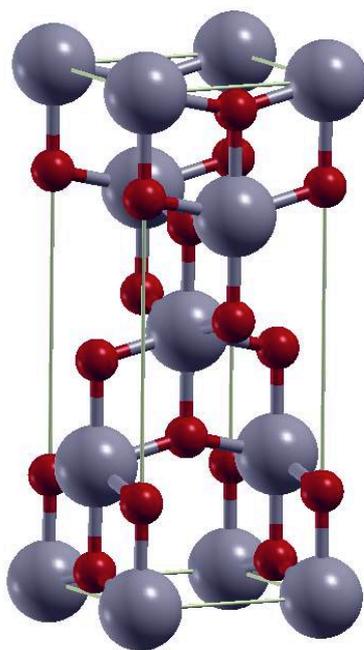
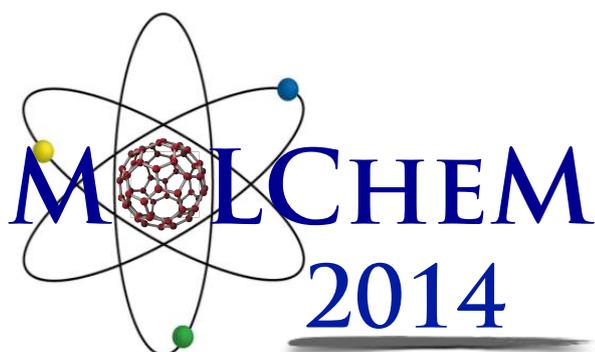


INTERNATIONAL
SYMPOSIUM ON MOLECULAR CHEMISTRY

DECEMBER 18-19, 2014 @ ISTANBUL

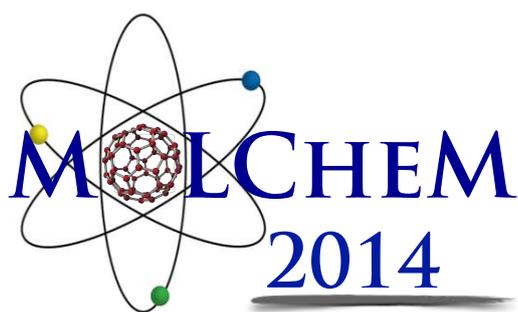


MOLCHEM2014

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MOLECULAR CHEMISTRY

18–19 DECEMBER 2014 @ ISTANBUL



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MOLCHEM2014 Ozet Kitabı Yıldız Teknik Üniversitesi Matbaası tarafından basılmıştır.

*This symposium is dedicated to
Prof. Dr. Zekiye ınar on the occasion of her 40 years in Science.*



MOLCHEM2014 Organizasyon Komitesi olarak katkılarından dolayı Yıldız Teknik Üniversitesi Rektörlüğü'ne ve Yıldız Teknik Üniversitesi Vakfı'na tesekkür ediyoruz.

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Invited Lectures

(alphabetical order according to the last name)

Idil Arslan-Alaton, Istanbul Technical University, Istanbul–Turkey
Viktorya Aviyente, Bogazici University, Istanbul–Turkey
Isil Balcioglu, Bogazici University, Istanbul–Turkey
Miray Bekbolet, Bogazici University, Istanbul–Turkey
Sondan Durukanoglu Feyiz, Sabanci University, Istanbul–Turkey
Burak Erman, Koc University, Istanbul–Turkey
Mirat D. Gurol, Gebze Technical University, Kocaeli–Turkey
Nilsun Ince, Bogazici University, Istanbul–Turkey
Cleva W. Ow-Yang, Sabanci University, Istanbul–Turkey
Emrah Ozensoy, Bilkent University, Ankara–Turkey
Yaron Paz, Israel Institute of Technology-Technion, Haifa-Israel
Pierre Pichat, CNRS (National Center for Scientific Research), Lyon-France
Davide Vione, Dipartimento di Chimica Analitica, Torino-Italy
Ersin Yurtsever, Koc University, Istanbul–Turkey
Mine Yurtsever, Istanbul Technical University, Istanbul–Turkey

- 15 Invited Speakers
- 11 Oral Presentations
- 141 Poster Presentations
- 241 Participants

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The members of the Organizing Committee express their sincerest gratitude to **Prof. Dr. Miray Bekbolet** (Bogazici University, Istanbul–Turkey). We greatly appreciate her encouragement, insightful guidance to organize MOLCHEM2014@Istanbul.

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MOLCHEM2014
MINI-SYMPOSIUM ON ADVANCED OXIDATION TECHNOLOGIES
DECEMBER 18, 2014

12:45–13:15 Registration

13:15–13:30 Opening Remarks

Session I Chairman: Miray Bekbolet — Moderator: Cemre Birben

13.30–14:00 Invited Lecture – Yaron Paz, Israel Institute of Technology, Israel
Preferential Photocatalytic Degradation of Contaminants

14.00–14:30 Invited Lecture – Nilsun Ince, Bogazici University, Turkey
Sonocatalytic destruction of paracetamol using Pd-supported TiO₂ nanoparticles

14.30–15:00 Invited Lecture – Idil Arslan-Alaton, Istanbul Technical University, Turkey
Toxicity of Common Quenching Agents used in Advanced Oxidation Processes

15:00–15:30 Coffee Break

Session II Chairman: Nilsun Ince — Moderator: Dila Kaya

15.30–16:00 Invited Lecture – Isil Balcioglu, Bogazici University, Turkey
Applicability of Advanced Oxidation Processes for Secondary Sludge to Reduce Micropollutants

16.00–16:30 Invited Lecture – Miray Bekbolet, Bogazici University, Turkey
Photocatalysis: Applications in drinking water treatment

