



# **ICNTC CONFERENCE**

INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

**9<sup>th</sup> INTERNATIONAL CONFERENCE ON  
NEW TRENDS IN CHEMISTRY  
19 – 21 MAY 2023**

## **9<sup>th</sup> ICNTC BOOK OF ABSTRACTS**

9th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

**19-21 MAY 2023 | Skopje, North Macedonia**



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**ICNTC Conference 2023**

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Chemistry Department

Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of “**9<sup>th</sup> International Conference on New Trends in Chemistry**”, to be held in Skopje, North Macedonia on the dates between May 19 – 21 , 2023

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

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

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

We kindly wait for your attendance to our conference to be held on 19 – 21 May 2023,

All informations are available in conference web site. For more information please do not hesitate to contact us. [info@icntcconference.com](mailto:info@icntcconference.com)

**Respectfully Yours,**

On Behalf of the Organization Committee of ICNTC Conference

**Prof. Dr. Dolunay SAKAR DASDAN**

*9<sup>th</sup> ICNTC 2023 | Conference Chair*

Yıldız Technical University – Istanbul / Turkey

Chemistry Department

## 19 MAY 2023 FRIDAY

10:00 – 10:10

Welcome Speech

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

10:10 – 11:00

Keynote Speech  
Speech Title

: Prof. Dr. Heikki TENHU  
: Polyelectrolytes – water soluble or not

### SESSION A

SESSION CHAIR	Prof. Dr. Sevil YUCEL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:00 – 11:20	HIGH RATE PROTOLYSIS ATTRACTORS ACTIVATE energy over zero $G_{(Pt)-GH_2O}=G_{CO_2gas}=0$ kJ/mol of indifferent (Pt), water and carbon dioxide FREE ENERGY CONTENT as BIOSPHERE Self-ORGANIZATION for PERFECT ORDER IRREVERSIBLE HOMEOSTASIS SUSTAINING the PROGRESS of BIOENERGETIC, EVOLUTION and SURVIVAL	Aris KAKSIS
11:20 – 11:40	VISIBLE LIGHT-DRIVEN PHOTOCATALYTIC HYDROGEN EVOLUTION ON DYE-SENSITIZED BISMUTH PHOSPHATE	Gizem YANALAK, Kübra Turgut, Adem Sarılmaz, Faruk Ozel, İmren Hatay Patır, Mustafa Ersöz
11:40 – 12:00	EFFECT OF NITROGEN FERTILIZER APPLICATION ON PLANT USABLE NITROGEN SPECIES IN SOIL DURING SORGHUM GROWING SEASON ON MARGINAL LANDS IN ONTARIO, CANADA	Julia LU
12:00 – 12:20	EXAMINATION OF THE CATALYTIC EFFECT OF CARBON DERIVATIVE METALLIC NANOMATERIALS ON POLLUTANTS IN WATER	Didem AYDIN, Ilkay Hilal GUBBUK, Mustafa ERSOZ
12:20 – 12:40	A SURFACE NETWORK BASED ON OXIDATIVE GRAPHENE OXIDE FOR THE DETERMINATION OF HYDROQUINONE AND CATECHOL IN GROUND AND WASTEWATER SAMPLES	Emad A. Khudaish
12:40 – 13:00	PREPARATION AND CHARACTERIZATION OF POLYSACCHARIDE BASED ORAL FILMS FOR QUETIAPINE FUMARATE RELEASE	Merve YAMAN AGIRMAN, Ilknur KUCUK

13:00 – 14:00	<b>LUNCH B R E AK</b> <b>LUNCH IS NOT INCLUDED INTO REGISTRATION FEE</b>
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### SESSION B

SESSION CHAIR	Prof. Dr. Nuriye AKBAY	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
14:00 – 14:20	DEGREDAATION REACTION KINETIC OF 6-APA	Seyda AYDOĞDU, Arzu Hatipoglu
14:20 – 14:40	DETERMINATION OF PHYSIOCHEMICAL PROPERTIES OF PRIMARY METABOLITES OF AN ANTIDEPRESSANT DRUG BY MOLECULAR MODELING	Simal KURUMOĞLU, Yelda YALÇIN GÜRKAN
14:40 – 15:00	CALCULATING ANALYSIS OF SEASONAL CHANGES AND DEGRADATION REACTIONS OF PESTICIDES IN SURFACE WATERS FEEDING SÜLEYMANPAŞA DISTRICT, TEKİRDAĞ	Cigdem SAYIKLI SIMSEK, Yelda YALCIN GURKAN
15:00 – 15:20	SCREENING OF SUPPORTED BIMETALLIC Fe CATALYSTS FOR LIGHT OLEFIN PRODUCTION in FTS: EFFECT OF SUPPORT MATERIALS	Deniz UYKUN MANGALOĞLU, Hüsnü ATAKÜL
15:20 – 15:40	A STUDY TO UNDERSTAND THIOFLAVIN-T INTERACTION WITH AB PEPTIDES AND FIBRILS	Pelin GUZEL, Dila KAYA, Nuriye AKBAY

15:40 – 16:00	<b>B R E AK</b>
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### SESSION C – POSTER SESSION

SESSION CHAIR	Prof. Dr. Julia LU, Prof. Dr. Sevil YUCEL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
16:00-17:00	SYNTHESIS OF CNT BASED METALLIC NANOPARTICLES AS EFFECTIVE CATALYSTS FOR THE DEGRADATION OF ORGANIC POLLUTANTS WITH NABH <sub>4</sub> IN WATER	İlkay Hilal GUBBUK, Didem AYDIN, Mustafa ERSOZ
	DEVELOPMENT OF METAL ORGANIC FRAMEWORK BASED MEMBRANES AND THEIR APPLICATION	Gülcihan ÖZDEM, Mustafa ERSÖZ, İlkay Hilal GUBBUK, Özlem ALTINTAŞ YILDIRIM, Hakan ERER
	DYE-SENSITIZED CALCIUM TUNGSTATE (CaWO <sub>4</sub> ) STRUCTURE FOR	İmren Hatay PATIR, Kübra Turgut, Gizem Yanalak, Adem Sarılmaz, Faruk Ozel, Mustafa



	PHOTOCATALYTIC HYDROGEN GENERATION WITH VISIBLE LIGHT	Ersöz
	REMOVAL of PYRACLOSTROBIN, PINOXADEN, GAMMA-CYHALOTHRIN PESTICIDES FROM GROUNDWATER BY DFT METHOD	Hidayet GUREL YORULMAZ, Burak GURKAN, <b>Yelda YALCIN GURKAN</b>
	ELECTRONIC PROPERTIES OF PLATIN-BASED ANTICANCER DRUGS	Mert Evirgen, Seyda Aydogdu, <b>Arzu HATIPOGLU</b>
	LaNiO <sub>3</sub> CATALYSED AMINATION OF PHENOLS	<b>Anna Adel ADAM</b> , Sándor Balázs NAGY, Szilveszter ZIEGENHEIM, Pál SIPOS, Gábor VARGA
	SYNTHESIS AND CHARACTERIZATION OF POLY(ETHYLENE-ALT-MALEIC-ANHYDRIDE)-PREGABALIN (1:1) RATIO CONTROLLED DRUG DELIVERY SYSTEM WITH CATALYST FREE MEDIA	<b>Ozge ESLEK</b> , Dolunay ŞAKAR
	CHOOSING A SECOND ADSORBENT TO SAMPLE VOLATILE ORGANIC COMPOUNDS IN BIOMASS GASIFICATION TAR	<b>Aleksandrs I. PUCKINS</b> , Sergejs D. OSIPOVS
	EFFECT OF ANIONIC/NONIONIC EMULGATOR SYSTEMS ON THE PROPERTIES OF WATER BASED STYRENE/ACRYLIC COPOLYMER PAINT BINDERS	Berfin Ceyda AYHAN, <b>Dolunay SAKAR</b> , Emine Cansu TARAKÇI
	CHEMICAL PVA HYDROGELS AS CLEANING DEVICE OF ANCIENT SURFACES	<b>Martina REDI</b> , Ozge ESLEK, Ester CHIESSI, Fabio DOMENICI, Gaio PARADOSSI
	COMPARATIVE TECHNO-ECONOMIC ANALYSIS OF INDUSTRIAL-SCALE BIOBUTANOL PRODUCTION PROCESSES FOR AN EFFICIENT WASTE MANAGEMENT	<b>Abdullah Bilal OZTURK</b> , Tulin OZBEK ,

### SESSION D – POSTER SESSION

SESSION CHAIR	Assoc. Prof. Dr. Emel AKYOL, Assoc. Prof. Dr. Azmi Seyhun KIPCAK	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
17:00-18:00	STUDY OF THE TOXICITY OF BENZANTHRONE LUMINESCENT DYES	<b>Jelena KIRILOVA</b> , Marina SAVICKA, Alise KIRILOVA, Armands MALECKIS, Tatjana GRIGORJEVA
	ANALYTICAL METHOD FOR THE DETERMINATION OF TAR PRODUCED	<b>Sergejs D. OSIPOVS</b> , Aleksandrs I. PUČKIN

	FROM THE PYROLYSIS OF WASTE TYRES	
	EVALUATION OF NOVEL DESIGNED DELICIOUS PEPTIDES FOR IMPROVING TASTE SENSATION	Ahmet Cenk ANDAÇ, Sevil YUCEL, Cem ÖZEL, Ceren KEÇECİLER, Kevser KÖKLÜ
	SYNTHESIS AND CHARACTERIZATION OF COBALT SULFIDE LAYERS	Asta BRONUSIENE, Skirma ZALENKIENE, Ingrida ANCUTIENE, Remigijus IVANAUSKAS
	SYNTHESIS AND CHARACTERIZATION OF TIN SULFIDE NANOPARTICLES	Asta BRONUSIENE
	ASSESSMENT OF OXIDATIVE STRESS BY DETECTION OF H <sub>2</sub> O <sub>2</sub> IN RYE SAMPLES USING A MULTIELECTRODE ELECTROCHEMICAL SENSOR	Irena MIHAILOVA, Vjaceslavs GERBREDERS, Marina KRASOVSKA, Valdis MIZERS, Eriks SLEDEVSKIS
	CONVOLUTIONAL NEURAL NETWORK-BASED EVALUATION OF CHEMICAL MAPS OBTAINED BY FAST RAMAN IMAGING FOR PREDICTION OF TABLET DISSOLUTION PROFILES	Boldizsár ZSIROS, Dorián László GALATA, Gábor KNYIHÁR, Orsolya PÉTERFI, Lilla Alexandra MÉSZÁROS, Ferenc RONKAY, Brigitta NAGY, Edina SZABÓ, Zsombor Kristóf NAGY, Attila FARKAS
	THE IMPACT OF STRUCTURE OF SELECTED CATIONIC LIPIDS ON PHYSICOCHEMICAL PROPERTIES OF MODEL MAMMALIAN MEMBRANES	Marzena MACH, Paweł WYDRO
	EFFECT OF ALKALINE EARTH IONS ON THE BEHAVIOUR OF ALKYL BENZENE SULFONATES	Szilveszter ZIEGENHEIM, Anna Adél ÁDÁM, Csaba BÚS, Bence KUTUS, Pál Sipos, László JANOVÁK, Imre DÉKÁNY

18:45 – 22:00	<b>GALA DINNER</b> Participants who registered as FULL PACKAGE has free Access to Dinner
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## 20 MAY 2023 SATURDAY

