

Editors

Ayhan Oral, Ph.D.
Ahmed Jashari, Ph.D.
Oğuz Gürsoy, Ph.D.

III. International
ISCMP
KOSOVO 2019

JOINT SCIENCE CONGRESS OF
MATERIALS AND POLYMERS

BOOK OF ABSTRACTS & PROCEEDINGS

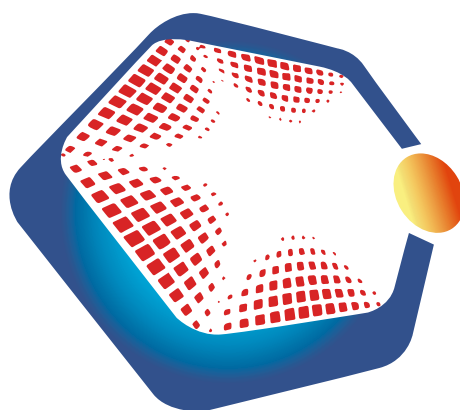
12 - 14 September 2019 - Pristina / KOSOVO

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BRK KİMYA VE
BİYOTEKNOLOJİ





III. International
ISCMP
KOSOVO 2019

ISCMP 2019

III. International Joint Science Congress of Materials & Polymers
12-14 September 2019 ■ Prishtina, Kosovo

BOOK of ABSTRACTS & PROCEEDINGS

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Editors:

Ayhan Oral, Çanakkale Onsekiz Mart University, Turkey

Ahmed Jashari, Tetova University, Macedonia

Oğuz Gürsoy, Burdur Mehmet Akif Ersoy University, Turkey

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Sidas Medya Ltd. Şti.: Fevzipaşa Blv. Çelik İş Merkezi Kat:3 D: 302 Çankaya, İzmir, Turkey

E-mail: sidasmedya@gmail.com

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Organized by
Çanakkale Onsekiz Mart University
Chemists Society
Turkish Cooperation and Coordination Agency
Tetova State University
Management Science University, Malaysia
Society of Chemists and Technologists of Macedonia
Prishtina University
Tunisian Chemical Society
Materials Research Society of North Macedonia

WELCOME ADDRESS

Dear participants,

Remarkable advances have been achieved in the science of materials and polymer over the last fifty years. A high quality of life away from environmental destruction has been set as a goal for a high level of human welfare and a sustainable future. As a result, more novel and functional materials have been introduced into everyday life. It is expected by not only sectoral and academic stakeholders but also end users that this process will last longer, producing more beneficial results.

Therefore, it is the primary aim of this scholarly gathering to transform research- and innovation-focused scientists, financial success promoting production, and social responsibility-oriented industry into strong stakeholders. To this end, an academic event will be jointly organized by the Chemists Society (Turkey), Çanakkale Onsekiz Mart University (Turkey), Republic of Turkey Prime Ministry-Turkish Cooperation and Coordination Agency, Tunisian Chemical Society (Tunisia), Prishtina University (Kosovo), Materials Research Society of North Macedonia (Macedonia), Management Science University (Malaysia), Tetova University (Macedonia) and Society of Chemists and Technologists of Macedonia (Macedonia) of four different countries with sectoral supports.

It is believed that the assembly of participants from different countries will allow them to share their knowledge, to exchange views, and to form various partnerships. Along with the scientific activities, a comprehensive social activities calendar was produced by the organizing committee to allow for fruitful interactions.

Although it is, broadly speaking, a scientific congress, it is different from other congresses in terms of such aspects as follows;

- (i) A collaboration protocol will be signed between the partners of the ICSMP following the completion of the Congress. Each partner will deliver a presentation on their strengths and interest in field of collaboration. Then, the partners will sign bilateral and multilateral agreements.
- (ii) Participants with posters will be allowed to deliver a four-minute presentation if they wish to and will be awarded a certificate of short oral presentation.

We would be more than happy to see you with us.

Assoc. Prof. Ayhan Oral
Prof. Jean-Francois Gerard

Chairpersons of of ISCMP 2019 Organizing Committee

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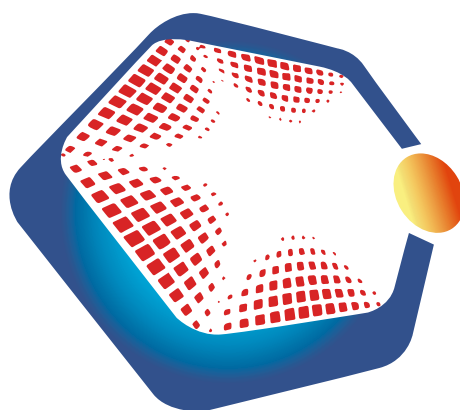
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**Sorted alphabetically by last name*



III. International
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KOSOVO 2019

ISCMP 2019 – SCIENTIFIC PROGRAM

September 11, 2019 (Wednesday)

| |
|---|
| Check-in to the Hotel (through the day) |
|---|

September 12, 2019 (Thursday)

| | | |
|----------------------|---|--|
| 09:00-17:00 | Registration | |
| 10:00-11:00 | Opening Remarks | |
| Section Chair | Metin Hayri Acar, Ph.D. | |
| 11:00-11:30 | Bruno Ameduri, Ph.D. | A Journey from the Synthesis of Functional 2-Trifluoromethacrylate Monomers to their Radical Copolymerizations with Vinylidene Fluoride, and Applications PLENARY SPEAKER |
| 11:30-11:50 | Jane Bogdan Bogdanov Ph.D. | Approaches for Design of Systems for Detection of Explosives Using Aromatic and Spiroconjugated Amines |
| 11:50-12:05 | Ana Holos Ph.D. Student | Influence of Carbon Nanotubes on ATRP Kinetics |
| 12:05-12:25 | Nazife Aslan Ph.D. | Investigation of Lead-210 Adsorption on Multi-Walled Carbon Nano Tube Modified with Onno Type Schiff Bases |
| 12:25-14:00 | Lunch | |
| Section Chair | Arianit Reka, Ph.D. | |
| 14:00-14:20 | Muhamad Nasir Ph.D. | Synthesis and Property of Quantum Carbon Dot/Polyvinyl Alcohol Nanofiber by Electrospinning |
| 14:20-14:40 | Avni Riza Berisha Ph.D. | First Principles Details into The Grafting of Aryl Radicals onto The Free-Standing and Borophene/Ag(111) Surfaces |
| 14:40-14:55 | Valbonë Veli Mehmeti Ph.D. Student | Exploring the Use of Nanomaterials as Corrosion Inhibitors. The Case of Carboxylated Graphene Oxide |
| 14:55-15:15 | Coffee Break | |
| Section Chair | Jean-Francois Gerard, Ph.D. | |
| 15:15-15:35 | Hasan Nazir Ph.D. | In Silico Analysis to Highlight the Effect of N1303K Mutation on CFTR Protein |
| 15:35-15:55 | Yavuz Emre Arslan Ph.D. | 3-Dimensional Bioscaffolds from Quince Seed Mucilage for Human Adipose-Derived Mesenchymal Stem Cells |
| 15:55-16:15 | Bashkim Ziberi Ph.D. | Use of Different Types and Environments of Smart Radiotherapy Biomaterials for Payload Release on Tumor Sites |
| 16:15-16:35 | Güliz Ak Ph.D. | Dual Drug Loaded Solid Lipid Nanoparticles for Glioblastoma Therapy via Intranasal Route: Development and Characterization of Nanoparticles |
| 16:35-16:55 | Asdren Zajmi Ph.D. | Effects of a Novel Chitosan-Loaded Bacteriophage Antibacterial Gel Against FusoBacterium Ulcerans for Tropical Skin Ulcer Treatment |
| 16:55-17:15 | Mustafa Alpaslan Ph.D. | Anticancer Effects of the Marine Extracts from Turkey |
| 17:15-17:30 | Hilal Deniz Yılmaz M.Sc. Student | Synthesis and Characterization of Si-Modified Quince Seed Mucilage based Bioscaffolds for Bone Tissue Engineering |
| 17:30-19:00 | POSTER SESSIONS | |

September 13, 2019 (Friday)

| | | |
|----------------------|---|--|
| Section Chair | Bruno Ameduri, Ph.D. | |
| 09:00- 09:30 | Mathias Destarac <i>Ph.D.</i> | Tailor-made polymers by aqueous RAFT polymerization (INVITED SPEAKER) |
| 09:30- 09:50 | Siddika Gamze Erzenin <i>Ph.D.</i> | New-Generation Superplasticizers for Concrete Industry |
| 09:50- 10:05 | Arta Veliu <i>Ph.D. Student</i> | New Nonstandard Method for Measuring Physical Properties of Homemade Polymer Filaments for 3D FFD printing |
| 10:05- 10:20 | Xheneta Zengo <i>M.Sc. Student</i> | Reinforcement of Gypsum with Polypropylene Fibers |
| 10:20-10:40 | Coffee Break | |
| Section Chair | Avni Riza Berisha, Ph.D. | |
| 10:40-11:10 | Traje Stafilov <i>Ph.D.</i> | Assessing the Environmental Impact of Metal Production. Case Study: The Republic of North Macedonia (INVITED SPEAKER) |
| 11:10-11:30 | Ahmed Jashari <i>Ph.D.</i> | Oxidation of Some Aldehydes to Acids with Jones Reagent Supported on The Diatomaceous Earth from The Republic of North Macedonia |
| 11:30-11:50 | Arianit Reka <i>Ph.D.</i> | Chemical, Mineralogical and Thermal Study of Rare Occurrence of Naturally Occuring Tridymite from Allchar |
| 11:50-12:05 | Gjani Hulaj <i>M.Sc. Student</i> | New Monograph Methods for Analysis of Some Small Anions in Three Different Pharmaceutical Formulations Using Suppressed Ion Chromatography |
| 12:05-12:20 | Omaira Anaya <i>Ph.D. Student</i> | Poly(1,2,3-triazolium imide)s Obtained Through AA+BB Click Polyaddition |
| 12:20-12:35 | Yalçın Coşkun <i>Ph.D.</i> | The Effect of Rose Essential Oil Component Phenyl Ethyl Alcohol on The Time-Dependent Mass Loss of Poly(Lactic Acid) |
| 12:35-14:00 | Lunch | |
| Section Chair | Jane Bogdan Bogdanov, Ph.D. | |
| 14:00-14:30 | Mahamadou Seydou <i>Ph.D.</i> | Understanding at Atomic Scale the Patterning of Some Substrates with Molecular Nanodomains Using the Self-Assembly Method (INVITED SPEAKER) |
| 14:30-14:50 | Elif Karacan Yeldir <i>Ph.D.</i> | Chitosan Microbeads for Encapsulation and Delivery of Essential Oils |
| 14:50-15:10 | Jean-Francois Gerard <i>Ph.D.</i> | Understanding Nanoscale Phenomena to Design High Performance Polymer-modified Bitumens |
| 15:10-15:30 | Tuğba Güngör Ertuğral <i>Ph.D.</i> | Functional Packaging Materials That Store Latent Heat in Food Safety |
| 15:30-15:45 | Eda Keskin Uslu <i>Ph.D. Student</i> | Rheological and Some Physicochemical Properties of Oleogels Prepared with Tallow and Partially Hydrolyzed Tallow Biomaterials |
| 15:45-16:00 | Nora Limani Bektashi <i>Ph.D. Student</i> | Characterization of Honey: Determination of Metal and Sugar Content |
| 16:00-16:20 | Coffee Break | |
| Section Chair | Traje Stafilov, Ph.D. | |
| 16:20-16:35 | Halime Çevikbaş <i>Ph.D. Student</i> | Investigation of Antibacterial and Antibiofilm Effects of Rose Essential Oil and Rose Absolute |
| 16:35-16:55 | Tülay Tütenocaklı <i>Ph.D.</i> | Salinity Threshold of Irrigation Water for Germination of Chickpea (<i>Cicer arietinum</i> L.) |
| 16:55-17:15 | Mustafa Akin <i>Ph.D. Student</i> | Edible Films Coating for Fruit Applications |
| 17:15-17:30 | Fatlında Rrahmani <i>M.Sc. Student</i> | Green Pesticides Based on Cinnamic Acid Dispersed in Hemp Fibers and Pectin |
| 17:30-19:00 | POSTER SESSIONS | |

September 14, 2019 (Saturday)

| | | |
|----------------------|---|---|
| Section Chair | Mathias Destarac, Ph.D. | |
| 09:00- 09:30 | Metin Hayri Acar <i>Ph.D.</i> | Thermally Induced Shape Memory Materials (INVITED SPEAKER) |
| 09:30- 09:50 | Serap Titretir Duran <i>Ph.D.</i> | Determination of Bisphenol A with Poly(p-Aminobenzoic Acid) Modified Gold Electrode by using Differential Pulse Voltammetry |
| 09:50- 10:05 | Muammer Burç <i>M.Sc. Student</i> | Voltammetric Determination of Diclofenac Sodium by using Poly(Beta-Cyclodextrin-co-2,4,6- Trimethylaniline) Modified Platinum Electrode |
| 10:05-10:35 | Coffee Break | |
| Section Chair | Mahamadou Seydou, Ph.D. | |
| 10:35-11:05 | Vural Bütün <i>Ph.D.</i> | Surface-Active and Stimuli-Responsive Polymers: Superb Sources for Various Polymeric Nanostructures and Applications (INVITED SPEAKER) |
| 11:05-11:20 | Veton Haziri <i>Ph.D. Student</i> | Electrochemistry of Oxygen Bubbles on Conductive and Non-Conductive Solids |
| 11:20-11:40 | Isa Degirmenci <i>Ph.D.</i> | The Thiol-Ene Polymerization of Natural Monomers: A DFT Study |
| 11:40-11:55 | Havva Yazar <i>M.Sc. Student</i> | Production of High Purity Alginate from Cystoseira Barbata Algae Collected out of Black Sea and Investigation of Usability As Biomaterial |
| 11:55-12:15 | CLOSING REMARKS | |
| 12:15-13:30 | Lunch | |
| 13:30-17:30 | SOCIAL ACTIVITY (PRIZREN EXCURSION) | |

ISCMP 2019 - POSTER PROGRAM

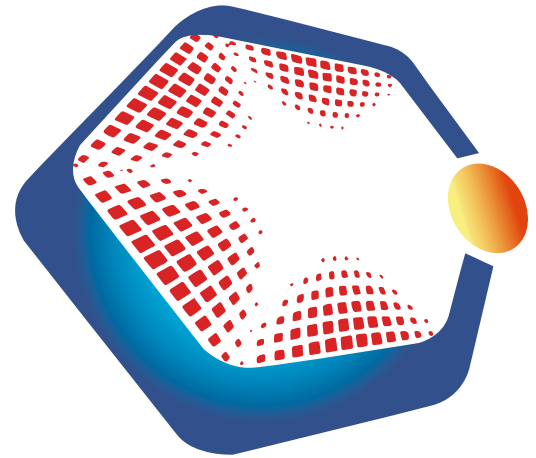
September 12, 2019

| NO | PRESENTER | TITLE |
|----|--------------------------|--|
| 1 | Admir Omaj | Docking Study of HIV-1 Reverse Transcriptase with a Virtual Library of Ligands |
| 2 | Admir Omaj | Structure Based Virtual Screening Studies to Identify Novel Potential Coumarin Derivatives for Cytochrome P450 14 Alpha-Sterol Demethylase |
| 3 | Senay Hamarat Sanlier | Dual Drug Loaded Solid Lipid Nanoparticles for Glioblastoma Therapy via Intranasal Route: Toxicological and Pharmacokinetic Studies |
| 4 | Fuat Shefqet Bislimi | A Study on Bacterial Adhesion of <i>Streptococcus</i> Mutans in Various Dental Ceramics: <i>In Vitro</i> Study |
| 5 | Merve Danisman | Investigation of Reaction Time and Enzyme Concentration Effects on Enzymatic Surface Modification of Hydroxyapatite |
| 6 | Emre Yilmaz | Biopolymer Production from Natural Sources and Usability as Biomaterials: Sodium Alginate and Collagen |
| 7 | Oğuz Gürsoy | Physicochemical and Rheological Properties of Commercial Kefir Drinks |
| 8 | Oğuz Gürsoy | Effect of Combined Application of Transglutaminase Enzyme and Ultrasonication Process on Physicochemical and Rheological Properties of Drinking Yogurt |
| 9 | Gülen Türker | Characterization of Polysaccharides from the Brown Algae <i>Colpomenia sinuosa</i> |
| 10 | Gülen Türker | Extraction and Characterization of Polysaccharides from the Red Algae <i>Gracilaria gracilis</i> |
| 11 | Seyhan Ulusoy | Antibacterial Cinnamaldehyde Loaded Nanofibers |
| 12 | Uğur Binbir | Allopathic Effects of Lavender Essential Oil on the Seed Germination and Seedling Development of Dent Corn (<i>Zea mays indentata</i> Sturt.) |
| 13 | Ali Sungur | Characterization of Biochar Produced from Green Walnut Shell |
| 14 | Beltina Iljazi | Stability of Alginate Gels in the Environments with Different pH Values |
| 15 | Güliz Ak | Preparation and Characterization of Antibiotic Nanocarrier from Aqueous Tillia Extract |
| 16 | Veprim Veli Thaçi | Recognizing Novel Potential Curcumin Derivatives for 6HDR Transferase Enzyme Based on Virtual Screening Studies |
| 17 | Ahmed Jashari | Green Surface Modification of Diatomaceous Earth from North Macedonia Using Olive Oil |
| 18 | Jane Bogdan Bogdanov | Development of Method for Detection of Volatile and Semivolatile Organic Compounds in Outdoor Urban Air in Skopje, Macedonia |
| 19 | Ljatifi R. Mahi | The Rise of the Coefficient Biosorption during Separation of Toxic Heavy Metals from Polluted Water by Modification of a Rise |
| 20 | Hamit Ismaili | Determination of Metals Mg, Ca, Zn, Fe, Cu, Ni, B, Pb, Mn, Cr, Vitamin C (Ascorbic acid), Sugar (Sucrose) to Vegetables (Potato- <i>Solanum toberosum</i> , Tomato – <i>Solanum lysopersicum</i> , Pepper – <i>Capsicum annum</i>) in Open Field and Greenhouse |
| 21 | Nimet Orgusha Sheqerxhiu | Grafting of the Gold Surface by Heterocyclic Moieties Derived through Electrochemical Oxidation of Amino Triazole-An Experimental and ab Initio Study |
| 22 | Egzon Ademi | Mineralogical Characterisation of Clayey Diatomite Sintered at 1200°C |
| 23 | Njomza Buxhaku | Characterization of the Porous Materials Obtained under Hydrothermal Procedure from Trepel and Portlandite |
| 24 | Milihate Xhafer Aliu | Occurrence and Enrichment Sources of Co, Cr and Ni in Soils of Mitrovica Region, Republic of Kosovo |

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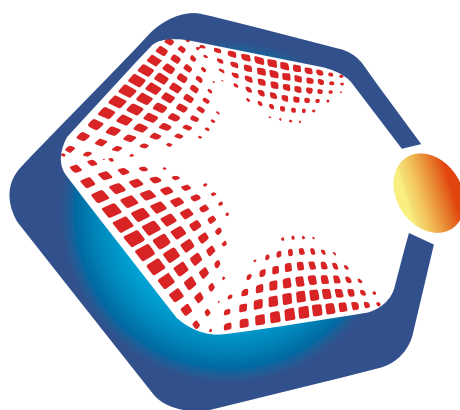
September 13, 2019

| NO | PRESENTER | TITLE |
|----|--------------------------|--|
| 24 | Avni Riza Berisha | The Attachment of Alkyl Groups onto a Graphene Monolayer. A DFT Study |
| 25 | Veton Haziri | Interaction of Oxygen Molecule onto Au(111) Surface Grafted by -Phenyl and -Carboxyphenyl Layers. A Theoretical Study |
| 26 | Rilinda Blerim Plakaj | The Adsorption of Ni(II) Ions onto Graphene Oxide: A Combined Experimental and Theoretical (DFT, Monte Carlo) Study |
| 27 | Rilinda Blerim Plakaj | Adsorptive Removal of Ni (II) Ions Using Graphene Oxide |
| 28 | Ardhmeri Arsim Alija | Graphene Oxide as an Effective Adsorbent for Methylene Blue Dye |
| 29 | Ardhmeri Arsim Alija | Monte Carlo Simulations and Experimental Study of the Methylene Blue Adsorption onto Graphene Surface |
| 30 | Drinisa Arsim Gashi | The Adsorption Performance of Graphene Oxide for Chromium Ions |
| 31 | Drinisa Arsim Gashi | Theoretical (Monte Carlo, DFT) and Experimental Study of the Adsorption of Chromium(VI) Ions onto Graphene Oxide |
| 32 | Veprim Veli Thaçi | Experimental and Theoretical Study of Some 2,5-Diarylidene-cyclopentanone Derivatives |
| 33 | Teonor Osmanaj | Synthesis, Characterization and Docking Studies of (4-(tert-butyl)-2,6-dimethylphenyl)boronic acid |
| 34 | Teonor Osmanaj | Adsorptive Behavior of Two 1,1'-binaphthalene Derivative onto the Pt Surface. A Combined Experimental and Theoretical Study |
| 35 | Sinecan Irem Bozkuş | New Trend in Energetic Materials Research; Co-Crystallization |
| 36 | Kübra Gürpınar | A Different Approach in Thermokinetic Analysis of Energetic Materials |
| 37 | Hasan Nazir | Theoretical Analysis of Fragment Contribution of Nitrogen-Reach Ligands and Bridge-Forming Co-Ligands to Molecular Orbitals of the Energetic Materials |
| 38 | Yaprak Gürsoy Tuncer | Effect of Electronegativity on Coordination Sphere in Coordination Compounds |
| 39 | Gjani Hulaj | The Impact of Covalent Surface Modification of the Active Carbon Powder in the Adsorption of Lindane |
| 40 | Songül Şen Gürsoy | A Novel Nonenzymatic Pesticide Sensor Based on Electropolymerized Polythiophene/TiO ₂ Nanocomposite |
| 41 | Kaltrina Avni Kastrati | Theoretical Study of Some Synthesized Carbazole-Pyridopyrimidine Derivative |
| 42 | Kaltrina Avni Kastrati | Synthesis and Characterization of Schiff Base Substituted Carbazole Bearing Pyridopyrimidine Compounds |
| 43 | Hasan Basri Karayel | The Effect of Natural Boron Mineral Use on the Essential Oil Ratio and Components of Musk Sage (<i>Salvia sclarea</i> L.) |
| 44 | Ljatifi R. Mahi | The Elimination of Aflatoxin B ₁ from the Pharmaceuticals Vegetative Raw Material Agnus Castus by Using Aluminium Oxide as an Adsorbent |
| 45 | Kaltrina Avni Kastrati | Theoretical Study of Some Synthesized Carbazole-Pyridopyrimidine Derivatives |
| 46 | Nimet Orgusha Sheqerxhiu | Electrochemical Grafting of Heterocyclic Amines on the Gold Surface |
| 47 | Nimet Orgusha Sheqerxhiu | Grafting of the Gold Surface by Heterocyclic Moieties Derived through Electrochemical Oxidation of Amino Triazole-An Experimental and ab Initio Study |
| 48 | Emira Fazlija | Characterization of the Porous Materials Obtained from Diatomite and Ca(OH) ₂ during Low-Temperature Hydrothermal Synthesis |
| 49 | Emira Fazlija | Effects of Thermal Treatment on Silica Phase Transition in Diatomite |
| 50 | Artan Gashi | Structure and stability of water clusters (H ₂ O) _n , n=2-30. Ab Initio Study |
| 51 | Artan Gashi | Comparison of the Performance of Different DFT Methods in the Calculations of the Stability and the Structure of Small |

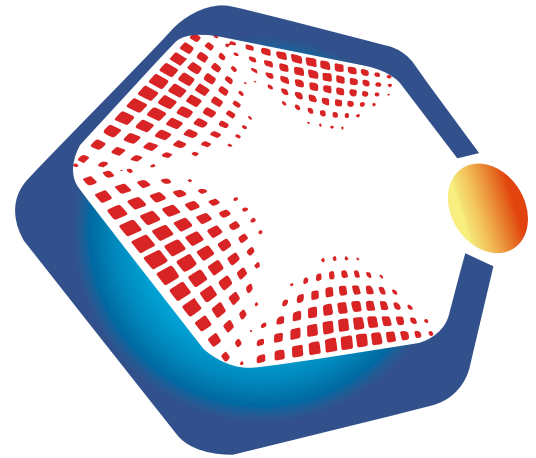


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**LIST OF
ABSTRACTS**



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III. International
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**INVITED
LECTURES**

Understanding Nanoscale Phenomena to Design High Performance Polymer-Modified Bitumens

J. F. Gerard*

Prof.
Ingénierie des Matériaux Polymères UMR CNRS
5223 , Université de Lyon, France

R. Gallu

Ingénierie des Matériaux Polymères UMR CNRS
5223 , Université Lyon, France

F. Dalmas

MATEIS UMR CNRS 5510, Université Lyon -INSA
Lyon, F-69621 Villeurbanne Cedex, France

F. Méchin

Ingénierie des Matériaux Polymères UMR CNRS
5223 , Université de Lyon, France

R. Perrin

14 rue de Saint-Nazaire, F-67025 Strasbourg Cedex
01, SOPREMA Co., France

F. Loup

8 rue du Dauphine, F-69964 Corbas Cedex,
EIFFAGE Co., France

Bitumen-based materials are widely used for waterproofing and road pavement applications. From a more fundamental point of view, bitumens are well-structured colloids based on asphaltenes peptized by resins suspended in aliphatic and aliphatic species. In fact, bitumens are based on their SARA fractions (Saturated, Aliphatic, Resins, and Asphaltenes) which are defined from the source and the grade of the selected bitumen. Bitumens are frequently used as blends with polymers in order to increase their thermo-mechanical properties over a wide range of temperatures, i.e. to reduce rutting (at high temperatures under large loads) and cracking (at low temperatures). Different types of polymers could be used to modify bitumens such as amorphous or semi-crystalline polymers, i.e. atactic polypropylene, semi-crystalline thermoplastics - for example, poly(ethylene-co-vinyl acetate) EVA -, linear and star block copolymers - for example, poly(styrene-b-butadiene-b-styrene) block copolymers (SBS) -, etc. The morphologies which govern the final properties of the polymer-modified bitumens (PMB), depend on the nature and content of the polymer and on the SARA composition of the bitumen. In fact, the morphologies, i.e. the shape, size, and phase composition of the multiphasic resulting blends result from the specific interactions between the polymer chains and the SARA fractions, i.e. the thermodynamics of mixing. In this lecture, we will first describe the bitumens colloidal structure and the interpretation of the rheological behavior of bitumens. From the analysis of the time-temperature superposition principle which is not able to describe the behavior of bitumens at high temperatures as well for high asphaltene and crystalline contents, a bimodal model is proposed based on the existence of a temperature dependent solid fraction within a liquid (or glassy) matrix. Such a model allows to predict the rheological behavior of aged bitumens, i.e. bitumens which undergo chemical changes of their SARA fractions. From the understanding and modelling of the behavior of these specific colloids, polymer-modified bitumens could be designed by using diblock poly(styrene-b-butadiene)(SB) and triblock poly(styrene-b-butadiene-styrene)(SBS) copolymers or thermoplastic elastomers. Nevertheless, SBS polymers display poor resistance to UV and therefore bring poor aging resistance to the polymer-modified bitumen blends. To overcome these drawbacks, thermoplastic polyurethanes (TPU) were synthesized according to their improved durability and better resistance to UV.

Keywords: Bitumens, Polymer, Colloidal Structure, Rheological Behavior

A Journey from the Synthesis of Functional 2-Trifluoromethacrylate Monomers to their Radical Copolymerizations with Vinylidene Fluoride, and Applications

M. Wehbi

Dr.

Macromolecular Engineering and Architectures
Team, Institut Charles Gerhardt, France

S. Banerjee

Dr.

Macromolecular Engineering and Architectures
Team, Institut Charles Gerhardt, France

A. Hachem

Dr.

CMOS Team, Institut Charles Gerhardt, France

A. Alaaeddine

Dr.

CMOS Team, Institut Charles Gerhardt, France

A. Mehdi

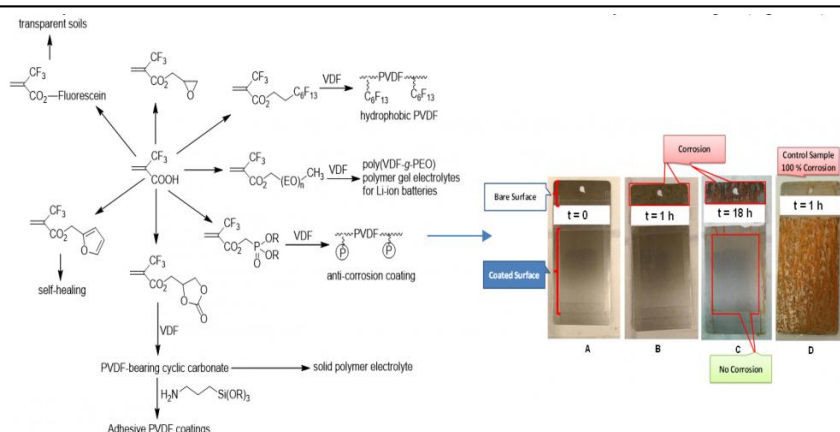
Dr.

Faculty of Sciences, Lebanese University, Lebanon

B. Ameduri*

Prof.

Macromolecular Engineering and Architectures
Team, Institut Charles Gerhardt, France



2-Trifluoromethacrylic acid (MAF) is a versatile building block for the synthesis of new functional monomers [1]. It can be homopolymerized by anionic initiation [2] but failed in the presence of any radical systems. However, its radical copolymerization with vinylidene fluoride (VDF) has been successful. This presentation reports overall strategies to synthesize novel functional 2-trifluoromethacrylate monomers and macromonomers as well as their radical copolymerization with VDF, leading to various materials such as higher thermal stable thermoplastics [3], polymer gel electrolytes for Lithium ion batteries [4-6], anticorrosion [7] and adhesive [8] hybrid coatings (Figure 1). Overall strategies to synthesize novel functional 2-trifluoromethyl monomers from 2-trifluoromethacrylic acid (MAF) and their radical copolymerization with VDF (left). Steel plates coated with poly(VDF-co-MAF Phosphonate) copolymer at the beginning of the experiment (A), after 1 h (B), and after 18 h (C). (D): Uncoated steel plate as reference sample after 1 h (right).) [3].

Keywords: 2-Trifluoromethacrylate, Radical Copolymerization, Vinylidene Fluoride

Acknowledgement: Tosoh FineChem Corporation (Shunan, Japan) is acknowledged for supplying MAF monomer.