16:30–16:45 Closing remarks

MOLCHEM2014
SYMPOSIUM ON MOLECULAR CHEMISTRY
DECEMBER 19, 2014

08:00–08:45 Registration

08:45–09:00 Opening Remarks

Session 1 – *Advanced Oxidation Technology*

Chairman: Miray Bekbolet — Moderator: Dila Kaya

09.00–09:30 Invited Lecture – Pierre Pichat, CNRS, France

Overview of Some Medical, Safety and Well-Being Applications of TiO₂ Photocatalysis

09.30–10:00 Invited Lecture – Yaron Paz, Israel Institute of Technology, Israel

On the Similarity and Dissimilarity between Photocatalytic Water Splitting and Photocatalytic Degradation of Pollutants

10.00–10:30 Invited Lecture – Davide Vione, University of Torino, Italy

The photochemistry of surface waters

10.30–11:00 Invited Lecture – Mirat Gurol, Gebze Technical University, Turkey

Biodiesel from Microalgal Biomass

11:00–11:20 Coffee Break

Session 2 – *Computational Chemistry & Biology*

Chairman: Viktorya Aviyente — Moderator: Cemre Birben

11.20–11:45 Invited Lecture – Viktorya Aviyente, Bogazici University, Turkey

How Good Can We Model the Kinetics in Free Radical Polymerization Reactions?

11.45–12:10 Invited Lecture – Burak Erman, Koc University, Turkey

Statistical Mechanics of Drug-Protein Interactions

12.10–12:35 Invited Lecture – Ersin Yurtsever, Koc University, Turkey

Modeling of Evaporation of Small Particles: Some Results, A Story and A Challenge!

12.35–13:00 Invited Lecture – Mine Yurtsever, Istanbul Technical University, Turkey

Theoretical Approach to Structure-Morphology Relationship in Segmented Polyurethane and Polyurea Copolymers

13:00–13:15 Oral Presentation – Nevin Uras-Aytemiz, Karabuk University, Turkey

Clathrate hydrates from all-vapor method: competition for small cage guest molecule occupancy

13:15–13:30 Oral Presentation – Cenk Selcuki, Ege University, Turkey

Interactions of Metal Ions with Biomolecules: A Density Functional Approach

13:30–14:30 Lunch

Session 3 – *Nanotechnology & Spectroscopy*

Chairman: Inci Sonmezoglu — Moderator: Nazli Turkten

14:30–14:55 Invited Lecture – Sondan Durukanoglu Feyiz, Sabanci University, Turkey

Growth of Silver Nanoclusters: An Atomistic View

14:55–15:20 Invited Lecture – Emrah Ozensoy, Bilkent University, Turkey

Understanding Catalytic Materials at the Molecular Level: From Thermal Chemistry to Photochemistry

15:20–15:45 Invited Lecture – Cleva W. Ow–Yang, Sabanci University, Turkey

Work Function Engineering of Transparent Conductive Electrodes at the Nanoscale

15:45–16:00 Oral Presentation – Seref Gucer, Uludag University, Turkey

Importance of Molecules in Environmental and Life Sciences: Metal Speciation & Fractionation

16:00–16:15 Oral Presentation – Cuneyt Berkdemir, Yildiz Technical University, Turkey

Exploring the Mimicry Materials for Catalytic Applications: Anion Photoelectron Imaging Spectroscopy of NbN and TaN

16:15–16:30 Coffee Break

Session 4 – *Molecular Modelling–Simulation & Experiment*

Chairman: Ersin Yurtsever — Moderator: Cagdas Buyukpinar

16:30–16:45 Oral Presentation – Gokhan Kacar, Technische Universiteit Eindhoven, Netherlands

Hierarchical multi-scale simulations for properties, metal adhesion, and self-healing ability of polymers

16:45–17:00 Oral Presentation – Saron Catak, Bogazici University, Turkey

Insight into the Polymerization of Conjugated Electroluminescent Polymer PPV: Diradical Character of Monomers and Dimers

17:00–17:15 Oral Presentation – Bulent Balta, Istanbul Technical University, Turkey

Conformational Rearrangements Triggering GTP Hydrolysis in EF–Tu

17:15–17:30 Oral Presentation – Namik Akkiloglu, University of Twente, Netherlands

Seeing biological macromolecules in action: From ensemble to single molecule

17:30–17:45 Oral Presentation – Dilek A. Boga, University of Utrecht, Netherlands

Renewable H₂ Production via Aqueous–Phase Reforming of Biomass–Derived Oxygenates

17:45–18:00 Oral Presentation – Enver Guler, Wetsus, Netherlands

Blue Energy-Ion exchange membranes for reverse electrodialysis

18:00–18:15 Oral Presentation – Aysu Yarman, University of Postdam, Germany

Molecular Imprinting: From Biology to Chemistry

18:15–18:30 Closing remarks

18:30–19:30 Poster Session

19:30 Dinner

*Symposium on
Molecular Chemistry*

INVITED LECTURES

IL – I

Preferential Photocatalytic Degradation of Contaminants

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Operating mostly by a radical mechanism, photocatalysis is considered to degrade contaminants in air and in water in a non-specific way. On one hand this non-specific way enable to treat large variety of contaminants. On the other hand, in cases where non-toxic compounds are presence together with less-toxic compounds, one would like to degrade specifically those contaminants that are most hazardous.

Based on our experience, we will discuss various ways to obtain specificity in photocatalysis, while mentioning the pros and cons of each method. These ways include:

- 1) Surface charge control
- 2) Molecular recognition 'Adsorb & suttle'
- 3) Molecular imprinting
- 4) Specificity by desorption control
- 5) Specificity by catalyst doping.