10:20 – 11:00

**Keynote Speech**

: **Prof. Dr. Sefik SUZER**

**Speech Title**

: XPS, A Chemical Analysis Tool for Exploring Electrical

Properties of

Liquid/Solid Interfaces

### SESSION E

SESSION CHAIR	Assoc. Prof. Dr. Emel AKYOL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:00 – 11:20	EFFECTS OF ALCOHOLS ON SODIUM DODECYLSULPHATE'S SOLUTION CHEMISTRY PROPERTIES AND DISSOLUTION OF CASDS <sub>2</sub> PRECIPITATES	<b>Csaba BUS</b> , Pál Sipos, Bence Kutus
11:20 – 11:40	DNA BINDING STUDIES FOR SOME SMALL MOLECULES	<b>Ayşegül GOLCU</b>
11:40 – 12:00	EFFECTS OF DRYING METHODS ON THE DRYING KINETICS OF BLANCHED BROWN CRAB MEAT	Zehra Ozden <b>OZYALCIN, Azmi Seyhun KIPCAK</b>
12:00 – 12:20	PHOTOCATALYTIC ACTIVITY of TiO <sub>2</sub> -Cu-METAL-ORGANIC FRAMEWORK (MOF)	Ayşenur KATIRCI, M. Efgan KİBAR, <b>Filiz UGUR NIGIZ</b>
12:20 – 12:40	PERVAPORATIVE DESALINATION BY PHOSPHOMOLYBDIC ACID/PVA HYBRID MEMBRANE	<b>Derya UNLU</b>
12:40 – 13:00	THE EFFECT OF ULTRASOUND PRETREATMENT ON THE OVEN AND VACUUM OVEN DRYING KINETICS OF BLUEBERRIES	Zeyd Emin TAŞÇI, <b>Ekin KIPCAK</b>

13:00 – 14:00	<b>LUNCH B R E A K</b> LUNCH IS NOT INCLUDED INTO REGISTRATION FEE
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### SESSION F

SESSION CHAIR	Prof. Dr. Aysegul GOLCU	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
14:00 – 14:20	POLYSACCAHARIDE BASED FILMS FOR A TRANSDERMAL DRUG DELIVERY SYSTEMS	<b>Deniz EKSI</b> , İlknur KÜÇÜK

14:20 – 14:40	ZR-BASED METAL ORGANIC FRAMEWORK FILLED MEMBRANE SYNTHESSES AND APPLICATION FOR CO <sub>2</sub> /N <sub>2</sub> SEPARATION	Filiz UGUR NIGIZ
14:40 – 15:00	2-(((3-CHLOROPHENYL)IMINO)METHYL)-4-NITROPHENOL: SYNTHESIS, MOLECULAR AND MEDICINAL STUDIES	Songul SAHIN, Necmi Dege
15:00 – 15:20	POLYACRYLIC ACID AND POLYACRYLIC ACID SODIUM SALT AS INHIBITORS OF CALCIUM OXALATE CRYSTAL FORMATION	Ahmed sadeq Abdo Esmail AL-DUBAI, Emel AKYOL

15:20 – 16:00	COFFEE B R E A K
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16:00 – 16:30	CLOSING CEREMONY
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**21 MAY 2023 SUNDAY**

	FREE DAY
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- [2] V. Baddam, V. Aseyev, S. Hietala; E. Karjalainen H. Tenhu; *Macromolecules* (2018), 51, 9681-9691
- [3] V. Baddam, R. Missonen, S. Hietala, H. Tenhu; *Macromolecules* (2019), 52, 6514-6522
- [4] V. Baddam, L. Valinen, H. Tenhu; *Macromolecules* (2021), 54, 4288-4299

**High rate protolysis Attractors activate over zero level of  $G_{(Pt)}=G_{H_2O}=G_{CO_2_{gas}}=0$  kJ/mol indifferent (Pt), water and carbon dioxide free energy content as Biosphere Self-Organization for perfect order irreversible homeostasis sustaining the progress for bioenergetic, evolution and survival.**

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**Abstract.** The quantitative studies for oxygen, carbon dioxide and water protolysis functional activity reveal multiply generated Self-Organization Attractors: pH=7.36, enzyme Carbonic Anhydrase reactivity, water  $[H_2O]=55.3$  mol/Liter concentration, air oxygen level 20.95 %, osmolar concentration 0.305 M, ionic strength 0.25 M, temperature 310.15 K degree etc.[1] High rate protolysis in water make oxygen fire safe , functionally activate  $CO_{2aqua}$  for Life Homeostasis. 2023 are hundred Years of Brønsted - Lowry protolysis, which high rate protonation stay at equilibria while homeostasis continues. Arterial dissolute oxygen [concentration](#)  $[O_{2aqua}]=6*10^{-5}$  M is safe Bioenergetic sustaining isooxia with air oxygen level 20.95 % Attractor 500 MYears. [14]

The perfect order irreversible non-equilibrium reactions of homeostasis are created by activation with high rate protolysis Attractors, which stay at equilibrium and activate molecules for progress of homeostasis. Those indispensably are for irreversible continuing homeostasis. Homeostasis generate bioenergetic concentration gradients for transport down and for osmosis against the gradients, which as Brownian molecular engines drive the organism homeostasis for evolution and for survival. [4] Deviation from high rate protolysis Attractor values disorder the Self-Organization perfect reaction order of homeostasis. The created Chaos disorders and stops the homeostasis which disappears as extinct from Biosphere. Zero energy  $G_{(Pt)}=G_{H_2O}=G_{CO_2_{gas}}=0$  kJ/mol belong to indifferent (Pt), water  $H_2O$  and  $CO_{2gas}$ . [Alberty](#) [8]

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

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## VISIBLE LIGHT-DRIVEN PHOTOCATALYTIC HYDROGEN EVOLUTION ON DYE-SENSITIZED BISMITE PHOSPHATE

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### Abstract

Nowadays, due to the increasing environmental pollution and growing population, many studies are carried out on environmentally friendly, clean, and renewable energy technologies. Photocatalytic hydrogen production by water separation method is recognized as a promising renewable energy [1]. For the ideal photocatalytic hydrogen evolution reaction (HER), low-cost and high-efficiency of catalysts should be used [2, 3]. Herein, the photocatalytic HER activity of the bismuth phosphate (BiPO<sub>4</sub>) catalyst was investigated in the presence of triethanolamine (TEOA) and Eosin-Y (EY) as an electron donor and dye sensitizer, respectively, with visible light illumination. The dye-sensitized photocatalytic hydrogen production activity of the BiPO<sub>4</sub> catalyst was calculated as 0.377 mmol g<sup>-1</sup> for 8h illumination. In addition, the photocatalytic HER activity of BiPO<sub>4</sub> was investigated by adding platinum as a cocatalyst under the same conditions in order to increase hydrogen efficiency. A comparative study demonstrated that EY-sensitized BiPO<sub>4</sub>/Pt catalyst have improved HER efficiency (4.589 mmol g<sup>-1</sup>) by nearly 12-fold due to the increased electron-transfer efficiency of Pt.

**Keywords:** *Photocatalytic; hydrogen evolution; bismuth phosphate; dye sensitized; cocatalyst*

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## **EFFECT OF NITROGEN FERTILIZER APPLICATION ON PLANT USABLE NITROGEN SPECIES IN SOIL DURING SORGHUM GROWING SEASON ON MARGINAL LANDS IN ONTARIO, CANADA.**

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Nitrogen can take various forms as it cycles through the environment (air, soil, and water). Fertilizer application is one of the most common agricultural practices that helps plant growth and increase crop yields. Plants, however, take up only a fraction of the fertilizer applied and the unused N can be released into the surface environment with unintended consequences for water and emitted to air, as nitrous oxide, contributing to global warming. This research focuses nitrogen species in soils during the sorghum growing season. Soil samples were collected from agricultural and marginal land fields at three different times during a growing season: Before Planting (BP), After Fertilizer Application (AFA), At Harvest (AH). Plant usable (water leachable  $\text{NO}_3^-$  and  $\text{NH}_4^+$ ) and unusable nitrogen species in the soil samples were analyzed using calorimetric and Kjeldahl methods. The results show the concentration of plant usable nitrogen varies with the land type and collection time; plant-usable nitrogen species, compared with unusable nitrogen species, only account for a small portion of the nitrogen in the soil; the level of plant usable nitrogen in the soil increased after N-fertilizer application but decreased to that in the soil before fertilizer application at harvest and the level of increase was as not proportional to the rate of fertilizer application.

## Examination of the catalytic effect of carbon derivative metallic nanomaterials on pollutants in water

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### Abstract

Pharmaceuticals are a group of various organic compounds that are continuously released into the environment and cause persistent organic micro-pollution in water environments such as sewage, surface, soil, and drinking water [1]. Ketoprofen, a commonly used non-steroidal anti-inflammatory drug for the treatment of pain syndromes in humans and animals, is not completely eliminated in wastewater treatment plants and can be found in waste and surface waters. Therefore, it is important to investigate the degradation and distribution of ketoprofen in terms of environmental pollution and to develop cost-effective and environmentally friendly treatment techniques to eliminate contamination[2]. Nanomaterials exhibit high catalytic activity due to their high surface area and chemical reactivity. They allow for rapid catalytic reactions and have great potential for environmental applications such as the treatment of wastewater and air [3]. In this study, carbon-based metallic nanomaterials were used to break down ketoprofen in water contaminated with NSAIDs. A metallic carbon-based material was synthesized at 550°C using a one-step method, which showed high catalytic activity and stability. The synthesized composites were extensively characterized using characterization methods such as IR, XRD, TGA, SEM to explore their development mechanisms. Ketoprofen degradation significantly increased with increasing metal percentage and was slightly affected by the amount of sodium borohydride. Almost complete elimination of ketoprofen within 60 minutes showed that the metallic carbon-based material was an effective method for degradation and promising for the removal of pharmaceuticals from wastewater.

**Key Words:** *nanomaterial, degradation, catalysis, ketoprofen, water treatment*

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## A surface network based on oxidative graphene oxide for the determination of hydroquinone and catechol in ground and wastewater samples

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### Abstract

A sensing network based on oxidative graphene oxide (OGO) fabricated onto a glassy carbon electrode (GCE) by consecutive anodic treatment of a native (virgin) synthesized graphene oxide (VGO). The proposed oxidative step is crucial to decrease stacking interactions and enrich the surface materials with oxygenated functionalities that play significant roles in improving the surface conductivity and electron transfer kinetics. A primary result achieved by electrochemical impedance spectroscopy (EIS) showed an exceptional reactivity of OGO interpreted by estimating the apparent rate constant ( $k_{app}$ ) of electron transfer kinetics that approaches 8.7 times over VGO. The differential pulse voltammetry (DPV) experimental data for the simultaneous determination of hydroquinone (HQ) and catechol (CC) verify the remarkable reactivity of the OGO compared to both bare GCE and VGO. The above supportive evidences underlines the significance of abundant oxygen functional groups for fast kinetics at OGO surface materials. The selectivity test of OGO-GCE in the determination of HQ and CC under optimal conditions was excellently achieved at which the detection limit ( $DL_{3\sigma}$ ) of HQ and CC were 0.114  $\mu\text{M}$  and 0.124  $\mu\text{M}$ , respectively. The successful analytical performance of OGO on two water samples suggested the application of robust, stable and promising materials for trace HQ and CC quantification.

**Key Words:** *Graphene Oxide; Oxidative Pre-treatment; Hydroquinone; Catechol; Water.*

## Preparation And Characterization of Polysaccharide Based Oral Films For Quetiapine Fumarate Release

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### Abstract

Orally dispersible films have gained significant interest as a drug delivery system due to their advantageous properties, such as faster drug absorption, higher bioavailability, and improved patient compliance, particularly in children, the elderly, and those with swallowing difficulties compared to traditional orally administered dosages [1]. This innovative drug delivery system, which is created by various polymers with suitable excipients, is designed to overcome the challenges associated with traditional oral drug administration [2-3].

Quetiapine fumarate, which was used as the active ingredient which is a new antipsychotic agent that responds to the positive and negative symptoms of bipolar disorder and schizophrenia. Also, in the case of bipolar disorder and schizophrenia, the use of oral films containing peppermint oil and rosemary could potentially provide a more effective and convenient treatment option for patients.

The aim of the present work was to formulate and characterize oral films based on polysaccharides containing quetiapine fumarate, peppermint oil and rosemary were prepared by using solvent casting technique. As oral film structures were confirmed by FTIR its physical properties such as thickness, homogeneity, disintegration time were determined. The dissolution rates of the films with the appropriate dosage of quetiapine fumarate in the oral, stomach and intestinal in vitro environments were investigated. Film dissolution studies were carried out on dissolution bath and drug release concentration was determined spectrophotometrically at a wavelength of 246 nm and with reference to an appropriate standard curve. It has been determined that oral films that is prepared present work exhibited maximal release in 10 min of quetiapine fumarate and it was between 80-90 %.

