BOOK OF ABSTRACTS

HELSINKI | 2017
ICNTC CONFERENCE
3rd INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

3rd International Conference on New Trends in Chemistry

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ICNTC CONFERENCE

3rd INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

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Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of "***3rd International Conference on New Trends in Chemistry***", to be held at Helsinki dates between 28–30th of April 2017

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

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

The most distinctive feature of ICNTC Conferences from other conference organizations is that the academicians working interdisciplinary can also attend to presentations performed in different speciality fields and they will also have the opportunity to meet with other academicians coming from various parts of the world.

Selected Papers presented as Oral Presentation in conference will be published in Special Issue Edition of Bulgarian Chemical Communications. (ISSN:0324-1130)

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Bulgarian Chemical Communications is indexed by Science Citation Index Expanded (SCI-E).

We kindly wait for your attendance to our congress to be held on April 28-30, 2017, with a hope to realize a satisfactory conference with it's social activities as well as the scientific ones and leaving a trace on your memories.

Respectfully Yours,
On Behalf of the Organization Committee of ICNTC Conference
Assoc. Prof. Dr. Dolunay SAKAR DASDAN

3rd ICNTC 2017 | Conference Chair

Yildiz Technical University – Istanbul / Turkey

Chemistry Department

SCIENTIFIC PROGRAM

27 APRIL 2017-THURSDAY

15:00 – 18:00 : REGISTRATION

28 APRIL 2017-FRIDAY

08:30 - 17:00 : REGISTRATION

MAIN HALL : GRAND OPENING CEREMONY

09:30 – 10:00 : CONCERT / Live Performance by Young Musicians

10:00 – 10:20	**BREAK**

HALL 1

10:20 – 11:20

Welcome Speech : Assoc. Prof. Dr. Dolunay SAKAR DASDAN / Yıldız Technical University

Conference Chair

KEYNOTE SPEAKER : **DR.AGNIESZKA KACZOR**

Title: NOVEL ANTIPSYCHOTICS IDENTIFIED IN STRUCTURE BASED VIRTUAL SCREENING

11:20 –11:40	**COFFEE/TEA BREAK**

HALL 1 / SESSION A

SESSION CHAIR	**DR.AGNIESZKA KACZOR**	
TIME	**TITLE**	**PRESENTER**
11:40 – 12:00	INVESTIGATION THERMAL AND MECHANICAL PROPERTIES OF PP/BEECH FLOUR COMPOSITE	**Çiğdem KADI** Hatice AKGÜL EVLEN Aslı ÖZMERT
12:00 – 12:20	ZETASIZER MEASUREMENTS OF POLYMER-DRUG DELIVERY SYSTEM: POLY (MALEIC ANHYDRITE-CO-VINYL ACETATE) -ACRIFLAVINE CONJUGATE	**Dolunay SAKAR DASDAN** Azize DIZDAR Gulderen KARAKUS
12:20 – 12:40	THE EFFECTS OF ADDITIVES ON PARTICLE SIZE AND MORPHOLOGY ON BASO4 CRYSTALS	**Emel AKYOL** Egemen OYMAN
12:40 – 13:00	REMOVAL OF COPPER BY HYBRID GEL BEADS BASED ON BİOPOLYMERS AND PERLITE	**Ilknur KUCUK** Irem Ulutas

13:00 – 14:00	**LUNCH**

HALL 1 / SESSION B

SESSION CHAIR	**ASSIST.PROF.DR.EMEL AKYOL**	
TIME	**TITLE**	**PRESENTER**
14:00 – 14:20	ADSORPTION-DESORPTION CHARACTERISTICS OF XAD-7 RESIN FOR THE REMOVAL OF 4-NITROPHENOL	Ozge YILDIRIM **Dila KAYA** Nevim SAN
14:20 – 14:40	THE CONTROLLED RELEASE OF BOVINE SERUM ALBUMIN FROM POLYSACCARIDE BASED HYDROGEL BEADS	Selin SARIYER Dilek DURANOGLU **Özlem DOGAN** Ilknur KÜCÜK
14:40 – 15:00	TUNING THE MORPHOLOGICAL PROPERTIES OF HIERARCHICAL POROUS POLYESTER/NANOCLAY COMPOSITES	**E. Hilal Mert**
15:00 – 15:20	THE COOPERATIVE EFFECT ON H_2SO_4...HNO_3...H_2O TERNARY SYSTEMS	**F.Mine BALCI**

15:20 –15:40	**COFFEE/TEA BREAK**

HALL 1 / SESSION C

SESSION CHAIR	**ASSIST.PROF.DR.OZLEM DOGAN**	
TIME	**TITLE**	**PRESENTER**
15:40 – 16:00	SOLID-STATE CHARACTERIZATION OF POLY(ETHYLENE GLYCOL) SAMPLES PREPARED BY SOLVENT CAST TECHNIQUE	**Cemile ÖZDEMİR DİNÇ** Ali GÜNER
16:00 – 16:20	ELECTROPOLYMERIZATION AND CHARACTERIZATION OF SALOPHEN DERIVATIVE SCHIFF BASE CO(II) AND NI(II) COMPLEXES ON THE GRAPHITE ELECTRODE AND ELECTROCATALYTIC INVESTIGATIONS	**Didem ÇAKMAK**
16:20 – 16:40	SYNTHESIS OF SiC FROM POLY(SILYNE-CO-CARBYNE) UNDER CO_2 ATMOSPHERE	**Yusuf NUR** Gizem Emine BAYOL
16:40 – 17:00	METAL COMPLEXES OF PERIMIDINE AND SCHIFF BASE LIGANDS BEARING BOTH NAPHTHALENE AND CHROMONE MOIETIES: SYNTHESIS AND CATALYTIC ACTIVITY	**Neslihan BEYAZİT** Cahit DEMETGÜL

29 APRIL 2017-SATURDAY

09:00 - 17:00 : REGISTRATION

09:15 – 10:00
KEYNOTE SPEAKER **: Prof Dr. Tenhu HEIKKI**

(Head of Chemistry Department, University of Helsinki)

Title: POLYMERIC HYBRID NANOMATERIALS

10:00 –10:10	**BREAK**

HALL 1 / SESSION D

SESSION CHAIR	Prof Dr. TENHU HEIKKI	
TIME	**TITLE**	**PRESENTER**
10:10 – 10:30	RGO/PEDOT NANOCOMPOSITE SYNTHESIS AND SUPERCAPACITOR APPLICATIONS	**Murat ATES** Sinan Caliskan Esin Ozten
10:30 – 10:50	INTERACTION OF PLATINUM BASED COMPLEXES WITH DNA AND DEVELOPMENT OF ELECTROCHEMICAL DNA BIOSENSORS	**İzzet KOÇAK** Ufuk YILDIZ Burak ÇOBAN Abdurrahman ŞENGÜL
10:50 – 11:10	MOLECULAR MODELLING OF 2-IMINOTHIAZOLES AS INSECTICIDAL ACTIVITY	**Asiye MERİÇ**

11:10 –11:30	**COFFEE/TEA BREAK**

HALL 1 / SESSION E

SESSION CHAIR	Dr.AGNIESZKA KACZOR	
TIME	**TITLE**	**PRESENTER**
11:30 –11:50	PREPARATION AND APPLICATION OF TRACK-ETCHED NANOPORE MEMBRANES AND THEIR SENSOR APPLICATIONS	**Dila KAYA** Kaan KECECI
11:50 –12:10	INVESTIGATION OF HYDROXYAPATITE MORPHOLOGY AT DIFFERENT EXPERIMENTAL CONDITIONS	**Özlem DOGAN** Büsra BODUR
12:10 –12:30	GREEN SYNTHESIS OF SOME NOVEL BIOACTIVE BENZIMIDAZOLE DERIVATIVES	**Mustafa Kemal GÜMÜŞ** İnci Selin Doğan Burak Barut Arzu Özel Bahittin Kahveci
12:30 –12:50	SYNTHESIS OF NEW RH(I) AND RU(III) COMPLEXES AND İNVESTIGATION OF THEIR CATALYTIC ACTIVITIES ON OLEFIN HYDROGENATION IN GREEN REACTION MEDIGUENA	**Hakan ÜNVER** Filiz YILMAZ
12:50 –13:10	[MN(CO)$_3$(BPY)(2-CHLOROBENZYLBENZIMIDAZOLE)]OTF COMPLEX AS A NEW PHOTOACTIVATABLE CO-RELEASING MOLECULE	**Elvan ÜSTÜN**

13:10 –14:00	**LUNCH**

HALL 1 / SESSION F

SESSION CHAIR	**Prof.Dr. MURAT ATES**	
TIME	**TITLE**	**PRESENTER**
14:00 – 14:20	INFLUENCE OF PH ON THE BIOFUNCTIONALIZATION LEVEL OF POLY(ACRYLONITRILE-CO-GLYCİDYLMETHACRYLATE) NANOFIBERS	**Zarie, E.S.** Botcha, N. K Homaeigohar, S. Abdelaziz, R. Elbahri, M.
14:20 – 14:40	PRETREATMENTS AND TEMPERATURE EFFECTS ON THE DRYING KINETICS OF PEAS	Ibrahim DOYMAZ **Ilknur KUCUK**
14:40 – 15:00	OUTDOOR AIR QUALITY SULPHUR DIOXIDE IN ISTANBUL	**Esin BOZKURT** Burak DİNÇER
15:00 – 15:20	SYNTHESES, STRUCTURAL CHARACTERIZATIONS OF *CIS*- AND *TRANS*-DISPIROCYCLIC FERROCENYLPHOSPHAZENES	**Yasemin TÜMER** Nuran ASMAFİLİZ Zeynel KILIÇ Tuncer HÖKELEK

15:20 –15:40	**COFFEE/TEA BREAK**

HALL 1 / SESSION G

SESSION CHAIR	**Assoc.Prof.Dr.E. HİLAL MERT**	
TIME	**TITLE**	**PRESENTER**
15:40 -16:00	A FIBROUS SOLID ELECTROLYTE FOR LITHIUM-ION BATTERIES	**Salim EROL**
16:00 – 16:20	RGO/PTH NANOCOMPOSITE SYNTHESIS AND ITS SUPERCAPACITOR PERFORMANCES	**Murat ATES** Sinan Caliskan Esin Ozten
16:20 – 16:40	CONTROLLED RELEASE OF DONEPEZIL HYDROCHLORIDE FROM HYDROGELS HAVING DIFFERENT PROPERTIES	**Emel AKYOL** Şebnem ŞENOL Özlem DOĞAN AYDENİZ

HALL 2 / SESSION H - POSTER

SESSION CHAIR	**Assoc.Prof.Dr.YELDA YALCIN GURKAN**	
TIME	**TITLE**	**PRESENTER**
16:40 – 17:40	A STUDY ON SOME MANGANESE (II) COMPLEXES	**Alaattin Güven** Esra Su İbrahim Kani
	SYNTHESIS AND ANTIMICROBIAL ACTIVITIES OF SOME NEW HYDRAZONES AND SEMICARBAZONES	Aysema SAYIK **Ayse Serguzel YUSUFOGLU**
	LIPASE AND TYROSINASE INHIBITORY ACTIVITIES OF AMARANTHUS LIVIDUS L.	Ozlem SACAN **Ayse CAN** Tugba YILMAZ OZDEN Refiye YANARDAG
	INFLUENCE OF STORAGE TIME AND TEMPERATURE ON THE ACTIVITY OF UREASE	Burcin Alev Sevim Tunalı Refiye Yanardag **Aysen Yarat**
	DEVELOPMENT OF PAPER-BASED COLORIMETRIC UREA STRIP	Burcin Alev Memet Vezir Kahraman **Aysen Yarat**
	OPTIMIZATION OF ULTRASOUND–ASSISTED EXTRACTION OF ANTIOXIDANTS FROM FENUGREEK SEEDS AND COMPARISION WITH CONVENTIONAL METHOD	Merve BAT **Ayşegül PEKSEL** Şule DİNÇ-ZOR Güzin ALPDOĞAN
	INVESTIGATION ON STRUCTURAL, ELASTIC AND THERMODYNAMIC PROPERTIES OF $MGNI_3$ INTERMETALLIC COMPOUND	**Boubeker OTHMANI** Said BOUCETTA
	ANTIBODY IMMOBILIZATION ON TO AMINE FUNCTIONAL MAGNETIC NANOPARTICLES	Makbule Pelin MUHSIR **Basak YUCE-DURSUN** Özkan DANIŞ Serap DEMIR Emrah CAKMAKCI
	IMMOBILIZATION OF LIPASE ONTO PHOTOCROSSLINKED INTERPENETRATING POLYMER NETWORK	**Basak YUCE-DURSUN** Asli Beyler CIGIL Özkan DANIŞ Serap DEMIR Memet Vezir KAHRAMAN
	DETERMINATION and VALIDATION of DIBUCAINE HCl, FLUOCORTOLONE PIVALATE and FLUOCORTOLONE CAPROATE in PHARMACEUTICAL PREPARATION by HPLC	**Bürge Aşçı** Mesut Koç

	SYNTHESIS AND CHARACTERİZATION OF SOME BENZO[A]PHENAZINE-5-ONES DERIVATIVES	**Cigdem SAYIL** Nahide Gulsah DENIZ
	CYCLIZATION REACTIONS OF NAPHTHOQUINONES TO BENZO[A]PHENOXAZIN-5-ONES	**Cigdem SAYIL** Nahide Gulsah DENIZ
	HIERARCHICAL POROUS POLYHIPE/CLAY COMPOSITES	**E. Hilal Mert** Sinan Şen
	DEVELOPMENT OF UPLC-ESI-MS/MS ANALYTICAL METHOD FOR QUINOLONE ANTIBIOTICS ANALYSIS IN HONEY	**Ece KÖK YETİMOĞLU** İsmail Emir AKYILDIZ
	ADSORPTIVE PROPERTIES OF METHACRYLATE BASED POLYHIPE COMPOSITES	**Elif YÜCE** E.Hilal Mert inan Şen Semih Saygi Nevim San
	HIGH MECHANICAL STRENGTH BIODEGRADABLE POLYMER FOAMS VIA COLLOIDAL TEMPLATING	**Fatma Nur PARIN** E. Hilal Mert
	REACTION MECHANISM OF STRONTIUM COBALTITE FORMATION DURING HEATING OF EQUIMOLAR MIXTURE OF STRONTIUM NITRATE AND COBALT NITRATE	**İbrahim YUSUFOGLU** Cemal ASLAN Cem KAHRUMAN
	PREVENTION OF VALPROIC ACID INDUCED GASTRIC DAMAGE BY ALPHA LIPOIC ACID	**Ismet Burcu TURKYILMAZ** Refiye YANARDAG
	RESVERATROL PROTECTS AGAINST IRRADIATION-INDUCED SMALL INTESTINE DAMAGE IN RATS	**Ismet Burcu TURKYILMAZ** Goksel SENER Refiye YANARDAG
	ANTIMICROBIAL ACTIVITIES OF SOME COMPOUNDS ANALOGOUS TO MORANTEL	**Kıymet GÜVEN** Asiye MERİÇ
	UV-CURABLE MICROENCAPSULATED ORGANIC-INORGANIC HYBRID PHASE CHANGE MATERIALS	**Memet Vezir KAHRAMAN** Emre BAŞTÜRK
	A NOVEL MAGNETIC POROUS RESIN FOR REMOVAL OF PHENOL FROM AQUEOUS SOLUTION	**Mustafa GAZI** Jalil HEYDARIPOUR Hayrettin Ozan GULCAN
	EXTRACTION OF COLLAGEN FROM FOOD WASTE AND THE PREPARATION OF POLYHYDROXYALKANOATE COMPOSITES	**Özkan DANIŞ** Mathias Wesamba WAFULA Basak YUCE-DURSUN Serap DEMIR Emrah CAKMAKCI
	IMMOBILIZATION OF PECTINASE VIA CLICK REACTION ON AMBERLITE XAD-4 RESINS	Emrah CAKMAKCI **Özkan DANIŞ** Dincer HOCAOGLU Basak YUCE-DURSUN

		Serap DEMIR
	INHIBITION OF ANTIACETYLCHOLINESTERASE ACTIVITIES OF SOME MEDICINAL PLANTS	**Refiye Yanardag** Nayat Orak
	EFFECTS OF EDARAVONE ON LENS INJURY INDUCED BY VALPROIC ACID	Hatice Alabak Neziha Hacıhasanoglu Çakmak **Refiye Yanardag**
	DEVELOPMENT OF FLUORESCENCE SENSOR FOR THE DETERMINATION OF ORGANOPHOSPHORUS BASED PESTICIDES	**Soner ÇUBUK** Ece KÖK YETİMOĞLU Memet Vezir KAHRAMAN
	THERAPEUTIC ROLE OF A-LIPOIC ACID, VITAMIN E AND SELENIUM COMBINATION IN LIVER OF DIABETIC MICE	Ayse KARATUG-KACAR Onur ERTIK Zeynep Mine COSKUN Sema BOLKENT Refiye YANARDAG **Sehnaz BOLKENT**
	EXAMINATION OF ANTIBACTERIAL AND PHOTODYNAMIC EFFECTS OF SOME PLANT EXTRACTS	**Serap Akyuz** Ozlem Moufti Chousein Ozlem Sacan Refiye Yanardag Sadık Kalaycı Aysen Yarat Fikrettin Sahin
	A GLASSY CARBON ELECTRODE MODIFIED WITH MWCNTS AND CALIX[4]ARENE FOR THE DETECTION OF TRACE CADMIUM (II)	**Semahat KÜÇÜKKOLBAŞI** Aygen DEMIR Serkan SAYIN Mustafa YILMAZ
	FIRST DERIVATIVE UV - SPECTROPHOTOMETRY FOR THE SIMULTANEOUS DETERMINATION OF AMLODIPIN BESILAT AND VALSARTAN IN COMBINED TABLET DOSAGE FORMS	**Semahat KÜÇÜKKOLBAŞI** Hasan UYSAL Zehra Özden ERDOĞAN

17:50 – 20:30	**CITY TOUR**

30 APRIL 2017-SUNDAY

09:00-14:00 : REGISTRATION

HALL 1 / SESSION I

SESSION CHAIR	**Prof.Dr. Onur ATAKISI**	
TIME	TITLE	PRESENTER
09:00 – 09:20	SYNTHESIS AND INVESTIGATION OF ANTIOXIDANT ACTIVITIES OF NOVEL 3-ALKYL(ARYL)-4-[4-METHOXY-3-(4-NITROBENZOXY)-BENZYLIDENAMINO]-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-5-ONES	**Şule BAHÇECİ** Özlem GÜRSOY KOL Murat BEYTUR Nuri YILDIRIM Haydar YÜKSEK
09:20 – 09:40	LIPOPOLYSACCHARIDE TREATMENT CHANGES PLASMA TOTAL OXIDANT AND ANTIOXIDANT CAPACITY ON A TIME DEPENDENT MANNER IN RABBITS	**Emine ATAKIŞI** Onur ATAKISI Canan GULMEZ Kezban YILDIZ DALGINLI
09:40 – 10:00	THEORETICAL STUDIES ON THE MOLECULAR STRUCTURE, CONFORMATIONAL AND VIBRATIONAL ANALYSIS OF 4-(METHOXYCARBONYL) PHENYLBORONIC ACID	**Güventürk UĞURLU** Hacali NECEFOĞLU
10:00 – 10:20	SYNTHESIS AND IN VITRO ANTIOXIDANT PROPERTIES OF NEW 3-ALKYL(ARYL)-4-[3-ETHOXY-4-(BENZENESULFONYLOXY)-BENZYLIDENAMINO]-4,5-DIHYDRO-1*H*-1,2,4-TRIAZOL-5-ONES	**Haydar YÜKSEK** Gül ÖZDEMİR Özlem GÜRSOY-KOL
10:20 – 10:40	THEORETICAL INVESTIGATIONS ON THE LINEAR, NONLINEAR OPTICAL, STRUCTURAL AND ELECTRONIC PROPERTİES OF NICOTINIC ACID AND ITS DERIVATIVES	**Hacali NECEFOĞLU** Güventürk UĞURLU
10:40 – 11:00	GAUSSIAN CALCULATIONS OF NOVEL 3-METHYL/ETHYL/n-PROPYL-4-[3-ETHOXY-4-(4-METHOXYBENZOXY)-BENZYLIDENAMINO)-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-5-ONES	**Hilal MEDETALIBEYOĞLU** Haydar YÜKSEK

11:00 –11:20	**COFFEE/TEA BREAK**

HALL 1 / SESSION J

SESSION CHAIR	**Prof. Dr. HAYDAR YÜKSEK**	
TIME	TITLE	PRESENTER
11:20 – 11:40	ACUTE PHASE PROTEINS and BIOCHEMICAL and OXIDATIVE STRESS PARAMETERS in *HYPODERMA Spp.* INFESTED CATTLE	Oguz MERHAN **Kadir BOZUKLUHAN** Halil Ibrahim GOKCE
11:40 – 12:00	SYNTHESIS, ANTIOXIDANT AND ANTIMICROBIAL PROPERTIES OF NEW MANNICH BASES CONTAINING 1,2,4-TRIAZOLE MOIETY	**Özlem GÜRSOY KOL** Haydar YÜKSEK Sevda MANAP Fevzi AYTEMİZ Muzaffer ALKAN
12:00 – 12:20	IN-VITRO ANTIOXIDANT AND BIOLOGICAL ACTIVITIES OF SOME NEW 1,2,4-TRIAZOLE DERIVATIVES WITH THEIR POTENTIOMETRIC TITRATIONS	**Özlem AKTAŞ YOKUŞ** Haydar YÜKSEK Sevda MANAP Fevzi AYTEMİZ Muzaffer ALKAN
12:20 – 12:40	EFFECTS OF DIETARY ZINC AND L-ARGININE SUPPLEMENTATION ON TOTAL ANTIOXIDANTS CAPACITY, LIPID PEROXIDATION, NITRIC OXIDE, EGG WEIGHT, AND BLOOD BIOCHEMICAL VALUES IN JAPANASE QUAILS	**Onur ATAKİŞİ** Emine ATAKİŞİ Asım KART
12:40 – 13:00	SYNTHESIS, NON-AQUEUS MEDIUM TITRATIONS, ANTIOXIDANT AND ANTIMICROBIAL ACTIVITIES OF SOME NEW 4-[(3-ALKYL(ARYL)-5-OXO-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-4-YL)-IMINOMETHYL]-PHENYL 3-METHOXYBENZOATES	**Murat BEYTUR** Haydar YÜKSEK Muzaffer ALKAN

13:00 14:00	**LUNCH**

HALL 1 / SESSION K - POSTER

SESSION CHAIR	**ASSOC.PROF.DR.DOLUNAY ŞAKAR DAŞDAN**	
TIME	**TITLE**	**PRESENTER**
14:00 – 15:00	VOLTAMMETRIC DETERMINATION OF SOME HEAVY METALS USING A CARBON PASTE ELECTRODE MODIFIED WITH ASPERGILLUS NIGER LOADED ON TiO$_2$ NANOPARTICLES	**Doruk AKDOĞAN** Hüsnü CANKURTARAN Ayşegül PEKSEL Güzin ALPDOĞAN
	AN INVESTIGATION ON THE STABILITY BEHAVIOUR OF POLY (MALEIC ANHYDRITE-CO-METHYL METHACRYLATE) COPOLYMER IN DIFFERENT pHs and MEDIUMS	Yesim KARAHAN Gamze TOSUN **Dolunay SAKAR DASDAN** Gulderen KARAKUS
	SYNTHESIS AND CHARACTERIZATION OF NOVEL HOMO AND HETERODINUCLEAR BALL-TYPE PHTHALOCYANINES*	**Esra KAKI** Ahmet ALTINDAL Bekir SALİH Özer BEKAROĞLU
	ZETASIZER MEASUREMENTS OF POLYMERS	**Gaye GUNGOR** Gamze TOSUN Yesim KARAHAN Dolunay SAKAR DASDAN Gulderen KARAKUS
	INVESTIGATION OF INHIBITION EFFECT OF S-(2-HYDROXETHYL)-4 METHYL-TRIAZOLE COMPOUND TOWARDS STAINLESS STEEL CORROSION IN ETHYLENE GLYCOL-WATER SOLUTION	Burcu TİMUR Mehmet ERBİL **İlyas DEHRİ**
	INHIBITION EFFICIENCY OF POLYACRYLIC ACID ON MILD STEEL CORROSION	Gökmen SIĞIRCIK Ayşen SARI Mehmet ERBİL **İlyas DEHRİ**
	DEVELOPMENT, VALIDATION AND QUANTITATION OF CANDESARTAN in HUMAN PLASMA BY LIQUID CHROMATOGRAPHY AND FLUORESCENCE DETECTION	**Mohammed F. ZAATER**
	THERMAL STABILITY AND ELASTIC PROPERTIES OF MG$_3$CUH$_{0.6}$ TERNARY HYDRIDE	**Said BOUCETTA** Boubakeur OTHMANI
	POLYURETHANE NANOCOMPOSITE MATERIALS CONTAINING PHOSPHORUS	**Sevim KARATAŞ**

	AND FLUORINE AND THEIR COATING APPLICATIONS	Gökhan TOPÇU
	SYNTHESIS AND CHARACTERIZATION OF 3-PHENYLOXYACETİC ACID SUBSTITUTED PHTHALOCYANINES	Betül KOCABIYIK **Ümit SALAN**
	COUMARIN SUBSTITUTED METAL-FREE, ZINC(II), COBALT(II) AND INDIUM(III) PHTHALOCYANINES: ELECTROCHEMICAL AND ELECTROCATALYTIC PROPERTIES	Efe B. Orman Asiye Gök Mustafa Bulut Ali R.Özkaya **Ümit SALAN**
	THE ANALYSIS of REACTION KINETICS of ACETAMIPRID MOLECULE THROUGH DFT CALCULATION METHOD	Bahar EREN **Yelda YALCIN GURKAN**
	DEGRADATION OF BENIDIPINE: EXPERIMENTAL AND THEORETICAL	**Yelda YALCIN GURKAN** Ayca KARASAKAL

Contents

NOVEL ANTIPSYCHOTICS IDENTIFIED IN STRUCTURE-BASED VIRTUAL SCREENING

Agnieszka A. KACZOR[1,2*], Katarzyna M. TARGOWSKA-DUDA[3], Marta KRUK-SŁOMKA[4], Andrea G. SILVA[5], Peter KOLB[6], Antti POSO[2], Grażyna BIAŁA[4], Marian CASTRO[5]

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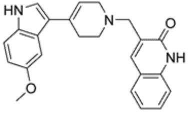
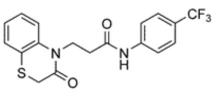
Abstract

Structure-based virtual screening using a D$_2$ receptor homology model was performed to identify D$_2$ receptor ligands as potential antipsychotics [1]. As a result of a screen of a library of 1.6 million compounds, we selected 21 compounds, which were subjected to experimental validation. From 21 compounds tested, we found ten D$_2$ ligands (47.6% success rate, among them D$_2$ receptor antagonists as expected) possessing additional affinity to other receptors tested, in particular to 5-HT$_{2A}$ receptors. The affinity of the compounds ranged from 58 nM to about 24 µM. Similarity and fragmental analysis indicated a significant structural novelty of the identified compounds. We found one D$_2$ receptor antagonist that did not have a protonatable nitrogen atom which is a key structural element of the classical D$_2$ pharmacophore model necessary to interact with the conserved Asp(3.32). This compound exhibited over 20-fold binding selectivity for the D$_2$ receptor compared to the D$_3$ receptor. We provide additional evidence that the amide hydrogen atom of this compound forms a hydrogen bond with Asp(3.32) by testing its derivatives which cannot maintain this interaction. We confirmed antagonistic/partial agonistic/agonistic properties of the compounds towards the receptors in *in vitro* assays and in *in silico* studies as the ligands affect the ionic lock interaction. The four best compounds (D2AAK1-D2AAK4) were subjected to *in vivo* evaluation [2]. All the compounds decreased amphetamine-induced hyperactivity (when compared to the amphetamine-treated group), measured as spontaneous locomotor activity in mice. In addition, a passive avoidance test demonstrated that all the compounds improved memory consolidation after acute treatment in mice. Elevated plus maze tests indicated that all the compounds induced anxiogenic activity 30 minutes after acute treatment. 60 minutes after administration D2AAK1 displayed anxiolytic activity, D2AAK3 lack of activity and the anxiogenic activity of D2AAK2 and D2AAK4 was still observable. In order to optimize the structures of the lead compounds, we designed, synthesized and tested their modifications.