IL – II

Sonocatalytic Destruction of Paracetamol using Pd-supported TiO₂ Nanoparticles

A. Ziylan , Y. Maeda , Nilsun Ince
ince@boun.edu.tr

¹Institute of Environmental Sciences, Bogazici University, Istanbul–Turkey

²Department of Applied Materials Science, Prefecture University, Osaka–Japan

Paracetamol (PCT) is a non-prescribed medication used widely for the relief of fever and anti-inflammatory pains. As such, it is one of the most frequently detected pharmaceutical in sewage treatment plant effluents and surface water as a 'high priority-trace pollutant' [1-3]. Destruction of pharmaceuticals (PhACs) in water by advanced oxidation processes (AOPs) involving reactive OH radicals and similar oxidizing species have lately received considerable attention due to the non-selective nature of these species for a wide range of organic compounds, including PhACs [4-6]. Sonolysis and sonocatalysis are viable AOP techniques, whereby organic compounds are effectively oxidized by cavitation-induced ·OH that is available in the bulk solution, the gas-liquid interface and on surfaces of solid catalysts. The current study aims to investigate the efficiency of Pd-supported TiO₂ nanoparticles (Pd-TiO₂) on sonocatalytical degradation of PCT by monitoring the rate of PCT decay, the extent of C-mineralization and the accumulation of H₂O₂ in solution as an indicator of ·OH formation. The results are compared with those obtained using commercial TiO₂ powder (Degusa P-25). The nanocomposite (Pd-TiO₂) was synthesized sonolytically using Na₂PdCl₄·3H₂O, powdered TiO₂ (Degusa P-25) and PEG-MS (polyethylene-glycol monostearate) in a multi-wave ultrasonic bath emitting at 200 kHz (Kaijo, 4021). PCT degradation was carried out in a multi-frequency reactor (Ultraschall/Meinhardt) optimized for a volume of 250 mL, a frequency of 861 kHz and a specific power of 0.23 W mL⁻¹. The tests were run at acidic, neutral and alkaline pH and with varying molar ratios of PCT to TiO₂ to select the optimum values of pH and catalyst dose. The stability of the nano-catalyst was tested by recovering and reusing it in 4-consecutive experiments. It was found that the rate of PCT degradation in the presence of Pd-TiO₂ was nearly pseudo-first order and increased with increasing doses of the catalyst and contact time, reaching a maximum at C₀=35 μM, Pd-TiO₂=5 mg L⁻¹ and pH=6.5. The efficiency of recovery and reuse of the nanoparticles was quite high, signifying the stability and superiority of immobilized TiO₂ as a catalyst over commercial P-25 powders.

References

- [1] M. D.G. de Luna, M. L. Veciana, C.C. Su, M.C. Lu, J. Haz. Mat. 217-218: 200-207. 2012. [2] Y. Kim, K. Choi, J. Jung, S. Park, P-G. Kim, J. Park, Environ. Int. 33:370-375.2007. [3] A. Ziylan, N.H. Ince, Chem. Engineer. J. 220:151-160.2013. [4] Q.P. Isariebel, J.L. Carine, J.H. Ulises-Javier, W. Anne-Marie, D. Henri, Ultrason. Sonochem. 16:610-616. 2009. [5] F. Mendez-Arriaga, R. Torres-Palma, C. Petrier, S. Esplugas, J. Gimenez, C. Pulgarin, Water Res. 42: 4243- 4248.2008. [6] L. Yang, L.E. Yu, M.B. Ray, Water Res. 42:3480-3488.2008.

IL – III

Toxicity of Common Quenching Agents used in Advanced Oxidation Processes

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The toxicity parameter serves as an important tool to judge the ecotoxicological safety and hence applicability of an advanced oxidation process (AOP) for water and wastewater treatment. In particular, the use of battery tests involving representative species from different trophic levels is highly recommended to follow-up ecotoxicological risks. Before measuring toxicity in reaction solutions being subjected to AOPs, residual oxidizing agents (ozone, hydrogen peroxide, persulfate, peroxymonosulfate, etc.) and (photo)catalysts have to be removed to eliminate their analytical as well as toxicological interferences with the reaction components. Several pretreatment procedures are available including quenching with (i) enzymes, (ii) reducing agents or (iii) metal oxides after pH adjustment and/or filtration steps if required.

In the present study, the acute toxicity of commonly used chemical oxidants (hydrogen peroxide, persulfate and peroxymonosulfate) and quenching agents (catalase enzyme, manganese dioxide, ascorbic acid, sodium thiosulfate, sodium nitrite and sodium sulfite) was examined by employing three different bioassays using the organisms *Vibrio fischeri* (marine photobacteria), *Daphnia magna* (freshwater cladoceran) and *Pseudokirchneriella subcapitata* (freshwater microalgae). Results have indicated that hydrogen peroxide toxicity could be effectively eliminated by adding catalase enzyme, whereas sodium thiosulfate and ascorbic acid were recommended as suitable quenching agents for the removal of persulfate and peroxymonosulfate in the *Vibrio fischeri* bioassay. None of the studied quenching agents was found to be suitable as persulfate and peroxymonosulfate quenchers in the *Daphnia magna* bioassay. In the case of *Pseudokirchneriella subcapitata*, manganese dioxide powder should be used as an alternative quenching agent to catalase, since catalase exhibited a high toxicity towards these microalgae. Sodium sulfite which is extensively used as a quenching agent in oxidative treatment processes, was not appropriate for quenching peroxymonosulfate in the studied bioassays.

In the present work it could be demonstrated that the selection of the most suitable quenching agent(s) to eliminate the interference of oxidants in bioassays is very critical for the correct interpretation of the obtained toxicity data. Selection of the most effective, non-toxic and hence appropriate quenching agent is crucial to decide whether an AOP application is ecotoxicologically safe and feasible.