**Key Words:** *Oral film, polysaccharide, sodium alginate, quetiapine fumarate, rosemary, mint*

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## DEGREDAATION REACTION KINETIC OF 6-APA

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### Abstract

Removal of medical wastes from water is of great importance in the field of environmental chemistry [1]. Antibiotics are important in medical waste because they are consumed around 200,000 tons per year worldwide. 6-aminopenicillanic acid (6-APA) is one of the widely used antibiotics for human medicine against bacterial infection and as a veterinary drug to prevent diseases [2-4]. As a consequence of excessive consumption of 6-APA, it is frequently detected in the aquatic environment [5]. In this study, the reaction kinetics of 6-APA with OH radical was investigated theoretically. It is very important to know the degradation kinetic mechanism of 6-APA in detail to remove them from the aquatic environment.

The quantum chemical calculations were performed with the DFT method B3LYP/ 6-31G (d,p) basis set within Gaussian 09 package. The solvation effects of water are computed using Conductor like Polarizable Continuum Model (CPCM) as the solvation model. Energy profile and thermodynamic calculations of the reaction were done. Among the reaction paths studied, the beta-lactam ring opening pathway was found to be the most probable path. Based on the results of the quantum mechanical calculations, the total rate constant was calculated as  $3.11 \times 10^{11} \text{ M}^{-1} \cdot \text{s}^{-1}$  by Transition State Theory.

**Key Words:** *Antibiotic, 6-APA, DFT, CPCM, water*

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# DETERMINATION OF PHYSIOCHEMICAL PROPERTIES OF PRIMARY METABOLITES OF AN ANTIDEPRESSANT DRUG BY MOLECULAR MODELING

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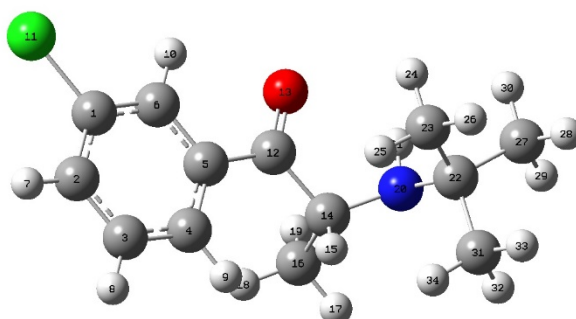
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## Abstract

Data from the Ministry of Health show that the amount of antidepressant use has increased by about 70 percent in the 11 years until 2020. According to the latest health statistics of the Ministry for 2020, while 29 antidepressant drugs per 1000 people per day decreased in 2009, this rate increased to 49 in 2020. In addition to its use as an antidepressant, bupropion is also used in the treatment of smoking cessation, methamphetamine and cocaine addiction, behavioral addictions such as pathological gambling, and attention deficit hyperactivity disorder.

Every substance (food, drug, etc.) taken into the body is excreted from the body because of enzymatic mechanisms and given to the natural environment and pollutes the nature. Our aim is to optimize the 3 primary metabolites with DFT method, which are formed because of enzymatic reactions after the drug is taken into the body. It is to theoretically explain the degradation pathways that metabolites given to the natural environment with urine may be exposed to.



**Figure 1.1.** Optimized structure of Antidepressant Drug (Bupropion) and the numbering system (grey, carbon; red, oxygen; blue, nitrogen; white, hydrogen; green, chlorine).

**Key Words:** Gaussian09, DFT, Antidepressant Drug, Primer Metabolites of Bupropion

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## CALCULATING ANALYSIS OF SEASONAL CHANGES AND DEGRADATION REACTIONS OF PESTICIDES IN SURFACE WATERS FEEDING SÜLEYMANPAŞA DISTRICT, TEKİRDAĞ

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In this study, the possible reaction paths of 2,3,4,5,6 pentachlorotoluene, Benzylbenzoate and Demeton molecules with OH radical. Optimized geometries are drawn with Gauss View 5. Later, with the Gaussian 09 program, geometric optimization was made and the lowest energy states were found. Geometric structure analysis was done and bond lengths and bond angles were calculated. The purpose of this study is to determine the most likely way of interaction of 2,3,4,5,6 pentachlorotoluene, Benzylbenzoate and Demeton molecules and OH in the gas phase and aqueous medium. The effect of solvent water, COSMO is used as the dissolution model and has a stabilizing effect in reducing the energy in the reactions. The lowest energy molecule has the most stable structure. Apart from these studies, the seasonal changes of the 3 pesticides mentioned in the water samples taken in 4 different seasons from the Naip Dam, which feeds the central neighborhoods of Süleymanpaşa District of Tekirdağ Province, were examined. These results will guide experimental studies and determine the fragmentation mechanism.

**Key words:** Pesticides, quantum mechanical methods, Gaussian09

# SCREENING OF SUPPORTED BIMETALLIC Fe CATALYSTS FOR LIGHT OLEFIN PRODUCTION in FTS: EFFECT OF SUPPORT MATERIALS.

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## Abstract

Fischer-Tropsch (FT) synthesis, which catalytically converts synthesis gas (CO and H<sub>2</sub>) into a large variety of fuels and chemicals, is an established technology. However, FT suffers from a broad product distribution which requires for costly follow on separation technologies. Recently the production of light olefins, e.g. ethylene, propylene, and butylene, by FT synthesis has been receiving considerable attention, besides the catalytic cracking of naphtha and the dehydrogenation of alkanes [1].

In this work the Fe-Co bimetallic catalysts for the production of light olefins from synthesis gas were studied. The main objective was to investigate the effect of support material on the catalyst performance. Seven different materials, namely  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>,  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, ZrO<sub>2</sub>, CeO<sub>2</sub>, Zeolite-Y and Zeolite-13X, were used as support materials in the preparation of the bimetallic catalysts. The iron and cobalt contents were kept constant for all catalysts in order to determine the most favorable support material for the light olefin production. The catalysts were synthesized by co-impregnation method. The activity tests of the synthesized catalysts were carried out by using a High Throughput Catalyst Performance Analyzer (CPA). The results showed that  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> and Zeolite-Y support materials were promising support materials for the light olefin production.

**Key Words:** *Fischer-Tropsch, Light Olefin, Bimetallic, Supported catalysts, Iron and Cobalt*

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## A STUDY TO UNDERSTAND THIOFLAVIN-T INTERACTION WITH A $\beta$ PEPTIDES AND FIBRILS

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### Abstract

Thioflavin-T (ThT) has been used as fluorescence probe to detect amyloids for over 50 years, thanks to its broad staining capacity, high sensitivity and practical use. As a fluorescence probe, ThT has extraordinary properties to detect and analyze amyloid fibril formation. Understanding the ThT-fibril interactions and comparing these interactions to ThT-protein interactions become important to investigate amyloid fibril formation, kinetics, structure, and pathogenesis. The information gathered from these studies will assist to design new inhibitors and therapeutics for amyloid related diseases. Before performing a comprehensive study on anti-amyloid therapies, a better understanding of ThT emission in different microenvironments and atomic details of interactions between ThT-peptides/ThT-fibrils are needed.

In this study, spectroscopic and computational approaches are utilized to understand ThT-amyloid interaction mechanisms. Firstly, UV-Vis absorption and fluorescence spectra of solely ThT, ThT-protein and ThT-fibril solutions were obtained and analyzed to screen and characterize amyloid fibril formation. In the experimental studies, lysozyme was selected as precursor protein to form amyloid fibrils. After observing the characteristic enhancement of ThT fluorescence upon binding to fibrils, we aimed to understand atomic details of interactions between ThT and A $\beta$  fibrils. For this reason, a protein-ligand docking procedure provided by HADDOCK<sup>1,2</sup> is applied to the peptides and fibrils of A $\beta$  structures retrieved from protein data bank<sup>3</sup>. The atomic structure of ThT is obtained from PubChem database<sup>4</sup>. According to the docking results, it is possible to say that ThT has a certain binding affinity to both A $\beta$  peptides and A $\beta$  fibrils. Statistical analysis of contacts between A $\beta$  fibrils and ThT showed that they are mostly interacted via the residues Met35 and Gly37 on the fibril surface in consistent with the data given in the literature.

In further studies, it is aimed to carry out molecular dynamics simulations for the selected ThT-peptide/ThT-fibril conformations obtained from docking studies. By this way, our investigations will provide new insights to design fluorescence probes for amyloid detection and to apply them in structure-guided design. Modulating the specificity of ThT to particular amyloid fibrils can also be possible after combining the findings from both experimental and computational approaches.

**Key Words:** *Fluorescence probes, amyloid fibrils, thioflavin-T, protein-ligand docking*

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## Synthesis of CNT based metallic nanoparticles as effective catalysts for the degradation of organic pollutants with NaBH<sub>4</sub> in water

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### Abstract

Nanomaterials offer desirable properties that are difficult to achieve with bulk materials. The nano sized porous catalyst particles offer a larger outer surface area and therefore increased catalytic activity. Research in the field of porous materials plays a vital role in research and industry. Pharmaceuticals and synthetic dyes are persistent pollutants commonly found in industrial wastewater. These organic compounds are toxic to aquatic organisms, so it is important to remove them from the water [1]. Dyes play a vital role in various branches of the dyeing and textile industries. Commercially available synthetic dyes are the dyes most commonly used in such industries. These paints are generally obtained from two main sources, namely coal tar and petroleum intermediates with a total annual production of more than  $7 \times 10^5$  tons [2]. Biodegradable textile dyes are discharged into natural streams and water bodies. The environment must be purified from this synthetic material. Environmental purification has increasingly become a global concern calling for considerable attention. In recent years, many strategies have been devised to remove these pollutants, including treatment methods such as oxidation, chemical and physical methods for degradation of these effluents. Recovery systems based on metallic nanoparticles are superior to conventional systems in terms of their efficiency. Carbon nanotubes (CNT) are known to be suitable support materials due to their affinity for metal cations [3]. Nanoparticle catalysis systems with lanthanide group metals, which have been little studied in the literature, are effective in turning into less harmful compounds through chemical reduction and decomposing dye molecules. Multi-walled CNT decorated with metal nanoparticle (CNTs/M nanocomposite) was prepared with clean, simple, and one-pot method as catalytic degradable material dyes [4].

In the study, commercially available CNT will be synthesized in thermal environment with metal salt after washing processes. This study reports the preparation of carbon nanotube supported metal catalyst and the results of characterization studies with FTIR, XRD, TGA. The catalyst system was effective in the catalytic reduction of the methyl yellow dye. The study is a model study in the field of using carbon nanotube supported metal nanoparticles for environmental remediation and protection.

**Key Words:** Carbon nanotubes, metal catalyst, dye degradation.

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## Development of metal organic framework based membranes and their application

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### Abstract

Water pollution although originated from different sources should be handled properly via environmental friendly materials and methods. Metal Organic Frameworks (MOFs) with tuneable porosity, high surface area/volume ratio and graphene oxide (GO) with different functional groups, as being prominent stars of material chemistry in the last decade were planned to be combined in a series of polyacrylonitrile (PAN) nanofiber membranes [1, 2]. Although, ZIF-8 was generally employed in gas separation and storage applications, it was preferred to be utilized in our novel nanofiber membranes to eliminate poisonous and carcinogenic methylene blue (MB) dye from an aqueous medium. Consequently, PAN nanofiber membranes with varying amounts of ZIF-8 and GO were prepared through the facile, material and cost effective electrospinning process over a nonwoven support in one step procedure. Involved in dye removal, adsorption isotherms and kinetics were investigated and the prepared membranes were characterized by contact angle, FTIR, SEM and EDX measurements. Also, the transport mechanism and kinetics of the prepared membranes were analyzed thorough a special diffusion cell. The results indicated that ZIF-8/GO/PAN nanofiber membranes have great potential for MB removal.

This study was carried out within the scope of the doctoral thesis project number 20211034 at Selçuk University.