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Assessing the Environmental Impact of Metal Production. Case Study: The Republic of North Macedonia

Trajce Stafilov*

Prof.

Institute of Chemistry, Ss Cyril and Methodius
University, Macedonia

Environmental impacts are the unwanted byproduct of economic activities. Inadvertently, humans alter environmental conditions such as pollution of soil, waters or food. Well-known assessments show that habitat change, the overexploitation of renewable resources, climate change, and particulate matter emissions are amongst the most important environmental problems. In addition, anthropogenic environmental changes, associated mainly with chemical pollution, lead to a degradation of the natural human environment. Among all chemical pollutants, trace elements are of a special ecological, biological and health significance. The production of metals results in the formation of emissions of unwanted solids, liquids and gases. The impacts are exacerbated by the use of various raw materials and fuel. There are toxicity concerns with a number of metals such as arsenic, cadmium, lead, mercury, etc. and even metals that are biologically essential may also become toxic at high levels. Therefore, detailed surveys of pollution with heavy metals of soil, waters, sediments, air and food on the entire territory of Northern Macedonia have been carried out. For that purposes various instrumental techniques such as atomic absorption spectrometry (AAS), inductively coupled plasma - atomic emission spectrometry (ICP-AES), inductively coupled plasma - mass spectrometry (ICP-MS) and neutron activation analysis (NAA) were applied. Air pollution was investigated by the application of moss biomonitoring and dust samples (attic dust and house-hold dust). Special attention was paid to the pollution with heavy metals in the regions with mining and metallurgical activities. It was found that the highest pollution is present in the areas with abounded or active mines (Pb, Zn, Cu, As, Sb, Ni, Cr), metallurgical plants (Pb, Zn, Cd, Fe-Ni, Fe-Cr, Fe-Si, Fe, steel) or thermoelectric power plants. High contents of some heavy metals were also found in the areas where their contents usually vary gradually across the geochemical landscape and depend on the geochemistry

Keywords: Metal Production, Pollution, Heavy Metals

Surface-Active and Stimuli-Responsive Polymers: Superb Sources for Various Polymeric Nanostructures and Applications

Vural Bütün*

Prof.

Department of Chemistry, Eskişehir Osmangazi
University, Turkey

Our researches are based on the synthesis and characterizations of different types of stimuli-responsive soluble copolymers which have great response to external conditions. They can self-assemble and form various nanostructures (micelles, gels, flocculates, etc) depending on a change of pH, temperature, ionic strength of the medium. They are getting more and more attention for various applications such as in biomedical technology (as antibacterial agents, drug carriers, controlled releasing systems etc), in sensor technology, in cosmetics. Recently, we have focused on poly(glycidyl methacrylate)-based block copolymers and their derivatizations with morpholine, piperazine and tertiary amine type reactants which provide a great way to tune surface activity, water solubility and response to external stimuli. Additionally, derivative polymers can also be converted into different structures with further reactions. They can self-assemble and form core-shell spherical micelles depending on solution conditions due to presence of a block with LCST behaviour. By using such diblock copolymers as stabilizers, we also succeeded to prepare a novel multi-responsive microgel of a water soluble monomer and "microgel-liposome" system having a potential in drug targeting/releasing applications. Important outcomes of these copolymers are their usage as (i) stabilizers in heterogeneous polymerizations, multi-responsive microgels, nanometal dispersions, (ii) source for novel cross-linked micelles, hydrogels, antibacterial materials, LbL nanofilms, etc.

Keywords: Self-Assembly, Stimuli-Responsive, Micelles, Microgels, Hydrogels, Cross-Linking

Thermally Induced Shape Memory Materials

Metin Hayri Acar*

Prof.

Chemistry Department, Istanbul Technical University
 Turkey

Gozde Aktas Eken

Other

Chemistry Department, Istanbul Technical University
 Turkey

Thermally induced shape memory polymers (SMPs) are an important class of smart materials which can switch their shape in a predefined way to respond to an external stimulus[1]. There has been significant interest to develop SMPs for the last two decades, especially for the ones that can be triggered by body temperature due to their great potential for biomedical applications such as cardiovascular stents[2], implants[3], self-healing coatings[4], actuators[5] and tissue engineering[6]. Until now, researchers mainly focused on copolymers of poly(lactide)[7], poly(glycolide)[8] and poly(ϵ -caprolactone)[3] and the polyurethane[9] to obtain SMPs that can be triggered around the body temperature[10]. Each application requires a different combination of material properties and functions. Therefore, SMPs with different characteristics are required to fulfill the demands of various applications. Herein, we describe PSf[11] and PVDF[12] based amphiphilic graft copolymers with thermally activated shape memory behavior. Atom transfer radical backbones with non-linear derivatives of PEG to obtain shape memory graft copolymers via "grafting from" strategy. Copolymers exhibited excellent shape memory properties around T_m of the soft segments and full recovery was achieved within seconds. These soluble and processable SMPs could potentially play an important role in biomedical applications.

Keywords: Shape Memory Material, Polymer, Smart Material

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Tailor-Made Polymers by Aqueous RAFT Polymerization

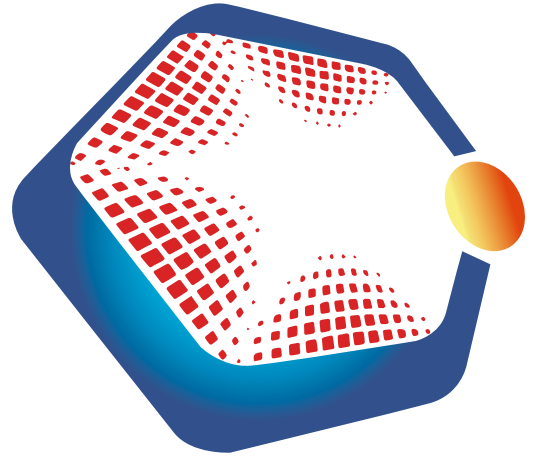
Mathias Destarac

Prof.

IMRCP, Université Toulouse 3 Paul Sabatier, France

Reversible-deactivation radical polymerization (RDRP) technologies allow the production of a large number of structurally complex functional copolymers, including diblock, graft, gradient, star and hyperbranched copolymers. Among the different RDRP strategies, reversible addition-fragmentation chain transfer (RAFT) polymerization is undoubtedly one of the most powerful and easy-to-implement. It can be carried out in water and already experienced industrial success. O-ethyl xanthates of general structure $R-S-(C=S)-OEt$ are well-suited to control the polymerization of monomers of disparate reactivities, typically from acrylates or acrylamides to vinyl monomers. This allowed the synthesis of many original block copolymers which will be exemplified. In particular, double hydrophilic block copolymers (DHBCs) made of neutral and charged blocks have been successfully synthesized and applied to the formation and stabilization of well-defined hybrid polymer-inorganic nanoparticles in aqueous media.

Keywords: Raft, Polymerization, Xanthate, Diblock Copolymer, Hybrid, Nanoparticle



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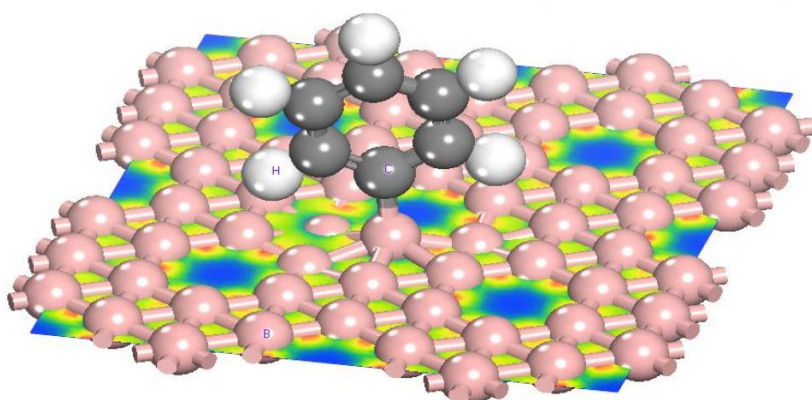
**ORAL
PRESENTATIONS**

First Principles Details into the Grafting of Aryl Radicals onto the Free-Standing and Borophene/Ag(111) Surfaces

Avni Riza Berisha*

Prof.

Department of Chemistry, The University of Pristina,
Kosovo



Borophene is an atomic two-dimensional allotrope of boron first synthesized in 2015. Even though this material is studied extensively due to its unique metallic, mechanical and optical properties, no study is focused toward its surface modification by the grafting reaction of the aryl radicals derived from diazonium cations. We suspect that a possible interaction of the aryl radicals with borophene surface is significant for the stabilization and functionalization of its surface. Therefore, the grafting of several para-substituted aryl radicals onto the borophene sheet is investigated by the means of the first principles calculations based on density functional theory. The binding energy of the phenyl radicals onto the borophene sheet, population analysis, and electron energy difference studies imply a covalent nature between the B atom of the borophene and the phenyl radical. The Electron Localization Function (ELF) analysis is applied to estimate the bonding nature amid the borophene and the grafted phenyl moiety. The Mulliken charge population is used to evaluate the possible electron transfer at the bond forming atoms (B and C) during this process. The obtained results contributed to shed light into the grafting mechanism, activation energy, stabilization and the nature of the formed chemical bonding between borophene and the para-substituted phenyl radicals.

Keywords: Borophene, Grafting, Aryl Radical, Diazonium Salt, Elf Analysis, Dft

Electrochemistry of Oxygen Bubbles on Conductive and Non-Conductive Solids

Veton Haziri*

Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

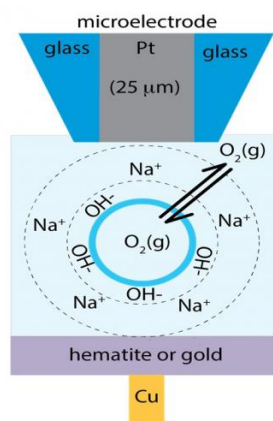
Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Jean François Boily

Prof.

Department of Chemistry, Umea University, Sweden



Gases emerged from electrochemical reactions at mineral surfaces are produced in the form of bubbles which are created within the reaction system. The electrical properties of gas bubbles are important in determining the interaction of bubbles and the way bubbles interact with other materials, to provide a basis for technical application in many fields. The study of water/gas bubble interface is essential to understand the behavior of the gas in aqueous solution and the interaction of the gas with mineral surfaces in the environment and in technological settings. One of such reactions of interest is the electrochemical splitting of water at hematite surfaces, from which oxygen bubbles are produced. In water or electrolyte condition, gas bubbles are observed to migrate against the direction of the electrical field, indicating them to be negatively charged. This is caused by the hydroxide layer at the bubble/water interface. An electrochemical system can be modeled by an equivalent circuit. In this study, electrochemical impedance spectroscopy (EIS) was used to extract electrochemical parameters affected by time, applied potential on the different substrates and the bubble size on measurements in different pH. By applying EIS, a technique that investigates the frequency-resolved impedance of charge carriers, knowledge about interesting electrochemical processes will be unfolded.

Keywords: Oxygen Bubble, Hematite, Gold, Electrochemical Impedance Spectroscopy

The Effect of Rose Essential Oil Component Phenyl Ethyl Alcohol on the Time-Dependent Mass Loss of Poly(Lactic Acid)

Yalçın Coşkun*

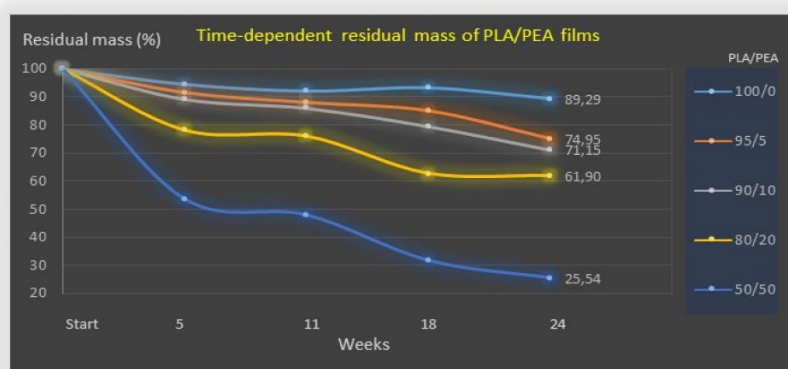
Dr.

Lapseki Vocational College, Canakkale Onsekiz Mart University, Turkey

Ayhan Oral

Assoc. Prof.

Department of Chemistry, Canakkale Onsekiz Mart University, Turkey



Polymeric materials are widely used materials today. The use of so much cause environmental problems such as waste problems. In addition to use for different purposes in accordance with the creatures also revealed the biocompatibility and biodegradability properties, such as the obligation of these materials. Therefore, applications of biopolymers, especially Poly (Lactic acid) (PLA) have increased in recent years. Hydrolytic biodegradation is one of the most important property for these kind of applications. The acceleration and control of this biodegradation process is an important argument for determining and increasing the usage areas of the material. In this study, a natural product Phenyl ethyl alcohol (PEA), which has no cytotoxic effect, mixed with PLA matrix as different proportions and the effect on the hydrolytic degradation process of PLA was investigated. For this purpose, the films were prepared according to the solution casting method by mixing the polymer and the natural component in different weight proportions. Samples were placed in the incubator at the human body temperature (37 °C) and pH (7.4) with Phosphate solution medium. The time-dependent mass loss of this material was investigated. As a result PEA has a time-dependent effect on the mass loss of PLA. The mass loss of PLA increased with the increase of waiting time. In the one-to-one PLA/PEA content (50/50), this loss rate has increased up to 74%.

Keywords: Poly(Lactic Acid), Biodegradation, Phenyl Ethyle Alcohol

Acknowledgement: This work was supported by Çanakkale Onsekiz Mart University Scientific Research Coordination Unit. Project number: FBA-2018-1368

Exploring the Use of Nanomaterials as Corrosion Inhibitors. The Case of Carboxylated Graphene Oxide

Valbonë Veli Mehmeti*

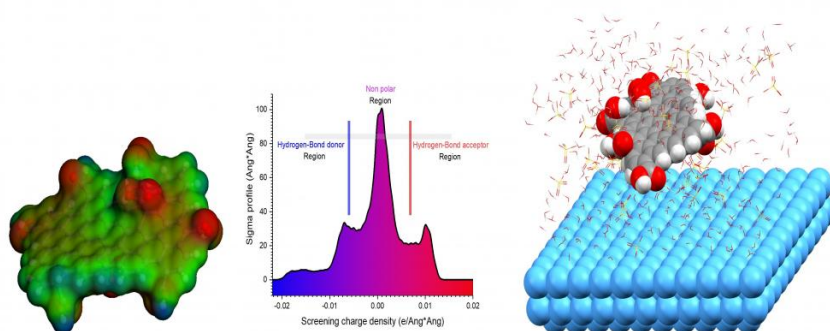
Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Fetah Podvorica

Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Metals are well-known to be predisposed to the oxidation when exposed to different aggressive solutions or even atmospheric conditions. Even though the use of coatings (from paints and polymers) offers a simple method to decrease the effect of corroding species on the surface, the key drawbacks of this method are the weak interactions between the metal surface and the coating layer so the physical organic barrier is weakened after a short time of exposure. The common method of the protection of metals against corrosion remains the use of inhibitors molecules. Graphene is considered as one of the most important classes of modern materials-nanomaterials, which are extensively explored for use in different fields of science (drug delivery to photovoltaics); nevertheless, graphene remains virtually unexplored towards applications aimed at the corrosion inhibition of materials. Theoretical computation methods are extensively employed for the study of the physicochemical properties of the inhibitors to understand at the molecular level their interaction with the metal surface. In this work, Molecular Dynamics and Monte Carlo simulation are used to assess the interaction between the oxidized and bare Niobium and Tantalum surfaces with graphene oxide.

Keywords: Graphene Oxide, Corrosion Inhibition, Monte Carlo, Niobium, Molecular Dynamics, Tantalum

Effects of A Novel Bacteriophage-Loaded Antibacterial Gel Against *Fusobacterium ulcerans* for Tropical Skin Ulcer Treatment

Asdren Zajmi*

Mr.

Department of Diagnostic and Allied Health Science,
Management & Science University, Malaysia

Maizatul Amalia Mohammad Ghazi

Mrs.

Department of Diagnostic and Allied Health Science,
Management & Science University, Malaysia

Mariam-Aisha Fatima

Dr.

Research Management Centre, Management &
Science University, Malaysia

This study aims to evaluate the chitosan-loaded bacteriophage gel (CLBG) for the treatment of tropical skin ulcer against *Fusobacterium ulcerans*. The sewage was collected, isolated and suspended to obtain the phage. The plaque formed from phage propagation was then collected and recorded. The chitosan gel was prepared and mixed with activated bacteriophage lysate and tested using the Minimum Inhibitory Concentration (MIC) and disc diffusion tests. Physico-chemical evaluation of the loaded gel was observed including viscosity, texture, TEM and pH. The plaque-forming units (PFU) of the bacteriophage were 6.8×10^4 PFU/ml, 2.3×10^4 PFU/ml, 1.1×10^4 PFU/ml and 4.0×10^4 PFU/ml. Physical evaluation revealed a milky yellowish formation of a gel texture with a pH of 4.63. Microscopic evaluation showed the morphology of chitosan and live tailless bacteriophage. The MIC values of CLBG against the selected pathogens were 1.0×10^{-5} ml/ml and 1.0×10^{-6} ml/ml, respectively. The zone of inhibition (ZI) for the CLBG was greater (>48 mm) compared to gentamycin (positive control; >25 mm). Statistical analysis using One-Way Anova showed the highly significant value of this study with $p < 0.001$. The CLBG demonstrated a greater synergism effect against the selected pathogen. Hence, the CLBG has a great potential to be a novel drug delivery for the treatment of tropical skin ulcer.

Keywords: *Fusobacterium ulcerans*, Bacteriophage, Tropical Skin Ulcer, Chitosan Gel, Tropical Phagedenic Ulcer

Acknowledgement: The author would like to thank Management and Science University (MSU) for supporting the research by providing financial assistance through the MSU Seed Grants (SG-382-0916-HLS & SG-358-0915-SPH).

Influence of Carbon Nanotubes on ATRP Kinetics

Ana Holos*

Ph.D. Student

Department of Synthesis and Characterization of
Polymers, Polymer Institute Slovak Academy of
Sciences, Slovakia

Jaroslav Mosnacek

Prof.

Department of Synthesis and Characterization of
Polymers, Polymer Institute Slovak Academy of
Sciences, Slovakia

Tomas Sedlacek

Prof.

Department of Polymer Engineering, Tomas Bata
University in Zlin, Faculty of Technology, Czech
Republic

Carbon nanotubes (CNTs) are of special interest for the industry, due to their unique chemical, physical and structure properties. To improve the manipulation of CNTs in organic polymer matrix, main focus is on their chemical modification. Atom Transfer Radical Polymerization (ATRP) is an effective method for synthesis of well-defined polymers. The carbon fillers have ability to trap the radicals, therefore the application of ATRP under ppm amounts of catalyst in the presence of carbon fillers is challenge. Trapping the radicals by CNTs during ATRP leads to accumulation of metal catalyst in higher oxidation state, which subsequently is not able to activate dormant polymer species and polymerization is stopped. In order to reduce the metal catalyst back to its lower oxidation state a high excess of reducing agent is needed. In this study the possibility of application photoATRP technique, which allows photochemical reduction of the deactivator, was investigated. PhotoATRP was performed without degassing the polymerization mixture, at room temperature. The effect of various CNTs concentrations has been investigated and the photoreduction of catalyst is slowed down with increasing the concentration of CNTs due to their ability to absorb the light. Also the effect of different intensity of irradiation was investigated. The ratio ligand to copper catalyst has impact on the kinetics and induction period where the excess of ligand can shorten the induction period, during which oxygen is consumed and increases kinetic of the photoATRP. The ARGET ATRP with the addition of 1000 ppm of reducing agent was also performed in the presence of CNTs. At higher CNTs concentration, i.e. > 0.5 wt%, the ARGET ATRP was faster at the beginning, but it stopped at 60 % of monomer conversion. The probable reason is trapping radicals by CNTs surface, which was confirmed by TGA showing the modification of CNTs by polymer.

Keywords: Carbon Nanotubes, Photo Atrp, Photoreduction, Trapping Radicals

Acknowledgement: This work was supported by the Slovak Research and Development Agency under the contract no. APVV-15-0545.

New Nonstandard Method for Measuring Physical Properties of Homemade Polymer Filaments for 3D FFD Printing

Arta Veliu*

Phd. Student

Department of Physics, University Ss. Cyril and
Methodius, Macedonia

Riste Popeski Dimovski

Prof.

Department of Physics, University Ss. Cyril and
Methodius, Macedonia

As desktop fused deposition modeling 3D printing becomes an everyday occurrence and 3D printing filament extrusion, a DIY makers practice, establishing a method for physical characterization of parts using only small amounts of homemade filament is of interest. Here is presented a new method for measuring change in physical properties of 3D printed part, printed with less than 1g of filament. Changes are observed due to material change (ABS, PLA, PET, recycled PLA 3D prints, recycled PET 3D prints, recycled PET), change in 3D printing procedures, changes in filament extrusion properties and changes in the thickness of the part. It was found out that the results obtained with this method are in correlation with the results from the standard test used in everyday practice. This is good because it allows fast characterization of exotic filament blends with very little material for research purposes, reducing the costs of production, and the possibility to implement fast changes in the filament blends.

Keywords: 3D Printing, Filaments, Extrusion

Investigation of Lead-210 Adsorption on Multi-Walled Carbon Nano Tube Modified with Onno Type Schiff Bases

Nazife Aslan*

Assoc. Prof.

Department of Chemistry, Ankara Hacı Bayram Veli University, Polatlı Science and Arts Faculty, Turkey

Orhan Atakol

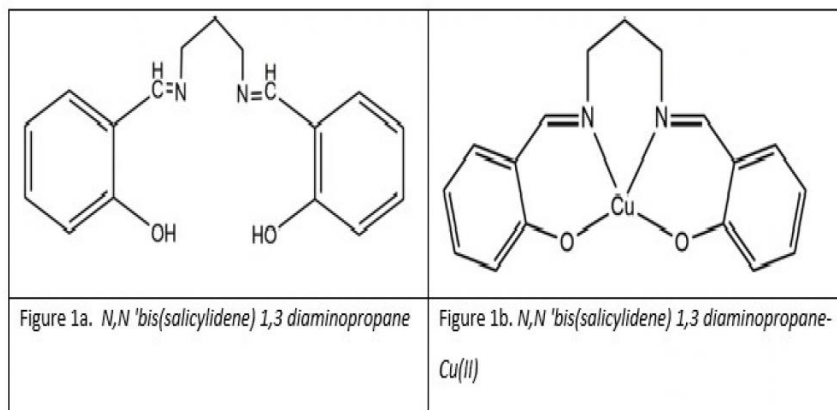
Prof.

Department of Chemistry, Ankara University, Science Faculty, Turkey

Nurdane Yılmaz

Dr.

Department of Chemistry, Kastamonu University, Education Faculty, Turkey



Lead-210 is one of the highly radiotoxic metals reaching the water supplies from nuclear power plants and mines. The chelating ability of Schiff bases enhances their application as a new adsorbent material for the removal of several toxic metals and their radioisotopes. In this study, multi-walled carbon nanotubes were modified using bis-*N,N'*-u(salicylidene)-1,3-diaminopropane and bis-*N,N'*(salicylidene)-1,3-diaminopropane-Cu(II). Schiff bases used for the modification of the multi-walled carbon nanotubes were syntheses according to our previous study [1]. The obtained SB-MWCNTs was characterized by scanning electron microscopy (SEM) analysis. The prepared adsorbent was used to adsorb lead (II) ions in aqueous solution. Various parameters such as adsorbent dose, initial pH, contact time and different initial concentration of lead (II) ions which influenced the adsorption capacity were investigated.

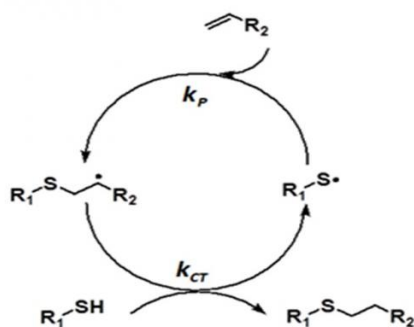
Keywords: Schiff Base, Multi-Walled Carbon Nanotubes, Pb-210 Removal

The Thiol-Ene Polymerization of Natural Monomers: A DFT Study

Isa Degirmenci*

Dr.

Chemical Engineering Department, Ondokuz Mayıs
University, Turkey



Scheme 1: Representation of the most significant steps of the thiol-ene reaction mechanism[1,2].

Recently, thiol-ene polymerisation (Scheme 1) have been getting growing attraction not only improved production of uniform polymer network, reduction of polymer shrinkage stress and obtaining narrow the Tg range but also providing a wide range of application areas from material science to bioorganic chemistry. Thiol-ene polymerization processes can pick up some advantages of both step growth and chain growth polymerizations. These processes are involved in the propagation and chain transfer steps [1]. Thiol-ene polymerization is mostly governed by the ratio of the propagation (k_p) and the chain transfer (k_{CT}) reaction rates (k_p/k_{CT}). The thiol-ene polymerization of natural monomers has not been well studied yet. Natural monomers such as isoprene, limonene, linalool and cinnamaldehyde considered one set of alkenes and some synthetic alkenes such as butadiene, styrene vinyl chloride as the other set of alkenes were quantum chemically studied in this study. Geometry and frequency calculations were carried out at M062X/6-311+G(3df,2p)//M062X/6-31+G(d) level. To investigate the influence of different thiol on the thiol-ene polymerization, methyl thiol and phenylthiol were chosen to represent aliphatic and aromatic thiols. This study has suggested that linalool can be suitable ene functional if aliphatic thiols are used for the thiol-ene polymerization while cinnamaldehyde should be used together with aromatic thiols for the same polymerization processes. In addition to this, these quantum chemical calculations can pave the way for tailoring and development of sustainable or renewable high-performance polymers in the industrial level.

Keywords: Thiol-Ene Polymerisation, DFT Study, Radical Polymerisation, Natural Monomers

Acknowledgement: I.D. acknowledges the TUBITAK research funding under grant no. 217Z073.

Reinforcement of Gypsum with Polypropylene Fibers

Xheneta Zengo*

Master Student

Department of Physics, University of Tetova,
Macedonia

Gypsum is a mineral belonging to the group of sulfates, i.e., sulfuric acid, which is often found in the earth's crust. The gypsum chemical name is calcium sulfate dihydrate ($\text{CaSO}_4 \times 2\text{H}_2\text{O}$). In this paper, two main types hemihydrates, hemihydrate alfa and beta with three different water contents during preparation, were prepared and studied in the shape of prisms. These hemihydrates are reinforced to see if the properties of the gypsum change, aiming to obtain a much stronger material than gypsum itself. The polypropylene fibers used to reinforce the gypsum is 8 mm long and 18 micro meters thick. The mass of fibers used is 0.5 %, 1 % and 1.5 % fibers of the mass of gypsum, with three water water factors for each hemihydrate. The testing methods used are in flexure and compression where it is measured the maximum tension of destruction. For the determination of elastic properties it is used the non destructive method of ultrasonic velocity test, a test made by sending a pulse through the structure, where it is measured the time needed for the pulse to pass through, a value from where the speed and the longitudinal module of elasticity can be determined. Also it is determined the porosity and the kinetic of water absorption of the new composition. The new composition, composed with grinded gypsum, water and polypropylene fibers, are tested to see: Does the porosity and water absorption change?, Is the gypsum going to be stronger or weaker? Is the maximum breaking point going to change? Since for gypsum the best drying point is 40°C, the new composition is tested to see if this point is going to be the same. The comparison of the obtained results of this composition and plain gypsum show different mechanical and physical properties.

Keywords: Gypsum Compositions, Mechanical Properties, Polypropylene, Flexure, Compression, Ultrasonic Velocity Test

New-Generation Superplasticizers For Concrete Industry

Siddika Gamze Erzengin*

Dr.

Department of Chemical Engineering, Süleyman
Demirel University, Turkey

'High-Performance Concrete' and the developments in this field are still one of the most important issues for concrete industry. New-generation superplasticizers (SPs) play key roles in production namely solve the fluidity and fluidity-retention problems of cement-based mixture, on the other hand, reduce water requirement of the system so cause high mechanical strength. Nowadays, various types of superplasticizers are synthesized to overcome the mentioned issues. Syntheses which are based on polycarboxylate chemistry dominate the chemical admixture sector and, polycarboxylate-type SPs (PCs) are known as 'new-generation SPs'. PCs have properties like, easiness of molecular structure change, the various properties by controlling the molecular weight and the structure, the excellent dispersion ability and stability and the small dosage to fit dispersibility in cement system. PC-type copolymers, terpolymers, polymers with different functional groups, polymers containing different side-chain lengths and side-chain densities, cross-linked polymers etc. are the some examples of production wide variety and they are effectively used in concrete mixtures. In this presentation, synthesis of PCs by radical polymerization and their characterization are expressed. Polymer structural characterization was achieved by Fourier Transform Infrared Spectroscopy. Molecular weights of synthesized superplasticizers were determined with Gel Permeation Chromatography. Here, polycarboxylates with different molecular architecture and molecular weight are introduced, the performances of these PCs by means of adsorption, workability, rheology, setting time and mechanical strength are comprehensively reported. Adsorption of PCs onto cement surface were determined by Total Organic Carbon analyses. Workability and rheology tests were achieved by a slump cone and a rheometer, respectively. Initial and final setting times of cement were determined by Vicat needle test. Knowing the fresh and hardened properties of cement system provide many advantages for designing better concrete. This study is a part of a completed national research project and, reflects a holistic approach of influences of PC-type superplasticizers in cement.

Keywords: Polycarboxylate, Superplasticizer, Workability, Rheology, Strength, Cement

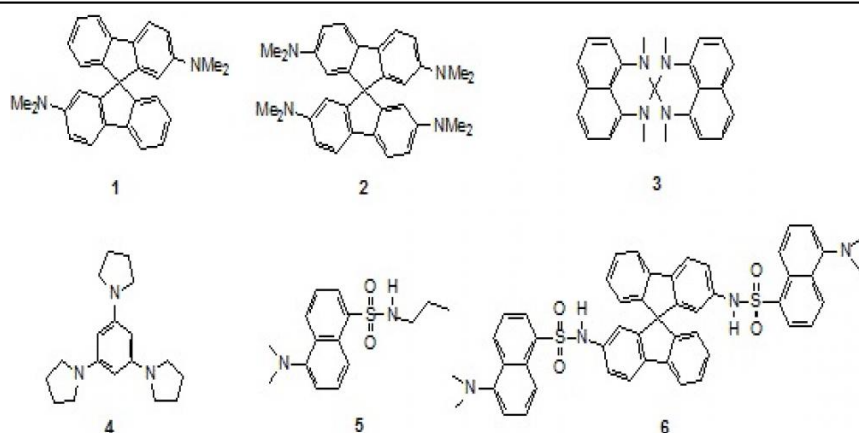
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Approaches for Design of Systems for Detection of Explosives Using Aromatic and Spiroconjugated Amines

Jane Bogdan Bogdanov*

Prof.

