemistry, and mechanical performance can be finely tailored [1]. Biopolymer-based aerogels, in particular, stand out for controlled drug delivery applications due to their sustainable origin and adjustable physicochemical behaviour [2]. In this study, a ternary biopolymer aerogel system composed of chitosan (CTS), pectin (PEC), and carboxymethyl cellulose (CMC) was fabricated and systematically optimized, with a primary focus on production parameters, structural stability, and future controlled release applications. The selection of this ternary polysaccharide system (CTS/PEC/CMC) was motivated by the complementary properties of each component and their ability to form synergistic three-dimensional networks.

Aerogel fabrication was achieved through gelation and chemical crosslinking, followed by solvent removal using freeze-drying that is a particularly effective method for preserving porous structures and maintaining the stability of incorporated active components. The optimization study focused on two key fabrication parameters as polymer concentration and crosslinking ratio. In this context, different polymer ratios and cross-linker concentrations were used to develop hybrid aerogels. Chemical crosslinking was employed as a critical strategy to enhance the usability of the biopolymers in aqueous environments and to improve the structural stability of the aerogels. By introducing covalent bonds between polymer chains, a three-dimensional network structure was formed, allowing precise control over solubility, swelling behaviour, and degradation characteristics. To avoid the use of conventional toxic cross-linking agents, citric acid (CA) was selected as a biocompatible, environmentally friendly, and water-soluble cross-linker capable of forming strong interactions with natural polymers due to its multifunctional structure [3].

Chemical structures were analysed using Fourier Transform Infrared Spectroscopy (FT-IR). Morphological characterization was investigated by scanning electron microscopy (SEM) revealing interconnected porous structures of the aerogels. Swelling and hydrolytic degradation studies were conducted to observe structural stability and to provide critical feedback for optimization of polymer concentration and crosslinking density. Additionally, mechanical performance of the aerogels was tested through compression tests.

All results were collectively evaluated to determine optimal fabrication conditions of CTS/PEC/CMC hybrid aerogels, which exhibited properties highly desirable for controlled drug delivery systems. While CTS contributed mechanical strength and cationic functionality, PEC enhanced the network flexibility and regulated swelling behaviour, and CMC improved hydrophilicity and structural uniformity. The integration of these components resulted in a balanced aerogel structure with enhanced features. Furthermore, the findings highlight the advantages of a ternary biopolymer approach and establish a strong basis for future application-oriented investigations into aerogel-based controlled drug delivery platforms.

Key Words: *Aerogel; chitosan; pectin; carboxymethyl cellulose; controlled drug delivery*

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References

[1] García-Gonzalez CA, Sosnik A, Kalmar J, De Marco I, Erkey C, Concheiro A, Alvarez-Lorenzo C (2021) Journal of Controlled Release 332:40-63.

[2] Yu S, Budtova, T (2024) Carbohydrate polymers, 332, 121925-121936.

[3] Lu H, Jiang X, Wang J, Hu R (2022) Frontiers in Materials, 9, 1093164-1093174.

SYNTHESIS AND CHARACTERIZATION OF ECO-FRIENDLY EDIBLE FILMS BASED ON PISTACHIO SHELL AND PEANUT OIL

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Abstract

The escalating environmental crisis triggered by the persistence of traditional petrochemical-derived packaging has made the transition toward biopolymer-based and biodegradable alternatives a critical imperative for sustainable development [1-4]. This study focuses on the strategic valorization of pistachio shells (Pistacia vera L.), a significant industrial agrowaste, by utilizing them as a lignocellulosic matrix to develop edible biofilm formulations with high-efficiency food preservation performance [5]. The methodology involved the systematic reduction of hard pistachio shells to a micronized powder size of 250 µm. These particles were subsequently integrated into a complex polymeric network composed of sodium alginate [6] and carrageenan, plasticized with glycerol, and further modified with peanut oil to optimize the overall barrier and mechanical performance.

Comprehensive characterization studies revealed the decisive role of plasticizer selection on film morphology and structural integrity. The utilization of glycerol demonstrated superior flexibility and microbial stability (specifically regarding fungal inhibition) compared to sorbitol-based formulations, which were found prone to micro-void formation and environmental degradation. Furthermore, the incorporation of peanut oil as a hydrophobic agent provided an extraordinary moisture barrier performance. By reducing the water vapor permeability (WVP) of the film matrix to a range of 0.704–2.593 g/m²·h, the developed films exhibited values considerably lower than those commonly reported in the literature, thereby effectively limiting moisture migration. Additionally, water solubility parameters presented a controllable and versatile profile ranging from 48.67% to 86.90%, allowing for tailored applications based on the specific moisture requirements of different food categories.

The protective efficacy of these edible coatings on fruit physiology was quantitatively confirmed through in vivo functional application tests. Following a 14-day storage period, critical weight losses of 70% in strawberries and 90% in apples observed in the control group (uncoated) samples were substantially suppressed to 40.48% and 70.07%, respectively, particularly when treated with the KG-3 (Carragenan-Glycerol-3) formulation. These results verify that the films act as an effective semi-permeable barrier, modulating gas diffusion to slow down metabolic activity while preserving the cellular structural integrity and firmness of the produce. The findings of this study contribute significantly to the literature by demonstrating that pistachio shell wastes can be successfully transformed into value-added active packaging materials, offering a scalable solution to extend shelf life while supporting circular economy principles.

Key Words: *Edible film; pistachio shell; peanut oil; biodegradable packaging; nut waste*

References

[1] Gigante, V., Dal Pont, B., Cavallero, A., Sbrana, C., Fabbri, L. P., Gabriele, M., & Aliotta, L. (2025). Designing eco-friendly edible coatings, valorising agro-wastes, to extend the shelf-life of post-hharvest strawberries. Carbohydrate Polymer Technologies and Applications, 11, 100984. https://doi.org/10.1016/j.carpta.2025.100984

[2] Usman, I., Sana, S., Jaffar, H. M., Munir, M., Afzal, A., Sukhera, S., Boateng, I. D., Afzaal, M., & Urugo, M. M. (2025). Recent progress in edible films and coatings: Toward green and sustainable food packaging technologies. Applied Food Research, 5(2), 101070. https://doi.org/10.1016/j.afres.2025.101070

[3] Kumar Gupta, R., AE Ali, E., Abd El Gawad, F., Mecheal Daood, V., Sabry, H., Karunanithi, S., & Prakash Srivastav, P. (2024). Valorization of fruits and vegetables waste byproducts for development of sustainable food packaging applications. Waste Management Bulletin, 2(4), 21–40. https://doi.org/10.1016/j.wmb.2024.08.005

[4] Gupta, D., Lall, A., Kumar, S., Patil, T. D., & Gaikwad, K. K. (2024). Plant-based edible films and coatings for food-packaging applications: Recent advances, applications, and trends. Sustainable Food Technology, *2*(5), 1428–1455. https://doi.org/10.1039/d4fb00110a

[5] Marzban Panah Maklavani, N., Maskani, M., & Karimi, S. (2025). Systematic review of pistachio shell waste: Environmental applications, sustainable approaches, and nanotechnology insights. Cleaner Waste Systems, 10, 100219. https://doi.org/10.1016/j.clwas.2025.100219

[6] Eslami, Z., Elkoun, S., Robert, M., & Adjallé, K. (2023). A review of the effect of plasticizers on the physical and mechanical properties of alginate-based films. Molecules, 28(18), 6637. https://doi.org/10.3390/molecules28186637

EFFECT OF HEMP FILLER ON THE MECHANICAL AND PHYSICAL PROPERTIES OF PLA/PBAT COMPOSITE FILMS

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Abstract

Increasing concerns over the sustainability of petroleum-based feedstocks have intensified efforts to develop renewable bio-based polymer systems. Compared to fossil-derived materials, bio-based alternatives offer reduced environmental burden, lower carbon footprint, and decreased reliance on finite fossil resources, aligning with sustainable material engineering principles. Renewable plastics offer significant potential to enhance resource efficiency while concurrently reducing environmental degradation, which remains a persistent global concern. In particular, biodegradable polymers that are susceptible to microbial degradation represent an effective strategy for mitigating plastic pollution. Among these materials, polylactic acid (PLA) and poly(butylene adipate-co-terephthalate) (PBAT) have attracted considerable attention for the development of sustainable products. PBAT is especially advantageous for food-contact applications due to its high biodegradability, excellent optical transparency, and superior flexibility. To further enhance its mechanical, barrier, and functional properties, various additives are frequently incorporated into PBAT formulations, thereby improving its overall performance and suitability for packaging applications. Hemp, which contains significant amounts of cellulose, hemicellulose, lignin, and pectin with numerous hydroxyl groups in its structure, highlights its potential for use as a modifying agent due to its high fiber content, lightness, and sustainability.

The aim of the present study is to formulate and to elaborate biodegradable polymer based on PLA-PBAT incorporated with hemp as a filler and to determine their morphological, physical, thermal and mechanical characterization for packing applications. Biofilms with varying PLA and PBAT ratios were prepared via the solution casting method, and alkalized hemp was incorporated into the matrix as a reinforcing filler.

The results indicate that incorporating the hemp as a filler significantly enhances the mechanical performance of the composites, particularly in terms of tensile strength and modulus.

Key Words: *PLA, PBAT, hemp, composite*

REFERENCES

[1] Abdullah AMH, Neogi S, Hossain S, Mohtasim FJ, Asaduzzaman R, Shahidur R, Shakib H, Jikrul A (2026) Journal of Hazardous Materials doi.org/10.1016/j.hazmp.2026.100042

[2] Florian F, Colin D, Olivier W, Manuel K, Luiz FDA (2015) Environmental Chemistry 12 (5): 582–591. doi.org/10.1071/EN14218

[3] Majibur RK, Ying C, Claude L, Hubert L, Qingjin P , Wen Z (2010) Biosystems Engineering 106(3) 315-323 doi.org/10.1016/j.biosystemseng.2010.04.004

[4] Asim S (2013) Materials Science And Engineering Article ID 325085 doi.org/10.1155/2013/325085

[5] Xiaokang J, Shujun L, Mengting Z, Zhaoning X, Zhengkun Y, Yuying M, Guoliang L, Enlong Z, Hai F, Shuhua Z (2025) International Journal Of Biolagical Macromolecules 332 (2) 148669 doi.org/10.1016/j.ijbiomac.2025.148669

[6] Jeannine B, Renan BP, Rodrigo VL, Ana MQBB, Paulo JAS (2020) International Journal Of Biolagical Macromolecules 164(1) 1399-1412 doi.org/10.1016/j.ijbiomac.2020.07.309

FROM ORANGE PEEL TO SUSTAINABLE BIOCOMPOSITE: PRODUCTION AND CHARACTERISATION OF PECTIN/CMC FILMS WITH MATCHA TEA EXTRACT

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Abstract

Global plastic output is projected to attain 600 metric tons by 2025. Petroleum-derived plastics have been chosen for their superior strength, excellent barrier characteristics, and economical large-scale manufacturing. However, consistent the EU Green Deal, the European Union aspires to become the first carbon neutrality by 2050, in this regard, promotes sustainable biopolymers as a viable alternative to petroleum-based plastics [1]. Citrus waste is now generated in substantial volumes worldwide and holds the potential to serve as a useful raw material for a sustainable circular economy model. The high expense and inefficacy of disposal techniques limit the complete utilization of these materials. Specifically, in the orange processing and fruit juice production industry, between 50-60% of the bulk of the orange fruit is waste [2]. Transforming this waste into value-added products is essential for the circular economy. Orange peel, a byproduct of citrus, comprises significant biopolymers like pectin (P), cellulose, and lignin. In this study pectin was extracted from orange peel using an acidic hot citric acid technique, with the extraction conducted by maintaining a solution at a 1:25 g/mL solid-liquid ratio at 80 °C for 1 hour. The yield of pectin was determined to be 51.55%. The objective of this study is to develop orange peel pectin-carboxy methyl cellulose (CMC) biocomposite films and to investigate the influence of Matcha tea extract on their structural and functional properties. To identify the optimal biopolymer film matrix, film solutions were formulated at various weight ratios (10:0, 9:1, 8:2, 7:3, 6:4, 5:5, w/w CMC:P) and generated via the casting technique. With an increase in pectin concentration, the mechanical strength of the films diminished, while their vapor permeability increased. Matcha was included in varying amounts (2,4, 6 mL) into the 8:2 CMC/P films, which exhibited optimal structural characteristics. Increased Matcha incorporation led to a reduction in mechanical strength and moisture content; conversely, a notable increase in water vapor permeability was observed. This phenomenon is attributed to the polyphenols in Matcha tea conferring hydrophobic properties to the film structure. Despite the reduction in mechanical strength, the developed films demonstrated enhanced functional properties, suggesting that Matcha tea infused CMC/P biocomposites hold great potential for active and eco-friendly packaging applications.

Key Words: *Film, Biopolymer, Orange peel pectin, Matcha tea*

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References

[1] Mocan M, Uncu SB (2024) Green Materials 12(4):237-252.

[2] Bátori V, Jabbari M, Åkesson D, Lennartsson PR, Taherzadeh MJ, Zamani A (2017) International Journal of Polymer Science 2017(1):9732329.

SYNTHESIS AND BILOGICAL ACTIVITY OF 1,2,3-TRIAZOLE–COUMARIN HYBRIDS

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Coumarins, characterized by a fused benzene-pyrone ring system, possess a high therapeutic index and strong affinity for diverse molecular targets, resulting in a broad spectrum of biological activities, including antiviral, antitumor and antimicrobial effects.[1] Their derivatives act through multiple mechanisms, such as free radical scavenging, induction of apoptosis, inhibition of angiogenesis, and suppression of tumor metastasis, and are also demonstrated efficacy in inhibiting viral entry and replication in susceptible host cells.[2] Additionally, 1,2,3-triazoles represent valuable heterocyclic pharmacophores in medicinal chemistry due to their bioisosteric relationship with the amide bond, a key structural motif in biomolecules such as proteins and nucleic acids.[3]

In this study, a series of coumarin–triazole hybrids were rationally designed and synthesized *via* three-step synthetic route. 4-*O*- and 7-*O*-propargylcoumarins were prepared by alkylation of hydroxycoumarin with propargyl bromide and were subsequently converted into 4- and 7-(1,2,3-triazole)–coumarin hybrids by copper(I)-catalyzed Huisgen 1,3-dipolar cycloaddition with the corresponding previously prepared 1-azidobenzenes under conventional and mechanochemical conditions. Mechanochemical synthesis generally afforded lower yields (7–79%), but offered advantages in terms of reduced solvent consumption and shorter reaction times. All synthesized compounds were evaluated *in vitro* for antitumor and antiviral activity. A 4-substituted coumarin derivative bearing a methoxy group at position 4 and a nitro group at position 2 of phenyl substituent attached to triazole ring exhibited pronounced activity against pancreatic adenocarcinoma (CAPAN-1, IC_{50} = 8.77 μM). The most potent antiviral activity against human coronavirus (HCoV-OC43, EC_{50} = 1.19 μM) was observed for a 4-substituted coumarin–triazole hybrid containing a chlorine atom at position 2 and a nitro group at position 5 of the phenyl ring.

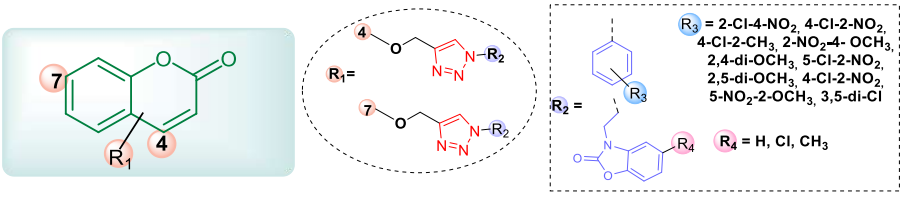

Figure 1. General structure of synthesized 1,2,3-triazole–coumarin hybrids

Key Words: coumarine; 1,2,3-triazole; antitumor activity; antiviral activity; mechanocehmistry

Acknowledgement: This work was supported by the Croatian Science Foundation under the project HRZZ-IP-2022-10-9420.

References

[1] Sinha S, Singh K, Ved A, Hasan Sm, Mujeeb S (2022) Mini-reviews In Medicinal Chemistry 22:1314.
[2] Flores-Morales V, Villasana-Ruiz AP, Garaza-Veloz I, González-Delgado S, Martinez-Fierro ML (2023) Molecules 28:2413.
[3] Gazivoda Kraljević T, Harej A, Sedić M, Kraljević Pavelić S, Stepanić V, Drenjančević D, Talapko J, Raić-Malić S (2016) European Journal Of Medicinal Chemistry 124:794.

EFFECT OF TANNIC ACID CONCENTRATION ON MECHANICAL AND STRUCTURAL PROPERTIES OF POLYVINYL ALCOHOL/CHITOSAN/POMEGRANATE PEEL POWDER BASED BIOCOMPOSITE FILMS

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Abstract

Tannic acid can act as a multifunctional natural crosslinker and active agent, significantly upgrading barrier, mechanical and functional performance of the biodegradable polymeric films through extensive hydrogen-bond interactions In this study, the effect of tannic acid (TA) addition at different ratios on the mechanical properties of polyvinyl alcohol (PVA), chitosan (CS), and pomegranate peel powder (PPP)–based biocomposite films was investigated. The films were produced by the solution casting method, and tannic acid was incorporated into the polymer matrix at 6-10% (w/w) ratios based on the total polymer weight. A film containing just pomegranate peel powder, PVA/CS/PPP, without tannic acid was used as the control sample.

The mechanical properties of the films were evaluated by tensile testing machine to determine elastic modulus, tensile strength, and elongation at break values. The results indicated that the incorporation of tannic acid led to an increase in elastic modulus and tensile strength of the films. The highest elastic modulus and tensile strength values were obtained for the films containing 10% tannic acid; however, a significant decrease in elongation at break was observed at this concentration. In contrast, films containing 6% and 8% tannic acid exhibited a more balanced mechanical performance, maintaining relatively high strength while preserving flexibility.

Structural interactions within the biocomposite films were analyzed using Fourier Transform Infrared Spectroscopy (FTIR). FTIR results revealed the formation of strong hydrogen bonding interactions between the phenolic –OH groups of tannic acid and the functional groups of PVA and chitosan. No new peaks related with covalent bond formation were detected, indicating that tannic acid acted as a physical crosslinking agent within the polymer matrix. These structural findings are consistent with the observed mechanical behavior, where enhanced intermolecular interactions contributed to increased stiffness and strength of the films.

In conclusion, this study demonstrates that tannic acid is an effective natural additive for developing the mechanical properties of PVA/CS/PPP-based biocomposite films, highlighting its potential for use in sustainable and biodegradable composite films.