IL – IV**Applicability of Advanced Oxidation Processes for Secondary Sludge to Reduce Micropollutants**

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Increased occurrence of antibiotics in sewage sludge raised concerns regarding the potential environmental and health impacts of these emerging micropollutants, which have not been previously a major subject of interest. The widespread antibiotic contamination is suspected to promote dissemination of antibiotic resistant pathogens, therefore contributing to the emergence of another important contaminant group. Since the problem is further aggravated by increased rates of worldwide sludge production, much powerful sludge management strategies can be required.

Although incineration is considered as an effective sludge reduction technology that can provide the destruction of various organic contaminants (e.g. antibiotics), its prevalent application can be limited by the high amount of energy consumption coupled with the release of potentially hazardous gases into the atmosphere. Anaerobic digestion is largely dictated in most countries due to the high biodegradability of sewage sludge and the valuable potential of biogas production. However, the accumulation of micropollutants including antibiotics in digested biosolids and the generation or the ineffective destruction of antibiotic resistance carriers is a current debate. Various sludge pre-treatment methods have been developed to accelerate anaerobic digestion. However, the fate of organic micro-contaminants during pre-treatment has been scarcely studied. Effective chemical oxidation processes and especially advanced oxidation processes (AOPs) that involve the generation of free radicals offer the advantage of short treatment periods already applied in order to support biological wastewater treatment. The findings of this study suggest that AOPs can be viable for the removal of problematic micropollutants from the sludge.

IL – V

Photocatalysis: Applications in Drinking Water Treatment**Miray Bekbolet**

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Drinking water resources contain substantial amounts of NOM mainly composed of humic substances of which the humic acids and fulvic acids constitute the major fractions. The presence of NOM adversely affects the drinking water quality through binding and complexing with inorganic and organic micropollutants, facilitating transport of contaminants, expressing undesirable color and taste, and most importantly serving as precursors for undesirable disinfection by-products. Besides conventional treatment methods, photocatalytic degradation of NOM has been investigated since decades. Oxidative removal of organic carbon matrix has been addressed by removal of dissolved organic carbon contents (DOC). Regarding the complex chemical nature of NOM, removal of DOC could not be visualized as adequate to express the functionality of the remaining carbon content (Uyguner-Demirel and Bekbolet, 2011). Most of the literature findings refer to the use of acid insoluble humic acid as the model compound of NOM.

Application of UV-vis and fluorescence spectroscopic techniques has been applied to elucidate the structural changes attained in humic matter by oxidation. UV-vis absorbance measurements express spectroscopic parameters displaying the behavior of color forming moieties (Color_{436} , Color_{400} and UV_{365}) and UV- absorbing centers (UV_{280} and UV_{254}). Fluorescence spectroscopic techniques either acquired in emission scan (FI_{emis}) or synchronous scan (FI_{syn}) modes represent the behavior of fluorophores of the organic matrix. Moreover, Excitation-Emission Matrix (EEM) fluorescence features bring about insight information on the removal, transformation and formation of new fluorophoric groups upon oxidation. With reference to the polydisperse nature of NOM composed of discrete molecular size fractions, the use of EEM features could be recognized as a useful tool in understanding of the humic structure. Photocatalytic degradation experiments were performed under intra-laboratory standardized conditions covering both the water matrix parameters as well as photocatalytic treatment operational parameters. Based on the specified humic parameters, an overview on the application of photocatalysis to drinking water would be presented.

References

Uyguner-Demirel, C.S., and Bekbolet, M., 2011. 'Significance of analytical parameters for the understanding of natural organic matter in relation to photocatalytic oxidation'. *Chemosphere*, 84, 1009-1031.

IL – 1

Overview of Some Medical, Safety and Well-Being Applications of TiO₂ Photocatalysis

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The capability of photo-excited TiO₂ to degrade organic matter, including that of microorganisms, is at the basis of its conventional environmental applications either commercialized or at the demonstration stage, viz. self-cleaning materials [1], purification of indoor air [2] and water [3]. In this communication, other much less-known potential applications - related to safety, health and well-being - will be presented, viz. food packaging, medical implants and progressive delivery of chemical compounds.

Regarding food packaging [4], photo-excited TiO₂ offers several assets: (1) inactivation/degradation of the microorganisms generating spoiling, ripening and other food alterations; (2) scavenging of O₂ capable of increasing food oxidation and inducing the growth of aerobic microorganisms; (3) oxidation of C₂H₄, a compound produced by fruits and vegetables which promotes ripening. The benefits of adding bactericide elements, such as Ag and Cu, to the packages have also been demonstrated. However, adverse effects must be taken into account, e.g., potential, gradual photocatalytic degradation of the food and the package, and possible release of TiO₂ particles.

Ti is a common component of medical implants. This metal is readily covered by layers of Ti oxides, among which TiO₂. These oxides have been shown to improve osseointegration of the implants, thus preventing implant loosening. Of particular interest in this respect is the fact that UV-irradiation of the future implant in a solution containing calcium and phosphate ions leads to the formation of a hydroxyapatite layer. This layer can induce bone formation around the implant, especially if it is functionalized with a protein that favors it [5]. Furthermore, because prevention of bacterial infections is obviously a major issue for implants, the effect of photo-excited TiO₂ on inactivation/degradation of bacteria and adhesion of biofilms is of high interest. Indeed, on-demand UV-irradiation can be applied in the case of dental implants. Interestingly, it has been observed that the antibacterial effect is maintained for several tens of minutes after the end of UV-irradiation [6].