Institute of Chemistry, Faculty of Natural Sciences and
 Mathematics, Ss. Cyril and Methodius University, Macedonia



The main component of any explosive device is the secondary explosive, so the detection of the "key ingredient" is of central importance. It has established that small quantities of explosives are transferred to the hands or deposited on outer surfaces of letter bombs or packages during the assembly of the explosive device. The bulk of the explosives used in such manner, have sufficient vapor pressure and traces of the explosive are released in the atmosphere. One common feature of the organic-based secondary explosives is the presence of the nitro group. The nitro group (NO₂) is electron-withdrawing and compounds that have one or more of them are expected to be good electron acceptors (A). In the presence of a good electron donor, D, (eg. aromatic amine) one can suspect a formation of electron donor-acceptor (EDA) complexes (also known as charge-transfer CT complexes). The goal of this project was to quantitatively explore the nature of the interaction between specially designed electron-rich aromatic amines Ar-NR₂ (1-6) and the secondary explosives (or appropriate model compounds and taggants). Their synthesis will be presented along with the purification. The compounds 1-3 are spiroconjugated aromatic amines with unique interaction of the two perpendicular pi-systems. From the obtained experimental results the compounds 2, 3 and 4 were too susceptible to oxidation for practical use. The most encouraging results were found with compound 5 (N-propyldansylamide) which is fluorescent and its fluorescence is quenched by volatile polynitroarenes and polynitrophenols. It also has a good solubility in dichloromethane and can be introduced in poly(methyl methacrylate) (PMMA) films. The PMMA films containing 5 are fluorescent and upon exposure of the vapors of taggant 2,3-dimethyl-2,3-dinitrobutane fluorescence quenching occurs.

Keywords: Detection, Explosives, Aromatic Amines, Spiroconjugated Amines

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Poly(1,2,3-triazolium imide)s Obtained Through AA+BB Click Polyaddition

Omaima Anaya*

Ph.D. Student

Departement of Chemistry, University of Tunis
El Manar, Tunisia

Imen Abdelhedi Miladi

Assoc. Prof.

Departement of Chemistry, University of Tunis
El Manar, Tunisia

Eric Drockenmuller

Prof.

Ingénierie des Matériaux Polymères (IMP - UMR
CNRS 5223), University Claud Bernard Lyon 1,
France

Hatem Ben Romdhane

Prof.

Departement of Chemistry, University of Tunis
El Manar, Tunisia

Poly(ionic liquid)s or polymeric ionic liquids (PILs) are a new class of polymer electrolytes which combines the properties of ionic liquids (ILs) and polymer architecture, and kept considerable attention in recent years.[1] Rapid advances in the chemistry, physics, and macromolecular architecture of PILs have prompted the development of new polyelectrolytes that have found applications in many fields, such as batteries, supercapacitors, solar cells, environment (water treatment), gas separation, catalysis, microelectronics (transistors, OLEDs), bio-related applications and so on...[2] 1,2,3-Triazolium-based poly(ionic liquid)s (TPILs) constitute the most recent addition to the pool of PIL materials.[3,4] Their synthesis benefits from the versatile, robust and orthogonal nature of CuAAC in combination with efficient quaternization and anion metathesis reactions. In this work, we report the synthesis of a new series of poly (imide-triazolium) via the post-polymerization modification of their precursor poly (imide-triazole). These different polymers were characterized by ¹H-NMR and their physico-chemical properties were determined by differential scanning calorimetry (DSC), thermogravimetric analysis (ATG) and steric exclusion chromatography (SEC). Those material can be considered as new candidate of solid polyelectrolytes for gas separation membranes.

Keywords: Poly(ionic liquid), CuAAC, Poly(imide-triazole), Poly(imide-triazolium)

Production of High Purity Alginate from *Cystoseira barbata* Algae Collected out of Black Sea and Investigation of Usability As Biomaterial

Nuray Emin

Dr.

Biomedical Engineering, Kastamonu University
Faculty of Engineering and Architecture, Turkey

Havva Yazar*

Master Student

Material Science and Engineering Department,
Kastamonu University, Faculty of Engineering
and Architecture, Turkey

Emre Yılmaz

Master Student

Material Science and Engineering Department,
Kastamonu University, Institute of Science, Turkey

Samet Özdemir

Other

Genetic and Bioengineering , Kastamonu University,
Faculty of Engineering and Architecture, Turkey

Algae are creatures with photosynthetic pigments that play a critical role in aquatic ecosystems. Especially brown and red algae contain important compounds such as agar, carrageenan and alginate, which are very important in industry and biotechnology. Sodium alginate, one of the varieties of alginic acid, is obtained from the cell wall of the algae and is the most common type of alginate used commercially. In this study, it was aimed to obtain high purity alginic acid sodium salt from *Cystoseira barbata* type brown algae collected from the coasts of Kastamonu province İnebolu district and to investigate the effectiveness of its uses as a biomaterial for tissue engineering applications. In this context firstly, different formaldehyde concentrations were tested during isolation of alginate from brown algae. In addition, changes in purity ratio and color tone were observed according to the number of repetitions of the purification process. The chemical structure of the alginate obtained was evaluated with FTIR analysis by the comparison with the commercially available high purification sodium alginate. Finally isolated alginate was tested for ability of forming different shapes in biomaterial productions. According to the results, higher purity but lower yield (23%) sodium alginate was obtained by using high concentration formaldehyde. It was observed that the purity ratio of sodium alginate increased as the number of repetitions of the purification step carried out by re-precipitation from solution increased, and the color tone turned from brown to light yellow. However, it was found that there was a decrease in yield contrary to increasing purity ratio.

Keywords: *Cystoseira barbata*, Algae, Sodium Alginate, Biomaterials, Tissue Engineering

1.Introduction

Algae are defined as primitive plant organisms with photosynthetic pigments that are critical in both aquatic and semi-aquatic ecosystems and which are structurally in both prokaryotic and eukaryotic classes. They are the primary producers in aquatic habitats and, because of the providing their own development, generate the first step of the food chain. Algae show different properties among themselves, but they are divided into different groups according to the color substances caused by the plastids in their structure. Algae contain iodine, bromine, monosaccharides, polysaccharides, sterols, protein, vitamins, alginic acid and agar. Due to the rich substance content, they are used as raw materials for meeting the needs of people. Especially brown and red algae owing to contain the important compounds such as agar, carrageenan and alginate are prominent in the fields of industry and biotechnology. Alginate, one of these raw materials, has a polysaccharide structure and is found in the cell walls of brown marine algae species (Phaeophyceae) in nature, but is also produced as an

extracellular matrix by some soil bacteria (*Azotobacter vinelandii* and *Pseudomonas aeruginosa*) (Akman,2011; Sze,1998; El-Gamal,2010; Yabanli,2009). Alginate has superior properties in terms of biocompatibility, biodegradability, chelating capability etc. Therefore, it attracts the attention of researchers due to its wide range of applications in biotechnology (Sun,2013). Alginate is a block copolymer composed of a-L-guluronic acid (G) and b-D-mannuronic acid (M) monomers. The guluronic acid molecules in the structure form hydrogel by coordinating with +2 metal cations, allowing the chains to be connected with each other and forming network structures. In this regard, which type of algae to be used commercially in the production of alginate is influenced by the cost of production, and also by the monomer composition of alginic acid. Depending on the type of brown algae, the structure and amount of alginate isolated varies. However, the type and degree of purity of the substances used for the extraction of algae also affect the properties of the isolated alginate. Therefore, the interactions of the substances used in the production of alginate and the impurities it contains should be well known (Haug, 1974). The goal of this study was to produce sodium salt of alginic acid, which has cell culture purity from the brown algae, obtained from Turkey's own resources. In this context, it was aimed to obtain high purity alginic acid from *Cystoseira barbata* type brown algae collected from the coasts of İnebolu district of Kastamonu province and then to investigate their hydrogel formation capacity to use as abiomaterial.

2. Materials and Methods

2.1 Collection of Samples The coast of İnebolu district of Kastamonu province was selected as the study area. In December, Algae were collected from the coast of İnebolu and brought to the laboratory. As a result of the investigations, it was determined that the collected algae material was *Cystoseira barbata* species. The algae were first washed under the tap water and cleaned from the unwanted substances (foreign bodies, mussels, seashepherds). The samples were stored on filter paper in a fume hood to remove excess water. After removal of the water, the samples were dried in the oven for 3 days at 45°C and 2 days at 22°C. The dried algae material was stored in room conditions until the time of use.

2.2 Alginate Production The methods and extraction procedures used were developed with reference to the methods given in "Percival and McDowell, 1967; McHugh, 1987". The algae material, which was previously prepared by drying, was divided into small pieces. 20 g of the sample was weighed into a beaker and 2% CH₂O (d: 1.09, 36.5%) solution was added and incubated in the oven at 45°C for 24 hours. After 24 hours, the samples were filtered with filter paper and washed twice with distilled water. 600 ml of 0.2 N HCl was added to the washed samples and incubated in an oven set at room temperature. The samples were then washed with distilled water and then extracted in a Soxhlet system in 1% Na₂CO₃ in a fume hood at 100°C for 3 hours. The resulting filtrate was centrifuged at 400 rpm for 30 minutes to separate from the colloids. then 60 ml of the supernatant was poured into the beaker and absolute C₂H₆O (Sigma, USA) was gradually added to complete the total volume of the solution to 300 ml. Sodium alginate was precipitated by stirring with baguette while adding ethanol. The resulting sodium alginate was filtered off and washed twice with 100 ml of absolute C₃H₆O (sigma, USA). The alginate solidified (S0: basic sample) from the gel form was placed in a petri dish and dried in an oven at 60°C. Dried alginate pieces were weighed and yield was calculated. It was then ground to powder. The ground alginate was separated according to the particle size (305-425 µm) by sieve.

2.3 Purification Process Purification was carried out by re-precipitating the alginate dissolved in water with ethanol. Purification was repeated twice (S1: 1st purification and S2: 2nd purification) and the purities of the alginates obtained were analyzed comparatively with the commercially available sodium alginate. The obtained alginate was tested for microsphere, fiber, film and scaffolding methods which are the most preferred methods in biomaterial production and the potential of these forms was investigated.

3.Result and Discussion

The effect of different concentrations of formaldehyde used on alginate isolation from brown algae on alginate yield was investigated. So, at the result of the analysis, it was determined that high concentration of sodium alginate was obtained by using high concentration formaldehyde. Sodium alginate samples obtained after purification gave similar results as control and color samples. The results of mannuronic acid and gluronic acid, which are characteristic of alginate, in the FTIR spectrum are similar among the samples. Although the peaks of gluronic acid and mannuronic acid on the FTIR spectrum vary according to the algae type obtained, gluronic acid in the reference alginate used in our thesis yielded a band of 1018.44 cm⁻¹, while mannuronic acid gave a band of 940.39 cm⁻¹. In S1, gluronic acid gave peak at 1021.22 cm⁻¹ and mannuronic acid gave peak at 944.11 cm⁻¹. Compared to the reference alginate, it was found that the peak values were generally the same in all samples, and the intensity of the peaks changed depending on the degree of purity. In addition, analyzes showed that peak shear of S2 treated with high concentration of formaldehyde were minimal compared to reference sodium alginate. Peak shifts in the FTIR spectra were found to decrease inversely with increasing purification. It was found that the transformation of the obtained sodium alginate from brown to lighter colors was correlated to the purification of sodium alginate. It has been found that as the purification steps are repeated, the color becomes even lighter. The biomaterial forming processes of the obtained sodium alginate were tested. In general, alginate was able to take standard biomaterial forms successfully. It was determined that the stability of the microspheres increased in relation to the residence time in CaCl₂ solution. This is interpreted as the cross-linking ratio increases with the alginate-Ca₂ + interaction time. On the other hand, in fiber formation, the thickness of the fiber was not always the same. This is thought to be caused by the non-homogeneity of mannuronic and gluronic acid block arrangements in the structure. In the film and scaffold structure formed using sodium alginate, it was determined that materials with sufficient morphology and mechanical strength can be produced when compared with standard samples.

4.Conclusion

In terms of the length of the seafront, Turkey, even though it takes place in the top row among the Mediterranean countries, algae-related works are less than those of the Western Mediterranean countries. In Turkey's seas, which are very rich in different species, the researches on algae to date indicate that there are nearly 1000 algae species in the sea flora. However, the industry based on algae on our coasts has not developed yet. Natural stocks are used only as raw products and only a few species are exported. Within the scope of the research, high purity alginic acid sodium salt was obtained by using the own resources of Turkey. It is thought that cell culture purity biopolymers can be obtained and commercialized economically if characterization is performed by advanced physical and chemical analyzes of sodium alginate produced. The methods and technology used to determine the stock quantities of algae species determined on the coasts of our country are gradually developing. Depending on the progress of the aquaculture sector, algae cultivation and the industry for these algae will also develop and become widespread in the next years.

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Functional Packaging Materials that Store Latent Heat in Food Safety

Tuğba Güngör Ertuğral*

Dr.

Canakkale School of Applied Sciences, Canakkale
Onsekiz Mart University, Turkey

Thermal preservation techniques in food safety take place at certain temperature (-18 - 60 ° C). Food packaging can developed to give specific properties and light-weight packaging materials that can provide cooling without use petroleum fuel. Phase change materials (PCM) that can storage latent heat thermal insulation materials. Containing solid-solid, solid-liquid PCM food packaging materials can protect foodstuffs from temperature fluctuations. Main PCMs, Polyethylene Glycol (PEG), Polytetramethylene Glycol (PTGM), fatty acids can be used as packaging material in food preservation. In this study, preservation properties of PEG bond; polyethylene terephthalate (PET) -PEG and maleic anhydride (MA) -PEG copolymers, caprylic acid -1-dodecanol eutectic mixtures in latent heat storage capacities and suitable microcapsule FDMs food packaging materials were investigated.

Keywords: Food Safety, PCM, Packaging Material, PEG, MA, Fatty Acid



Fig. 1. Classification of energy storage materials (Pielichowska and Pielichowski 2014)

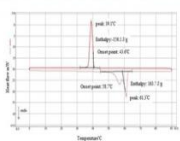


Fig. 2. MA-PEG (Mw 4000) copolymer DSC curve (Günger Ertuğral 2016)

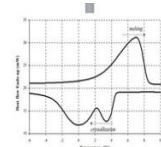


Fig. 4. RT5 encapsulated in polyurethane (PU) DSC curve (Wilson et al., 2017)

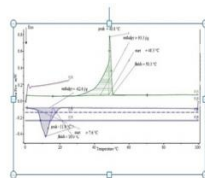


Fig. 3. PET-PEG (Mw 6000) block copolymer DSC curve (0-100 °C) (Günger Ertuğral 2016)

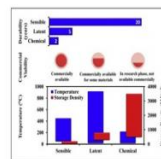


Fig. 5. Storage capacities, commercial viabilities and durability aspects of PCMs for thermal energy storage (Günger et al., 2019)

1. INTRODUCTION Packaging; It is a tool that ensures delivery, promotion of foodstuffs to consumers in a high quality and reliable manner with minimum total cost (Üçüncü, 2011). Packaging can play an active role in temperature control of perishable foods but thermal comfort properties of these standard materials (paper, glass, tin, plastic, wood, aluminum, etc.) are not sufficient. Storage temperatures vary according to food processing and type. According to the storage temperatures of foodstuffs that are packaged since production; -Hot foods (60 ° C and above), -Fresh foods (10 - 18 ° C), -Cold foods (0 ° C- 7 ° C) -Chilled food products (-2 ° C to $+2$ ° C) -Frozen food (-18 ° C and below) It is possible to classify frozen foods (-30 ° C and below) (Shih and Wang, 2015) . Phase-changing substances, phase change temperature known as the temperature range from one phase to another phase (Mattila, 2006). They can store heat at high enthalpy during phase change. During melting and crystallization, system stores heat but its temperature remains constant. FDMs can generate heat energy emissions in event of sudden temperature drops or increases (Pielichowska and Pielichowski, 2014) . Thermal preservation techniques in food safety are carried out at a specific temperature range (-18 - 60 ° C).

Industrial Usage Areas of FDM Applied Food Packaging can be classified by 5 processes (Güngör Ertuğral 2016); -Storage of fresh fruits and vegetables (5-10°C) -Catering (fast food) (60 °C) -Storage of dried food products (20-25°C) -Cold storage with cold air transport (-5-10°C) -Food production line requiring thermal storage. The application of thermal energy storage through formulation and use of PCMs is a feasible solution for storage/release of energy. In this study, heat storage thermal capacities of phase change materials that they (fatty acid) caprylic acid /1-dodecanol eutectic mixture, solid-solid phase exchange material PEG linked PET so PET-PEG copolymer, MA-PEG copolymers and microcapsule FDMs. Also compatibility of FDM in food packaging production processes was investigated.

2. MATERIAL and METHOD

2.1. PCM Copolymers for Food Packaging

Some foods should be marketed and storage under freezing, chilling or refrigerating conditions because low temperatures improve the chemical, physical and microbial safety of food. In order to extend food products shelf-life and prevent their spoilage, preservation of the during cold chain. For the food industry, PCMs have been generally used for heat storage and transportation systems. Synthesis of latent heat storage material and microcapsule latent heat storage material studies for food packaging have increased. Furthermore, latent heat storage values are higher than chemical heat storage (Fig.5) (Nazir et al., 2019). MA-PEG copolymer: MA monomer and solid-solid phase exchange material PEG (Mw: 4000) formed copolymer is straight chain structure. It showed melting temperature at 18 °C in measurements made by DSC (Fig. 3). Further, PEG was attached to PET polymer by fisher esterification and according to DSC results, melting temperature was 18°C and melting enthalpy was 72 Jg⁻¹, solidification temperature was 18°C and solidification enthalpy value was -81 Jg⁻¹ as measured (Fig.2) (Güngör Ertuğral, 2016). Eutectic Mixture of Caprylic Acid and 1-Dodecanol; It can be used as a solid-liquid phase change material in packaging materials in food applications (milk, fruits and vegetables etc.) due to the low phase change temperature especially in eutectic mixtures. The melting temperature is 6.52 °C and has a heat storage capacity of 171.06 J g⁻¹ (Jiang et al., 2011). It is suitable to be used as in wall material in double walled food storage and transportation tank. Rubitherm RT5 encapsulated in polycaprolactone (PCL), heat transfer behavior of a plate made from encapsulated PCM (Rubitherm RT5 encapsulated in polycaprolactone PCL) model phase transition of the PCM. The numerical result demonstrated a better thermal capacitance of the encapsulated PCM material compared to a standard one (cardboard) (Hoang et al., 2014). PS/RT5 microencapsulation, RT5 (a blend of paraffins with a transition temperature at 5 °C) heat management PS foam tray containing an ultrathin fiber-structured PS/PCM coating was prepared by using high throughput electrohydrodynamic processing. For this purpose, polystyrene (PS) was used as the encapsulating matrix of a commercial PCM called RT5, by using the electrospinning technique. Electrohydrodynamic processing seems to be a promising alternative to develop heat management materials, further works will be focused on the improvement of heat storage capacity and efficiency of the developed packaging materials along cold storage time. (Wilson et al., 2017). Microcapsules containing n-hexadecane (C16) with a melamine-urea-formaldehyde (MUF) shell were synthesized by emulsion polymerization and microcapsules melting temperature 14.7 °C and melting enthalpy 167.4 Jg⁻¹ as determined (Alehosseini and Jafari, 2019).

3. RESULT AND DISCUSSION

When the DSC curve of MA - PEG 4000 copolymer was examined, melting and solidification temperature difference was measured as 18.1 °C and melting and solidification enthalpy difference was measured as 8 Jg⁻¹ (Fig.2). Two different DSC measurements of the PET-PEG multiblock copolymer were performed. In Figure 3, the solidification temperature is 7.6 °C and the melting temperature is 48.3 °C. The melting enthalpy is 93.3 Jg⁻¹ and the enthalpy of solidification -62.6 Jg⁻¹. (Fig 3.) Analysis of a DSC thermogram enables the determination of two important parameters: the phase transition temperature range and denaturation enthalpy (or phase change enthalpy-ΔH). Hysteresis was observed: the crystallization began at a lower temperature (about 4°C) compared to the end of the melting (about 8°C) (Fig. 4).

4. CONCLUSION

PCMs can be classified into organic, inorganic, and eutectic materials. Moreover, there are several techniques for encapsulation of PCMs such as emulsion polymerization, coacervation, sol-gel encapsulation, spray drying, electrohydrodynamic processes, etc. Some studies have

revealed that besides improvements in the thermal storage capacity of the thermal transfer fluids, the thermal conductivity efficiency of the fluids could be increased by adding nano PCMs. Recently, PCFs, as fibrous forms of PCMs, have been considered by researchers. These innovative PCMs are of interest as energy storage/release systems to adequately coat or control temperature sensitive products in various conditions (i.e. refrigeration equipment), and can be applied in smart food/pharmaceutical packaging (Alehosseini and Jafari, 2019). PET is a packaging material commonly used in the food industry. The solid-solid phase exchange material obtained by PEG bonding starts the phase change in PET-PEG copolymer 18? and provides thermal insulation when used in food packaging materials. However, solid-liquid packaging materials can be applied to packaging materials by microencapsulation. In particular, phase change of RT5 encapsulated in polycaprolactone (PCL) at 4 ? prevent microbial and chemical degradation in foodstuffs. Food packages that store latent heat protect food in case of temperature fluctuations in cold chain applications. Solid-solid phase change materials preferred, especially because that doesn't leak in food packaging materials. It is possible to provide insulation in food packaging materials with hidden heat storage.

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In Silico Analysis to Highlight the Effect of N1303K Mutation on CFTR Protein

Ali Oztuna

Dr.

Department of Medical Genetics, Gulhane Training
and Research Hospital, Turkey

Hasan Nazir*

Assoc. Prof.

Department of Chemistry, Ankara University,
Science Faculty, Turkey

Cystic Fibrosis is a life-threatening autosomal recessive genetic disease of the Caucasians. Progressive lung disease is still the main cause of the mortality and median survival age for the disease is forty years with available conventional therapies. Mutations in the CFTR (cystic fibrosis transmembrane conductance regulator) gene which encodes CFTR protein are the cause of disease. F508del and N1303K are the most two common mutations in Turkey which resides in the two ATP binding domains namely NBD1 and NBD2 (Nucleotide Binding Domain) respectively. Knowing and understanding the impact of mutations on the protein will help to understand the disease mechanisms and also to propose novel mutations specific therapies. In this study, effect of the N1303K mutation on CFTR protein was investigated by molecular dynamics and docking analysis. In this content, physicochemical, dynamic properties of the wild type and mutant protein and also mutational effect on the protein stability and ATP binding affinity were evaluated.

Keywords: Cystic Fibrosis, Cfr, N103K, Molecular Docking, Molecular Dynamics

Edible Films Coating for Fruit Applications

Mustafa Akin*

Ph.D. Student

R&D, Petro Yag Ve Kimyasallar San. ve Tic. A.Ş.,
Turkey

Elif Kahraman

Mrs.

R&D, Petro Yag Ve Kimyasallar San. ve Tic. A.Ş.,
Turkey

An edible film is defined as a thin layer, which can be consumed, coated on a food or placed as barrier between the food and the surrounding environment. Degradation results in processed fruits because of water loss, softening, increased respiration and microbial contamination. For this reason, edible films have a great deal of prominence in fruit surface coatings [1]. When fruit is separated by a barrier, such as a coating or packaging, from exchange of gases with the atmosphere, there is the possibility for respiration to become anaerobic with the associated development of off-flavor [2]. Thus, it is expected that edible film coatings will have certain properties like respiration, antimicrobial activity, water loss prevention. For this study, we selected four coating (FX6-FJ9-FJ7-FX11) treatments with a wide range of barriers to gas exchange, from non-coated control to shellac, a strong barrier coating. These coating products are commercial products that have been stretched in the R & D laboratory of PETRO YAG ve KİMYASALLAR SAN. ve TİC. A.Ş. The effects of coating products were investigated on peach, orange, lemon and apple fruits under the room temperature and fridge storage conditions. In studies on coated and uncoated fruit, moisture content of coating films, water solubility of dry films, antimicrobial activity, and weight loss measurements were investigated. According to the moisture contents of dry films comparison of carnauba wax, shellac and CW-Shellac solutions dry films did not significantly vary from each other. Solubility of dry films in water 42.3; 37.83; 44.9 % for FJ9, FX6, FJ7 and 100% for FX11 respectively. Only FX6 showed antimicrobial activity against *Staphylococcus aureus* (ATCC 25923) and *Escherichia coli* (ATCC 25922). When the weight loss test results are examined, it is determined that different formulas have different effects on the fruits.

Keywords: Shellac, Carnauba Wax, Surface Coating, Edible Film

Salinity Threshold of Irrigation Water for Germination of Chickpea (*Cicer arietinum* L.)

Tülay Tütenocaklı*

Dr.

Lapseki Vocational School, Canakkale Onsekiz Mart
University, Turkey

Yalçın Coşkun

Dr.

Lapseki Vocational School, Canakkale Onsekiz Mart
University, Turkey

Ismail Tas

Assoc. Prof.

Irrigation Engineering, Canakkale Onsekiz Mart
University, Turkey

Mevlut Akcura

Prof.

Department of Field Crops, Canakkale Onsekiz Mart
University, Turkey

Chickpea (*Cicer arietinum* L.) is considered as animal feed in human nutrition in certain parts of the world. Chickpea is a good food source in terms of high protein content. Chickpea has the highest salt tolerance among legumes. As in all plants, chickpea can tolerate some degree of irrigation water salinity. Determining the response of the plant to salinity and increasing the tolerance level is of great importance for sustainable production. In order to meet the future needs, production should be increased with yield and quality. The economic value of product losses caused by environmental pressures is increasing day by day. Environmental conditions are largely difficult and costly to adjust to plants. Therefore, efforts to obtain tolerant plants by using genetic technologies are rapidly increasing. Increasing tolerance of plants to environmental pressures and especially irrigation water salt stress is one of the most important features for the varieties to be developed. The results of germination study are among the basic information needed in cell and tissue culture techniques, genetic engineering methods and classical breeding methods. Germinating of 9 chickpea variety, which are producing of Turkey, was tested performed for irrigation water salinity. Sodium Adsorption Ratio rate (SAR) of irrigation water was under 3. At the same time different electrical conductivity (0, 6, 8, 10, 12 and 16 dS/m) was used for germinating test. As a result of the study, the most tolerant varieties for irrigation water salinity are varieties 1 and 2. Sensitive varieties are determined as 7 and 9 varieties. Varieties 1 and 2 can be used as breeding material for tolerance to irrigation water salinity and drought stress.

Keywords: Chickpea, Irrigation Water Salinity, Electrical Conductivity, SAR

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Synthesis and Property of Quantum Carbon Dot/Polyvinyl Alcohol Nanofiber by Electrospinning

Muhamad Nasir*

Dr.

Research Unit for Clean Technology, Indonesian
Institute of Sciences, Indonesia

Rihlatul Adni

Other

Research Unit for Clean Technology, Indonesian
Institute of Sciences, Indonesia

Indriyati Indriyati

Mrs.

Research Unit for Clean Technology, Indonesia
nInstitute of Sciences, Indonesia

Muhamad Suhaeimi

Other

Research Unit for Clean Technology, Indonesian
Institute of Sciences, Indonesia

Fitri Dara

Dr.

Research Unit for Clean Technology, Indonesia
nInstitute of Sciences, Indonesia

Indah Primadona

Dr.

Research Unit for Clean Technology, Indonesia
nInstitute of Sciences, Indonesia

Quantum Carbon Dot/Polyvinyl Alcohol nanofiber has been synthesis by electrospinning process. Electrospinning solution was prepared by mixing of quantum carbon dot and polyvinyl alcohol in water as solvent. The optimum condition to prepare nanofiber as follow: flow rate 0.01 ml/minute, distance between nozzle to collector 15 cm and applied voltage 22 kV. Morphology of quantum carbon dot/polyvinyl alcohol nanofiber was characterized by using scanning electron microscopy. Nanofiber has smooth and homogenously morphology without bead on nanofiber string with average diameter 275 nm. Structure of nanofiber was characterized by using FTIR. Quantum carbon dot/Polyvinyl alcohol nanofiber has water contact angle 60. This water contact measurement showed that quantum carbon dot/polyvinyl alcohol nanofiber has hydrophilic character.

Keywords: Quantum Carbon Dot/Polyvinyl Alcohol Nanofiber, Electrospinning, Hydrophylic Nanofiber

Dual Drug Loaded Solid Lipid Nanoparticles for Glioblastoma Therapy via Intranasal Route: Development and Characterization of Nanoparticles

Güliz Ak*

Dr.

Ege University, Faculty of Science, Department of Biochemistry / Ege University ARGEFAR , Turkey

Tuğba Karakayalı

Master Student

Ege University, Faculty of Science, Department of Biochemistry, Turkey

Ayşe Ünal

Master Student

Ege University, Faculty of Science, Department of Biochemistry / Ege University ARGEFAR, Turkey

Şenay Hamarat Şanlıer

Prof.

Ege University, Faculty of Science, Department of Biochemistry / Ege University ARGEFAR, Turkey

Glioblastoma is the most common form of brain cancer. Solid lipid nanoparticles can also be used via intranasal route to across blood brain barrier (BBB) and enhance drug delivery to the brain. β -hydroxybutyrate is a substrate of monocarboxylic acid transporter that is expressed on BBB to transport across the barrier. Temozolomide and carmustine are used for brain tumors but they have short half life and lead systemic side effects. In this study we aimed to develop carmustine and temozolomide encapsulated solid lipid nanoparticles for glioblastoma therapy via intranasal administration. Solid lipid nanoparticles were prepared using cetyl palmitate, polysorbate80 and the previously synthesized conjugate consisting of stearylamine and β -hydroxybutyrate through hot homogenization technique. Conjugate was chemically analyzed with FTIR and ¹HNMR. Carmustine and temozolomide were added before homogenization so as to encapsulate the drugs into nanoparticles. Drug loaded nanoparticles were characterized with FTIR, TGA, SEM, TEM and zetasizer. In vitro drug release and biocompatibility tests were performed. According to data, conjugate was successfully prepared with amide bond. Carmustine and temozolomide were encapsulated into nanoparticles with efficiency of 78% and 90.77%, respectively. Dual drug loaded nanoparticles were spherical in shape, had size of 227 nm and zeta potential of -25.6 mV. Drug delivery from nanoparticles were in controlled manner. Furthermore, dual drug loaded nanoparticles had no hemolysis effect on erythrocytes and bound to serum proteins with 21-28%. According to all data, carmustine and temozolomide loaded solid lipid nanoparticles could have potential for glioblastoma therapy via intranasal route.