D2AAK1



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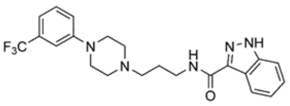
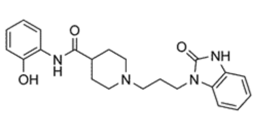


D2AAK3



D2AAK4

Key Words: *behavioural studies, in vitro studies, molecular modelling, organic synthesis*

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POLYMERIC HYBRID NANOMATERIALS

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Rapid development of polymerization techniques has given chemists possibilities to synthesize polymers with complex architectures in a controlled manner. Atom transfer radical polymerization (ATRP) and reversible addition-fragmentation chain transfer polymerization (RAFT) are methods to synthesize block copolymers, star-like polymers etc with narrow molecular mass distributions and predetermined molar masses. These techniques enable also the creation of hybrid materials where organic polymers are bound to inorganic entities.

In this presentation, some recently prepared hybrid nanomaterials will be discussed. Special attention is paid on polymer-protected gold nanoparticles. Other cases include polymeric derivatives of other metals, silica, and montmorillonite.

Key Words: *controlled radical polymerization; hybrid materials; nanoparticles*

DEVELOPMENT, VALIDATION AND QUANTITATION OF CANDESARTAN IN HUMAN PLASMA BY LIQUID CHROMATOGRAPHY AND FLUORESCENCE DETECTION

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Abstract

A simple, fast, selective and stability indicating assay for quantitation of candesartan in presence of naproxen as an internal standard in human plasma is presented and validated. The method involved liquid liquid extraction of the drug from plasma followed by chromatographic separation on a Lichrosphere C-18 column, at room temperature.

The mobile phase consisted from acetonitrile: Methanol (30:70, V/V) buffered to pH 3.5 with 10 mM KH_2PO_4. The mobile phase pumped isocratically at a flow rate of 1.0 mL/min. Fluorescence detection was used for identification and quantitation with wave lengths set at $\lambda_{250/400}$ nm for excitation and emission, respectively. Linearity measurement over a concentration range of 3.0-120.0 ng/mL was verified as indicated by a correlation coefficient of 0.9997. The overall intra- and inter- day accuracies were close to 100% with precisions of 4.6% and 5.2%, respectively. The mean relative recovery of candesartan was (97.87 ± 2.95) %. The method was able to estimate 3.0 ng/mL of the drug within less than five minutes. Stability testing reveled that candesartan and naproxen were stable for short and long periods of storage and handling at room temperature and – 20 c°, as well as after three cycles of freeze and thaw.

Keywords: *Candesartan, Naproxen, Liquid chromatography, Human plasma and Fluorometry.*

ANTIBODY IMMOBILIZATION ON TO AMINE FUNCTIONAL MAGNETIC NANOPARTICLES

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Abstract

Cancer of the prostate is one of the most prevalent medical problems among men [1]. The prostate specific antigen in the serum has been used as a cancer marker for initial diagnosis, surveying treatment and outcome. A number of key limitations with prostate specific antigen, currently the standard detection test, have justified evaluation of new biomarkers [2]. Engrailed-2 is a potential biomarker for several cancers, including prostate cancer. In particular, it has been reported that the expression level of engrailed-2 increases in prostate cancer tissue and that urinary engrailed-2 is more specific and sensitive to prostate cancer than prostate specific antigen [3].

In this study, for the first time water-borne thiol-ene suspension photo polymerization was performed in the presence of magnetic nanoparticles. Neat magnetic nanoparticles were coated and *in situ* functionalized with amine groups by using thiol-ene chemistry. Anti engrailed-2 antibodies were immobilized onto these magnetic nanoparticles by physical adsorption and glutaraldehyde activated covalent bonding methods, respectively. Covalent bonding antibodies (1.775 mg/g) were found to be higher than physically immobilized antibodies (0.54 mg/g). Engrailed-2 concentration was analyzed by enzyme-linked immunosorbent assay. Magnetic nanoparticles were characterized by different techniques. After thiol-ene suspension photo polymerization, the average diameter of the neat magnetite nanoparticles increased from ~15 nm to ~32 nm.

We would like to thank Marmara University, Commission of Scientific Research Project for financial support of the project FEN-C-YLP-100616-0279.

Key Words: *Antibody immobilization; Engrailed-2; Magnetite nanoparticle; Prostate cancer; Thiol-ene.*

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SYNTHESIS AND CHARACTERIZATION OF SOME BENZO[A]PHENAZINE-5-ONES DERIVATIVES

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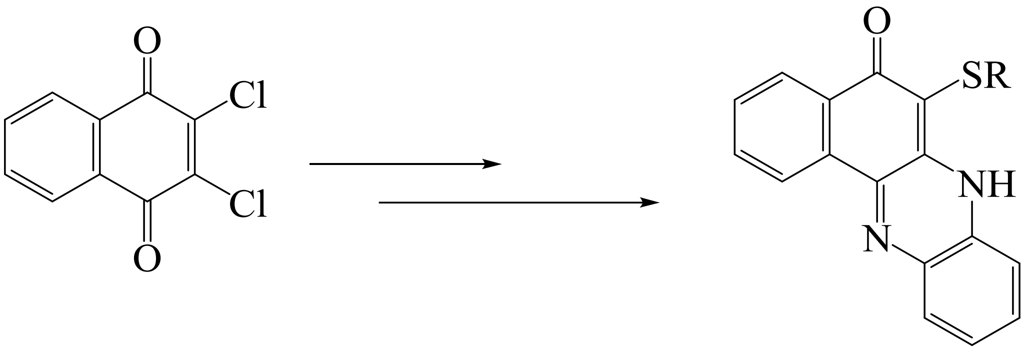
imines are useful for medicine, dyestuffs and others in the wide of industries. Some phenoxazone and phenothiazone derivatives containing stable quinone imine systems have been synthesized to study the biological and pharmaceutical activities, e.g. antitumor activities, and to obtain the useful pigments [1-3].

In this work, we synthesized 6-(alkylthio)benzo[a]phenazine-5(7H)-ones by the condensation of phenyl-1,2-diamine or 2-aminophenol with 2-(alkylthio)-3-chloro-1,4-naphthoquinone compounds.

The conversion of the substituents of the resulting products, the reduction and the dehalogenation were carried out. All new compounds were characterized on the basis of nuclear magnetic resonance spectroscopy (^{1}H- and ^{13}C-NMR), mass spectrometry (MS), and fourier transform infrared spectroscopy (FT-IR).



Key Words: 1,4-Naphthoquinones; Spectroscopy; Benzo[a]phenazines

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SYNTHESIS AND CHARACTERIZATION OF NOVEL HOMO AND HETERODINUCLEAR BALL-TYPE PHTHALOCYANINES*

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Abstract:

These Pcs have four bridged substituents on the periphery of each benzene ring of the two Pc monomers. The chemical and physical properties of these complexes change significantly due to the distance between the two Pc monomers. The ball-type Pcs show different and interesting properties, such as electrical, gas sensing, electrocatalytic and electrochemical, in comparison to their parent monomers [1,2].

In this study, new ball-type homodinuclear Co(II)–Co(II) phthalocyanine and ball-type heterodinuclear Co(II)–Fe(II) phthalocyanine were synthesized from the corresponding [2,10,16,24-tetrakis{4,4’-cyclohexylidenebis(2-cyclohexyphenoxyphthalonitrile)} phthalocyaninatocobalt(II)]. The novel compounds have been characterized by elemental analysis, IR, UV-Vis and MALDI-TOF mass spectroscopy [3].

* This study is supported by a grant (Project No: Science-A-100713-0329) from Marmara University The Commission of Scientific Research Projects.

Key Words: *Synthesis, phthalocyanine, homonuclear, heterodinuclear, characterization*

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INHIBITION EFFICIENCY OF POLYACRYLIC ACID ON MILD STEEL CORROSION

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Abstract

Metallic materials, especially mild steel are extensively used in industrial applications for many purposes from construction material to storage tanks and pipelines. These materials are generally exposed to hydrochloric and sulphuric acid solutions for the purpose of pickling, cleaning and descaling in industries. Most attempts have been investigated to protect metals against corrosion for such industrial procedures. Among them, organic compounds are widely preferred as corrosion inhibitor to get under control corrosion. These compounds have significant potential to form protective layer on metal surface via their adsorptive groups. Furthermore, corrosion inhibitors should have several properties such as low cost, environment friendly and good efficiency in aqueous solution [1-3].

In present study, the inhibition efficiency of polyacrylic acid has been studied for mild steel corrosion in 0.5 M HCl acid media. Electrochemical impedance spectroscopy and potentiodynamic measurements were realized to get information about corrosion, for various inhibitor concentration and temperature conditions. Surface analysis was carried out by scanning electron microscopy method, too. Polyacrylic acid presents good adsorptive capability via -OH groups and high hydrophobicity characteristic on the top of protective film. The obtained results depicted that polyacrylic acid exhibit good inhibition efficiency on mild steel corrosion in 0.5 M HCl acid solution.

Key Words: *Polyacrylic acid, corrosion inhibitor*

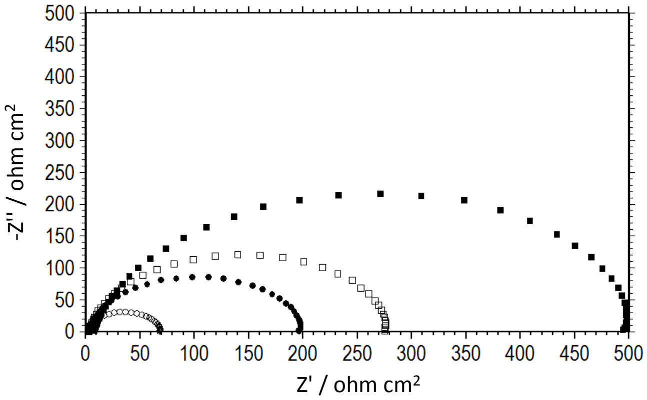

Figure 1. The Nyquist plot of mild steel in 0.5 M HCl solution (○) and containing inhibitor;
% 3 (●), % 5 (□) and % 10 (■).

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PREVENTION OF VALPROIC ACID INDUCED GASTRIC DAMAGE BY ALPHA LIPOIC ACID

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Valproic acid (VPA, 2-propyl valeric acid), is a widely used anti-epileptic drug all around the world. However, its usage brings some important side effects on many organs and systems like liver and gastrointestinal systems by producing free radicals [1,2]. Alpha lipoic acid is a sulphur containing compound which is naturally occurred in all living systems. It is also reported as a potent free radical scavenger which regenerates endogenous and exogenous antioxidants [3,4]. In this study, we aimed to investigate possible protective effects of alpha lipoic acid on valproic acid induced gastric damage. Rats were divided into four groups. Group 1 is control group, Group 2 is rats given alpha lipoic acid (50 mg/kg), Group 3 is rats receiving VPA (0.5 g/kg), Group 4 is rats given VPA and alpha lipoic acid. While VPA was applied by intraperitoneally, alpha lipoic acid was administered by gavage technique for fifteen days. On the 16th day, all the animals were sacrificed under anesthesia. Stomach tissues were taken, homogenized in saline to make 10% (w/v) homogenate and centrifuged. In supernatants, reduced glutathione (GSH), lipid peroxidation (LPO), advanced oxidized protein products (AOPP), nitric oxide (NO) and protein levels were determined. According to the results, GSH levels were found to be decreased while LPO, AOPP and NO levels were increased in VPA group when compared to control group. Administration of alpha lipoic acid reversed these effects in VPA group. We may suggest that alpha lipoic acid prevents gastric tissue against VPA-induced damage.

Key Words: *Valproic acid; Alpha lipoic acid; Gastric damage*

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EXTRACTION OF COLLAGEN FROM FOOD WASTE AND THE PREPARATION OF POLYHYDROXYALKANOATE COMPOSITES

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Abstract

Food waste is a composition of both raw and cooked food materials and annualy a great amount of food has been discarded as commercial and domestic waste. The management of these wastes is an economically and environmentally challenging problem [1]. In accordance with the environmental concerns, utilization of these wastes for development of biodegradable bio-based materials is becoming increasingly important [2]. One important ingredient is collagen which can be obtained from the meat, and poultry industry. However various health concerns such as spongiform encephalopathy, foot and mouth disease, and allergic reactions, restricts the use of collagen from these sources as well as due to religious reasons [3]. Therefore, alternative sources such as fish waste should be considered for overcoming these issues.

In this study, in order to make more effective use of under-utilized resources, we isolated and characterized type-I collagen from fish waste. Nanofibrous mats were obtained by electrospinning a combination of poly(3-hydroxybutyrate) and type-I collagen and their surfaces were characterized by attenuated total reflection Fourier transform infrared spectroscopy, electron spectroscopy for chemical analysis and atomic force microscopy. Biodegradation of poly(3-hydroxybutyrate)/collagen nanofibrous scaffold were investigated. Surface wettability of the nanofiber mats were evaluated by contact angle measurements. The thermal stability and crystallinity of the nanofibrous mats were determined by thermal gravimetric analysis and differential scanning calorimetry, respectively. By taking advantage of the biological properties of both collagen and poly(3-hydroxybutyrate), we are planning to prepare new materials for wound dressing applications.

Key Words: *Collagen; Polyhydroxybutyrate; Composite; Biodegradation; Nanofiber.*

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INHIBITION OF ANTIACETYLCHOLINESTERASE ACTIVITIES OF SOME MEDICINAL PLANTS

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Age-related neurodegenerative diseases such as Alzheimer’s disease and Parkinson’s disease are increasing in prevalence with the rise in long evity of populations world-wide. Alzheimer's disease (AD), the most common form of dementia, is a neurodegenerative disease characterized by progressive cognitive deterioration together with declining activities of daily living and neuropsychiatric symptoms or behavioural changes [1]. The oldest, on which most currently available drug therapies are based, is known as the "cholinergic hypothesis" and suggests that AD begins as a deficiency in the production of the neurotransmitter acetylcholine. Therefore, acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) inhibitors have gained a great popularity for the treatment of AD. In our study, we have examined different plant extracts which are thought to have direct or indirect effects on brain and nervous system on acetylcholinesterase enzyme activity. Plant materials were washed with distilled water and dried at room temperature.The extracts were prepared by using water and ethyl alcohol. Acetylcholinesterase inhibitory activities of the different plant extracts were increasing in a dose dependent manner. As a result all the plants showed acetylcholinesterase inhibitor activity. Among the extracts studies sage leaf, onion and melissa officinalis showed the highest inhibitor activity and it was concluded that they could be useful in the prevention and treatment of Alzheimer’s and other related diseases.

Key Words: *Acetylcholinesterase;inhibition;plant extracts*

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A GLASSY CARBON ELECTRODE MODIFIED WITH MWCNTs AND CALIX[4]ARENE FOR THE DETECTION OF TRACE CADMIUM (II)

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Abstract

In recent years, the heavy metal ion discharge into the environment has been paid attention by scientists because of their high toxic effects for the living organisms even at trace concentrations[1]. Because heavy metal ions are toxic even at trace concentrations, they should be found at limited values in environmental, and biological materials.

Calixarenes constituting of a condensation of phenol and formaldehyde display immerse fundamental role as receptors of large variety of molecular and ionic guest systems and have the fascinating framework. In the past few years, different calixarene derivatives, which were functionalized with cation, anion, organic/bimolecular-binding groups, have shown outstanding vehicle properties for the extraction or recognition of cation, anion and organic/biomolecules [2].

A novel modified carbon paste electrode was constructed and used for rapid, simple, accurate, selective and highly sensitive simultaneous determination of Cd(II) using differential pulse anodic stripping voltammetry (DPASV). The carbon paste electrode was modified multi-walled carbon nanotubes (MWCNTs) and calix[4]arene derivative (Calix-CrA) [3].

For comparison a modified glassy carbon electrode was also prepared and used for rapid, simple, accurate, selective and highly sensitive simultaneous determination of trace metal using differential pulse anodic stripping voltammetry (DPASV). The electrode was modified with calix[4]arene derivative grafted multi-walled carbon nanotubes (CNT-Calix-CrA). Both modified electrodes (Calix-CrA/CPE and Calix-CrA/GC) had an excellent selectivity and stability for Cd(II). Compared with unmodified electrodes, the stripping peak currents had a significant increase at the modified electrodes. Operational parameters such as pH; deposition potential, deposition time, resting time, pulse amplitude were optimized for the determination Cd(II). Under the optimal conditions, the linear range, the detection limit and limit of quantification were calculated and evaluated statistically.

Key Words: Stripping voltametry , MWCNTs , Modified elektrode

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COUMARIN SUBSTITUTED METAL-FREE, ZINC(II), COBALT(II) AND INDIUM(III) PHTHALOCYANINES: ELECTROCHEMICAL AND ELECTROCATALYTIC PROPERTIES

***Efe B. Orman*[a]*, Asiye Gök*[a]*, Mustafa Bulut*[a]*, Ali R.Özkaya**[a]*, Ümit Salan*[a]**

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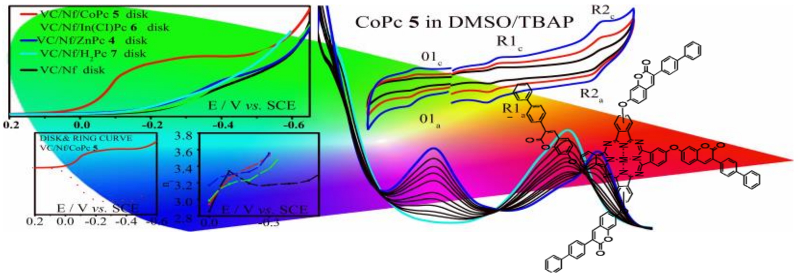
Phthalocyanines (Pcs) are aromatic eight nitrogen atoms containing heterocyclic conjugated macrocycles with 18π-electrons cloud delocalized over an arrangement of alternated carbon and nitrogen atoms. Coumarin derivatives of Pcs remarkably affect photochemical, photophysical, spectral and electrochemical properties of Pcs [**1**].

In this paper peripheral/non-peripheral 7-oxy-3-biphenylcoumarin substituents were introduced in the place of the phenyl group at the third position of the coumarin ring. The redox properties of the newly synthesized compounds were also identified by voltammetric methods. However, it is not possible to completely distinguish the electron transfer processes of the compounds by voltammetry alone [**2**]. Thus, the nature of the redox processes and the effect of substituents position on the formation of aggregated species were examined by voltammetry and in situ spectroelectrochemistry. In addition, the electrocatalytic performances of the complexes have been examined by hydrodynamic rotating disk electrode (RDE) and bipotentiostatic rotating ring-disk electrode (RRDE) voltammetry measurements.



***Key words**: Phthalocyanine, Coumarin, Electrochemistry, Spectroelectrochemistry, and oxygen electrocatalys.*

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DEGRADATION OF BENIDIPINE: EXPERIMENTAL AND THEORETICAL

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Abstract

Benidipine hydrochloride, being the derivate of 1,4-dihydropyridine is a calcium channel blocker antihypertensive drug. In this study, the active ingredient benidipine has been exposed to acidic, basic, neutral and oxidative decomposition in various concentrations and different time periods and its percentage of decomposition was calculated. By developing a spectrophotometric method that is sensitive for benidipine determination in tablet dosage form, quantitative analysis has been made on pharmaceutical tablet comprising active ingredient benidipine. Possible reaction pathways of benidipine have been examined theoretically. Benidipine molecule has been drawn with Gauss View 5 for theoretical analysis and the calculations have been made on Gaussian09 package. The quantum mechanical calculations have been made by using the method of gas phase density functional theory DFT / B3LYP / 631G*. Optimal geometric parameters, thermodynamic and electronic properties.

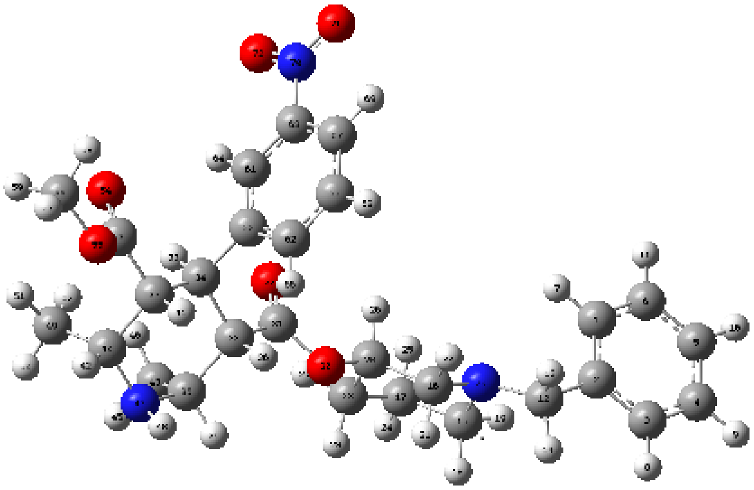

Fig. 1. Optimized structure of benidipine

Key Words: *Benidipine, DFT, molecular modelling*

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DEVELOPMENT OF PAPER-BASED COLORIMETRIC UREA STRIP

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Urea is the end product of protein metabolism. Increased urea level in the body fluids indicates kidney dysfunction. The current urea determination methods require an analytical device and expert [1, 2]. In this work, for the simple, cheap and rapid urea determination, a paper-based colorimetric strip has been developed.

The urea determination was based on enzymatic reaction between urease and urea in the system involving chromogen mix sensitive to pH changes [3]. The chromogen solution was prepared by mixing 4,4'-Bis(4-amino-1-naphthylazo)-2,2'-stilbenesulfonic acid, phenol red, m-cresol purple and thymol blue dyes. The filter paper was coated with chromogen solution and dried at room temperature. Then the paper was wetted with urease solution (500 U/mL) and dried again at room temperature. To prepare color-urea concentration scale,test paper having immobilized urease and chromogen, was reacted with urea solutions at different concentration (10-500 mg/dL). The colors on test paper changed from yellow to purple. Urea concentration and corresponding color were evaluated qualitatively with the naked eye, and quantitatively by using a color analyzer. In addition, the developed paper-based colorimetric urea strip was tested using by biologic samples.

By this way urea concentration can be measured up to 500 mg/dL. It is convenient for individuals, physicians, emergency centres and rural areas without sophisticated facilities.

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Keywords: *Urea determination; paper- based colorimetric sensor ; body fluids*

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IMMOBILIZATION OF LIPASE ONTO PHOTOCROSSLINKED INTERPENETRATING POLYMER NETWORK

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Abstract

Lipases (triacylglycerol ester hydrolases, EC 3.1.1.3) are unusual enzymes that can catalyze the hydrolysis and formation of the ester linkage between glycerol and long-chain fatty acids. They are used in various industries such as dairy, food, textile, pharmaceutical, cosmetic and biotechnology [1]. Enzyme immobilization is one of the essential parts of modern biotechnology. This process allow repeated use and frequently overcome structural instability problems. For this purpose, the native enzyme can be immobilized on different support materials using various techniques and provides long-term use of the biocatalyst [2].

In the present study, we immobilized lipase enzyme from *Candida rugosa* onto a polymeric support material which was obtained by simultaneous photopolymerization of trimethylolpropane triacrylate and hydroxyethyl methacrylate and 1,6-hexandioldiglycidylether where a full interpenetrating polymer network was formed [3,4]. Scanning electron microscopy and Fourier transform infrared spectroscopy performed for the characterization of polymeric support. The immobilized and free enzyme was studied with two different reaction systems, hydrolytic and synthetically: hydrolysis of *p*-nitrophenyl palmitate in aqueous medium and synthesis of *p*-nitrophenyl linoleate in *n*-hexane medium. The optimum pH value for both native and immobilized *Candida rugosa* lipase was 6.5, in the attempt to study the pH effect on the hydrolytic activity. The effect of temperature on the immobilized lipase enzyme was studied for hydrolytic and synthetic activity and found to be 55 and 50°C, respectively. K_m values of the hydrolytic and synthetic activities for the free enzyme are found to be 0.71 and 1.12 mM, respectively, while for the immobilized enzyme, the values are 0.2 mM and 0.1 mM. Storage stability and reusability of immobilized lipase were also studied.