Key Words: *Tannic acid; Biocomposite films; Mechanical properties; FTIR; Solution casting*

Acknowledgement: This work has been supported by the Research Fund of Bursa Technical University (Project Number: 230D014).

Synergistic Thermal–UV Stress Accelerates HBCD Release From Back-Coated Textiles: Volatile And Nanoscale Particulate Pathways

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Abstract-Hexabromocyclododecane (HBCD) is a persistent organic pollutant (POP) in legacy textiles. This study quantifies its emissions from back-coated fabrics under thermal aging, UVA-340 exposure, and mechanical abrasion, explicitly evaluating synergistic thermal–UV interactions. Emissions were measured via kinetic modeling, headspace VOC sampling, and size-resolved particulate analysis. Thermal aging at 90 °C yielded **0.167 ± 0.01 %** volatilization; UV exposure produced **0.162 ± 0.02 %** while combined thermal–UV stress accelerated emissions (**synergy factor S = 1.92**) with a cumulative release of **0.233 ± 0.03 %**, nearly doubling the additive prediction. Mechanical abrasion released **6.53 µg m^{-2} cycle^{-1}** particulates, dominated by **30–260 nm** nanoscale fractions following UV pre-aging. Average airborne concentrations were **≈250 µg m^{-3} for unaged** and **0.8–60 µg m^{-3} for UV-aged** textiles. This work introduces the first quantitative kinetic synergy factor (S) for HBCD, demonstrating that combined thermal–UV stress nearly doubles the release rate predicted by additive models. Furthermore, we establish a novel link between photochemical aging and the generation of respirable, nanoscale particulate emissions, a critical pathway overlooked in current risk assessments. These findings provide essential parameters for exposure models and highlight the necessity of multi-stressor frameworks in regulatory design

Keywords: Hexabromocyclododecane (HBCD); flame retardants; thermal–UV aging; photothermal synergy; particulate emissions; diffusion-controlled release.

PHENYLBORONIC ACID-ENHANCED BENZOXAZINE RESINS AS PROMISING MATRICES FOR THERMAL PROTECTION COMPOSITES

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Abstract

The high speeds reached by spacecraft and aircraft during their journeys through the atmosphere cause these vehicles to be subjected to significant stresses from the external environment. Factors such as high temperature resulting from aerodynamic friction, oxidative environment, high pressure, and plasma effect threaten the structural and thermal integrity of the system [1]. The simultaneous effect of multiple challenging environmental factors has made the development of innovative engineering materials in this field necessary. Therefore, the development of composite materials with high thermal resistance, resistance to mechanical impact, flame retardant properties, low thermal expansion coefficient, and lightweight characteristics is aimed. Such composites are called thermal protection systems (TPS). TPS acts as a heat shield by preventing the transfer of excessive heat generated on the outer surface of vehicles exceeding hypersonic speeds to the internal structure [2]. The composite materials used in these systems are generally in the form of multi-phase structures containing a reinforcement phase (carbon, glass, or Kevlar fiber) and a matrix phase (resin, ceramic, or polymer) that provide high mechanical strength. One of the determining factors in the performance of this multi-component structure is the matrix phase, which is directly affected at high temperatures. Since the matrix material is the part most damaged due to ablation and surface friction under hyperthermal conditions, the correct selection of the polymer type to be used is of critical importance [3]. Phenolic resins have been preferred as matrix materials in many spacecraft designs due to their advantages such as low thermal conductivity, high coal residue yields, and the capacity of gases released during thermal decomposition to absorb heat. Polybenzoxazine (PBz) resin is a type of thermoset polymer that has been developed in this context and can be an alternative to the phenolic structure [4]. Benzoxazine resins have the potential to reduce problems such as brittleness, harmful compounds released during hardening, and the use of acidic catalysts compared to traditional phenolic systems. In this study, the aim is to evaluate the results obtained using a modification method to improve the thermal properties of the benzoxazine resin group. Boron modification was applied to the synthesized benzoxazine resins. It was determined that benzoxazine resins with phenylboronic acid additive provided a significant increase in coal residue yield compared to the benzoxazine system without additive. Differential scanning calorimetry (DSC) analysis of the benzoxazine resin revealed two characteristic peak temperatures. The first peak occurred at 118.71°C, and this transition is associated with a preceding thermal event occurring at a low temperature. The second and more significant peak was observed at 198.80°C, and this temperature represents the point where the curing reaction of the resin shows maximum activity. The obtained DSC data reveal that the benzoxazine resin is activated by a heat-triggered polymerization mechanism and gains chemical stability at high temperatures. These properties support the usability of benzoxazine-based systems in high-performance applications requiring thermal resistance and structural integrity [6].

Key Words: *Benzoxazine, Phenolic resin, Thermal properties, Phenylboronic acid*

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References

[1] Daniel A, Badhe Y, Srikanth I, Gokhale S, Balasubramanian K (2016) Industrial and Engineering Chemistry Research 55:10645-10655.
[2] Cheng H, Fan Z, Hong C, Zhang X (2021) Composites Part A: Applied Science and Manufacturing 143, 106313.
[3] Zhang Y, Shen Q, Li X, Wang L, Nie C (2021) Materials Chemistry Frontiers 5(11):4214-4224.
[4] Guo T, Fan Y, Bo C, Qi Z, Tao H, Ziran C, Youhui X (2021) High Performance Polymers 33(7):825-831.
[5] Deliballi Z, Kiskan B, Yagci Y. (2020) Macromolecules 53(7):2354-2361.
[6] Yin R, Cheng H, Hong C, Zhang X (2017) Composites Part A: Applied Science and Manufacturing 101: 500-510.

Production and Characterization of a Double-Layered Wound Dressing Containing Electrospun Polylactic Acid and Hypericum-Infused Alginate Hydrogel

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Abstract

This study involves the development of a double-layered, natural-based wound dressing using advanced production techniques to accelerate the wound healing process and minimize the risk of infection. The goal is to combine the properties expected of an ideal wound dressing—moist environment maintenance, high absorption capacity, appropriate porosity, and antimicrobial protection—into a single structure [1],[2]. The outer layer of the wound dressing was produced using the electrospinning method with polylactic acid (PLA), a synthetic polymer with high biocompatibility [3]. The produced PLA nanofibers were found to have a porosity of over 85%. Contact angle measurements showed a value of 128°, indicating that the outer layer exhibits hydrophobic characteristics. This feature protects the wound area from external fluids while also allowing gas transmission. Mechanical tests revealed that the PLA layer exhibits a tensile strength of approximately 4 MPa and provides sufficient mechanical resistance for wound dressing applications. When SEM and optical microscope images were evaluated together, it was observed that the nanofibers had a homogeneous distribution and that structural integrity was maintained. FT-IR analyses showed that the electrospinning process did not cause any degradation or unwanted side reactions in the basic chemical bond structure of PLA. In the inner layer, alginate hydrogel, a natural biopolymer, was chosen to support tissue regeneration by keeping the wound moist [4],[5]. This hydrogel structure was enriched with Hypericum perforatum extract, known for its wound-healing and anti-inflammatory properties, at concentrations ranging from 1% to 4%. Swelling analyses revealed that the hydrogel containing 2% Hypericum perforatum showed the highest performance, reaching a swelling rate of approximately 652%. The same formulation was found to have a lower hardness value and offer a more flexible structure. FT-IR analyses confirmed that the Hypericum perforatum components were successfully integrated into the alginate network structure. As a result, a functional double-layered wound dressing was developed by combining the mechanical strength and protective barrier properties of PLA nanofibers produced by the electrospinning method with the high liquid absorption capacity and biological activity of Hypericum perforatum-enhanced alginate hydrogel. The findings indicate that this structure offers an effective and promising alternative for modern biomedical applications and tissue engineering studies.

Key Words: *Polylactic acid, Electrospinning, Alginate hydrogel, Hypericum perforatum extract, Bilayer wound dressing*

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References

[1] Dhivya, S., Padma, V.V., Santhini, E. (2015). Wound dressings-A review. BioMedicine, 5(4), 22-28.
[2] Tiwari, N., Kumar, D., Priyadarshani, A., Jain, G.K., Mittal, G., Kesharwani, P., Aggarwal, G. (2023). Recent progress in polymeric biomaterials and their potential applications in skin regeneration and wound care management. Journal of Drug Delivery Science and Technology, 82, 104319.
[3] Khouri, N. G., Bahú, J. O., Blanco-Llamero, C., Severino, P., Concha, V. O., & Souto, E. B. (2024). Polylactic acid (PLA): Properties, synthesis, and biomedical applications–A review of the literature. *Journal of Molecular Structure*, *1309*, 138243.
[4] Veld, R. C. O., Walboomers, F., Jansen, J. A., Wagener, F. A. D. T. G. (2020). Design Considerations for Hydrogel Wound Dressings: Strategic and Molecular Advances, Tissue Engineering Part B: Reviews, 26, 3.
[5] K. Varaprasad, T. Jayaramudu, V. Kanikireddy, C. Toro, E.R. Sadiku, Alginate-based composite materials for wound dressing application: a mini review, Carbohydr. Polym. 236 (2020).

A NEW APPROACH TO THE SYNTHESIS OF A SELENIUM-DOPED BIOACTIVE GLASS SYSTEM: IMPLICATIONS FOR BIOACTIVITY AND DEGRADATION BEHAVIOR

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Abstract

Bioactive glasses are very prominent in both hard and soft tissue applications. In the glass network, various elements from the periodic table can be incorporated to impart specific bioactive properties to the material [1]. Selenium is an essential trace element and a component found in bone and muscle tissues. The element is known to possess antioxidant, anticancer, antibacterial, and anti-inflammatory activities, regulate interleukin-6, reactive oxygen species, and pro-inflammatory gene expression, macrophage migration activity, and mitochondrial functions of cells in inflammatory processes [2, 3]. Despite these properties of selenium, studies on selenium-doped bioactive glass are limited in the literature [4]. Accordingly, the present study reports on the synthesis and *in vitro* characterization of monodispersed, spherical bioactive glass nanoparticles in the system: SiO_2–P_2O_5–CaO–SeO_2.

The bioactive glass nanoparticles were synthesized with some additional steps to a modified Stöber Method by Miola et. al. The process is a base catalysed sol-gel method and individual, non-agglomerated particles can be obtained with the help of high pH in the basic synthesis avoiding the use of surfactants [5]. The obtained particles were then characterized by X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, X-ray fluorescence (XRF) spectroscopy, scanning electron microscopy coupled with energy-dispersive X-ray spectroscopy (SEM–EDS), and thermogravimetric and differential thermal analysis (TG/DTA) etc. Afterward, the *in vitro* bioactivity was evaluated by measuring the ions exchanged between the bioactive glass particles and simulated body fluid over a period of up to 14 days using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). Furthermore, the *in vitro* biodegradability was also evaluated by incubating the produced particles in TRIS-HCl buffer solution at 37 ˚C for different time intervals up to 24 h. In this context, changes in the pH of the incubation medium and the percentage weight loss of the particles were determined.

The characterization results showed that Se-doped, nanoscale, monodispersed, spherical bioactive glass particles were successfully synthesized using a modified Stöber method. The *in vitro* bioactivity results indicate that selenium incorporation had no detrimental effect on the bioactivity of the bioactive glass compared with the undoped sample, in terms of ion release and hydroxyapatite precipitation. The bioactive and biodegradable behavior of the particles make them very promising for both soft and hard tissue engineering applications.

The potential use of these particles as dermal filler materials is currently being investigated within an ongoing research and development project.

Key Words: *Bioactive Glass; Stöber Method; Selenium, Bioactivity; Biodegradability*

Acknowledgement: This work has been supported by The Scientific and Technological Research Council of Türkiye (TÜBİTAK) under project number 224M333.

References

[1] Mehrabi T, Mesgar AS, Mohammadi Z (2020) ACS biomaterials science & engineering, 6:5399-5430.
[2] Chen D, Liang Z, Su Z, Huang J, Pi Y, Ouyang Y, ... Guo L (2023) ACS Applied Materials & Interfaces, 15:34378-34396.
[3] El-Kady AM, Ali AA, El-Fiqi A (2020) Journal of Non-Crystalline Solids, 534:119889.
[4] Swetha R, Priyangha PT (2024) Cureus, 16:e61728.
[5] Miola M, Piatti E, Sartori P, Verné E (2023) Journal of Non-Crystalline Solids 622:122653.

Synthesis and In Vitro Characterization of Quercetin-Loaded Alginate-Keratin Composite Hydrogels for Enhanced Wound Healing Applications

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Abstract

This study involves the effective management of cutaneous wounds remains a significant clinical challenge, primarily because traditional dressing materials, such as cotton gauze, often fail to maintain an optimal moisture balance. This deficiency can lead to secondary tissue trauma during dressing changes and delay the natural regeneration process. Consequently, contemporary biomedical research has increasingly focused on the development of "smart" biomaterials that mimic the extracellular matrix to facilitate superior healing. This study details the synthesis and comprehensive characterization of a novel hybrid hydrogel system designed to serve as a bioactive component within multilayered wound dressings. By synergistically combining the exceptional water-retention capacity of sodium alginate with the biological affinity of keratin, a functional matrix was engineered to provide both structural support and the controlled delivery of therapeutic agents.

The fabrication protocol involved the preparation of a 1% (w/v) sodium alginate solution, which was subsequently blended with keratin at varying concentrations (1%, 2%, and 3% w/v) at a controlled temperature of 45 0 C to ensure homogeneity. The resulting composite mixture was subjected to ionic cross-linking using calcium chloride (CaCl2), establishing a stable three-dimensional network through the interaction between calcium ions and alginate chains. To impart specific antioxidant and anti-inflammatory properties to the scaffold, quercetin—a potent natural polyphenol—was encapsulated within the matrix at a precise concentration of 0.1% .

The structural integrity and chemical composition of the synthesized hydrogels were rigorously evaluated using Fourier Transform Infrared (FTIR) spectroscopy. The spectral analysis confirmed the successful molecular entrapment of quercetin, evidenced by the appearance of a distinctive aryl ether (C-O-C) peak at 1271 cm-1. This specific molecular signature indicates that the bioactive molecule remained chemically stable within the polymeric network without degradation. A pivotal aspect of the investigation was the assessment of the hydrogel's swelling behavior, a critical parameter for the effective management of wound exudates. Experimental data revealed that the formulation containing 2% keratin achieved an optimal swelling ratio of 293% after a 48-hour period. This substantial absorption capacity suggests that the hydrogel can effectively regulate fluid balance at the wound site, thereby preventing maceration while maintaining sufficient hydration to support cellular migration.

Furthermore, in vitro release studies conducted in a phosphate-buffered saline (PBS) environment at pH 7.4 demonstrated a sophisticated, time-dependent release kinetic profile. The results indicated that increasing the keratin content significantly modulated the diffusion rate of quercetin, with the formulation containing 3% keratin exhibiting the highest cumulative release efficiency over the test period. This controlled release mechanism provides

a dual benefit: an initial burst release to mitigate immediate oxidative stress and infection risks, followed by a sustained delivery phase to support long-term tissue regeneration. In conclusion, the alginate-keratin-quercetin hydrogel system developed in this work offers a highly biocompatible, mechanically stable, and therapeutically active alternative for advanced wound care applications.

Key Words: *Hydrogel, Sodium Alginate, Keratin, Quercetin, Drug Release, Wound Care.*

Acknowledgement: *This research was supported by the Çanakkale Onsekiz Mart University Scientific Research Projects Coordination Unit (BAP) and Grant Number FBA-2025-5202.*

Enzyme-Assisted Soxhlet Extraction of Helichrysum Arenarium and Investigation of the Effect of Enzymes (Cellulase, Pectinase, Xylanase) on Total Flavonoid Content

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Abstract

Medicinal plants were widely used in the treatment of diseases throughout history [1,2]. *Helichrysum arenarium* is one of the promising resource rich in bioactive chemicals, especially flavonoids [3]. Flavonoids have been used in the treatment of various diseases due to their many health benefits, such as antioxidant, anti-inflammatory, anti-aging, antibacterial, antiviral, anticancer, neuroprotective, and antitumor properties [4,5]. Extraction technology is the most important step in the recovery of bioactive chemicals from plants. Flavonoids has been mainly extracted by traditional extraction methods such as soxhlet extraction method and waterbath immersion [6]. Today, the application enzyme-assisted extraction (EAE) to extract active substances from plants has increasingly emerged as a new trend. EAE is an extraction method that uses enzymes such as cellulase, hemicellulase, pectinase, xylanase, xylase, a-amylase and polygalacturonase for the extraction of valuable compounds from plants [7].

In the present work, the flavonoid extraction from Helichrysum arenarium using soxhlet extraction alone and in combination with enzyme-assisted methods was investigated and the influence of enzimes types (cellulase, pectinase, and xylanase) was explored. The total flavonoid content was determined based on the aluminum chloride colorimetric method [9] in terms of quercetin equivalent (mg QE/mL). The results indicate that the highest yield obtained in the presence of xylanase enzyme. The enzyme-assisted extraction method has demonstrated higher extraction capacity compared to traditional soxhlet extraction, offering high efficient.