The use of photo-excited TiO₂ has also been investigated for progressive delivery of chemical compounds (e.g., drugs, personal care products, repellents, insecticides, etc.). Depending on its chemical structure, the compound can be (1) directly attached to TiO₂ (as was proposed for TiO₂ nanotubes [7]) via a coupling agent designed to be eliminated on photo-exciting TiO₂; (2) contained in microcapsules made of polymers easily degradable by photocatalysis and deposited on a TiO₂ film [8]. Although the principle is attracting, studies are still at the early stage with model compounds. Complex adjustments are obviously necessary regarding proper release without photocatalytic degradation of the compound. See for example the following articles:

(1) P. Pichat, Self-cleaning materials based on solar photocatalysis in 'New and future developments in catalysis', Vol. 7 'Solar catalysis', S.L. Suib (Ed.), Elsevier, pp. 167-190, 2013. (2) P. Pichat, Appl. Catal. B, 99 (2010) 428-434. (3) Photocatalysis and water purification, P. Pichat (Ed.), Wiley-VCH, Weinheim, 2013. (4) A. Llorens et al., Trends Food Sci. Technol., 24 (2012) 19-29. (5) S. Piskounova et al., J. Biomed. Mater. Res. B, 91 (2009) 780-787. (6) Y. Cai et al., Plos One, 8 (10), (2013) e75929. (7) N. K. Shrestha et al., Angew. Chem., 120 (2008) 1-5. (8) J. Marques et al., Int. J. Photoenergy, Article ID 712603, 2013.

IL – 2

On the Similarity and Dissimilarity between Photocatalytic Water Splitting and Photocatalytic Degradation of Pollutants

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The last four decades have shown a remarkable increase in the scientific interest in photocatalysis, as a tool for tackling the world's energy and waste problems. The apparent similarity between photocatalytic water splitting and photocatalytic degradation of pollutants, studied so far by two different scientific communities, raises a question regarding the extent by which one may utilize the knowledge obtained in one field for the benefit of the other. This review examines the common features as well as the differences between the two areas. The main similarities stem from the common dependence on the absorption of photons and on subsequent charge carrier dynamics. The main dissimilarities are linked to thermodynamics, to the type of reactants and end-products and no less important, to the role of adsorption and desorption. At present the fundamental differences between storing energy versus using it in order to solve environmental issues affects practical solutions. Yet, easy transfer of knowledge, research resources and personnel between the two is not only possible but should be encouraged.

IL – 3

The photochemistry of surface waters

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Chemical reactions driven by sunlight are important processes in surface freshwaters, where they are involved in the transformation of xenobiotic molecules and of naturally occurring compounds. The relevant reactions are generally distinguished into direct photolysis and indirect photodegradation. Direct photolysis involves molecules that absorb sunlight and are transformed as a consequence. Indirect phototransformation involves reactive transients such as $\cdot\text{OH}$, $\text{CO}_3^{\cdot-}$, $^1\text{O}_2$ and the triplet states of chromophoric dissolved organic matter ($^3\text{CDOM}^*$). They are generated by irradiation of photosensitisers such as CDOM (producing $^3\text{CDOM}^*$, $^1\text{O}_2$ and $\cdot\text{OH}$), nitrate and nitrite ($\cdot\text{OH}$). The radical $\text{CO}_3^{\cdot-}$ is produced via oxidation of carbonate/bicarbonate by $\cdot\text{OH}$ and, at a lesser extent, upon oxidation of carbonate by $^3\text{CDOM}^*$. The transient species formed by irradiated photosensitisers can induce the degradation of naturally occurring compounds and of pollutants. Photochemical transformation kinetics in surface waters can be modelled, on the basis of photochemical reactivity parameters of the relevant molecules (direct photolysis quantum yield and second-order reaction rate constants with $\cdot\text{OH}$, $\text{CO}_3^{\cdot-}$, $^1\text{O}_2$ and $^3\text{CDOM}^*$) and of water chemical composition. The model predictions have been validated against field data of pollutant phototransformation.

A software tool has recently been derived from the model (APEX: Aqueous Photochemistry of Environmentally-occurring Xenobiotics), and it is available for free download. The approach based on the measurement of photochemical reactivity parameters, followed by APEX modelling, has been applied to several pollutants including pesticides, pharmaceuticals and personal care products. In some cases, it could also be applied to the prediction of the environmental photogeneration of toxic intermediates.

Here two examples will be considered of the application of this approach, the first being the reaction between toluene and $\cdot\text{OH}$ that accounts for the majority of toluene photochemical removal from surface waters. The importance of the $\cdot\text{OH}$ reaction compared to biodegradation was assessed, and the reaction mechanism was investigated by combining experiments and quantum mechanical calculations. The second example is the photochemical formation of dioxins from the antibacterial agent triclosan.

IL – 4

Biodiesel from Microalgal Biomass

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The production of biodiesel, a renewable energy, from microalgae has the potential of simultaneously addressing the growing energy need and partially mitigating the global warming by capturing carbon dioxide from the atmosphere through algal photosynthesis. However, growing microalgae is costly because of the need for large amounts of water and nutrients, including nitrogen (N), phosphorus (P) and trace elements. Yet, these requirements can easily be met by domestic and some industrial wastewaters.

The objective of this study was to grow a mixed microalgal culture in wastewater medium and convert the lipids extracted from microalgal biomass into biodiesel. The wastewater effluent from the Omerli Biological Wastewater Treatment Plant (operated by Istanbul Water and Sewerage Administration) was used as the growth medium for a mixed microalgal culture, which was cultivated from various natural water sources and acclimated to a biologically-treated wastewater. The culture in 20 liter glass tanks was then continuously fed by CO₂ gas, illuminated by artificial light and maintained at 25°C. The wastewater contained 19.6 mg/L of NO₃⁻-N and 1.9 mg/L of PO₄⁻³-P, and N and P were removed by more than 90% during the process of growing microalgae.

The microalgal biomass was separated and concentrated by using a submerged microfiltration membrane device. Various membrane types were tested to investigate the variation of water flux with time and the mechanisms of membrane bio-fouling due to algal biomass. In addition, physical cleaning was performed to observe the recoveries in water flux.