Keywords: Solid Lipid Nanoparticle, Temozolomide, Carmustine, Glioblastoma, β -hydroxybutyrate, Intranasal

Acknowledgement: We would like to thank for financial support received from The Scientific and Technological Research Council of Turkey (TUBITAK) (Grant number: 117S241).

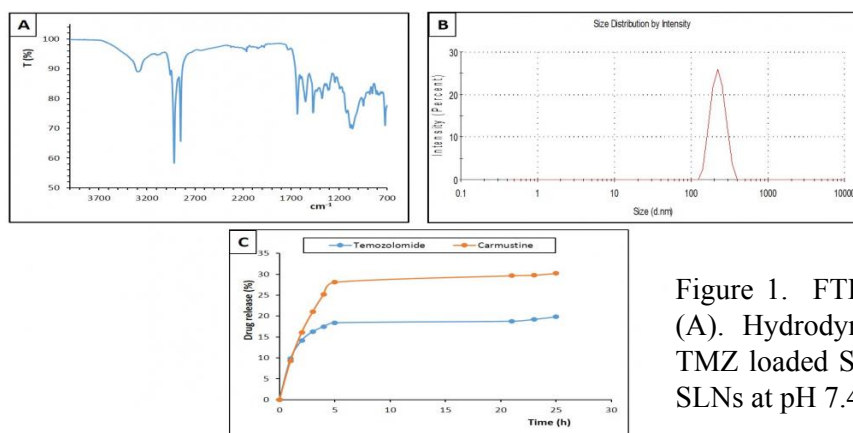


Figure 1. FTIR spectrum of SA and HBA conjugate (A). Hydrodynamic size distribution of BCNU and TMZ loaded SLNs (B). BCNU and TMZ release from SLNs at pH 7.4 (C)

1.Introduction

Glioblastoma which is a grade IV astrocytoma is the most common brain tumors in adults, accounting for 54% of all gliomas. The median survival of this cancer is 7-15 months after its initial diagnosis. Conventional treatment includes tumor resection, radiotherapy and chemotherapy (especially with temozolomide). Nanotechnological drug delivery could promise more effective therapy with minimal side effects (Michael et al., 2018). Crossing the BBB is a major problem in drug delivery. Solid lipid nanoparticles which are nanospheres consist of solid lipid matrix can also be used to cross the BBB and enhance drug delivery to the brain (Gastaldi et al., 2014). β -hydroxybutyrate (HBA) is one of the substrates for monocarboxylic acid transporter (MCT) that is expressed on BBB to transport across the barrier. HBA can be used for decoration of solid lipid nanoparticles to improve drug delivery to brain. (Venishetty et al., 2013). Intranasal administration is direct (mainly extracellular and transcellular) transport of agents from the nasal cavity to the brain and these pharmacological substances can bypass the blood brain barrier (BBB). There are a lot of advantages of intranasal administration such as non-invasiveness, avoidance of the systemic circulation, reducing the systemic toxic effects, self-administration by patients etc (Van Woensel et al., 2013). Temozolomide is an alkylating agent, most effective in glioblastoma, however it must be given to patients in high doses owing to its short half life. In addition it has a number of side effects. Carmustine is a nitrosourea compound and is known to be an effective anticancer agent for brain tumors. It has also short half life and leads to systemic side effects. The purpose of this study is development of temozolomide and carmustine loaded solid lipid nanoparticles for glioblastoma therapy via intranasal route in order to transport drugs across the BBB, enhance drug efficiency and minimize side effects. Nanoparticles were characterized and *in vitro* tests were performed.

2.Materials and Methods

Stearylamine (SA), β -hydroxybutyrate (HBA), 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC), N-hydroxysuccinimide (NHS), cetyl palmitate, polysorbate 80, carmustine (BCNU), temozolomide (TMZ) were purchased from Sigma-Aldrich. Other chemicals were analytical grade. SA and HBA were conjugated with amide bond utilizing EDC/NHS chemistry. The conjugate was filtered, purified and verified with FTIR and ¹H-NMR analyses (Venishetty et al., 2013). Hot homogenization technique was used for solid lipid nanoparticle (SLN) synthesis (Martins et al., 2012; 2013, Venishetty et al., 2013). Briefly, for empty (no drug containing) nanoparticles cetyl palmitate was heated up to 65°C, then the conjugate and polysorbate 80 were added into it. Pre-emulsion was prepared and homogenized with high shear dispersing machine and sonicator, respectively at 65°C. Obtained emulsion was cooled down to 4°C and settled to 25°C. Nanoparticles were purified and obtained through centrifugation as pellet phase. In order to encapsulate drugs into nanoparticles, varying

amounts of carmustine and temozolomid (0.1-0.5%, (w/w)) were added before homogenization. FTIR, TGA, SEM, TEM, hydrodynamic size, zeta potential analyzes of nanoparticles were performed to characterize nanoparticles. Drug loading amounts were determined by HPLC. Drug release tests were carried out in pH 7.4 phosphate buffer at 37°C using dialysis membrane tubings. Hemolysis and protein binding assay were performed via mixing and incubating nanoparticles with erythrocytes (2%) and fetal bovine serum at 37°C for 2 h.

3.Result and Discussion

SA and HBA was linked for enhanced uptake through MCT-1 receptor to transport across the BBB. The structure of SA-HBA conjugate was checked for band signals with FTIR (Figure1A) (peak at 1633 cm^{-1} demonstrated amide bond) and $^1\text{H-NMR}$. Solid lipid nanoparticles formed with cetyl palmitate as lipid phase, polysorbate80 as aqueous phase surfactant and also conjugate as target molecule. Conjugate consisted of two molecules: SA that was used as lipid group and HBA that was selected for transportation via MCT1. Moreover, polysorbate 80 as surface material was known to enhance transport potential of nanoparticles across the BBB (Tian et al., 2011). Obtained and optimized unloaded SLNs were characterized and found as thermally stable up to 200°C and nearly spherical. SLNs had hydrodynamic size (220.9 nm) and zeta potential (-7.55 mV). Optimum drug loading efficiencies were dedected as 78% for BCNU and 90.77% for TMZ. In addition to these data, BCNU and TMZ loaded nanoparticles had similar properties to empty nanoparticles. Dual drug loaded SLNs had size of 227 nm (polydispersity index was 0.455) (Figure 1B) and nanoparticles were revealed as anionic particles (zeta potential was -25.6 mV). It is known that the brain uptake rates of anionic nanoparticles are superior to cationic or neutral nanoparticles (Lockman et al., 2004) and higher zeta potential value make a great contribution to physical stability (Heurtault et al., 2003). Furthermore hydrodynamic size of nanoparticles were proper for intranasal delivery. Drug release percent was dedected as 19.82 for TMZ and 30.22 for BCNU (Figure 1C) implying controlled drug delivery. Hemolysis and protein binding assay were applied for identifying biocompatibility of nanoparticles. It was suggested that bound serum protein amount which was in a range of 21-28% could not effect drug delivery and SLNs could not bring about damage to red blood cells. These results meant that dual drug loaded SLNs were biocompatible.

4.Conclusion

In this work, dual drug (carmustine and temozolomide) loaded solid lipid nanoparticles were developed. Nanoparticles had spherical shape and proper characteristics for intranasal drug delivery. Moreover, drug delivery from nanoparticles were in controlled manner and nanoparticles had biocompatible properties. It was thought that BCNU and TMZ loaded SLNs could have potential for further studies in terms of glioblastoma therapy via intranasal administration.

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3-Dimensional Bioscaffolds from Quince Seed Mucilage for Human Adipose-Derived Mesenchymal Stem Cells

Yavuz Emre Arslan*

Dr.

Department of Bioengineering, Canakkale Onsekiz
Mart University, Turkey

Ekin Simsek

Master Student

Department of Bioengineering, Canakkale Onsekiz
Mart University, Turkey

Polysaccharides have attracted the considerable attention of researchers in the field of tissue engineering due to not only their biocompatible and biodegradable features but also their abundance in nature. Plant mucilage, a new source of polysaccharide, can be obtained from seeds, roots, and leaves of several plants. Here, we aimed at producing a three-dimensional (3D) novel bioscaffold from quince seed mucilage (QSM) for regenerative medicine applications. In the first stage, mucilage was extracted from, molded and lyophilized (referred as to QSM-dS). The structural integrity, this is to say microarchitecture of QSM-dS, was kept using 1-Ethyl-3-(3-dimethylaminopropyl)-carbodiimide/N-hydroxysuccinimide. The crosslinked scaffolds (referred as to cQSM-dS) were characterized via scanning electron microscopy, Fourier transform infrared spectroscopy, Brunauere-Emmette-Teller analysis, thermogravimetric analysis (TGA), dynamic mechanical analysis (DMA) in addition to the swelling, liquid uptake, and porosity tests. Extraction yield of QSM was calculated to be $6.28 \pm 0.40\%$ ($n=3$). The total surface areas of the QSM-dS and cQSM-dS were found to be $9.416 \text{ m}^2/\text{g}$ and $27.195 \text{ m}^2/\text{g}$ by BET analysis. SEM analysis indicated that bioscaffolds had an interconnected porous structure, and pore size increased by crosslinking process. DMA and TGA were fulfilled to understand the effect of the crosslinking process on the prepared scaffolds. These tests proved that the mechanical and thermal features were improved after the crosslinking process. In vitro biocompatibility of the cQSM-dS was assessed by the 3-[4,5-dimethylthiazole-2-yl]-2,5-diphenyltetrazolium bromide (MTT) assay. The assay showed that the prepared scaffolds had no cytotoxic effect on human adipose-derived mesenchymal stem cells (hAMSCs). hAMSCs attached, migrated and proliferated in/on the surface of the cQSM-dS, which was proved by SEM and histochemistry studies. Furthermore, the cells formed cluster-like morphology at the late stage of the culture. In conclusion, we believe that cQSM-dS, which can provide a 3D microenvironment for the cells, have the potential to repair damaged tissue sites.

Keywords: Quince (*Cydonia oblonga* Miller) seeds, Mucilage, Human Adipose-Derived Mesenchymal Stemcells, Bioengineered 3D Scaffolds, Tissue Engineering

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Determination of Bisphenol A with Poly(p-Aminobenzoic Acid) Modified Gold Electrode by using Differential Pulse Voltammetry

Serap Titretir Duran*

Assoc. Prof.

Department of Chemistry, İnönü University, Turkey

Bisphenol A (BPA) is an important matter in chemical industry used in the produce of some food contact materials such as plastics, adhesives and coatings. But BPA has also some toxic effects for human endocrine system and environment. Therefore, novel sensitive and selective methods for determination the level of BPA in environmental, foods and medical samples need to be developed. In this study, a novel, sensitive, simple and cheap electrochemical sensor based on poly (p-aminobenzoic acid) p(p-ABA) modified gold electrode (AuE) was developed for the measurement of BPA in water samples. Firstly, AuEs were modified with polymerization of the p-ABA as a monomer by using bulk electrolysis in 0.01 M HCl at -250 mV. Then the electrochemical oxidation of BPA carried out in 0.1 M phosphate buffer solution (PBS) pH=6 on p(p-ABA) modified AuE. The effects of various electrochemical parameters, such as scan rate, electrolyte type and electrolyte pH were examined. Differential pulse voltammetry (DPV) was used as an ideal analytical method for the qualitative and quantitative detect of BPA in water samples. The developed electrochemical sensor has linear signal to BPA in the range of 2-100 uM. The detection limit (LOD) of the developed method was 0.26 uM and correlation coefficient was 0.999. Additionally, the developed sensor was used to determination the BPA in bottled drinking water sold in Turkish markets by using DPV, and obtains satisfactory results. The recovery values of the bottle water samples waited in the freezer, at room temperature and in the car were calculated as 102.22%, 104.68% and 106.06% respectively.

Keywords: Bisphenol A, Sensor, Bottled Water, Poly (p-aminobenzoic acid)

Characterization of Honey: Determination of Metal and Sugar Content

Nora Limani Bektashi*

Ph.D. Student

Faculty of Technological Sciences, Mother Teresa
University, Macedonia

Olga Popovska

Prof.

Faculty of Technological Sciences, Mother Teresa
University, Macedonia

Arianit Reka

Prof.

Faculty of Natural Science and Mathematics,
University of Tetova, Macedonia

Drita Abazi

Ph.D. Student

Faculty of Technological Sciences, Mother Teresa
University, Macedonia

Arif Latifi

Dr.

Medical Faculty, Department of Hematology,
Macedonia

In this study, five samples of honey (4 from various beekeepers and 1 from a local supermarket) were analyzed to determine the presence of Pb, Fe, Mn, Al, Cu, Cr, Zn, Cd, As, Ni and Se content using atomic absorption spectrometry. Samples were collected from the following locations: 2 from Skopje, 2 from Kumanovo and 1 from Preshevo. HPLC was applied to determine sugars in honey samples. Acid and moisture were also determined. The average values of concentration were from 0.033 to 0.055 mg/kg, 0.610 to 2.498 mg/kg, 0.052 to 0.377 mg/kg, 2.133 to 3.474 mg/kg, 0.060 to 1.034 mg/kg, 0.005 to 0.019 mg/kg, and 0.067 to 0.085 mg/kg for Pb, Fe, Mn, Al, Cu, Cr, and Zn, respectively. Cadmium was determined in one sample (0.040 mg/kg), while the presence of arsenic, nickel and selen were not observed. The total amount of reductive sugars were within the standard value of min 60 g/100 g honey. The moisture was from 16.6 to 17.6% (max 20%). The acid content was recorded from 9 to 28 mEq/1 kg honey (max 50 mEq/1 kg honey). The results were compared with the safety standards established from the Ministry of Agriculture, Forestry and Water Economy. In general, the analyzed parameters are within the standards and honey can serve as good dietary source.

Keywords: AAS, Honey, HPLC, Rid, Sugars,

Oxidation of Some Aldehydes to Acids with Jones Reagent Supported on the Diatomaceous Earth from The Republic of North Macedonia

Ahmed Jashari*

Assoc. Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Rina Cami

Other

Department of Chemistry, University of Tetovo,
Macedonia

Agim Shabani

Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Fatlinda Rrahmani

Master Student

Department of Chemistry, University of Tetovo,
Macedonia

Mirjeta Rramani

Other

Department of Chemistry, University of Tetovo,
Macedonia

Arianit Reka

Assoc. Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Traditionally, conversion of aldehydes to corresponding carboxylic acids has been realized by Jones reagents, oxone, potassium permanganate etc. But, unfortunately these methods fails to produce satisfactory results, because in general the reactions are slow, uncontrolled, time-consuming and a lot of byproducts are created, that makes difficulties in the isolation of the main product. To avoid all of this, transformation of aldehydes to carboxylic acids was developed by oxidizing agents using solid supports. Solid supports have advantages over the traditionally methods, they modify activity of the reagent, improve selectivity and the most important make product isolation easier. In objective of this study was the oxidation of some aldehydes to corresponding carboxylic acids utilizing diatomaceous earth from North Macedonia as solid support for the Jones Reagents. Experimental parts have shown a successfully oxidation of those aldehydes to the corresponding carboxylic acids when used North Macedonia diatomaceous earth as solid support for Jones reagent, at room temperature for 30 min, in the presence of dichloromethane as solvent. Acids were isolated as very pure products, without need of further purification and in moderate to high yields. Other benefit of this procedure is that all of the constituents can be recycled and the process is scalable.

Keywords: Oxidation, Aldehydes, Carboxylic Acids, Jones Reagent, Solid Support, Diatomaceous Earth

Investigation of Antibacterial and Antibiofilm Effects of Rose Essential Oil and Rose Absolute

Halime Çevikbaş*

Ph.D. Student

Department of Biology, Süleyman Demirel
University, Turkey

Seyhan Ulusoy

Assoc. Prof.

Department of Biology, Süleyman Demirel
University, Turkey

Rose essential oils possess a wide range of biochemical activities, such as analgesic, hypnotic, antispasmodic, anti-inflammatory and anticonvulsant. Also, rose essential oils have some other activities such as antioxidant, antibacterial, antibiofilm. *Pseudomonas aeruginosa* is an opportunistic human pathogen which forms biofilm through quorum sensing system. Repressing biofilm formation will be a treatment approach that looks promising especially for the immunocompromised patients. In this research, rose essential oil and rose absolute that are natural products and have been used for conventional medicine for a long time were tested. Minimum inhibitory concentrations (MICs) were determined by broth dilution assay and biofilm formation were investigated in *P. aeruginosa* PA01 strains. In conclusion, MIC values for rose essential oils were determined while as $> 2\%$, for rose absolute was determined as 1% in *P. aeruginosa* PA01. Also, it was observed that the rose essential oil and rose absolute (by 1% concentration) inhibited biofilm formation by 16% and 51% in *P. aeruginosa* PA01, respectively. At the end of this research, it was proved that rose essential oil and rose absolute can be a significant anti-biofilm agent.

Keywords: Rose Essential Oil, Rose Absolute, Antibacterial, Antibiofilm

Acknowledgement: This work was financially supported by a Project No FDK-2019-6862 from Research Foundation of Süleyman Demirel University, Isparta, Turkey.

Chemical, Mineralogical and Thermal Study of Rare Occurrence of Naturally Occuring Tridymite from Allchar

Arianit Reka*

Prof.

Department of Chemistry, State University of
Tetovo, Macedonia

Petre Makreski

Prof.

Faculty of Technology and Metallurgy, Ss. Cyril and
Methodius University, Macedonia

Blagoj Pavlovski

Prof.

Faculty of Technology and Metallurgy, Ss. Cyril and
Methodius University, Macedonia

Njomza Buxhaku

Master Student

Department of Chemistry, State University of
Tetovo, Macedonia

The samples of naturally occurring tridymitic earth (tridymite) are collected from the Allchar Caldera, Republic of North Macedonia, and they represent a very loose, weak and soft rock almost entirely white that very much resembles diatomaceous earth. The chemical composition of the samples was determined by classical silicate analysis and shows that the raw material (tridymite) contains of the following oxides (wt%): SiO₂ (90.17), Al₂O₃ (1.79), Fe₂O₃ (0.328), MnO (0.0004), TiO₂ (0.055), CaO (0.132), MgO (0.20), K₂O (0.52), Na₂O (0.25), and LOI (6.15). Results from the X-ray diffraction examination clearly show presence of predominant tridymite crystalline phase, associated with quartz and muscovite. The IR spectrum of the tridymitic earth exhibits absorption bands at 791 cm⁻¹ and 1100 cm⁻¹ ascribed to the stretching Si-O-Si vibrations. The bands at 3650 and 1640 cm⁻¹ are assigned to the stretching and bending vibrations from the absorbed water, respectively. SEM investigations show characteristic hexagonal crystals of tridymite and globular forms present in the raw material. Results from the TEM investigations show globular forms present in the samples.

Keywords: Natural Tridymite, XRPD, FTIR, SEM

Green Pesticides Based on Cinnamic Acid Dispersed in Hemp Fibers and Pectin

Fatlinda Rrahmani*

Master Student

Department of Chemistry, University of Tetovo,
Macedonia

Federica Zuppari

Dr.

Department of Industrial Engineering, University of
Salerno, Italy

Giuliana Gorrasi

Prof.

Department of Industrial Engineering, University of
Salerno, Italy

Gianluca Viscusi

Ph.D. Student

Department of Industrial Engineering, University of
Salerno, Italy

Ahmed Jashari

Assoc. Prof.

Department of Chemistry, University of Tetovo,
Macedonia

The long-term use of synthetic pesticides has evidenced a damage environment and a toxicological residues accumulation. Also, they have shown adverse effects in intimidation on human health and ecosystems. Therefore, looking for alternative bio-pesticides are a viable solution also called "green pesticides". This study reports the preparation of green pesticides based on pectin composed with hemp fibers untreated, hemp fibers treated with alkali solution and cinnamic acid. The dispersion of cinnamic acid and hemp fibers into a pectin matrix was obtained using high energy ball milling. Structure and physical properties of the matrix were evaluated. Also the release of cinnamic acid was followed using UV spectrophotometry. The results have show that in the first 15 minutes about the 90% of CA is released for pectin and HF untreated pectin samples, while it is evident that, for treated HF pectin composites, a lower amount of filler (from 60 to 75%) has been released.

Keywords: Pectin, Hemp Fibers, Cinnamic Acid, Green Pesticides, Solid Support

Use of Different Types and Environments of Smart Radiotherapy Biomaterials for Payloadrelease on Tumor Sites

Bashkim Ziberi*

Assoc. Prof.

Department of Physics, University of Tetova,
Macedonia

Michele Moreau

Mrs.

Radiation Oncology, Dana Farber Cancer
Institute/University of Massachusetts Lowell, Boston,
MA, United States

Wilfred Ngwa

Dr.

Radiation Oncology , Brigham and Women's Hospital,
Dana-Farber Cancer Institute, Harvard Medical School,
Boston, MA, United States

Reports show that acidic pH mimicking tumor pH levels causes alterable anergy in both human and mouse CD8+ T lymphocytes in vitro. The hypothesis of this study is to introduce an alkaline agent such as smart radiotherapy biomaterials (a-SRBs) to cause apoptosis in tumor cells. For this purpose the optimal release kinetics of drugs from SRBs was monitored by varying: radiation (RT) dose, types of polymers used, and pH level of media to enhance therapeutic outcomes. SRB matrices were developed respectively as high-capacity payload poly-(lactic-co-glycolic)-acid (PLGA) and Polycaprolactone (PCL) 4mm-length spacers loaded with 5ug Fluorescein (FITC) dye to slowly release the drug-depot for simultaneous localized radiotherapy. FITC_SRBs were placed in varying pH of PBS media (e.g. pH 7.4, 6.8, and 8) to examine the effect of media pH on the SRBs. A comparison of PLGA and PCL SRB_FITC release kinetics was performed. Results show at RT doses of 6 and 20Gy, acidic media degrades SRBs faster than alkaline media. At 12Gy, PLGA_SRBs showed up to 59% higher release at pH 8 compared to pH 7.4. Results showed higher than 50% payload release for all RT doses at pH 8. PLGA_SRBs released faster than PCL_SRBs over 15-day span. These results confirm that acidic medium mimicking the tumor microenvironment boosts the release of drugs from SRBs. These findings showed differing pH can influence the release of payload from SRBs. Therefore, further studies could investigate how alkaline SRBs (a-SRBs) can intensify the therapeutic efficiency of T-cell based immunotherapies.

Keywords: Radioimmunotherapy, Polymers

Synthesis and Characterization of Si-Modified Quince Seed Mucilage Based Bioscaffolds for Bone Tissue Engineering

Hilal Deniz Yilmaz*

Master Student

Department of Bioengineering, Canakkale Onsekiz
Mart University, Turkey

Ugur Cengiz

Assoc. Prof.

Department of Chemical Engineering, Canakkale
Onsekiz Mart University, Turkey

Yavuz Emre Arslan

Dr.

Department of Bioengineering, Canakkale Onsekiz
Mart University, Turkey

In the field of bone tissue engineering, natural hydrogels are the crucial players due to their biodegradable, bioactive, and bio-mimicking features. Although there are many natural hydrogels, quince seed mucilage (QSM), which is a well-known polysaccharide, was used to construct an osteoregenerative bioscaffolds because of its remarkable wound healing and regenerative capacity. The bioactive and biodegradable properties of the mucilage were enriched with silica molecules to mimic better the nature of bone structure and boost bone regeneration. Silicon modification of the QSM was fulfilled using tetraethyl orthosilicate (TEOS) with sol-gel technique, which is a relatively inexpensive, non-toxic, and well-known way that offers synthesis state-of-the-art hybrid gels under mild conditions. The morphological structure of the Si-modified QSM bioscaffolds was investigated under a stereomicroscope, and the presence of silica molecules was proven by energy dispersive spectroscopy analysis in addition to scanning electron microscopy micrographs. The thermal features of the prepared bioscaffolds were determined by differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The morphological analyses indicated that Si-modified QSM bioscaffolds possessed interconnected 3D networks, which is required for cell hosting and growth. The average pore size of the Si-modified QSM scaffolds was measured to be 66.8 μm . With respect to TGA analysis, it was seen that 80.55% of the total mass was lost at 328.72°C. Also, DSC analysis implied that there is a Td (degradation) point around ~300°C, which supports the TGA data. In conclusion, the mucilage from quince seed, and the silica molecules from TEOS has been successfully reacted to create a durable and highly porous hydrogel. We believe that the novel hybrid material could be used in further cell culture studies, especially as an osteoregenerative material for bone tissue engineering applications.

Keywords: Quince Seed Mucilage, Hydrogel, TEOS, Sol-Gel, Bioscaffold, Bone Tissue Engineering

Rheological and Some Physicochemical Properties of Oleogels Prepared with Tallow and Partially Hydrolyzed Tallow Biomaterials

Eda Keskin Uslu*

Ph.D. Student

Department of Food Engineering, Canakkale Onsekiz
Mart University, Turkey

Emin Yılmaz

Prof.

Department of Food Engineering, Canakkale Onsekiz
Mart University, Turkey

The biomaterials saturated monoglyceride (MG), saturated monoglyceride + diglyceride mixture (MDG), tallow fat (TF), and partially hydrolyzed tallow fat (HTF) were used to prepare sunflower seed oil oleogels. While MG, MDG, and HTF created oleogel at 10% addition level, it was about 30% for TF to yields table oleogel. Oil binding capacity (OBC), gel formation time (GFT) and L, a*, b* values were performed to determine physicochemical properties of oleogels. For four oleogels oil binding capacity values were around 99%, gel formation time with TF and HTF was longer (35.0 and 33.3 min) than those of the MG and MDG oleogels (8.33 and 0.34 min) and the expected differences in color values were observed according to stock oil and organogelator type used. Frequency sweep, time sweep and temperature ramp tests were accomplished to investigate rheological properties of oleogels. After determining the linear viscoelastic region (LVR) for each sample, a frequency-sweep test was performed. For all samples, storage modulus (G') values were higher than those of the loss modulus (G'') values, indicating the exact gelled consistency. Then a time-sweep test was completed with strain at LVR, strain higher than LVR, and strain at rest (lower than LVR). These tests were proved that, all gels deform under higher strain, but reformed at rest region. This is an essential property for oleogels to come back after mechanical deformation. Finally, a temperature-ramp test was done. The test showed that all oleogels were protected their gelled consistency at around 55°C temperature, then the gel deformed. This result suggest that these oleogels could be used temperatures up to 50°C with out any loss of structure. In conclusion, especially HTF could be a successful organogelator to create oleogels similar to those oleogels created with MG and MDG organogelators.

Keywords: Partially Hydrolyzed Tallow Fat, Biomaterials, Oleogels, Rheology, Stability

Anticancer Effects of the Marine Extracts from Turkey

Salih Can Suner

Phd. Student

Chemical and Chemical Processing Technologies,
Canakkale Onsekiz Mart University Lapseki
Vocational School, Turkey

Halil I Ciftçi

Prof.

Department of Drug Discovery, Kumamoto
University, Japan

Doha E Ellakwa

Prof.

Department of Biochemistry, Al-Azhar University,
Egypt

Ayhan ORAL

Assoc. Prof.

Department of Chemistry, Çanakkale Onsekiz Mart
University, Turkey

Masami Otsuka

Prof.

Faculty of Life Sciences, Kumamoto University,
Japan

Mikako Fujita

Prof.

Faculty of Life Sciences, Kumamoto University,
Japan

Bariş Hasan Ozalp

Assoc. Prof.

Vehicles and Transportation Technologies,
Canakkale Onsekiz Mart University Vocational
School of Marine Technologies, Turkey

Mustafa Can

Assoc. Prof.

Department of Engineering, Katip Celebi University,
Turkey

Mustafa Alparslan*

Prof.

Marine Biology, İzmir Katip Çelebi Üniversitesi,
Turkey

Marine natural products have received great attention to the world as an important source of new drugs for the last five decades. However, the marine organisms found in the seas surrounding Turkey (the Black Sea, the Aegean Sea, and the Mediterranean Sea) have not been yet extensively studied. In this study, three marine organisms (Sponge: A, Füska: B and Sea star: C) were sampled from the Dardanelles (Turkish Straits System, Western Turkey) by Scientific Divers, transferred to the laboratory and then were extracted with ethanol, which were investigated for their anticancer effects against A549 human lung adenocarcinoma, MCF-7 human breast cancer, A375 human melanoma, HCT116 human colon cancer, K562 human chronic myeloid leukemia and multiple myeloma cell lines (H929 and KMS-12PE). The cytotoxic effects of these extracts on normal blood cells PBMCs (Peripheral Blood Mononuclear Cell) were also investigated to determine their selectivity. Among them, (A) was found to be the most effective anticancer marine extract against all cancer cell lines; H929, K562, KMS-12PE, MCF-7, HCT116, A549 and A375 with IC50 value of 2.91g/mL, 7.17 g/mL, 9.55 g/mL, 11.51 g/mL, 17.54 g/mL, 20.88 g/mL and 25.15 g/mL respectively. Conversely, extract B and C showed no significant activity on all cells at 100 g/mL concentration. While extract A did not show cytotoxicity on normal cells (PBMC) at 100 g/mL and 300 g/mL, it showed cytotoxicity at 30 g/mL. These results pointed out that extract A contains various types of bioactive compounds. The identification of the active compound from the Turkish sponge and its mechanism of action is ongoing in our lab.

Keywords: Anticancer, Marine Products, Lung Adenocarcinoma,

Voltammetric Determination of Diclofenac Sodium by using Poly(beta-Cyclodextrin-co-2,4,6- Trimethylaniline) Modified Platinum Electrode

Muammer Burç*

Master Student

Department of Chemistry, Inonu University, Turkey

Oznur Güngör

Dr.

Department of Chemistry, Inonu University, Turkey

Serap Titretir Duran

Assoc. Prof.