Key Words: *Helichrysum arenarium, Flavonoid, Soxhlet Extraction, Enzyme-assisted Extraction, Xylanase.*

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References

[1] A Cetinkaya, A., Yayla, S., Hurkul, M. M., & Ozkan, S. A. (2025). The sample preparation techniques and their application in the extraction of bioactive compounds from medicinal plants. Critical Reviews in Analytical Chemistry, Advance online publication, 1–36. https://doi.org/10.1080/10408347.2025.2503437

[2] Chaves, J. O., de Souza, M. C., da Silva, L. C., Lachos-Perez, D., Torres-Mayanga, P. C., Machado, A. P. D. F., Forster-Carneiro, T., Vázquez-Espinosa, M., González-de-Peredo, A. V., Barbero, G. F., & Rostagno, M. A. (2020). Extraction of flavonoids from natural sources using modern techniques. Frontiers in Chemistry, 8, 507887. https://doi.org/10.3389/fchem.2020.507887

[3] de Luna, F. C. F., Ferreira, W. A. S., Casseb, S. M. M., & de Oliveira, E. H. C. (2023). Anticancer potential of flavonoids: An overview with an emphasis on tangeretin. Pharmaceuticals, 16(9), 1229. https://doi.org/10.3390/ph16091229

[4] Ivanović, M., Albreht, A., Krajnc, P., Vovk, I., & Razboršek, M. I. (2021). Sustainable ultrasound-assisted extraction of valuable phenolics from inflorescences of Helichrysum arenarium L. using natural deep eutectic solvents. Industrial Crops and Products, 160, 113102. https://doi.org/10.1016/j.indcrop.2020.113102

[5] Klein-Junior, L. C., de Souza, M. R., Viaene, J., Bresolin, T. M. B., de Gasper, A. L., Henriques, A. T., & Van Heyden, Y. (2021). Quality control of herbal medicines: From traditional techniques to state-of-the-art approaches. Planta Medica, 87, 964–988. https://doi.org/10.1055/a-1529-8339

[6] Łubek-Nguyen, A., Ziemichód, W., & Olech, M. (2022). Application of enzyme-assisted extraction for the recovery of natural bioactive compounds for nutraceutical and pharmaceutical applications. Applied Sciences, 12(7), 3232. https://doi.org/10.3390/app12073232

[7] Simsek, S., Akyol, E., & Kucuk, İ. (2025). Development of a high-performance liquid chromatography (HPLC) method for coumarin quantification in medicinal plants extracted via Soxhlet. Bulgarian Chemical Communications, 57(3), 202. https://doi.org/10.34049/bcc.57.3.SS-EA-IK

SESAMOL-FUNCTIONALIZED CYCLOPHOSPHAZENES: SYNTHESIS, STRUCTURAL CHARACTERIZATION, AND BIOLOGICAL EVALUATION

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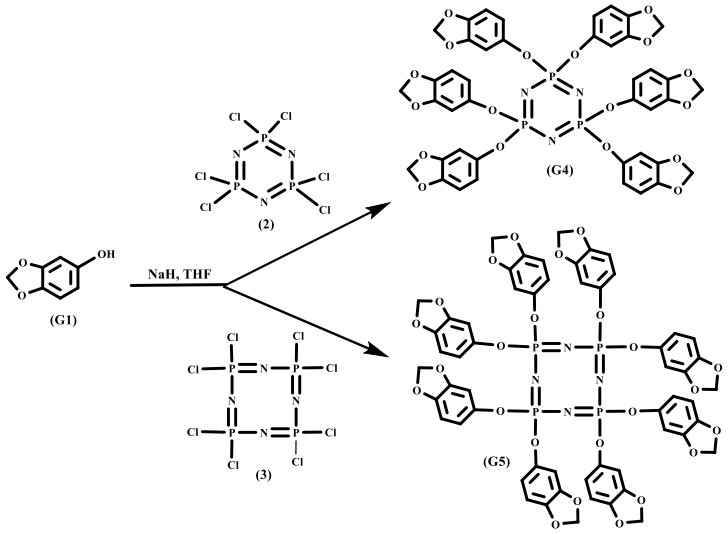
Abstract

In the present study, sesamol-appended cyclophosphazene derivatives (**G4** and **G5**) were synthesized and characterized by elemental analysis, mass spectrometry and (^{1}H, ^{13}C and ^{31}P) NMR spectroscopy. The crystal structure of **G4** was determined and reported for the first time.



The biological activities (amylolytic, DNA cleavage, antimicrobial, and antioxidant activities) of sesamol and the cyclophosphazenes derivatives were systematically evaluated. The synthesized compounds demonstrate a promising potential for diverse applications within the enzyme, pharmaceutical and environmental industries after in vitro, in vivo and in situ toxicologic test systems [1].

Key Words: *Sesamol, Cyclophosphazene, Antimicrobial, Amylolytic activity, DNA cleavage*

References

[1] Ibisoglu H, Sahin Ün S, Zorlu Y, Atilla D, Tollu G, Kılınç E, Ozdemir S, **(2026)** Journal of Molecular Structure, 1357, 145199.

Nickel Sulfide Quantum Dots Anchored on ZIF-67 as an Efficient Electrocatalyst for Hydrogen Evolution Reaction

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Abstract

Sustainable hydrogen production by water electrolysis requires efficient and cost-effective noble-metal-free electrocatalysts. Pt-based catalysts have excellent hydrogen evolution reaction (HER) activity, but their scarcity and expense prevent widespread use. Thus, transition-metal-based catalysts with controllable nanoscale structures and good interfacial charge-transfer properties remain a research priority. In this study, a hybrid electrocatalyst with in-situ generated nickel sulfide quantum dots (NiS_x QDs) on a ZIF-67 scaffold was produced rapidly using microwave irradiation and tested for acidic HER in 0.5 M H_2SO_4 [1].

NiS_x QDs were directly nucleated and generated on pre-synthesized ZIF-67 utilizing nickel precursors and ammonium sulfide ($(NH_4)_2S$) as the sulfur source in polar solvents under microwave irradiation. Fast heating and uniform nucleation reduce particle agglomeration and create ultrasmall NiS_x domains and intimate interfacial contact with the porous MOF substrate. For uniform catalyst loading and repeatable electrochemical testing, the NiS_x QDs@ZIF-67 composite was processed into a stable catalytic ink with the proper binder/solvent mixture and drop-cast onto a glassy carbon electrode (GCE). The synthesis conditions were optimized to enable rapid quantum dot formation while preserving the structural integrity of the ZIF-67 framework. The porous architecture enhances reactant and product transport due to increased surface area [2].

Electrocatalytic performance in 0.5 M H_2SO_4 was evaluated by LSV, Tafel analysis, EIS, and stability studies. The NiS_x QDs@ZIF-67-modified GCE showed faster HER kinetics and improved interfacial electron transport, with a low overpotential at 10 mA cm^{-2} and a decreased Tafel slope. EIS results indicated lower charge-transfer resistance compared to reference electrodes, accelerating catalyst–electrolyte reaction kinetics. Operating stability under acidic environments was tested using long-term chronoamperometry. The large dispersion of NiS_x QDs provides many active sites, robust interfacial coupling from in-situ development, and porous support for electrolyte accessibility and gas release, improving activity. This study demonstrates that microwave-assisted in-situ synthesis of nickel sulfide quantum dots on MOF platforms is an effective strategy for constructing noble-metal-free electrocatalysts for acidic hydrogen evolution and scalable hydrogen production.

Key Words: *Hydrogen evolution reaction; quantum dots; ZIF-67; MOF-based electrocatalyst; water electrolysis.*

References

[1] Li, Cha, Hao Zhang, Ming Liu, Fei-Fan Lang, Jiandong Pang, and Xian-He Bu (2023) Industrial Chemistry & Materials, 1: 9-38.
[2] Vetti, K.J. and A. Koca (2025) International Journal of Hydrogen Energy, 97: p. 214-225.

THE EFFECTS OF H_2O:TEOS RATIO ON THE COMPOSITION AND MORPHOLOGY OF BIOACTIVE GLASSES SYNTHESIZED BY THE STÖBER METHOD

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Abstract

The sol-gel method was reported for synthesis of bioactive glasses with advances than melt-quenching method in the early stage of 90's, for the first time. It has been determined that reducing the size of bioactive glasses, especially at the nanoscale, increases the surface area and consequently increases surface reactivity and bioactivity [1, 2]. It is highly important for increased protein adhesion, enhanced biomineralization and osteoblast proliferation or differentiation, improved properties such as antimicrobial, anti-inflammatory etc. [1]. On the other hand, spherical bioactive glasses have more uniform distribution when they are used in matrix materials, with improved mechanical features and increased bioactivity [3]. However, it is ambitious to produce spherical, monodispersed and nanoscaled bioactive glass particles with the basic sol-gel method [1].

In this study, bioactive glass samples were synthesized by the Stöber Method which is a base catalysed sol-gel method. Agglomeration of the particles were prevented by a modification as adding a centrifuge step after the formation of the silica nanoparticles [4]. Furthermore, it is known that H_2O:TEOS mole ratio is also an important parameter for particle aggregation, the ratio should be at least 4:1 [5]. Thus, several bioactive glass samples were synthesized with same composition (54% SiO_2 – 33% CaO – 13% P_2O_5) by changing H_2O:TEOS mole ratios from 4:1-62:1 to investigate the effects on the composition and morphology within this research. After that, Scanning Electron Microscopy coupled with Energy Dispersive X-Ray Spectrometry (SEM-EDS) was used to identify morphological properties, X-Ray Diffraction (XRD) was used to investigate crystallization, Fourier Transform Infrared (FTIR) Spectroscopy was used to observe functional groups. In addition, thermal behavior and properties were analysed by Thermogravimetry Differential Thermal Analysis (TG/DTA).

In conclusion, spherical bioactive glass particles were produced. The characterization results clearly demonstrate that the increasing H_2O:TEOS mole ratio affects the composition and morphology of the synthesized samples. For example, the findings showed that the expected composition was more closely achieved when production was carried out using a 62:1 H_2O:TEOS ratio. The result obtained implies that the gap between theoretical and experimental compositions can be decreased by increasing H_2O:TEOS ratio. Furthermore, the particles were non-agglomerated and well-dispersed compared to others.

Key Words: *Bioactive Glass; Sol-Gel; Stöber Method; H_2O:TEOS; Monodispersity*

Acknowledgement: This work has been supported by The Scientific and Technological Research Council of Türkiye (TÜBİTAK) under project number 224M333.

References

[1] Lukowiak A, Lao J, Lacroix J, Nedelec JM (2013) Chemical Communications 49:6620-6622.
[2] Kesse X, Vichery C, Nedelec JM (2019) Acs Omega, 4:5768-5775.
[3] Zheng K, Lu M, Liu Y, Chen Q, Taccardi N, Hüser N, Boccaccini AR (2016) Biomedical Materials 11:035012.
[4] Miola M, Piatti E, Sartori P, Verné E (2023) Journal of Non-Crystalline Solids 622:122653.
[5] Bourebrab MA, Oben DT, Durand GG, Taylor PG, Bruce JI, Bassindale AR, Taylor A (2018) Journal of Sol-Gel Science and Technology, 88:430-441.

SYNTHESIS AND APPLICATION OF PENTAAMMINEACETATOCOBALT(III) NITRATE AS A LOW-TEMPERATURE BLEACHING CATALYST IN DISHWASHING DETERGENTS

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The primary challenge in the formulation of automatic dishwashing detergents (ADWD) is the removal of polyphenolic stains (e.g., tea and coffee) at reduced temperatures to meet energy efficiency standards. Sodium percarbonate, the standard oxygen source, typically requires temperatures 60^{o}C for effective activation. Transition metal catalysts, specifically Cobalt(III) complexes, offer a superior alternative by lowering the activation energy barrier for perhydrolysis, thereby enabling robust oxidation performance at 30-40^{o}C. This study investigates the synthesis and catalytic efficiency of Pentaammineacetatocobalt(III) Nitrate, $[Co(NH_3)_5(OAc)](NO_3)_2$.

The complex was synthesized via one-pot oxidative ligand substitution route with $Co(NO3)_2.6H_2O$, H_2O_2 and CH_3COOH. The structure was confirmed using UV-Vis spectroscopy (d-d transitions) and FT-IR (noting the characteristic acetate carbonyl stretch at 1610 cm-1). The synthesized complex was incorporated into a standard "all-in-one" ADWD matrix at a concentration of 200 ppm (0.02% w/w). Upon dissolution, the Cobalt(III) center interacts with the perhydroxyl anions (HOO^-) released by the percarbonate. This interaction generates highly reactive hydroxyl and superoxide radials, which oxidatively cleave the chromophores in polyphenolic stains, rendering them colorless and water-soluble. Performance was evaluated at 40^{o}C using DM-14 Tea soil (soiled melamine resin tile) in a standard cycle (water hardness: 250 ppm $CaCO_3$).

Detergents containing the Cobalt catalyst showed a 35% increase in remission on tea stains at 40^{o}C compared to catalyst-free formulations. The performance achieved by Cobalt-catalyzed systems at 35-40^{o}C was found to be statistically equivalent to standard TAED-based systems at 60^{o}C. The nitrate salt variant exhibited excellent chemical stability within the alkaline detergent matrix, maintaining its catalytic activity after 3 months of accelerated storage testing at 40^{o}C. Pentaammineacetatocobalt(III) Nitrate is a highly efficient bleach catalyst that bridges the performance gap in cold-water dishwashing. By facilitating rapid oxidation at lower temperatures, this technology enables significant energy savings and shorter wash cycles without compromising hygiene or cleanliness standards.

Keywords: *Coordination Chemistry, Cobalt(III) Complexes, Bleach Catalyst, Dishwashing Performance, Low-Temperature Hygiene.*

Effect of Aromatic Ring Number and Substituent Arrangement on the Properties of Phenanthro[9,10-d]imidazole Derivatives for OLEDs

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Abstract

Does the number and arrangement of aromatic rings in a substituent affect the properties and OLED applicability of phenanthro[9,10-d]imidazole derivatives? To address this issue, we synthesized ten phenanthro[9,10-d]imidazole derivatives (0A–0J) via a condensation reaction. The compounds differ in the aromatic substituent at the C2 position, selected to provide a systematic increase in the number of aromatic rings and differences in the attachment position of the substituents: phenyl (0A), biphenyl-1-yl (0B), naphthalen-1-yl (0C), naphthalen-2-yl (0D), anthracen-9-yl (0E), phenanthren-9-yl (0F), anthracen-2-yl (0G), triphenylen-2-yl (0H), pyren-1-yl (0I), and perylen-3-yl (0J). All phenanthro[9,10-d]imidazole derivatives exhibit thermal stability above 290 ºC. However, this parameter is not strictly related to the increasing number of aromatic rings in the substituent. Electrochemical studies revealed that the oxidation process is strongly associated with the substituent at the C2 position. The reduction process takes place on the phenanthro[9,10-d]imidazole core. Interestingly, in the case of systems with a larger conjugated system, the reduction occurs much more easily (0E, 0G, 0I). The absorption spectra of 0A–0D, 0F, and 0H are largely independent of the aromatic substituent, whereas 0E, 0G, and 0J show absorption features characteristic of anthracene or perylene substituents. The emission spectra of 0A–0D, 0H, and 0F indicate emission from a locally excited singlet emission state (^{1}LE), while compounds 0E, 0G, 0I, and 0J exhibit stronger substituent-dependent emission behavior. Electroluminescence studies have shown that the emission color and efficiency can be fine-tuned by changing the aromatic substituent at the C2 position. Compounds 0E, 0I, and 0J combine favorable energy alignment, moderately delayed fluorescence, and strong solid-state emission, with 0J achieving an EQE of 4.3% and a luminance reaching 8960 cd·m^{-2}.

Key Words: *phenanthroimidazole derivatives; electroluminescence; organic light emitting diode; OLED; light emitting devices;*

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SYNTHESIS AND SUBSTITUENT-DEPENDENT TAUTOMERISM OF BENZOTHIAZOLYL AZO DYES DERIVED FROM 2-NAPHTHOL

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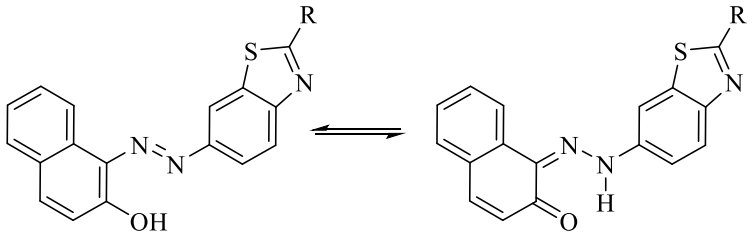
Azo dyes containing both a hydroxyl group and an azo chromophore are known to undergo azo-hydrazone tautomerism, which involves proton transfer between oxygen and nitrogen atoms. This process is of considerable interest from both theoretical and applied perspectives. The position of the tautomeric equilibrium has a significant influence on key characteristics of azo dyes, including their colour, hue, photostability and technological performance. In our previous work, azo-hydrazone tautomerism of 6-[(2-hydroxy-1-naphthyl)diazenyl]benzothiazole and its 2-methyl-substituted analogue was examined using a combination of ^{13}C NMR spectroscopy and DFT calculations. The observed *K*azo-hydrazone(H)/*K*azo-hydrazone(CH_3) ratio of 1.3 indicated that electron-donating substituents favour a shift of the equilibrium towards the azo tautomer [1,2].

In the present study, we describe the synthesis and investigate the tautomerism in solutions of a series of new 2-substituted derivatives which exhibit more pronounced equilibrium shift (Figure 1). A detailed DFT calculations were carried out to determine the relative stabilities of tautomers, predict NMR and UV/Vis spectroscopic parameters and evaluate the kinetic parameters of the proton transfer reaction.



R = -CF_3, -Cl, -$N(CH_3)_2$, -Ph

Figure 1. 2-substituted benzothiazolyl azo-derivatives

Key Words: *Azo dyes; benzothiazole, azo-hydrazone tautomerism; 13C NMR spectroscopy; DFT calculations*

Acknowledgement: *This work is funded by the European Union – NextGenerationEU (SIMBA-6, TTF-IIP-07)*

References:

[1] Pavlović G, Racané L, Čičak H, Tralić-Kulenović V. (2009) Dyes and Pigments 83:354-362.
[2] Racané L, Mihalić Z, Cerić H, Popović J, Tralić-Kulenović V. (2013) Dyes and Pigments 96:672-678.

SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION AND TITRATIONS WITH METAL CATIONS OF PYRIDINE HYDRAZONES

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As parts of numerous natural and synthetic compounds, heterocycles such as pyridine are often used as useful building blocks in medicinal chemistry. Their structural similarity to naturally occurring nucleotides allows their modification and optimization in order to obtain more selective compounds for rational drug design [1]. Besides pyridine derivatives, hydrazone-based compounds have attracted significant attention due to their wide range of biological activities, including antimicrobial, antioxidant, and anticancer activity. Hydrazones contain carbonyl and imine functional groups, which enable them to coordinate metal ions and form stable complexes while the presence of the NH group enables hydrogen bonding interactions [2,3]. Metals such as K, Zn, Co, Cu and Fe, as essential biogenic elements, play vital roles in the human body, and their deficiency or excess can lead to various pathological effects [4]. In this work, we report the synthesis and structural characterization of substituted pyridine hydrazones prepared in order to investigate their potential application as metal ion sensors in solutions. The target compounds were synthesized via condensation reactions between substituted hydrazines and aromatic aldehydes. The structures of the prepared compounds were confirmed using ^{1}H and ^{13}C NMR spectroscopy and MS spectrometry. UV-Vis titrations with aqueous solutions of metal cations K^{+}, Li^{+}, Zn^{2+}, Co^{2+}, Cu^{2+}, Fe^{3+} were performed to evaluate the potential applicability of the synthesized hydrazones for metal ion sensing purposes.

Key Words: *pyridine; hydrazone; biogenic elements; metal cations; UV/Vis spectroscopy*

Acknowledgement: This research was conducted within the project OsKomLiMe (112104) financed by the European Union's- NextGenerationEU fund from the source 581 – The recovery and resilience mechanism, in the frame of Programme financing of public higher education institutions and public scientific institutes.