The microalgal cells were collected and treated by Ultrasound at intensities of 0,01 – 0,5 kWh/L at a frequency of 30 kHz and for durations of 5–60 minutes. The level of cell disintegration increased with increasing sonication power intensity; the highest release of intracellular material due to cell disruption was achieved at an intensity of 0.4 kWh/L. In solution, total protein, carbohydrate and the lipids concentrations increased respectively by 9 times, 5 times and twice at that intensity.

The lipids were extracted by solvents and subjected to Gas Chromatographic analysis. The lipids were then subjected to esterification for conversion to biodiesel.

Acknowledgement

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IL – 5

How Good Can We Model the Kinetics in Free Radical Polymerization Reactions?

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Free radical polymerization is favored in industry due to its independence from extensive purification step. It can be applied to a wide variety of vinyl monomers and it is possible to obtain high molecular weight polymers with free radical polymerization.[1] Well-defined polymers with controlled molecular weights can be obtained with living/controlled radical polymerization.[2-3] In the first part of the study, the kinetics of the copolymerization of ST/HEMA system will be presented. Quantum-chemical calculations have been performed to monitor the solvent effects on the free-radical copolymer composition and propagation rate coefficients of styrene (ST) with hydroxyethylmethacrylate (HEMA) in polar aprotic N,N-dimethylformamide (DMF) and nonpolar toluene. These solvents have an impact on the copolymer composition (and monomer reactivity ratios) of the ST/HEMA system. Variations in the propagation rate in different media affect the monomer reactivity ratios, which in turn affect the copolymer composition.[4] In the second part of this presentation, the role of tacticity in free radical polymerization will be discussed. Tacticity is a measure of stereoregularity of a polymer chain and many of the polymer properties such as tensile strength, melting point, and solubility depend on it. The tacticity of the polymer chain is determined by the regularity in the configuration of the pseudochiral centers and can be controlled by means of Lewis acids and solvents.[5] In this study the role of Lewis acids in enhancing the stereoregulation of N,N-dimethylacrylamide will be discussed.

In the last part of this talk the relationship between free radical polymerization rates of methacrylates and chemical properties of their monomeric radicals will be presented. In this part, the rate of photopolymerization of 21 alkyl methacrylates is correlated with chemical properties of their monomeric radicals by making use of the enthalpic and polar effects of these radicals.[6-7]

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IL – 6

Statistical Mechanics of Drug–Protein Interactions

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Atoms of a protein exhibit well defined thermal fluctuations, referred to as B-factors or Debye-factors. These fluctuations are of the order of an [U+FFFD] gstrom. Binding of a ligand molecule, which may be a drug molecule, changes the B-factors of the given protein. The new values of the fluctuations are not arbitrary and have to satisfy certain conditions that must be compatible with the stability of the ligand-protein complex, and more importantly with the structure-function relations of the protein which is closely related to the phenomenon of allosteric activity. Thus, in addition to the thermodynamic stability of the ligand- protein complex, the function of the new system, which is the result of evolution, is of importance, and may be studied by the tools of statistical mechanics.

IL – 7**Modeling of Evaporation of Small Particles:
Some Results, A Story and A Challenge!**

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In this study, Molecular Dynamics simulations of single particle evaporation of small binary clusters will be presented. Morse potential functions with varying range parameters are chosen for the interaction between constituents so that effect of the range of interaction on both thermodynamical and dynamical properties can be analyzed. To study the structural motifs of the global minima and the extent of the mixing various measured are introduced. Then the evaporation of these clusters are studied by the Molecular Dynamics simulations. The possible existence of the broken ergodicity is argued and the simulations are shown to provide a test for detecting it. Finally some peculiar behavior of thermodynamics and dynamics of these processes will be discussed.

IL – 8

Growth of Silver Nanoclusters: An Atomistic View

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We have investigated the growth processes of various Ag nanoclusters with different shape and morphology. In order to understand the shape evolution of nanocluster at the atomistic level, the energy barriers and reaction rates of different pathways are determined using nudged elastic band method and molecular dynamic simulations based on the potentials extracted from embedded atom method. Growth processes are controlled using varying initial nucleation conditions: deposition angle and rate, temperature, cluster size and shape. Our results show that the reaction conditions control the formation of atoms into clusters and determine the shape of nanocrystals. We also discuss our simulation results with the experimental studies based on the shape-controlled synthesis.

IL – 9**Understanding Catalytic Materials at the Molecular Level: From Thermal Chemistry to Photochemistry****Emrah Ozensoy**

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In this talk, two different genres of TiO₂-promoted DeNO_x catalysts with NO_x storage capabilities will be discussed. The first genre of catalysts to be discussed is TiO₂-promoted NO_x-Storage Reduction (NSR) catalysts for automotive applications, which function through thermally activated surface processes. Experimental results from ultra-high vacuum (UHV) applications on atomically well-defined planar model catalysts as well as realistic high-surface area (mesoporous) materials will be combined with theoretical Density Functional Theory (DFT) modeling results. Through these results, surface functionalization of conventional NSR materials (i.e. BaO/Al₂O₃) with TiO₂ is presented as an effective strategy to 'fine-tune' the surface dispersion of the catalytically active nano-domains, obtain superior NO_x storage capacity and enhance tolerance against catalytic sulfur poisoning. Inspired by the thermally-activated automotive catalysts given above, a new genre of photochemically-activated TiO₂-promoted DeNO_x catalysts will also be introduced. These novel photochemically activated systems called 'Photocatalytic NO_x Oxidation and Storage' (PHONOS) systems, operate under ambient conditions (25 °C) and offer a hybrid platform combining thermal catalysis and photocatalysis.