***Key Words:** Candida rugosa, Enzyme immobilization, IPN, Lipase, Photocrosslinked*

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CYCLIZATION REACTIONS OF NAPHTHOQUINONES TO BENZO[A]PHENOXAZIN-5-ONES

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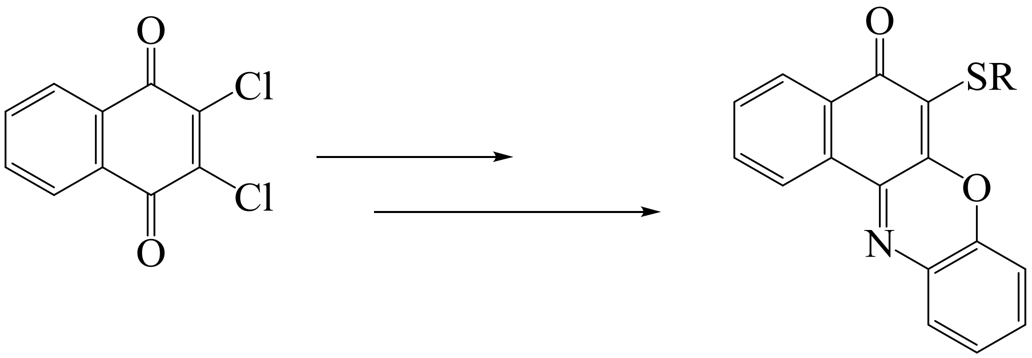
In this work, we synthesized 6-(alkylthio)-5H-benzo[a]phenoxazine-5-ones by the condensation of phenyl-1,2-diamine or 2-aminophenol with 2-(alkylthio)-3-chloro-1,4-naphthoquinone compounds. Their structures were characterizated by micro analysis, FT-IR, ^{1}H-NMR, ^{13}C-NMR, MS spectroscopy.



Key Words: Quinones; Sulfur Compounds; Benzo[a]phenoxazones

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INVESTIGATION OF INHIBITION EFFECT OF S-(2-HYDROXETHYL)-4 METHYL-TRIAZOLE COMPOUND TOWARDS STAINLESS STEEL CORROSION IN ETHYLENE GLYCOL-WATER SOLUTION

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Abstract

Ethylene glycol is widely used as coolant is automotive heat exchanger (namely antifreeze), mixed with water, in a pH range between 7 and 8 due to its great heat absorption capacity. Corrosion is a major problem in the coolant system of an engine block. To deal with this problem, inhibitors have become essential components in most brands of commercial coolants currently [1], the main composition of conventional coolant is 30-70 vol % ethylene glycol, and the added inhibitors normally include molbydate, phosphate, borate, nitrate, tolylthriazole, benzoate and silicate [2]. And in addition of these inhibitors, organic compounds can be used in order to produce the most long-lived antifreeze. Organic compounds containing heteroatoms with electronic lone pair (N, O, S and P) or π system, or conjugated bonds, or aromatic ring, are generally considered to be effective corrosion inhibitors. The inhibition ability of S-(2-hydroxethyl)-4 methyl-triazole towards stainless steel corrosion in ethylene glycol-water solution was studied at various concentration using electrochemical impedance spectroscopy (EIS) and electrochemical polarization curve techniques. According to this measurement inhibition effect of S-(2-hydroxethyl)-4 methyl-triazole has given in vol 50 % etylene glycol-water solution and increased with inhibitor concentration is given.

Key Words: *Ethylene glycol, corrosion inhibition*

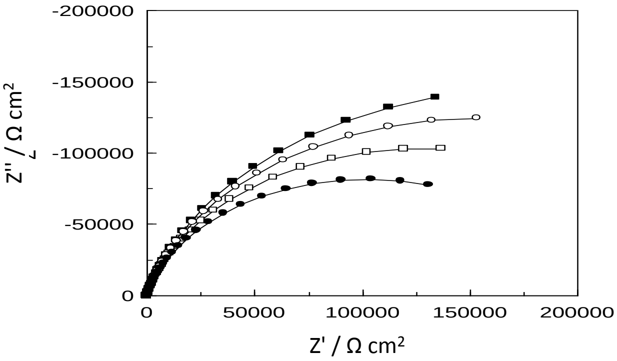

Figure 1. Nyquist plots of stainless steel electrode obtained in ethylene glycol-water solution (●) (inset) and containing 0.01(■), 0.001 (○), 0.001(□) S-(2-hydroxethyl)-4 methyl-triazole (solid line show fitted result).

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RESVERATROL PROTECTS AGAINST IRRADIATION-INDUCED SMALL INTESTINE DAMAGE IN RATS

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Radiotherapy is one of the most important and preferred treatment for malignancies and ionizing radiation can induce cell damage and cell death through the reactive oxygen species generated by radiolytic hydrolysis. It is well known that while radiotherapy mainly affects the area with the neoplastic tissue, various side effects at the adjacent tissues are occurred because of scattered-radiation-caused oxidative stress [1, 2]. Since gastrointestinal side effects are common in patients receiving prostate radiotherapy we aimed to investigate the potential protective effects of resveratrol, a well-known antioxidant and present in many plants, red wine, grapes and peanuts [3] against radiation induced intestinal tissue injury. Sprague-Dawley rats were exposed to a single dose of 20 Gy prostate-confined irradiation and given either vehicle or resveratrol (10 mg/kg, orally) once daily. Rats were decapitated at either one week or ten weeks following irradiation. Small intestine tissues were taken for for the determination of protein, reduced glutathione (GSH), lipid peroxidation (LPO), nitric oxide (NO) levels and myeloperoxidase (MPO) activity. GSH levels were found to be increased in early radiation group and decreased in late radiation group. LPO, NO levels and MPO activities were increased both in early and late radiation group. Administration of resveratrol reversed these effects in these groups. The present data demonstrated that resveratrol, through its free radical scavenging and antioxidant properties, attenuates irradiation-induced oxidative organ injury, suggesting that resveratrol may have a potential benefit in radiotherapy by minimizing the adverse effects and will improve patient care.

Key Words: *Resveratrol, Small Intestine, Radiation*

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IMMOBILIZATION OF PECTINASE VIA CLICK REACTION ON AMBERLITE XAD-4 RESINS

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Abstract

Pectinases catalyze the hydrolysis of α-1,4-glycosidic linkage of polygalacturonic acid [1]. These enzymes are utilized as a part of the fruit juice industry in operations, for example, illumination and the decrease of thickness and turbidity [2]. Despite their superior catalytic properties, free enzymes are faced with high cost, instability and lack of continuous use in industrial operations. Enzyme immobilization is a standout amongst the most famous methodologies to enhance enzyme stability, easy recovery and allow repeated use and also, staying away from protein contamination of the last product [1].

In this work, an acetylene-functionalized pectinase was attached to azide-functionalized amberlite via click reactions. The morphology of the polymeric support was characterized by scanning electron microscopy and Fourier Transform Infrared Spectroscopy. Immobilization enhanced the thermal stability of the pectinase. Kinetic activity, repeated use and storage stability of the free and immobilized enzyme were also studied. Contrasted and native pectinase, the immobilized catalysts were found to display better resistance of varieties in pH and temperature, and additionally enhanced storage stability. The V_{max} and K_m values of immobilized pectinase were found to be nearly equal to native form which indicated that conformational flexibility of pectinase was retained even after immobilization. The residual activity of immobilized pectinase was 75% after nine cycles of reuse.

This work was supported by Marmara University, Commission of Scientific Research Project under grants FEN-C-YLP-131216-0552.

Key Words: *Enzyme immobilization; pectinase; amberlite; click reaction.*

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EFFECTS OF EDARAVONE ON LENS INJURY INDUCED BY VALPROIC ACID

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Valproic acid (VPA, 2-propyl pentanoic acid), a branched short-chain fatty acid, is an antiepileptic drug which is widely used for the treatment of certain types of seizures, migraine, and other disorders as mania in bipolar patients [1,2]. Besides the beneficial effects, it is reported that valproic acid damages many tissue and organs at the end of the long-term theraphy. The enhancement in the free radical production because of VPA is indicated as one of the reason for damages in tissue and organs. Edaravone (3-methyl-1-phenyl-2-pyrazylone-5-one) is a powerful antioxidant which can show its protective effect on many oxidative stress conditions via its free radical scavenging property. The aim of the study was to investigate the protective effects of edaravone against valproic acid-induced lens injury in rats. Male Sprague Dawley rats were used in the study. The rats were randomly distributed into 4 groups. Group I; control rats. Group II; rats receiving intraperitoneally 0.5 g/kg valproic acid, daily for 7 days.Group III; rats receiving 30 mg/kg edaravone for 7 days, intraperitoneally, daily. Group IV; rats receiving 0.5 g/kg valproic acid, 2 h prior to the administration of 30 mg/kg edaravone for 7 days, intraperitoneally, daily. At 16 h after valproic acid and edaravone administration, all the animals were sacrificed under anesthesia and lens tissue samples were taken. Lens tissue samples were homogenized in saline to make 10 % (w/v) homogenate and were centrifuged. The administration of valproic acid caused a decrease in the levels of glutathione content, superoxide dismutase, glutathione peroxidase, glutathione reductase, glutathione-S-transferase activities and an increase in the levels of lipid peroxidation and protein carbonyl content, aldose reductase and sorbitol dehydrogenase activities. Administration of edaravone reversed these effects. According to the results, the protective effect of edaravone may be put forward against valproic acid induced lens injury.

Key Words: *Valproic acid:edaravone:lens*

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FIRST DERIVATIVE UV -SPECTROPHOTOMETRY FOR THE SIMULTANEOUS DETERMINATION OF AMLODIPIN BESILAT AND VALSARTAN IN COMBINED TABLET DOSAGE FORMS

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Abstract

A simple, rapid and reproducible first derivative UV spectrophotometric method was developed for the simultaneous determination of amlodipin besilat and valsartan in combined tablets[1]. Solutions of standart and samples in methanol derivative absorbance (dA/dλ) values were measured at 243,6 and 248,8 nm' for amlodipin besilat and 237,2 and 289 nm's for valsartan, respectively. Calibration graphics plooting and standard addition method were used to determine drug active compoundsat 243,6 nm's for amlodipine besylat and 289 nm's for valsartan. In this method, the calibration curve for amlodipine besylat and valsartan demonstrated linearity in the range 3,0 – 10,0 mg/L and 10,0 – 60 mg/L, respectively. The correlation coefficent were calculated as 0,9997 and 0,9965 for amlodipine besylat, 0,9992 and 0,9979 for valsartan by calibration graphic plooting technique; 0,9973 for amlodipine besylat and 0,9973 for valsartan by standard addition technique. The recovery test was succesfully applied from laboratory-prepared mixtures. The developed method was applied successfully for quality control assay in combined tablets and in vitro dissolution.

Key Words: *Amlodipine besylat, First derivative spectrophotometry, valsartan, drug.*

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SYNTHESIS AND CHARACTERIZATION OF 3-PHENYLOXYACETIC ACID SUBSTITUTED PHTHALOCYANINES

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Abstract

Phthalocyanines are 18 π-electron macrocyclic aromatic compounds consisting of four isoindolin units linked together by nitrogen atoms. The particular two-dimensional π-electron delocalization over these macrocycles gives rise to a great number of unique physical properties. Thus, phthalocyanines are chemically and thermally stable compounds that exhibiting exceptional optical and electrical behavior. For this reasons, they find a wide application in the area of metarials science. Up to now, about 70 different elements have been used as central atoms in phthalocyanines. It is also possible to attach a wide variety of substituents at the periphery of the macrocycle, which can alter the electronic structure of the system.

In this study, 3-phenyloxyacetic acid substituted novel metallo phthalocyanines were synthesized. The ligands and complexes were characterized by elemental and spectroscopic analysis, including ^{1}H–NMR, mass spectra, FT–IR, UV–*Vis* spectral and MALDI–TOF mass data.

Key Words: *metallo phthalocyanines; spectroscopy; metarials science; macrocyclic aromatic compounds; 3-phenyloxyaceticacid substituted phthalocyanines*

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THE ANALYSIS of REACTION KINETICS of ACETAMIPRID MOLECULE THROUGH DFT CALCULATION METHOD

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Abstract

Structural features and selected physicochemical properties of Acetamiprid (neonicotinoid) has been investigated by Density Functional Theory quantum chemical calculations. This study aims to predict degradation mechanism of Acetamiprid molecule in gas phase and solvation phase. The probable reaction pathes of Acetamiprid molecule with OH radical have been analyzed. The optimized geometry was calculated via Gauss View 5. Subsequently, the lowest energy status were found out through geometric optimization via Gaussian 09 programme. With the aim to determine the intermediates occurring at the photocatalytic degradation mechanism of Acetamipirid, geometric optimization of molecule was realized through Density Functional Theory (DFT) method. Activation energy for probable reaction path was calculated, and their most stable state from the thermodynamic perspective for the gas phase and solvation phase. The impact of ethanol, chloroform and toluene solvents were investigated by using COSMO as the solvation model. The predicted mechanism was confirmed by comparison with the experimental results on simple structures reported in the literature.

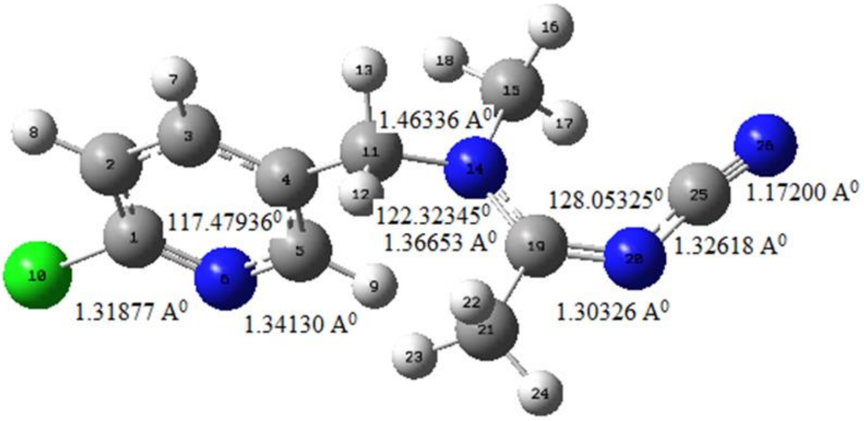

Fig. 1. Optimized structure of acetamiprid

Key Words: *Acetamiprid, DFT, molecular modelling, Gaussian09*

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A STUDY ON SOME MANGANESE (II) COMPLEXES

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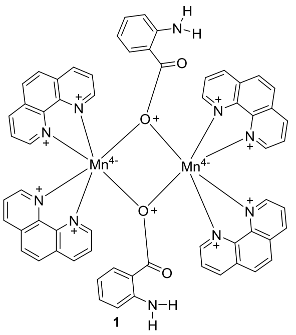
ABSTRACT

Metal based agents are continuously gaining increasing attention as potential drug candidates or as tools in diagnostic applications [1-2]. Combination of unique intrinsic properties of metal ions and complexes, e.g. redox-properties, radioactivity, magnetism or reactivity, with the multiplicity of various organic and bioorganic ligands afforded an inconceivable number of potential molecules.

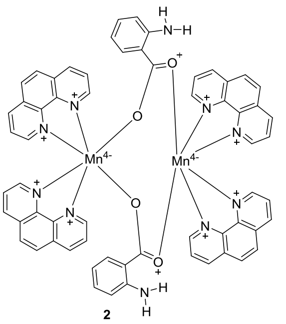
In this study, we examined the structures and infrared and UV-VIS spectroscopic properties of some manganese (II) complexes, which are [Mn2(µO-2-$NH_2C_6H_4COO$)2(bipy)4]·2(ClO_4) (**1**), [Mn2(µOO-2-$NH_2C_6H_4COO$)2(phen)4]·2(ClO_4) (**2**), Mn2(µO-2 $NH_2C_6H_4COO$)2(bipy)4] ·2(ClO_4) (**3**), and [Mn2(µOO-2-$NH_2C_6H_4COO$)2(bipy)4]·2(ClO_4) (**4**) by using experimental and quantum chemical computational methods [3].

Compounds **1** and **4** have been synthesized in methanol at 50°C and characterized by single crystal X-ray diffraction [4-5] technique.



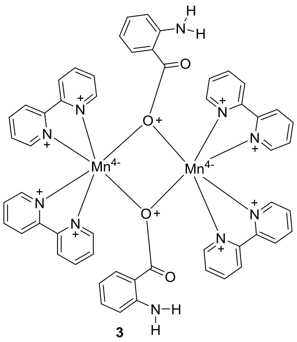
1

[Mn2(μ_O-2-$NH_2C_6H_4COO)_2$(bipy)4]·2(ClO_4)



2

[Mn2(μ_{OO}-2-$NH_2C_6H_4COO)_2$(phen)4]·2(ClO_4)



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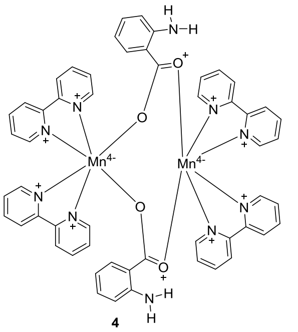
[Mn2(μ_O-2-$NH_2C_6H_4COO)_2$(bipy)4]·2(ClO_4)



4

[Mn2(μ_{OO}-2-$NH_2C_6H_4COO)_2$(bipy)4]·2(ClO_4)

Key Words: Infrared-ultraviolet-Vis spectroscopy; computational chemistry; manganese (II) complexes; X-ray diffraction.

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LIPASE AND TYROSINASE INHIBITORY ACTIVITIES OF *AMARANTHUS LIVIDUS* L.

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Abstract

Amaranthus species are widely distributed throughout the world and they are able to produce grains and leafy vegetables [1]. *Amaranthus lividus* L. is used as a vegetable in Black Sea Region of Turkey. *In vitro* antioxidant potential and *in vivo* hepatoprotective effects of *A. lividus* were studied previously in our laboratory [2,3]. Obesity called the metabolic disease of the century is an increasing public health problem. Obesity is also a major risk factor for important diseases including hypertension, diabetes, degenerative arthritis and myocardial infarction [4]. Between among the multiple studies that have been made for the treatment of obesity, pancreatic lipase inhibition has been investigated for the identification of potential antiobesity agents in plants [5]. Tyrosinase is an enzyme present in plant and animal tissues that catalyzes the production of melanin and other pigments from tyrosine by oxidation. Tyrosinase inhibitors from plant origin have been tested as cosmetics and pharmaceuticals to prevent overproduction of melanin in edipermal layers or as whitening agents [6]. In this study, we have investigated lipase and tyrosinase inhibitory activities of water extract from *A. lividus*. It was found that *A. lividus* exhibits antilipase and antityrosinase activities increasing in a dose dependent manner. According to these results, *A. lividus* may be considered as a potential drug for pharmaceutical and cosmetic industries due to its antilipase and antityrosinase activities.

Key Words: *Amaranthus lividus L., lipase, tyrosinase, inhibitory activity*

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SYNTHESIS AND ANTIMICROBIAL ACTIVITIES OF SOME NEW HYDRAZONES AND SEMICARBAZONES

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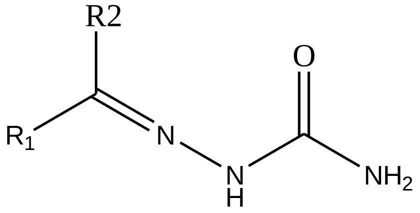
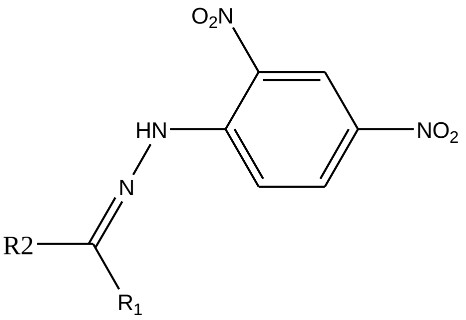
Abstract

Hydrazones and semicarbazones have many applications in derivatization processes and medicine, organic and analytical chemistry. These are also used as plasticizer, stabilizer, antioxidant and polymerization initiators for polymers. In addition to spectrophotometric, fluorimetric, gravimetric and potentiometric applications, hydrazones and semicarbazones are also used as indicator and spot test reactives. [1] According to the literature, these compounds can be widely used in the herbicide and pesticide production to rodent and regulate the growth of plants due to their antibacterial and antifungal properties. They can be widely used in the treatment of various diseases such as tuberculosis, leprosy, mental disorders and malignant tumors. [2] [3] Different structural original ketones were synthesized and hydrazone, semicarbazone dervatives of these ketones were obtained. Hydrazones and semicarbazones were identified by IR, 1H-NMR, 13C-NMR, mass and chromatographic methods. Synthesized compounds were as below.



Semicarbazones



Hydrazones

Escherichia coli ATCC 25922, *Klebsiella pneumoniae* ATCC 4352, *Proteus mirabilis* ATCC 14153, *Pseudomonas aeruginosa* ATCC 27853, *Enterococcus faecalis* ATCC 29212, *Staphylococcus aureus* ATCC 29213, *Staphylococcus epidermidis* ATCC 12228**,** *Candida parapsilosis* ATCC 22019, *Candida tropicalis* ATCC 750, *Candida albicans* ATCC 10231 were used for antimicrobial studies. MIC values were determined. According to the obtained results hydrazones' antimicrobial activities were found higher than semicarbazones' antimicrobial activities.

Key Words: *hydrazone; semicarbazone; antimicrobial activity*

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OPTIMIZATION OF ULTRASOUND–ASSISTED EXTRACTION OF ANTIOXIDANTS FROM FENUGREEK SEEDS AND COMPARISION WITH CONVENTIONAL METHOD

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Abstract

Free radicals can be generated from metabolic pathways within body tissues, and they can also be introduced from external sources such as drugs, food, UV radiation, smoke and environmental pollution. Free radicals have been implicated in the cause of several diseases such as liver cirrhosis, atherosclerosis, cancer, and diabetes and they play an important role in ageing. Oxidative stress can also contribute to the development of neuro-degenerative disorders, such as Alzheimer's and Parkinson's as well as other diseases. Antioxidants are capable of scavenging free radicals and effectively reducing the extent of oxidation. A great number of plant worldwide show a strong antioxidant activity and a powerful scavenger activity against free radicals. This antioxidant capacity can be explored in food industry by using plants as a source of low-cost antioxidants that can replace synthetic additives. Plants constitute an important source of active natural products which differ widely in terms of structure and biological properties. The prevention of cancer, neurodegenerative and cardiovascular diseases has been associated with the ingestion of fresh fruits, vegetables or plants rich in natural antioxidants [1-2].

Fenugreek (*Trigonella foenum graecum*) is an annual plant belongs to the Leguminosae family. The seeds are used to flavor many foods mostly curry powders, teas and spice blend. Seeds of fenugreek spices have also medicinal properties. Fenugreek paste, locally termed as "Cemen"is a popular food in Turkey which is prepared from ground fenugreek seeds [3].

This study aims to improve the extraction of antioxidants from fenugreek seeds by testing different conditions such as solvent, extraction time and pH. The effects of extraction process parameters were evaluated in order to optimise extraction methods. Antioxidant activities of the fenugreek seeds extract were also tested for radical scavenging capacities. Antioxidant activities were compared to standard synthetic antioxidants such as butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT), α-tocopherol and epicatechin.

Key Words: *Fenugreek seed; Antioxidant; Free-radical scavenging; Ultrasound-assisted extraction; Experimental design.*

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INFLUENCE OF STORAGE TIME AND TEMPERATURE ON THE ACTIVITY OF UREASE

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Urease (urea amidohydrolases, EC 3.5.1.5) that is a nickel-dependent metalloenzyme, is synthesized by plants, some bacteria, and fungi. It plays primary role in nitrogen metabolism in nature and catalyses the hydrolysis of urea to carbon dioxide and ammonia [1]. Apart from its natural significance, urease offers potential for many applications [2]. Like all other enzymes, urease is made of protein, that is why it is sensitive molecule and is affected by storage conditions [3]. A small change in enzyme activity during storage may cause a big error in analysis results. The aim of the present study was to evaluate the effects of storage time and temperature on urease activity.

Urease solutions at seven different activities (from 100 to 2000 U/mL) were prepared. They were stored at room temperature, in the refrigerator (4°C), in the deep freezer (-18°C and -80°C), to examine the effects of storage temperature. At 0, 1, 4, 7, 11, 14, 17, 21, 24, 28 days, to determine the effects of storage time, urease activities were measured in all samples by modified Weatherburn method [4].

The relative activities of solutions of 100-1000 U/mL were 75% and below after 4 days for all storage temperatures. Therefore the enzyme activities were continued to measure for 2000 U/mL urease solutions on other days. At the end of 14 day, the relative activities of 2000 U/mL urease solutions, kept at all storage temperatures, were 84% and over. After day 14 till day 28, only at room temperature, the relative activity reduced to 37%, while at other storage temperatures, the relative activities were above 80%.

Since urease enzyme can be maintained at 4°C for almost a month without losing its activity too much, it has practical importance. At the laboratories having no deep freezer, the urease enzyme studies can be done accurately. For short or long term storage, low activities urease solutions (such as 100-1000 U/mL) should be stored at room temperature or at 4°C, should not be stored at -18 or -80°C.

Keywords: *Urease activity; storage time; storage temperature*

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INVESTIGATION ON STRUCTURAL, ELASTIC AND THERMODYNAMIC PROPERTIES OF MGNI$_3$ INTERMETALLIC COMPOUND

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Abstract

In this work, we have used the density functional theory (DFT) plane-wave pseudo potential method, with generalized gradient approximation (GGA) to investigate the structural, elastic, and thermodynamic properties of the intermetallic compound $MgNi_3$. Comparison of the calculated equilibrium lattice constant and experimental data shows very good agreement. The elastic constants were determined from a linear fit of the calculated stress-strain function according to Hooke's law. From the elastic constants, the bulk modulus B, shear modulus G, Young's modulus E, Poisson's ratio σ, anisotropy factor A, and the ratio B/G for $MgNi_3$ compound are obtained. Our calculated elastic constants indicate that the ground state structure of $MgNi_3$ is mechanically stable. The calculation results show that this intermetallic crystal is stiff, elastically anisotropic and ductile material. The Debye temperature is also predicted from elastic constants. The temperature dependence of the enthalpy H, free energy F, entropy S, and heat capacity at constant volume C_v of $MgNi_3$ crystal in a quasi-harmonic approximation have been obtained from phonon density of states and discussed for the first report.