References

[1] Villa-Reyna AL, Perez-Velazquez M, Gonzalez-Felix ML, Galvez-Ruiz JC, Gonzalez-Mosquera DM, Valencia D, Ballesteros-Monreal MG, Aguilar-Martinez M, Leyva-Peralta MA (2024) International Journal of Molecular Sciences 25:7640-7670
[2] Czyżewska I, Mazur L, Popiołek Ł (2024) Chemical Biology & Drug Design 104: 14590-
[3] Tafere DA, Gebrezgiabher M, Elemo F, Sani T, Atisme TB, Ashebr TG, Ahmed IN (2025) RSC Advances 15:6191-6207
[4] Kostova I (2023) Inorganics 11:56-86

Production of Desalination Membranes From Recycled PVDF Polymers

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Abstract

Water is not only an essential resource for life but also a crucial input in industry. Water sources around the world vary in their levels of pollution and salinity. Advanced technologies have been developed for the use of water in industrial applications. The aim of this study is to investigate the separation of saline water using an innovative membrane distillation method for use in process and cooling water. A key point of the study is the use of a membrane regenerated from waste polymer in the membrane distillation system. This will ensure waste disposal by reusing waste without mixing it into nature, and will contribute to the country's economy by recycling waste instead of using a new product. In addition, the study will involve the direct use of real seawater on an industrial scale.

Within the scope of the study, polyvinylidene fluoride (PVDF), a commercial membrane material, was obtained from waste membranes and reused. This enabled the production of a recycled domestic membrane. The recovered PVDF was produced as a porous membrane using the electrospinning technique. Characterization tests such as FTIR, porosity-water retention, and mechanical strength were performed on the membrane. The porosity value of 78% is consistent with the structure reported in the literature for recycled PVDF. The stress value of the membrane obtained using recycled PVDF polymer was measured as 10.09 MPa, while the strain value was 0.64. This indicates that the membrane exhibits flexible mechanical behavior. Finally, salt rejection of 99% and above was achieved.

Key Words: *Desalination; Membrane Distillation; PVDF; Recycling*

Acknowledgement: *This study was supported by Çanakkale Onsekiz Mart University Scientific Research Projects Coordination Unit with Project Code of FBA-2025-4996.*

CHEMICAL CHARACTERISATION OF MADDER (*Rubia tinctorum* L.), DETERMİNATION OF ANTIOXIDANT ACTIVITY AND DFT STUDIES ON SELECTED COMPOUNDS

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Abstract

This study aimed to characterize the above-ground (root) and above-ground parts of the Rubia tinctorum plant growing in the Havsa region of Thrace, and to experimentally determine its antioxidant activities. The study also aimed to theoretically investigate the compounds and fragments characterized by experimental results using the DFT/B3LYP/6-31G(d) basis set of Quantum Mechanical Density Functional Theory (DFT). Ultimately, the goal was to reveal the relationship between theoretical and experimental data.

R. tinctorum was extracted using hexane, chloroform, and water. The phenolic content was determined by LC-MS/MS, and the volatile/semi-volatile compound composition by GC-MS. LC-MS/MS revealed 10 phenolic acids and 8 flavonoid compounds in the above-ground water extract, while 4 phenolic acids and 5 flavonoids were detected in the root water extract. GC-MS analysis of the plant revealed fatty acids and esters, alkanes, and anthraquinones as the main compounds.

Total phenolic content and antioxidant activities of all extracts were investigated using DPPH, FRAP, and ABTS methods. Chloroform extracts showed the highest antioxidant activity in all methods except DPPH. In addition, theoretical studies were conducted with selected compounds and anthraquinones present in high amounts in above-ground water, subsurface chloroform, and subsurface hexane extracts. The degradation pathways of the main compounds used as natural dyes and the starting molecules and fragments obtained from the extractions were determined.

Keywords: Antioxidant, anthraquinone, DFT, *Rubia tinctorum*, chromatography

References

[1] Krishnan Marg KS (1985) The Wealth of India: Raw Materials, National Institute of Science Communication and Information Resources CSIR, New Delhi-110 012.

INVESTIGATION OF THE CORRELATION BETWEEN SKIN PERMEATION AND GLOBAL REACTIVITY DESCRIPTORS IN PHENOLIC ANTIOXIDANTS: A COMPARATIVE DFT AND ADMET STUDY

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Abstract

This study investigates the correlation between the skin permeation potential and global reactivity descriptors of four structurally distinct phenolic compounds: Ethyl Guaiacol, Carvacrol Acetate, Caffeic Acid, and Syringic Acid. Molecular geometries were optimized using Density Functional Theory (DFT) at the B3LYP/6-311G(d,p) level. Global reactivity descriptors, including chemical hardness, softness, and electrophilicity index, were derived from the Frontier Molecular Orbitals (FMO). The electronic structure and stability of the derivatives were evaluated through Partial Density of States (PDOS), vibrational analysis, and global reactivity descriptors. Additionally, Atoms-in-Molecules (AIM) and Non-Covalent Interaction (NCI) topological analyses were employed to characterize intramolecular hydrogen bonding and electronic delocalization. Percutaneous permeability coefficients, pharmacokinetic parameters, and toxicological profiles were predicted using SwissADME and ProTox-3.0 computational platforms. A significant contrast in skin permeation was observed between the alkylated/esterified derivatives and their carboxylic acid counterparts. Carvacrol Acetate and Ethyl Guaiacol exhibited superior permeability, whereas Caffeic and Syringic Acids demonstrated limited barrier penetration. DFT analysis revealed that low chemical hardness and reduced dipole moments are critical electronic factors facilitating diffusion through the lipophilic stratum corneum. All compounds were predicted to be in Toxicity Class 4 or 5, confirming their safety for topical applications. The findings indicate that skin permeability is governed not only by lipophilicity but also by intrinsic electronic "softness." This "Quantum-Permeability" approach provides a predictive framework for the rational design of bioactive molecules in cosmeceutical and transdermal drug delivery systems. The study also highlights the utility of DFT combined with ADMET analysis for evaluating their pharmacological potential. [1]

Key Words: *ADMET, DFT, Phenolic Antioxidants, PDOS, Protox-3.0*

References

[1] Hammami, M., Chaabani, E., Yeddes, W., Wannes, W. A., & Bourgou, S. (2023). Phenolic compounds and skin permeability: An in silico investigation..

Synthesis and Characterization of *N*-Methyl-D-Glucamine Using Pd/C-Supported Raney Nickel Catalyst

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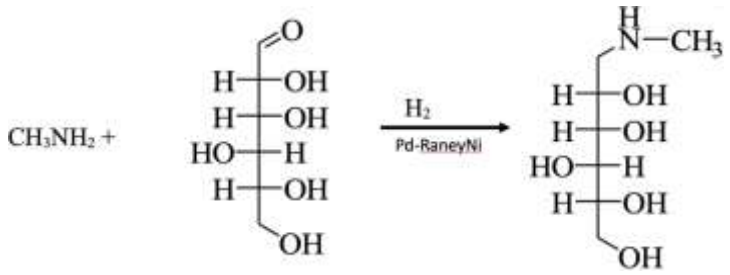
This study examines a hybrid catalyst system developed to achieve high efficiency and selectivity in the synthesis of *N*-Methyl-D-Glucamine (Meglumine), a vital pharmaceutical excipient. The reductive amination of D-Glucose with methylamine was performed using a Pd/C-supported Raney Nickel catalyst. The chemical structure of the resulting product was rigorously verified through FTIR and 1H NMR spectroscopy. In industrial Meglumine synthesis, Raney Nickel is traditionally used as the sole catalyst; however, this method can sometimes lead to issues such as low selectivity and catalyst deactivation. The Pd/C-supported Raney Nickel (Raney Ni-Pd/C) system used in this study aims to create a synergistic effect by combining the high hydrogenation capacity of nickel with the superior selectivity of palladium for imine hydrogenation at lower temperatures.



Experimental methods and Analytical Results: The reaction was carried out in a controlled autoclave reactor according to the following stages: D-Glucose was dissolved in a methanol/water mixture and mixed with monomethylamine (CH3NH2). The Pd/C-supported Raney Nickel catalyst was added to the mixture. The system was agitated at temperatures of 50−70∘C and under H2 pressure of 60−80 bar. The presence of Pd ensured rapid saturation of the imine intermediate, thereby minimizing the formation of by-products such as sorbitol. The structural integrity and purity of the synthesized Meglumine were confirmed by FTIR an 1H NMR. The aldehyde C=O stretching band observed in the 1720−1740 cm−1 region of the starting material (glucose) completely disappeared. Characteristic O−H and N−H bands around 3280cm−1 and 3350cm−1 indicate the amino sugar alcohol structure. A sharp singlet peak belonging to the methyl group(δ 2.65 ppm) directly attached to the nitrogen (−NCH3) was observed.

Conclusion: The Pd/C-supported Raney Ni catalyst system provided high conversion rates and crystalline purity in the synthesis of Meglumine. The Pd support allowed the reaction to proceed under milder conditions while improving the color and overall quality of the product. Characterization studies (FTIR, NMR) prove that the targeted molecular structure was obtained with high precision.

Keywords: Meglumine, Raney Ni-Pd/C, Reductive Amination, Hydrogenation,

SYNTHESIS OF BIO-POLYOLS FROM AGRICULTURAL WASTE FOR SUSTAINABLE INSULATION PANEL APPLICATIONS

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Polyurethane (PU)-based polymers are essential materials across diverse industries, including construction, automotive, and textiles, due to their superior mechanical and thermal insulation properties. However, the reliance on petroleum-derived polyols and isocyanurates poses significant environmental challenges, such as high carbon emissions and resource depletion. This study aims to develop an eco-friendly alternative by synthesizing bio-polyols from olive pomace through an acid-catalyzed liquefaction process.

To prepare the biomass, olive pomace was dried at 80°C for 24 hours to remove moisture. The liquefaction was performed using polyhydric alcohols, specifically PEG 400 and glycerin; glycerin facilitated the swelling and increased cross-linking density, while PEG 400 ensured low viscosity. The resulting bio-polyols exhibited an OH value of 300–500 mg KOH/g and a viscosity below 1000 cP. These synthesized polyols were blended with petroleum-based counterparts at ratios of 10%–30% to produce rigid insulation panels. The performance of the panels was evaluated through standardized testing: Compressive Strength : 0.095 MPa, Tensile Strength: 0.085 MPa , Apparent Density: 38 kg/m³, Thermal Conductivity : 0.0023 W/mK.

The results shoows that biomass-derived foams achieve mechanical strength values comparable to traditional petroleum-based polyurethanes. By substituting a portion of fossil-based inputs with renewable biomass, this approach effectively reduces the carbon footprint and promotes sustainable material production in the insulation industry. Overall, the synthesized bio-polyols show promising potential for industrial-scale polyurethane applications.

Keywords: Polyurethane, Bio-polyol, Olive Pomace, Insulation Panels, Sustainability, Liquefaction.

REMOVAL OF ACETAMIPRID FROM WATER BY ADVANCED TREATMENT PROCESSES: EFFICIENCY AND ECOTOXICOLOGICAL ASPECTS

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Abstract

Acetamiprid, a neonicotinoid insecticide widely used in agriculture, is increasingly detected in surface waters and wastewater due to its high solubility, chemical stability, and poor biodegradability. Conventional water treatment processes have proven insufficient for its effective removal, posing a significant ecotoxicological risk. This study aimed to compare the efficiency of photolysis, direct oxidation with hydrogen peroxide (H_2O_2), photolysis in the presence of H_2O_2, and membrane separation processes (ultrafiltration (UF), nanofiltration (NF), and reverse osmosis (RO)) in removing acetamiprid from aqueous solutions, while simultaneously assessing ecotoxicity and the formation of degradation/transformation products.

The results showed that acetamiprid is an extremely stable compound, exhibiting limited degradation during photolysis alone, even under prolonged illumination with simulated solar radiation. Direct oxidation with H_2O_2 resulted in negligible removal, confirming that without H_2O_2 activation, no significant oxidation of acetamiprid occurs. A significant improvement in removal efficiency was achieved by using photolysis in the presence of H_2O_2 due to the generation of hydroxyl radicals. Degradation kinetics strongly depended on pH-value, with acidic conditions favoring faster transformation of the compound. LC-MS/MS analysis identified numerous degradation and transformation products formed during photochemical processes, indicating complex degradation pathways for acetamiprid. Ecotoxicological assessment using the *Vibrio fischeri* bioluminescence inhibition test showed that removal of the parent compound does not necessarily result in reduced toxicity. In some cases, an increase in ecotoxicological effect was observed, attributed to the formation of more reactive and biologically active transformation products.

Membrane separation processes showed a clear increase in in the order UF < NF < RO. Ultrafiltration did not result in significant retention of acetamiprid, while NF enabled partial removal. Reverse osmosis was the most efficient technology, achieving more than 90% removal.

These results clearly confirm that acetamiprid is a highly challenging pollutant for water treatment and that no single process ensures both complete removal and toxicity reduction. The synergistic use of membrane and photochemical processes, combined with required identification of degradation products and ecotoxicological evaluation, is necessary for developing efficient and safe technologies for treat neonicotinoid-contaminated waters.

Key Words: *acetamiprid; advanced treatment processes; photolysis; membrane separation; ecotoxicity*

Acknowledgement: **This research was funded by the NATO Science for Peace and Security Programme under grant id. G6087**

DIETARY FIBER CONTENT AND THERAPEUTIC POTENTIAL OF FRUITS AND NON-EDIBLE PARTS OF *ARONIA MELANOCARPA* (MICHX.) ELLIOT

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Introduction. *A. melanocarpa* is currently an intensively studied plant species due to the exceptional biological value of its fruits, which are rich in phenolic compounds with strong antioxidant activity, as well as hypotensive, vasoprotective, anticancer, antibacterial, and antiviral effects. In contrast, other plant parts of *A. melanocarpa* remain poorly investigated, and scientific data focusing on dietary fiber content are still limited. Dietary fibers play an essential role in metabolic regulation, gastrointestinal health, detoxification processes, and in the reduction of blood glucose and cholesterol levels. Therefore, exploring dietary fibers not only in fruits but also in non-edible plant parts may contribute to their efficient valorization.
Objectives. Comparative study of dietary fiber in fruits and non-edible parts of *A. melanocarpa.* This approach may open new perspectives for the therapeutic and functional use of *A. melanocarpa* plant products.
Materials and Methods. For the comparative assessment of dietary fiber content, plant materials of *A. melanocarpa*, including leaves collected at pre-flowering, flowering, and post-flowering stages, inflorescences, fruits, and one- and three-year-old twigs with their bark, were harvested from the plant collection of *Nicolae Testemitanu* State University of Medicine and Pharmacy. The study was carried out using standardized gravimetric methods. Dietary fiber fractions were determined using neutral detergent fiber (NDF) and acid detergent fiber (ADF) methods. NDF includes cellulose, hemicellulose, and lignin, ADF comprises cellulose and lignin, ADL (acid detergent lignin) specifically quantifies lignin, while neutral detergent solubles (NDS) represent soluble components such as soluble carbohydrates and pectins.
Results. The NDF content followed the descending order: three-year-old shoots with bark > one-year-old shoots with bark > mature leaves > pre-flowering leaves = flowering leaves > fruits = flowers. A similar descending trend was observed for ADF content, with minor variations in individual values; however, an exception was noted, as the ADF content in fruits exceeded that of flowers. In contrast, the distribution of ADL content differed and was ranked as follows: three-year-old shoots > one-year-old shoots > three-year-old bark = one-year-old bark > mature leaves > flowering leaves > pre-flowering leaves > fruits > flowers. A distinct distribution pattern was observed for NDS, with the highest values recorded in flowers, followed by pre-flowering leaves, fruits, flowering leaves, mature leaves, one-year-old shoots, and one- and three-year-old bark, while the lowest content was observed in three-year-old shoots.
Conclusions. These results indicate that, in addition to fruits, non-edible parts of *A. melanocarpa* are valuable sources of dietary fibers. Woody tissues exhibited the highest content of structural fibers, while fruits and flowers contained lower but still relevant fractions. These findings support the targeted valorization of non-edible aronia biomass for potential therapeutic and functional applications.

Key Words: *Aronia melanocarpa*; fruits; non-edible parts; dietary fibers; therapeutic potential
Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P8-8.3-ROMD-2023-0307, within PNCDI IV.

BRAIN PENETRATION IN CNS AND NON-CNS DRUGS USING MOLECULAR ELECTRONIC PARAMETERS

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Abstract

The Blood-Brain Barrier (BBB) is a selective biological filter that protects the central nervous system (CNS), and some drugs need to enter the brain while others do not. BBB permeability is conventionally predicted based on physicochemical parameters, including logP, molecular weight, and total polar surface area (TPSA). However, only a limited number of studies have investigated the effect of a molecule's electronic structure and reactivity on this process. The objective of this study is to ascertain the correlation between BBB permeability, as determined by DFT (Density Functional Theory), and global reactivity parameters (η, ω, dipole moment, polarizability). A comparative analysis with classical ADMET parameters was also performed. Four small molecules that have been clinically approved were selected for further investigation: Diazepam and carbamazepine exhibit high BBB permeability, while atenolol and metformin demonstrate low BBB permeability. The molecules were optimised at the M06-2X/6-31G(d,p) DFT level, and parameters such as the HOMO-LUMO energy difference, chemical hardness, softness, electrophilic index, dipole moment, and polarizability were calculated. BBB parameters were evaluated using SwissADME and pkCSM via logBB, logP, and TPSA. The objective of this study was to establish a comparison that would reveal the reactivity and classical parameter differences between molecules that successfully pass the BBB and those that do not. Preliminary analyses indicate that molecules with high BBB passage exhibit reduced dipole moments and enhanced polarizability. Furthermore, it is hypothesised that the energy range and electrophilic indices may offer a superior explanation for BBB passage in comparison to classical logP and TPSA. The present study demonstrates that BBB permeability can be evaluated as a potential additional marker, alongside reactivity parameters, in molecular electronic parameter-based reactivity assessments, and as a criterion in CNS drug design. [1]

Key Words: *ADMET, Blood–brain barrier, CNS drugs, DFT, Electronic reactivity, LogBB*

References

[1] Afridi, M. B., Sardar, H., Serdaroğlu, G., Shah, S. W. A., Alsharif, K. F., & Khan, H. (2024). SwissADME studies and Density Functional Theory (DFT) approaches of methyl substituted curcumin derivatives. Computational Biology and Chemistry, 112, 108153.

INFLUENCE OF EXTRACTION TECHNIQUE ON THE POLYPHENOLIC COMPOSITION OF *SOLIDAGO CANADENSIS* L. AERIAL PARTS

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Introduction. *Solidago canadensis* L. is a medicinal plant widely recognized for its high content of phenolic compounds, particularly flavonoids and phenolic acids. These bioactive constituents are largely responsible for the plant's documented therapeutic properties, such as anti-inflammatory, antioxidant, antimicrobial, and diuretic activities, which support its use in modern phytotherapy. Consequently, there is increasing interest in standardized phytopharmaceutical products derived from *S. canadensis*, highlighting the need for optimized extraction and analytical methods to ensure consistent quality and efficacy.