**Key Words:** *membrane removal, ZIF-8, electrospinning, dye, PAN.*

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# DYE-SENSITIZED CALCIUM TUNGSTATE (CaWO<sub>4</sub>) STRUCTURE FOR PHOTOCATALYTIC HYDROGEN GENERATION WITH VISIBLE LIGHT

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## Abstract

Photocatalytic hydrogen production using sunlight is recognized as a promising approach for today's energy problem, which can be considered artificial photosynthesis [1]. This solar light-driven photocatalysis process has received increasing attention owing to its potential to be an environmental friendly process [2, 3]. Herein, low-cost, easily synthesized, highly efficient, and stability of photo/catalysts should be preferred for the photocatalytic hydrogen production reaction [4, 5]. Therefore, the Calcium tungstate (CaWO<sub>4</sub>) photocatalyst was studied for photocatalytic hydrogen evolution systems in the presence of a triethanolamine (TEOA) electron donor and EY dye sensitizer under visible light illumination. The HER activity of the dye-sensitized CaWO<sub>4</sub> photocatalyst was calculated as 1.173 mmol g<sup>-1</sup> for 8h visible light irradiation. Moreover, the dye-sensitized photocatalytic HER activity of the CaWO<sub>4</sub> catalyst was investigated by using platinum cocatalyst under the same conditions, and the yield of photocatalytic hydrogen production of the catalyst was reached 21.143 mmol g<sup>-1</sup> for 8h. Here, Pt acted as the active site for proton reduction leading to high photocatalytic activity of hydrogen production.

**Keywords:** Photocatalyst; hydrogen evolution; calcium tungstate; dye sensitized; cocatalyst

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## REMOVAL of PYRACLOSTROBIN, PINOXADEN, GAMMA-CYHALOTHRIN PESTICIDES FROM GROUNDWATER BY DFT METHOD

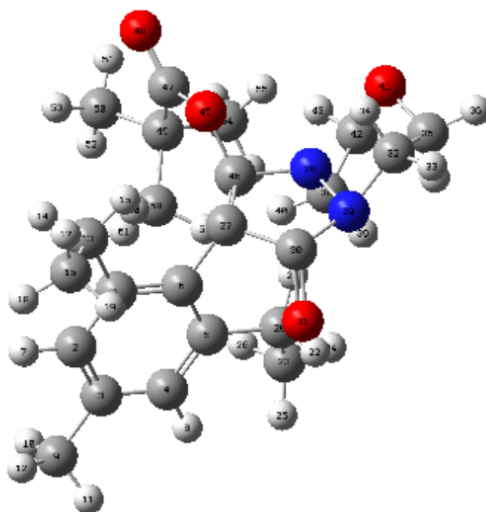
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### Abstract

Today, there is a shortage of food due to the increase in the world population. For this reason, pesticides are used to remove plant pests in order not to cause product loss in agriculture. Especially in agriculture, synthetic pesticides created to achieve high efficiency are increasing day by day. The pesticides used get into the soil and then into the groundwater. In this study, the ways of decomposition of pesticides Pyraclostrobin from the fungicide variety, Pinoxaden from the herbicide variety, and Gamma-cyhalothrin from the insecticide variety in groundwater were investigated theoretically. Optimized geometries were drawn with Gauss View 5.0, and then geometric optimization was carried out using the Gaussian 09W program using Functional Density Theory (DFT) and Hartree-Fock methods. The geometrical structure (bond angles and bond lengths) of all three molecules and their possible degradation products were calculated at the level of B3LYP theory within the Hartree-Fock (HF) method and density function theory (DFT) in the basic set of 6-31G(d). Thus, the possible degradation mechanisms of these three pesticide molecules in water were determined. These results will guide experimental studies.



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

**Key Words:** Pesticid, Fungicide, Herbicide, Gaussian 09W, DFT

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## LaNiO<sub>3</sub> catalysed amination of phenols

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### Abstract

Perovskites are mixed metal-oxides with low price and various thermal stability which depends on their bulk and surface characteristics and composition. They are extensively researched for their catalytic, optical, and magnetic *etc.* properties.

In this study, we investigated the structure and catalytic properties of a number of La-Ni containing perovskites with various metal ratio. The catalytic test reaction was the direct amination of phenols with hydrazine monohydrate under different reaction conditions in liquid phase.

Traditionally, anilines and their C-and/or N-substituted variants originate from petrochemical sources, extracted by two-step nitration-reduction. However, due to their importance, various methods were explored to synthesize these molecules.

Previously, these methods were carried out under hard conditions (Pd/C catalyst, high temperature and gas phase amination).

However, in our work, anilines were prepared with LaNiO<sub>3</sub> catalyst in liquid phase phenols amination at reflux temperature, using hydrazine monohydrate as aminating agent. The properties of the catalysts, their structure, composition, the acidity/basicity of their surface were thoroughly investigated as they influence the catalytic behaviour of these materials.

During the optimization of the amination reactions, different amounts of hydrazine was used, the effect of various solvents were also studied and the composition of catalyst was also changed (LaNiO<sub>3</sub>, La<sub>2</sub>NiO<sub>4</sub>, La<sub>3</sub>Ni<sub>2</sub>O<sub>7</sub> and La<sub>4</sub>Ni<sub>3</sub>O<sub>10</sub>) along with the catalyst loading.

As a result, we developed a new method for direct amination of phenols to aniline and their derivatives in liquid phase with LaNiO<sub>3</sub> catalyst.

**Key Words:** *perovskites; LaNi-perovskite; catalysis; amination of phenols; hydrazine monohydrate*

## ELECTRONIC PROPERTIES OF PLATIN-BASED ANTICANCER DRUGS

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### Abstract

The discovery of the anticancer properties of cisplatin has made it the pioneer of metal-based anticancer drugs that have been used from the past to the present [1]. However, cisplatin lacks tumor tissue selectivity and renders target cells resistant to cisplatin over time [2]. Therefore, scientists have synthesized new cisplatin analogs such as carboplatin, oxaliplatin, nedaplatin, lobaplatin, and heptaplatin. These platinum-based chemotherapeutic drugs are the most widely used in the treatment of different cancer diseases such as testicular, colon, stomach, breast, prostate, and small cell and non-small cell lung [3,4]. Besides the great benefits of platinum chemotherapeutics, they also have various side effects such as nephrotoxicity and negative effects on the kidneys [5]. In addition to the toxicities of the drug, long-term use of cisplatin causes cisplatin resistance.

In this study, the electronic and physicochemical properties of cisplatin and its derivatives have been investigated. All calculations were performed with the Density Functional Theory (DFT) method within Gaussian 09W software. DFT calculations were carried out by using the three parameter Becke-Lee-Yang-Parr (B3LYP) exchange-correlation functional with the LanL2DZ basis set. Solvent effects were computed by using Conductor like Polarizable Continuum Model (CPCM) as the solvation model and the solvent was water with a dielectric constant is  $\epsilon=78.355$ . Frontier orbital energies, global and local descriptors, and frequencies were calculated for both vacuum and aqueous media.

**Key Words:** anticancer drug, global descriptors, local descriptors, DFT, CPCM

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## Synthesis and Characterization of Poly(ethylene-alt-maleic-anhydride)-Pregabalin (1:1) Ratio Controlled Drug Delivery System with Catalyst Free Media

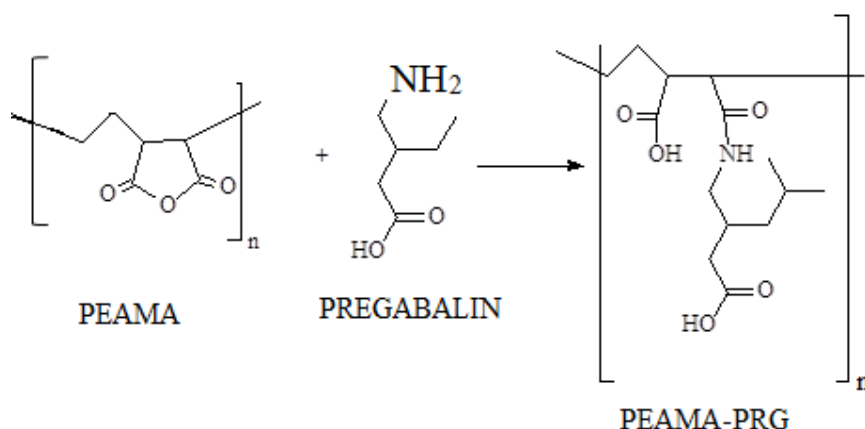
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### Abstract

The main purpose of controlled drug delivery systems is to release the drug to the target tissue or organ. The system leads the release with maximum therapeutic effect by controlling the amount of the drug and the duration of treatment. Maleic anhydride can be used in drug delivery systems via the maleic anhydride-copolymer formula. Amide, ester and carboxylic structures containing amino and hydroxyl groups can be bounded with a covalently bound to maleic anhydride group by ring-opening of the maleic anhydride [1]. Pregabalin is a medication commonly used to treat epilepsy, fibromyalgia, pain, and anxiety. Pregabalin has a half-life of approximately 6 hours. It is observed with an average hour after 1.5 hours and it can be taken frequently. This reason can lead to the development of controlled drug delivery system through conjugating with polymers [2].

In this work, it was aimed pregabalin drug active material bounded covalently with maleic anhydride copolymer to release controlled in order to prevent the drug leaving from polymer matrix. Also, it was aimed increase stability and activity of drug, and reducing frequent drug intake. For this purpose, Poly(ethylene-alt-maleic anhydride) (PEAMA) and Pregabalin (PRG) with (1:1) ratio copolymer-drug delivery system (PEAMA-PRG) was synthesized in catalyst free media and was characterized by <sup>1</sup>H NMR and FTIR/ATR. The stability and activity of PEAMA-PRG (1:1) ratio copolymer-drug delivery system were determined in different pH environments and different artificial body fluids at 37 °C via zeta sizer measurements and UV/VIS, respectively.



Scheme 1 Synthesis of PEAMA-PRG (1:1) Copolymer-Drug Delivery System in Catalyst Free Media

**Key Words:** *Controlled drug delivery system, poly(ethylene-alt-maleic-anhydride), pregabalin, stability and activity*

**Acknowledgement:** This work was supported by the Scientific Research Project Coordination Center of Yıldız Technical University, Turkey (Project No:FYL-2022-4874).

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## CHOOSING A SECOND ADSORBENT TO SAMPLE VOLATILE ORGANIC COMPOUNDS IN BIOMASS GASIFICATION TAR

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### Abstract

Biomass constitutes a noteworthy proportion of renewable energy and accounts for roughly 12% of the primary energy consumption worldwide. When subjected to gasification, biomass yields a mixture of gases including hydrogen, carbon monoxide, carbon dioxide, water, methane, and light hydrocarbons. This gas, referred to as producer gas, also contains some undesirable elements such as dust and tar. Tar, which is a complicated blend of aromatic compounds comprising polycyclic aromatic hydrocarbons, can impede the gasification process by condensing and clogging equipment like fuel lines, filters, engines, and turbines. As a result, much emphasis is placed on minimizing the tar content in the producer gas.

For the purposes of the current investigation, a specialized apparatus was constructed to sample volatile organic compounds. This device consists of a column filled with adsorbents. Specifically, a 1 mL solid phase extraction (SPE) adsorbent cartridge (Alltech) containing 100 mg of loosely packed sorbent was used. Three different sorbents were evaluated in the column, namely: a) Carbopack B (with a surface area of approximately 100 m<sup>2</sup> g<sup>-1</sup> and a particle size of 60/80 mesh, obtained from Supelco); b) Carbotrap (with a particle size of 20/40 mesh, from Supelco); and c) activated coconut charcoal (with a surface area of 1070 m<sup>2</sup> g<sup>-1</sup> and a particle size of 20/40 mesh, obtained from Supelco). To inject the solution under examination, a small piece of glass tubing was attached in front of the adsorbent cartridge. This tubing was heated using insulated heating tape to promote rapid evaporation of the solution.