Department of Chemistry, Inonu University, Turkey

Diclofenac sodium (DC) is a phenylacetic acid derivative nonsteroidal anti-inflammatory drug. It is used for the musculoskeletal and joint disorders such as rheumatoid arthritis, osteoarthritis, and ankylosing spondylitis. DC is well absorbed after oral administration. This compound exhibits a terminal half-life of 1-2 h, volume of distribution of 0.17 L/kg, and 99% protein binding and enters the synovial fluid. The determination of small amounts of DC in pharmaceutical preparations is very important for medical and pharmaceutical needs where it is used for the treatment of various diseases. Several analytical methods have been described in the literature for the determination of DC in pharmaceutical and biological samples. These methods include gravimetry, spectrometry, and partial least-squares (PLS), univariate second derivative spectroscopy, fluorescence spectroscopy, GC, HPLC, and densitometry. In the study, electrode modifications was carried out electrochemically with cyclic voltammetry (CV) method. For this purpose; a solution of 2.5 mM beta-Cyclodextrin and 1.5 mM 2,4,6- Trimethylaniline in Britton Robinson buffer (BRB) solution adjusted to pH 7.5 was used. Then, electrochemical behaviour of DC at the poly(beta-Cyclodextrin-co-2,4,6- Trimethylaniline) film modified Pt electrode was investigated by CV and differential pulse voltammetry (DPV) method. Optimization of parameters such as film thickness, pH, and electrolyte type were examined. The voltammetric results indicate that the beta-Cyclodextrin-co-2,4,6-Trimethylaniline coated platinum electrode shows excellent analytical performance for the determination of DC in terms of a detection limit, high sensitivity, accuracy and reproducibility. This method could be used for the accurate detection of DC in clinical and pharmaceutical industries in the future.

Keywords: Diclofenac Sodium, Copolymer, Beta-Cyclodextrin, 2,4,6- Trimethylaniline, Sensor, Voltammetry

Chitosan Microbeads for Encapsulation and Delivery of Essential Oils

Elif Karacan Yeldir*

Dr.

Department of Chemistry, Canakkale Onsekiz Mart
University, Turkey

Ayhan Oral

Assoc. Prof.

Department of Chemistry, Canakkale Onsekiz Mart
University, Turkey

Chitosan is a biodegradable and biocompatible linear polysaccharide that derived from alkaline deacetylation of chitin which is the second most abundant natural polymer after cellulose .Due to its non-toxicity, anti-microbial property, solubility in water, chitosan is a good candidate especially for biomedical applications. In this study, Cinnamaldehyde (CIN) encapsulate in chitosan beads, and release of CIN from beads are investigated. Chitosan solution was prepared in 7% acetic acid solution. Chitosan beads were obtained by dropping the chitosan solution in 10% NaOH solution. These beads were washed with distilled water and preserved in PBS. After it was mixed with CIN methanol in the amount of 50% of the used chitosan, 7% acetic acid solution and chitosan are added and mixed till a homogenous mixture was obtained. Chitosan/CIN beads were obtained by dropping this solution in 10% NaOH solution , and they were washed with distilled water. PBS was used at 37 °C to perform the study on the relaese of the antibacterial substances from chitosan containing those. The prepared chitosan/CIN beads within PBS solution were being mixed for 5 days at 400 rpm, samples were taken periodically. The amount of CIN released from the chitosan/CIN spheres was determined by both UV-Vis spectrophotometer and GC-MS and the results obtained with both methods were observed to be compatible with each other. Accordingly, the amount of CIN released from the chitosan/CIN spheres reached 8 ppm, the maximum amount, in PBS buffer at 37°C after approximately 60 minutes.

Keywords: Chitosan, Cinnamaldehyde, Encapsulation, Essential Oil, Controlled Release,

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New Monograph Methods for Analysis of Some Small Anions in Three Different Pharmaceutical Formulations using Suppressed Ion Chromatography

Gjani Hulaj*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Ngoc Phuoc Dinhc

Dr.

Uminova, Diduco AB, Sweden

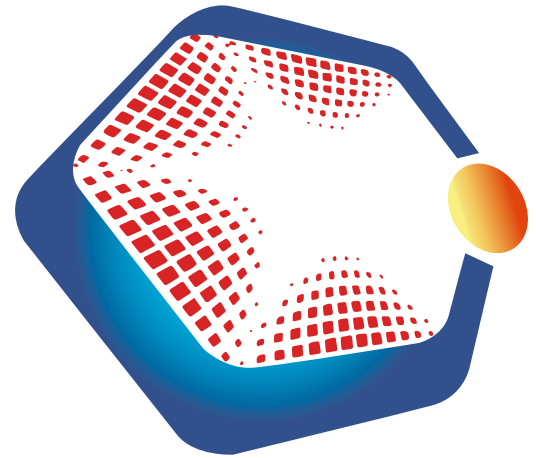
Tobias Jonsson

Dr.

Uminova, Diduco AB, Sweden

Small anionic substances have been commonly used in pharmaceutical formulations as active pharmaceutical ingredients and also as excipients. In many cases, the impurities in pharmaceuticals are also anionic compounds. Conventionally, titration and photo-spectroscopic techniques have been used in pharmacopeia methods for analysis of these ions. However, these methods suffer from limited specificity and selectivity, as well in their ability for simultaneous analysis of multiple compounds. Ion chromatography has been emphasized as an appropriate technique that allows for both specificity control and quantification of ionic substances in pharmaceuticals. We have used suppressed ion chromatography to develop a universal method to separate and quantify pharmaceutical counterions. Various stationary phases and mobile phases were exploited during method development and optimization. This resulted in a method that successfully allowed simultaneous analysis of 14 of the most used anions in pharmaceutical formulations.

Keywords: Ion Chromatography, Pharmacopeia, Pharmaceutical Counterions, Stationary Phases, Pharmaceutical Formulations, Quantification of Ionic Substances



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**POSTER
PRESENTATIONS**

Docking Study of HIV-1 Reverse Transcriptase with a Virtual Library of Ligands

Admir Omaj*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Human immunodeficiency virus (HIV) is a lentivirus that causes developed immunodeficiency syndrome (AIDS), a condition in humans in which the immune system begins to fail, leading to deadly opportunistic infections. For its exclusive catalytic properties, Reverse Transcriptase (RT) has been the target enzyme for many antiviral therapeutic agents used in the treatment of AIDS, including a number of different compounds. In this study, we report the structure based virtual screening to identify the hit compounds which can be developed as suitable ligands for the HIV-1 reverse transcriptase. A structure based in silico procedure was applied to discover the binding modes of most active compounds from an anti HIV drug database of ligands containing 339 entries (retrieved from ChEMBL). The crystal structure of enzyme (PDB ID: 1REV ? HIV-1 reverse transcriptase), crystallized with the complexed molecule of 9-chloro-TIBO, was acquired from the Protein Data Bank server (<http://www.pdb.org>). The structure of ligands were prepared (using LigPrep with protonation states assignment at pH 7.0 ± 2.0) for docking using the Schrödinger Maestro software and then was submitted to the Protein Preparation Wizard. The grid generation was formed using Glide program and docking runs were performed with extra precision docking mode (XP). Most active ligands were analyzed in terms of docking score and non-covalent interactions to understand better which structural features reveals the best docking properties toward the HIV-1 reverse transcriptase.

Keywords: Docking, HIV-1, Non-Covalent Interactions, HIV Drug Database , Virtual Screening , Aids

Voltammetric Determination of Nitrite in situ Derivatized with Ranitidine at Electrochemical Reduced Graphene Oxide using Anionic Surfactants

Majlinda Ganimet Haliti*

Master Student

Department of Chemistry, University of Prishtina
"Hasan Prishtina", Kosovo

Arsim Maloku

Dr.

Department of Chemistry, University of Prishtina
"Hasan Prishtina", Kosovo

Tahir Arbneshi

Prof.

Department of Chemistry, University of Prishtina
"Hasan Prishtina", Kosovo

Vullnet Veseli

Master Student

Department of Chemistry, University of Prishtina
"Hasan Prishtina", Kosovo

Liridon Berisha

Prof.

Department of Chemistry, University of Prishtina
"Hasan Prishtina", Kosovo

Nitrites are one of the most toxic and dangerous components for human health and the environment. Therefore, many determination methods have been developed. Surface modification of glassy carbon paste electrode (GCPE) with electrochemical reduced graphene oxide (ERGO) was performed in cyclic voltammetry. Hydrophobic chain of anionic surfactants adsorbed on electrode surface by drop casting increased reduction peak of derivatized nitrite ion with ranitidine in acidic medium. For determination of nitrite ion were optimized different parameters, such as pH, surfactant concentration, ranitidine concentration, equilibration time etc. Furthermore, square wave voltammetric (SWV) parameters were optimized such as amplitude, frequency and step potential to find better electrode response to nitrite ion. New method showed good linearity up to $275\text{ }\mu\text{M}$ with detection limit (LOD) $1.89\text{ }\mu\text{M}$ and quantitation limit (LOQ) $6.32\text{ }\mu\text{M}$ and recovery test for nitrite ion was 94%.

Keywords: Nitrite, Square Wave Voltammetry, Electrochemical Reduced Graphene Oxide, Anionic Surfactants

Theoretical Study of Some Synthesized Carbazole-Pyridopyrimidine Derivatives

Kaltrina Avni Kastrati*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Mustafa Arslan

Prof.

Department of Chemistry, Sakarya University,
Turkey

Several carbazole-pyridopyrimidine derivatives were synthesized and structurally characterized using FTIR and NMR spectroscopy. The theoretical calculations with the aim to better understand the structural characteristics, electronic excitations and the reactivity of the synthesized molecules were performed. The lowest energy conformers of the carbazol-pirimidine in the first calculation step were exposed to several Annealing Dynamics cycles. The IR and UV-VIS spectra were computed using the DFT/TDDFT (Time-Dependent Density-Functional Theory) method with the B3LYP (Becke, 3-parameter, Lee?Yang?Parr) functional with Grimme dispersion correction and 6-311g basis set by Gaussian 16 software. The computed parameters such as: IP, EA, E(HOMO), E(LUMO) , etc. - offered a full insight to the regard of the influence of the substituents on the electronic properties of the molecules.

Keywords: Carbazole, DFT/TDDFT, IP, EA, B3LYP, Gaussian 16 software

Structure Based Virtual Screening Studies to Identify Novel Potential Coumarin Derivatives for Cytochrome P450 14 Alpha-Sterol Demethylase

Admir Omaj*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Veprim Thaçi

Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

In this study, we report the structure based virtual screening to identify the hit compounds which can be developed as suitable ligands for the 1EA1 enzyme. A structure based in silico procedure was applied to discover the binding modes of most active compounds from a coumarin database containing 469 entries of chemical database of bioactive molecules with drug-like properties (retrieved from ChEMBL). The crystal structure of enzyme (PDB ID:1EA1 from Cytochrome P450 14 alpha-sterol demethylase (CYP51) from *Mycobacterium tuberculosis*), crystallized with the reference drug (fluconazole) of antifungal activity assay, was acquired from the Protein Data Bank server (<http://www.pdb.org>). The structure of ligand was prepared (using LigPrep with protonation states assignment at pH 7.0 ± 2.0) for docking using the Schrödinger Maestro interface and then was submitted to the Protein Preparation Wizard. Prior docking, the grid generation was formed using Glide program and docking runs were performed with single precision docking mode (SP). Most active ligands were analyzed in terms of non-covalent interactions to understand better which structural features reflects best docking properties of the coumarin derivatives toward the docking site of the 1EA1 enzyme.

Keywords: 1EA1 Enzyme, Coumarin Database, ChEMBL, Docking, Virtual Screening, In Silico

Dual Drug Loaded Solid Lipid Nanoparticles for Glioblastoma Therapy via Intranasal Route: Toxicological and Pharmacokinetic Studies

Ayşe Ünal

Master Student

Ege University, Department of Biochemistry / Ege University ARGEFAR, Turkey

Güliz Ak

Dr.

Ege University, Department of Biochemistry / Ege University ARGEFAR, Turkey

Buket Bakan

Dr.

Ege University, Department of Biology, Turkey

Senay Hamarat Sanher*

Prof.

Ege University, Dept. of Biochemistry / Ege University ARGEFAR, Turkey

Tuğba Karakayalı

Master Student

Ege University, Department of Biochemistry, Turkey

Özge Sarı

Mrs.

Ege University ARGEFAR, Turkey

Nefise Ülkü Karabay Yavaşoğlu

Prof.

Ege University, Department of Biology, Turkey

According to the American Brain Tumor Association, the most common type of cancer after leukemia is brain tumor in individuals aged 0 to 19 years. Glioblastoma(GB), which is a grade IV astrocytoma, is more common than grade III anaplastic astrocytoma. Although treatment approach consisting of maximum safe neurosurgical resection, radiation and chemotherapy is standard multimodal treatment for newly diagnosed GB, prognosis is poor and median survival is 14.6 months. Patients receive radiotherapy and chemotherapy and can receive Temozolomide (TMZ) treatment as primary or adjuvant chemotherapy. In treatment of recurrent glioblastoma, recommendation of FDA is to use Carmustine (BCNU) together with radiotherapy. Carmustine is an oral alkylating agent that acts by binding to DNA with reactive alkyl radicals by stopping transcription and replication. However, survival rate of glioblastoma can be increased by 2.5 months on average. For this reason, new drug delivery system for treatment of glioblastoma was developed and then TMZ and BCNU drugs were loaded. In addition, dual drug system for the treatment of glioblastoma, preparation was thought to easily cross the blood brain barrier. Because of the lipophilic character of the drugs, firstly, organic phase was prepared by dissolving in cetyl palmitate and then conjugated with γ -hydroxybutyrate ketonkorate stearyl amine to allow interaction with MCT-1 receptor in brain endothelial cells to pass the blood-brain barrier into this organic phase. The aqueous phase needed for synthesis of solid lipid nanoparticles was prepared with polysorbate 80, which is known to aid in crossing blood brain barrier, and surface of solid lipid nanoparticles was coated with polysorbate 80 to make the system ready for application. Solid lipid nanoparticles containing dual drug system were applied intranasally to reach the brain with higher concentration. As a result of pharmacokinetic and toxicological studies, it was determined that drugs accumulated in brain in high ratio.

Keywords: Solid Lipid Nanoparticle, Temozolomide, Carmustine, Glioblastoma, Intranasal Application, Blood Brain Barrier

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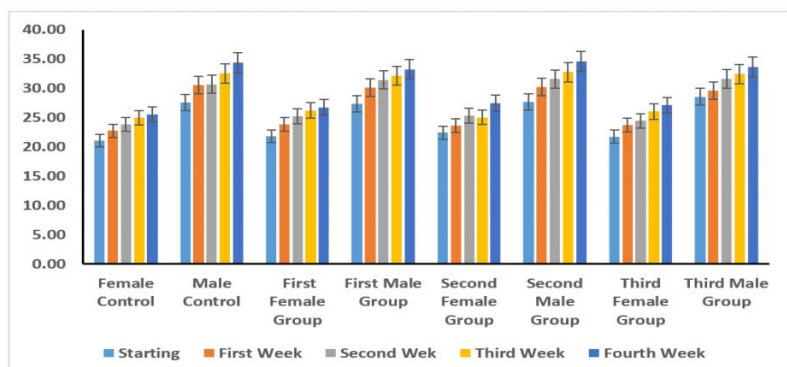


Figure 1. 28 days subacute toxicity weight change graph

1.Introduction

According to the American Brain Tumor Association, the most common cancer type after leukemia in individuals aged 0 to 19 years is brain tumor. Grade IV astrocytoma which is a type of glioblastoma (GB) is approximately four times more common than grade III anaplastic astrocytoma. Although treatment approach consisting of maximum safe neurosurgical resection, radiation and chemotherapy is standard multimodal therapy for newly diagnosed GB, the prognosis is poor and median survival is 14.6 months. In treatment of recurrent glioblastoma, FDA's recommendation is to administer radiotherapy treatment regimen together with BCNU. Carmustine is an oral alkylating agent that binds to DNA with reactive alkyl radicals and shows activity by stopping transcription and replication. However even in this case, the mean survival time for glioblastoma treatment may increase by 2.5 months. Therefore, it is important to develop new treatment approaches for glioblastoma, which involves a high proportion of malignant brain tumors. In the project, initially, we aimed to prepare solid lipid nanoparticles (SLN) containing BCNU and TMZ. Due to the lipophilic character of the drugs, the drugs will first be dissolved in cetyl palmitate and the organic phase will be prepared. γ -hydroxybutyrate ketone will be conjugated with stearyl amine and added to organic phase to provide interaction with the MCT-1 receptor present in the brain endothelial cells in order to have an ability pass the blood-brain barrier. The aqueous phase needed for the synthesis of SLN will be prepared with polysorbate 80, which is also known to help cross the blood brain barrier, and the surface of the SLN will be coated with polysorbate 80. It will be formulated for intranasal administration to achieve higher concentration of prepared SLN in brain which containing the dual drug system. In recent years, many methods have been tried to overcome the blood-brain barrier to provide effective treatment for brain diseases, and intranasal administration is prominent in this sense. It is expected that temozolomide and carmustine will damage glioblastoma cells by creating cytotoxic effect after the prepared final formulation taken into and cleared by destruction in tumor cells,. The efficacy of the nano-carrier in the treatment of brain tumors will be investigated by preclinical experiments.

2.Materials and Methods

Stearylamine (SA), beta-hydroxybutyrate (HBA), 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide (EDC), N-hydroxysuccinimide (NHS), cetyl palmitate, polysorbate80, carmustine (BCNU), temozolomide (TMZ) were purchased from Sigma-Aldrich. Other chemicals were analytical grade. For pharmacokinetic studies, SLN with 10.60 $\mu\text{g/ml}$ BCNU and 9.16 $\mu\text{g/ml}$ TMZ were used in pharmacinetic studies. Drug loaded SLN we readministered i.n. route into mice (Hanson, et al., 2013). Then, the mice were placed in metabolism cages and mice were sacrificed after a certain period of time to remove heart, liver, spleen, kidney and brain tissues.

Tissues and feces samples were washed with cold PBS and then weighed and homogenized by adding 10 mM pH: 7.4 phosphate buffer per mg (Sharma et al., 2018). Determination of drugs in homogenates was performed by HPLC method. In addition, drug analyzes were performed in plasma samples obtained from blood taken from EDTA tube and urine samples collected. For toxicological studies, for single dose acute toxicity, the highest dose of the drug delivery system, 500 µg/mL, was administered intravenously to 1 male and 1 female CD1 mouse and mice were observed for 48 hours. As the result of the experiment was observed that the mice did not die, the substance was considered non-toxic and repeated dose toxicity was administered. In the repeated dose toxicity study, 6-8 weeks old female and male CD1 mice were used. BCNU and TMZ-bearing SLN in 3 separate doses; 100 µg/mL, 300 µg/mL and 500 µg/mL were distributed in 10 mM pH 7.4 phosphate buffer. The dose groups were administered by i.n route for 4 weeks. Mice were weighed each week during the application and their condition was monitored. When the study was completed, the rats were sacrificed and their blood was taken into lithium heparinized tubes and blood parameters were analyzed on Vetscan VS2 device using Comprehensive Diagnostic Profile rotor. Toxicological evaluation was performed using all data obtained.

3.Result and Discussion

Based on the TMZ determination, the distribution of SLN given to the mouse by the i.n route in the average organs was examined, it was observed that approximately 49% accumulation in the brain and kidney as the organ where the most drugs were found. When the literature data were examined, it was stated that the plasma half-life of TMZ was approximately 1.8 hours and its elimination was mainly in the kidneys (Portnow et al., 2009). Based on the BCNU determination, the distribution of SLN in the average organs was found to be approximately 60% accumulation in the brain and the brain and then the kidney as the organ where the drug was most accumulated. In spleen, heart and lung samples, both drugs could not be detected in HPLC determination and it can be said that the drugs and thus SLN are not distributed to these organs. In the acute dose toxicity studies, there was no acute toxic effect at 500µg/mL concentration. Following this experiment, repeated dose (subacute) toxicity studies were started. During the 28-day repeated dose toxicology studies, all mice were weighed regularly every week. According to the results, it was clear that there were no weight loss and weight gain in the threedrug and control groups. After the repeated dose toxicity trial was completed, approximately 0.7 to 1.0 ml of cardiac blood was taken from each mouse under ketamine + xylazine an esthesia and blood analyzes were performed on a bi ochemistry analyzer. Whenbiochemical parameters were examined, no significant difference was observed in terms of i.n applicationcompared to healthy control group. No significant difference was observed between ALT enzyme activity anddose groups in healthy mice. While ALB levels decrease in liver diseases, GLOB levels are known to increase in liver diseases (Serfilippi, 2003). TMZ shows low hematological toxicity with rapid reversible and non-cumulative thrombocytopenia and only rarely leukopenia. In addition, it ca uses bone marrow suppression (Mamaati, 2006). BCNU as a nitrosurea derivative of amino acids in the carbamollen by causing various key enzymatic reactions inhibits and nephrotoxic (Uyanikgil, 2006). In addition, Na +, K +, BUN and CRE values were examined and dose groups were compared with healthy mice to determine whethe r there was any impairment of renal function. Since no significant difference was observed in the trial, it could be said that nephrotoxicity did not occur as a side effect of carmustine. As a result of repeated dose toxicity studies, BCNU- TMZ-SLN structure synthesized has no toxic effect.

4.Conclusion

In this study, dual drug loaded SLN were synthesized and applied mice via i.n. route. The nanoparticles were

mostly accumulated in brain. It was thought that BCNU and TMZ loaded SLN could have potential for further studies.

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A Study on Bacterial Adhesion of *Streptococcus mutans* in Various Dental Ceramics : *In Vitro* Study

Fuat Shefqet Bislimi **

Ph.D. Student

Department of Prosthodontics, Dental Clinic "Dr Fuati", Boris Kidric 49, Kumanovo, Republic of North Macedonia, Macedonia

Metodija Najdoski

Prof.

Department of Chemistry , Institute of Chemistry, Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, Arhimedova 5, 1000 Skopje, Republic of Macedonia , Macedonia

Jagoda Bajevska

Prof.

Department of Prosthodontics, Faculty of Dentistry, Ss. Cyril and Methodius University, Skopje, Republic of North Macedonia, Macedonia

Arianit Agron Reka

Assoc. Prof.

Department of Chemistry , Faculty of Natural Sciences and Mathematics, University of Tetovo, Ilinden n.n., 1200 Tetovo, Republic of North Macedonia, Macedonia

Streptococcus mutans has been identified as a major etiologic agent of human dental caries and forms a significant proportion of oral streptococci in carious lesions. This study investigates the correlation of surface properties (effect of contact angle and free surface energy) on three restorative materials (zirconia, nickel-chromium-molybdenum alloy and composites) used in dental prosthetics with bacterial adhesion to *Streptococcus mutans*. 10 samples of each material (zirconia, nickel-chromium-molybdenum alloys and composites) of 8 mm diameter and 2.5 mm thickness were used. Aqueous contact angle measurements, free surface energy and bacterial adhesion to the sample surfaces were performed. Bacterial adhesion is determined by planting samples in blood agar cultures and using an electron microscope (SEM). The highest values of bacterial adhesion are found in composites, followed with the metal alloys, while the lowest values are found in zirconia. Measurements show that zirconia has 17 colonies, Ni-Cr-Co alloy has 65 and composites 80 colonies. The composites showed the highest degree of bacterial adhesion, compared to the other investigated materials, which correlates with the free surface energy of the samples (24.31 mJ/m² for zirconia, 31.78 mJ/m² for Ni-Cr- Co alloy and 48.82 mJ/m² for the composite).

Keywords: *Streptococcus mutans*, Bacterial Adhesion, Hydrophobicity, Free Surface Energy, SEM

Investigation of Reaction Time and Enzyme Concentration Effects on Enzymatic Surface Modification of Hydroxyapatite

Merve Danisman*

Ph.D. Student

Department of Chemistry, Canakkale Onsekiz Mart
University, Turkey

Ayhan Oral

Assoc. Prof.

Department of Chemistry, Canakkale Onsekiz Mart
University, Turkey

Hydroxyapatite (HAP), which is the prime component of bone and teeth, can be characterized as osteoconductive, biocompatible, noninflammatory, nontoxic and bioactive. Due to its superior bio-properties it has found a wide range in biomaterial applications. In addition, with surface modification of hydroxyapatite its poor properties such as low toughness, poor mechanical resistance etc., can be improved and thus its potential applications can be extended. Enzymes can catalyze reactions, do not produce by-products, use a small amount, save energy and time, and do not harm human health and the environment. In addition, the amount of chemical waste in the reactions with enzymes is much less than the chemical surface modification methods. Therefore, studies on enzymatic surface modification methods, which are more modern and environmentalist and advantageous compared to chemical techniques, have become increasingly important in recent years. Besides all these, enzymes show optimum activity and stability at certain conditions. Therefore, to optimize the surface modification reaction, the investigation of the effect of reaction variables is key importance. Because of these reasons in this study, the effects of reaction time and enzyme concentration on HAP surface modification with enzyme catalyzed reaction were investigated.

Keywords: Surface Modification, Enzyme, Hydroxyapatite, Reaction Time

DFT Study of Some Carbazole Bearing Pyridopirimidine-Substituted Sulfonamides Derivatives

Fatjonë Bedri Krasniqi*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Mustafa Arslan

Prof.

Department of Chemistry, University of Sakarya,
Turkey

Arleta Rifati Nixha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Several carbazol-benzenesulfonamide derivatives were synthesized and structurally characterized. For theoretical calculations, the conformational space search for the studied molecules is performed using Molecular Mechanics (MM). The lowest energy conformers obtained from MM, were further subjected to several Annealing Dynamics cycles (using an initial temperature of 300 K and a mid-cycle temperature of 500K) to ensure the lowest possible energy structures, which were used as the initial starting structure in the DFT calculations. The IR and UV-VIS spectra were computed using the DFT/TDDFT (Time-Dependent Density-Functional Theory) method with the B3LYP ((Becke, 3-parameter, Lee-Yang-Parr) functional with Grimme dispersion correction (empirical dispersi and 6-311g basis set by Gaussian 16 software. The computed electrostatic potentials on concentric vdw surface grids (ESP maps) , E(HOMO), E(LUMO), UV-VIS spectra etc. permitted better to understand the structural characteristics, electronic excitations and the reactivity of the synthesized molecules.

Keywords: Carbazole, DfT, Molecular Mechanics, B3LYP, Gaussian 16 software,

Preparing Electrospun Polylactic Acid-Sulfanil Amide Nanofibers as Drug Delivery Systems

Sallih C. Suner*

Ph.D. Student

Chemical and Chemical Processing Technologies,
Canakkale Onsekiz Mart University Lapseki
Vocational School, Turkey

Ayhan Oral

Assoc. Prof.

Department of Chemistry, Canakkale Onsekiz Mart
University, Turkey

Electrospinning is the best way to obtain nanofibers that can be prepared micro and nano size with this method and as a drug delivery system nanofibers can be designed for a wide range drug release kinetics. Polylactic acid (PLA) is a biodegradable polymer which can be successfully electrospun and so many materials can be loaded PLA nanofibers for different applications such as food packaging, wound healing, drug delivery. In this study, different amounts of Sulfanilamide (SA) between 2.5 and 15% weight ratio of PLA were loaded to PLA nanofiber during the preparation of nanofibers by electrospinning technique as drug delivery system. The morphological structure of PLA and drug loaded PLA-SA nanofibers were determined by using scanning electron microscope-energy dispersing X-Ray (SEM-EDX). The width of PLA-SA nanofiber was measured from 230 nm to 860 nm. From the EDX results, C, O, N and S ratio of PLA-SA nanofiber were found as 82.9, 14.7, 1.4 % and 1 %, respectively. According to the FT-IR spectroscopy of PLA-SA, the peaks of amine and sulfonyl groups were gradually increased by increasing the SA concentration into PLA-SA nanofiber structure. These results show that SA was successfully entrapped into PLA nanofiber at different weight ratios between 2.5 and 15% for controllable drug delivery system. The SA release amounts from 2.5, 5, 7.5, and 15 % drug loaded PLA-SA nanofibers were determined in phosphate buffer solution (PBS) at pH 7.4 by using UV-Vis spectroscopy at 248 nm wavelength. The experimental results show that drug release rate increases with the increasing drug percentage in the PLA nanofibers and long-term drug releasing can be obtained for PLA-SA nanofiber. The nanofiber successfully delivered SA for 505 h.

Keywords: Nanofibers, Drug Delivery, Electrospinning, Polylactic Acid, Sulfanilamide

Biopolymer Production from Natural Sources and Usability as Biomaterials: Sodium Alginate and Collagen

Emre Yilmaz*

Master Student

Sustainable Agriculture and Natural Plant Resources
Department, Kastamonu University, Turkey

Havva Yazar

Master Student

Material Science and Engineering Department,
Kastamonu University, Turkey

Salma A. Taher Mohamed

Ph.D. Student

Material Science and Engineering Department,
Kastamonu University, Turkey

Nuray Emin

Dr.

Biomedical Engineering, Kastamonu University
Turkey

Polymers are considered in two basic classes as natural (polymers produced by biological-systems) and synthetic (chemically synthesized from starting materials). They are widely used in food, textile, pharmaceutical and biomedical industries. Although synthetic polymers have a widespread use, the uses of natural polymers is increasing day by day. Biopolymers in class of natural-polymers are naturally occurring polymers in the life process of living-organisms. They are obtained from biomass and natural and/or genetically modified organisms. Their synthesis is usually based on enzyme-catalyzed-reactions and chain-growth from activated monomers by complex metabolic processes within cells. They are light, inexpensive, easy-shape, excellent mechanical-properties, chemically inert and corrosion-resistant macromolecules. In this respect, biopolymers have become more preferred in recent years, especially in biomimetic-approaches in field of tissue-engineering. Polymeric biomaterials, which are identical to geometrically damaged tissue for tissue regeneration and serve as matrix to which cells can adhere, are used as scaffold. Biopolymers can be synthesized commercially in reactive purity and, in addition can be obtained by isolation from natural sources under laboratory conditions. Commonly used in biomaterial production; alginic acid is obtained from brown-red algae, while collagen is generally obtained from tendons of bovine/ovine-animals, rat-tail tendons and the like. The aim of this study was to isolate sodium alginate from brown-sea algae, and collagen from rat-tail tendons and purify them for ready to use in cell-culture. The scaffolding-formation potential of the biopolymeric-structures by lyophilization was also investigated. As a result, it was found that sodium-salt of alginicacid can be obtained with high purity by step-fractionation. Collagen was obtained as type-1-collagen molecule from the tendons, and had been purified by dissolving and filtered tendons in acidic solution. In conclusion, the biodegradability analysis of lyophilized collagen and alginate scaffolds in HANK's solution showed that scaffolds have durability to allow new tissue formation for tissue engineering applications.

Keywords: Biopolymers, Biomaterials, Sodium Alginate, Collagen, Brown-Red Algae, Rat-Tendons

Physicochemical and Rheological Properties of Commercial Kefir Drinks

Oguz Gursoy*

Prof.

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

Kübra Kocatürk

Master Student

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

Hasne Nazlı Yakalı

Master Student

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

Yusuf Yilmaz

Prof.