Objectives. Influence of extraction technique on the polyphenolic composition of *S. canadensis* aerial parts.

Materials and Methods. Flowering aerial parts of *S. canadensis* were collected from the plant collection of the *Nicolae Testemitanu* State University of Medicine and Pharmacy. Extracts were obtained using thermal maceration (TM) and microwave-assisted extraction (MAE), with variations in ethanol-water ratios, plant-to-solvent ratios, and extraction temperature. The resulting extracts were lyophilized to enhance stability and facilitate pharmaceutical processing. Polyphenolic characterization was performed using high-performance liquid chromatography (HPLC) coupled with UV–diode array detection (DAD). Chromatographic separation was achieved on an Eclipse Plus C18 column using gradient elution with 0.2% trifluoroacetic acid in water and acetonitrile as mobile phases, while detection was conducted at multiple wavelengths specific for distinct phenolic subclasses.

Results. The chromatographic profile revealed the presence of rutin hydrate, hyperoside, quercetin-3-O-glucopyranoside, quercetin-3-O-galactoside, kaempferol-3-O-rutinoside, and kaempferol-3-O-glucoside as major flavonoid constituents. The total polyphenol content ranged from 23.99 to 56.24 mg/g DW for MAE-derived extracts and from 36.28 to 55.70 mg/g DW for TM-derived extracts, highlighting the influence of extraction technique and operational parameters on polyphenol yield. Comparatively, MAE enabled rapid processing and high polyphenol recovery, albeit with greater variability depending on extraction conditions, whereas TM yielded more consistent results with slightly higher minimum values; overall, both methods were effective for extracting flavonoid-rich fractions, with MAE offering improved efficiency and reduced processing time, and TM ensuring greater reproducibility and robustness.

Conclusions. The high levels of polyphenolic compounds obtained through both extraction methods, confirm *S. canadensis* species as a rich source of these bioactive compounds. The optimized and lyophilized extracts provide a stable, flavonoid-rich matrix suitable for further formulation and quality standardization, supporting their potential use as raw materials in the development of phytopharmaceutical products.

Key Words: *Solidago canadensis*, HPLC analysis, phenolic compounds, extraction methods

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P8-8.3-ROMD-2023-0307, within PNCDI IV.

REMOVAL OF BISPHENOL A FROM WATER

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Abstract

Adsorption is one of the most widely used water treatment techniques due to its simplicity, cost-effectiveness, and high efficiency, typically employing adsorbent materials such as clay minerals, activated carbon, or polymer-based adsorbents [1]. Bisphenol A (BPA) is a synthetic compound widely used in the production of polycarbonate plastics and epoxy resins found in many consumer products [1]. Due to its widespread use, BPA is frequently detected in water sources and poses significant environmental and health risks because of its potential endocrine-disrupting effects [2].

In this study, batch adsorption experiments were conducted to investigate the removal of BPA from aqueous solutions using bituminous coal-based microporous activated carbon (C1300) and styrene-divinylbenzene-based hypercrosslinked ion exchange resin (MN-200). Adsorption experiments were conducted at 298 K in batch mode. Preliminary adsorption tests were performed using a constant adsorbent of 10 mg with 20 mL of 100 mg/L BPA solution. For isotherm studies, varying amounts of MN-200 and C-1300 (2 to 20 mg) were agitated with BPA solution until equilibrium.

Experimental results revealed that C-1300 activated carbon reached the highest adsorption capacity of 193.29 mg/g. Notably, the MN-200 polymer achieved a competitive adsorption capacity of 151.65 mg/g. The equilibrium data were modeled using Langmuir, Freundlich, and Temkin isotherms. The Freundlich model best described the adsorption behavior of MN-200 (R^2=0.97), suggesting heterogeneous surface interactions, whereas the Temkin model provided the best fit for C-1300 (R^2 = 0.96). The results demonstrate that adsorption behavior is significantly affected by the structural characteristics and surface functional groups of the materials.

Key Words: *Bisphenol A (BPA), adsorption, activated carbon, polymeric adsorbent, adsorption isotherms, water treatment*

References

[1] Bhatnagar, A., & Anastopoulos, I. (2017). Adsorptive removal of bisphenol A (BPA) from aqueous solution: A review. Chemosphere, 168, 885–902. https://doi.org/10.1016/j.chemosphere.2016.10.121

[2] Loganathan, P., Vigneswaran, S., Kandasamy, J., Nguyen, T. V., Cuprys, A. K., & Ratnaweera, H. (2023). Bisphenols in water: Occurrence, effects, and mitigation strategies. Chemosphere, 328, 138560. https://doi.org/10.1016/j.chemosphere.2023.138560

Removal of Flutamide from Aqueous Solutions Using Activated Carbon Derived from Lavender: An Adsorption Study

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Abstract

Water is one of the most fundamental needs of living organisms, and all vital biochemical reactions occur in an aqueous environment. Water is an indispensable resource not only for humans but also for all living organisms at every level of the ecosystem to sustain their existence. However, certain pharmaceutical active compounds present in drinking and utility water cannot be completely removed by conventional water treatment methods, posing a significant threat to living organisms [1]. In this study, the potential use of lavender biomass, from which essential oil had been extracted, as an adsorbent for the removal of the pharmaceutical active compound Flutamide from aqueous solutions in wastewater was investigated. In the adsorption experiments, activated carbon derived from lavender biomass was used. During the production of activated carbon, a pyrolysis process was carried out at 750 °C, followed by chemical activation using $ZnCl_2$ as the activating agent. As a result of the experimental studies, the maximum removal efficiency of the pharmaceutical active compound was determined to be 92.47%, which was achieved under the conditions of pH 6, 5 g/L adsorbent dosage, 120 rpm stirring speed, and 25 °C temperature. The obtained findings indicate that activated carbon derived from lavender biomass is an effective and reusable adsorbent for the removal of the active pharmaceutical compound Flutamide from aqueous solutions.

Key Words: Flutamide**, **lavender, biomass, adsorption, wastewater.

References

[1] Della-Flora A, Wilde ML, Thue PS, Lima D, Lima EC, Sirtori C (2020) Combination of solar photo-fenton and adsorption process for removal of the anticancer drug flutamide and its transformation products from hospital wastewater. Journal of Hazardous Materials 396-122699.

Forensic Identification of Pen Ink Pigments Using Dual-Wavelength Raman Spectroscopy Combined with Chemometrics

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Abstract

The identification of the chemical structures of pen inks (gel and ballpoint pens) is of critical importance, particularly in forensic document examination, counterfeit detection, and ink age determination [1-3]. However, the different pigment matrices used in ink formulations complicate standard spectroscopic analyses [4-6]. The aim of this study is to identify commonly used derivatives of Methyl Violet, Crystal Violet, and Pigment Blue using dual-wavelength confocal Raman spectroscopy at 532 nm and 785 nm and to classify the obtained data using chemometric methods. In the study, a Raman system equipped with a 532 nm (green) diode laser with 50 mW power and an 1800 line/mm grating and a 785 nm (red) air-cooled diode laser with 300 mW power and a 1200 line/mm grating was used. Methyl Violet (MV), Crystal Violet (CV), Victoria Blue, and Phthalocyanine derivatives (PB 15:1, 15:3, 15:4, PB 15:4 Mallak) were selected as analytes. 1 mg of pigment was prepared in 2 ml of phenoxyethanol, determined to be the most suitable solvent, and applied to the paper surface using a glass pipette. During the spectral data collection process, the exposure time, laser power, and accumulation parameters were optimized. “Baseline subtraction” and Savitzky–Golay (Window: 9, Degree: 2) smoothing algorithms were applied to the raw data, followed by Principal Component Analysis (PCA) using OriginLab software. In the analyses conducted, characteristic spectra were successfully obtained for the Phthalocyanine group Pigment Blue (PB 15:1, 15:3, 15:4) derivatives commonly found in gel pens using a 785 nm laser source in static mode (Center: 1100, Exposure: 25 sec, Laser Power: 0.0001%). However, it was determined that the triarylmethane-based pigments Methyl Violet (MV) and Crystal Violet (CV) exhibited intense fluorescence interference at the 785 nm wavelength due to their chromophore structures, and their spectra could not be obtained. For these pigments, a 532 nm laser source was integrated into the system, the parameters were revised (Static mode, Center: 1100, Exposure: 5 s, Laser Power: 0.5%), and distinctive peaks were observed by suppressing the fluorescence effect. As a result of PCA analysis, successful clustering was achieved based on the variations in the spectral data of different pigment classes. This study has demonstrated that a single laser wavelength is insufficient for analyzing all pigment types in ink analysis, and that wavelength optimization is essential depending on the chemical structure of the analyte (particularly the difference between triarylmethane and phthalocyanine groups). The use of complementary 532 nm and 785 nm lasers has eliminated the fluorescence problem. Supported by chemometric approaches, this method provides a fast, accurate, and reliable analytical method for characterizing pigments present in ink for forensic chemistry applications.

Key Words:*Pigment Analysis, Raman Spectroscopy, Forensic Chemistry, Principal Component Analysis (PCA)*

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References

[1] Grechukha, N. M., Gorshkova, K. O., Panov, M. S., Tumkin, I. I., Kirillova, E. O., Lukianov, V. V., ... & Kochemirovsky, V. A. (2017). Analysis of the Aging Processes of Writing Ink: Raman Spectroscopy Versus Gas Chromatography Aspects. Applied Sciences, 7(10), 991

[2] Gorshkova, K. O., Tumkin, I. I., Myund, L. A., Tverjanovich, A. S., Mereshchenko, A. S., Panov, M. S., & Kochemirovsky, V. A. (2016). The Investigation of Dye Aging Dynamics in Writing Inks Using Raman Spectroscopy. Dyes and Pigments, 131, 239-245.

[3] Braz, A., López-López, M., & García-Ruiz, C. (2013). Raman Spectroscopy for Forensic Analysis of Inks in Questioned Documents. Forensic Science International, 232(1-3), 206-212.

[4] Raza, A., & Saha, B. (2013). Application of Raman Spectroscopy in Forensic Investigation of Questioned Documents Involving Stamp Inks. Science & Justice, 53(3), 332-338.

[5] Teixeira, C. A., & Poppi, R. J. (2019). Discriminating Blue Ballpoint Pens Inks In Questioned Documents by Raman Imaging and Mean-Field Approach Independent Component Analysis (Mf-Ica). Microchemical Journal, 144, 411-418.

[6] Adamos, M. V., Rickard, W. D., Van Bronswijk, W., & Sauzier, G. (2025). In-Situ Profiling of Pen Ink Degradation on Paper Using Raman Spectroscopy and Tof-Sims. Applied Surface Science, 705, 163500.

REMOVING DISPERSE ORANGE 30 DYE FROM SIMULATED WASTEWATER WITH QUINCE LEAVES BIOADSORBENT

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Abstract

Bioadsorbents made from natural materials have drawn a lot of attention lately because of their potential to remove dyes from wastewater in an environmentally friendly manner. These materials are inexpensive, renewable, biodegradable, and require little processing. Because of their abundance, inherent surface functionality, and efficiency in binding dye molecules, plant-based adsorbents in particular have been thoroughly investigated due to high adsorption capacities because of their lignocellulosic structure and porous surfaces. As a novel, inexpensive, and eco-friendly biosorbent for efficiently eliminating safranin dye from wastewater, quince leaves have the potential to support sustainable treatment approaches.[1,2]

In this work, quince leaves, which are a natural adsorbent, were used in their pure form without any chemical treatment. The leaves were subjected sequentially to washing, air drying, and oven drying processes. After oven drying, the quince leaves were crushed into small pieces to increase their surface area. The prepared adsorbent was used to determine the optimum conditions for the adsorption of Disperse Orange 30 from synthetic wastewater. Within this scope, parameters such as adsorbent dosage (0.8 g and 1 g), contact time (10, 30, 60, 90, and 120 min), temperature (25, 30, 40, 50, and 60 °C), and initial dye concentration (50, 100, 150, 200, 250, 300 mg/L) were investigated. Based on the experimental data obtained, the adsorption behavior of Disperse Orange 30 onto quince leaves was evaluated. Langmuir, Freundlich, and Temkin isotherm models were applied to analyze the adsorption equilibrium, while the pseudo-first-order, pseudo-second-order, and intraparticle diffusion models were used to examine the adsorption kinetics. In addition, the thermodynamic properties of the adsorption process were also investigated.

Key Words: *Quince Leaves; Bioadsorbent; Disperse Orange 30; Dye removal*

References

[1]] Babakhouya N., Benammar S., Hamitouche A.Y.E., Boudjemaa A., Messaoud-Boureghda M.Z., Bachari K. (2024) Chem. Prod. Process Model. 19(2):297–314.
[2] Caylak O (2025) Journal of Molecular Liquids 433:127960

PREPARATION AND ANALYSIS OF A HERBAL EXTRACT SOLUTION HAVING RESTORATIVE EFFECTS POTENTIAL AGAINST RADIATION DERMATITIS

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Cancer is a serious disease in which unusual cells grow quickly, divide uncontrollably and can spread from where they start to other organs. Different methods are used to treat cancer and one of these is radiotherapy. Radiotherapy uses ionizing radiation. While these rays target cancer cells, they can also damage healthy cells. Because of this, patients may develop skin problems such as redness, flaking, or crusting. Radiation-induced dermatitis (RID) is the most frequent side effect of radiotherapy [1] The medications used for skin wounds caused by radiotherapy often contain strong chemical substances. Since cancer patients are already exposed to many chemicals during their treatment, using these chemical-based products can be difficult for them. Herbs have been used for centuries to promote wound healing. Although empirical use is centuries old, the scientific evidence for their efficacy and their active compounds has only recently been investigated by researchers and their effects have been published [2] Instead of chemical ingredients, plant-based materials can be used to help heal the wounds that appear after radiotherapy.[3]

In our study, we prepared a plant-based solution in PBS containing *Plantago lanceolata* (Allantoin), *Cistus* (Cistus creticus;laden), *Centella asiatica(*Gotu Kola*)* and *Aloe vera* to help the skin wounds that develop in patients receiving radiotherapy heal faster. Allantoin supports wound healing and cell vitality. Laden helps prevent infections and supports the healing process. Centella Asiatica has wound-healing and moisturizing effects, and it also prevents deeper cracks that may form when the wound becomes too dry. Aloe Vera moisturizes the skin and helps the wounds heal. For the treatment of the skin wounds that appear in cancer patients undergoing radiotherapy, these plant-based ingredients were combined to obtain the solution. It was integrated this solution into cotton pads for ease of use. The solution-infused cotton pads were tested using UV/VIS spectrophotometry, microscopy and zetasizer analysis. The obtained results showed that this solution may have the potential to benefit wounds in patients undergoing radiotherapy.

Key Words: *Plantago lanceolata (Allantoin); Cistus (Cistus creticus;laden); Centella asiatica(Gotu Kola) Aloe vera*

References

[1] Ren S, Jin J, Wu X, Han B, Zhang W, Rong F, Hou W, Shi Q, Lin H, Liu J (2025) Journal of Dermatological treatment 36(1).
[2] Aygül D, Kılıç D, Özkan F, Yağan Uzuner Y (2025) Pharmaceutics 17(7), 941.
[3] [3] Olszowy-Tomczyk,M. and Wianowska, D. (2024). An in vitro study on the antioxidant properties od Cistus incanus extract, Agriculture, 14(9),1559.

INVESTIGATION OF THE EFFECT OF ULTRASONIC PRETREATMENTS ON THE OVEN DRYING OF ARONIA BERRIES

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Abstract

Aronia berry *(Aronia melanocarpa)* is characterized as a "super fruit" due to its high antioxidant content; however, it is a fruit with a high moisture content of approximately 70%, which leads to rapid spoilage. Drying is of great importance to extend the shelf life and preserve the economic value of the product. Nevertheless, the waxy and tough skin structure of aronia berries creates a significant resistance to mass transfer during traditional hot air (oven) drying processes. This skin resistance increases energy costs by extending the drying time and leads to the degradation of quality attributes such as color and nutritional value, due to prolonged exposure to high heat. Ultrasonic pretreatment is an innovative method that accelerates mass transfer and shortens drying time by creating micro-channels in the fruit skin through the cavitation effect. In this study, it was aimed to determine the optimum processing time and perform mathematical modeling of the data during the oven drying of aronia berries assisted by ultrasonic pretreatment. Experimental studies were carried out at temperatures of 60°C, 70°C, and 80°C. Ultrasonic pretreatment durations were determined as a control group (no pretreatment), 1, 3, 5, 10, 15, and 20 minutes. The effects of the aforementioned pretreatments on the drying behavior of aronia berries were investigated in comparison with the untreated samples. Within the scope of the study, the kinetic parameters of effective moisture diffusivity (D_{eff}) values were calculated, and the drying curves were described using the most common mathematical modeling equations in the literature, by using Statistica 8.0 software. As a result, it was observed that ultrasonic pretreatment applied for a moderate duration significantly reduced the drying time of aronia berries and optimized the process.

Key Words: *Aronia berry; oven drying; drying kinetics; ultrasonic pretreatment; mathematical modelling*

Hydrothermal Synthesis and Structural Characterization of Amino-Functionalized Zr-Based MOFs for Electrochemical Membrane Applications

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Abstract

The performance of proton exchange membranes used in vanadium redox flow batteries (VRFB) largely depends on the structural and surface properties of the additive materials. Therefore, in recent years, Zr-based metal-organic framework (MOF) structures with high chemical stability and tunable pore structures have emerged as promising additives in membrane systems [1, 2]. Especially Zr-based MOFs that are resistant to acidic environments have the potential to support proton transport while limiting the passage of highly valuable vanadium ions.

In this study, UiO-66, MOF-801, MOF-808, and MIL-140 structures, along with their amine-functionalized derivatives, were synthesized using the hydrothermal method. Pure and NH_2-functionalized variants were obtained in a controlled manner through ligand modification. The structural integrity and crystal phase verification of the synthesized MOFs were carried out using X-ray diffraction (XRD) analyses, and the chemical bond structures were examined using Fourier-transform infrared spectroscopy (FTIR). Morphological properties were evaluated using scanning electron microscopy (SEM); specific surface area and pore parameters were determined through Brunauer–Emmett–Teller (BET) analyses. Additionally, the particle surface charge and colloidal stability properties were determined through zeta potential measurements.

The obtained results show that all Zr-based MOF structures successfully formed their characteristic crystal phases and that the amine-functionalized derivatives provided significant changes in surface chemistry. It has been evaluated that in NH_2-functionalized MOFs, the surface polarity increases, the zeta potential values reflect the surface charge differentiation, and this situation could positively affect the interaction with the polymer matrix in the later stages. BET analyses have confirmed the high surface area and microporous character of the MOF structures.