***Key Words**: MgNi$_3$; Elastic properties; Thermodynamic properties; DFT*

DETERMINATION and VALIDATION of DIBUCAINE HCl, FLUOCORTOLONE PIVALATE and FLUOCORTOLONE CAPROATE in PHARMACEUTICAL PREPARATION by HPLC

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Abstract

The present paper presents the development and validation HPLC method for the quantitative determination of dibucaine HCl (DB), fluocortolone pivalate (FP) and fluocortolone caproate(FC) in pharmaceutical preparations. The optimum separation of analytes was achieved with a isocratically mobile phase at a flow rate of 1.3 mL min^{-1}. The mobile phase system consisted of methanol/water/acetic acid (71.6/26.4/2). Analytical method validation was made by the examination of the linearity, repeatability, accuracy, limit of quantification and detection and stabilitiy parameters. The correlation between the peak areas and the concentrations DB, FP and FC was examined for linearity parameter. The correlation coefficients were found 0,999; 0,996; 0,999 respectively. The solutions which were prepared at 3 different concentrations of each substance were analyzed 3 times within the same day and 4 times on different days for the repeatability. The intra-day and inter-day RSD values were less than 2 %. In order to calculate accuracy, analyses were performed by the addition of 3 different concentrations of DB, FP and FC into the examined samples which contain the substances. The proposed method resulted in satisfactory recoveries for all pharmaceuticals, ranging from 97.67 to 105.50. The limit of detection values were calculated as 0,128 ; 0,142 ; 0,203 μg mL^{-1}, and the limit of quantification values were calculated as 0,428;0,477;0,677 μg mL^{-1} for DB, FP and FC respectively. Under refrigerated and room temperature conditions, all componantes in the mobile phase and water were stable for at least 1 month The development method was applied to the determination of DB, FP and FC in pharmaceutical preparations. The recoveries were found as reasonably good in view of the usual limits of 90–110% established by regulatory agencies [1]

Key Words: *HPLC,validation dibucaine HCl fluocortolone pivalat an fluocortolone caproate*

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INVESTIGATION THERMAL AND MECHANICAL PROPERTIES OF PP/BEECH FLOUR COMPOSITE

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ABSTRACT

Composite materials are put into use while their properties are improved by the researchers each passing day due to the advantages they provide and their variety in the application fields.

One such renewable material is wood flour which is one of the most common forms of reinforcement in thermoplastics. Wood plastic composites (WPCs) are preferred in our study due to their advantages such as good resistance, low costs, availability and low wear on the processing equipment.

In this study beech tree flour and polypropylene (PP) composites were produced and this composites thermal and mechanical properties were investigated.

It has been observed that 5 composites which were produced by increasing the beech flour by 5%, have increased in Elasticity module and hardness based on the ratio of the beech flour but on the other hand, its elongation and tensile strength has decreased. PP-20% beech flour mixture is seen to have the highest Elasticity module and hardness. 61% decrease has been observed in tensile strength with the increasing flour ratio. Characterization of PP and PP-beech flour composites has been carried out via thermal analysis and SEM methods.

Key Words: *Polypropylene; Thermoplastic; Wood-Polymer Composites (WPCs); Thermal and mechanical properties.*

AN INVESTIGATION ON THE STABILITY BEHAVIOUR OF POLY (MALEIC ANHYDRITE-CO-METHYL METHACRYLATE) COPOLYMER IN DIFFERENT pHs and MEDIUMS

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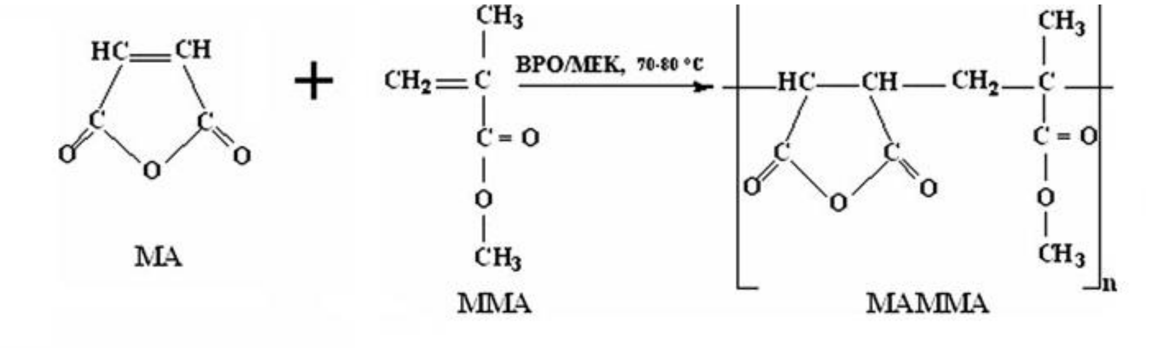
Abstract

Maleic anhydride (MA) copolymers show various biological activities. The action of MA copolymers as mitotic inhibitors, drug delivery system, their functional role in neoplastic processes and in immunology, and their resistance to viruses have been reported [1,2]

In this study, poly (maleic anhydrite-co-methyl methacrylate) copolymer (MAMMA) which can be used as drug delivery system was freshly synthesized by free radical copolymerization of MA and MMA using BPO as the initiator in methyl ethyl ketone according to following reaction:[3]



The stability of MAMMA has been examined by using Zetasizer Measurements which are zeta potential, mobility and particle size. For this purpose, the Zeta Potential Analyzer was used and stability behavior of MAMMA was determined in different pHs and as function of time in dekstrose and PBS solutions.

Key Words: stability, zetasizer, maleic anhydride copolymer, bioactive polymer

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VOLTAMMETRIC DETERMINATION OF SOME HEAVY METALS USING A CARBON PASTE ELECTRODE MODIFIED WITH ASPERGILLUS NIGER LOADED ON TIO2 NANOPARTICLES

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The most frequently used methods for the determination of trace amounts of heavy metal ions are based on atomic absorption/emission spectrometry and chromatography. However, these techniques are relatively expensive and, in most cases, require a complex and rigorous pretreatment of the sample prior to analysis. The low-cost and the highly precise electroanalytical techniques may be alternative to these methods for the determination of heavy metals and suitable for onsite monitoring. Generally, various mercury based electrodes are used for the electrochemical determination of trace amounts of metal ions. However, mercury electrodes do not serve selectivity, and the toxicity and disposal of mercury are important issues. Hence, the application of modified electrodes for the sensitive and selective determination of heavy metal ions has remarkable development [1]. When the chemically modified electrodes are used for this purpose, both the preconcentration and the electrochemical measurement steps can be achieved without the need for an elution procedure. Various chemical modifiers including complex forming ligands, chelating/ion exchanger resins have been introduced into the modified electrodes for heavy metal determination [2, 3]. In recent years, various biomass based adsorbents such as plant tissues, algae, enzymes and microbial moieties have been largely applied for the preconcentration and remediation of heavy metal ions and the other chemicals [4, 5]. However, a few electroanalytical studies have been conducted on biomass modified materials [6, 7].

In this study, a carbon paste electrode modified with Aspergillus Niger loaded on TiO_2 nanoparticles was used to determine the heavy metal ions such as cadmium, lead and copper. The applied anodic stripping method includes successive preconcentration, reduction and square wave anodic stripping steps on the modified electrode. The effect of some parameters such as paste composition, pH, preconcentration time, reduction potential and time, type of supporting electrolyte and potential scan regime of the stripping step were investigated to find the optimal conditions for the trace determination of the studied metal ions.

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HIERARCHICAL POROUS POLYHIPE/CLAY COMPOSITES

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Abstract

In recent years, porous polymer monoliths have been attracting attention on the fields of adsorption, ion exchange, catalysis, and tissue engineering. In this respect, wide variety of materials with miscellaneous properties based on template-assisted processes has been developed by scientists. Among these, emulsion template polymer monoliths have a particular importance as a result of their hierarchical porous structure and low-density [1,2].

Emulsion templating is a simple and effective route for the preparation of macroporous and open-cellular polymers through high internal phase emulsions (HIPEs). HIPEs are usually defined as concentrated emulsions consisting of a high ratio of internal or dispersed phase. The volume fraction (ø) of the internal phase of a HIPE is usually greater than 0.74. In case of, either one or both phases of a HIPE contain monomers, polymerization of the monomer containing phases resulted in polyHIPE polymers which exhibit a well-defined morphology.

In this study, we demonstrate the effect of using a surface modified organoclay in the morphological, mechanical and thermal properties of polystyrene polyHIPEs. With this respect, we used an oil-based intercalant, which is a reactive methacryl derivative of quaternized methyl oleate (QMQ), in order to render the montmorillonite (MMT) organophilic character. Organically and functionally modified OrgMMT clay was added into the continuous phase of the emulsions as a reinforcer in three different loading degrees (1, 2, and 3 wt %). The contribution of presence of OrgMMT used in the polymer matrix on the properties of resulting polyHIPE composites were discussed in terms of morphological, thermal and mechanical properties.

Key Words: *emulsion templating, polyHIPE composite, OrgMMT*

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DEVELOPMENT OF UPLC-ESI-MS/MS ANALYTICAL METHOD FOR QUINOLONE ANTIBIOTICS ANALYSIS IN HONEY

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Abstract

The fluoroquinolones are a family of broad spectrum, systemic antibacterial agents that have been used widely as therapy of respiratory and urinary tract infections. Fluoroquinolones are active against a wide range of aerobic gram-positive and gram-negative organisms. The fluoroquinolones are believed to act by inhibition of type II DNA topoisomerases (gyrases) that are required for synthesis of bacterial mRNAs (transcription) and DNA replication. The fluoroquinolones are indicated for treatment of several bacterial infections, including bacterial bronchitis, pneumonia, sinusitis, urinary tract infections, septicemia and intraabdominal infections, joint and bone infections, soft tissue and skin infections, typhoid fever, bacterial gastroenteritis, urethral and gynecological infections, and pelvic inflammatory disease and several other infectious conditions. The common side effects of the fluoroquinolones are gastrointestinal disturbances, headaches, skin rash and allergic reactions. Less common but more severe side effects include QT prolongation, seizures, hallucinations, tendon rupture, angioedema and photosensitivity.

Quinolones may be directly toxic or be a source of resistant human pathogens, representing a possible risk to human health. The use of antibiotics in food producing animals has generated a considerable interest. The accumulated scientific evidence is that certain uses of antibiotics in food (milk, tissue, honey, egg) producing animals can lead to antibiotic resistance in intestinal bacteria, and this resistance can then be transmitted to the general population, causing treatment-resistant illness. These uses of antibiotics can also create antibiotic resistance in non-pathogenic bacteria. The resistance genes can be transferred to disease causing bacteria, resulting in antibiotic-resistant infections for humans. It is recognized that a major route of transmission of resistant microorganisms from animals to humans is through the food chain.

Developing method will increase the repeatability, sensitivity with minimal and cost efficient sample preparation procedures. Using technique UPLC-ESI-MS/MS, gives faster run times and resolutions according to classical LC-MS/MS methods. Development of multifunctional screening method at honey samples will also contribute very low detection limits and comprehensive compound library for fluoroquinolone residue analysis with additional 14 quinolone derivatives beside typical analytes like ciprofloxacin and enrofloxacin.

This work was supported by Marmara University, Commission of Scientific Research Project (M.Ü. BAPKO) under grant FEN-C-YLP-090217-0061.

Key Words: *Fluoroquinolone, Antibiotics, UPLC-MS/MS, Honey*

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ADSORPTIVE PROPERTIES OF METHACRYLATE BASED POLYHIPE COMPOSITES

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Abstract

Adsorption is an economical and efficient technique used for the removal of pollutants from contaminated water. In this context, porous adsorbents with large surface area and hierarchical porosity are attracting specific interest of the scientists. There are several methods used for preparation of porous polymer composites as adsorbents. However, emulsion templating have been studied extensively as compared to other methods due to the unique morphological properties of resulting materials.

Emulsion templating is basically a method which uses emulsion droplets for the creation of hierarchical porosity. In this context, high internal phase emulsions (HIPEs), which are defined as concentrated emulsions having high volume fraction of internal phase, are often preferred as templates. If the continuous phase or both phases of a HIPE contains monomer(s) polymerization of the monomer containing phase(s) resulted in poly(HIPEs). These are the polymers with well-defined morphology, hierarchical open porous structure, and low density [1,2].

In this study, polyHIPE composites were prepared by the polymerization of HIPE templates consisting of 1,3-butanediol dimethacrylate (1,3-BDDMA) and surface modified montmorillonite (SM-MMT). In order to render the clay organophilic and compatible with the continuous phase, a reactive intercalant – quaternary cocoamine salt having a styryl group – was used for surface modification [3]. The morphological and mechanical properties of the obtained materials were investigated by means of clay loading. Hierarchical porous structure of the resulting polyHIPE composites was confirmed by SEM. On the other hand, the variation of mechanical strength was determined by applying uniaxial compression load. Moreover, exfoliation and intercalation of clays in polymer matrix was confirmed by XRD analyses. In order to demonstrate the adsorptive properties of the obtained composites batch adsorption experiments were performed for methyl violet 2B (MV) as a function of their SM-MMT loading.

Key Words*: polyHIPE composite, reactive intercalant, nanoclay, adsorption, methyl violet 2B*

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HIGH MECHANICAL STRENGTH BIODEGRADABLE POLYMER FOAMS VIA COLLOIDAL TEMPLATING

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Abstract

Biodegradable polymers have been attracting attention of the scientists as scaffolds for tissue engineering applications with diverse cell types. The concept of bone tissue engineering is to produce alternating viable synthetic tissue scaffolds to be used in the treatment of tissue loss caused by traumas and accidents. The most important issue in these applications is to harvest osteogenic cells, seed them on biodegradable foam and allow them to proliferate and differentiate to create a new tissue. At this point, an ideal tissue should exhibit interconnected porous structure as well as biocompatibility. In this respect, colloidal templating is attracting considerable interest in the field of tissue engineering due to the advantage of forming hierarchical porous materials accompanied with high chemical resistance, permeability properties and low density.

In this study, colloidal templating for the preparation of porous polymer composites based on 1,3-diglyceroate diacrylate (GDA), 2-ethylhexyl acrylate (2-EHA), and hydroxyapatite is presented. Diverse morphological, mechanical and thermal properties were obtained by changing hydroxyapatite amount used in the emulsification process. The resulting foams were characterized by scanning electron microscopy (SEM) and their surface areas were measured by applying the Brunauer–Emmet–Teller (BET) equation on N_2 adsorption/desorption isotherms. In order to demonstrate the mechanical strength, resulting composites were tested in terms of uniaxial compression stress. Thermal stability of the obtained foams was investigated by thermal gravimetric analysis (TGA). Moreover, in vitro degradation behavior was followed via the experiments conducted in stimulated body fluid (SBF) and the degradation of the obtained foams was demonstrated by measuring changes in mass and morphology.

Key Words: *biodegradable polymer, colloidal templating, hydroxyapatite, mechanical properties*

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ZETASIZER MEASUREMENTS OF POLYMERS

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Abstract

The presence of the polymers has a significant influence on the colloidal system stability. The adsorption of natural or synthetic polymers at the solid–liquid interface is a very sophisticated process determined by many factors such as macromolecule structure, solution pH, temperature, and surface properties of the adsorbent. As a result, polymer chain presence on the solid surface modifies the stability of aqueous suspensions causing increase of their stabilization (steric, electrosteric stabilization) or a complete destabilization (bridging flocculation, depletion interactions, or charge neutralization) [1, 2]. Stabilization of the dispersed systems is particularly desirable in the production of high-quality paints, cosmetics, and medicines. Surface properties of drug carrier systems are responsible for their interactions with plasma proteins. Zetasizer measurements which are zeta potential, particle size and mobility provide valuable properties of particles or molecules in liquid medium. Zeta potential is a scientific term for electrokinetic potential in colloidal systems, i.e., electric potential in the interfacial double layer at the location of the slipping plane versus a point in the bulk fluid away from the interface [3]

In this work, zetasizer measurements (zeta potential, mobility and particle size) of poly (maleic anhydrite-co-vinyl acetate) copolymer which is an alternative polymer for drug delivery system were determined by using the Zeta Potential Analyzer with different pHs and as function of time in dekstrose and PBS solutions.

Key Words: zeta potential, mobility, particle size, poly (maleic anhydrite-co-vinyl acetate) copolymer

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Reaction Mechanism of Strontium Cobaltite Formation During Heating of Equimolar Mixture of Strontium Nitrate and Cobalt Nitrate*

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Abstract

Strontium cobaltite is a promising material for the fabrication of dense ceramic membranes for oxygen separation, solid electrolytes, solid oxide fuel cells and electrocatalytic reactors for high electronic and oxygen ionic conductivity and high electrochemical activity and high level oxygen diffusivity. Strontium cobaltite has a wide range of oxygen stoichiometry and exists in different crystal structures depending on the valence states of cobalt, temperature, oxygen partial pressure and the method of thermal treatment. The importance of strontium cobaltite has been increasing due to the electrical, magnetic and catalytic properties of crystal structures. Although there are many studies about the investigation of various strontium cobaltites, production of new strontium cobaltites by addition of some additive elements and investigation of electrical, chemical, magnetic and optical properties of these oxides, it could not be seen any studies about the characterization of the intermediate and final products occurred during the production of strontium cobaltite from their nitrate salts at elevated temperatures in the literature [1, 2].

In this study, chemical grade $Sr(NO_3)_2$ and $Co(NO_3)_2•6H_2O$ were used as starting materials to produce strontium cobaltite with equimolar amounts of Sr and Co. Simultaneous Thermogravimetric, Differential Thermal and Mass Spectrometry Analyses (TGA/DTA-MS) were carried out under dry air atmosphere to determine the reaction mechanism of strontium cobaltite production process. The characterization of the intermediate and final products was made by using X-Ray Powder Diffraction (XRD) and Fourier Transform - Infrared Spectroscopy (FT-IR) analytical techniques.

$Co(NO_3)_2 \cdot 6H_2O$ in the initial mixture decomposed to Co_3O_4 gradually from room temperature to 558 K via formation of $Co(NO_3)_2 \cdot 4H_2O$, $Co(NO_3)_2 \cdot 2H_2O$, $Co(NO_3)_2 \cdot H_2O$, $Co(NO_3)_2$, $CoONO_3$ and Co_2O_3 intermediate compounds. $Sr(NO_3)_2$ remained stable and was not decomposed in this temperature range. 1 mole of non-stoichiometric $Sr_6Co_5O_{15-\delta}$ (δ=2.20) is formed with together 1/3 mole of Co_3O_4 during the decomposition of $Sr(NO_3)_2$ between 753 and 902 K. $Sr_6Co_5O_{15-\delta}$ (δ=3.07) and non-stoichiometric $Sr_2Co_2O_{5-\delta}$ (δ=0.70) and $Sr_2Co_2O_{5-\delta}$ (δ=0.89) are formed between the temperature intervals of 902 and 1182, 1182 and 1198 and 1198 and 1465 K, respectively.

*This study is supported by a grant (Project Number: 50961) from Istanbul University Scientific Research Projects

Key Words: *Strontium cobaltite; thermal decomposition; characterization*

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ANTIMICROBIAL POTENTIAL OF SOME COMPOUNDS ANOLOGOUS TO MORANTEL

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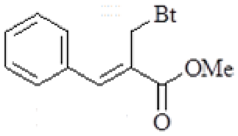
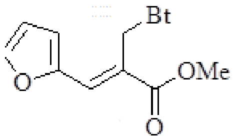
Abstract

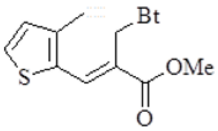
Endoparasitary and antiprotozoal drugs, *i.e.* carrying both heterocyclics such as quinazole, imidazothiazole, benzimidazole, imidazole, thiazole, thiophene, pyrimidine, pyridine, pyrazole or furan and functionalities such as amide (-CO-NH-) or urea (-NH-CO-NH-) residues are synthesized as novel compounds which contain different heterocyclics like benzotriazole [1-5]. In this study, some compounds (6a, 6b, 6c and 6d) which contain Bt-CH=C- (ethen)(vinyl) similar to Morantel were screened for their antimicrobial activity.



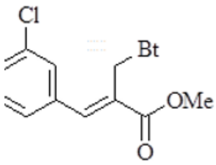
6a



6b



6c



6d

Antimicrobial activities of compounds were tested using the microbroth dilution method (Koneman *et al*., 1997) by using *Staphylococcus aureus* NRRL B-767, *Ps. aeroginosa* ATCC 27853, *Klebsiella pneumoniae*, *E.coli* ATCC 25922, *E. faecalis*, *P. vulgaris*, *C. albicans* ATCC 10231 and *C. Globrata*. MICs were recorded as the minimum concentration of a compound that inhibits the growth of tested microorganisms. All of the compounds tested were illustrated significant antibacterial and antifungal activity when compared with reference drugs.

Key Words: Antimicrobial activity, Morantel, microbroth dilution

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UV-CURABLE MICROENCAPSULATED ORGANIC-INORGANIC HYBRID PHASE CHANGE MATERIALS

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Abstract

Phase change materials (PCMs) are materials that undergo the solid-liquid and solid-solid phase transformation, more commonly known as the melting-solidification cycle, at a temperature within the operating range of a selected thermal application. PCMs are designed to store latent heat and also regulate temperature since they can absorb and dispense thermal energy during phase transition process. There are many different types of PCMs available, but the vast majority fall into three main classifications: organics, inorganic and liquid metals. The organic PCMs have a leakage problem. However, this leakage problem can be eliminated by modifying the PCMs. For this purpose, microencapsulation is used for the best solution. The various advantages of microencapsulated PCMs are avoiding leakage of organic materials during a melting process, reduction of volume changes during phase transition, growing heat-transfer area and decreasing reactivity with the outside environment [1].

In this study, UV-curable microencapsulated organic-inorganic hybrid phase change materials (micro-PCMs) were prepared; the micro-PCMs, which are based on a fatty alcohol core and a methacrylated polyacrylic acid (m-PAA) shell, were prepared by the sol–gel and UV-curing techniques. The differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) result showed that the micro-PCMs have the best phase change and thermal stability properties between 20°C and 70°C working temperature range. The melting latent heat enthalpy was measured between 100 and 140 J/g, and the freezing latent heat enthalpy is found between 90 and 130 J/g. The decomposition temperatures of the organic-inorganic hybrid micro-PCMs increase by increasing the sol-gel content in the sample formulation. The obtained results indicated that these organic-inorganic hybrid micro-PCMs promise a great potential for the thermal energy storage application.

This work was supported by Marmara University, Scientific Research Commission (BAPKO no. FEN-A-110316-0096).

Key Words: Microencapsulation, sol-gel, phase change material, uv curing, polyacrylic acid.

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DEVELOPMENT, VALIDATION AND QUANTITATION OF CANDESARTAN IN HUMAN PLASMA BY LIQUID CHROMATOGRAPHY AND FLUORESCENCE DETECTION

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Abstract

A simple, fast, selective and stability indicating assay for quantitation of candesartan in presence of naproxen as an internal standard in human plasma is presented and validated. The method involved liquid liquid extraction of the drug from plasma followed by chromatographic separation on a Lichrosphere C-18 column, at room temperature.

The mobile phase consisted from acetonitrile: Methanol (30:70, V/V) buffered to pH 3.5 with 10 mM $KH2PO4$. The mobile phase pumped isocratically at a flow rate of 1.0 mL/min. Fluorescence detection was used for identification and quantitation with wave lengths set at λ250/400 nm for excitation and emission, respectively. Linearity measurement over a concentration range of 3.0-120.0 ng/mL was verified as indicated by a correlation coefficient of 0.9997. The overall intra- and inter- day accuracies were close to 100% with precisions of 4.6% and 5.2%, respectively. The mean relative recovery of candesartan was (97.87 ± 2.95) %. The method was able to estimate 3.0 ng/mL of the drug within less than five minutes. Stability testing reveled that candesartan and naproxen were stable for short and long periods of storage and handling at room temperature and – 20 c°, as well as after three cycles of freeze and thaw.

Key Words: *Candesartan, Naproxen, Liquid chromatography, Human plasma and Fluorometry.*

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A NOVEL MAGNETIC POROUS RESIN FOR REMOVAL OF PHENOL FROM AQUEOUS SOLUTION

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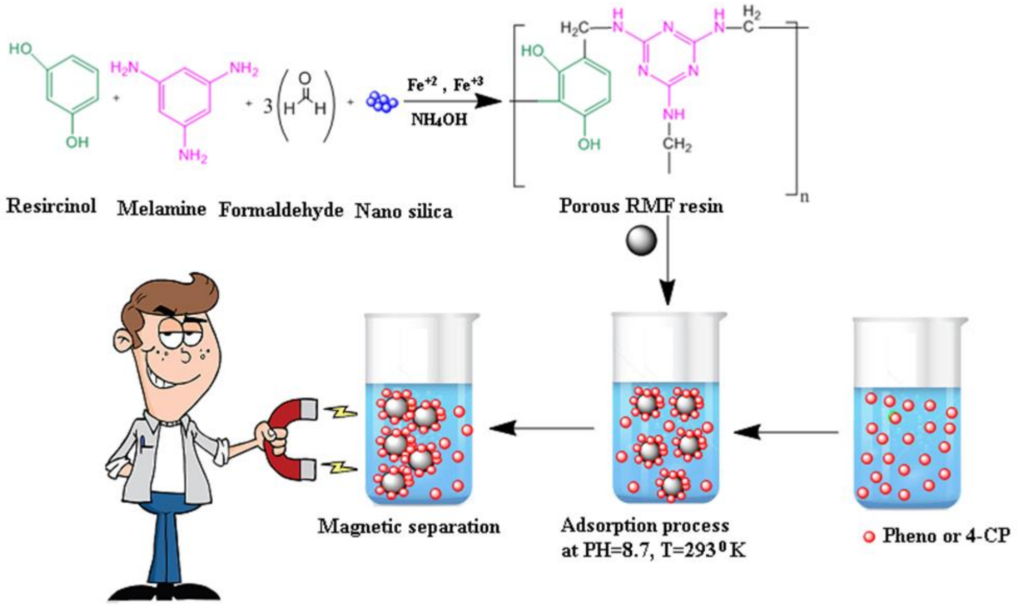
Abstract

The past decade has seen a revolution in the science of porous materials. Porous resin polymers (PRPs) with high thermal, chemical stability and developed inner space are widely used in industry, environmental protection, and chemical analysis [1]. In this study characterize a novel porous magnetic resin (PM-RMF) which was synthesized using resorcinol, melamine, formaldehyde and then its ability for phenol and 4-chlorophenol adsorption was investigated. The resin obtained was characterized by Fourier Transfer Infrared (FT-IR), scanning electronic microscopy (SEM), vibrating sample magnetometer (VSM), Thermogravimetric (TG) and derivative thermogravimetric (DTG) analysis and specific surface area (BET). The effect of initial concentration, adsorbate dose, pH, and contact time were studied in the batch adsorption. The equilibrium adsorption isotherm of phenol and 4-chlorophenol (4-CP) were fitted to the Freundlich equation (R^2>0.99). Adsorption studies showed that the uptake of phenol (q_{max}= 2.34) was higher than 4-CP (1.56mmol/g). The adsorption kinetic results indicated that pseudo-second- order could be better describe adsorption behaviour (R^2>0.9905).



Scheme 1. Synthesis of porous magnetic resin (PM-RMF) and its phenol removal applications.