The research focused on investigating the adsorption efficacy of benzene, toluene, and xylenes on Carbopack B, Carbotrap, and activated coconut charcoal at various temperatures. To accomplish this, fixed amounts of stock solutions were introduced into a heated glass tube located before the adsorbent cartridge. An air pump was used to pull air through the heated tubing and adsorbent cartridge at a flow rate of 100 mL per minute for a duration of one minute, allowing 100 mL of air to pass through the adsorbent. The temperature of the glass tube, into which the stock solution was injected, was increased to 100, 150, and 200°C, with the air temperature passing through the adsorbent cartridge rising correspondingly. Carbopack B and Carbotrap sorbents are not practical for adsorbing volatile organic compounds in synthesis gas at temperatures higher than room temperature. As the temperature of the glass tube used for introducing the stock solution increases, the adsorption of the studied compounds on these sorbents decreases. In addition, a clear relationship is observed between the increase in air temperature, the amount of unabsorbed compounds, and their boiling points. As the temperature rises, compounds with lower boiling points tend to adsorb less effectively than those with higher boiling points. Conversely, the adsorption of the studied compounds on activated coconut charcoal remains consistently high regardless of the temperature.

**Key Words:** biomass; gasification; tar; adsorbent; solid-phase adsorption

## EFFECT OF ANIONIC/NONIONIC EMULGATOR SYSTEMS ON THE PROPERTIES OF WATER BASED STYRENE/ACRYLIC COPOLYMER PAINT BINDERS

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### Abstract

Paint binders are one of the main materials of paint. It ensures that the paint has good adhesion and that the pigment is spread evenly over the entire surface. The surfactants used in the synthesis of paint binders, on the other hand, play a role in the regulation of viscosity by affecting the stable polymerization and particle size, while reducing the surface tension. Each of the surfactant groups classified as cationic, anionic, nonionic and amphoteric has a different effect on polymerization. [1,2]

In this study, it is aimed to investigate the effect of anionic, nonionic and anionic/nonionic surfactants on the reaction during the emulsion copolymerization of styrene and acrylic monomers. For this purpose, the effect of anionic, nonionic and anionic/nonionic surfactant systems at different ratios on the emulsion copolymerization of styrene with butyl acrylate, acrylic acid and acryl amide in the presence of ammonium persulfate initiator to obtain water-based styrene copolymer-based paint binders will be examined and characterized via solid substance analysis, FTIR/ATR, DSC and viscosity. Then, after the results are compared with each other, the optimum anionic/nonionic surfactant system will be created and water-based emulsion paint binders will contribute to the properties such as better bonding of the paint to the surface to be applied and better distribution of the pigment in the system.

**Key Words:** Paint binder; water based styrene/acrylic copolymer; surfactant

**Acknowledgement:** This study was supported by TUBITAK BİDEB 2209-B (1139B412201959)

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## Chemical PVA hydrogels as cleaning device of ancient surfaces

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### Abstract

Poly(vinyl alcohol), PVA, hydrogels can be used as platforms for many biomedical applications due to PVA biocompatibility and chemical versatility. Freeze-thaw process, exploiting the PVA tendency to crystallize, is probably the most known method to obtain PVA-based hydrogels. However, chemical crosslinking of PVA allows for several applications in injectable micro- and nano-devices as well as in monolithic hydrogels. The latter are receiving increasing attention as a tool for the sustainable and “green” cleaning and maintenance of ancient paper artifacts [1,2].

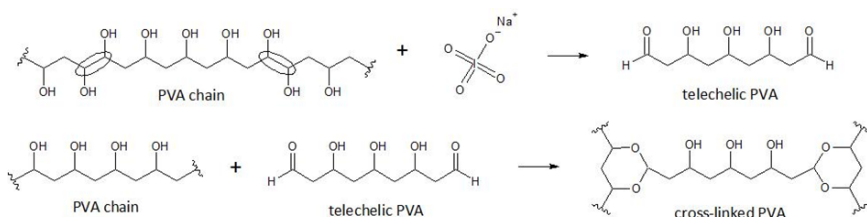
In this contribution we focus on the detailed study of the influence of chemical crosslinking in PVA hydrogels generated by the oxidation of the head-to-head sequences, with the splitting of the PVA backbone into shorter chains having an aldehyde group at each end. The crosslinks are the condensation product of these aldehydes with the hydroxyl moiety of the PVA main chains and the crosslinking degree is controlled by the amount of oxidant deployed, i.e. by the number of split PVA chains.

The elastic modulus,  $G'$ , viscous modulus,  $G''$ , and the polymer volume fraction after swelling,  $\Phi_{2s}$ , were used to assess the number of elastically active crosslinks in the polymer network according to Flory-Renher and Peppas theories [3,4]. From such a study, we could assess a linear correlation between the oxidant amount (%) and the crosslinks of the network.

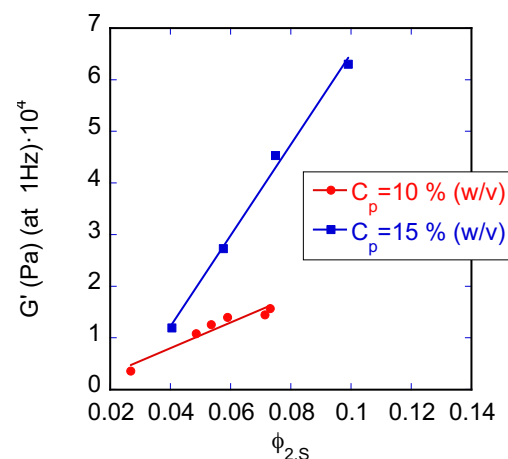
For all crosslinking degree values explored such PVA hydrogels displayed a  $G' > G''$  for strain sweeps ranging from 0.1% to 10%, confirming their gel behavior.

The extent of crystalline domains was assessed by differential scanning calorimetry, DSC, the enthalpy of melting detected on freeze-dried samples was related to the network crosslinking degrees. Addition of water to  $\Phi_{2s} = 0.17$ , caused the complete disappearance of a melting point for all samples, confirming the role of water as plasticizer for PVA. Based on this evidence we can rule out the presence of crystallinity at the maximum swelling reached by our PVA hydrogels, i.e. at  $\Phi_{2s} \ll 0.17$ .

$G'$  and  $G''$  dynamic frequency sweeps revealed, quite unexpectedly, a crossover frequency typical of a self-healing material, dependent from the crosslinking degree, which can explain some of the properties that make these materials perfect candidates for the performing of cleaning treatments on paper or wooden surfaces.



Scheme of the synthesis of PVA chemical hydrogels using telechelic PVA as crosslinker agent



Correlation of the elastic modulus,  $G'$ , with the polymer volume fraction after swelling,  $\Phi_{2s}$

**Key words:** Hydrogels, rheology, polyvinyl alcohol, Cultural heritage conservation, Swelling

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# COMPARATIVE TECHNO-ECONOMIC ANALYSIS OF INDUSTRIAL-SCALE BIOBUTANOL PRODUCTION PROCESSES FOR AN EFFICIENT WASTE MANAGEMENT

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## Abstract

Global warming and increasing greenhouse gas (GHG) emissions are the major concerns in the globalized world. The contributions of fossil fuel usage to these destructive issues are crucial and can not be underestimated. For achieving the net-zero carbon emissions pointed out by the United Nations (UN), the usage of liquid-based biofuels, i.e., biodiesel, bioethanol, and biobutanol, in transportation has significant importance for the environment. Among those biofuels, biobutanol possesses the most similar physical and fuel properties to gasoline, and it can be accepted as a promising candidate for replacement in the future [1]. Moreover, these chemicals also important in the several industry including plastics, polymers, lubricants, brake fluids, and synthetic rubber. Biobutanol can be produced through a biological process called Acetone-Butanol-Ethanol (ABE) fermentation utilizing carbon sources by fermentative Clostridium species. Although ABE fermentation is accepted as an environmentally friendly process, the process is still struggling with challenges for industrial-scale production. Feedstock costs, low fermentation yield, butanol toxicity on the microorganism, and long fermentation duration are some of the challenges that must be overcome [2]. For that purpose, the usage of low-cost lignocellulosic biomass as a feedstock and applying various fermentation processes can be accepted as a promising approach for reducing both capital and operational expenses [3]. In this study, process simulation and techno-economic analysis were applied by using fed-batch and batch fermentation results for biobutanol production from lignocellulosic biomass. The results were evaluated in SuperPro Designer<sup>®</sup> (v11) to find out the effect of production methods on process feasibility and to determine basic economic notions such as cash flows, net present value (NPV), internal rate of return (IRR%), and payback period (PB) [4]. According to simulation results, despite reaching the higher ABE titer in the fermentation broth in the fed-batch process, fermentation duration and additional feedstock costs directly affect (more than 12%) both operational expenses and the profitability of the plant.

**Key Words:** *Biobutanol, Sustainable Environment, Lignocellulosic Biomass, Techno-economic Analysis*

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## STUDY OF THE TOXICITY OF BENZANTHRONE LUMINESCENT DYES

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### Abstract

Many dyes, including luminescent ones, are widely used in our everyday consumption, therefore they are potentially dangerous for the environment, as they can get into sewage and groundwater. In this regard, a sensitive, fast, reliable and inexpensive toxicity assay is needed to assess toxicity to living cells. Current microbial and biochemical assays to evaluate chemical toxicity of various substances include insects, fish, *Daphnia magna*, and tumor cell lines to assess molecular toxicity to eukaryotic cells and tissues. To identify the toxicity of compounds, it is necessary to use various bioassay methods that complement each other in the spectrum of analytes.

For this purpose, we evaluated the toxicological effect of new benzanthrone amino phosphonates using wheat germ (*Triticum aestivum*) as a test organism and found that the studied compounds exhibit toxic effects on wheat seedling growth. The experiments performed, namely the determination of morphology, leakage of electrolytes, the content of malonic aldehyde and pigments, showed that benzanthrone  $\alpha$ -aminophosphonates exhibit a toxic effect on the growth of wheat seedlings to varying degrees, depending on the concentration and substituent on  $\alpha$ -carbon.

We then extended the biotoxicity study to a new test object. As the test organism, yeast *Saccharomyces cerevisiae* was used. Their great advantage is that they can be stored dry for a long time, then when water is added, the yeast revives and is ready to be used in a toxicity test.

The biological toxicity test used, is based on the detection of changes in yeast viability. To distinguish living cells from dead cells, they were examined under a microscope using methylene blue: dead cells were stained blue, while living cells were not stained. The studied dyes in various concentrations were exposed to yeast cells for various durations. After the selected exposure time, the number of live (colorless) and dead (stained) cells was counted and analyzed to assess the toxicity of the studied luminescent dyes.

**Key Words:** Luminescent dyes; Toxicity; Viability; Benzanthrone derivatives; *Saccharomyces cerevisiae*

## ANALYTICAL METHOD FOR THE DETERMINATION OF TAR PRODUCED FROM THE PYROLYSIS OF WASTE TYRES

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### Abstract

The environmental problem of disposing of worn-out tyres is becoming increasingly significant due to population growth, an increase in the number of vehicles, and rapid industrialization. About 1.5 billion used tyres are discarded each year, and they have the potential to cause serious waste and environmental issues when they end up in the waste stream. Approximately 75-80% of these used tyres become waste in the environment. Due to the thermostatic polymer structure of used tyres, they have a service life of 80-100 years in landfills as they don't melt and don't break down into their chemical components. Rubber found in tyres has a high calorific value of 33-34 MJ kg<sup>-1</sup>, making it an excellent raw material for the production of fuel. Researchers have conducted thermal analysis on the separate components of discarded tyres to find ways to improve their efficiency in producing energy. Recovering both energy and materials from these tyres is regarded as an effective method of utilizing the waste tyres.