This study presents the synthesis and versatile characterization of Zr-based MOFs, which serve as the foundation for composite membrane systems to be developed for VRFB applications. The advantages provided by the surface chemistry and charge properties of amine-functionalized derivatives present significant potential in terms of supporting proton conduction pathways and optimizing ion selectivity [3–6].

Key Words: *Zr-based MOF; UiO-66; MOF-801; MOF-808; MIL-140; amino functionalization; hydrothermal synthesis; zeta potential*

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References

[1] Nor NAM, Jaafar J, Ismail AF, Mohamed MA, Rahman MA, Othman MHD (2020) Journal of Membrane Science 595:117579.

[2] Zhang H, Li X, Zhang H (2018) Energy Storage Materials 15:324–350.

[3] Xin Q, Zhang Y, Wang S, Li X (2021) Chemical Engineering Journal 420:129743.

[4] Tambat SN, et al. (2018) Journal of Materials Chemistry A 6:10235–10245.

[5] Nguyen VH, et al. (2023) Journal of Energy Storage 62:106915.

[6] Henrique A, et al. (2020) Microporous and Mesoporous Materials 305:110329.

Sustainable Heavy Metal Ion Detection of Waste-Based Carbon Quantum Dots

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Abstract

Environmental pollution, particularly heavy metal contamination, represents a major global challenge due to its persistence, toxicity, and adverse effects on ecosystems and human health [1]. Conventional detection methods often involve complex procedures, high costs, and limited sustainability, highlighting the need for environmentally friendly and efficient sensing technologies. In recent years, carbon quantum dots (CQDs) have emerged as promising fluorescent nanomaterials owing to their strong photoluminescence, low toxicity, high biocompatibility, and the presence of surface functional groups that enable effective interactions with metal ions [2].

In this thesis, carbon quantum dots were sustainably synthesized from olive-derived agricultural waste, which mainly consists of holocellulose, lignin, and proteins [3], using a green hydrothermal synthesis route. This approach aims to valorize biomass residues while minimizing environmental impact. The synthesized CQDs were systematically characterized to evaluate their physicochemical, structural, and optical properties using techniques such as UV–Vis spectroscopy, photoluminescence spectroscopy, and transmission electron microscopy (TEM). Owing to their abundant surface functional groups and strong fluorescence emission, the CQDs were investigated as fluorescent probes for the sensitive and selective detection of ferric ions (Fe^{3+}) in aqueous media. The interaction between CQDs and Fe^{3+} ions induced pronounced photoluminescence quenching, enabling sensitive detection at environmentally relevant concentrations. These results demonstrate that olive-waste-derived CQDs are low-cost and sustainable sensing platforms for water quality monitoring, supporting agricultural waste valorization and environmentally responsible approaches to heavy metal pollution control.

Key Words: *Carbon Quantum Dots (Cqds), Heavy Metal Contamination, Olive-Derived Agricultural Waste, Fluorescence Emission, Photoluminescence Quenching.*

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References

[1] Torres Landa, S. D., Bogireddy, N. K. R., Kaur, I., Batra, V., & Agarwal, V. (2022). Heavy metal ion detection using green precursor derived carbon dots. iScience, 25(2), 103816. https://doi.org/10.1016/j.isci.2022.103816

[2] Hamed, M., Chinnam, S., Bedair, A., Emara, S., & Mansour, F. R. (2024). Carbon quantum dots from natural sources as sustainable probes for metal ion sensing: Preparation, characterizations and applications. Talanta Open, 10, 100348. https://doi.org/10.1016/j.talo.2024.100348

[3] Sousa, D. A., Ferreira, L. F. V., Fedorov, A. A., do Rego, A. M. B., Ferraria, A. M., Cruz, A. B., Berberan-Santos, M. N., & Prata, J. V. (2022). Luminescent carbon dots from wet olive pomace: Structural insights, photophysical properties and cytotoxicity. Molecules, 27(19), 6768. https://doi.org/10.3390/molecules27196768

Performance Assessment of Faujasite Variants for Multi-Metal Adsorption: Impact of Mineral Type and Competitive Heavy Metal Interactions

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Abstract

Industrial wastewater containing heavy metals requires an effective treatment strategy. The ion-exchange method with high surface area adsorbents and high exchange capacity is a widely used approach. Faujasite (FAU), Zeolite X, is one of the best candidates in this regard. However, studies assessing different variants of FAU for multi-metal adsorption and competitive interactions remain limited in literature. This study assessed the adsorption of Pb^{2+}, Cd^{2+}, Zn^{2+}, Cu^{2+}, Ni^{2+}, and Cr^{3+} on three different FAU types (Natural [Nat-FAU], Synthetic [Syn-FAU], and Na-Loaded [Na-FAU]) by Atomic Absorption Spectroscopy for concentration determinations. Adsorption behavior was analyzed under single-metal and binary-metal systems to mimic competitive interactions and optimize multi-metal removal. Mineral characterization was performed before the adsorption tests: XRD analysis confirmed that the crystalline FAU framework has maintained its structure. SEM micrographs showed that Syn-FAU has a more uniform morphology with better crystalline definition than Nat-FAU and Na-FAU samples. Also, XRF and CEC analyses indicated that Syn-FAU has a lower Si/Al ratio and higher cation-exchange capacity in comparison to Nat-FAU and Na-FAU.

A major similarity among all three variants was almost total uptake of Pb^{2+} (~100%). These results confirm a general high affinity for lead in the FAU framework. However, significant performance differences were noted for the other metals. Syn-FAU showed the highest overall performance with 95–100% uptake for Cd^{2+}, Zn^{2+}, Cu^{2+}, and Cr^{3+}, which is in line with its higher cation exchange capacity (CEC). On the other hand, Nat-FAU showed a small drop in effectiveness for most cations but had a special advantage in getting rid of Ni^{2+}, going beyond 80% and doing better than Syn-FAU (70%). This indicates that surface diversity and extra mineral phases in the natural matrix offer greater attraction for the very hydrated Ni^{2+} compared to the pure crystalline framework. Also, in comparison with Nat-FAU, the Na-FAU form showed almost no benefits and was characterized by strong inhibition of Ni^{2+}, Cr^{3+}, and Cu^{2+} (uptake decreased from about 11% to about 24%). These results suggest that Syn-FAU gives the best overall treatment for multiple metals whereas the natural mineral provides a good and cheaper option for specific lead and nickel removal.

The three FAU variants were tested in binary competitive conditions to check their practical applicability. The binary-mixture tests showed synergistic promotion ($R > 1$), antagonistic inhibition ($R < 1$), and noninteraction ($R \sim 1$) compared to single-ion systems, where R is the binary-to-single uptake ratio. In Syn-FAU, the removal of Pb^{2+} and Cd^{2+}, as well as in Nat-FAU for Cd^{2+} and Zn^{2+}, did not depend on competing ions ($R \sim 1$). The lack of a competitive effect indicates that, under the conditions studied, the co-ions did not significantly compete for exchange sites in the FAU framework[1], probably because there

were enough sites available and/or uptake was selective. It is important to note that synergistic promotion was seen among frameworks: Pb^{2+} as a co-ion greatly enhanced Cr^{3+} removal ($R > 1.50$) in both Syn-FAU and Nat-FAU, while Cd^{2+} improved Ni^{2+} removal ($R > 1.10$) within the Syn-FAU. In the case of Na-FAU, this synergy shifted, as the presence of Pb^{2+} significantly enhanced the removal of Ni^{2+} ($R > 1.45$). This synergistic removal might be due to cooperative adsorption in multicomponent systems combined with changes in mass transfer kinetics, leading to increased uptake of co-ions like Cr^{3+} and Ni^{2+}[2]. On the other hand, antagonistic inhibition was noted for Ni^{2+} extraction ($R < 0.50$) when Cu^{2+} was present (Syn-FAU and Nat-FAU) or Cr^{3+} was present (Nat-FAU and Na-FAU); competitive site occupation resulted in a significant decrease in the efficiency of Ni^{2+} removal. In this situation, Cu^{2+} or Cr^{3+} might compete for adsorption/ion-exchange sites, with the effect being further enhanced by mass-transfer limitations such as film and intraparticle/pore diffusion[3]. All other binary pairs exhibited no more than mild interference ($0.50 < R \leq 1.00$), indicating weak competitive interactions for shared adsorption/ion-exchange sites, with removal largely unaltered or only slightly diminished in the presence of co-ions.

Keywords: Faujasite, Competitive Adsorption, Synergistic Promotion, Ion-Exchange Selectivity, Heavy Metal Removal, Wastewater Treatment.

References

[1] X. Liu, R. Tian, W. Ding, Y. He, and H. Li, “Adsorption selectivity of heavy metals by Na - clinoptilolite in aqueous solutions,” *Adsorption*, no. 0123456789, 2019, doi: 10.1007/s10450-019-00081-x.

[2] S. Mustafa, S. Khan, M. Iqbal, and S. Yar, “Applied Surface Science The role of Pb 2 + ions doping in the mechanism of chromate adsorption by goethite,” vol. 255, pp. 8722–8729, 2009, doi: 10.1016/j.apsusc.2009.05.169.

[3] A. Zendelska, M. Golomeova, B. Golomeov, and B. Krstev, “Effect of Competing Cations (Cu , Zn , Mn , Pb) Adsorbed by Zeolite Bearing Tuff from Macedonia, vol. 17, no. 1, pp. 21–24, 2018.

INFLUENCE OF EXTRACTION TECHNIQUE ON THE POLYPHENOLIC COMPOSITION OF *SOLIDAGO CANADENSIS* L. AERIAL PARTS

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Introduction. *Solidago canadensis* L. is a medicinal plant widely recognized for its high content of phenolic compounds, particularly flavonoids and phenolic acids. These bioactive constituents are largely responsible for the plant's documented therapeutic properties, such as anti-inflammatory, antioxidant, antimicrobial, and diuretic activities, which support its use in modern phytotherapy. Consequently, there is increasing interest in standardized phytopharmaceutical products derived from *S. canadensis*, highlighting the need for optimized extraction and analytical methods to ensure consistent quality and efficacy.

Objectives. Influence of extraction technique on the polyphenolic composition of *S. canadensis* aerial parts.

Materials and Methods. Flowering aerial parts of *S. canadensis* were collected from the plant collection of the *Nicolae Testemitanu* State University of Medicine and Pharmacy. Extracts were obtained using thermal maceration (TM) and microwave-assisted extraction (MAE), with variations in ethanol-water ratios, plant-to-solvent ratios, and extraction temperature. The resulting extracts were lyophilized to enhance stability and facilitate pharmaceutical processing. Polyphenolic characterization was performed using high-performance liquid chromatography (HPLC) coupled with UV–diode array detection (DAD). Chromatographic separation was achieved on an Eclipse Plus C18 column using gradient elution with 0.2% trifluoroacetic acid in water and acetonitrile as mobile phases, while detection was conducted at multiple wavelengths specific for distinct phenolic subclasses.

Results. The chromatographic profile revealed the presence of rutin hydrate, hyperoside, quercetin-3-O-glucopyranoside, quercetin-3-O-galactoside, kaempferol-3-O-rutinoside, and kaempferol-3-O-glucoside as major flavonoid constituents. The total polyphenol content ranged from 23.99 to 56.24 mg/g DW for MAE-derived extracts and from 36.28 to 55.70 mg/g DW for TM-derived extracts, highlighting the influence of extraction technique and operational parameters on polyphenol yield. Comparatively, MAE enabled rapid processing and high polyphenol recovery, albeit with greater variability depending on extraction conditions, whereas TM yielded more consistent results with slightly higher minimum values; overall, both methods were effective for extracting flavonoid-rich fractions, with MAE offering improved efficiency and reduced processing time, and TM ensuring greater reproducibility and robustness.

Conclusions. The high levels of polyphenolic compounds obtained through both extraction methods, confirm *S. canadensis* species as a rich source of these bioactive compounds. The optimized and lyophilized extracts provide a stable, flavonoid-rich matrix suitable for further formulation and quality standardization, supporting their potential use as raw materials in the development of phytopharmaceutical products.

Key Words: *Solidago canadensis*, HPLC analysis, phenolic compounds, extraction methods

Acknowledgement: This work was supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-IV-P8-8.3-ROMD-2023-0307, within PNCDI IV.

SYNTHESIS OF A NOVEL SYMMETRICAL SILICON PHTHALOCYANINE PHOTOSENSITIZERS CONTAINING CARBOXYLIC ACID BASED AXIAL ANCHORING GROUPS

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Abstract

Increasing demands for global energy and electronic materials together with technological advances necessitates energy transformation today. Although many industrial and technological studies are carried out for this purpose, one of these studies is dye-sensitized solar cells (DSSCs) in the field of photovoltaic technology. Efficiency in DSSCs depends on the counter electrode, photoanode, the formation of sensitizers with the electrolyte and their compatibility in operating performance [1]. Phthalocyanines (Pcs) with high thermal, chemical and light stability are very important macrocyclic compounds [2-4]. In this study, a novel silicon phthalocyanine (SiPc) carrying bisdibutyl phenoxy acrylic acid and having axial anchoring groups are synthesized as the photosensitizers of dye sensitized solar cells (DSSCs). The obtained novel photosensitizers are elucidated by using ^{1}H-NMR, MALDI-TOF, FT-IR, UV–Vis spectroscopy and elemental analysis.

Key Words: *Synthesis, Symmetric, Phthalocyanine, Acrylic acid, Spectroscopy*

References

[1] Alsudairi A, Li J, Ramaswamy N, Mukerjee S, Abraham K, Jia Q (2017) The Journal of Physical Chemistry Letters 8:2881–2886.
[2] Koca A (2009) Electrochemistry Communications11:838–841.
[3] Ozoemena KI, Nyokong T (2006) Electrochimica Acta 51:5131–5136.
[4] Mani V, Devasenathipathy R, Chen SM, Huang ST, Vasantha V (2014) Enzyme and Microbial Technology 66:60–66.

SYNTHESIS AND CHARACTERIZATION OF A NOVEL SILICON PHTHALOCYANINE CONTAINING CARBOXYLIC ACID GROUPS

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Abstract

Owing to growing global energy, technological developments and increasing use of electronic equipment, energy conversion has become very important in our lives. Many advanced studies have been done by scientists to have this transformation. One of the works that have been done by the scientist is dye-sensitized solar cells (DSSC), which are actively used in photovoltaic technology. DSSC performance depends on the formation of the sensitizers used, the photoanode, the counter-electrode, the electrolyte used and the harmonious operation of all these equipment [1-3]. For this purpose, tert-butyl moieties containing carboxylic acid anchoring groups substituted novel diaxially silicon (IV) phthalocyanines were synthesized. The obtained novel photosensitizers are elucidated by using ^{1}H-NMR, MALDI-TOF, FT-IR, UV–Vis spectroscopy and elemental analysis.

Key Words: *Synthesis, Characterization, Phthalocyanine, Carboxylic acid, Silicon*

References

[1] Urbani M, Ragoussi ME, Nazeeruddin MK, Torres T (2019) Coordination Chemistry Reviews 381:1-64.
[2] Koca A (2009) Electrochemistry Communications 11:838–841.
[3] Güzel E, Baş H, Bıyıklıoğlu Z, Şişman İ (2020) Applied Organometalic Chemistry 35:e6214.

MODIFICATION OF BITUMEN BY ADDING REACTIVE TERPOLYMER, POLYOLEFIN ELASTOMER, AND THERMOPLASTIC

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Abstract

In this study, 50/70 penetration grade TÜPRAŞ bitumen was modified. The reactive elastomeric terpolymer of DuPont (Elvaloy RET), Dow Engage 8411 polyolefin elastomer, and Atactic Polypropylene (PP) polymers were used for bitumen modification [1,2]. Each of the polymers—Elastomeric terpolymer (Elvaloy RET), Engage 8411 polyolefin elastomer, and Atactic Polypropylene (PP)—was added to the 50/70 penetration grade bitumen at proportions of 0.5%, 1%, 1.5%, 2%, and 2.5% by weight. Additionally, 1% by weight of the other two polymers was added to obtain modified bitumen samples. The samples were subjected to Penetration (TS 118 EN 1426) and Softening Point (TS 120 EN 1427) tests in accordance with the Turkish General Directorate of Highways Modified Bitumen Specification. With the decrease in penetration values and the increase in softening point values, modified bitumen that is more resistant to stress, shock waves, and impacts was obtained. Moreover, the modified bitumen exhibited greater resistance in regions with high air temperatures [3].

Key Words: *Bitumen modification; penetration value; softening point; reactive; elastomeric terpolymer; polyolefin elastomer*

References

[1] Selvavathi V, Sekar VA, Sriram V, Sairam B (2002) Petroleum Science and Technology, 20:535-547.
[2] Polacco G, Stastna J, Vlachovicova Z, Biondi D, Zanzotto L (2004) Polymer Engineering and Science 44(2):2185–2193.
[3] Geçkil T, Seloğlu M (2018) Construction and Building Materials 173:262–271.

REMOVAL OF SELECTED POLLUTANTS FROM TEXTILE WASTEWATER USING A HYBRID MBR–NF SYSTEM

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Abstract

Nanofiltration is increasingly applied as a polishing step following biological treatment for textile wastewater due to its ability to remove organic matter and color while allowing partial salt passage. This study investigates the removal efficiency of selected pollutants in a hybrid membrane bioreactor–nanofiltration (NF) system treating textile wastewater (TWW). The performance of NF was evaluated using MBR effluent as feed under operating pressures ranging from 8 to 12 bar. Influent and permeate samples were analyzed for chemical oxygen demand (COD), turbidity (NTU), total nitrogen (TN_b), and absorbance (color), allowing assessment of pollutant removal under realistic operating conditions.

The NF process achieved substantial removal of organic matter, with COD decreasing from approximately 67–68 mg/L in the MBR effluent to 11–14 mg/L in the permeate, corresponding to removal efficiencies of 79–83%. Turbidity was effectively reduced from 1.1–1.3 NTU to below 0.5 NTU, resulting in removal efficiencies between 65–82%. Significant color removal was observed, with absorbance reduced from approximately 3.3–3.6 to 2.8–3.0, corresponding to removal efficiencies of up to 56%. In contrast, nitrogen removal across the NF membrane was limited. TN_b concentrations decreased only marginally, with removal efficiencies below 25%, indicating that dissolved nitrogen species readily passed through the NF membrane. These results highlight the selective separation behavior of NF membranes, which effectively retain organic compounds and colloidal matter while allowing partial passage of low molecular weight inorganic species. The findings demonstrate that the hybrid MBR–NF system provides effective polishing of biologically treated TWW, particularly in terms of organic matter, turbidity, and color reduction [1,2]. However, limited nitrogen removal suggests that additional treatment steps may be required where strict nutrient discharge or reuse criteria apply.