Key Words: *Phenol, 4-chlorophenol, resorcinol-melamine-formaldehyde resin, magnetic removal*

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THERMAL STABILITY AND ELASTIC PROPERTIES OF $MG_3CUH_{0.6}$ TERNARY HYDRIDE

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Abstract

Theoretical study of thermal stability and elastic properties of a new intermetallic hydride compound $Mg_3CuH_{0.6}$ have been carried out based on density functional theory (DFT), within local density approximation (LDA). The calculated structural parameter of $Mg_3CuH_{0.6}$ compound is consistent with the experimental data. The calculated heat of formation shows that this compound has strongest alloying ability and structural stability. The elastic constants were determined from a linear fit of the calculated stress-strain function according to Hooke's law. From the elastic constants, the bulk modulus B, shear modulus G, Young's modulus E, Poisson's ratio σ, anisotropy factor A and the ratio B/G for $Mg_3CuH_{0.6}$ compound are obtained. The sound velocities and Debye temperature are also predicted from elastic constants and discussed for the first report. This is the first quantitative theoretical prediction of these properties.

Key Words: *Intermetallic hydride; Structural properties; Thermal stability; Elastic properties; DFT*

THERAPEUTIC ROLE OF α-LIPOIC ACID, VITAMIN E AND SELENIUM COMBINATION IN LIVER OF DIABETIC MICE

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Abstract

Diabetes mellitus is a chronic metabolic disease characterized by anomalies forming in carbohydrate, lipid, protein metabolisms [1]. We have been previously studied positive effects of α-lipoic acid + vitamin E + selenium combination on pancreatic tissues of streptozotocin-diabetic mice [2]. The aim of this study was examined the role of α-lipoic acid (ALA) + vitamin E (Vit E) + selenium (Se) combination on endocannabinoid system, morphological and biochemical changes in diabetes. The mice were divided into five groups. 1-Citrate buffer, 2-The solvents of the antioxidants, 3-The antioxidants [ALA (50 mg/kg), Vit E (100 mg/kg) and Se (0.25 mg/kg)], 4-Streptozotocin (STZ) (as five consecutive daily doses of 40 mg/kg for diabetes), 5-The antioxidants+STZ. Sections of liver tissues were stained with Masson's trichrome and Hematoxilin-Eosine for histochemical analyses. Also, we determined immunopositive cell number and the density for cannabinoid receptors (CB1R and CB2R) in liver. Liver tissue homogenates were used for enzyme analyses and fucose, hexose and advanced oxidation protein product (AOPP) levels. The degenerative changes such as picnotic nuclei and necrotic cell, hyperemia and sinusoidal dilation increased in diabetic group, but all of them decreased in the antioxidants+STZ mice. CB2R immunopositive cell number and the density significantly decreased in diabetic group compared to the citrate buffer group, while a significant change was not observed in CB1R, statistically. Liver catalase and paraoxonase activities were decreased while fucose, hexose and AOPP levels were increased in diabetic group. As a result, triple antioxidant treatment was not affect the regulation of cannabinoid receptor expressions heavily. However, triple antioxidant treatment reversed negative effects induced diabetes, morphologically and biochemically.

Key Words: Lipoic acid, Vitamin E, Selenium, Liver, Diabetes

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EXAMINATION OF ANTIBACTERIAL AND PHOTODYNAMIC EFFECTS OF SOME PLANT EXTRACTS

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In current dentistry treatments, with the aim of preventive approach it is argued that removing only the infected layer of dentin is sufficient for cavity preparation [1]. However it is impossible to be sure with bare eyes that infected layer was completely removed or not. In addition, the cause of secondary caries and post operative sensitivities has been reported as residual bacteria in some studies [2]. In the light of this information cavity disinfection needs have emerged. The aim of this study is to investigate the antibacterial and photo-active properties of *Cotinus coggygria* Scop., *Rumex cristatus* DC., *Petroselinum crispum*, *Beta vulgaris* L.var.cicla and *Eruca sativa* aqueous extracts [3-5]., and to investigate their usefulness for cavity disinfection in dentistry.

The aqueous solutions of plant extracts were prepared to be at a maximum concentration and the *Streptococcus mutans* (*S. mutans)* solutions mixed with Phosphate buffered saline (PBS) to give 10^8 cfu/mL. A 430-480 nm wavelength light source was used for the irradiation. Three different applications were made: 1) Plant extracts + *S. mutans* mixture that was not exposed to light, 2) Plant extracts + *S. mutans* mixture exposed to light, 3) *S. mutans* exposed to light. No antibacterial effect was found for the first and third applications. In the second application, however, irradiation with extract + *S. mutans* mixture reduced the number of microorganisms in the beginning by 99 % for only *Rumex cristatus* DC. extract (log 2). *Rumex cristatus* DC. aqueous extracts can be used as an alternative in photo-active disinfection of cavities in dentistry.

Key Words: *Plant extracts; antibacterial, photo-active; cavity disinfection; dentistry*

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POLYURETHANE NANOCOMPOSITE MATERIALS CONTAINING PHOSPHORUS AND FLUORINE AND THEIR COATING APPLICATIONS

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ABSTRACT

In this study, bis (4-(ß-hydroxy propoxy) pheyl) phosphine oxide (BHPPPO) was synthesized as a monomer which was used 20%wt., 40%wt. and 60%wt. in polyurethane acrylate oligomers (PUA's). UV-curable PUA oligomers were obtained by using isophorone diisocyanate (IPDI), polyethylene glycol (PEG1500), BHPPPO and 2-hydroxyethyl methacrylate (HEMA). The structures characterization of oligomers were performed by ^{1}H-NMR and ATR-FTIR spectroscopy. Triethoxyethylsilane terminated perfluoro component (Si-PF) was synthesized using 1H,1H,9H,9H-perfluoro nonanediol and 3-(isocyanato propyl) trimethoxysilane as a silane-coupling agent to improve the compatibility of the organic and inorganic phases. A series of UV-curable organic-inorganic hybrid coating materials was prepared to include different amount of PUA's and Si-PF. Physical and mechanical properties such as modulus, elongation at break, water resistance and gloss of materials were characterized. On the other hand, effect of synthesized compounds to thermal properties of nanocomposite coating materials were measured thermal gravimetric analysis (TGA) and limiting oxygen ındex (LOI). Surface propeties such as hydrophobic and oleophobic behaviour were observed with deionized water and ethylene glycol by contact angle test. The surface morphology of the nanocomposite coating was characterized by scanning electron microscopy (SEM). Improvement in properties were presented with proportional to amount of BHPPPO and Si-PF.

Key Words: *nanocomposite, uv-curable, phosphine oxide, fluorinated sol-gel*

Acknowledgement: This work was supported by Marmara University Science Fund.(BAP No: FEN-A-120616-0270 and FEN-C-YLP-080415-0121).

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DEVELOPMENT OF FLUORESCENCE SENSOR FOR THE DETERMINATION OF ORGANOPHOSPHORUS BASED PESTICIDES

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Abstract

Pesticides are biologically active chemicals that cause problems, such as insects, animals, microorganisms, weeds, and other harm, to die or change their behaviour, and present a potential health risk for humans. In addition to being toxic, these compounds also cause cancer-causing agents. Some of these traditional chemical and biochemical applications are resistant to natural conditions and are strictly forbidden. However, pesticides are transported by the food chain, concentrated by bioaccumulation in the bodies of the creatures, and when progressing in this chain, they reach a greater extent at each stage.

Pesticide analysis is very important for the accurate assessment of how people are exposed to pesticides in various matrices, including food. For this reason, it is important to determine the residue levels and analyse it at very low concentrations using the analytical methods used.

In our study, a fluorescence polymeric sensor was prepared by photopolymerization for the analysis of organophosphorus pesticides. In addition, parameters such as pH, concentration range, sensitivity, selectivity, precision, response time and reproducibility required for determination has been systematically examined. After method validation, the method was applied to real samples.

This work was supported by Marmara University, Commission of Scientific Research Project (M.Ü. BAPKO) under grant FEN-A- 110117-0018.

***Key Words:** Fluorescence, Sensor, Organophosphorus, Pesticides, UV-curing.*

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PREPARATION AND APPLICATION OF TRACK-ETCHED NANOPORE MEMBRANES AND THEIR SENSOR APPLICATIONS

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Abstract

There is an ever-growing interest for analysis of molecules using resistive-pulse sensing, which is an effective method for the detection of molecules [1]. Resistive-pulse sensors basically rely on particles' passage from one compartment to the other through a nano- or micro-pore and measuring the current-drops during the translocation of molecules. These momentary changes in current are used for the detection and identification of molecules. This sensing paradigm can be based on biological or synthetic nanopores. The synthetic nanopores fabricated in solid-state materials present several advantages over biological ones such as chemical, mechanical, and thermal robustness and control over shape and size [2].

Compared to other techniques of fabricating synthetic nanopores, the track-etch method emerges as an applicable and easy alternative by means of obtaining nanopores with controlled size, shape and density [3]. This technique also allows preparing nanopores with different geometries by varying the etching conditions which, is basically based on the irradiation of membranes with accelerated heavy ions to create latent tracks inside the membranes. Following this process, multiple nanopores, or even a single nanopore in polymer membranes can be prepared. An example SEM image of a multiporous poly(ethylene terephthalate) (PET) membrane surface is given in Figure 1.

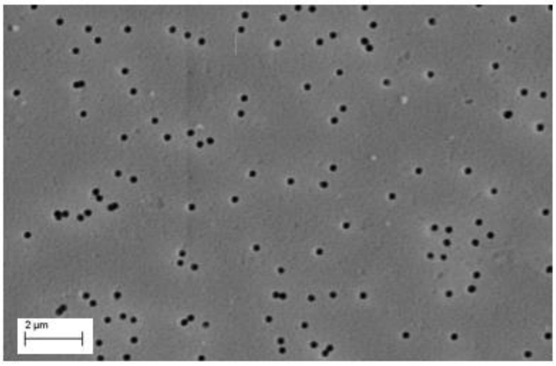

Figure 1. SEM image of a multiporous PET membrane

In this study, we showed the fabrication of nanoporous membranes using track-etch method. The geometry and dimensions of the nanopores were characterized by SEM and electrochemical measurements (i.e., current-voltage (I-V) curves). The resistive-pulse sensing paradigm was demonstrated using PET nanopore and divalent metal ion(s) was chosen as analyte.

Key Words: *Resistive-pulse sensing; divalent ion detection; track-etched PET membrane; nanopore sensor*

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CONTROLLED RELEASE OF DONEPEZIL HYDROCHLORIDE FROM HYDROGELS HAVING DIFFERENT PROPERTIES

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Abstract

Drug delivery systems have been of great interest for the past few decades to realize the effective and targeted drug delivery and minimize the side effects in the field of pharmaceutics [1]. Alzheimer's disease is a degenerative disorder, in which there is a progressive deteriorative of intellectual and social functions, memory loss, personality changes and inability for self care, and has become the fourth leading cause of death in developed countries [2]. Donepezil Hydrochloride is a second-generation cholinesterase inhibitor, used for the treatment of Alzheimer's disease having greater specificity for the brain acetyl cholinesterase enzyme [3]. Hydrogels represent a key means of controlled or sustained delivery [4]. Alginates are natural polysaccharides that have shown many uses in biomedical and pharmaceutical applications due to their low cost, low toxicity, biocompatibility and biodegradability [5].

In the work presented, synthesis drug carrying hydrogels having different properties and drug release experiments are performed. For this pupose, gelatin, α-cellulose, natural zeolite: clinoptilolite, activated clinoptilolite and 4-acryloyl morpholine are combined with sodium alginate (Na-alg). Hydrogels were characterized by Fourier transform infrared spectroscopy and scanning electron microscopy. In vitro release studies have been performed for donepezil hydrochloride loaded hydrogels in water, 1.2, 6.8 and 7.4 pH media. The results showed that these hydrogels can be used as very useful materials for drug delivery systems.

Key Words: *Drug delivery systems, Hydrogels, Sodium alginate, Donepezil hydrochloride*

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PRETREATMENTS AND TEMPERATURE EFFECTS ON THE DRYING KINETICS OF PEAS

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Abstract

In this study, peas were dried in convection dryer at a temperature range of 55-75°C with a constant air velocity of 2 m/s. The peas were pre-treated with ethyl oleate and blanched with hot water at 85°C before drying. Drying process continued until sample moisture fell down to 0.11 kg water/kg dry matter. The blanched samples dried faster than the other pre-treatment and control conditions. Besides, drying rate increased with increasing temperature. The experimental results illustrated the absence of constant-rate drying period and drying took place in the falling-rate period. Four well-known thin-layer models were used to predict drying kinetics by nonlinear analysis of regression. The Midilli and Kucuk model best fitted the experimental data for the whole range of temperatures. The moisture diffusivity coefficient at each temperature was determined by Fick's second law of diffusion, in which their value varied from 7.66×10-11 m^2/s to 2.44×10-10 over the mentioned temperature range. The dependence of effective diffusivity coefficient on temperature was expressed by an Arrhenius type equation. The calculated values of the activation energy of moisture diffusion were 36.75, 38.11 and 43.25 kJ/mol for pre-treated with ethyl oleate, blanched samples and control samples, respectively.

Key Words: *Activation energy; Drying; Effective diffusivity; Pea; Pre-treatments.*

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RGO/PEDOT NANOCOMPOSITE SYNTHESIS AND SUPERCAPACITOR APPLICATIONS

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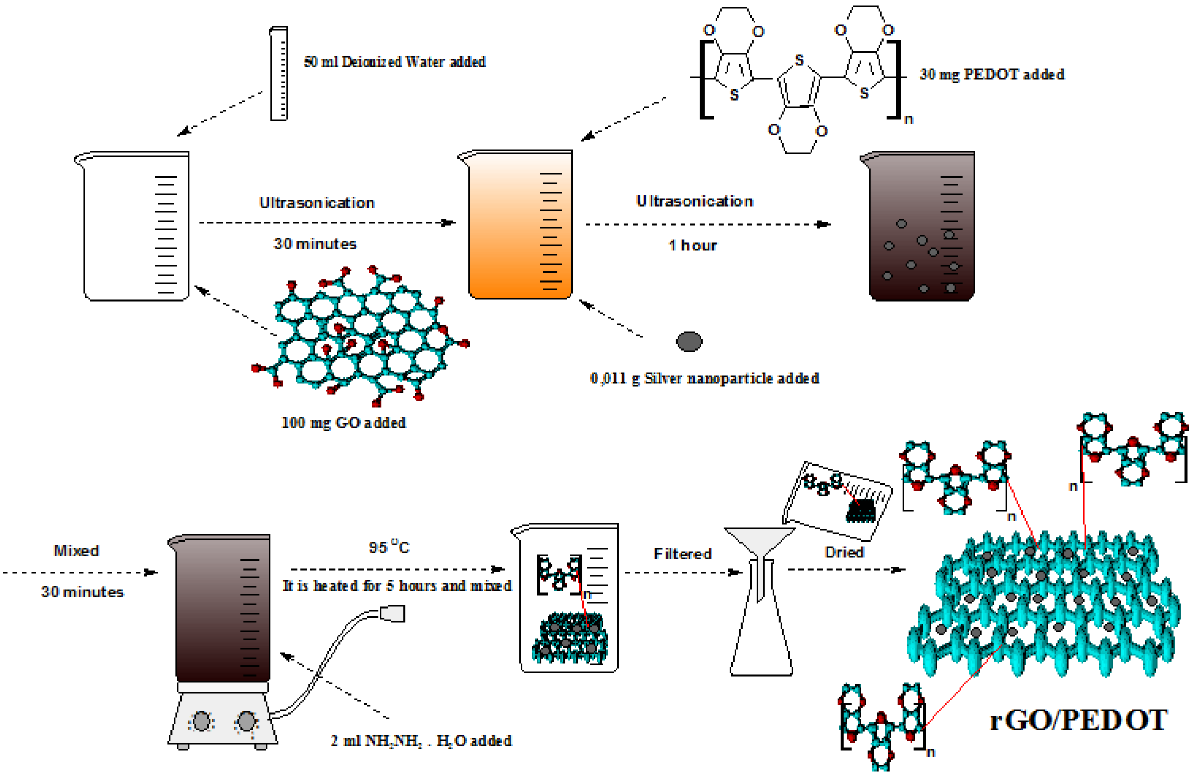
Abstract

rGO/PEDOT nanocomposite was prepared from graphene oxide, resulting via reduction of hydrazine with poly(3,4-ethylenedioxythiophene) [1]. Ag nanoparticles were added to the composite material to increase the conductivity of the material. Therefore, the higher homogeneous polymer matrix film was obtained on graphene sheets. The GO/PEDOT nanocomposite films were characterized by CV, SEM-EDX, FTIR-ATR, EIS analysis. The active electrode materials were designed by two electrode configuration for supercapacitor performances. CV, CC and EIS analysis were performed to measure capacitance, energy and power densities. Ragon and stability plots were given in this study.



Scheme 1. The synthesis steps of rGO/PEDOT nanocomposite.

Key Words: *reduced graphene oxide, PEDOT, supercapacitor, nanocomposite, electrochemistry.*

Acknowledgements: The financial support from Namik Kemal University, Tekirdag, Turkey, project number: NKUBAP. 01.GA.16.076 gratefullfy acknowledged.

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INVESTIGATION OF HYDROXYAPATITE MORPHOLOGY AT DIFFERENT EXPERIMENTAL CONDITIONS

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Abstract

The controlled synthesis of inorganic crystals is important on material fabrication which requires particles of specific size, shape and morphology. The calcium phosphate salts is of particular interest because of its importance in various fields such as industrial water systems, wastewater treatment processes, agriculture fertilizers, and biological calcification processes.

The thermodynamically most stable phase of calcium phosphate salt is hydroxyapatite (HAP, $Ca_5(PO_4)_3OH$). HAP properties depend on its stoichiometry and morphological characteristics especially its crystal size distribution, crystallinity, porosity and shape. Therefore recently, the study of controlling these parameters has gained great scientific and industrial interest. It was reported that small changes in these properties had significantly effects on the mechanical properties of HAP crystals.

In this work, the effects of temperature and polymeric additives on HAP crystallization were investigated by wet chemical synthesis. Polyacrylic acid homopolymer and styrene-acrylic copolymer were used as additive. The obtained crystals were characterized by SEM, BET, FT-IR and X-Ray powder diffraction methods. The result showed that the morphological characteristics changed depending on the experimental conditions.

Keywords: *Hydroxyapatite; polymeric additives; crystallization; morphology; chemical synthesis.*

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ADSORPTION-DESORPTION CHARACTERISTICS OF XAD-7 RESIN FOR THE REMOVAL OF 4-NITROPHENOL

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Abstract

Organic pollutants released in water present a major threat to the environment and human health. Among these pollutants are phenols and its derivatives that can be found in the wastewaters of industries such as oil, medicine, pesticides, plastics, disinfectants etc. [1]. Since the removal of such substances from water is very important environmentally and ecologically, there are a variety of methods developed for this purpose such as advanced oxidation processes, membrane technologies and biological degradation. All these methods have some disadvantages such as limited field of applications, energy requirement, expensiveness or creating secondary pollutants. Therefore, adsorption based cleansing of wastewaters emerged as a very applicable alternative [2]. A variety of natural or synthetic materials can be used as adsorbents [3]. In this study Amberlite XAD-7, was selected as the adsorbent. This commercially available, polar, polymeric resin was chosen because of its high surface area, aliphatic structure and excellent physical and thermal stability.

The aim of this study was to determine whether Amberlite XAD-7 resin was an appropriate adsorbent for the removal of 4-nitrophenol (4-NP) from aqueous mediums. For this purpose, adsorption and desorption experiments were conducted using a horizontal shaker water bath at constant temperature in batch system. The effects of contact time, the amount of adsorbent, initial concentration of 4-NP, pH, the point of zero charge of the adsorbent and temperature on the adsorption process were investigated.

Adsorption isotherms were applied using the equilibrium data of the adsorption process and Freundlich isotherm was found to explain the adsorption phenomena. Kinetic and thermodynamic data were also analyzed. It was shown that the adsorption kinetics fitted the pseudo second order kinetic model and intra-particle diffusion model carried out in three steps. ΔG^0 was calculated as -5412.03 J mol^{-1} for 1x10^{-4} mol.L^{-1} initial concentration of 4-NP, 3 g L^{-1} adsorbent dose and 293 K. At the same conditions, ΔH^0 was found to be -20.0 kJ mol^{-1} and ΔS^0 was calculated as -49.89 J mol^{-1} K^{-1}. The thermodynamic data revealed that the adsorption of 4-NP on XAD-7 was spontaneous and exothermic which was in agreement with the experimental results.

Desorption process was performed five times using NaOH solutions in certain concentrations and the use of NaOH as desorption solution was found to be a very suitable choice for these five cycles. As a result of all these studies, it was shown that adsorption is a useful method for the removal of 4-NP from aqueous solutions and XAD-7 can be used repeatedly without deterioration after desorption processes.

Key Words: *adsorption, 4-nitrophenol, XAD-7, adsorption kinetics, adsorption isotherms*

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THE EFFECTS OF ADDITIVES ON PARTICLE SIZE AND MORPHOLOGY ON $BaSO_4$ CRYSTALS

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Abstract

Today, the production of small particles in research and development fields has become an important subject[1]. These nano-particles have wide application potential in many areas such as heterogeneous catalysis, semiconductors, microelectronics, data storage, pharmaceutical, paint and ceramic industrial applications. When the crystals are reduced to very small dimensions, a large increase in surface area occurs and this can earn them many new different features. With the increase of surface area of the barium sulfat synthesized in a nanometer range, improved benefits are provided to the properties of a material such as thermal stability of the materials, the crystallization rate, resistance activity and thermoluminescence properties[2]. The resulting surface activity of these nano particles is quite high due to the high surface area to volume ratio of the particles and as a result they tend to agglomerate which decreases their applicability. In order to obtain the barium sulfate particles with the appropriate properties for the material that it is used, avoiding the agglomeration and having a controlled size and morphology during the production is of critical importance[3-5].

In this study the effects of alginate, polyacrylic acid and polyvinyl sulfonic acid on barium sulfate crystallization which has a great importance for industries such as pharmaceuticals, paint, plastic and especially the oil industry were investigated. The barium sulfate crystals synthesized with the additives used in different concentrations and the effects of these additives on the properties of the crystals such as particle size, morphology and tendency to agglomerate were investigated.

Key Words: *Barium sulfate; nano, alginate, polyacrylic acid, polyvinyl sulfonic acid*

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REMOVAL OF COPPER BY HYBRID GEL BEADS BASED ON BIOPOLYMERS AND PERLITE

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Abstract

Heavy metal pollution is one of the most important environmental problems and threatening to human health and ecological systems. A wide range of techniques have been developed for the removal metal ions from aqueous solution such as chemical precipitation, filtration, ion exchange, electrochemical treatment, membrane technologies, adsorption. Among them, adsorption is a promising and widely applied method as sorbent plays a key role in the removal of heavy metals from aqueous solution.

In this work, novel hybrid gel beads with a well defined and controlled size formed by alginate biopolymer, and perlite were designed, prepared and characterized for heavy metals removal. Also, different types of carrageenan were used as a second biopolymer to vary functional groups of hybrid beads. The different formulations of alginate, carrageenan hydrogels with perlite and different processing parameters were considered to determine the best conditions required to achieve the most adequate response in terms of the shape stability and functionality of the developed systems. Physical and chemical properties of the hybrid beads were characterized by using several techniques such as FTIR, SEM, TG. Heavy metal removal efficiency of hybrid gel beads was studied for aqueous copper solution. The equilibrium experiments were investigated over the range of 0-50 mgL^{-1} of copper using a dosage of the hybrid beads of 0.5 gL^{-1}. The kinetic study indicates the copper adsorption equilibrium time was obtained in 4 h. The results showed the adsorption performance of hybrid beads is greatly affected by ratio of biopolymers and perlite as well as carrageenan type.

Key Words: *Alginate, carrageenan, perlite, hybrid beads, adsorption*

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RGO/PTH NANOCOMPOSITE SYNTHESIS AND ITS SUPERCAPACITOR PERFORMANCES

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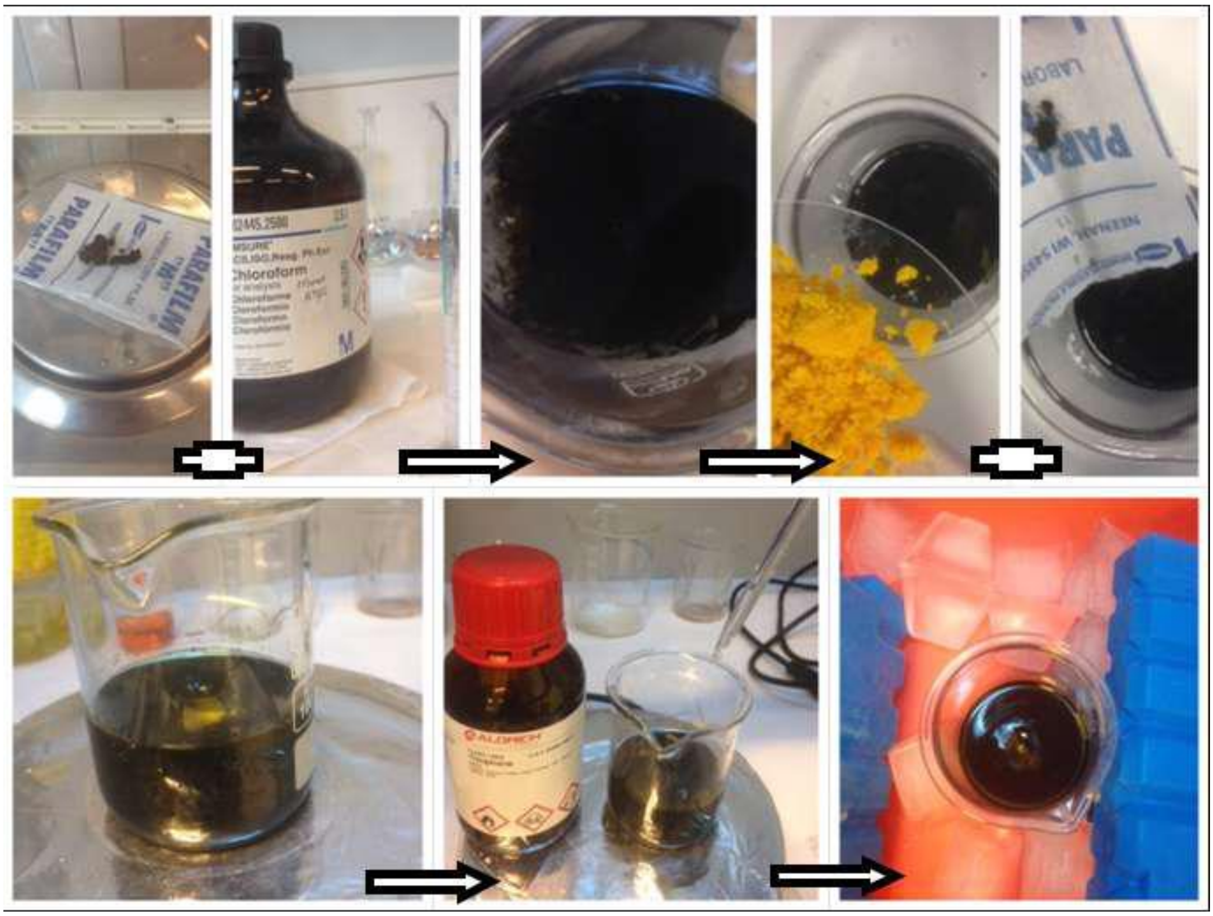
Abstract

0.2 g graphene added to the 50 ml chloroform and dispersed for 1 h in ultrasonication. 1 g Thiophene was added to the solution and stirred at 5 $_o$C for 6 h. After that, solution was filtrated and added DI water up to pH ~7. rGO/PTh nanocomposite was obtained at 60 $_o$C under vacuum atmosphere [1]. Ag nanoparticles were added to the composite material to increase the conductivity of the material. The rGO/PEDOT nanocomposite films were characterized by CV, SEM-EDX, FTIR-ATR, EIS analysis. The active electrode materials were designed by two electrode configuration for supercapacitor performances. CV, CC and EIS analysis were performed to measure capacitance, energy and power densities.