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

Hande Özge Güler

Ph.D. Student

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

Kefir is one of the most preferred fermented beverages, and its production constitutes a significant portion of the dairy industry. In this study, the physicochemical and rheological properties of commercial (plain) kefir drinks were compared. Kefir drinks of different brands ($n=5$) were purchased from national markets in Turkey, and the samples with different expiration dates for each brand were used as replications. The ranges for the dry matter, protein and fat contents (%) of the commercial kefir drinks were 9.54-11.58, 1.55-3.08 and 2.50-3.34%, respectively. Moreover, the pH values of the samples were in the range of 3.80-4.11 while total titratable acidity (%) values ranged from 0.65 to 0.93% (lactic acid). Insignificant differences in pH values were determined among different brands of commercial kefir drinks ($p>0.05$) while significant changes were obtained among other physicochemical properties ($p<0.05$). In rheological analyses conducted at 4.0, 8.0 and $12.0\pm 0.3^{\circ}\text{C}$, the power law model was used to interpret the rheological characteristics of kefir drinks, which resulted in higher R^2 values. Besides, the apparent viscosity values of the samples (111.6-186.0 1/s) were observed to be inversely related to the temperature and varied between 0.97 and 124.50 mPa.s ($p<0.05$). Results showed that significant differences in the physicochemical and rheological properties were present among the commercial kefir samples of different brands and expiration dates, indicating the compositional variations of raw materials and kefir cultures used in the production.

Keywords: Kefir, Fermented Milk, Consistency, Rheological Behavior, Viscosity

Effect of Combined Application of Transglutaminase Enzyme and Ultrasonication Process on Physicochemical and Rheological Properties of Drinking Yogurt

Serdar Duman

Master Student

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

Oğuz Gürsoy*

Prof.

Department of Food Engineering, Burdur
Mehmet Akif Ersoy University, Turkey

Yusuf Yilmaz

Prof.

Department of Food Engineering, Burdur Mehmet
Akif Ersoy University, Turkey

In this study, drinking yogurt samples were produced by using milk samples either treated with ultrasonication (150W, 5 min), transglutaminase enzyme added at the ratio of 0.01%, 0.02% and 0.03% without ultrasonication treatment or treated by both applications. Some physicochemical, rheological, sensory and microbiological properties of drinking yogurt samples were determined during 10 days storage at + 4°C, and the effects of the applications on drinking yogurt samples were determined. Individual or combined applications of ultrasonication and transglutaminase treatments during drinking yogurt production did not have a significant effect on dry matter, fat and protein contents and CIELAB color parameters (L^* , a^* and b^*) of drinking yogurt samples. Ultrasonication of milk and treatment with transglutaminase enzyme did not influence the starter culture growth during storage. The total lactobacilli and total streptococci counts of drinking yogurt samples did not fall below 7 log cfu/mL during storage. Treatment with ultrasonication+transglutaminase enzyme did not lead to a change in the pH value of drinking yogurt samples ($p < 0.05$) but decreased the acidity values (%) of the samples compared to the control sample ($p < 0.05$). In comparison to the control group, all applications (ultrasonication treatment, transglutaminase enzyme addition and their combination) decreased serum separation values significantly in drinking yogurt samples and also increased their apparent viscosities ($p < 0.05$). According to the results, the addition of 0.01% transglutaminase enzyme and ultrasonication may be more effective to decrease the serum separation of drinking yogurt samples and to increase their apparent viscosity at the same time. Similarly, the results of sensory analysis showed that the combined application of ultrasonication treatment and 0.01% transglutaminase enzyme addition, instead of their individual use, resulted in higher sensory flavor scores. In conclusion, the combined use of transglutaminase enzyme and ultrasonication treatment may have a significant contribution to the reduction of the use of this enzyme in dairy industry.

Keywords: Drinking Yoghurt, Ultrasonication, Transglutaminase, Serum Separation, Rheology

Characterization of Polysaccharides from the Brown Algae *Colpomenia sinuosa*

Gülen Türker*

Assoc. Prof.

Canakkale Applied Science Collage, Canakkale
Onsekiz Mart University, Turkey

Ilknur Ak

Assoc. Prof.

Department of Aquaculture, Canakkale Onsekiz
Mart University, Faculty of Marine Sciences and
Technology, Turkey

The polysaccharides of brown algae which called phycocolloids can be used commercially as gelling agent, stabilizers and thickeners for suspension and emulsions. Among the brown algae *Colpomenia sinuosa* possess sulfated polysaccharides such as fucoidan and laminarian. Fucoidan is the most abundant sulfated polysaccharides that is extracted from marine brown seaweeds and it is important in cosmeceutical and food production as it is possible to extract from cheap resources and used in novel drugs and functional food production. In this study, thallus of *C. sinuosa* were collected from İzmir Bay (İzmir) and Dardanelles Strait (Çanakkale). The sulfated polysaccharides extracted from collected samples. The characterization of polysaccharide contents were determined with NMR, FTIR and X-RD. The FTIR results showed that, *C. sinuosa* exhibit a broad band around 1220-1260 cm^{-1} , assigned to the presence of sulfate ester groups (S-O), which is a characteristic component in fucoidan and sulfated polysaccharides in brown seaweeds. We found that, the ^1H NMR spectrum contained several intense signals in the alpha anomeric (4.9-5.6 ppm) and high-field (1.0-3.5 ppm) regions. Signals at 5.601-5.027 ppm were assigned mainly to H1 alpha-L-fucopyranose residues. According to our results, *C. sinuosa* contain heterofucans such as fucoidan and little amounts of laminarian.

Keywords: Polysaccharide, Brown Algae, *Colpomenia sinuosa*, Fucoidan, Laminarian, Characterization

Acknowledgement: The authors thank the Çanakkale Onsekiz Mart University Science and Technology Application and Research Center for providing laboratory facilities for our experiments.

Extraction and Characterization of Polysaccharides from the Red Algae *Gracilaria gracilis*

Gülen Türker*

Assoc. Prof.

Canakkale Applied Science Collage, Canakkale
Onsekiz Mart University, Turkey

Ilknur Ak

Assoc. Prof.

Department of Aquaculture, Canakkale Onsekiz Mart
University, Faculty of Marine Sciences and
Technology, Turkey

Phycocolloids (e.g., carrageenan, agar and alginic acid) are special polysaccharides produced by several seaweed species. Carrageenan and agar are sulfated polysaccharides extracted from some red algae (Rhodophyta). These phycocolloids have a range of different and special properties which is generating an increasingly commercial and scientific interest. Also, seaweeds are very important natural resources which are employed and as sources of polysaccharides (mainly alginates, carrageenans and agar) for use in food and pharmaceutical industry. The phycocolloid "carrageenan" is a family of linear sulfated polysaccharides which differ in their degree of sulfation. In this study, thallus of *Gracilaria gracilis* were collected from Dardanelles Strait (Çanakkale). The sulfated polysaccharides extracted from collected samples. The characterization of polysaccharide contents were determined with NMR, FTIR and X-RD. The FTIR spectra of *G. gracilis* extract exhibited sharp peaks at 1409 cm^{-1} correspond to C-O stretching and O-H bending. FTIR spectrum of the extracted polysaccharide fraction, expanded in the region between 1400 and 700 cm^{-1} the sulfate groups bands. The bands found at 1370 and 1251 cm^{-1} may be attributed to sulfate ester groups, the band at 1080 cm^{-1} corresponds to galactan, the band at 830 cm^{-1} refers v-carrageenan. The ^1H NMR spectrum showed the signals from the alfa-anomeric proton at δ 5.64, 5.32 and 5.02 (assigned, respectively, to 3,6-alfa-L-anhydro galactose linked to beta-D-galactose, alfa-L galactose-6-sulfate linked to beta-D-galactose and alfa-D galactose linked to 3,6-alfa-L anhydro galactose), and from the H-1 of beta-D-galactose linked to 3,6-alfa-L-anhydro galactose with a signal at δ 4.33. Our results showed that, *G. gracilis* have different types of carrageenan such as v-carrageenan and little amounts of K-carrageenan.

Keywords: Red Algae, *Gracilaria gracilis*, Polysaccharide, Carrageenan, Phycocolloid, Characterization

Acknowledgement: The authors thank the Çanakkale Onsekiz Mart University Science and Technology Application and Research Center for providing laboratory facilities for our experiments.

Antibacterial Cinnamaldehyde Loaded Nanofibers

Zeynep Akpınar

Master Student

Department of Biology, Süleyman Demirel
University, Turkey

Seyhan Ulusoy*

Assoc. Prof.

Department of Biology, Süleyman Demirel
University, Turkey

Mert Akgün

Master Student

Department of Chemistry, Çanakkale Onsekiz Mart
University, Turkey

Ayhan Oral

Assoc. Prof.

Department of Chemistry, Çanakkale Onsekiz Mart
University, Turkey

Cinnamaldehyde is a GRAS molecule with antibacterial properties. Cinnamaldehyde was added PLA and gelatin polymers at different concentrations to obtain nanofibers by electro-spinning technique. The nanofibers were characterized by FT-IR, SEM, HPLC, TGA and their antibacterial properties were investigated. The diameters of PLA-Gel-Sinam1; PLA-Gel-Sinam2; PLA-Gel-Sinam3 nanofibers were 294.9 ± 46.8 nm; 254 ± 58.3 nm; 728.5 ± 98.3 nm respectively. Nanofibers showed antibacterial effect for all strains used in this study. The results of this study showed that the cinnamaldehyde nanofibers have the potential to be used for infections caused by human pathogenic bacteria.

Keywords: Cinnamaldehyde, Antibacterial, Nanofiber

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Allopathic Effects of Lavender Essential Oil on the Seed Germination and Seedling Development of Dent Corn (*Zea mays indentata* Sturt.)

Uğur Binbir*

Master Student

Dept. of Soil Sci. and Plant Nutr., Canakkale Onsekiz
Mart University, Turkey

Cafer Türkmen

Assoc. Prof.

Dept. of Soil Sci. and Plant Nutr., Canakkale Onsekiz
Mart University, Turkey

İsmail Taş

Assoc. Prof.

Departments of Agricultural Structures and Irrigation,
Canakkale Onsekiz Mart University, Turkey

Yalçın Coşkun

Dr.

Lapseki Vocational College, Canakkale Onsekiz
Mart University, Turkey

Yakup Cikili

Dr.

Dept. of Soil Sci. and Plant Nutr., Canakkale Onsekiz
Mart University, Turkey

Medicinal and aromatic plant oils contain many components. Many of these components have allopathic effects on other living organisms. These components may have positive and negative effects on agricultural production. The development of new agricultural practices is very important for sustainable agriculture in order to reduce their disadvantages and benefit from their positive aspects. The lack of safe food, which has been shown to be one of the main causes of increasing health problems in recent years, may be reduced to some extent by studies of such natural compounds. In a sustainable agricultural production, reliable food, reliable water, the highest yield and quality are targeted by satisfying all the needs of the plants in the period from sowing to harvest from natural sources. Increasing and evolving technology is increasing research on the use of chemical preparations derived from naturally occurring plants. In this study, investigated the allopathic effects of lavender essential oil on the seed germination and seedling development of dent corn. For this purpose, lavender essential oil was added to each petri dish at different doses [control (0), 2, 4, 6 and 8 ?L/9 cm diameter petri dish]. At the end of 11th day, the effects of bio-chemicals on the germination ratio loss, seedling dry weight, relative humidity of seedling, root length, seedling length, and seedling wet weight were measured and calculated. As results of variance analysis essential oil treatment of lavender has a significantly affect across of control treatment ($p<0.05$) on all investigated characters. Germination ratio loss and seedling dry weight increased with increase of essential oil dose. Relative humidity, root length, seedling length and seedling wet weight decreased with increase of essential oil dose. In conclusion, it was found that lavender residues of corn plant can tolerate up to a certain content of essential oil. It can be said that there is no harm in applying lavender residues to the corn fields since the essential oil contains a very small amount of essential oil. As a result of this research, it was necessary to examine the possibilities of lavender wastes to be given to the soil with different applications.

Keywords: Lavender, Corn, Germination, Allopathic Affect, Seedling Development

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Characterization of Biochar Produced from Green Walnut Shell

Ali Sungur*

Assoc. Prof.

Department of Soil Science & Plant Nutrition,
Canakkale Onsekiz Mart University, Turkey

Yasemin Kavdır

Prof.

Department of Soil Science & Plant Nutrition,
Canakkale Onsekiz Mart University, Turkey

Mustafa Soylak

Prof.

Department of Chemistry, Erciyes University,
Turkey

Özgür Özay

Assoc. Prof.

Department of Chemistry, Canakkale Onsekiz Mart
University, Turkey

Remzi İlay

Dr.

Department of Soil Science & Plant Nutrition,
Canakkale Onsekiz Mart University, Turkey

Biochar is a carbon-rich organic material obtained by burning biomass (plant resources, animal, urban and industrial wastes) either under limited oxygen or in non-oxygen media (pyrolysis). Biochar reduces metal bioavailability by absorbing metal ions on their surfaces. Biochar can be produced using poultry wastes, plant and industrial wastes. Some biochar does not completely carbonize during production, so it contains carbonized and amorphous organic matter in different proportions. Therefore, biochar can function in soil as soil organic matter. In the literature, there are studies on the removal of various metal ions from aqueous media with biochar obtained from biological sources. In this study, biochar was obtained by pyrolysis at 300, 400 and 600°C from green walnut shell which was used for the first time in biochar production. The produced biochar was acidified with 2% HNO₃ to increase the surface area. Pore size and surface area of biochar were measured by BET (Brunauer-Emmett-Teller) method. When the BET results were examined, the surface areas of the biochar obtained by pyrolysis at 400 and 600°C were 1.3 m²/g while the surface areas of the acidified biochar were increased approximately 40 times. SEM (Scanning Electron Microscope) images of both acidified and non-acidified samples of biochar produced by pyrolysis (600 °C) were obtained. According to the analyzes, acidification process dissolved structures such as metallic oxide, metals and formed pores on the surface of biochar. We continue to study on the removal of heavy metals from aqueous media with biochar produced.

Keywords: Biochar, Green Walnut Shell, SEM, BET

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Stability of Alginate Gels in the Environments with Different pH Values

Beltina Iljazi*

Master Student

Department of Physics, University of Tetovo,
Macedonia

Ahmed Jashari

Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Naim Mahmudi

Prof.

Department of Physics, University of Tetovo,
Macedonia

Alginate is a biomaterial that has found numerous application in biomedical science and engineering due to its favorable properties. Alginate can be easily modified via chemical and physical reactions to obtain derivatives having various structures, properties, functions and applications. Alginate-based biomaterials can be utilized as drug delivery systems, wound dressing and cell carriers for tissue engineering. In this project is investigated stability of Ca_2^+ cross linked alginate gels in media with acidic, neutral and basic pH and the stability of alginate gels depending on the different ratios of CaCO_3/GDL . We have seen that alginate gels are more stable and keep their form for more than a week in acidic environment and are destroyed within half an hour in basic environment. Also we have concluded that the ratio of $\text{CaCO}_3/\text{GDL}=1/3$ gives better properties of alginate gels than the others ratios like 1:1 that gives very soft gels and 1:4 that gives very fragile gels. It is important to mention that the ratio $\text{CaCO}_3/\text{GDL}=1:2$ also gives good properties similar with the ratio 1:3. During this research we have used the gravimetric method, measuring the mass of alginate gels kept in environment with different pH values for short time intervals.

Keywords: Alginate, pH, Wound Dressing, Biomaterial

Preparation and Characterization of Antibiotic Nanocarrier from Aqueous *Tilia* Extract

Güliz Ak*

Dr.

Ege University, Faculty of Science, Department
of Biochemistry, Turkey

Bahar Şeker

Mrs.

Ege University, Faculty of Science, Department
of Biochemistry, Turkey

Asunur Erkan

Other

Ege University, Faculty of Science, Department
of Biochemistry, Turkey

Green chemistry enables nanoparticle production utilizing plant extract, microbial cells etc. This approach is easy, cost-effective and environmentally friendly. *Tilia* plant extract contains natural substances such as bioflavonoids and phenolic compounds which are reducing, capping and coating agents. Amoxicillin is used in the treatment of a number of infectious diseases, however drug has short half-life and low bioavailability. Nanoparticulate systems could promise more effective therapy through targeted drug delivery. Magnetic (iron oxide) nanoparticles have great advantages as drug carriers since drugs can be addressed to target area with external magnetic field thus increases bioavailability and decreases side effects of drugs. In this work, the main objective is to synthesis of iron oxide nanoparticles from *Tilia* extract and investigate the potential as amoxicillin nanocarrier. Magnetic nanoparticles were prepared using aqueous *Tilia* extract and FeCl₃ solution at different ratios. These nanostructures were characterized with FTIR, SEM, XRD and zetasizer. Amoxicillin solutions at varying concentrations were incubated with magnetic nanoparticles for drug adsorption and *in vitro* drug release from nanoparticles at pH 7.4 and 37°C was studied. It was found that nanoparticles had spherical morphology (70-80 nm), magnetite core and capped with flavanoids. Optimum amoxicillin amount in magnetic nanoparticles was determined as 100.17 µg drug/ mg nanoparticle with 85.14% loading efficiency. Drug release was faster in the first hours and proceeded in controlled manner. It can be suggested that nanoparticles could have potential as amoxicillin nanocarrier with low cost and ecofriendly production.

Keywords: Green Synthesis, *Tilia* Extract, Magnetic Nanoparticle, Amoxicillin, Drug Delivery, Adsorption

Recognizing Novel Potential Curcumin Derivatives for 6HDR Transferase Enzyme Based on Virtual Screening Studies

Veprim Veli Thaçi*

Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Riza Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Jane Bogdanov

Assoc. Prof.

Institute of Chemistry, Faculty of Natural Sciences
and Mathematics, Ss. Cyril and Methodius University,
Macedonia

In this study, we report the structure based virtual screening to pinpoint the hit compounds which can be developed as suitable ligands for the 6HDR transferase enzyme. A structure established in silico procedure was applied to find out the binding modes of most active compounds from a curcumin database containing 55 entries of chemical database of bioactive molecules with drug-like properties (retrieved from ChEMBL). The crystal structure of the enzyme (PDB ID: 6HDR ? Dual specificity tyrosine-phosphorylation-regulated kinase from Homo sapiens), bound to curcumin [(1E,6E)-1,7-bis(4-hydroxy-3-methoxyphenyl)hepta-1,6-diene-3,5-dione] , was acquired from the Protein Data Bank server (<http://www.pdb.org>). The structure of ligand was prepared (using LigPrep with protonation states assignment at pH 7.0 ± 2.0) for docking using the Schrödinger Maestro interface and then was submitted to the Protein Preparation Wizard. Prior docking, the grid generation was formed using Glide program and docking runs were performed with extra precision docking mode (XP). Most active ligands were analyzed in terms of non-covalent interactions to understand better which structural features reflect best docking properties of the curcumin derivatives toward the docking site of the 16HDR transferase enzyme. Moreover, the physicochemical and pharmaceutical properties such as miLogP value, molecular weight, number of hydrogen bond acceptors, number of hydrogen bond donors, and number of rotatable bonds for each strongest curcumin docking molecules were analyzed. These properties were evaluated against Lipinski's rule of five that predicts drug-likeness of the potential drug compound. Lipinski's rule of five states that most of the molecules with good membrane permeability will have LogP ≤ 5 , molecular weight ≤ 500 , the number of hydrogen bond acceptors ≤ 10 , and the number of hydrogen bond donors ≤ 5 .

Keywords: Curcumin, Enzyme, Bioactive Molecules, Physicochemical, Docking Molecules, Pharmaceutical Properties

Green Surface Modification of Diatomaceous Earth from The North Macedonia Using Olive Oil

Belma Ademi*

Mrs.

Department of Chemistry, University of Tetovo,
Macedonia

Agim Shabani

Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Blazo Boev

Prof.

Faculty of Natural and Technical Sciences,
University In Stip, Macedonia

Fatlinda Rrahmani

Master Student

Department of Chemistry, University of Tetovo,
Macedonia

Arianit Reka

Assoc. Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Ahmed Jashari

Prof.

Department of Chemistry, University of Tetovo,
Macedonia

Diatomite is comprised of sedimentary remains of diatoms, a class of unicellular algae in both fresh and seawater. The chemistry and morphology of diatomite products provide the high porosity, high surface area and low bulk density. Republic of North Macedonia posses few types of diatomite, classified in class I, class II and class III. More important, in North Macedonian there is a large amount of class I diatomite that contains over 95% SiO₂ and only few percentage of the other metals, which was confirmed by ICP-MS and ICP-AOS analysis. Because of this purity this material is versatile for various application. On the other side, his strongly hydrophilic surface due to the large number of free OH groups, can be used to make surface modification in order to obtain novel materials. Therefore, some fatty acids produced from olive oil were used in order to develop esterification. Thus, long nonpolar tails were covalently bonded to the surface of the diatomite, obtaining much less polar material with different physical-chemical properties. Afterwards, the characterization of the modified material was performed. Methods used for characterization of the modified material and comparison with the unmodified material were: SEM, FTIR, XRPD. This material will be employed in hydrothermal reaction in order to obtain novel ceramic materials.

Keywords: Diatomite, Surface Modification, Olive Oil, Ceramics

Development of Method for Detection of Volatile and Semivolatile Organic Compounds in Outdoor Urban Air in Skopje, Macedonia

Jane Bogdan Bogdanov*

Prof.

Institute of Chemistry, Faculty of Natural Sciences
and MAThematics, Ss. Cyril and Methodius
University, Macedonia

Katerina Baceva Andonovska

Dr.

Research Center for Environment and Materials,
Macedonian Academy of Sciences and Arts,
Macedonia

Jasmina Petreska Stanoeva

Prof.

Institute of Chemistry, Faculty of Natural Sciences
and Mathematics, Ss. Cyril and Methodius
University, Macedonia

The goal of this study was introduction of appropriate methods for detection and determination of volatile organic compounds (VOC) and semivolatile organic compounds (SVOC) in outdoor urban air in Skopje, Macedonia. A method involving Radiello® passive/diffusive samplers for environmental monitoring of outdoor air monitoring. The unique radial design offers higher capacity and faster uptake/sampling rates than traditional passive methods. The sampling time, the proper desorption method and analytical methods were optimized. The Radiello® passive/diffusive samplers were placed in several municipalities in Skopje and the organic compounds were monitored monthly over period of several months. Using gas chromatography coupled to mass spectrometry (GC-MS) we were able to detect and quantify over 20 compounds. Most of the VOCs and SVOCs originate from transport fuels and derivatives such as BTEX (benzene, toluene, ethyl benzene and xylenes) and tetradecane. Also in many samples naturally occurring monoterpenes were detected (alpha-pinene, beta-pinene and limonene), even though they can originate from turpentine oil or cleaning products. Based on the results from analyses and identification of major components the sources of these compounds were pinpointed (natural vs. anthropogenic). Especially worrisome was the aerial presence of phthalate esters (dibutyl phthalate and bis(2-ethylhexyl) phthalate), which were detected in winter and which most likely originate from burning polymeric materials. Certain compounds were proposed as markers for urban areal pollution. The long term goal is to set up quantitative analyses of these "control" VOCs and SVOCs and to monitor their concentrations throughout the year. The ultimate goal is to pinpoint the sources of areal outdoor urban pollution and to devise control measures for their reduction or elimination.

Keywords: Outdoor Urban Air, Volatile Organic Compounds, Semivolatile Organic Compounds, GC-MS, Passive Sampling

The Rise of the Coefficient Biosorption During Separation of Toxic Heavy Metals from Polluted Water by Modification of a Rise

Mahi Ljatifi*

Dr.

Chemical Engineering, Max Zeller Söhne, AG
Pflanzliche Heilmittel Romanshorn, Switzerland

Arianit Reka

Prof.

Faculty of Natural Sciences and Mathematics,
State University of Tetova, Macedonia

Ejup Latifi*

Others

Ministry of Economics, Skopje, Macedonia

In the group of conventional methods for separation of heavy metals from water resources are oxydation/precipitation and concentration/precipitation. Adsorption has many advantages in controlling polluted waters, these are as follow: investments are insufficient, simple project, there are no side effects from toxic substances, and superior elimination of heavy metals. The rise husk used as a biosorbent shows very good facilities for separation of a large number of heavy metals from polluted waters especially metals which are eliminated very difficult through other methods such as Cr 6+. Using the rise husk as a natural biosorbent for elimination of Cr6+ ions, there are reached very good results, with a high coefficient of biosorption but it is not enough yet, therefore it is necessary to do a modification of the biosorbent in order to rise the biosorption coefficient. The rise husk undergoes the process of oxydation, and a result of this comes to the change of the morphology of biosorbent surface depending on the reproductivity of the structure creating in this way spaces with a regular orientation which represent a structure in the form of a sphere well organized, rising the active surface of biosorbent and makes easier the adsorption of metal ions Cr6+ within the biosorbent. Carbonisation of the rise husk is made on 400 °C. By modifying the rise husk apparently rises the biosorption coefficient, the biosorption time is shortened, and the amount of biosorbent is lowered as well.

Keywords: Rise Husk, Biosorbent, Carbonisation

The Interaction of Some Alkyl Phosphonic Acids with the Cu(111) Surface in Aqueous Acid and Ethanol Media - a Monte Carlo Study

Valbonë Veli Mehmeti*

Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Ramë Vataj

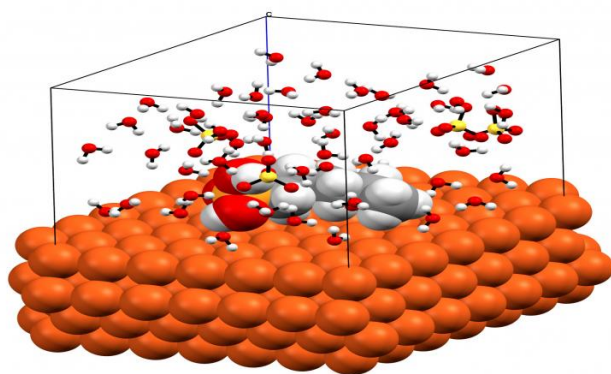
Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Fetah Podvorica

Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Alkyl phosphonic acids are a class of molecules that are well known for their self-assembly onto the hydroxide surfaces. This feature allow a simple yet a covalent bonding for the creation of organic bonded monolayer onto different surfaces. These surfaces have a wide applications ranging from corrosion protection of materials to Dye-sensitized solar cells. A crucial step to enhance and to fundamentally understand how these surfaces are created is the elucidation of the interaction process that leads to such interface creation. Although, experimentally this is rather hard to accomplish, using theoretical computation methods one can acquire a good understanding how this interaction takes place at the surface. In this study we employed Monte Carlo and Molecular Dynamics to understand this process. A Cu(111) model (Periodic Boundary Conditions) with dimensions: 15.336 * 15.336 * 15 Å vacuum layer at the C axis is used as a surface. The interaction with the Cu(111) surface of three different alkyl phosphonic acids (hexyl-, octyl- and decylphosphonic acids) both: in aqueous acidic media and ethanol one is evaluated by Monte Carlo and Molecular Dynamics simulations. The MD simulations with the Forcite Module (Materials Studio) were performed using COMPASS II. Prior to the use of MD simulations, the surfaces were optimized using the Smart optimization algorithm with the energy convergence criteria of 10⁻⁴ kcal/mol and force criteria of 5 × 10⁻³ kcal/mol/Å. The atom charges for the calculations were assigned using the DFT calculations (level of theory: GGA/PBE, DNP 3.5 basis set). The MD was conducted using an NVT (constant-temperature, constant-volume) canonical ensemble at 298 K. The time step for MD was 1 fs with a total simulation time of 500 ps. The system temperature was controlled using a Berendsen Thermostat. For the data analysis, 500 ps of trajectory frames were used.

Keywords: Surface Modification, Alkyl Phosphonic Acids, Monte Carlo, Molecular Dynamics, Corrosion, DFT

Determination of Metals Mg, Ca, Zn, Fe, Cu, Ni, B, Pb, Mn, Cr, Vitamin C (Ascorbic Acid), Sugar (Sucrose) to Vegetables (Potato-*Solanum tuberosum*, Tomato-*Solanum lycopersicum*, pepper-*Capsicum annum*) in Open Field and Greenhouse

Hamit Ismaili

Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Veprim Thaçi*

Phd. Student

Department of Chemistry, University of Prishtina,
Kosovo

Donjeta Demelezi

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Ramiz Hoti

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Vegetable crops represent important components in people's nutrition. Vegetable crops provide about 12% of the energy value in human food. In vegetables, carbohydrates are represented in quantity various, in the form of monosaccharides, disaccharides, polysaccharides, chitin, cellulose hemicellulose. Mostly in tomatoes, melons, potatoes, peas, etc. These represent energy source, but also participate in certain metabolic processes. Albums are a little represented, which are very important. Albumins of plant origin are important for the construction of cells. In 1 gram albumin has 16.8 J energy. While greases are represented in the form of acids saturated and unsaturated fatty acids and represent energy compounds. Vitamins are especially represented in fruits and vegetables. In vegetables are represented almost all vitamins, in particular vitamin C, beta-carotene, and vitamins from group B. The content of vitamins is different and depends on the type of vegetables. Mineral matter in vegetables are represented by about 50 elements. Vegetables are most commonly represented by calcium, magnesium, iron, potassium, phosphorus and other minerals. The content depends on the type, variety and manner of cultivation of vegetables.

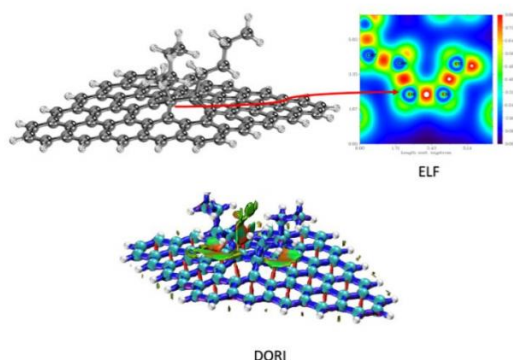
Keywords: Carbohydrate, Vitamins, Minerals, Fatty Acids, Vegetables, Beta-Carotene

The Attachment of Alkyl Groups onto a Graphene Monolayer. A DFT Study

Avni Riza Berisha*

Prof.