Key Words: *nanofiltration; textile wastewater; membrane; membrane bioreactor; removal*

Acknowledgement: *This research was supported by the NATO Science for Peace and Security Programme (WaRMem project, MYP G6087).*

[1] Grilli S, et al (2011) *Performance evaluation of an MBR–NF hybrid system treating textile wastewater*. Membrane Water Treatment 5(3):197–204.
[2] Li K, Liu Q, Fang F, Wu X, Xin J, Sun S, Wei Y, Ruan R, Chen P, Wang Y, et al (2020) *Influence of nanofiltration concentrate recirculation on performance and economic feasibility of a pilot-scale MBR–NF hybrid process for textile wastewater treatment with high water recovery*. Journal of Cleaner Production 261:121067.

Synthesis, Characterization, Molecular Docking and Biological Activity of New Schiff Bases Containing Pyrazole Arylhydrazone-Based Moieties as Antitumor Agents

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Abstract:

Pyrazole arylhydrazones have been designed as mixed-hybrid isosteres of two known dual inhibitors of prostaglandin synthase and 5-lipoxygenase, BW-755c and CBS-1108. Several derivatives within this class have been reported to inhibit *in vitro* platelet aggregation in citrated platelet-rich rabbit plasma. Moreover, numerous pyrazole derivatives have exhibited significant antiproliferative activity against various cancer cell lines. In the present study, a novel series of Schiff bases incorporating pyrazole arylhydrazone-based moieties was designed and synthesized via condensation of 5-hydrazino-1,3-dimethyl-4-nitro-1H-pyrazole with different aromatic aldehydes and ketones, including thiophene-2-carbaldehyde, furan-2-carbaldehyde, benzo[b]thiophene-2-carbaldehyde, phenyl(pyridin-2-yl)methanone, and 1,1'-(pyridine-2,6-diyl)bis(ethan-1-one). The isolated compounds were characterized by their physical properties, elemental analysis, IR-, MS (EI)- and NMR-spectroscopy. Molecular docking studies were conducted to assess the binding affinity of the compounds toward selected cancer-related protein targets. Furthermore, the cytotoxic effects were evaluated against human colorectal carcinoma (HCT-116) and breast adenocarcinoma (MCF-7) cell lines has been studied.

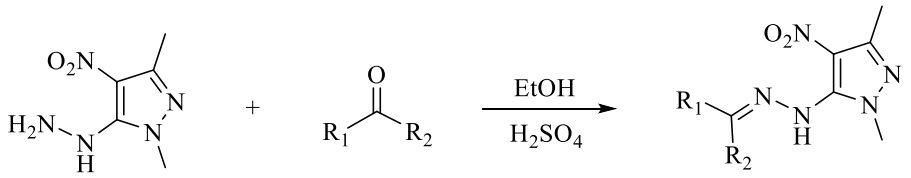

Figure: Pathway for the synthesis of the pyrazole arylhydrazone-based Schiff bases (R_1= thiophen-2-ylmethylene, furan-2-ylmethylene, benzo[b]thiophene-2-ylmethylene, pyridin-2-ylmethylene, and (*E*)-*N*((1,3-dimethyl-4-nitro-1*H*-pyrazol-5-yl)methyl)-1-(pyridine-2,6-yl)ethan-1-imine , R_2= H, Ph, Me)

Photoinducible decarboxylation in reactions with alkynes: regioselective addition of alkyl radicals to the triple bond

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Abstract

Visible-light photocatalysis should be considered as catalysis based on chemical processes initiated by the absorption of electromagnetic radiation from the visible range (380-750 nm). This technique has received growing interest due to its considerably milder and more economical reaction conditions when compared to thermal methods.[1] Recently, this approach has gained immense popularity, leading to significant progress in the area.[2] Numerous transformations initiated by visible light have been reported, including the decarboxylation of carboxylic acids, which generates free radicals that can react with alkynes, enabling the formation of C–C bonds.[3,4,5]

In this research, we examined the application of light-initiated radical decarboxylation of proline in reactions with unsaturated compounds while utilising external photocatalysts (**3**). The reaction conditions were optimised by examining the effect of various factors (solvent, photocatalyst, base) on the desired product (**4**) yield and the isomers **4a**/**4b** ratio. Preliminary findings suggest that the presence of a Lewis acid (LA) may play a role in favouring the formation of a single isomer of the product. Consequently, we also analysed the impact of various additives and LA, including metal salts (i.e. zinc, copper, scandium, ytterbium). The optimised conditions were subsequently employed to promote the addition of the resulting alkyl radical from **1** to a range of substrates bearing triple carbon-carbon bonds.

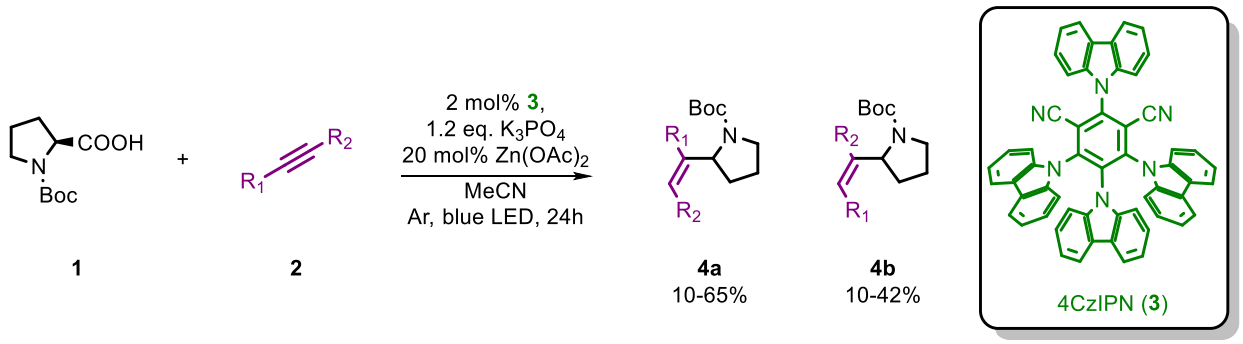

Figure 1: Light-induced decarboxylation of Boc-*L*-proline (**1**) with alkynes (**2**) leading to compound (**4**).

Key Words: *photochemistry, decarboxylation, alkynes, radicals, addition*

Acknowledgement: The research has been supported by the grant SONATA17 number UMO2021/43/D/ST4/02948 from the Polish National Science Center (NCN).

References

[1] T. Patra, D. Maiti; *Chem. Eur. J.*, **2017**, *23*, 7382−7401

[2] N. A. Romero, D. A. Nicewicz; *Chem. Rev.*, **2016**, *116*, *17*, 10075–10166

[3] N. A. Till, R. T. Smith, D. W. C. *MacMillan; J. Am. Chem. Soc*. **2018**, *140*, 5701−5705

[4] M. M. Mastandrea, S. Cañellas X. Caldentey, M. A. Pericàs**;** *ACS Catal.*, **2020**, *10*, *11*, 6402−6408

[5] H. Yue, Ch. Zhu, R. Kancherla, F. Liu, M. Rueping; *Angew. Chem*. **2020**, *132*, 5787−5795

DOUBLE-SIDED CONTROL OF PRODUCT TYPE PREFERENCE IN THE VISIBLE-LIGHT INITIATED REACTION OF 1,3-DICARBONYL COMPOUNDS WITH ALKENES

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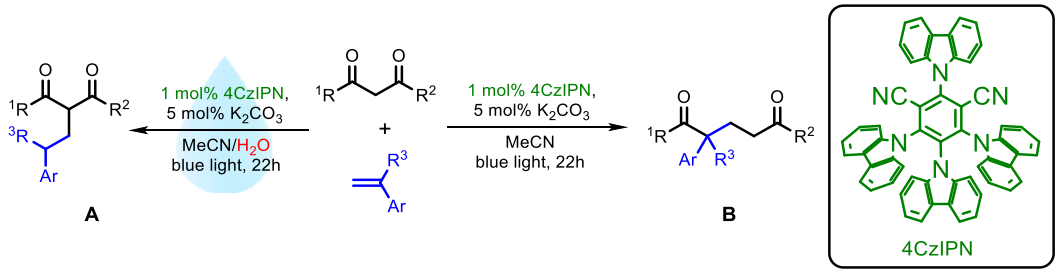
Abstract

Visible-light-driven photocatalysis has emerged as a major focus in modern organic chemistry due to its alignment with Green Chemistry principles. By utilizing milder and more sustainable reaction environments, this approach offers a cost-effective alternative to traditional methods while significantly reducing environmental impact [1]. These advantages have been showcased in several studies centered on the formation of C-C bonds between olefins and molecules with activated methylene group [2-4].



This study investigates the 4CzIPN catalyzed reaction between alkenes and 1,3-dicarbonyl compounds under visible-light irradiation. The findings demonstrate that the specific reaction conditions - most notably the inclusion or exclusion of water - determine the final result. Depending on the parameters, the reaction produces either radical addition products (**A**) or 1,5-dicarbonyl compounds (**B**).

By examining the effects of multiple variables on yield and selectivity, this work establishes the optimal parameters required for peak regioselectivity. Furthermore, the versatility of the method was tested through a substrate scope that included a wide array of esters, diketones, and alkenes. Additionally, the mechanistic data were analysed to gain a deeper understanding of the experimental outcomes and to further streamline the process.

Key Words: *photoredox; radical reactions; De Mayo reaction; visible-light; solvent effect*

***Acknowledgement*: This work was supported by Strategic Program Excellence Initiative at the Jagiellonian University and the Polish National Science Centre.**

References

[1] Marzo L, Pagire SK, Reiser O, König B (2018), Angew. Chem. 130, 10188–10228.
[2] Baś S, Yamashita Y, Kobayashi S (2020) ACS Catal. 10, 10546–10550.
[3] Martinez-Haya R, Marzo L, König B (2018) Chem. Comm. 54, 11602–11605.
[4] Ohashi M, Nakatani K, Maeda H, Mizuno K (2010) J. of Photochem. Photobiol. A: Chem. 214, 161–170

CHEMICAL CHARACTERIZATION OF $PM_{2.5}$ IN THE URBAN AIR OF TIRANA: SOURCES, CHEMICAL MARKERS AND ATMOSPHERIC SECONDARY PROCESSES

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Abstract

This pilot study presents a detailed chemical characterization of fine particulate matter with an aerodynamic diameter of 2.5 micrometres collected in an urban area in Tirana, aiming to identify the sources and atmospheric processes influencing its composition. The analyses of water-soluble ions and carbohydrates indicates that this particulate matter consists of a combination of primary sources and products of secondary transformations. Elevated concentrations of sulphates, nitrates and various organic acids indicate advanced oxidation of organic and inorganic matter. The presence of specific markers such as levoglucosan, mannosan and mannitol suggest contributions from biomass combustion, biological activity, and plant materials. The results demonstrate the complexity of urban particulate matter and highlight the importance of chemical analysis for the assessment of pollutant sources, as well as for supporting receptor models such as positive matrix factorisation in understanding the dynamics of particulate matter with an aerodynamic diameter of 2.5 micrometres in the atmosphere.

Key Words: *Fine particulate matter; chemical composition; water-soluble ions and carbohydrates; primary sources; secondary transformations.*

Acknowledgement: The author gratefully acknowledges ACTRIS SAMU (ACTRIS Head Office Italy, CNR-IMAA) for funding support and CNR-ISAC (Italian National Research Council, Lecce, Italy) for laboratory analyses of fine particulate matter with an aerodynamic diameter of 2.5 micrometres.

DEVELOPMENT OF A NOVEL POLYMER-BASED SPE METHOD FOR TRICLOSAN

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Abstract

Triclosan (TCS), a synthetic compound belonging to the EPC group, has broad-spectrum antibacterial properties [1]. Annual TCS production exceeds 1500 tons, and it is widely used in personal care, medical, household, veterinary, and daily consumer products such as mouthwashes, toothpastes, soaps, detergents, disinfectants, plastic additives, shampoos, and deodorants [1, 2]. Due to its low metabolism in animal and human bodies, the majority of TCS is released into the environment. Therefore, TCS accumulates in the environment, becoming a major source of pollution.

In this study, a polymer-based solid-phase extraction (SPE) cartridge was developed using cross-linked polymeric microspheres to extract TCS from water. The chemical and morphological properties of the microspheres were characterized using Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and Brunauer–Emmett–Teller (BET) analysis. Various parameters, such as the type and volume of elution solvent, the sample pH, and the sorbent amount, were investigated to assess the effect of SPE. TCS analysis was performed using a high performance liquid chromatography-diode array detector. The applicability to a real water matrix under optimum SPE conditions was evaluated, and a new SPE cartridge was developed as an alternative to commercial SPE cartridges.

Key Words: *Triclosan, solid phase extraction, microspheres, high performance liquid chromatography*

References

[1] Milanović M, Đurić L, Milošević N, Milić N (2023) Environmental Science and Pollution Research 30:25119-25140.
[2] Luo Z, He Y, Zhi D, Luo L, Sun Y, Khan E, Tsang DC (2019) Science of the Total Environment 696:133990.

THE INFLUENCE OF THE EXPANSION OF THIOPHENE SUBSTITUENTS ON THE PHYSICOCHEMICAL PROPERTIES AND APPLICATION POSSIBILITIES OF FLUORENE DERIVATIVES

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Abstract

The dynamic development of technology and the economy leads to an increasing demand for electrical energy. Therefore, reducing electricity consumption and promoting its green production constitute major challenges for modern science. Particularly interesting solutions to this problem include smart windows [1][2] and perovskite solar cells [2]. Smart windows use electrochromic compounds as "smart" materials that change color in response to an applied external voltage [2][3]. This enables the selective blocking of near-infrared radiation and visible light, which can directly translate into increased energy savings in building heating and air-conditioning. In turn, perovskite solar cells, alleviate the burden on conventional energy-generation methods and are closely linked to the green transition of energy sources. However, the development of such applications requires chemical compounds that meet numerous stringent requirements. Among the many families of organic compounds, thiophene derivatives deserve special attention with regard to electrochromic properties [1][2][3]. Compounds of this type are durable, stable, and often exhibit multistep electrochromism [1][2][3].
The aim of this work was to synthesize and investigate the influence of alkyl groups and thiophene substituents on the physicochemical properties of six fluorene derivatives. The structures of the obtained compounds were confirmed using NMR spectroscopic methods. Thermal, optical, electrochemical, and spectroelectrochemical studies were carried out, enabling assessment of the effect of substituents on molecular properties. The results show that modifying fluorene with acetylene-linked thiophene derivatives significantly affects absorption, emission, and electrochromic properties, confirming the potential of these materials for practical applications.

Key Words: *smart windows; perovskite solar cells; electrochromism; thiophene derivatives; fluorene derivatives;*

Acknowledgement: **This work was co-funded by the project: „jUŚt transition – Potencjał Uniwersytetu Śląskiego podstawą Sprawiedliwej Transformacji regionu" (FESL.10.25-IZ.01.0369/23-003). The project is implemented under the European Funds for Silesia 2021-2027. Program co-financed by the Just Transition.**

References

[1] Zangoli M, Monti F, Zanelli A, Marinelli M, Flammini S, Spallacci N, Zakrzewska A, Lanzi M, Salatelli E, Pierini F, Di Maria F (2024) Chemistry A European Journal 30:e202303590.
[2] Kula S, Szlapa-Kula A, Krompiec S, Gancarz P, Filapek M (2019) Synthetic Metals 247:202-211.
[3] Nicolini T, Frontana-Uribe B A, Kuhn A, Salinas G (2023) ChemElectroChem 10:e202300346.

A NOVEL AZULENE–BODIPY FLUOROPHORE: SYNTHESIS AND PHOTOPHYSICAL PROPERTIES

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Abstract

Azulene–BODIPY conjugates have attracted growing interest due to the combination of the excellent photophysical properties of BODIPY dyes such as high molar absorptivity, sharp emission bands, and good photostability with the unique nonalternant aromatic structure and unusual electronic characteristics of azulene. Previous studies on azulene-BODIPY systems have demonstrated that varying the connectivity between azulene and the BODIPY core can modulate electronic conjugation and optoelectronic properties [1,2]. Additionally, azulene-modified BODIPYs have been shown to exhibit large, red-shifted absorption into the near-infrared region and sensitivity to aggregation and protonation stimuli, highlighting the impact of azulene incorporation on photophysical behaviour [3,4].

In this study, a novel azulene-linked BODIPY derivative was synthesized, and its photophysical properties were systematically investigated. The molecular structure was unambiguously confirmed by single-crystal X-ray diffraction analysis. UV–vis absorption and steady-state fluorescence spectra were recorded in a range of solvents to evaluate solvent-dependent behaviour. The compound displayed intense visible absorption characteristic of BODIPY chromophores, along with additional spectral features attributable to the azulene unit. Collectively, these findings further demonstrate that azulene conjugation represents an effective and versatile strategy for fine-tuning the photophysical properties of BODIPY-based fluorescent materials.

Key Words: *BODIPY, azulene, fluorescent molecule, photosensitiser, photophysical property.*

References

[1] Kumar RN, Agraval AA, Debnath S, Chodhury A, Zade SS (2023) New Journal of Chemistry 47:2456.
[2] Gai L, Chen J, Zhao Y, Mack J, Lu H, Shen Z (2016) RSC Advances 6:32124.
[3] Zhao C, Wu B, Yang J, Baryshnikov GV, Zhou UY, Ågren H, Zou Q, Zhu L (2022) Dyes and Pigments 197:109867.
[4] Nishimura K, Kato M, Fukui T, Miura K, Tsuda M, Okada S, Fukushima T, Nakamura H (2025) Molecular Pharmacuetics 22:2660-2670.

Preparation Of A Phytohydrogel Containing Medicinal And Aromatic Plant Extracts

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Abstract

With the increasing global interest in natural products, the importance and utilization of medicinal and aromatic plants have expanded significantly. Population growth, advancements in the healthcare sector, and increased awareness of the adverse effects of synthetic products on human health have further enhanced the demand for these plants. Medicinal and aromatic plants are widely used in various fields, including medicine, cosmetics, food, and environmental applications. In this study, total phenolic content and antioxidant activities of extracts obtained from selected medicinal and aromatic plants through solvent extraction under specific conditions were investigated. Phytohydrogels based on chitosan and xanthan gum were prepared using these plant extracts, and their characterization was carried out through FTIR analysis, swelling behavior, and surface morphology examinations. According to the experimental results, the highest total phenolic content was determined as 3.93 mg GAE/10 g DM in the ethanol extract of green tea. Antioxidant activity results revealed that the antioxidant capacity of juniper seed extracts ranged between 85.06% and 99.07 %, depending on the solvent used. Swelling tests indicated that the highest swelling ratio (96.22 %) was obtained from the third synthesis method incorporating both plant extract and quercetin. Quercetin release studies demonstrated that the release from the phytohydrogels was relatively low. FTIR analysis confirmed the presence of hydroxyl (O–H), amine (N–H), carbonyl (C=O), and carboxylate (COO^-) groups, as well as C–O and C–O–C bonds in the chemical structure of the phytohydrogels. Overall, the findings suggest that the synthesized phytohydrogels have strong potential for application in various high value-added sectors, particularly in cosmetics.