To conduct practical research, a technology was chosen that involves quickly heating finely-ground oil shale. This is done by using a solid heat carrier, like hot ash, in a rotary drum reactor. A rotary kiln reactor located in Daugavpils, Latvia was used for the pyrolysis experiments. During the investigation of tar sampling from non-condensable gas produced during tyre pyrolysis, researchers discovered that the most effective sampling device contained 500 mg of an amino-phase sorbent and 100 mg of activated coconut charcoal. This device was successful in capturing tar and the volatile organic compounds associated with it. The first column used was a 3 mL ISOLUTE® single fritted reservoir (Biotage), which contained 500 mg of aminopropyl-bonded silica adsorbent (ISOLUTE® NH<sub>2</sub>) with an exchange capacity of 0.6 meq g<sup>-1</sup>, a particle size of 50 µm, and an average pore size of 60 Å. The second column was a 1 mL ISOLUTE® single fritted reservoir (Biotage) containing 100 mg of activated coconut charcoal with a surface area of 1070 m<sup>2</sup> g<sup>-1</sup> and a particle size of 20/40 mesh, 420-840 µm.

The method suggested in this research for measuring the concentration of tar compounds requires less sampling time compared to existing methods. This enables faster monitoring of pyrolysis conditions based on tar analysis results in pyrolytic gas. Moreover, unlike other techniques, the proposed method can measure both heavy tar compounds and light tar compounds like benzene and toluene. There was no significant difference observed in the total amount of tar and its component compounds with the increase in the volume of pyrolytic gas. However, an increase was noted in the quantity of lighter compounds like benzene and toluene that passed through the amino-phase adsorbent and were collected on the activated coconut charcoal as the gas volume increased. As the volume of pyrolytic gas increased, more compounds were detected and identified on the amino-phase adsorbent. It is crucial to consider the concentration of tar in the pyrolytic gas while determining the sampled gas volume and identifying individual tar compounds with low concentrations.

**Key Words:** SPA method; tar; gas chromatography; tyres; pyrolysis

## EVALUATION OF NOVEL DESIGNED DELICIOUS PEPTIDES FOR IMPROVING TASTE SENSATION

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### Abstract

The term "flavor" refers to the sensitivity that mostly consists of volatile components and that allows taste and smell to be sensed simultaneously [1]. To enhance the flavors of meals, a wide variety of additives are utilized in the modern food industry. Peptides are frequently utilized as organic flavors. It is possible to extract the flavoring ingredient from natural sources or to create it artificially. The building blocks of peptides, amino acids, each have a distinctive flavor. These amino acids may be combined to produce various flavors [2].

This work used the microwave-assisted solid phase peptide synthesis (SPPS) technique to synthesized the delicious (umami) peptide, which has the amino acid sequence Lys-Gly-Asp-Glu-Glu-Ser-Leu-Ala and different peptides from umami peptide. Through LCMS, peptides are identified, and by an HPLC apparatus, they are purified. Homology modeling, molecular docking, and molecular dynamics (MD) studies were carried out umami taste receptor T1R1/T1R3 in complex in hopes of understanding at a molecular level the mechanism of action of the delicious taste sensation. Peptides were successfully synthesised and purified. The extracellular Venus flytrap domains (VFTD) of the T1R1/T1R3 receptor appear to have several binding sites that peptides can bind to, according to MD findings. In addition, peptides did not have *in vitro* toxic effect on cells.

**Key Words:** *Delicious peptide, flavor, Molecular docking, Molecular Dynamics, Umami*

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## SYNTHESIS AND CHARACTERIZATION OF COBALT SULFIDE LAYERS

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Composite materials, which are made from a combination of different components, play an important role in modern technology. Polymers with layers of binary d-metals chalcogenides on the surface are also called composites. The study of these composites in recent years has attracted considerable interest due to their new properties, which are a combination of the properties of the original inorganic and polymeric materials. Group II–VIA chalcogenides are direct-gap semiconductors with a sharp optical absorption edge and large absorption coefficients [1]. Therefore, due to their unique physical and electro-optical properties, they can be used in various optoelectronic devices, lasers, light emitting diodes, thin film transistors and photovoltaic cells, including photoconductive and photovoltaic solar cells [2]. One of the representatives of this family is cobalt sulfide, which exists in a number of metal chalcogenide phases (such as  $\text{Co}_9\text{S}_8$ ,  $\text{Co}_3\text{S}_4$ ,  $\text{CoS}_2$ , and  $\text{CoS}$ ) and is complex due to its chemical composition [3]. Depending on the stoichiometric composition of cobalt chalcogenides, these compounds have different physical properties. Therefore, it is very important to obtain the compositions of cobalt sulfide layer having the desired physical properties.

The goal of the present work was to study the formation of the layers of cobalt sulfide ( $\text{Co}_x\text{S}$ ) on polyamide PA 6 films when the solution of dodecathionic acid ( $\text{H}_2\text{S}_{12}\text{O}_6$ ) as precursor of sulfur was used. The  $\text{Co}_x\text{S}$  layers were formed on pieces of PA film  $15 \times 70$  mm in size and  $70 \mu\text{m}$  thick by a technologically simple and inexpensive sorption-diffusion method, carried out in two stages. At the first stage, polymer was treated in solution of dodecathionic acid, then washed with distilled water and dried over  $\text{CaCl}_2$  for 24 h. In the second stage, the sulfurized PA samples were treated with cobalt(II) ammonia complex solution, than rinsed with distilled water and as in the first stage. The total amount of cobalt and sulfur in the cobalt sulfide layers was studied by optical emission spectroscopy on a PerkinElmer Optima 8000 instrument. The phase composition of the obtained layers was investigated using a DRON-6 diffractometer. Surface elemental analysis of the  $\text{Co}_x\text{S}$  layers was performed using a custom-designed Kratos Axis Ultra X-ray photoelectron spectroscopy system.

**Key Words:** *cobalt sulphide layers; polythionic acids; chalcogenide; polyamide.*

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## SYNTHESIS AND CHARACTERIZATION OF TIN SULFIDE NANOPARTICLES

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The novel synthesis of *tin sulfide* films was used for deposition directly from abundant and biodegradable precursors via a simple **SILAR** method.

Increased energy consumption stimulates the development of various types of energy [1]. Energy is an urgent issue for the economic and social development of the world and approximately 65% of the global energy demand is driven by non-renewable fossil fuels [2]. To deal with a reduction in the supply of fossil fuels, it is necessary to use more renewable energy sources [3]. The most feasible and effective method for the storage and conversion of renewable energy is some energy storage devices based on electrochemical technologies, such as the *supercapacitor* (SC). Due to the high-power density and long-life cycle compared to batteries and the better energy density compared to traditional capacitors, SCs are one of the most promising energy storage devices.

Metal *chalcogenides*, as a class of materials, have shown somewhat superior performance. Tin sulfides are almost non-toxic and abundant in nature. They all have energy-related applications because of their strong structure, excellent electrical and optical properties, etc. The main motivation of this paper is the development of thin films based on an inexpensive, safe, and simple process using materials of high abundance. Thin films of tin sulfide were deposited on *FTO* glass slides by applying the SILAR method and using "green" precursors, aqueous solutions, low deposition temperature, and environmental safety reducing agent, namely L-ascorbic acid. The morphology, phase composition, optical properties, and electrochemical calculations of thin films were determined. The application of tin sulfide in supercapacitors was explored. Deposited films were annealed in the range of 200-400 ° C. After the *annealing* films become thicker and are formed of more densely packed particles. Results of the XRD analysis of annealed films show the typically reported structure of herzenbergite. It could be seen that after annealing, all diffraction peaks are enhanced. Raman analysis together with XRD confirms the growth of single-phase SnS. Scanning electron microscopy (SEM) images allowed us to examine the microstructure of the samples. Annealing has a significant effect on grain size and surface roughness, and also improve electrochemical results. The specific capacitance lies between 1.02-39 F/g, with a specific energy from 1.84 to 50.06 Wh/kg. All of the values depend on the quantity of L-ascorbic acid and the annealing temperature.

In this paper, we describe a simple, eco-friendly method for the synthesis of tin sulfide nanoparticles stabilized with L-ascorbic acid. The results obtained showed that SnS thin films after annealing in an inert atmosphere demonstrate the possibility of using them in electrochemical capacitors.

**Key Words:** *tin sulphide; SILAR; supercapacitor; chalcogenides; annealing.*

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## Assessment of oxidative stress by detection of H<sub>2</sub>O<sub>2</sub> in rye samples using a multielectrode electrochemical sensor

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### Abstract

Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is a crucial signalling molecule in plants that regulates various physiological processes such as growth, development, and stress responses. However, excessive production of H<sub>2</sub>O<sub>2</sub> can lead to oxidative stress, a condition in which there is an imbalance between the production of reactive oxygen species (ROS) and antioxidant defense mechanisms. Generally, many abiotic stressors (such as high temperatures, drought, salinity, herbicides and heavy metal exposure) and biotic stressors (such as pathogen infection and herbivory) can lead to an increase in ROS production in plant cells. This can cause damage to cellular components such as proteins, lipids, and DNA, ultimately leading to cell death and plant damage [1]. Plants have evolved various mechanisms to regulate the production of H<sub>2</sub>O<sub>2</sub> and manage oxidative stress, including the activity of enzymes such as catalase, peroxidases, and superoxide dismutase. Understanding the role of H<sub>2</sub>O<sub>2</sub> in plants and the mechanisms underlying oxidative stress can provide insights into developing strategies to improve plant growth, productivity and tolerance to various environmental stressors.

Several methods are available to determine the concentration of H<sub>2</sub>O<sub>2</sub> in plants, including optical interferometry, spectrophotometric, fluorimetric, chemiluminescence and electrochemical methods [2]. Electrochemical methods have several benefits compared to other methods. Electrochemical sensors have high sensitivity and selective, and can detect low concentrations of H<sub>2</sub>O<sub>2</sub>, typically in the nanomolar or micromolar range [3]. This makes them suitable for detecting small changes in H<sub>2</sub>O<sub>2</sub> levels in response to saline stress.

Previously, our laboratory successfully used Co<sub>3</sub>O<sub>4</sub> and CuO nanostructures as coatings for working electrodes to detect H<sub>2</sub>O<sub>2</sub> in real samples with high sensitivity and selectivity to the main interferents [4]. This research aims to develop an electrochemical device that can measure using these materials simultaneously. The working electrodes were coated with Co<sub>3</sub>O<sub>4</sub> and CuO nanostructures using a low-temperature hydrothermal synthesis process optimized for high adhesion level to the wire surface and high sensing performance. The device is then integrated with a readout circuit that can measure and analyze the signals from each electrode simultaneously. To test the performance of the electrochemical device, experiments were conducted using solutions containing various concentrations of H<sub>2</sub>O<sub>2</sub> and interferents. The results demonstrate that the device can accurately detect H<sub>2</sub>O<sub>2</sub> in the presence of interferents with high sensitivity and selectivity. The proposed electrochemical device, with multiple working electrodes modified with Co<sub>3</sub>O<sub>4</sub> and CuO nanostructures, demonstrates high sensitivity and selectivity for detecting H<sub>2</sub>O<sub>2</sub> in real rye samples.

**Key Words:** *electrochemical sensor; hydrogen peroxide; oxidative stress; CuO; Co<sub>3</sub>O<sub>4</sub>.*

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## Convolutional neural network-based evaluation of chemical maps obtained by fast Raman imaging for prediction of tablet dissolution profiles

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### Abstract

In the research work our poster is based on, the capabilities of a state-of-the-art fast Raman imaging apparatus are exploited to gain information about the concentration and particle size of hydroxypropyl methylcellulose (HPMC) in sustained release tablets. The extracted information is utilized to predict the in vitro dissolution profile of the tablets. For the first time, convolutional neural networks (CNNs) are used for the processing of the chemical images of HPMC distribution and to directly predict the dissolution profile based on the image. This new method is compared to wavelet analysis, which gives a quantification of the texture of HPMC distribution, carrying information regarding both concentration and particle size. A total of 112 training and 32 validation tablets were used, when using a CNN to characterize the particle size of HPMC, the dissolution profile of the validation tablets was predicted with an average f2 similarity value of 62.95. Direct prediction based on the image had an f2 value of 54.2, this demonstrates that the CNN is capable of recognizing the patterns in the data on its own. The presented methods can facilitate a better understanding of the manufacturing processes, as detailed as detailed information becomes available with fast measurements.