IL – 10

Work Function Engineering of Transparent Conductive Electrodes at the NanoscaleCleva W. Ow-Yang¹**Hasan Kurt**¹, **Junjun Jia**², **Oguzhan Gurlu**³, **Yuzo Shigesato**²

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While the design of new materials and device architectures will lead to enhanced organic electronic device performance, the interfaces arising from adjacent layers offer an additional degree of engineering optimization. To this end, one approach is to improve energy level alignment, while another is to modify surface properties. With the goal of improving charge collection efficiency in organic photovoltaics, we use nanoparticle-based interlayers to engineer the work function of transparent conductive electrodes in P3TH:PC60BM solar cells. Through varying the surface coverage by lithium fluoride (LiF) nanoparticles systematically, the work function of indium tin oxide (ITO) can be tuned and correlated to an improvement in device performance. Solution-processing of LiF (sol-LiF) is achieved by using polymeric micelle reactors for two purposes: (i) as vessels for size-monodisperse nanoparticle synthesis and (ii) for tailoring the 2-D distribution of the sol-LiF nanoparticles during deposition. The sol-LiF interlayer was formed by spin coating and subsequent oxygen plasma-etch removal of the polymer. Polymer-based solar cell devices were fabricated using the conventional architecture of ITO/(interlayer)/P3HT:PCBM/thermal-LiF/Al. An optimum in device efficiency was associated with a sol-LiF surface coverage of 5.3% on modified ITO electrodes with a surface workfunction of 5.08 eV, implying an improvement in energy level alignment with PEDOT:PSS. The successful proof-of-concept devices suggest a new route for surface work function modification for new transparent conductive materials. Moreover, increased flexibility in materials processing of interlayers enriches the possible methods for interfacial engineering, particularly when incorporating new transparent conductive materials into existing device architectures.

IL – 11

Theoretical Approach to Structure-Morphology Relationship in Segmented Polyurethane and Polyurea Copolymers

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Segmented copolymers consist of alternating hard and soft segments along their backbone. These systems generally possess a microphase separated morphology due to the chemical incompatibility between the segments and the crystallinity of the PU and PU hard segments. The hard segments are held together due to strong H- bonding interactions [1] and dispersed as isolated microdomains in a continuous soft segment matrix. Macrophase separation is prevented due to the covalent linkages between the segments [2]. The influence of hydrogen bonding and the symmetry of the diisocyanate group contained in the hard segments on the morphology and thus properties of the copolymers were studied at different time and length scales computationally. Structures and intersegmental interactions at the molecular scale were studied by the density functional theory (DFT) method at M06-2X/6-31g(d,p) levels. Different morphologies arising from the structural changes were studied at the meso scale by the dissipative particle dynamics (DPD) method. We showed that size and shape of the micro phase domains in these systems can be controlled by varying the type and weight percentage of the soft segments as well as symmetry and planarity of the diisocyanate groups [3]. Computational results obtained strongly supported the experimental observations reported on the morphology and thermal and mechanical properties of these segmented polyurethanes and polyureas [4].

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ORAL PRESENTATIONS

OP – 1

Clathrate Hydrates from All-Vapor Method: Competition for Small Cage Guest Molecule Occupancy

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Clathrate hydrates are non-stoichiometric crystalline compounds that contain guest molecules of suitable sizes and shapes trapped in well-defined cavities formed by water molecules. Recently, a simple method was developed for the formation of aerosols of gas-hydrate nanoparticles that one is able to measure high quality FTIR spectra.[1-5] Analysis of the FTIR data provides a measure of kinetic data of competition of the small cage guests. In this talk, I will briefly review the experimental and computational results of competing gas molecules to the small cage of structure II hydrates.

Acknowledgement

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OP – 2**Interactions of Metal Ions with Biomolecules: A Density Functional Approach****Cenk Selcuki**

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Metal ions are essential for living cells and even the nonessential ones are required for metabolic processes. They mainly act as co-factors or as main components of prosthetic groups for metalloproteins; but, they are also potentially toxic when their concentrations exceed tolerated limits. Recent studies indicate that some metal ions also play important role in metabolic process regulations in microorganisms.

This work will summarize some of the model systems investigated in our group in order to understand the mechanism(s) of metal ion-biomolecule interactions by using computational tools, mainly quantum chemical techniques based on Density Functional Theory (DFT). A better understanding of the interaction mechanisms not only will enable us to minimize the effects of metal toxicity but also will help us to improve new hybrid systems that can be used in many different fields from health to bionanotechnology.

Our preliminary results indicate that metal ions mostly bind to specific sites with a high selectivity in the investigated model systems. The studies will be extended to include implicit and explicit solvent models to understand the effects of the medium.

OP – 3

Importance of Molecules in Environmental and Life Sciences: Metal Speciation & Fractionation

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The bioavailability or toxicity of elements are strongly species-dependent and related with its chemical forms.[1-3] Additionally, elements can be found as a part of biomacromolecules in food, biological or environmental samples and these structures represent valuable informations about their different actions.[3] For example, some metalloproteins are produced under heavy metal stress in environmental pollution.[4] Identification and characterization of chemically transformed species in metallodrugs are important for its activity as therapeutic agent.[1] So, speciation studies has therefore become an important topic of research and plays important role in many areas such as quality control of food products, examination of occupational exposure, clinical analysis, environmental monitoring, etc. [5] In some cases defining chemical species i.e. speciation analysis are difficult and the term fractionation is defined achemicalnd applied in these fields. Structure of matter is the key parameter that influences the physical and chemical properties. In this respect, fractionation is a process of the separation of an analyte or a group of analytes from a given sample according to physical or chemical properties.[2] In terms of food and nutrition, the elemental composition of plant foods together with the fractionation studies will give valuable insights as beneficial and toxic levels of the elements may be closer. Our presentation is related with the fractionation of the manganese and copper associated macromolecules from plant derived foods; spinach (*Spinacia oleracea L.*), wheat (*Triticum aestivum L.*) flour and hazelnut (*Corylus avellana L.*) to understand the bioavailability affects and risk assessments. Inductively coupled plasma mass spectrometry was used for the determinations.