Key Words: *Extraction, FTIR, Determination of Total Phenolic Content (TPC), Antioxidant Activity Assay, Quercetin Relese Test, Chitosan, Xantham Gum*

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SESAMOL-FUNCTIONALIZED CYCLOPHOSPHAZENES: SYNTHESIS, STRUCTURAL CHARACTERIZATION, AND BIOLOGICAL EVALUATION

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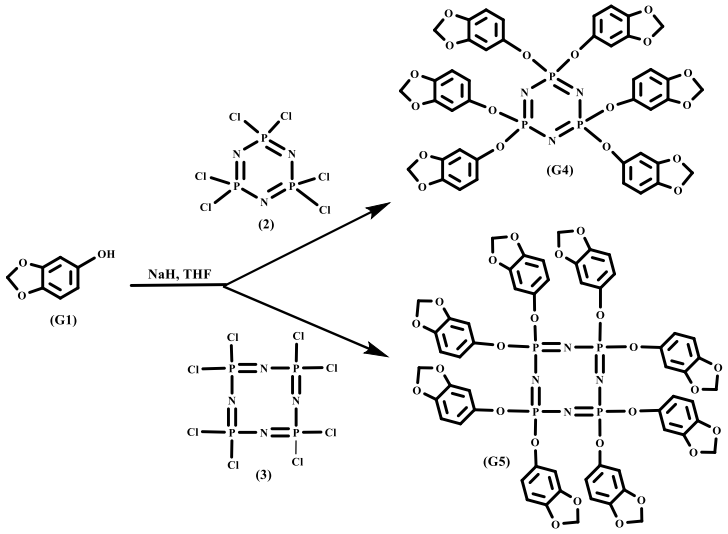
Abstract

In the present study, sesamol-appended cyclophosphazene derivatives (**G4** and **G5**) were synthesized and characterized by elemental analysis, mass spectrometry and (^{1}H, ^{13}C and ^{31}P) NMR spectroscopy. The crystal structure of **G4** was determined and reported for the first time.



The biological activities (amylolytic, DNA cleavage, antimicrobial, and antioxidant activities) of sesamol and the cyclophosphazenes derivatives were systematically evaluated. The synthesized compounds demonstrate a promising potential for diverse applications within the enzyme, pharmaceutical and environmental industries after in vitro, in vivo and in situ toxicologic test systems [1].

Key Words: *Sesamol, Cyclophosphazene, Antimicrobial, Amylolytic activity, DNA cleavage*

References

[1] Ibisoglu H, Sahin Ün S, Zorlu Y, Atilla D, Tollu G, Kılınç E, Ozdemir S, **(2026)** Journal of Molecular Structure, 1357, 145199.

DETERMINATION OF THE CHEMICAL COMPOSITION OF THE ESSENTIAL OIL OF THE RUBIA TINCTORUM PLANT

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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 [1]. The genus *Rubia* belongs to the Rubiaceae family, which comprises approximately 450 genera and around 6,500 species [2]. *Rubia tinctorum* L. (Rubiaceae) has a long history of traditional use as a diuretic and in the treatment of conditions such as jaundice, sciatica, and paralysis. It has also been employed as a postpartum menstrual regulator and in the management of rheumatism, eczema, and fungal infections [3]. Moreover, *R. tinctorum* serves as an important natural source of dye raw materials utilized in the cosmetic, textile, food, and pharmaceutical sectors. Beyond its industrial applications, the species is also well known for its diverse and beneficial biological activities [4].

In this study, the essential oil of *Rubia tinctorum* was obtained by the hydrodistillation method, and the volatile and semi-volatile compounds it contains were identified using the GC–MS technique. GC–MS analysis revealed the presence of 21 compounds in the essential oil extract of *R. tinctorum*. The chemical profile was determined by fatty acids, accounting for 89.29% of the total composition, followed by alkanes (5.32%), terpenoids (4.57%), alcohols (0.5%), and aldehydes.

Key Words: *Plant; Rubia tinctorum; essential oil; gas chromatography (GC)*

References

[1] Türkan Ş, Malyer H, Öz Aydın S, Tümen G (2006) Ordu İli ve Çevresinde Yetişen Bazı Bitkilerin Etnobotanik Özellikler. Süleyman Demirel Üniversitesi, Fen Bilimleri Enstitüsü Dergisi, 10(2): 162-166.

[2] Krishnan Marg KS (1985) The Wealth of India: Raw Materials, National Institute of Science Communication and Information Resources CSIR, New Delhi-110 012.

[3] Güzel Y, Güzelşemme M, Miski M (2015) Ethnobotany of medicinal plants used in Antakya: A multicultural district in Hatay Province of Turkey. Journal of Ethnopharmacology 174:118-152.

[4] Kabaalioğlu N, Tezcan H (2021) The important of root dyeing in the ottoman period, The positive and negative effects of chemical dyes on the textile industry. International Social Sciences Studies Journal 7(86):3573-3578.

SYNTHESIS OF N-METHYL-GLUCAMINE VIA REDUCTIVE AMINATION OF GLUCOSE USING CARBON NANOTUBE-SUPPORTED PALLADIUM CATALYST

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Amino-sugars and their derivatives possess a broad range of applications in biochemical processes and the pharmaceutical industry, particularly as contrast agents and solubility enhancers. Schiff bases resulting from the reaction of glucose with primary amines are highly susceptible to side processes such as the Maillard reaction and Amadori rearrangement. In this study, a nanostructured Pd/CNT catalyst system is proposed to saturate these unstable intermediates with high selectivity. This work focuses on the selective hydrogenation of the Schiff base formed by the condensation of glucose and methylamine, utilizing a carbon nanotube-supported palladium catalyst. Offering superior stability and reusability compared to traditional methods, the Pd/CNT catalyst achieved high yields in the synthesis of N-methyl-glucamine (Meglumine), a compound of critical pharmaceutical importance. Reaction conditions, catalytic efficiency, and product characterization have been detailed extensively.

Pd nanoparticles were loaded onto functionalized multi-walled carbon nanotubes (MWCNTs) using the impregnation method. Glucose and methylamine were stirred in a methanol/water medium at a 1:1.15 molar ratio at room temperature for 60 minutes to ensure Schiff base formation. The mixture was transferred to an autoclave reactor in the presence of the Pd/CNT catalyst. The reaction was conducted at a temperature of 70°C and under 60 bar of H_2 pressure for a duration of 2 hours. Product yield and purity were monitored using HPLC and FTIR spectroscopy. The Pd/CNT catalyst was observed to selectively target the formed imine bond (C=N) rather than the direct reduction of the carbonyl group, which would result in sorbitol formation. An N-methyl-glucamine selectivity exceeding 89% was achieved using Pd/CNT. The high surface area of the CNT support minimized mass transfer limitations, thereby shortening the reaction time. It was determined that the catalyst maintained its activity without significant loss even after 8 usage cycles.

This study demonstrates the efficacy of the Pd/CNT catalyst in converting bio-based raw materials into value-added chemicals. Maintaining low requirements for high pressure and temperature is promising for the industrial scalability and sustainability of the process.

Keywords: *Pd/CNT, Reductive Amination, Glucose, Schiff Base, Meglumine*

References:

COMPUTATIONAL TOXICOLOGY of FLUFENAUXIRIM and AMINOCYCLOPYRACHLOR: A DFT REACTIVITY and ECOTOXICITY COMPARISON

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Abstract

Comprehensive experimental toxicological data are currently unavailable for Flufenauxirim, a novel pyrimidine carboxylic acid herbicide introduced in 2025. In this study, an integrated in silico toxicological assessment was performed by combining Density Functional Theory (DFT), QSAR modeling, and read-across approaches.

Quantum chemical calculations were carried out at the B3LYP/6-31G(d) level using Gaussian to obtain global reactivity descriptors (HOMO–LUMO energy gap, electrophilicity index, chemical hardness/softness) and local reactivity parameters (Fukui functions) for Flufenauxirim and the reference compound Aminocyclopyrachlor. Aquatic toxicity endpoints (fish LC_{50} and Daphnia EC_{50}) were estimated through OECD QSAR Toolbox category formation and read-across workflows. Multiple linear regression analysis was applied to correlate DFT-derived descriptors with predicted toxicity values. Comparative analysis revealed differences in electrophilic/nucleophilic character and reactivity patterns between the two compounds, providing insight into their potential genotoxic and ecotoxic behavior. External validation confirmed the robustness and predictive performance of the DFT-QSAR model. The estimated aquatic toxicity values were evaluated in the context of regulatory safety thresholds. This integrative computational framework addresses critical data gaps and supports early-stage environmental risk assessment for newly introduced herbicidal active substances [1].

Key Words: *Computational Toxicology, Density Functional Theory (DFT), Ecotoxicity Prediction, QSAR Modeling, Reactivity Descriptors)*

References

[1] Chen W, Li Y, Zhang Q, Jiang L (2018) Pesticide Biochemistry and Physiology 142;81-89.

ANTIOXIDANT ACTIVITY OF BLACK CABBAGE (*Brassica oleracea* L. var. *sabellica*) FLOWERS

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Phenolic compounds are common plant secondary metabolites which have not only physiological functions in plants but also positive effects for human health because they can act as antioxidants. The phytochemical-rich cabbages are one of the most economically important plant families in the world. They are very significant global contributors to the foodscape from both a nutritional perspective and a culinary perspective, being viewed variously as vegetables, starchy staples, condiments, or even medical foods (1,2).

Black cabbage (*Brassica oleracea* L. var. *sabellica*) is one of the most important vegetables grown around the world for consumption. For many years, it has also been used for therapeutic purposes . Its flowers are yellow and flowers are used to produce flower roast (3).

The aim of the present study was to determine the total phenolic and flavonoid contents of black cabbage flower extracts and to evaluate their biological activity especially as antioxidant agent. Water, acetone and methanol extracts of the black cabbage flowers collected from Akçakoca (Düzce, Turkey) was prepared.

The antioxidant activity of these extracts was investigated by using different tests. The results showed that extracts exhibited different levels of polyphenols contents and antioxidant activity. Thus, solvents with different polarities had significant effect on antioxidant activity.

References

1-Y. Yesiloglu and L. Sit, *Spectrochim. Acta A*, **95**, 100 (2012).
2-Y.Yesiloglu and S. Gulen, *Bulgarian Chem. Comm*., **48**, 9 (2016).
3-B. Tohidi, M. Rahimmalek, A. Arzani, *Food Chem*., **220**, 153 (2017).

FREEZE DRYING OF COCKLE: DRYING KINETICS AND MATHEMATICAL MODELLING

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Abstract

This study investigates the freeze-drying kinetics and mathematical modeling of cockles (*Tapes philippinarum*), a highly valued seafood species. While freeze-drying is a premier preservation method that maintains the physical and chemical integrity of food by removing water through sublimation, its high operational costs due to long processing times necessitate the use of pretreatments. The primary objective of this research was to examine the impact of various pretreatment parameters, including ultrasonication, blanching, and saltwater immersion, on drying rates and moisture diffusivity to optimize the dehydration process. Samples were subjected to ten different pretreatment conditions: ultrasonication (1 and 5 min), blanching (1 and 5 min), blanching in 10% and 20% saltwater (1 min), and saltwater immersion (5 and 10 min at 10% and 20% concentrations). The drying data were fitted against 13 mathematical models to determine the most accurate predictive framework for each method. The experimental results revealed that the drying processes were completed within 240 to 480 minutes, with all samples exhibiting a dominant falling rate period. Effective moisture diffusivity ($D_{eff)}$ values were found to range between 3.47 and 6.89 × 10^{-10} m^2/s. Notably, blanching emerged as the most effective pretreatment for minimizing drying time and achieving the highest D_{eff} values, with performance improving as treatment duration increased. In the saltwater immersion groups, D_{eff} increased proportionally with both salt concentration and immersion time. Statistical analysis indicated that the Verma model provided the best fit for the control, ultrasonic, and blanching groups (R^2 values up to 0.999997), while the Aghbashlo et al. model was most suitable for the saltwater immersion samples (R^2 values up to 0.999967). These findings provide a technical foundation for enhancing the efficiency of industrial freeze-drying processes for cockles through targeted thermal and osmotic pretreatments.

Key Words: *Blanching; lyophilization; modelling; seafood; shell*

SWELLING CHARACTERISTIC OF FREEZE DRIED MUSSEL, SHRIMP AND SQUID

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Abstract

This study investigates the effect of the freeze-drying method and ultrasonic (US) pretreatment on the rehydration behavior, effective diffusion coefficients (D_{eff}), and color characteristics of blue mussels, red shrimps, and European squids. Seafood is a vital nutrient source, but its high perishability necessitates efficient preservation methods like drying. While traditional drying often impairs quality, freeze-drying preserves the pore structure by removing ice through sublimation, facilitating rapid reabsorption of water. The primary objective was to determine the experimental rehydration kinetics as a function of time and temperature (25, 40, and 60°C). Samples were prepared in two groups: those with a 5-minute ultrasonic water bath pretreatment and those without. Rehydration data were analyzed using Peleg and Two-Term Exponential mathematical models to evaluate their fit and predictive accuracy. Additionally, D_{eff} values were calculated based on Fick's second law of diffusion, and color changes were measured to assess physical quality. The results demonstrated that rehydration occurred rapidly in the initial stages, with mussels and shrimps reaching maximum rates within 10 minutes, while squids peaked at 20 minutes. Ultrasonic pretreatment generally enhances water absorption capacity by expanding the pore structure. For mussels, US-pretreated samples at 25°C showed the highest rehydration ratio (2.32 g/g). Conversely, for shrimps and squids at 25°C, untreated samples absorbed more water, a deviation attributed to their specific biological structures. Across all species, increasing the rehydration temperature led to a decrease in the final rehydration ratio. Mathematical modeling revealed that the Peleg model provided the most accurate fit for all species across various temperatures, yielding the highest R^2 and lowest RMSE and χ^2 values. Calculated D_{eff} values ranged from 1.21×10^{-9} to 5.59×10^{-9} m^2/s. Color analysis indicated that US pretreatment generally resulted in higher lightness values for rehydrated squids and shrimps. In conclusion, freeze-drying combined with ultrasonic pretreatment effectively preserves the structural integrity and improves the rehydration performance of seafood

Key Words: *lyophilization; modelling; seafood; shell; ultrasonication*

REMOVAL OF CHROMIUM (VI) FROM AQUEOUS SOLUTION USING POMEGRANATE PEEL BASED BIOSORBENT

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Abstract

Pomegranate peel, which constitutes approximately 40-50 % of the total weight of the pomegranate, is widely regarded as an agricultural waste product. However, owing to its rich organic composition and high cellulose content, it has emerged as a promising raw material for the selective adsorption of heavy metal ions [1]. Pomegranate peel waste has significant potential as an environmentally friendly and low-cost alternative raw material to produce sustainable adsorbents.

In this study, adsorption of hexavalent chromium [Cr (VI)] ions on a natural biosorbent derived from pomegranate peel was investigated. Pomegranate peels produced at different carbonization temperatures, nitrogen flow rates and heating rates were utilized in the adsorption process, to investigate the effect of production parameters on the hexavalent chromium adsorption capacity of pomegranate peel. The effects of key operational parameters such as pH and adsorbent dosage were also examined. The experimental data were analyzed using Langmuir and Freundlich isotherm models along with kinetic modeling to better understand the adsorption mechanism.

The results showed that the adsorbent which was carbonized at 950 °C with 3 L/h nitrogen flow rate and 5 ˚C/min heating rate, achieved the highest Cr (VI) removal efficiency (97.98 %) and adsorption capacity under optimal conditions at pH 2. The adsorption process was found to be better described by the Freundlich adsorption isotherm model ($R^2 = 0.984$).

This study demonstrates that thermally produced carbon from pomegranate peel can be effectively used for the removal of heavy metals, offering an environmentally sustainable solution for utilizing agricultural waste.

Key Words: *Pomegranate peel, biosorbent, chromium, adsorption, adsorption isotherm.*

References

[1] Chen, Y., Yang, J., & Abbas, A. (2023). Enhanced Chromium (VI) Adsorption onto Waste Pomegranate-Peel-Derived Biochar for Wastewater Treatment: Performance and Mechanism. Toxics, 11(5), 440.

Fluorocarbon Free Water Repellent Additives for Outdoor Polypropylene Yarns: Development and Performance Evaluation

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Abstract

Fluorocarbon based water repellent finishes are widely used in outdoor textiles; however, increasing environmental concerns related to perfluorinated compounds (PFAS) have driven the need for more sustainable alternatives. In this study, fluorocarbon free water repellent polypropylene (PP) filament yarns were developed using silicone based additives incorporated during the melt spinning process.

Different additive systems and dosage levels were evaluated in terms of processability, water repellency, and durability. Water repellency performance was assessed through contact angle measurements and standard spray tests (ISO 4920, AATCC 22), while UV resistance and color stability were evaluated using accelerated aging tests (ASTM G154, ISO 105-B04).

The results demonstrated that silicone based additives can significantly improve water repellency, with no water uptake observed in treated samples compared to untreated fabrics. However, increasing additive concentration led to higher spinning pressures, indicating processing limitations. Alternative additive systems, such as powder based solutions, did not achieve the targeted performance.

Overall, the study highlights the potential of silicone based masterbatch systems as a viable fluorocarbon free solution for outdoor PP yarns, while emphasizing the need for optimization in processing conditions and additive compatibility to ensure stable and scalable production.

Mechanistic Analysis and Control of Phenolic Yellowing in Polypropylene and Polyester Fibers: A Chemical Approach to Prevent Discoloration

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Abstract

This study focuses on the mechanistic analysis and control of phenolic yellowing in polypropylene (PP) and polyester (PES) filament yarns under controlled laboratory conditions. Both dope dyed and raw white yarns were evaluated to understand the influence of material composition and processing parameters on discoloration behavior.

The effects of flame retardant (FR) systems, UV stabilizers, and their combined use were systematically investigated. Accelerated aging tests, including phenolic yellowing tests (ISO 105-X18), UV exposure, and Xenon arc weathering (ISO 105-B04), were conducted to assess color stability and identify critical degradation pathways.

Results indicate that phenolic yellowing is strongly influenced by additive interactions, particularly under combined FR and UV stabilization systems, which tend to intensify discoloration. Polyester fibers showed higher sensitivity compared to polypropylene, likely due to deeper diffusion of reactive species.

The findings highlight the importance of optimizing additive formulations and controlling processing conditions to improve long term color stability. This study provides practical insights for the development of more stable formulations in outdoor and technical textile applications.