**Key Words:** *fast Raman imaging; convolutional neural network; dissolution prediction; sustained release tablets; process analytical technology*

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## The impact of structure of selected cationic lipids on physicochemical properties of model mammalian membranes

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### Abstract

In recent years, many studies have focused on the search for new carriers of drugs or genetic material. A relatively new class of compounds used in drug delivery systems is cationic lipids. Cationic lipids are synthetic bioactive molecules of lipid-like structure, which causes that similarly to natural lipids they possess amphiphilic character. Many of them, however, show strong toxicity which hampers their *in vivo* application [1-3]. Therefore novel cationic lipids are still synthesized and investigated. The triesters of phosphatidylcholine (Et-PC) are a particular group of cationic lipids which as derivatives of natural phosphocholines exhibit significantly reduced toxicity [4]. The exact mechanisms of lipofection and drug delivery by cationic lipids are probably a multi-step process and so far there have been not fully elucidated. However, the biological membrane is the first place of action of these bioactive molecules either as a target or as a barrier that protects the interior of the cell.

The aim of the studies was to determine the impact of two derivatives of triesters of phosphatidylcholine (1,2-dipalmitoyl-sn-glycero-3-ethylphosphocholine - EDPPC and 1,2-dioleoyl-sn-glycero-3-ethylphosphocholine - EDOPC) differing in the length and saturation of the acyl chains on the properties of model mammalian membranes. The investigations included the analysis of the influence of selected cationic lipids on the molecular organization of mixed phosphatidylcholine/ sphingomyelin/cholesterol system in which the molar ratio of lipids reflected the proportion of these lipids in the lipid rafts. In studies were used Langmuir monolayer technique in combination with Brewster angle microscopy and liposomal systems with the application of dynamic light scattering (DLS), zeta potential measurements, the experiments concerning the release of calcein entrapped in the liposomes after titration with surfactant solution and steady-state fluorescence anisotropy of DPH.

The obtained results indicated that the structure of hydrophobic part of selected cationic lipids exerts a huge effect on the properties of the investigated mammalian membranes. The incorporation of cationic lipids leads to the weakness of intermolecular interaction in model lipid rafts wherein EDOPC exerts a more unfavorable impact on membrane components than EDPPC. Furthermore, cationic lipids with unsaturated bindings in acyl chains destabilize more model membranes by greater reduction of condensation and ordering degree. Moreover, the changes of structure in hydrophobic part also contribute to the emergence of differences in the fluidity and permeability of model lipid rafts.

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## Effect of alkaline earth ions on the behaviour of alkylbenzene sulfonates

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### Abstract

Sodium dodecylbenzene sulfonate (SDBS) is a widely used anionic surfactant often utilized by different industrial fields but also by households and agriculture. However, usually the commercially available SDBS consist of not purely one component but different homologues of alkyl benzene sulfonates. As the anionic head group can bind to alkaline-earth metal ions, their presence influences the behaviour of these surfactants considerably.

In our work, different properties of solutions with varying surfactant contents were studied in the presence of Ca<sup>2+</sup> ions, along with the examination of the solids precipitating from the solutions, in some cases comparing the results obtained by the addition of Mg<sup>2+</sup> instead of Ca<sup>2+</sup>.

The changes caused by the cations include the critical micelle concentration the micelle sizes and surface tension, which were thoroughly studied. Strikingly, beside the rapidly decreasing surface tension known in the literature earlier, another systematical change was found in the studied systems indicating another micellar equilibrium.

The cation tolerance of the surfactant was also determined, along with the composition of the amorphous, gel-like precipitates.

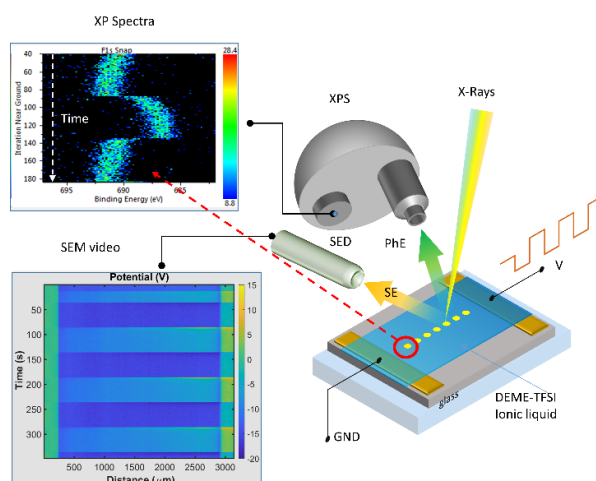
**Key Words:** Alkylbenzene sulfonate; surfactant; alkaline earth ion tolerance; second critical micelle concentration; Ca-DBS;

## XPS, A Chemical Analysis Tool for Exploring Electrical Properties of Liquid/Solid Interfaces

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Electrochemical devices are based on the fundamental process of ion migration and accumulation on surfaces. Complex interplay of molecular properties of ions and device dimensions control the entire process and define the overall dynamics of the system. Particularly, for ionic liquid-based electrolytes it is often not clear which property and to what extent contributes to the overall performance of the device. Herein we use X-ray photoelectron spectroscopy (XPS), while the device is under electrical bias. Such a procedure reveals localized electrical potential developments, through binding energy shifts of the atomic core levels, in a chemically specific fashion. Combining it with Square-Wave AC Modulation, the information can also be extended to time domain, and investigate devices configured as a coplanar capacitor, having an ionic liquid as the electrolyte, in macro-dimensions. Our analysis reveals that nonlinear voltage profile across the device emerge from spatially nonuniform electrical double layer formation on electrode surfaces. Interestingly coplanar capacitor has extremely slow time response which is particularly controlled by IL film thickness. XPS measurements can capture the ion dynamics in tens of seconds to microseconds range, and reveal that ionic motion is all over the device, including those on metallic electrode regions. This behavior can only be attributed to motion in more than one dimension. The ion dynamics can also be faithfully simulated by using a modified PNP equation, taking into account steric effects, and device dimensions. XPS measurements on two devices with different dimensions corroborated with and validated the simulation results. We propose a new experimental approach and provide new insights into the dynamics of ions across electrochemical devices.

M. Basaran, E. Oz, S. Ergoktas, C. Kocabas, B. Ulgut, A. Kocabas, S. Süzer (2022), *Faraday Discussions* **236**, 86.

## Effects of alcohols on sodium dodecylsulphate's solution chemistry properties and dissolution of CaSDS<sub>2</sub> precipitates

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### Abstract

Anionic surfactants are commonly used materials in the chemical and pharmaceutical industries, where their main role is the reduction of the interfacial tension between two immiscible phases (IFT). The presence of divalent cations, especially Ca<sup>2+</sup> and Mg<sup>2+</sup>, in the aqueous phase may cause a decrease in surfactant concentration because of precipitation [1]. The use of alcohols as co-solvents were reported to enhance the solubility of surfactant-metal-ion precipitates [2]. However, the underlying alcohol-water interactions and their effect on solubility are still not completely understood.

In the present study, the interactions between sodium dodecylsulphate (SDS) and alcohols (methanol, ethanol, *n*-propanol and *n*-butanol) were characterised by using spectrophotometry, dynamic light scattering (DLS) and interfacial tension measurements. The concentration of Ca<sup>2+</sup> ions was varied between 3 and 10 g/L at 5 g/L SDS, whereas the amount of alcohols added to solutions varied between 5–20 vol%, depending on the alcohol. (For *n*-butanol, mixtures with > 5.0 vol% were found to be non-miscible.) Our experimental data show that precipitation occurred also in the presence of methanol and ethanol while *n*-propanol and *n*-butanol enhanced the solubility of the CaSDS<sub>2</sub> salt. That is, solutions remained transparent up to a concentration of 10.0 g/L Ca<sup>2+</sup>.

Our results suggest that the increase in solubility is strongly correlated with the chain length and thus the polarity of the alcohol molecule.

**Keywords:** *anionic surfactant, Ca<sup>2+</sup> ion, alcohol, precipitation, UV-Vis spectroscopy*

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### Acknowledgement

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## DNA Binding Studies for Some Small Molecules

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### Abstract

DNA is the pharmacological target for many drugs in clinical use and further clinical trials. Because DNA is the executive molecule of the cell, it directs all life activities such as nutrition, respiration, and reproduction. It also regulates cell functions through DNA transcription (RNA synthesis) and copies itself (replication) during preparations for cell division<sup>1</sup>. When the drug interacts with DNA, it either artificially alters or inhibits the functions of DNA<sup>2</sup>. The drug's process of altering and inhibiting the function of DNA is very important for the control and treatment of the disease. In this study, the interaction mechanism of some small molecules such as newly synthesized ligand molecules, plant extract, and its derivatives, and some drug molecules, with double-stranded DNA was investigated by analytical (spectrophotometric and voltammetric) techniques. In addition, the binding constants (K<sub>b</sub>) of each small molecule showing the ability to bind to DNA were compared with those in the commercial and literature.

**Key Words:** *DNA, binding mechanisms, ligand, plant extract, drug, spectroscopy, voltammetry*

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## EFFECTS OF DRYING METHODS ON THE DRYING KINETICS OF BLANCHED BROWN CRAB MEAT

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### Abstract

The study was conducted to examine various drying methods on the drying kinetics of brown crab meat pre-treated with blanching in a 5% brine solution. The drying methods used in this study included oven drying, infrared (IR) drying, and microwave (MW) drying. The results obtained from these drying methods were analyzed and evaluated through statistical and color analyses. To conduct the study, oven and IR drying were carried out at varying temperatures between 60°C - 80°C, while MW drying was performed at different power settings between 140 W - 350 W. The data collected from these experiments were analyzed to determine the drying rates, effective moisture diffusivities ( $D_{eff}$ ), and activation energies ( $E_a$ ). Mathematical models were used to compare the drying times, and graphical representations were created to present the findings. The outcomes of the study showed that the microwave drying method had the highest  $D_{eff}$  value, which ranged between  $2.83 \times 10^{-9}$  and  $9.76 \times 10^{-9}$  m<sup>2</sup>/s, while the oven drying method had the lowest  $D_{eff}$  value, which ranged between  $1.90 \times 10^{-10}$  and  $2.62 \times 10^{-10}$  m<sup>2</sup>/s. The  $E_a$  values for the oven, IR, and MW methods were calculated as 15.74 kJ/mol, 37.55 kJ/mol, and 72.71 kW/kg, respectively. Furthermore, the highest R<sup>2</sup> value was obtained with Aghbashlo et al. model for the oven and Alibas model for IR and MW. In addition, the color analysis showed that the MW drying method caused the highest total color change ( $\Delta E$ ), followed by IR and oven drying.

**Key Words:** *Activation energy, brown crab, color change, effective moisture diffusivity*

## Zr-based metal organic framework filled membrane syntheses and application for CO<sub>2</sub>/N<sub>2</sub> separation

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### Abstract

Carbon dioxide is a polluting gas in the atmosphere that has a greenhouse effect and directly leads to global warming. There are many natural and artificial sources of carbon dioxide in the world. When carbon dioxide from these sources is not used properly, it is released into the atmosphere and the concentration in the atmosphere increases [1,2]. This change in the atmosphere changes global warming and climatic conditions in the world. Therefore, it is vital to reduce carbon dioxide emissions in the atmosphere. Carbon dioxide released from sources is captured, separated and stored or converted to reduce emissions. In particular, carbon dioxide from the flue gas mixes with nitrogen to a large extent. Adsorption, absorption, pressure scavenging processes and cryogenic processes are used to separate carbon dioxide from nitrogen and other mixtures. Membrane separation is the most efficient method to separate carbon dioxide and nitrogen gas after combustion. In this study, it was aimed to separate carbon dioxide and nitrogen by membrane gas separation method and for this, zirconium-based metal organic cage was synthesized and added to polyvinyl alcohol polymeric matrix and MOF doped nanocomposite membranes were produced. Characterization of the synthesized MOF material was performed. Accordingly, the surface area was obtained over 480 m<sup>2</sup>/g, and its high microstructure was proven according to the XRD results. The image of the membrane with MOF added is given in Figure 1. MOF additive increased gas permeability and especially CO<sub>2</sub> selectivity. As a result, it has been proven that the porous and latticed structure increases the diffusion selectivity, and the membrane can be used as a potential gas separation membrane. In the next step, the effect of MOF additive ratio and pressure conditions on the separation performance will be examined.