Scheme 1. rGO/PTh nanocomposite synthesis experiments.

Key Words: *polythiophene, supercapacitor, galvanostatic charge-discharge, nanocomposite, energy density.*

Acknowledgements: The financial support from Namik Kemal University, Tekirdag, Turkey, project number: NKUBAP. 01.GA.16.076 gratefullfy acknowledged.

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THE CONTROLLED RELEASE OF BOVINE SERUM ALBUMIN FROM POLYSACCARIDE BASED HYDROGEL BEADS

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Abstract

The polymeric delivery systems are of interest for many biomedical and food applications such as drug delivery systems, development of scaffold and incorporation of bioactive proteins into food products. Therefore, the studies of the encapsulation and release of protein have attracted as a model in drug delivery systems. Natural and synthetic polymers have been used in order to produce hydrogel beads suitable for protein encapsulation. Alginate and kappa-carrageenan are natural polymers that have found numerous implementation in biomedical and engineering fields due to its favorable properties, including biocompatibility and ease of gelation.

In this study, the encapsulation of Bovine Serum Albumin (BSA) in hydrogel beads was performed at different process conditions. Physically crosslinked hydrogel beads were prepared by crosslinking of the mixture of sodium alginate and kappa-carrageenan by using Ca^{+2} and K^{+1}. The effects of [Ca]/[K] ratio, pH and the ratio of alginate and kappa-carrageenan on encapsulation efficiency were investigated. Release experiments were done in simulated gastric fluid (SGF pH 1.2) and subsequently in simulated intestinal fluid (SIF pH 7.5).

BSA-loaded beads became smaller in gastric fluid. Transferring beads from gastric fluid to intestinal fluid led to burst, and released BSA.

Keywords: *Bovine serum albumin; polysaccharide; hydrogel beads; gastric; intestinal; encapsulation;*

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MOLECULAR MODELLING OF 2-IMINOTHIAZOLES AS INSECTICIDAL ACTIVITY

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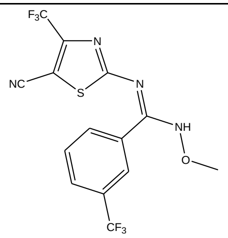
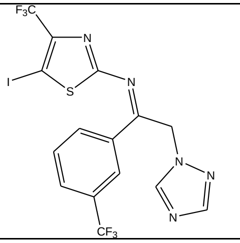
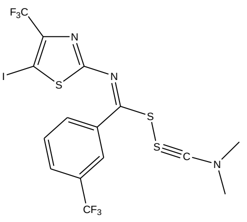
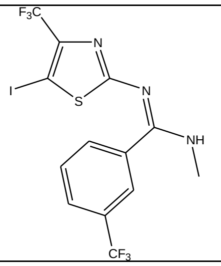
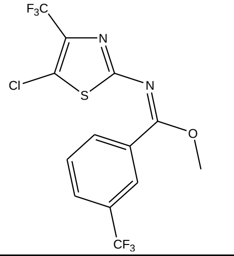
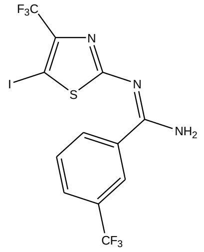
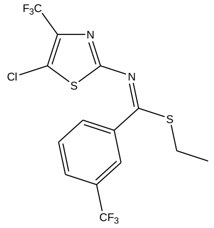
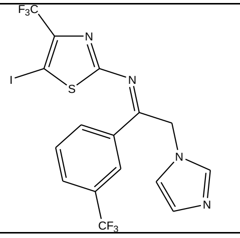
Abstract

Insecticides are used in agriculture, medicine, industry and by consumers, indoor. Insecticides are also claimed to be a major factor behind the increase in agricultural 20th century's productivity. On the other hand, modes of their action is important in understanding whether an insecticide will be toxic to unrelated species, such as fish, birds and mammals.

Docking, a new way of illuminating the effect mechanisms of biologically active chemicals offer a new green chemistry field.

Although 2-iminothiazoles are designed, synthesized and tested as protein tyrosine phosphatase 1B inhibitors [1], cannabinoid receptor ligands [2], pifithrin-α p53 inactivators [3], etc. there is not any remarkably record on their insecticidal docking study.
Present work introduce the molecular modelling and mapping of active site of previously synthesized by us insectisidal 2-iminothiazole derivatives [4], by using classical docking techniques, *i.e.* MOE, etc. [5].

Tested comp.	The structures of tested compounds	Tested comp.	The structures of tested compounds	Tested comp.	The structures of tested compounds
6		9		26	
95		98		99	
121		143			

Key Words: *Molecular modelling; docking; insecticide; 2-iminothiazole.*

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SOLID-STATE CHARACTERIZATION of POLY(ETHYLENE GLYCOL) SAMPLES PREPARED by SOLVENT CAST TECHNIQUE

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Abstract

The effect of solvents (water, methanol, dimethyl sulfoxide, chloroform and tetrahydrofuran) casted on the poly(ethylene glycol) (PEG) samples with varying molecular weights (PEG 2000, PEG 4600, PEG 8000 and PEG 10000) was performed solid-state characterization by FTIR, Raman and X-ray Diffraction in submitted study.

FTIR and Raman spectra have been used in literature [1-4] as solid evidence for the direct association of the solvents with the etheric oxygen of PEG. In this study, spectral differences were classified with respect to stretching, bending, rocking, angle bending and internal rotation frequencies and low-frequency Raman region according to functional groups and thus crystallinity as related with solvent character and polymer molecular weight were evaluated. Crystalline and amorphous regions in the XRD diffractograms have been found by Polynomial Regression method through Microsoft Office Excel program and subsequently, crystallinity percentages were evaluated. From XRD spectra of PEG/solvent systems, the highest decrease in crystallinity percent has been detected in the sample cast from tetrahydrofuran. On the other hand, the largest frequency shifts of various stretching and bending vibrations of PEG have been observed for the samples cast from chloroform and especially tetrahydrofuran in FTIR and Raman spectra. The parallelism of both computation [5] and thermodynamic [6] and spectroscopic data about solubility profiles of PEG/solvent systems has been determined. In the end of trio study, the parallelism of both computation and thermodynamic and spectroscopic data about solubility profiles of PEG/solvent systems has been determined.

The results indicated that association/solvency power of solvents for poly(ethylene glycol) samples prepared by solvent cast technique was decreased below order: tetrahydrofuran > chloroform > dimethyl sulfoxide > methanol > water.

Key Words: *Poly(ethylene glycol); solvent cast technique; Fourier Transform Infrared Spectroscopy; Raman; X-ray Diffraction.*

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ELECTROPOLYMERIZATION AND CHARACTERIZATION OF SALOPHEN DERIVATIVE SCHIFF BASE CO(II) AND NI(II) COMPLEXES ON THE GRAPHITE ELECTRODE AND ELECTROCATALYTIC INVESTIGATIONS

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Abstract

Recently, modified electrodes and its applications have attracted more attention in electrochemistry studies because of their high selectivity and sensitivity, rapid response and low cost [1]. These electrodes have acquired wide applications in electroanalysis, fuel cells, biosensors and protection against corrosion [2]. Redox active organic or inorganic molecules that contain heteroatom have been mostly used as modifiers at study of surface modification. Modification process of surfaces has been performed by different methods particularly physical, chemical or electrochemical.

In this study, electropolymerization of Salophen derivative Schiff base Co(II) and Ni(II) complexes was carried out on the graphite electrode in 0,15 M $LiClO_4$ supporting electrolyte medium by electrochemical methods. Modified surfaces were characterized by CV, UV-Vis, SEM-EDAX, EIS, FTIR and ICP-MS techniques. The electrocatalytic activity of modified electrodes was investigated upon various biochemical species such as dopamine, chatechol, glucose.

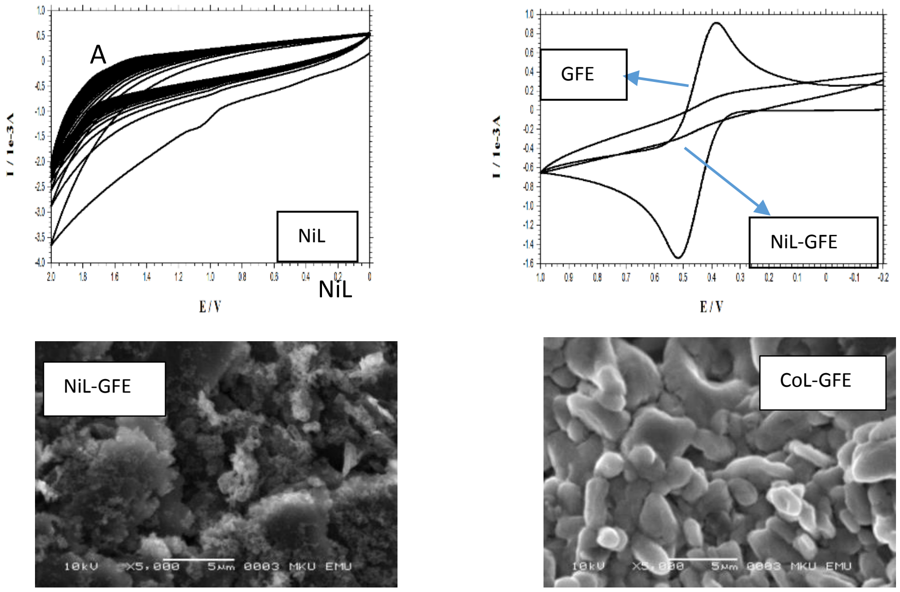

Figure.1. A. The multi-cycle CVs of immobilization of Schiff base Ni(II) complex on graphite electrode vs. Ag/AgCl, ν:100 mVs^{-1}, B. Electrochemical characterization of NiL-GFE. And SEM images of CoL-GFE and NiL-GFE surfaces.

Key Words: *modification; characterization; graphite electrode; Schiff base metal complex; electropolymerization.*

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ZETASIZER MEASUREMENTS OF POLYMER-DRUG DELIVERY SYSTEM: POLY (MALEIC ANHYDRITE-CO-VINYL ACETATE) - ACRIFLAVINE CONJUGATE

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Abstract

The presence of the polymers has a significant influence on the colloidal system stability. The adsorption of natural or synthetic polymers at the solid–liquid interface is a very sophisticated process determined by many factors such as macromolecule structure, solution pH, temperature, and surface properties of the adsorbent. As a result, polymer chain presence on the solid surface modifies the stability of aqueous suspensions causing increase of their stabilization (steric, electrosteric stabilization) or a complete destabilization (bridging flocculation, depletion interactions, or charge neutralization) [1, 2]. Stabilization of the dispersed systems is particularly desirable in the production of high-quality paints, cosmetics, and medicines. Surface properties of drug carrier systems are responsible for their interactions with plasma proteins. Zetasizer measurements which are zeta potential, particle size and mobility provide valuable properties of particles or molecules in liquid medium. Zeta potential is a scientific term for electrokinetic potential in colloidal systems, i.e., electric potential in the interfacial double layer at the location of the slipping plane versus a point in the bulk fluid away from the interface [3]

In this work, zetasizer measurements (zeta potential, mobility and particle size) of poly (maleic anhydrite-co-vinyl acetate)-akrifilavine polymer-drug conjugate were determined by using the Zeta Potential Analyzer with different pHs and as function of time in dekstrose and PBS solutions. Absorption and permeability of MAVA/AF, MAVA and AF were also determined by UV Spectrophotometer.

Key Words: zeta potential, mobility, particle size, poly (maleic anhydrite-co-vinyl acetate)-acrifilavine conjugate

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TUNING THE MORPHOLOGICAL PROPERTIES OF HIERARCHICAL POROUS POLYESTER/NANOCLAY COMPOSITES

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Abstract

Emulsion templating is a versatile method for the preparation of porous polymer monoliths which offers the advantageous of hierarchical and open porous morphology. In a typical emulsion templating application, a concentrated emulsion is first generated and then the continuous phase is polymerized. By this way, internal phase droplets serve as a tool for the creation of porosity in the resulting polymer. The main advantage of emulsion templating is the ability of controlling pore morphology and physical properties of the obtained materials by altering the composition of continuous phase. Polymers formed via emulsion templating are defined by using the type of the emulsions. In most cases, high internal phase emulsions (HIPEs) are used as templates for the creation of highly porous polymer monoliths. Polymers synthesized within HIPEs are named as polyHIPEs [1,2].

In this study, hierarchical porous polyester/nanoclay polyHIPE composites were synthesized within HIPE templates consisting of unsaturated polyester resin, divinylbenzene, and surface modified montmorillonite. In order to tailor pore diameters and pore size distribution, surfactant amount and internal phase ratio was varied during emulsion preparation. It was found that depending on the internal phase ratio of the emulsion templates, average surface areas of resulting composites are change between 59.87 m^2 g^1 and 161.20 m^2 g^{-1}. Moreover, the influence of nanoclay loading was investigated. It was found that increasing amount of nanoclay loading contributes to the formation of cells which are interconnected with pore throats [3].

Key Words: *emulsion templating, polyHIPE composite, unsaturated polyester resin, nanoclay*

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[MN(CO)$_3$(BPY)(2-CHLOROBENZYLBENZIMIDAZOLE)]OTF COMPLEX AS

A NEW PHOTOACTIVATABLE CO-RELEASING MOLECULE

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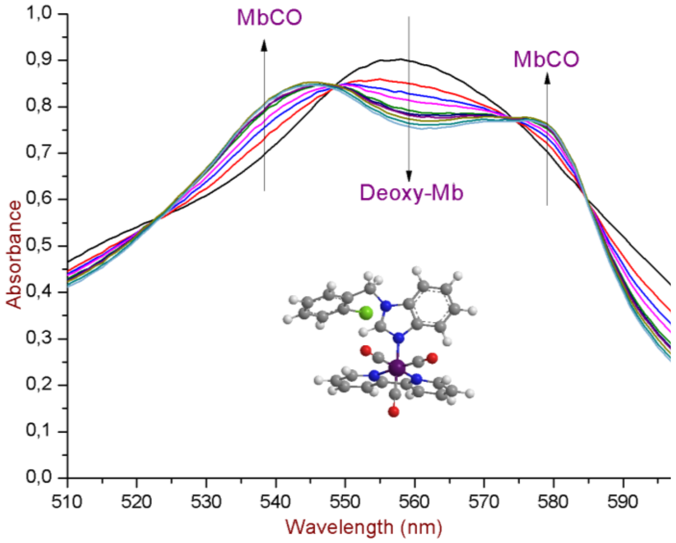
Abstract

Carbon monoxide (CO), which is a colorless, odorless, tasteless gas, is actually toxic due to its interaction with transporting oxygen in blood for the humans over certain amount. However, it is synthesized endogenously in human body course of hemoglobin degradation, and the ratio of the CO increases in case of illness [1]. The scientist paid attention to this increment and studied about therapeutic effects of carbon monoxide at the beginning of 2000s such as the other small messenger molecules, NO and H_2S [2].

The investigations about CO have divided into two ways. The first group of scientists have been studying the bio-effects and were analyzed anti-inflammatory, anti-apoptotic, anti-oxidant, anti-cancer and anti-proliferative properties, and founded that CO protects tissues against hypoxia or ischemia–reperfusion injury, causes vasodilatation, and had an appreciable role in preclinical animal models of cardiovascular disease, inflammatory disorders, and organ transplantation [2]. But, CO has to release to tissue with controllable amount in controllable time and the second group have been trying to synthesize the best CO-releaser. Metal carbonyl complexes have been synthesized as effective CO-Releasing Molecules (CORMs).



Photoactivatable CO-releasing molecules, entitled photoCORMs [3], is well-described. Novel [Mn(CO)$_3$(bpy)(N-2-chlorobenzylbenzimidazole)]PF_6 complex has been synthesized as photoCORMs. The structure of the compound has enlightened by ^{1}H NMR, ^{13}C NMR, IR, LC-MS, and elemental analysis. CO-releasing properties of the compound has been investigated. Also DFT/TDDFT analysis of complex has been made with ORCA package program by BP86 functional for obtaining the optimized geometries, MO electron densities and having insights electronic transitions that promote CO-release.

Key Words: *photoCORMs, manganese complexes, benzimidazole, MYO-assay, DFT/TDDFT*

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LIPOPOLYSACCHARIDE TREATMENT CHANGES PLASMA TOTAL OXIDANT AND ANTIOXIDANT CAPACITY ON A TIME DEPENDENT MANNER IN RABBITS

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Abstract

It is well known that lipopolysaccharide (LPS), an outer-membrane component of gram-negative bacteria has frequently been used in experimental models of inflammation and oxidative stress [1-3]. Oxidative stress is described as an imbalance between reactive oxygen species (ROS) and scavenger systems (antioxidants). It can be caused by the inflammatory response to sepsis. [4]

In this study, it was aimed to investigate the dose and time dependent effects of bacterial LPS on antioxidant status by evaluating total antioxidant capacity (TAC), total oxidant capacity (TOC)) and other biochemical parameters (total protein, albumin, globulin, albumin/globulin ratio in rabbits. Prior to LPS injection, blood samples were collected from 15 New Zealand rabbits (weighing 3-3.5 kg, at the age of 20-24 months) and these samples were named as 0th h. Then, 150 µg/kg LPS was intravenously injected through ear veins to the Group I (n=7) and 300 µg/kg LPS to the Group II (n=8). Following injections, plasma samples were separated after taking blood samples into heparinized pits at 0st, 1st, 2nd and 3rd h. Biochemical parameters were measured by colorimetrically using commercial kits. While TAC level was decreased 2nd and 3rd h, TOC level was increased in 3rd h in group I ($p<0.005$ and $p<0.01$ respectively) compared to the 0th h. Although TAC level was decreased in 1st, 2nd and 3rd h in group II, TOC level was increased in 2nd and 3rd h ($p<0.00$, $p<0.05$) compared to the 0th h. No significant difference was found in other biochemical parameters.

In conclusion, while some blood biochemical parameters (total protein, albumin, globulin, albumin/globulin ratio) was unchanged but TAC and TOC levels were significantly changed with intravenous LPS injections to the rabbits. Findings also indicated that the effect of intravenous LPS was not dose dependent. LPS increased TOC level and decreased TAC level by inducing destructive effect in the blood plasma within two hours.

Key Words: *Rabbit, Lipopolysaccharide, Total Antioxidant Capacity, Total Oxidant Capacity, Blood.*

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OUTDOOR AIR QUALITY SULPHUR DIOXIDE IN ISTANBUL

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Abstract

The oxidation of sulphur dioxide (SO_2) emitted by natural processes or human activity affects atmosphere. If oxidation processes are not efficient, chemical composition of the atmosphere and biosphere can change. The oxidation of SO_2 produces H_2SO_4. SO_2 gases in atmosphere are removed by oxidizing chemical reactions naturally. Human activity may affect oxidation capacity because of increasing these gases in atmosphere. OH reaction destroys these gases. Therefore these gases are removed by reaction with OH. OH oxidizes SO_2 to sulfuric acid (H_2SO_4). H_2SO_4 reaches to biosphere or hydrosphere through rain. Free radicals in atmosphere have small amount but react fast and spread throughout atmosphere. SO_2 is one of the reactive radicals and has effect on the oxidation processes. It is important for atmospheric composition balance. From Marmara Clean Air Centre in Istanbul, SO_2 measurement values in Kandilli, Sultanbeyli, and Umraniye between March 1, 2013 and April 30, 2016 are evaluated in this study. The results obtained for SO2 were below the limit value in the air recommended by Turkish Government. Air quality is considered satisfactory, and air pollution poses little or no risk. The temperature was found to be significant factor compared to wind velocity and humidity influencing SO_2. SO_2 concentrations were increasing in winters compared to other seasons.

Key Words: *outdoor air quality; SO_2; oxidation; Istanbul*

Acknowledgements

This study was supported by the Marmara University, Scientific Research Projects Committee (BAPKO) with the project number FEN-D-120417-0189. The Study data was supported by Marmara Clean Air Centre in Ministry of Environment and Urban Planning and Istanbul Regional Directorate of Meteorology.

THE COOPERATIVE EFFECT ON H_2SO_4…HNO_3…H_2O TERNARY SYSTEMS

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Abstract

H_2SO_4, HNO_3 and H_2O molecules are found in abundance in our environment are important molecules from atmospheric perspective. These molecules take place in heterogeneous reactions, which cause ozone depletion that is one of the important events of today’s world. Most of these reactions have occurred at the Polar Stratospheric Clouds (PSC), which is on the Stratosphere layer of the atmosphere. One part of the PSC clouds formed from $H_2SO_4/HNO_3/H_2O$ supercooled ternary solutions (STS) [1,2].

The aim of this study is to investigate the interaction of the hydrogen-bonded H_2SO_4…HNO_3…H_2O ternary systems by using ab initio calculations. All calculations were performed by Gaussian 09 package program [3]. The results are discussed in terms of structure, energetic and spectroscopic perspectives.

Key Words: *hydrogen bond, cooperative effect, ternary systems, ab initio calculations, molecular interaction*

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THEORETICAL STUDIES ON THE MOLECULAR STRUCTURE, CONFORMATIONAL AND VIBRATIONAL ANALYSIS OF 4-(METHOXYCARBONYL) PHENYLBORONIC ACID

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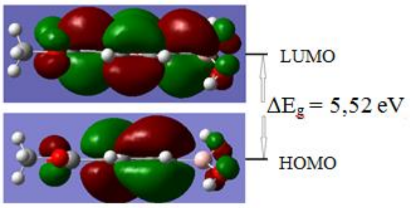
Abstract

Boronic acids containing organic compounds and their derivatives have found increasing attention due to their possible application potentials in the field of science like supramolecular chemistry, analytical chemistry, medicine, biology, catalysis, organic synthesis and crystal engineering [1-3]. Organic compounds containing boron shows unique neutron bombardment behavior and due to their preferential localization properties in tumor including tissues, they make possible boron-10 neutron capture therapy. The phenylboronic acid and its derivatives were investigated by several authors. Flanagan et al. [4] experimentally determined the crystal structure of 4- (methoxycarbonyl) phenylboronic acid. Recently, interesting studies have been devoted to the synthesis, characterization, physical and chemical properties and variety of these molecules. To the best of our knowledge, there is no theoretical and experimental study on 4-(methoxycarbonyl) phenylboronic acid except for molecular structure. In this work, a quantum-chemical investigation on the structural and non-linear optical properties of 4-(methoxycarbonyl) phenylboronic acid is carried out. We have studied the ground state geometrical energy, vibrational frequencies, conformational analysis, dipole moment, polarizability and first static hyperpolarizability, E_{HOMO} (the highest occupied molecular orbital energy), E_{LUMO} (the lowest unoccupied molecular orbital energy) and HOMO-LUMO energy gap (ΔEg) of title molecule by DFT/B3LYP and HF level of theory using the 6-311++G(d, p) basis set, in gas phase. Also, HOMO-LUMO energy gaps, dipole moment, polarizabilities, and static hyperpolarizabilities were calculated as a function of both dihedral angle (C3-C4-C7-O10) between methoxycarbonyl group and benzene ring and dihedral angle (C2-C1-B8-O11) between boronic acid OH groups and benzene ring. For the conformational analysis, torsion potentials were obtained for the molecule by performing a constrained geometry optimization of the structure as a function dihedral angles C3-C4-C7-O4 and C2-C1-B8-O11 which were from 0˚ to 180˚ by steps of 10˚ the B3LYP/6-311G(d,p) and HF/6-311G(d,p) methods. Structural parameters such as bond lengths, bond angles and dihedral angles of title molecules compared with data in the literature



Energy gap (ΔEg) of title molecule in theB3LYP/6-311++G (d, p)

Key Words: *4- (methoxycarbonyl) phenylboronic acid; polarizability; HOMO-LUMO.*

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THEORETICAL INVESTIGATIONS ON THE LINEAR, NONLINEAR OPTICAL, STRUCTURAL AND ELECTRONIC PROPERTİES OF NICOTINIC ACID AND ITS DERIVATIVES

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Abstract

Nicotinic acid (**I**) used in the treatment of diseases such as hypercholesterolemia and pellagra is known as niacin or B3 vitamin [1, 2]. Nicotinamide (**II**), which is a part of the same vitamin B group, is also used both as a dietary supplement and as a medicine [3]. Diethylnicotinamide (**III**), a derivative of **II**, is an important respiratory stimulant [4]. Nicotinohydrazide (**IV**), another derivative of **I**, is an efficient peroxidase-activated inhibitor of the POX activity of PGHS-2 [5]. Methyl nicotinate (**V**) is used in the synthesis of **IV**, one of the isomers of isonicotinic hydrazide, the most efficient antituberculosis drag [6].