Department of Chemistry, The University of Pristina,
Kosovo



The grafting of alkyl groups onto the graphene surface remains an unanswered question with regard to their geometry, binding strength, nature of the formed bond and the activation energy for such a process to take place. To elucidate the process of the grafting we employed the Density Functional Theory (DFT). As a study model for this purpose served a 5x5 armchair hydrogen passivated graphene monolayer. The surface concentration and the distance of the attached alkyl groups gave important information with the regard of the influence of such effects on the interaction strengthening resulting from the cooperative effects of the first grafted group onto the second one. When the attached alkyl moieties own terminal functional groups: -hydroxyl, -fluorine, -carboxyl, -methyl; as revealed from Molecular Dynamics, this results as a facile opportunity to tune the dispersion properties of graphene. For the visualization of both covalent and non-covalent interaction regions simultaneously by a real space function, the Density Overlap Regions Indicator (DORI) analysis was carried out. The 2D Electron Localization Function (ELF) plot and 3D DORI surface evidence clearly the covalent bonding between the attached alkyl radical and the graphene surface. The equal conclusion is also drawn from the computed Laplacian Bond Order (LBO), thus undoubtedly confirming once more time the covalent nature of the formed bond.

Keywords: Alkyl Radical, Alkyl Diazonium Salt, Bond Strength, Elf Analysis, Dori Analysis, Laplacian Bond Order

Interaction of Oxygen Molecule onto Au(111) Surface Grafted by -Phenyl and-Carboxyphenyl Layers. A Theoretical Study

Veton Haziri*

Phd. Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

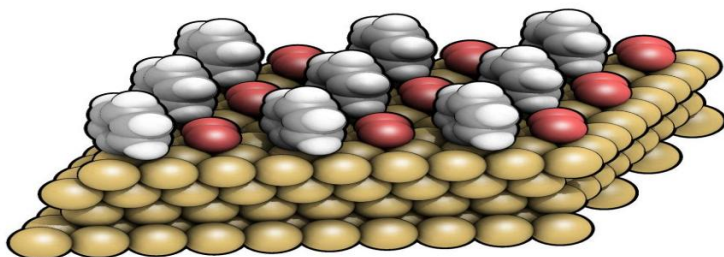
Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Jean François Boily

Prof.

Department of Chemistry, Umea University, Sweden



Surface modification via the aryl radicals derived from the de-diazotization reaction of aryldiazonium salts permits an elegant way to modify/functionalize different surfaces. In contrast to other methods (thiols, phosphonic acids, etc) it remains the only general one vis-à-vis the surface types (metals, semiconductors, and insulators) that it can be applied. Although the structure of the modified surfaces by aryl layers is up to now well characterized experimentally by a number of different methods (XPS, Raman, IRRAS, AFM . . .), the interaction of molecules such as oxygen with the formed interface remains up to now unknown. To elucidate how the oxygen molecule interact on the Au(1 1 1) modified surfaces by aryl groups (phenyl or carboxyphenyl), a Force Field Simulation using The General Utility Lattice Program (GULP) software is performed. Au (111) 4 layer model (at Periodic Boundary Conditions - grafted by one or two aryl groups, either phenyl or carboxyphenyl + oxygen molecule) with dimensions: 8.649 * 8.649 * 20 Å vacuum layer at the C axis is used as a surface. The MD simulations with the GULP were performed using ReaxFF 6.0 forcefield, NVT (constant-temperature, constant-volume) canonical ensemble at 298 K. The time step for MD was 1 fs with a total simulation time of 50 ps. For the data analysis, the whole trajectory frames of the MD simulations were used.

Keywords: Surface Modification, Aryl Layer, GULP, Molecular Dynamics, Oxygen

The Adsorption of Ni(II) Ions onto Graphene Oxide : A Combined Experimental and Theoretical (DFT, Monte Carlo) Study

Rilinda Blerim Plakaj*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Ardhmeri Alija

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Fetah Podvorica

Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Drinisa Gashi

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Valbonë Mehmeti

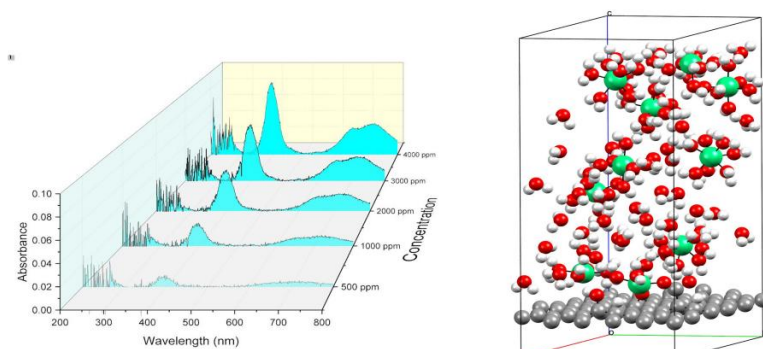
Phd. Student

Department of Chemistry, University of Prishtina,
Kosovo

Veprim Thaçi

Phd. Student

Department of Chemistry, University of Prishtina,
Kosovo



Graphene oxide (GO) represents a nanomaterial of immense interest for the adsorption of different chemical species ranging from small ions to relatively huge molecules such as peptides and even proteins. For the adsorption from aqueous solutions GO is material of choice as it is hydrophilic (contains oxygenated functional groups) and possess huge surface. For the evaluation of its adsorption properties (both experimentally and theoretically) the nickel (II) ions were selected in this study. The adsorption energies for different adsorption sites of Ni(II) ions onto GO model (with an epoxy, carboxy and hydroxyl functional groups on its surface) were evaluated via the use of DFT [through the Generalized Gradient Approximation (GGA)/ PBE (using all-electron core treatment / DNP 4.4 basis set) in combination with the Tkatchenko-Scheffler dispersion correction]. Multiwfn software is used to analyze and plot the Non-covalent interactions between the Ni(II) ions and GO surface. Monte Carlo (MC) calculation was performed using Periodic Boundary Conditions (PCB). The GO model served for the adsorption study consisted of 5x5 GO layer. For the simulation, 1 ? 10 Ni(II) ions + 100 water molecules (as a solvent) were used (the system charges were assigned using QEq method). The MC is

accomplished by using several cycles of simulated annealing. The adsorption configurations were obtained as the temperature was gradually decreased.

Keywords: Nickel (II) Ions, Monte Carlo, DFT, Graphene Oxide, Adsorption, Generalized Gradient Approximation

Adsorptive Removal of Ni (II) Ions Using Graphene Oxide

Rilinda Blerim Plakaj*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Ardhmeri Alija

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Arsim Maloku

Dr.

Department of Chemistry, University of Prishtina,
Kosovo

Drinisa Gashi

Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Albert Maxhuni

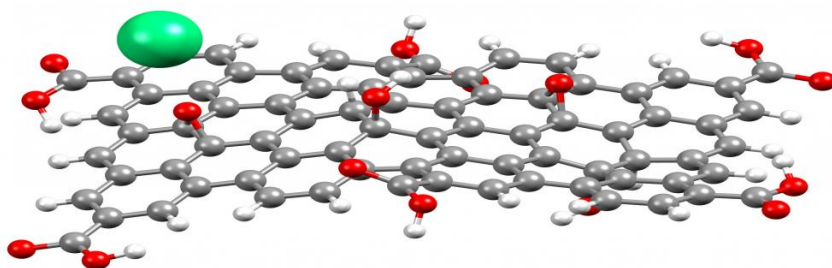
Dr.

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Graphene oxide (GO) obtained from graphite (using Hummers method) was used to adsorb nickel ions from an aqueous solution. The GO was characterized using UV-VIS spectroscopy and X-ray powder diffraction (XRD). Furthermore, the use of Density Functional Theory [using Generalized Gradient Approximation (GGA)/ PBE (using all-electron core treatment / DNP 4.4 basis set)] provided key details concerning the adsorption energy of Ni (II) ions and its dependence on the adsorption site of graphene oxide. For the highest energy adsorption site, the computation of Non-Covalent Interaction plots permits to analyze the type of interaction that takes place during this process.

Keywords: Nickel (II) Ions, Graphene Oxide, Nn-Covalent Interactions, DFT, Adsorption, UV-VIS Spectroscopy

Graphene Oxide as An Effective Adsorbent for Methylene Blue Dye

Ardhmeri Arsim Alija*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Drinisa Gashi

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Rilinda Plakaj

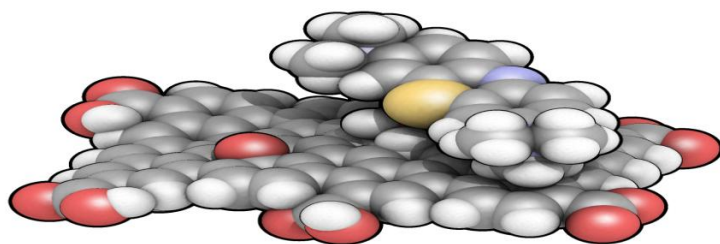
Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Graphene Oxide represents an interesting and important nanomaterial that reflects diverse properties. As a result, many practical applications oriented toward energy storage, photovoltaics, corrosion protection, adsorption, etc., take advantage of its outstanding properties. As graphene oxide not only own a huge surface are but also polar oxygenated groups (-hydroxyl, -epoxy, -carboxyl), its adsorptive properties toward different chemical species are exceptional. The synthesized Graphene oxide by using the Hummers method is evaluated as adsorbent toward the Methylene Blue (MB) molecule. The adsorption performance of the material was assessed through the use of UV-VIS spectroscopy. Moreover, the use of theoretical computation methods (DFT) permitted a detailed geometrical description and energetics on how such adsorption takes place. The computation of Non-Covalent Interaction plots clearly evidences how the MB molecule adsorbs onto the graphene oxide surface.

Keywords: Methylene Blue, Graphene Oxide, Adsorption, Non-Covalent Interactions, UV-VIS Spectroscopy, DFT

DFT, Monte Carlo Simulations and Experimental Study of the Methylene Blue Adsorption onto Graphene Surface

Ardhmeri Arsim Alija*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Drinisa Gashi

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Veprim Thaçi

Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Rilinda Plakaj

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Valbonë Mehmeti

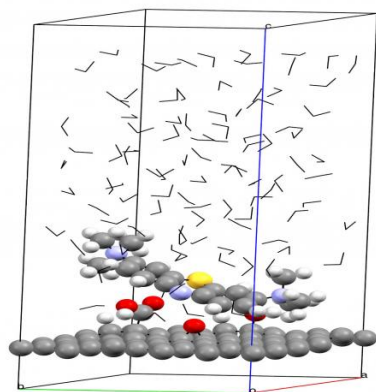
Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Graphene oxide (GO) has attracted the interest of many scientists due to its extraordinary properties. Moreover, its hydrophilicity combined with the huge surface area makes him an effective adsorbent for different chemical species. In this work, the synthesis of RGO was done by sonication-assisted oxidation of graphite in a solution of potassium permanganate and concentrated sulfuric acid. To study both experimentally (at pH=7 and pH=2, using UV-VIS spectroscopy) and theoretically the adsorption properties of this material, as an adsorbent Methylene Blue (MB) dye is used. DFT calculations were carried out using the DFT code implemented in the Dmol3 software (BIOVIA). The Generalized Gradient Approximation (GGA) in the form of Perdew et al. (PBE) [using all-electron core treatment / DNP 4.4 basis set / energy convergence criteria of 1.0e-5 Ha and 1.0e-6 SCF tolerance] in combination with the Tkatchenko-Scheffler (TS) dispersion correction schemes was used to compute the adsorption energies. Monte Carlo (MC) calculation was performed using Periodic Boundary Conditions (PCB). The GO model served for the adsorption study consisted of 5x5 graphene layer (11.138 x 9.905 angstrom + 20-angstrom vacuum layer at C axis) with an epoxy, carboxy and hydroxyl functional groups on its surface. For the simulation, one MB + 100 water molecules (as a solvent) were used. The MC is performed by using 5 cycles of simulated annealing with 50000 steps for each process. The temperature of the annealing process was set automatically at 10000 to 100 K for each cycle. Possible adsorption configurations were obtained as the temperature was slowly decreased.

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Keywords: Methylene Blue, Adsorption, Graphene Oxide, DFT, Monte Carlo, Periodic Boundary Conditions (PCB)

The Adsorption Performance of Graphene Oxide for Chromium Ions

Drinisa Arsim Gashi*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Rilinda Plakaj

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Ardhmeri Alija

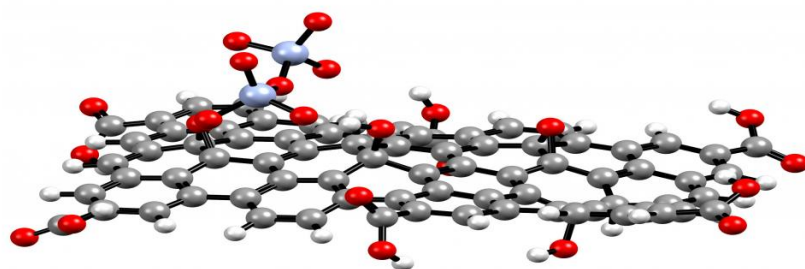
Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Many adsorbents have relatively low capacity and slow adsorption kinetics for chromium(IV) ions, so to overcome these limits graphene oxide (GO) is synthesized and evaluated as an adsorbent for these ions. The selection of GO as an adsorbent is based upon its huge surface, the facile synthesis and its hydrophilic character. Graphene oxide is synthesized using the Hummers method. Its adsorption performance toward the chromium (VI) ions is evaluated experimentally through the use of UV-VIS spectroscopy. Additionally, the applications of Density Functional Theory (DFT) gave important details regarding the adsorption energy and its dependence on the adsorption site of graphene oxide. For the highest energy adsorption site, the computation of Non-Covalent Interaction plots permits to analyze the type of interaction that takes place during this process.

Keywords: Dichromate Ions, Graphene Oxide, Non-Covalent Interactions, DFT, Hummers Method, Adsorption

Theoretical (Monte Carlo, DFT) and Experimental Study of the Adsorption of Chromium (VI) Ions onto Graphene Oxide

Drinisa Arsim Gashi*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Rilinda Plakaj

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Fidaim Saihiti

Other

Kosovo Geological Survey, Ministry of Economic
Development, Kosovo

Ardhmeri Alija

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Epir Qeriqi

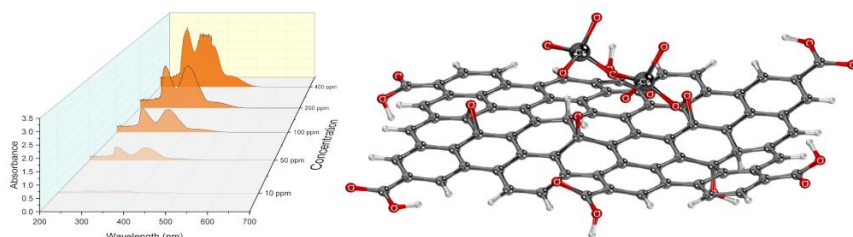
Other

Kosovo Geological Survey, Ministry of Economic
Development, Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Due to its extraordinary properties Graphene oxide (GO) represents a special nanomaterial with immense scientific interest. In contrast to graphene, GO is hydrophilic, this feature, combined with the enormous surface area, gives this materials exceptional adsorptive properties. To evaluate both experimentally and theoretically the adsorptive behavior of this material, as an adsorbent chromium (VI) ions are used. Monte Carlo (MC) calculation was performed using Periodic Boundary Conditions (PCB). The GO model served for the adsorption study consisted of 5x5 graphene layer (with an epoxy, carboxy and hydroxyl functional groups on its surface). For the simulation, one potassium dichromate + 100 water molecules (as a solvent) were used (the system charges were assigned using QEq method). The MC is performed by using several cycles of simulated annealing. During the annealing process the temperature was set automatically at 10000 to 100 K for each annealing cycle. The adsorption configurations were acquired as the temperature was slowly decreased. DFT calculations were carried out using the DFT Materials Studio (Biovia). The Generalized Gradient Approximation (GGA)/ PBE [using all-electron core treatment / DNP 4.4 basis set] in combination with the Tkatchenko-Scheffler (TS) dispersion correction schemes was used to compute the adsorption energies. Non-covalent interaction were obtained by performing a single point geometry optimization and were plotted using Multiwfn software.

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Keywords: Adsorption, Chromium (VI) Ions, Monte Carlo, DFT, Graphene Oxide, Simulated Annealing

Experimental and Theoretical Study of Some 2,5-Diarylidencyclopentanone Derivatives

Veprim Veli Thaçi*

Ph.D. Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

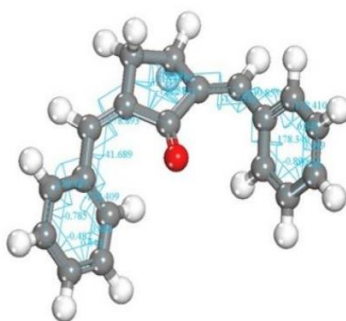
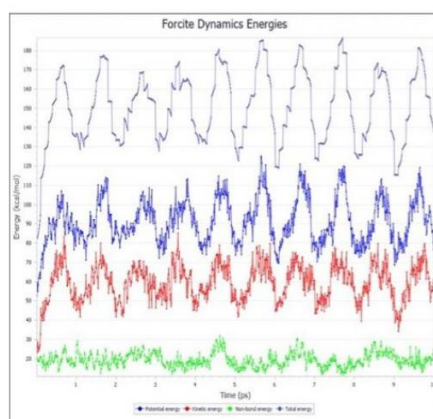
Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Jane Bogdanov

Assoc. Prof.

Institute of Chemistry, Faculty of Natural Sciences and
Mathematics, Ss. Cyril and Methodius University,
Macedonia



Four 2,5-diarylidencyclopentanone derivatives containing substituted phenyl moieties were synthesized. The products were characterized by mass spectrometry, FTIR and UV-VIS spectroscopy and comparison to literature data. These derivatives have interesting photochemical properties and exhibit biological activity. They are known Michael-acceptors especially with biological relevant thiols. The first step towards deeper understanding of the activity is to carry out theoretical calculations on the structural features. For theoretical calculations, in the first step the conformational space search for the studied molecules was to sample reasonable low energy conformations and this was performed by means of Molecular Mechanics (MM) calculations via the COMPASS II (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies) force field. The low energy conformer was subjected to several Annealing cycles (using Molecular Dynamics; initial temperature 300 K, mid-cycle temperature 500K) to ensure the lowest possible energy structure, which served as a starting point for DFT calculations. All DFT calculations were accomplished using the DFT/TDDFT (Time-Dependent Density-Functional Theory) method with the Austin-Frisch-Petersson (APFD) functional with dispersion and 6-311+g(d,p) basis set by Gaussian 16 software. The solvent effects were included using the integral equation formalism (IEF) version of polarizable continuum model (PCM).

Keywords: 2,5-Diarylidencyclopentanone Derivatives, DFT, Austin-Frisch-Petersson, COMPASS II, Molecular Mechanics, Quantum Mechanics

Synthesis, Characterization and Docking Studies of (4-(Tert-Butyl)-2,6-Dimethylphenyl)Boronic Acid

Teonor Osmanaj*

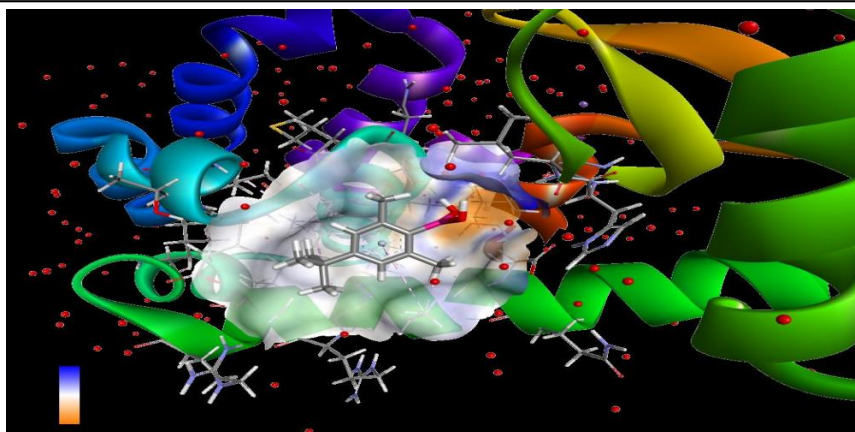
Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



Boronic acids are an important class of organic compounds that find widespread uses for: as Suzuki coupling agents (in organic synthetic reactions due to their distinctive properties and reactivity as mild organic Lewis acids), in chemotherapy, as inhibitors, in construction of chemical sensors, etc. In this work, the synthesis of (4-(tert-butyl)-2,6-dimethylphenyl)boronic acid is achieved from the reaction of 2-bromo-5-(tert-butyl)-1,3-dimethylbenzene with Trimethyl borate in the presence of magnesium as catalyst to give the product in good selectivity and medium-to-good yield (50-75%) . The obtained product is structurally characterized using NMR spectroscopy. Molecular Docking is used with the objective to predict the interaction of (4-(tert-butyl)-2,6-dimethylphenyl)boronic acid (and other designed molecules) and the T4 lysozyme L99A protein molecule, (pdb 3HH3) , thereby generating the three dimensional structures of interest. Docking produces acceptable candidate structures. These structures are further ranked using methods known as scoring functions to identify structures that are most likely to occur in the interaction between the molecule and protein. The best ranked docking were subjected to careful analysis to elucidate Non Covalent Interactions (NCI) between the molecule and protein, enabling not only a deeper understanding of the docking process but also providing important hints how to increase the interaction (through designing particular functional moieties or groups onto the molecule).

Keywords: Non Covalent Interactions , Docking, Boronic Acids, Ccoring, Nmr, T4 Lysozyme L99A

Adsorptive Behavior of Two 1,1'-Binaphthalene Derivative onto the Pt Surface. Acombined Experimental and Theoretical Study

Teonor Osmanaj*

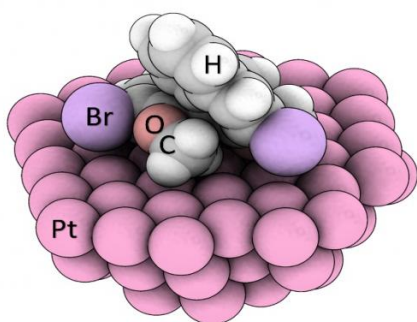
Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



The adsorptive behavior of 3,3'-diiodo-2,2'-dimethoxy-1,1'-binaphthalene and 2,2'-dimethoxy-1,1'-binaphthalene toward the Pt surface is evaluated by using Linear Sweep Voltammetry. The study is conducted by using a PalmSens3 potentiostat connected with a three-electrode cell at 298K. A graphite rod ($d = 3$ mm, $l = 4$ cm) served as an auxiliary electrode and the saturated calomel electrode (SCE) as a reference electrode. The current decrease on the Tafel plot of the Pt electrode in the presence of the studied compounds in comparison to the blank solution clearly supports the adsorption of these molecules takes place on the Pt. Furthermore, the use of Monte Carlo (MC) and Molecular Dynamics (MD) simulations permitted to elucidate at the molecular level how the adsorption of these molecules takes place onto the Pt surface.

Keywords: Binaphthalene, Adsorption, Pt Surface, Monte Carlo, Linear Sweep Voltammetry, Molecular Dynamics

New Trend in Energetic Materials Research; Co-crystallization

Sinecan Irem Bozkuş*

Master Student

Forensic Science Institute, Turkish National Police
Academy, Turkey

Kübra Gürpınar

Ph.D. Student

Department of Chemistry , Ankara University ,
Turkey

Orhan Atakol

Prof.

Department of Chemistry, Ankara University,
Turkey

Yaprak Gürsoy Tuncer

Master Student

Department of Chemistry, Ankara University,
Turkey

Nurcan Acar

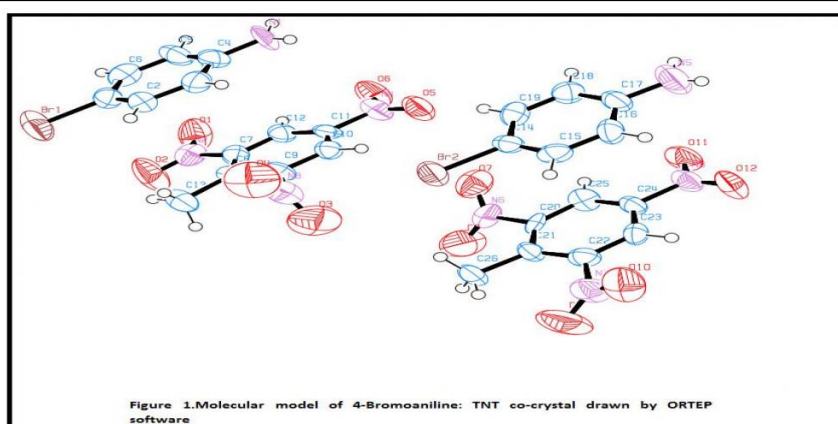
Assoc. Prof.

Department of Chemistry, Ankara University,
Turkey

Nilgün ŞEN

Dr.

Forensic Science Institute, Turkish National Police
Academy, Turkey



this aim, the new formed between TNT and 4-bromoaniline were chosen for characterisation.

Keywords: Co-Crystallization, Tnt, 4-Bromoaniline, Explosive Sensitivity, Explosive Performance, Energetic Materials

A Different Approach in Thermokinetic Analysis of Energetic Materials

Kübra Gürpınar*

Ph.D. Student

Department of Chemistry, Ankara University,
Turkey

Mehmet Abdülkadir Akay

Prof.

Department of Chemistry, Ankara University,
Turkey

Yaprak Gürsoy Tuncer

Master Student

Department of Chemistry, Ankara University,
Turkey

Orhan Atakol

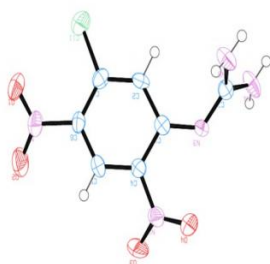
Prof.

Department of Chemistry, Ankara University,
Turkey

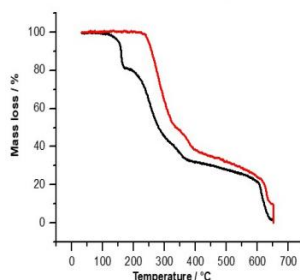
Nurcan Acar

Assoc. Prof.

Department of Chemistry, Ankara University,
Turkey



The Ortep drawing of N(2,4-dinitro-5-chlorophenyl)guanidin



TG curves of N(2,4-dinitro-5-chlorophenyl)guanidin (II) at different heating rate, black: 5 °C/min, red: 15 °C/min. heating rate

Thermokinetic analysis is usually a collection of methods applied to polymeric materials, but it can also be applied to energetic materials and others. Energetic substances are explosives, which have been known as energetic substances for the last 30 years and thermokinetic analysis gives useful results to estimate the lifetime and safety of energetic substances. The methods used on thermokinetic analysis are two classes, isothermal and nonisothermal methods. The most commonly used isothermal method is Coats-Redfern method and this method is the basis of many other methods. Nonisothermal methods are more confident methods and the most commonly used nonisothermal methods are Ozawa and Kissinger methods, [1,2]. All methods used for thermokinetic analysis are graphical semiempirical methods and different parameters are plotted against $1/T$ value in all methods. Semi-experimental thermodynamic parameters of the thermal reaction are calculated from the slopes and shifts of the obtained lines. Thermal decomposition reactions of energetic substances occur in the form of detonation and as estimated detonation reactions are very quickly. Therefore in highly heating rates such as 10, 15, 20, 25 °C / min. , the reaction can be observed as one-step reaction. However, the detonation reaction may be two or more steps and the reaction mechanism is very important for the estimation of the reaction products. For this reason the steps of detonation reactions can only be observed at low heating rates, such as 0.5, 0.75, 1.0. In Ozawa and other Ozawa-based methods, $\log B$ (B = heating rate) versus $1/T$ value is plotted and if the B value is less than 1 °C / min, $\log B$ is negative and cannot be calculated thermodynamic parameters. In this study, three new energetic substances were prepared from 1,3-dinitro-4,6-dichlorobenzene

and thermokinetic analysis of these substances were performed with CR, OFW

Keywords: Energetic Material, Thermokinetic Analysis, TGA, DSC

Theoretical Analysis of Fragment Contribution of Nitrogen-Rich Ligands and Bridge-Forming Co-Ligands to Molecular Orbitals of the Energetic Materials

Arda Atakol

Ph.D. Student

Fire Testing Laboratory, Turkish Standards
Institution, Turkey

Hasan Nazir*

Assoc. Prof.

Department of Chemistry, Ankara University
Science Faculty, Turkey

There have been many studies recently about new nitrogen and oxygen rich energetic materials which will have controllable explosive properties. It has been aimed for these new energetic materials that have high thermal decay temperature, high pulse sensitivity and also high explosion temperature and gas phase for the majority of reaction products. We are suggesting that metal complex energetic materials bearing nitrogen-rich ligands and bridge-forming co-ligands will have high detonation pressure and thermal decomposition temperature. In the light of this prediction, two pyrazolyl pyridine ligands, Bis-2,6(Pyrazol-1-yl)pyridine (pp) and Bis-2,6(3,5-dimethylpyrazol-1-yl)pyridine (dmpp), were prepared and their Ag (I) complexes, namely [AgppNO₃] (I), [AgdmppNO₃] (II), [AgppClO₃] (III), [AgdmppClO₃] (IV), [AgppClO₄] (V), [AgdmppClO₄] (VI), were synthesized by using AgNO₃, AgClO₃ and AgClO₄. Molecular structures of the complexes were determined by X-Ray diffraction method. The fragment contributions to HOMO and LUMO energy levels and formation enthalpies of the complexes were calculated by using Gaussian 09 software package. The pressure and velocity of detonation of the complexes were calculated according to Kamlet-Jacobs equation by using formation enthalpy values. Finally, the fragment contribution to the pressure and velocity of detonation were discussed.

Keywords: Energetic Materials, Silver Complexes, Bridge Ligands, Fragment Contribution

Effect of Electronegativity on Coordination Sphere in Coordination Compounds

Yaprak Gürsoy Tuncer*

Master Student

Department of Chemistry, Ankara University,
Turkey

Nurcan Acar

Assoc. Prof.

Department of Chemistry, Ankara University,
Turkey

Sinecan Irem Bozkuş

Master Student

Department of Forensic Science, Turkish National
Police Academy, Turkey

Orhan Atakol

Prof.