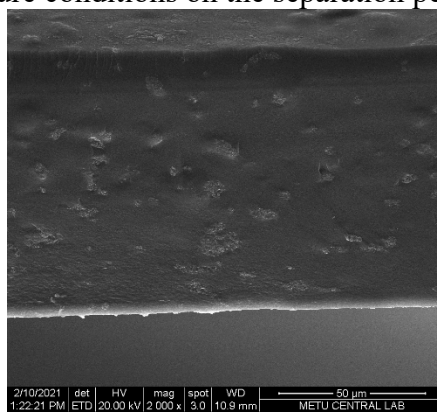


Figure 1. MOF loaded membrane

**Keywords:** Zr-MOF, MIL 140B, nanocomposite membrane, CO<sub>2</sub> separation

**Acknowledgements:** This work has been supported by Çanakkale On Sekiz Mart Universty Scientific Research Projects Coordination Unit (FBA-2022-4068).

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## Photocatalytic Activity of TiO<sub>2</sub>-Cu-Metal-Organic Framework (MOF)

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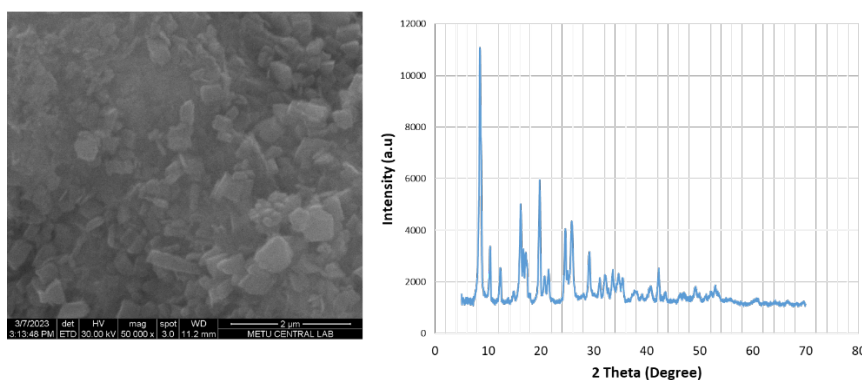
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### Abstract

The accumulation of greenhouse gases and carbon dioxide (CO<sub>2</sub>) in the atmosphere has greatly increased with industrialization. The accumulation of greenhouse gases and carbon dioxide (CO<sub>2</sub>) creates serious problems on our environment such as global warming, melting of glaciers, sea level rise, and extinction of species [1]. One of the solutions developed is CO<sub>2</sub> reduction. CO<sub>2</sub> conversion can be achieved in a sustainable and environmentally safe way with the light-based photocatalytic method [2]. In this study, a titanium dioxide doped copper metal organic framework (Cu-MOF) based photocatalyst was prepared for the photocatalytic reduction of CO<sub>2</sub>. MOFs are effective photocatalysts with their photocatalytic activity, surface modification, structuring with other semiconductors, and doping with metal nanoparticles [3]. The activity of the photocatalyst was determined by means of synthetic dye reduction reaction. In order to improve the photocatalytic activity, Cu-MOF and TiO<sub>2</sub>/Cu-MOF MOF photocatalysts were synthesized and compared. The photocatalyst was characterized using Fourier Transform Infrared Spectroscopy, scanning electron microscopy, and X-Ray diffraction test. According to the SEM and X-Ray results (Fig.1) the Cu-based MOF was successfully synthesized. Both the SEM and XRD results are met with the reported literature results. The MB reaction also showed that the catalyst had photocatalytic activity on use of dye reduction.



Şekil 1. Cu-MOF characterization result

**Keywords:** CO<sub>2</sub> Reduction, Metal-Organic Framework (MOF), Photocatalyst

**Acknowledgements:** This work has been supported by Çanakkale On Sekiz Mart Universty Scientific Research Projects Coordination Unit (Grant number: FYL-2023-4326)

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# PERVAPORATIVE DESALINATION BY PHOSPHOMOLYBDIC ACID/PVA HYBRID MEMBRANE

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## Abstract

Water is a rather important demand for the survival of all living things on earth. Considering that 75% of the world and 65% of the human body form from water, the importance of water is appeared once again. Most water sources are non-potable water sources such as oceans and seas. Potable water resources constitute only 0.3% of the total amount of water. One of the most important problems facing the world is the providing of clean drinking water for human consumption. As the human population and industrialization increase, the demand for water increases. In addition to the demand, increasing population and industrialization also result in the pollution of water resources [1-3].

Desalination applications are usually conduct by heat treatments such as multistage flash distillation and multiprocess distillation and membrane processes such as reverse osmosis and pervaporation [4]. Membrane processes in desalination applications has many advantages such as high separation performance, low energy consumption, easy to integration to industrial systems. Among these membrane processes, pervaporation has an important position [5]. Dense, homogeneous membranes are used in pervaporation and separation is occurred by permeation and evaporation steps. Pervaporation is an important alternative in desalination applications with its energy saving, being resistant to pollution, and high separation performance considering the flux and salt retention rates [6].

In this study, the pervaporation process is chosen for desalination application. Hydrophilic polymer is used for the membrane synthesis in desalination. For that purpose, Polyvinyl alcohol as the polymeric material was chosen. The reason of the chosen the Polyvinyl alcohol as membrane material is high water affinity, ease of film formation and high mechanical and thermal stability. Polymeric membranes are easy to production and relatively inexpensive compared to other types of membranes. However, polymeric membranes show swelling properties and result in high flux and low selectivity. To overcome this problem, new types of organic-inorganic composite membranes called hybrid membranes have been developed in recent years. In this study, phosphomolybdic acid was also chosen as additive material. The effects of phosphomolybdic acid amount, salt concentration and operation temperature on the desalination performance were examined. Optimum operation conditions have been determined and under these conditons, salt rejection of 99.99% and flux value of 2.45 kg/m<sup>2</sup> h were obtained.

**Key Words:** *Desalination; Membrane; Pervaporation; Phosphomolybdic Acid; Water*

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## THE EFFECT OF ULTRASOUND PRETREATMENT ON THE OVEN AND VACUUM OVEN DRYING KINETICS OF BLUEBERRIES

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### Abstract

Blueberries (*Vaccinium corymbosum*) are small, perishable fruits with blue color, which are cultivated mostly in North and South America. They contain a lot of healthy nutrients, polyphenols, organic acids and minerals. Moreover, blueberries are very good antioxidant sources, having the potential to reduce the adverse impacts of some diseases like memory loss and cancer. However, they are seasonal fruits with very short shelf lives. Hence drying can be used as a way of preserving this important fruit. In the literature, although there are numerous articles focusing on the antioxidant capacities and nutritional contents of blueberries, studies investigating their drying kinetics and the effects of various pretreatments on the process are still scarce. Therefore, in this study, the effect of ultrasound pretreatment on the oven drying and vacuum oven drying of blueberries is investigated. During the experiments, the drying temperatures were selected as 60, 70 and 80°C. For both methods, experiments were conducted with 30 s and 60 s prior ultrasound pretreatments and the results were compared with the untreated dried sample data. The kinetic parameters of effective moisture diffusivities ( $D_{eff}$ ) and activation energy ( $E_a$ ) values were calculated. Moreover, the drying curves were modelled with the most known mathematical modelling equations given in the literature. The drying times were seen to decrease by increasing the drying temperature and with the effect of vacuum. However, ultrasound pretreatment was seen to have an adverse effect on the drying duration of blueberries.

**Key Words:** *Blueberry; oven drying; vacuum oven drying; ultrasound; pretreatment*

## POLYSACCAHARIDE BASED FILMS FOR A TRANSDERMAL DRUG DELIVERY SYSTEMS

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### Abstract

Alzheimer's disease is a progressive neurodegenerative condition that predominantly affects the elderly population. While most of the treatment for Alzheimer's disease is administered orally, this treatment method has disadvantages for elderly patient groups with forgetting and swallowing difficulties. Transdermal drug delivery systems provide for the management of various diseases, due to the advantages they offer in comparison with oral dosage forms [1-3].

The aim of this study to investigate the potential of various polysaccharide as a transdermal film to control the release of donepezil hydrochloride, a drug commonly used to treat Alzheimer's disease. Pectin and guar gum were used as polysaccharide based polymer matrix for the transdermal films were prepared by using the solvent casting method. The effect of concentration of polysaccharides and drug, film thickness, and time on drug release was investigated using Franz diffusion cells, which simulate human skin. The drug release kinetics was determined by analyzing samples taken at various time intervals using a UV spectrophotometer. The findings of the study indicated that transdermal films containing pectin and guar gum were able to control the release of donepezil hydrochloride effectively, and they also had suitable mechanical properties for drug release applications. Therefore, the study's results suggest that pectin and guar gum have potential as new materials for developing treatments for Alzheimer's disease and other diseases that require continuous drug release.

**Key Words:** Drug Delivery, Donepezil Hydrochloride, Polysaccharide, Alzheimer

**Acknowledgement :** This study was financially supported by the Research Fund of the Yıldız Technical University with Project No. FBA-2021-4491.

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## 2-(((3-CHLOROPHENYL)IMINO)METHYL)-4-NITROPHENOL: SYNTHESIS, MOLECULAR AND MEDICINAL STUDIES

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### Abstract (Times New Roman, 12pt, Bold)

In this study, an organic compound with Schiff base structure, 2-(((3-chlorophenyl) imino) methyl)-4-nitrophenol (CISB) was synthesized and its structure elucidation was performed by X-ray analysis. The molecular properties were investigated both structurally and electronically. The physicochemical properties and ADME parameters were investigated using a web server to evaluate the medicinal efficacy. The potential targets of the title compound were determined using the LigTMap server based on ligand similarity and binding similarity scores. We found potential targets in these enzyme classes: Hydrolase, kinase, and transferase. Based on these results, the seven most potential targets were selected based on the docking scores obtained ( $\Delta G \geq -7$  kcal mol<sup>-1</sup>). Among all targets, tankyrase 2 was determined to be the most effective target for our compound with docking scores of -9.266 and -8.621 kcal mol<sup>-1</sup>. Gastrointestinal absorption and blood-brain barrier permeability of the title compound were also determined.

**Keywords:** Chlorine compound; Schiff base; FMOs; ADME; Docking

# POLYACRYLIC ACID AND POLYACRYLIC ACID SODIUM SALT AS INHIBITORS OF CALCIUM OXALATE CRYSTAL FORMATION

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## Abstract

In both industrial machinery and the medical field, calcium oxalate (CaOx) crystal formation is a significant issue[1-2]. This formation must be minimized to avoid problems and ensure optimal equipment performance in industries[3-4]. To contribute to the development of preventative measures, this research aimed to examine the inhibitory effects of polyacrylic acid (PAA) and polyacrylic acid sodium salt (PAANa) on CaOx crystal formation. A batch crystallization technique was used to investigate the inhibitory effects of PAA and PAANa on CaOx crystal formation at four different concentrations (0.5, 0.75, 1, and 2 ppm) in aqueous solutions at 37°C. The Langmuir adsorption isotherm was utilized to investigate the adsorption mechanism of the inhibitors. The study found that PAA prevented crystal growth by 50–90%, while PAANa was more effective, reducing it by 95–98%. Additionally, the differential heat of adsorption of  $Q_{diff}$  for the kink Langmuir adsorption isotherm for PAA and PAANa were 41.56 and 49.28 KJ/mol, respectively.

The findings demonstrate the potential use of PAA and PAANa as inhibitors and advance our understanding of the fundamental principles underlying CaOx crystal formation. Therefore, this research contributes to the development of preventative measures to avoid these problems and ensure optimal equipment performance in industries and prevent kidney stone formation in the medical field.

**Key Words:** *Calcium oxalate; Scale formation; Inhibitors; Polyacrylic acid sodium salt; Medical field.*

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