We report the electrostatic potential, electronic energy, molecular structure and nonlinear optical properties of **I** - **V** and ethyl nicotinate (**VI**). Molecular properties were calculated by Hartree Fock (HF) and density functional theory (DFT) methods with the various basis sets. ^{1}H NMR and ^{13}C NMR chemical shifts calculations have been performed by using the DFT with B3LYP functional and HF methods, where the 6-311+G (2d, p) and 6-31G (d) basis sets were employed. The highest occupied molecular orbital (HOMO) energy, the lowest unoccupied molecular orbital (LUMO) energy values and non-linear optical properties such as dipole moment, polarizability and first order hyper polarizability of **I** - **VI** have been calculated with HF/ 6-311++G(d,p) and B3LYP/6-311++G(d,p) levels of DFT theory. The dipole moment for **I** - **VI** are calculated at 0.718, 1.445, 3.492, 0.993, 0.511 and 0.737 Debye, respectively with DFT/B3LYP level of theory the 6-311++G (d, p) basis set. The dipole moment value of **III** was the highest the dipole moment values in the studied molecules. Structural values of some of these molecules compared with data in the literature. All computational studies have been performed with the Gaussian 09W program package

Key Words: *Nicotinic acid; nicotinamide; nicotinohydrazide; non-linear optic; hyperpolarizability.*

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SYNTHESIS OF NEW RH(I) AND RU(III) COMPLEXES AND INVESTIGATION OF THEIR CATALYTIC ACTIVITIES ON OLEFIN HYDROGENATION IN GREEN REACTION MEDIA

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Abstract

Ionic liquids have better advantages in comparison with conventional organic solvent systems [1]. They can be used as biphasic catalytic systems with a suitable organic solvent with hosting the catalyst inside. In this study, two new Ru(III) and Rh(I) complexes of N-acyl benzotriazole derivative ligand have been synthesized and characterized. Complexes catalytic hydrogenation activities were tested on styrene and 1-octene under different reaction conditions in both [bmim][BF_4] and organic solvent. 100 % ethyl benzene conversion was obtained with Rh(I) and 86.6 % was found to be with Ru(III) complex. The catalytic experiments was also conducted in DMSO and toluene to make comparison with ionic liquid under the same conditions (393 K and 6h). In addition, 1-octene conversion was found to be 94.5 % with Rh(I) complex at 373 K for 1h. Hydrogen pressure and catalyst amount effect was also tested. Reusability tests of complexes was investigated in [bmim][BF_4] for five cycles under 10 bar H_2. In styrene hydrogenation, no activity loss was observed during five cycle with Rh complex (Figure 1).

Keywords: *N-acyl benzotriazole, ionic liquid, hydrogenation, Rhodium, Ruthenium.*

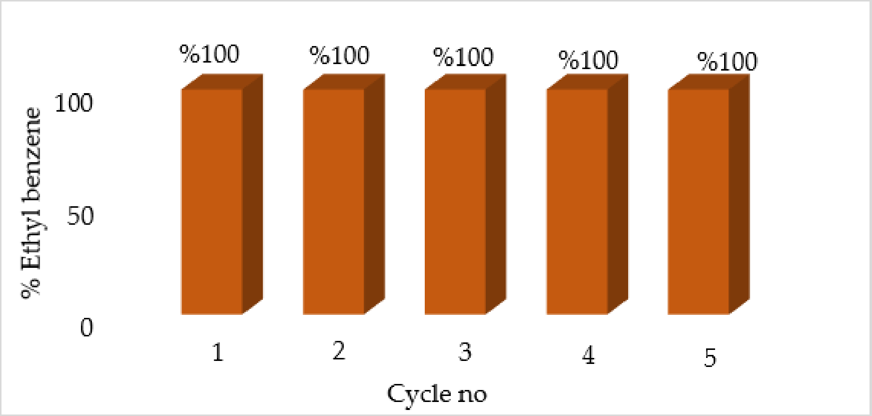

Figure 1. Reusability of [RhL(COD)]Cl catalyst in styrene hydrogenation

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SYNTHESIS AND IN VITRO ANTIOXIDANT PROPERTIES OF NEW 3-ALKYL(ARYL)-4-[3-ETHOXY-4-(BENZENESULFONYLOXY)-BENZYLIDENAMINO]-4,5-DIHYDRO-1*H*-1,2,4-TRIAZOL-5-ONES

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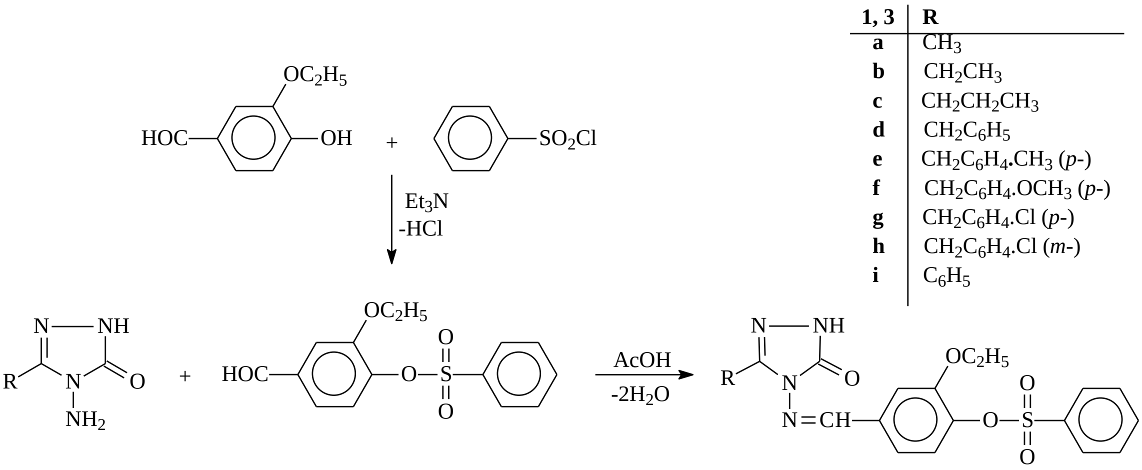
Abstract

Antioxidants are extensively studied for their capacity to protect organism and cell from damage that is induced by the oxidative stress. A great deal of research has been devoted to the study of different types of natural and synthetic antioxidant. A large number of heterocyclic compounds, containing the 1,2,4-triazole ring, are associated with diverse biological properties such as antioxidant, anti-inflammatory, antimicrobial and antiviral activity. Exogenous chemicals and endogenous metabolic processes in human body or in food system might produce highly reactive free radicals, especially oxygen derived radicals, which are capable of oxidizing biomolecules by resulting in cell death and tissue damage. Oxidative damages play a significantly pathological role in human diseases.

In this study, the reactions of 3-alkyl(aryl)-4-amino-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**1**) with 3-ethoxy-(4-benzenesulfonyloxy)-benzaldehyde (**2**) were investigated and nine novel 3-alkyl(aryl)-4-[3-ethoxy-4-(benzenesulfonyloxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**3**) were obtained. The structures of nine new compounds are established from the spectral data. Then, the antioxidant properties of **3** type compounds were studied and evaluated using different three antioxidant assays; including reducing power, free radical scavenging and metal chelating activity [2-4].

Key Words: *Schiff base; 1,2,4-triazole; synthesis; antioxidant; chelating activity*



1, 3	**R**
a	CH_3
b	CH_2CH_3
c	$CH_2CH_2CH_3$
d	$CH_2C_6H_5$
e	$CH_2C_6H_4.CH_3$ (*p*-)
f	$CH_2C_6H_4.OCH_3$ (*p*-)
g	$CH_2C_6H_4.Cl$ (*p*-)
h	$CH_2C_6H_4.Cl$ (*m*-)
i	C_6H_5

1 **2** **3**

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GAUSSIAN CALCULATIONS OF NOVEL 3-METHYL/ETHYL/n-PROPYL-4-[3-ETHOXY-4-(4-METHOXYBENZOXY)-BENZYLIDENAMINO)-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-5-ONES

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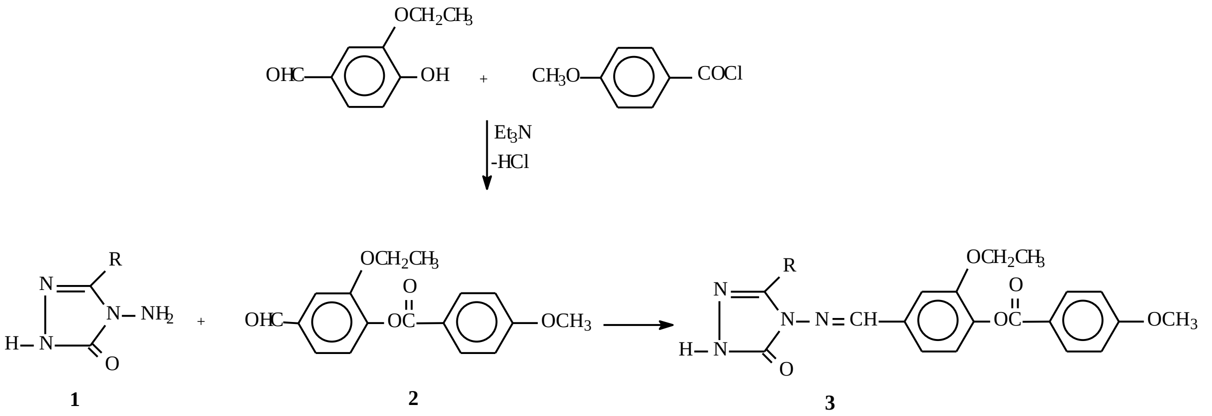
Abstract

In this study, three new 3-alkyl-4-[3-ethoxy-4-(4-methoxybenzoxy)-benzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**3a-c**) were synthesized by the reaction of 3-alkyl-4-amino-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**1a-c**) with 3-ethoxy-4-(4-methoxybenzoxy)-benzaldehyde (**2**), which was synthesized by the reaction of 3-ethoxy-4-hydroxybenzaldehyde with 4-methoxybenzoyl chloride by using triethylamine. The compounds synthesized were characterized by IR, ^{1}H-NMR,^{13}C-NMR and UV spectral data. These compounds were optimized by using the B3LYP/6-31G (d,p) and HF/6-31G (d,p) basis sets [1,2]. ^{1}H-NMR and ^{13}C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 [2]. Experimental and theoretical values were inserted into the grafic according to equatation of δ exp=a+b. δ calc. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. IR absorption frequencies of analysed molecules were calculated by two methods. The veda4f program was used in defining IR data which were calculated theoretically [3]. The experimental and the obtained theoretical values were compared and found by regression analysis that are accurete. Furthermore, geometric properties (bond angles, bond lengths and dihedral angles), thermodynamic parameters, electronic properties (total energy, dipole moment), the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), Mulliken atomic charges of 3-alkyl-4-[3-ethoxy-4-(4-methoxybenzoxy)-benzylidenamino)-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**3a-c**) have been investigated by using Gaussian 09W program. The structural data of these compounds have been calculated by using 6-31G(d,p) basis set with density functional method (DFT/B3LYP) and Hartree-Fock method (HF).

Key Words: *4,5-Dihydro-1H-1,2,4-triazol-5-one, Gaussian 09W, 6-31G(d,p) basis set, molecular structure analysis, vibrational frequencies*



a) R=CH_3; **b)** R=CH_2CH_3; **c)** R=$CH_2CH_2CH_3$

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INTERACTION OF PLATINUM BASED COMPLEXES WİTH DNA AND DEVELOPMENT OF ELECTROCHEMICAl DNA BIOSENSORS

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Abstract

The electrochemical behaviour and the interaction of $[Pt(bpy)(pip)]^{2+}$ **(1)**, $[Pt(bpy)(hpip)]^{2+}$, **(2)**, $[Pt(bpy)(iip)](PF_6)$ **(3)** and $[Pt(bpy)(miip)](PF6)_2$ (4) with DNA were investigated. These platinum (II) complexes have exhibited to interact with DNA through intercalation mode. For the cyclic voltammetry experiments, since a larger decrease in the peak current and more positive shift in the peak potential were observed in the presence of 4, it can be concluded that 4 possesses higher intercalative binding affinity towards DNA with respect to the other platinum compounds[1-3]. Electrochemical DNA biosensor based on the immobilization of ds-DNA and ss-DNA probe and **1** and **2** onto electrochemically activated glassy carbon (GC) electrode were also accomplished. The immobilization of ds-DNA and ss-DNA probe and hybridization experiments were studied through differential pulse voltammetry using **1** and **2** as hybridization indicators. Platinum complexes, **1** and **2**, showed larger electrochemical signals for the hybridized probe ds-DNA with respect to ss-DNA immobilized on glassy carbon electrode. The developed electrochemical DNA biosensor was found to have good selectivity and analytical performance for the complementary target nucleotide with limit of detection of 1.23×10^{-8} mol L^{-1} and 8.05×10^{-9} mol L^{-1} for the complex **1** and **2**, respectively.

Key Words: *Platinum complexes; DNA binding; Intercalation; DNA biosensor*

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ACUTE PHASE PROTEINS and BIOCHEMICAL and OXIDATIVE STRESS PARAMETERS in *HYPODERMA Spp.* INFESTED CATTLE

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Abstract

The aim of the present study was to determine concentrations of acute phase proteins (APP), oxidative stress and some biochemical parameters in naturally infested cattle with *Hypoderma spp*. For this purpose, 10 clinically healthy cattle as controls and 25 Brown Swiss cattle with *Hypoderma spp.* were used. Blood samples were collected to tubes from jugular vein. Parts of blood samples were stored without any process as a whole blood. The serum was separated from the remaining blood samples. The reduced glutathione (GSH) in whole blood and the level of malondialdehyde (MDA), haptoglobin (Hp), ceruloplasmin, serum amyloid A (SAA), AST, GGT, ALP, CK, albumin, urea and total protein levels in serum were colorimetrically determined. The present study indicated that the concentrations of Hp, SAA, ceruloplasmin, AST, GGT, ALP, CK, and MDA were significantly increased, and albumin, total protein, GSH concentrations were significantly decreased in the *Hypoderma spp.* infested group compared to the control group. In conclusion, the production of APP increased in a response to acute phase response in animals with subcutaneous warbles. Furthermore, liver functions were also shown to be impaired and oxidative stress developed as a result of metabolic products of the parasite in *Hypoderma spp.* infested cattle.

Key Words: *Acute Phase Proteins, Biochemical Parameters, Cattle, Hypoderma spp., Oxidative Stress*

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THE EFFECT OF MAGNETIC FIELD ON THE THERMOELECTRIC PROPERTIES OF POLYTHIOPHENE

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Abstract

Conducting polymers have attracted much attention in various fields owing to their potential applications in flexible and transparent devices because of attractive properties such as easy synthesis, low intrinsic thermal conductivity, high electrical conductivity, cost effectiveness, the ability to be mass produced by use of straightforward synthetic methods, and the ability to be deposited over large areas compared to the inorganic semiconducting materials. It was observed the molar mass and mechanical properties of polymers increase when the polymer synthesis under magnetic field [1]. It was expected to increase the thermoelectric properties of polythiophene (PTH) because of the increased chain length under magnetic field.

PTH was synthesized under various magnetic field intensities in order to reveal the effect of magnetic field to electrical conductivity and Seebeck coefficient in this study. PTH was synthesized by chemical oxidation using the emulsion polymerization process with or without the presence of a continuous magnetic field. The particle sizes of the nanoparticles in the colloidal aqueous solutions were measured by dynamic light scattering and scanning electron microscopy. The electrical conductivities of the samples were measured by four-point-probe technique. The electrical conductivity of the samples increased approximately one order but the Seebeck coefficient did not changed considerably with increasing magnetic field intensity. Dynamic light scattering, FTIR-ATR and UV-visible spectroscopy techniques were also used for the characterization.

Key Words: *Conducting polymer, Polythiophene, Seebeck coefficient, magnetic field, thermoelectric.*

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SYNTHESIS, NON-AQUEUS MEDIUM TITRATIONS, ANTIOXIDANT AND ANTIMICROBIAL ACTIVITIES OF SOME NEW 4-[(3-ALKYL(ARYL)-5-OXO-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-4-YL)-IMINOMETHYL]-PHENYL 3-METHOXYBENZOATES

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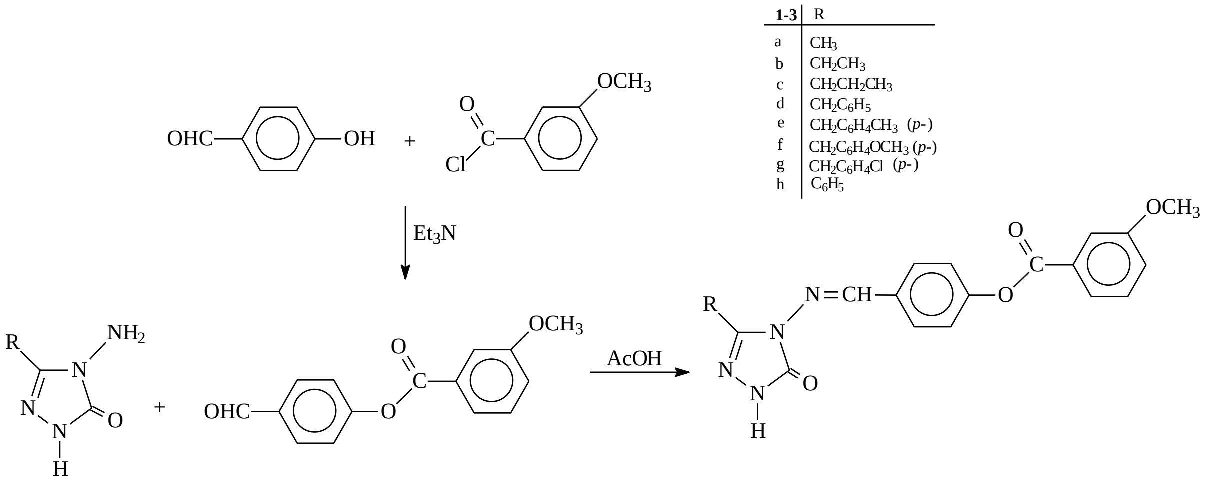
Abstract

In the present study, nine novel 4-[(3-alkyl(aryl)-5-oxo-4,5-dihydro-1*H*-1,2,4-triazol-4-yl)-iminomethyl]-phenyl 3-methoxybenzoates (**3**) were synthesized from the reactions of the corresponding 3-alkyl(aryl)-4-amino-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**1**) with 4-formylphenyl 3-methoxybenzoate (**2**), which was obtained from the reaction of 4-hydroxybenzaldehyde with 3-methoxybenzoyl chloride by using triethylamine. The new compounds synthesized were characterized by using IR and ^{1}H-NMR, ^{13}C-NMR spectral data. The second part of the study, nine novel 4-[(3-alkyl(aryl)-5-oxo-4,5-dihydro-1*H*-1,2,4-triazol-4-yl)-iminomethyl]-phenyl 3-methoxybenzoates (**3**) were titrated potentiometrically with TBAH in non-aqueous solvents (isopropyl alcohol, tert-butyl alcohol, acetone and N,N-dimethylformamide) and graphs were drawn for all cases. The half notralization potentials and pK_a values were determined by half neutralization method [1].

In the third part of the study, the antioxidant properties of the compounds **3** were studied using by three antioxidant assays (reducing power, free radical scavenging and metal chelating activity). For the measurement of the reductive ability, Fe^{3+}-Fe^{2+} transformation was investigated in the presence of title compound [2]. The hydrogen atoms or electrons donation ability of the synthesized compounds were measured by DPPH$^·$ [3]. The chelating effect of ferrous ions by the compounds were determined [4]. BHT, BHA and α-tocopherol were used as reference antioxidant compounds.

In the last part of the work, antimicrobial activities of compounds **3** were measured by using an agar well diffusion method [5] and the results obtained were evaluated.



1-3	R
a	CH_3
b	CH_2CH_3
c	$CH_2CH_2CH_3$
d	$CH_2C_6H_5$
e	$CH_2C_6H_4CH_3$ (*p*-)
f	$CH_2C_6H_4OCH_3$ (*p*-)
g	$CH_2C_6H_4Cl$ (*p*-)
h	C_6H_5

1 **2** **3**

Key Words: *1,2,4-Triazole, synthesis, pK$_a$, antioxidant, antimicrobial activity*

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GREEN SYNTHESIS OF SOME NOVEL BIOACTIVE BENZIMIDAZOLE DERIVATIVES

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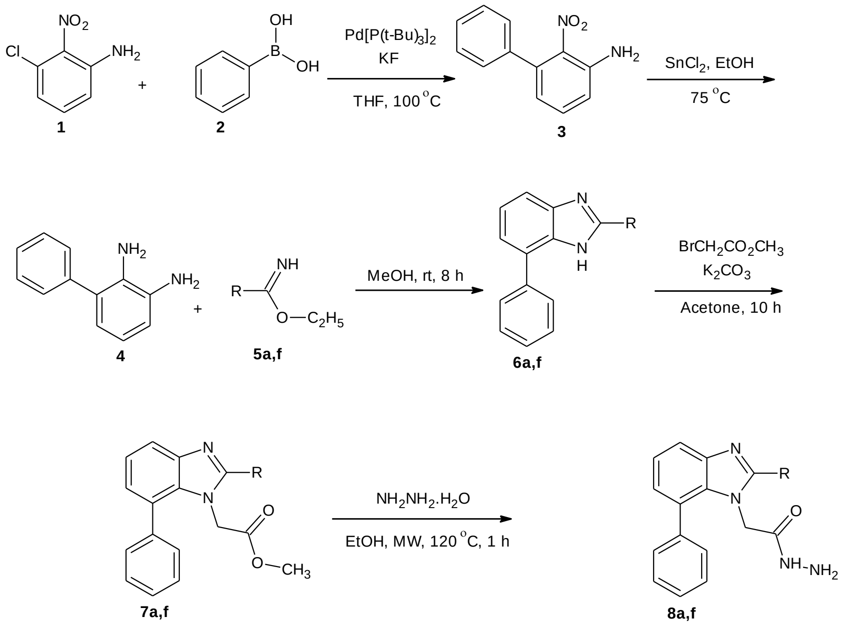
Abstract

Benzimidazole derivatives are represented by a wide variety of medicines, such as albendazole, thiabendazole, omeprazole, carbendazim, mebendazole, and timoprazole [1-3], while in nature the benzimidazole moiety is found in the structure of vitamin B12 [4].

In our previous studies, we have synthesized some bioactive benzimidazole derivatives. Some of the compounds were shown to demonstrate important antitumor, antioxidant, and lipase inhibition activities [5-8].

In the last of these studies we focused on the synthesis of novel benzimidazole (6a-f) as potent anti-tyrosinase and antioxidant agents [8]. In the current study we synthesized, with a green approach, from these benzimidazoles (6a-f) to benzimidazole-acetates (7a-f) and benzimidazole-acetohydrazides (8a-f) derivatives. These 12 new derivatives (7a-f and 8a-f) have been screened for their enzyme inhibition and antioxidant activities.



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Thermoelectric Properties of THE poly(3,4-ethylene dioxythiophene) AND BINARY ZINC Copper SULFIDE COMPOSITES

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Abstract

A thermoelectric (TE) material can be used to generate electricity or temperature difference. The TE materials used in the state-of-the-art technology are rigid, toxic and expensive inorganic semi-conductive metal alloys. Conducting polymers have a great potential to produce more preferable TE materials since they have superior properties such as flexibility, lightness, low cost, non-toxicity, easy synthesis and processibility in comparison to inorganic materials. The studies suggest that poly(3,4-ethylene dioxythiophene) (PEDOT) is the most promising among the conductive polymers because of its high conductivity, stability and flexibility although its own figure-of-merit is not high enough, yet [1]. It would appear that the most preferable way to improve the TE properties of PEDOT is to prepare its inorganic hybrid nanocomposites with high Seebeck coefficient. Metal sulfides were started to be investigated as TE materials because of their low costs, low toxicity, and optimizable TE properties in recent years [2].

In this work, we first report a facile method for preparation of $Zn_xCu_{1-x}S$ by co-precipitation in solution and then preparation of $Zn_xCu_{1-x}S$/PEDOT composite films and their microstructure and TE properties. To the best of our knowledge, TE properties of this composite have not been reported in literature.

Key Words: *Thermoelectric****,*** *zinc sulfide, PEDOT, composite, zinc copper sulfide*

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METAL COMPLEXES OF PERIMIDINE AND SCHIFF BASE LIGANDS BEARING BOTH NAPHTHALENE AND CHROMONE MOIETIES: SYNTHESIS AND CATALYTIC ACTIVITY

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Abstract

The synthesis and characterization of transition metal complexes with various ligand systems containing nitrogen and oxygen donor atoms has been the subject of great interest because of their wide applications in various fields. Among these ligand systems, while Schiff bases have been studied extensively for decades, in recent years considerable attention has been drawn to perimidines as they have electron affinity, reduction potential and also exhibit diverse range of biological activities [1,2]. Usually the product of the condensation reaction of primer amines with various carbonyl groups is Schiff base, however when 1,8-diaminonaphthalene is used as primer amine it can be obtained perimidine derivatives [3].

In this study, a new Schiff base and a new 2,3-dihydro-*1H*-perimidine derivative were synthesized from the condensation reaction of same carbonyl compound (6-formyl-7-hydroxy-5-methoxy-2-methylbenzopyran-4-one) with 2,3-diaminonaphthalene and 1,8-diaminonaphthalene, respectively. Cu(II) and Fe(II) complexes of the ligands were obtained by using appropriate metal salts. The prepared compounds were characterized by UV-Vis, FT-IR, NMR and mass spectroscopy, elemental, AAS and TGA analyses, molar conductivity and magnetic susceptibility. The catecholase activity of the complexes was performed for the oxidation of 3,5-di-*tert*-butylcatechol in methanol at 25°C by monitoring the increase of the absorption band at 390-400 nm of the product 3,5-di-*tert*-butylcatequinone. The compatibility of catalytic reaction with Michaelis-Menten kinetics also investigated by the method of initial rates.

Key Words: *Perimidine; Schiff Base; Metal Complexes; Catecholase Activity; Michaelis-Menten kinetics.*

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EFFECTS OF DIETARY ZINC AND L-ARGININE SUPPLEMENTATION ON TOTAL ANTIOXIDANTS CAPACITY, LIPID PEROXIDATION, NITRIC OXIDE, EGG WEIGHT, AND BLOOD BIOCHEMICAL VALUES IN JAPANASE QUAILS

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Abstract

Zinc is a hydrophilic metal which is found in the structure of more than 300 enzymes and molecules in the body. It is an essential element in many physiological functions including growth, immune response, reproduction, and antioxidant defense [1–4]. In addition, zinc plays an important role in pregnancy, bone growth, milk production, and egg production [5, 6].
The aim of this study was to evaluate effects of dietary zinc and L-arginine supplementation on blood total antioxidant capacity (TAC), malondialdehyde (MDA), nitric oxide (NO), some blood chemistry parameters, and egg weights of laying quails. Three groups of Japanese quails were fed with a diet containing L-arginine (5 mg/kg), zinc (60 mg/kg), and normal basal diet (control) for 30 days. TAC, lipid peroxidation, and biochemical analysis were performed in the blood of animals. L-Arginine and zinc supplementation improved TAC and reduced MDA concentrations compared to the control ($P<0.05$). In comparison to the control, blood NO concentrations were increased by Larginine ($P<0.01$) and zinc treatment ($P<0.05$). Both zinc ($P<0.001$) and L-arginine ($P< 0.01$) supplementation significantly increased egg weight in laying quails. Some of the blood chemistry parameters were also altered by the treatment of L-arginine and zinc supplementation. No difference was found in blood albumin and creatinine levels among the groups. Blood glucose ($P=0.833$) and total protein ($P=0.264$) levels in control and Larginine-treated groups were found to be similar. Glucose and total protein levels were decreased in zinc-supplemented animals compared to the control and L-arginine groups ($P< 0.05$). No difference was found in triglyceride levels between control and zinc-applied groups ($P=0.197$). However, L-arginine treatment reduced the blood triglyceride levels compared to the control ($P<0.05$). In conclusion, L-arginine and zinc supplementation could be beneficial and effective for decreasing oxidative stress, boosting antioxidant capacity, and improving egg weight in the blood of the animals.