Department of Chemistry, Ankara University,
Turkey

Kübra Gürpınar

Phd. Student

Department of Chemistry, Ankara University,
Turkey

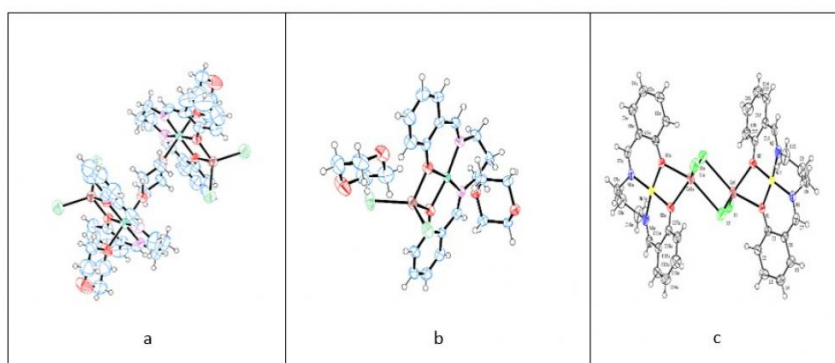


Figure 1. Three different coordination in the prepared complexes a: $[(NiL.ZnI_2)_2.(C_4H_8O_2)_3]$ Octahedral coordination, b: $[(NiL.ZnI_2).(C_4H_8O_2)].(C_4H_8O_2)$, Square pyramid, c: $[(NiL.CdI_2)_2]$ Square Planar

Bis-N, N'(salicylidene)-1,3-diaminopropane(LH2) has been a common ligand since 1947 in Coordination chemistry literature.[1] In particular, the polynuclear complex has a high tendency to form. [2] Therefore, mononuclear complex could not be prepared with this ligand for a long time. The first mononuclear Ni(II) and Cu(II) complexes were prepared in 1985. Mononuclear CuL and NiL complexes from homo or heterodi nuclear complexes with lewis bases in the medium. The electronegativity value of the lewis base can change coordination spheres of NiL and CuL complex. In the study, the NiL complex prepared (M= Zn (II) or Cd (II) , X: Cl, Br, and I) was reacted with lewis acids in non-aqueous solvents and M metal ion and X halide ions change the coordination spherin around the electronegativities Ni(II) was determined. Around the NiL mononuclear complexes, there are squared planes, square piramides or oktahedral coordination spheres.

Keywords: Schiff Bases, L H2, Ni Complex, Cu Complex, Coordination Spheres, Mononuclear Complex

The Impact of Covalent Surface Modification of the Active Carbon Powder in the Adsorption of Lindane

Gjani Hulaj*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Besart Shatri

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Manjola Kelmendi

Master Student

Department of Biology, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Water pollution remains a serious problem. Adsorption technology is currently being used in large scale for the removal of such pollutants from wastewaters. Among the different existing systems adsorbent for the removal of pollutants from wastewaters, activated carbon powder (ACP) is the most widely used one in developed countries. The adsorption of organochlorine pesticides onto ACPs, is established to be the most effective and reliable method for the removal of organic pesticides. We used ACP for the adsorption of Lindane from hexane solutions as a first step in order to gain some insights about the sorption ability of this material and to compare it after the surface modification step with organic layer. The ACP powder modified by the reduction of different synthesized diazonium salts. The adsorption performance of ACP and covalently modified ACP toward the Lindane (gamma-hexachlorocyclohexane, γ -HCH) was evaluated through the use of GC-ECD technique. The obtained results point out that ACP is a very promising adsorbent for the wastewater treatment.

Keywords: Diazonium Salts, Lindane, GC-ECD Phenyl Radicals, Adsorption, Quantification

A Novel Nonenzymatic Pesticide Sensor Based on Electropolymerized Polythiophene/TiO₂ Nanocomposite

Songül Şen Gürsoy*

Prof.

Department of Chemistry, Burdur Mehmet Akif Ersoy University, Turkey

Derya Kahraman

Ph.D. Student

Department of Chemistry, Burdur Mehmet Akif Ersoy University, Turkey

In this study, a novel nonenzymatic pesticide sensor was developed by using electropolymerized polythiophene/TiO₂ (PTh/TiO₂) composite material. The structural and morphological analysis of composite were made by FTIR and SEM, respectively. The response of the pesticide sensor was measured by CV in the range of -1-2.3 V versus SCE which was due to the electroreduction of malathion. The PTh/TiO₂ nanocomposite was sensitive for malathion. The operational conditions such as pH, thiophene amount, coating cycle were optimized.

Keywords: Polythiophene, Composite, Pesticide, Sensor

Acknowledgement: This research was supported by Burdur Mehmet Akif Ersoy University, Scientific Research Projects Commission for Scientific Research from Turkey (Project Number: 0407-MP-17)

Differential Pulse Voltammetric Determination of Endocrine-Disrupting Chemical: Trifluralin at a Disposable Electrode

Ümit Gege*

Master Student

Department of Chemistry, Çanakkale Onsekiz Mart
University, Turkey

Serkan Karakaya

Dr.

Department of Chemistry, Çanakkale Onsekiz Mart
University, Turkey

Yusuf Dilgin

Prof.

Department of Chemistry, Çanakkale Onsekiz Mart
University, Turkey

Trifluralin (TRF) has been generally used as a selective herbicide in agricultural applications in wide variety of plant cultures [1] and it is one of the major source of pollutant in soils and waste waters with significant concentration ($> 5 \times 10^{-9}$ M). Electrochemical methods have been found great attention in routine analytical determinations of pesticides because of their advantageous properties such as simple, low cost, short analysis time, high sensitivity and simple instrumentation [2]. In this study, electrochemical determination of TRF has been performed at Pencil Graphite Electrode (PGE) using differential pulse voltammetry (DPV) based on both its reduction and oxidation. Step potential, modulation amplitude, modulation time and interval time in DPV method have been optimized as 7.5 mV, 100 mV, 3.0 ms and 50 ms for oxidation and -7.5 mV, 100 mV, 50 ms and 70 ms for reduction, respectively. Linear responses for oxidation and reduction of TRF have been found as 1.0 - 75 μ M and 1.0 - 100 μ M, respectively. LOD values for oxidation and reduction studies were found to be 0.31 μ M and 0.33 μ M, respectively. Proposed sensor was successfully applied to various water sources.

This study was produced from MSc thesis of Ümit Gege.

References [1] M. Irabdoust, M. Haghighi, A.A. Taherpour, M. Jafarzadeh, Journal of the Iranian Chemical Society, 2018, 15(3): 719-732. [2] É. Castro Ferro, C.A.L. Cardoso, G.J. Arruda, Journal of Environmental Science and Health, Part B, 2017, 52(10): 762 -769.

Keywords: Trifluralin, Pesticide, Herbicide, Pencil Graphite Electrode, Differential Pulse Voltammetry, Electrochemical Sensor

Electrochemical Grafting of Heterocyclic Amines on the Gold Surface

Nimet Sheqerxhiu*

Ph.D. Student

Department of Chemistry, Unuversity of Prishtina,
Kosovo**Sereilakhena Phal**

Ph.D. Student

Department of Chemistry SE 90187 Umeå, Umeå
University, Faculty of Science and Technology,
Sweden**Azem Lajci**

Prof.

Department of Chemistry, University of Prishtina
Hasan Prishtina FNMS, Kosovo**Nardi Sheqerxhiu**

Mr.

Forensic Toxicology, Institution of Forensic
Medicine, Kosovo**Solomon Tesfalidet**

Prof.

Department of Chemistry SE 90187 Umeå, Umeå
University, Faculty of Science and Technology,
Sweden**Avni Berisha**

Assoc. Prof.

Department of Chemistry, University of Prishtina
Hasan Prishtina FNMS, Kosovo

The electrochemical properties of Au electrode grafted with amino-triazole (AT) groups have been studied. In the first step, gold electrode was covalently grafted with a layer of AT via the formation of aminyl radicals under electrochemical oxidation reaction of corresponding AT molecule. The surface modification of gold electrode via aminyl radicals is initiated by using cyclicvoltammetry (several scan cycles in the potential range +0.2 and +1.6 V) through the electro-oxidation of AT solution in acetonitrile. The presence of AT groups on the modified electrode surface was studied by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) and compared with the electrochemical behaviour of the bare gold. The barrier proprieties of the deposited layer on the gold surface was investigated in the presence of an electroactive Fe(CN)₆^{3-/4-} redox probe. The results indicate the presence of the amino-triazole groups on the gold surface - confirming a successful grafting reaction.

Keywords: Amino Triazole, Aminyl Radicals, Electrochemical Oxidation, Electrochemical Impedance Spectroscopy, Grafting, Cyclic Voltammetry

Grafting of the Gold Surface by Heterocyclic Moieties Derived through Electrochemical Oxidation of Amino Triazole: An Experimental and Ab Initio Study

Nimet Sheqerxhiu

Phd. Student

Department of Chemistry, Unuversity of Prishtina, Kosovo

Sereilakhena Phal

Phd. Student

Department of Chemistry SE 90187 Umeå, Umeå University, Faculty of Science and Technology, Sweden

Azem Lajci

Prof.

Department of Chemistry, University of Prishtina
Hasan Prishtina FNMS, Kosovo

Nardi Sheqerxhiu

Mr.

Forensic Toxicology, Institution of Forensic
Medicine, Kosovo

Solomon Tesfalidet

Prof.

Department of Chemistry SE 90187 Umeå, Umeå University, Faculty of Science and Technology, Sweden

Avni Berisha*

Assoc. Prof.

Department of Chemistry, University of Prishtina
Hasan Prishtina FNMS, Kosovo

Surface modification of gold is accomplished by using the aminyl radicals formed through the electrochemical oxidation of the amino-triazole molecule dissolved in organic media (acetonitrile). The electrochemistry of the grafting process and the redox behavior of the grafted heterocyclic layer is similar to that of the aliphatic amines [1]. The capability of the modified surfaces for blocking redox reaction was assessed using ferrocyanide-ferricyanide redox couple and displayed important differences. The redox probes display a decrease electron transfer rate. The increase of the charge transfer resistance of the grafted layer is suggestive for a compact layer formation. Furthermore, the Au₁₃ cluster was used to compute BDE (Bond dissociation energies) and a number of other important parameters such as bond strength and length of the interface, etc. These parameters were computed using ONTEP software [Order-N Total Energy Package - a software intended specifically for calculations on large systems, it employs density functional theory (DFT) in the density matrix formulation.

Keywords: Amino Triazole, Grafting, ONTEP, Electrochemical Oxidation, Au₁₃ Cluster

Characterization of the Porous Materials Obtained from Diatomite and $\text{Ca}(\text{OH})_2$ during Low-Temperature Hydrothermal Synthesis

Emira Fazlija*

Master Student

Faculty of Natural Sciences and Mathematics,
University of Tetova, Macedonia

Ahmed Jashari

Prof.

Faculty of Natural Sciences and Mathematics,
University of Tetova, Macedonia

Ivan Boev

Prof.

Faculty of Natural and Technical Sciences, Goce
Delcev University, Macedonia

Arianit A. Reka

Prof.

Faculty of Natural Sciences and Mathematics,
University of Tetova, Macedonia

Blagoj Pavlovski

Prof.

Faculty of Technology and Metallurgy, Ss. Cyril and
Methodius University, Macedonia

Blazo Boev

Prof.

Faculty of Natural and Technical Sciences, Goce
Delcev University, Macedonia

Petre Makreski

Prof.

Institute of Chemistry, Ss. Cyril and Methodius
University, Macedonia

The diatomaceous earth that is used in this research was collected from the Mariovo region (Republic of North Macedonia). From a physical-mechanical point of view, diatomaceous earth represents soft, light and brownish-gray sedimentary fine porous rock. Just like the other inorganic materials that contain amorphous SiO_2 , diatomaceous earth is convenient and promising material for the production of porous materials (ceramics) due to its natural porosity, low density and mineralogical composition. The aim of study was to test this diatomaceous earth as a raw material for production of porous ceramics under low-temperature hydrothermal procedure and also to determine its physical-mechanical properties of products and determine its mineralogical composition. Various mixtures of diatomite and portlandite were prepared (8%, 11%, 14%, 17%, 20%, 23%, 26% portlandite), while the moisture was 40%. Hydrothermal synthesis of porous ceramics has been carried out under saturated steam pressure at 130 °C for a period of 3 h. The compressive strength of products obtained during low- temperature hydrothermal reaction ranging from 7.74 to 19.99 MPa and the bulk density ranged from 0.95 to 1.007 g/cm³.

Keywords: Diatomite, Hydrothermal Synthesis, Porous Ceramics

Effects of Thermal Treatment on Silica Phase Transition in Diatomite

Arianit A. Reka*

Prof.

Faculty of Natural Sciences and Mathematics,
University of Tetovo, Macedonia

Emira Fazlija

Master Student

Faculty of Natural Sciences and Mathematics,
University of Tetovo, Macedonia

Blazo Boev

Prof.

Faculty of Natural and Technical Sciences, Goce
Delcev University, Macedonia

Petre Makreski

Prof.

Institute of Chemistry, Ss. Cyril and Methodius
University, Macedonia

Blagoj Pavlovski

Prof.

Faculty of Technology and Metallurgy, Ss. Cyril and
Methodius University, Macedonia

Ahmed Jashari

Prof.

Faculty of Natural Sciences and Mathematics,
University of Tetovo, Macedonia

Ivan Boev

Prof.

Faculty of Natural and Technical Sciences, Goce
Delcev University, Macedonia

The diatomite subject in this research was been collected form the Mariovo region (village of Besiste, Republic of North Macedonia). The raw material is a sedimentary fine porous rock, soft, light with brownish grey colour, with specific gravity 2.01 g/cm³. The chemical analysis revealed the following chemical composition: SiO₂ (86.33 wt%), Al₂O₃ (3.01 wt%), Fe₂O₃ (2.79 wt%), MnO (0.06 wt%), TiO₂ (0.139 wt%), CaO (0.76 wt%), MgO (0.28 wt%), P₂O₅ (1.39 wt%), K₂O (0.68 wt%), Na₂O (0.191 wt%), and LOI (5.66 %). The X-ray powder diffraction results shows presence of the amorphous phase as well as the following crystalline phases in the raw material: quartz and muscovite. While the thermally treated diatomite at 1000°C for a period of 1 hour shows significant change, the "bump" which indicates the amorphous phase has been significantly reduced. Evident is the decrease of the peaks for muscovite while at the same time there is a significant increase of the cristobalite peaks. Results for the SEM analysis depicted morphological changes expressed by shrinkage of the pore diameters in comparison to the initial material.

Keywords: Diatomite, XRPD, Phase Transition, SEM

Mineralogical Characterisation of Clayey Diatomite Sintered at 1200°C

Egzon Ademi*

Mr.

Department of Chemistry, University of Tetova,
Macedonia

Blagoj Pavlovski

Prof.

Department of Chemistry, Faculty of Technology and
Metallurgy, Ss. Cyril and Methodius University,
Macedonia

Petre Makreski

Prof.

Department of Chemistry, Institute of Chemistry,
Faculty of Natural Sciences and Mathematics, Ss.
Cyril and Methodius University, Macedonia

Arianit A. Reka

Prof.

Department of Chemistry, University of Tetova,
Macedonia

Ahmed Jashari

Prof.

Department of Chemistry, University of Tetova,
Macedonia

Bujar Durmishi

Prof.

Department of Chemistry, University of Tetova,
Macedonia

Clayey diatomite represents a grayish, soft, very light, weakly cemented, finely biogenetic opal sedimentary rock found in southern part of Republic of North Macedonia, more precisely near the city of Bitola. The aim of this work was the analysis and comparison of raw inorganic material clayey diatomite from the Bitola region with the treated sample of the same material at 1200°C. SEM allows in depth-analysis of the surface and FTIR spectroscopy proves the phase and surfacial modifications of the sample. The analysed sample shows the following chemical composition: SiO₂ (63.65 wt%), Al₂O₃ (11.76 wt%), Fe₂O₃ (5.93 wt%), MnO (0.13 wt%), TiO₂ (0.63 wt%), CaO (1.42 wt%), MgO (2.22 wt%), P₂O₅ (0.11 wt%), K₂O (1.63 wt%), Na₂O (0.92 wt%), LOI (11.50 %). Compression strength proved that clayey diatomite treated during heating at specific temperature makes a great material with 32.48 MPa, while the initial sample of natural clayey diatomite had compression strength of 4.4MPa. The X-ray powder diffraction shows presence of amorphous phase as well as presence of crystalline phases: quartz, cristobalite, illite, hydromuscovite, chlorites, kaolinite and biotite. With the temperature increase during sintering, the treated material changes colour into darker brown, as well as increases the bulk density. SEM of the treated sample shows morphological changes as well reduction of the diameters of the pores compared to the untreated natural clayey diatomite. It also shows the well-defined biogenic origin of fossil diatoms skeletons. The FTIR spectrum of natural clayey diatomite prove the presence of water in the sample, while the spectrum of treated clayey diatomite at 1200°C prove it's absence.

Keywords: Clayey Diatomite, SEM, FTIR, Compression Strength

Characterization of Porous Materials Obtained Under Hydrothermal Procedure from Trepel and Portlandite

Njomza Buxhaku*

Master Student

Department of Chemistry, State University of
Tetovo, Macedonia

Arianit Reka

Prof.

Department of Chemistry, State University of
Tetovo, Macedonia

Ahmed Jashari

Prof.

Department of Chemistry, State University of
Tetovo, Macedonia

The aim of this research is to obtain light porous materials, products from the reaction of trepel and portlandite. Trepel represents a natural mixture of diatomaceous earth and clay minerals. Trepel is a raw materials with high porosity, which makes is suitable material for production of porous products. The raw material show a bulk density of 0.8 g/cm³, water absorption 67.99% and specific mass 1.94 g/cm³, while the chemical composition is as follows: SiO₂ (55.80%wt), Al₂O₂ (15.15%wt), Fe₂O₃ (8.34% wt), CaO (2.94% wt.) SO₃ (0.95% wt.), K₂O (2.01% wt.), Na₂O (2.34% wt.) and LOI 9.50 %. During the hydrothermal reaction of trepel with portlandite new phases are formed. The probes were prepared while mixing 80% trepel with 20% portlandite, with the help of a cylindrical mold (10 mm x 15 mm) and were pressed on a mechanical press at compressive strength from 2-10 kN. Probes obtained from the hydrothermal reaction of mixtures of trepel and portlandite show bulk density 0.85 - 0.90 g/cm³. The products of the hydrothermal reaction are lightweight materials, yet materials with high compressive strength ranging from 15 - 20 MPa.

Keywords: Material Characterization, Trepel, XRPD

Occurrence and Enrichment Sources of Co, Cr and Ni in Soils of Mitrovica Region, Republic of Kosovo

Milihate Xhafer Aliu*

Assoc. Prof.

Department of Industrial Engineering with
Informatics, University of Applied Sciences In
Ferizaj, Kosovo

Robert Sajn

Dr.

Department of Geology, Geological Survey of
Slovenia, Slovenia

Milihate Xhafer Aliu

Assoc. Prof.

Department of Industrial Engineering with
Informatics, University of Applied Sciences In
Ferizaj, Kosovo

Traje Stafilov

Prof.

Department of Chemistry, Ss Cyril and Methodius
University, Macedonia

Intense lead and zinc mining and smelting activities in the Mitrovica environs, Republic of Kosovo brings out huge amount of mining and metallurgical waste to the environment. To evaluate its environmental quality the metal contents were determined in the 156 topsoil samples (depth 0-5 cm) using inductively coupled plasma - atomic emission spectrometry (ICP-AES) and inductively coupled plasma - mass spectrometry (ICP-MS). The methods of parametric and nonparametric statistics were used for the data analysis. The universal kriging with linear variogram interpolation method was applied to construct the maps of areal distribution of heavy metals in soil. The obtained results show that the average content of Cr, Co and Ni in soil for the entire study area amounts to 60 mg/kg in range 7.0-1100 mg/kg, 2.2 mg/kg in range from 2.7 to 160 mg/kg, and 96 mg/kg in range 7.6-2600 mg/kg, respectively. Spatial distribution maps of Co, Cr and Ni shows their predominance in the area of Triassic serpentinites on the North-eastern and Western parts of study area. The lowest contents are found on the outcropping of Miocene latites and quartz-latites and Miocene pyroclastites. Therefore, it could be concluded that the increased content of Co, Cr and Ni in soils from this area is of lithogenic origin. It is shown that content of Co, Cr and Ni exceeds the target Dutch value in 173 km², 82 km² and 256 km², respectively, while the content of Cr and Ni exceeds the intervention Dutch value in 17 km² and 63 km², respectively.

Keywords: Cobalt, Chromium, Nickel, Soil, Natural Pollution, Spatial Distribution, Mitrovica, Republic of Kosovo

Structure and Stability of Water Clusters (H₂O)_n, n=2-30. An Ab Initio Study

Artan Gashi*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

The group of water molecules "clusters" that holds together through hydrogen bonding, is a focus point of many researches worldwide. This research interest it's relies on the fact that this study enables the deeper understanding of solution chemistry, ice and many other biochemical processes that have a profound importance. The exploration of structural and binding properties of water clusters is the first step to understand the behavior of water on the macroscopic level. Ab initio calculations were performed on water clusters (H₂O)_n, n=2-30 were performed using two different approaches: a) Molecular Mechanics, using the MMFF94s force field (MM) and b) quantum mechanics (QM) calculations by employing Generalized Gradient Approximation (GGA) with Perdew-Burke-Ernzerhof functional. The MM calculations served as a starting point (in order to decrease computation time) for MM calculations. Different important parameters such as: first and second energy of dissociation, fragmentation energy, dipolar moment, etc. were evaluated for the water clusters, enabling a deeper understanding of their stability.

Keywords: Perdew-Burke-Ernzerhof, Dft, Water Clusters, MMFF94s , Molecular Mechanics, Quantum Mechanics

Comparison of the Performance of Different DFT Methods in the Calculations of the Stability and the Structure of Small

Artan Gashi*

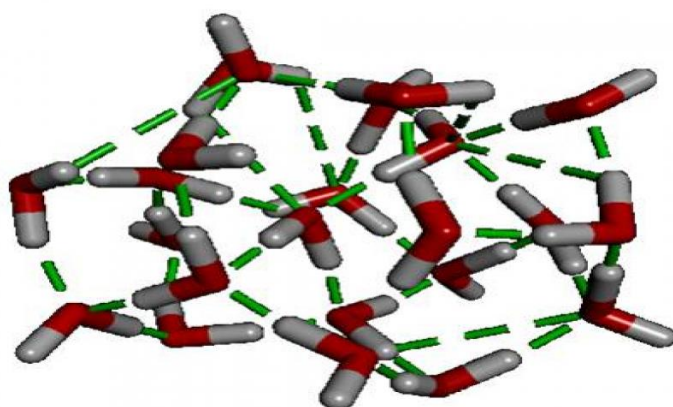
Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo



The evaluation of the performance of different theoretical calculation methods with regard to the: first and second energy of dissociation, fragmentation energy, dipolar moment, etc. for the water clusters $(\text{H}_2\text{O})_n$, $n=2-30$ were performed. The initial cluster geometries were constructed using Molecular Mechanics (using Avogadro software and the Merck Molecular Force Field MMFF94s). In the second step, the comparative performance of different density functional theory (DFT) methods in predicting the molecular structure of the water clusters is reported. The DFT calculations permitted to understand at the molecular level the stability and the structural organization of the studied water clusters.

Keywords: Water Cluster, Dft, Quantum Mechanics, Molecular Mechanics, Fragmentation Energy, First and Second Energy of Dissociation

Synthesis of Carbazole Bearing Pyridopyrimidine-Substituted Sulfonamide Derivatives

Fatjonë Bedri Krasniqi*

Master Student

Department of Chemistry, University of Prishtina,
Kosovo

Mustafa Arslan

Prof.

Department of Chemistry, University of Sakarya,
Turkey

Arleta Rifati Nixha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Avni Berisha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Kosovo

Heterocyclic compounds are biologically active molecules in the development of new medicinal agents due to their essential roles in vitamins, enzymes, and nucleic acids. The synthesis and characterization of carbazole containing pyridopyrimidine-substituted sulfonamide derivatives (3a-c) were studied. The obtained structures are confirmed based on IR, ¹H NMR and ¹³C NMR spectra and the results obtained from the elemental analysis have been consistent with the composition of the newly synthesized compounds.

Keywords: Carbazole, Sulfonamide, Pyridopyrimidine

Theoretical Study of Some Synthesized Carbazole-Pyridopyrimidine Derivative

Kaltrina Avni Kastrati*

Master Student

Department of Chemistry, University of Prishtina,
Faculty of Mathematical & Natural Sciences, Kosovo

Mustafa Arslan

Prof.

Department of Chemistry, Sakarya University,
Faculty of Art and Sciences, Turkey

Arleta Rifati Nixha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Faculty of Mathematical & Natural Sciences , Kosovo

Avni Berisha

Prof.

Department of Chemistry, University of Prishtina,
Faculty of Mathematical & Natural Sciences , Kosovo

Several carbazole-pyridopyrimidine derivatives were synthesized and structurally characterized using FTIR and NMR spectroscopy. The theoretical calculations with the aim to better understand the structural characteristics, electronic excitations and the reactivity of the synthesized molecules were performed. The lowest energy conformers of the carbazol-pirimidine in the first calculation step were exposed to several Annealing Dynamics cycles. The IR and UV-VIS spectra were computed using the DFT/TDDFT (Time-Dependent Density-Functional Theory) method with the B3LYP (Becke, 3-parameter, Lee?Yang?Parr) functional with Grimme dispersion correction and 6-311g basis set by Gaussian 16 software. The computed parameters such as: IP, EA, E(HOMO), E(LUMO) , etc. - offered a full insight to the regard of the influence of the substituents on the electronic properties of the molecules.

Keywords: Carbazole, DFT/TDDFT, IP, EA, B3LYP, Gaussian 16 Software

Synthesis and Characterization of Schiff Base Substituted Carbazole Bearing Pyridopyrimidine Compounds

Kaltrina Avni Kastrati*

Master Student

Department of Chemistry, University of Prishtina,
Faculty of Mathematical & Natural Sciences, Kosovo

Qëndresa Istrefi

Master Student

Department of Chemistry, University of Prishtina,
Faculty of Mathematical & Natural Sciences, Kosovo

Mustafa Arslan

Prof.

Department of Chemistry, Sakarya University,
Faculty of Art and Sciences, Turkey

Arleta Rifati Nixha

Assoc. Prof.

Department of Chemistry, University of Prishtina,
Faculty of Mathematical & Natural Sciences, Kosovo

The Schiff bases formation which are useful molecules both biologically and synthetically, is one of the most important reactions in organic and medicinal chemistry. In basic conditions were efficiently synthesized Schiff base substituted carbazole bearing pyridopyrimidine compounds (3a-c) through corresponding benzaldehyde derivatives on treatment with 7- (4-amino-phenyl)- 5-(9-ethyl-9H carbazol-3-yl)- 1,3-dimethyl- 1H-pyrido [2,3-d] pyrimidine-2,4-dione in tetra- hydrofuran under reflux. The obtained structures are confirmed based on IR, ¹H NMR and ¹³C NMR spectra and the results obtained from the elemental analysis have been consistent with the composition of the newly synthesized compounds.

Keywords: Carbazole Containing Pyridopyrimidine, Imine, Benzaldehyde, Schiff Bases

The Effect of Natural Boron Mineral Use on the Essential Oil Ratio and Components of Musk Sage (*Salvia sclarea* L.)

Hasan Basri Karayel*

Dr.

Dept. of Medicinal and Aromatic Plants, Kütahya
Dumlupınar University, Gediz Vocational School, Turkey

This study was carried out in Dumlupınar University, Gediz Vocational School, Medical and Aromatic Plants Department's application field in 2016 and 2017 in order to determine the effect of different boron doses (0, pure and 1/8 kg/decare) on the rate and quality of volatile oil in musk (*Salvia sclarea* L.) species grown in Kütahya-Gediz conditions. This extract was used both in pure form and in 1/8 ratio which was diluted with pure water. This plant's volatile oil was obtained by hydrodistillation method (GC-MS/FID). In the analyzes carried out in 2017, the rate of essential oil was found to be 0.11% in the plant growing without boron, while it was 0.44% in the plant grown with pure boron. However this rate was found as 0.23% in the 1/8 boron ratio application. As a result of the analysis of the essential oil of Musk Sage (*Salvia sclarea* L.) exposed to different boron doses (No boron, Pure boron and 1/8 kg / da) 19, 17, 17 components were defined respectively in the drug flower in the second year. The main components of *Salvia sclarea* L. species were found as follows: For the boron-free application; Spathulenol 23.75%, Caryophyllene oxide 19.41%, Linalool 10.10%, Sclareoloxide 9.92% For the pure dose application; Spathulenol 26.67%, Sclareoloxide 18.81%, Caryophyllene oxide 16.13%. For the 1/8 ratio boron dose application; Spathulenol 24.82%, Sclareoloxide 16.68%, Caryophyllene oxide 14.86%. It has been observed that pure boron dose has a positive effect on the essential oil ratio and components of Musk Sage (*Salvia sclarea* L.).

Keywords: Boron, Essential oil, *Salvia sclarea* L.

The Elimination of Aflatoxin Bacteria from the Pharmaceuticals Vegetative Raw Material *Agnus Castus* by using Aluminium Oxide as an Adsorbent

Ljatif R. Mahi*

Dr.

Chemistry Engineering, Max Zeller Söhne
AG, Pflanzliche Heilmittel Romanshorn,
Switzerland

Arianit Reka

Prof.

Faculty of Natural Sciences and
Mathematics, State University of Tetova,
Macedonia

Ejup Ljatif

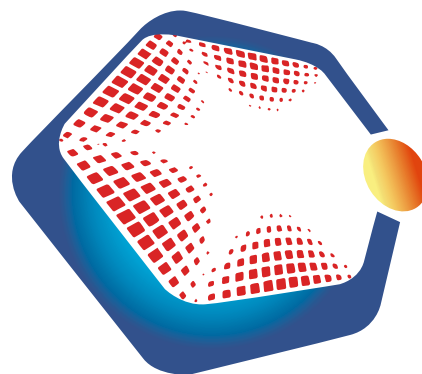
Other

Ministry of Economics, Skopje, Macedonia

Aflatoxin is created from the family of *Aspergillus* bacteria such as *Aspergillus flavus*, *A. parasiticus* and *A. nomius*. The optimal conditions for creating of Aflatoxin are the high amount of moisture above 18% as well as the vegetative raw material the temperature is between 25-30°C. The presence of Aflatoxin is evident in the seeds and fruits of the plants, mainly before harvesting. The aflatoxins penetrate very fast into the skin and during the transformation in Aflatoxin B1, B2 and other penetrate in the liver which are very dangerous, poisonous, toxic, carcinogenic and deadly. At the pharmaceutical vegetative material *Agnus Castus*, Aflatoxins at first appears in its fruits first with not great amount but during the raw material is prepared respectively during the grinding the amount of Aflatoxins is rising because of releasing of the heat during grinding. The elimination of Aflatoxin is a very difficult process and it is very hard to realise but by using the clay - Tonerde Tonsil Standard 318 FF, as an adsorbent, comes to a decrease of its concentration at vegetative raw material pharmaceuticals *Agnus Castus*, at very low levels under the maximum allowed level which makes possible further processing and getting extracts for pharmaceuticals purposes. The advantages of this adsorbent are multiple in economic and ecological aspects as well.

Keywords: Aflatoxin, Extraction, Clay, Dry Mass, Extract





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