Key Words: *Zinc, L-Arginine,Totalantioxidant capacity, Nitric oxide, Egg weight*

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IN-VITRO ANTIOXIDANT AND BIOLOGICAL ACTIVITIES OF SOME NEW 1,2,4-TRIAZOLE DERIVATIVES WITH THEIR POTENTIOMETRIC TITRATIONS

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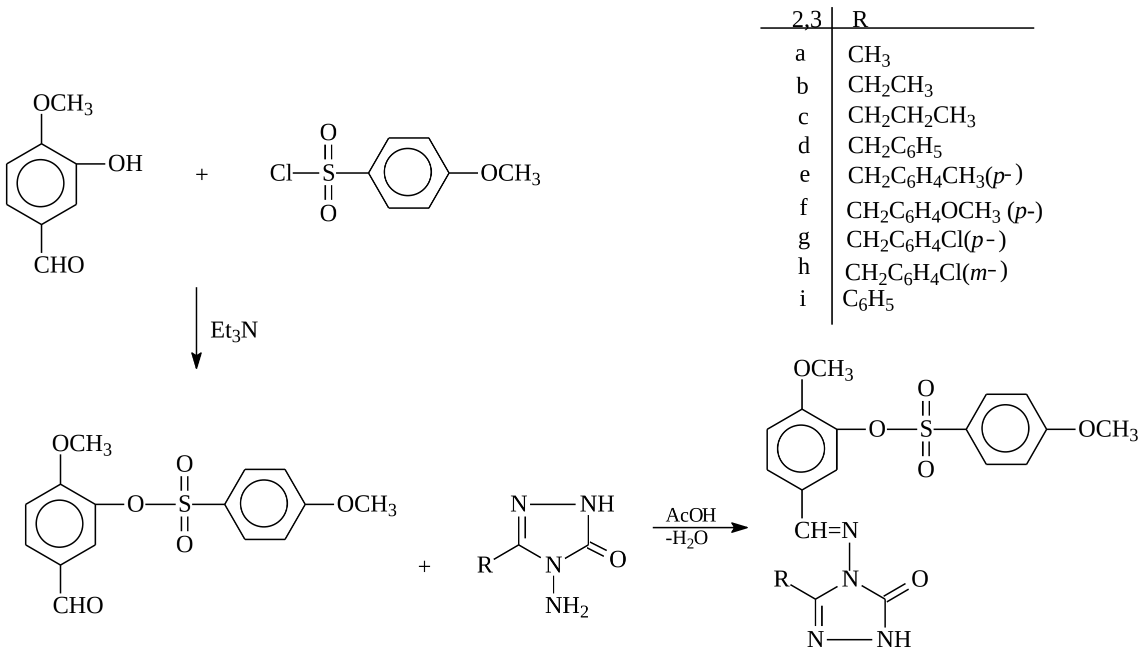
Abstract

1,2,4-Triazole derivatives have drawn considerable attention for the past few decades due to their diverse biological properties. Many 1,2,4-triazole derivatives are found to be potent antioxidant, anti-inflammatory, antimicrobial and antiviral agents [1]. On the other hand, it is known that 1,2,4-triazole and 4,5-dihydro-1H-1,2,4-triazol-5-one rings have weak acidic properties, so that some 1,2,4-triazole and 4,5-dihydro-1H-1,2,4-triazol-5-one derivatives were titrated potentiometrically with tetrabutylammonium hydroxide in non-aqueous solvents, and the pK_a values of these compounds for each non-aqueous solvent [2].

This study was planned as four parts. The first part contains that synthesis of new compounds. In this section, nine new 3-alkyl(aryl)-4-[3-(4-methoxybenzenesulfonyloxy)-4-methoxybenzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**3**) were synthesized from the reactions of 3-alkyl(aryl)-4-amino-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (**2**) with 3-(4-methoxybenzenesulfonyloxy)-4-methoxybenzaldehyde (**1**), which was synthesized by the reaction of 3-hydroxy-4-methoxybenzaldehyde with 4-methoxybenzenesulfonyl chloride by using triethylamine. In the second part of the study, the antioxidant activity of **3** type compounds were tested by ferric-reducing antioxidant power, 1,1-diphenyl-2-picrylhydrazyl (DPPH) assays and Fe^{2+} – metal chelating assay [3-5]. And then, the antimicrobial activity of compounds **3** were investigated by used agar well diffusion method [6]. At the end of the study, the newly synthesized compounds **3** were titrated potentiometrically with tetrabutylammonium hydroxide in isopropyl alcohol, tert-butyl alcohol, acetonitrile and N,N-dimethylformamide and the half-neutralization potential values and the corresponding pK_a values were determined for all cases.

Key Words: *Synthesis; antioxidant; antimicrobial; pK_a; acidity*



2,3	R
a	CH_3
b	CH_2CH_3
c	$CH_2CH_2CH_3$
d	$CH_2C_6H_5$
e	$CH_2C_6H_4CH_3$(*p*-)
f	$CH_2C_6H_4OCH_3$ (*p*-)
g	$CH_2C_6H_4Cl$(*p*-)
h	$CH_2C_6H_4Cl$(*m*-)
i	C_6H_5

1 **2** **3**

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SYNTHESIS, ANTIOXIDANT AND ANTIMICROBIAL PROPERTIES OF NEW MANNICH BASES CONTAINING 1,2,4-TRIAZOLE MOIETY

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Abstract

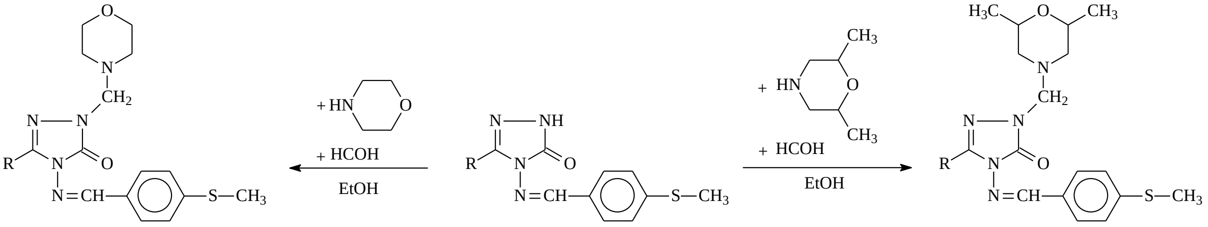
Triazoles are heterocyclic compounds that contain three nitrogen atoms. 1,2,4-Triazole and 4,5-dihydro-1H-1,2,4-triazol-5-one derivatives are reported to possess a broad spectrum of biological activities such as analgesic, antibacterial, antioxidant and antiparasitic properties [1-3]. Considering about the development of new hetero moieties by combining potential biological active scaffolds, an attempt was made here to obtain 1,2,4-triazoles bearing morpholine ring and to evaluate their antioxidant activity.

In this regard, eight new 1-(morpholine-4-yl-methyl)-3-alkyl(aryl)-4-(4-methylthiobenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-ones (**2**) and seven new 1-(2,6-dimethylmorpholine-4-yl-methyl)-3-alkyl(aryl)-4-(4-methylthiobenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-ones (**3**) were synthesized by the reactions of 3-alkyl(aryl)-4-(4-methylthiobenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-ones (**1**) with formaldehyde and morpholine, 2,6-dimethylmorpholine, respectively. 3-alkyl(aryl)-4-(4-methylthiobenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-ones (**1**) were synthesized according to literature [4]. The titled compounds were characterized by IR, ^{1}H NMR and ^{13}C NMR spectral data.

In the second part of the study, the antibacterial properties of the compounds **2** and **3** investigated by using Agar well diffusion methods against some different strains and data were recorded.

In the last part of the study, the antioxidant properties of the compounds **2** and **3** were studied and evaluated using different three antioxidant assays; including reducing power, free radical scavenging and metal chelating activity.

Key Words: *Mannich base; 1,2,4-triazole; synthesis; antioxidant; antimicrobial*



2 **1** **3**

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A FIBROUS SOLID ELECTROLYTE FOR LITHIUM-ION BATTERIES

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Abstract

Lithium-ion batteries are the preferred system for large-scale energy storage, particularly in automobiles. Most common rechargeable Li-ion batteries are made using organic liquid electrolytes, which is currently the major constraint for design and production of these batteries for large-scale applications. The liquid electrolyte can leak through the containment walls of the battery and can catch fire or cause an explosion due to the flammability of lithium exposing to air. The replacement of the organic liquid electrolyte with a more reliable inorganic solid electrolyte in all-solid-state Li-ion batteries simplifies the design of these batteries and improves their durability. Compared to liquid electrolytes, nonflammable solid electrolytes significantly improve the safety of the batteries. Moreover, direct stacking of all-solid-state cells in one package yields a high operating voltage in a smaller volume and provides higher energy density. In order to achieve the potential advantages of solid-state batteries and to commercialize this class of batteries, thin films of the solid electrolytes were developed to provide low resistance for lithium-ion transfer. Current vacuum-based deposition techniques such as pulsed-laser deposition, atomic layer deposition, and magnetron sputtering that are used in laboratory environments and electronics industry are too costly and therefore do not allow for scale-up of the process and commercial production of large-scale batteries. Furthermore, a good contact between the solid electrolyte and electrode materials cannot be readily obtained, making it difficult to fabricate an all-solid-state battery.

The new methodology proposed in this work uses oxide filaments/fibers instead of a dense thin film electrolyte, allowing: (i) straightforward fabrication without the use of costly thin film production techniques, (ii) minor changes in the existing Li-ion battery production lines, and (iii) better mechanical stability and electrochemical performance. $Li_7La_3Zr_2O_{12}$ (LLZO) fibers as an electrolyte were prepared using the electrospinning technique. This technique is widely used for fabricating fibers from a wide range of materials, including oxysalts, oxides, and sulfides, with diameters ranging from several nanometers to micrometers and lengths up to several millimeters. The process is based on the unidirectional elongation of a spinnable viscoelastic solution by considering various parameters involved in the electrospinning process [1]. The crystallographic phase and morphology of the products was studied X-ray diffraction (XRD) patterns and scanning electron microscopy (SEM), respectively.

The results indicated that the produced electrolyte would be a good alternative of all-solid-state batteries for electric vehicles in terms battery of safety and performance.

Key Words: *All-solid-state Li-ion battery; fiber electrolyte; LLZO, battery safety; battery performance*

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SYNTHESIS AND INVESTIGATION OF ANTIOXIDANT ACTIVITIES OF NOVEL 3-ALKYL(ARYL)-4-[4-METHOXY-3-(4-NITROBENZOXY)-BENZYLIDENAMINO]-4,5-DIHYDRO-1*H*-1,2,4-TRIAZOL-5-ONES

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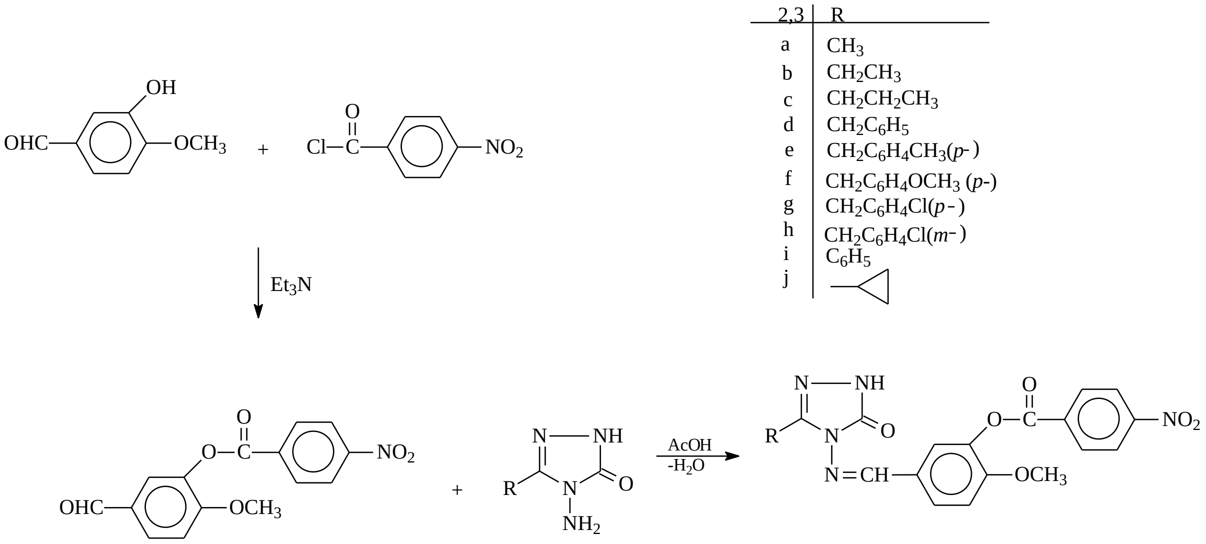
Abstract

Antioxidants are extensively studied for their capacity to protect organism and cell from damage that is induced by the oxidative stress. A great deal of research has been devoted to the study of different types of natural and synthetic antioxidant. A large number of heterocyclic compounds, containing the 1,2,4-triazole ring, are associated with diverse biological properties such as antioxidant, anti-inflammatory, antimicrobial and antiviral activity. Exogenous chemicals and endogenous metabolic processes in human body or in food system might produce highly reactive free radicals, especially oxygen derived radicals, which are capable of oxidizing biomolecules by resulting in cell death and tissue damage. Oxidative damages play a significantly pathological role in human diseases.

In this study, ten novel 3-alkyl(aryl)-4-[4-methoxy-3-(4-nitrobenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (3a-j) were synthesized by the reactions of 3-alkyl(aryl)-4-amino-4,5-dihydro-1*H*-1,2,4-triazol-5-ones (2a-j) with 4-methoxy-3-(4-nitrobenzoxy)-benzaldehyde (1) and characterized by IR, ^{1}H NMR, ^{13}C NMR and UV spectral data. Then the antioxidant properties of the compounds were studied and evaluated using different three antioxidant assays, including reducing power, free radical scavenging and metal chelating activity. For the measurement of the reductive ability, Fe^{3+}-Fe^{2+} transformation was investigated in the presence of compound using by the method of Oyaizu [1]. The hydrogen atoms or electrons donation ability of the synthesized compound was measured by DPPH· using the method of Blois [2]. The chelating effect of ferrous ions by the compound was determined according to the method of Dinis et al [3]. BHT, BHA and α-tocopherol were used as reference antioxidant compounds.

Key Words: 1,2,4-Triazole, *Synthesis; antioxidant*



1 **2** **3**

2,3	R
a	CH_3
b	CH_2CH_3
c	$CH_2CH_2CH_3$
d	$CH_2C_6H_5$
e	$CH_2C_6H_4CH_3$(*p*-)
f	$CH_2C_6H_4OCH_3$ (*p*-)
g	$CH_2C_6H_4Cl$(*p*-)
h	$CH_2C_6H_4Cl$(*m*-)
i	C_6H_5
j	

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SYNTHESES, STRUCTURAL CHARACTERIZATIONS OF *cis*- AND *trans*- DISPIROCYCLIC FERROCENYLPHOSPHAZENES

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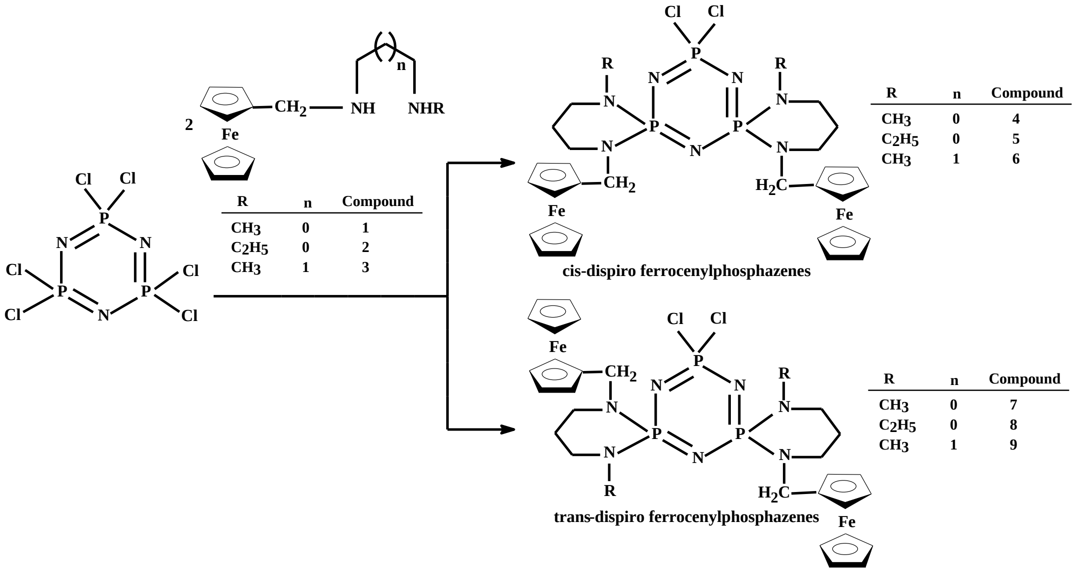
Abstract

Hexachlorocyclotriphosphazene (trimer; $N_3P_3Cl_6$) is a renowned phosphorus-nitrogen compound that has a wide range utility for the syntheses of trimeric phosphazene derivatives [1-3]. The condensation reactions of hexachlorocyclotriphosphazene, $N_3P_3Cl_6$, with N-alkly-N-monoferrocenyl-diamines, $FcCH_2NH(CH_2)_nNHR$ [n = 0, R = CH_3 (**1**); n = 0, R = C_2H_5 (**2**) and n = 1, R = CH_3 (**3**)] produced mainly new *cis*- (**4**, **5** and **6**) and *trans*- (**7**, **8** and **9**) dispirocyclic ferrocenylphosphazenes (Scheme1). The FTIR, ^{1}H, ^{13}C and ^{31}P NMR techniques were used for the characterization of these compounds. In addition, the molecular and solid state structures of **5**, **6**, **7** and **9** were evaluated using X-ray crystallography.



Scheme 1 Syntheses route of *cis*- (4-6) and *trans*- (7-9) dispirocyclic ferrocenylphosphazenes

Key Words: *Dispiroferrocenylphosphazenes, hexachlorocyclotriphosphazene, ferrocene, crystal structure, spectral analysis.*

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SYNTHESIS OF SIC FROM POLY(SILYNE-CO-CARBYNE) UNDER CO_2 ATMOSPHERE

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Abstract

A broad class of ceramics, called as polymer derived ceramics (PDCs), are prepared by the pyrolysis of polymer precursors in an ambient atmosphere. The common members of PDCs are secondary systems such as SiC, SiO_2, Si_3N_4, BN etc, ternary systems such as SiOC, SiCN and BCN, and quaternary SiBOC, SiOCN, SiBCN [1]. Owing to the solubility of polymer precursors, PDCs can also be processed in different structural forms as fibers, coatings, thin films etc. There are two types of polymer precursors; polysilynes and polycarbynes. Polysilynes include poly(methyl silyne) (PMSi), poly(phenyl silyne) and poly(hexyl silyne) [2]. Silicon carbide (SiC) is formed via thermal process of them under inert gas [3]. Poly(methyl carbyne), poly(phenylcarbyne) and poly(hydridocarbyne) (PHC) are the main members of polycarbynes, which are formed diamond and DLC upon pyrolysis [4]. As a result, the nature and chemistry of these organo-silicon polymeric precursors determine the composition of ceramic that will forms [5]. Poly(silyne-co-hydridocarbyne) (PSH) is one of these polymeric precursor and already contains silicon and organic carbon on its backbone, or is the combination of silyne and carbyne in one polymer [5]. Therefore it can be easily converted to silicon carbide with high yield and without requiring additional carbon species or any catalyst. In the study, it is reported the electrochemical synthesis of poly(silyne-co-hydridocarbyne) and the production of SiC from PSH upon thermal process under CO_2 and ambient atmosphere, which is the first attempt to produce SiC under CO_2 atmosphere. The electrochemical synthesis of PSH was accomplished electrochemical in 50 ml of an undivided cell, which contains trichloro(dichloro methyl) silane monomer (0.007 M, in 30 ml DME) and TBAFB (0.01 M, in 30 ml DME). −8.0 V potential was applied for the electrolysis during 8 h at room temperature and under an Ar atmosphere as reported in ref 5. The resulting PSH was characterized via UV/Vis, ^{1}HNMR, and FTIR spectroscopy. Then, PSH samples were heated to produce ceramics at 1000^{o}C, at 750^{o}C and at 500^{o}C in a tube furnace under a constant flow of CO_2, at a ramp rate of 10^{o}C/min, held for 24 h and then cooled to room temperature. The resulting ceramic, SiC, was characterized with Raman, FTIR, SEM, optical microscope and X-ray spectroscopy. The X-ray analysis of ceramic was showed that various SiC phases can be produced at different process temperatures. The material formed at 1000^{o}C is the mixture of Moissanite-5H, Moissanite-8H and Moissanite-84R while Moissanite-5H was obtained at 750^{o}C and amorphous phase was formed at 500^{o}C.

Key Words: electropolymerization; pre-ceramic polymer; silicon carbide; ceramic

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INFLUENCE OF PH ON THE BIOFUNCTIONALIZATION LEVEL OF POLY(ACRYLONITRILE-CO- GLYCIDYLMETHACRYLATE) NANOFIBERS

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Abstract

Nano-engineering materials are designed to illustrate novel and significantly improved physical and chemical properties. Nanofibers are an important class of such materials which have drawn considerable attention in the past decades because of their interesting properties such as high surface-to-mass (or volume) ratio that could be beneficial for advanced applications e.g. biomedicine, energy, filtration etc.. Electrospun nanofiber membranes (ENMs) possess high porosity, interconnected open pore structure and small tunable pore size. Such structural features nominate them as an excellent candidate for water and air filtration. Yet, they are highly hydrophobic and as low selective as microfiltration membranes. One solution to address such challenges is biofunctionalization of the nanofibers.[1,2] The protein ligands immobilized on the nanofibers not only hydrophilize them but also enhance selectivity and separation ability to ultrafiltration area. These outcomes are

influenced by the biofunctionalization level of the nanofibers. This level itself is impacted largely by environmental parameters such as pH of the medium wherein the biofunctionalization takes place. In the current study, we aim to evaluate the effect of this particular parameter on the biofunctionalization extent of a polymeric nanofiber mat of poly(acrylonuitrile-co-glycidylmethacrylate) (PANGMA). This polymer possess epoxide groups that can readily interact with amine groups of proteins, here, bovine serum albumin (BSA).

Keywords: *Electrospinning; Nanofibers; Membranes; Bio functionalization*

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2,3,4-TRIMETHOXY-5-IODOPHENYLBORONIC ACID AS EFFICIENT, GREEN AND ROOM TEMPERATURE CATALYST FOR DIRECT PEPTIDE SYNTHESIS

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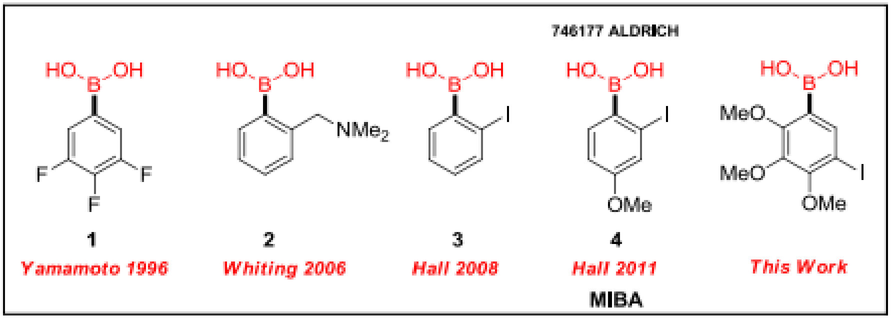
The peptide bond formation directly between carboxylic acids and amines is a fundamental transformation and one of the most commonly used in organic synthesis. Amides/peptides are presented in range of bioactive and synthetic compounds such as agricultures, insecticides and pharmaceutical drugs. [1] It has been estimated that 25% of synthetic pharmaceuticals contain a minimum of one amide bond.[2] Although amide bond formation is one of the most studied reaction in organic synthesis and is deeply employed by industry,[1a] an efficient method for direct coupling between carboxylic acids and amines continues to be an important scientific pursuit. A large number of methods for the formation of amides have been developed and reported, including: direct condensation of carboxylic acids with amines;[3] reaction of acid halides or anhydrides with amines;[4] and the reaction of activated carboxylic acids with amines using coupling reagents[1a, 5]and other approaches.[6] Most of these reported methods, with the exception of direct amide bond formation, are usually considered to be unstable, expensive, toxic and poorly atom-economic.[7] A direct condensation of carboxylic acids involving nucleophilic substitution by an amine nucleophile is known to be distinctively hard under acidic or basic conditions. Recent advances in this field include the use of arylboronic acids [ArB(OH)2] and boric acid [B(OH)3] as catalysts for direct amide bond formation. Some of the most efficient arylboronic acid catalysts are shown. In 1996, Yamamoto and co-workers reported the first catalytic use of electron deficient arylboronic acid, 3,4,5-trifluorophenylboronic acid 1. In 2006, Whiting and co-workers reported that 2-[(diisopropylamino)methyl]phenylb oronic acid 2 is also an effective catalyst. Ishihara and co-workers reported that Primary alkylboronic acids are active catalysts for amide bond formation of α-hydroxycarboxylic acids.[8] These catalysts required refluxing solvent at temperatures between 80- 110 °C for several hours. More recently, Hall and co-workers in 2008 demonstrated that 2-iodophenylboronic acids 3 and later on the second generation, 3-methoxy-2-iodophenylboronic acid, MIBA, 4 as catalytically active catalysts under mild conditions at room temperature in the presence of 4A° molecular sieves. It has been hypothesized that ortho substituent is essential for catalytic activity. The importance of ortho substituent has been confirmed by the poor activity of para-isomer whereas the meta-isomer has not been examined. Herein, we report the ability of 5-iodo-2,3,4-trimethoxyphenylboronic acid as the first meta-isomer to serve as an efficient and waste-free catalyst for direct amide bond formation of carboxylic acids at room temperature



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