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OP – 4

Exploring the Mimicry Materials for Catalytic Applications: Anion Photoelectron Imaging Spectroscopy of NbN and TaN

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This study was undertaken to produce anion NbN and TaN that are partially similar to the electron binding energy spectra of anion Pd and Pt, respectively. As we know that Pd and Pt metals have been actively used for many catalytic applications but unfortunately they are exceptionally expensive materials. The identification of an alternative less expensive catalyst will be economically beneficial. Gas-phase spectroscopic studies are one of the alternatives to open up a new approach to forming nanoscale materials from the bottom up via cluster assembly. In this respect, we have investigated the ground electronic states and electron affinities of anion NbN and TaN by obtaining their electron binding energies and photoelectron angular distributions via a photoelectron imaging spectroscopy. The detachment energies of anion NbN and TaN are measured from the X band maximum which defines the 0-0 transition between ground states of anion and neutral species. To explore an analogy, we compared the electronic properties of NbN and TaN with that of Pd and Pt because they have the same number of valence electrons.

OP – 5

Hierarchical Multi-scale Simulations for Properties, Metal Adhesion, and Self-healing Ability of Polymers

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In this work, we strive to perform molecular simulations to study the properties of cross-linked polymers either in bulk or in contact with a solid metal substrate. The polymer is a cross-linked one where some functional groups react with each other leading to a stiff network structure. Due to the relevant time scales inherent in a cross-link formation process, this cannot be simulated at the atomic level. Therefore, performing calculations at higher scales is needed to build and relax the cross-linked polymer either in bulk or at presence of a metal substrate. For this purpose, we use a mesoscopic simulation method referred as Dissipative Particle Dynamics (DPD). This method is proven to be successful in predicting the structure of polymers; and was recently used in a combined experimental-simulation approach to study the surface segregation of low surface energy dangling chains on cross-linked polymer films, the self-replenishing ability, which allows the recovery of the initial hydrophobicity of cross-linked polymeric films upon multiple surface damages and to reveal the role of interfaces on self-healing of surface-structure composites.

Recently, we extended this method by implementing a generalized parameterization procedure for variable DPD bead volumes. For the correct polymer structure, the representation of the actual bead sizes in the simulations is needed. By using this procedure we later studied the network properties and structure of a cross-linked polymer. A multi-scale approach bridging the coarse-grained and atomistic scales is constructed for quantification of polymer-metal DPD interactions. This procedure is later implemented to DPD simulations for the structure of a polymer near a metal-oxide surface. The mesoscopic structures of the polymer are fine-grained for atomic MD simulations to compute the material and interfacial properties. The mechanical properties such as Poisson's ratio, elastic modulus and glass transition temperature; and the interaction energies between the polymer and surface alumina are found to match well with the experimental measurements.

OP – 6

Insight into the Polymerization of Conjugated Electroluminescent Polymer PPV: Diradical Character of Monomers and Dimers

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Despite various studies on the polymerization of PPV through different precursor routes,⁽¹⁾ detailed mechanistic insight on the level of the individual reactions and intermediates is still incomplete. The present study employs DFT, DMRG⁽²⁾ (Density Matrix Renormalization Group) and CAS calculations to gain more insight into the polymerization of PPV via the Gilch route⁽³⁾ –known to exclusively occur through a radical mechanism– and identify reactions that lead to side products, such as the p– cyclophane system. Furthermore, the effect of the nature of the p–quinodimethane system on PPV polymerization is assessed with respect to the size of the aromatic core as well as heteroatoms in the conjugated system. The nature of the aromatic core and the specific substituents alter the electronic structure of the p– quinodimethane monomers and in turn affect the polymerization mechanism.

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OP – 7

Conformational Rearrangements Triggering GTP Hydrolysis in EF-Tu

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Elongation Factor Tu is responsible of the accuracy of the ribosomal protein synthesis. It forms a ternary complex with GTP and aminoacyl-tRNA. Correct codon- anticodon pairing triggers the hydrolysis of GTP to GDP. The GDP bound form of EF- Tu has a low affinity to aa-tRNA, hence releases the aa-tRNA in the ribosome and dissociates from the ribosome. The information about the codon-anticodon matching is thought to be relayed via conformational changes on the ribosome and EF-Tu.

In this study, molecular dynamics simulations have been carried out to get insight about the conformational behavior of the GTP bound EF-Tu in the absence of the ribosome. EF-Tu from *E. coli* and *T. aquaticus* have been simulated at 310 and 343 K respectively. Thermodynamic integration simulations have been used to determine the pKa of His85, an essential residue for catalysis. The role of the protonation state of this residue has been investigated via simulations with His85 being either protonated or neutral. In addition to the simulations of wild type EF-Tu, several mutants have also been studied.

Thermodynamic integration simulations yield pKa values of 8, 9 and 10 for the I61A mutant, wild type and D87E mutant proteins. These results indicate that His85 is mostly protonated at physiological pH and its pKa is regulated by the hydrophobicity of its environment and by its contact with a negatively charged residue. In both its protonated and neutral forms, His85 can be oriented into the active site or away from the active site. Protonated His85 is mostly situated in the active site whereas neutral His85 is usually at the outside.

In all simulations on EF-Tu from *T. aquaticus* in the absence of tRNA, the Switch I region is very mobile and orients Arg57 into the active site. This position of Arg57 is similar to that of the catalytic arginine in other G-proteins. The presence of tRNA reduces the mobility of Switch I which remains in a conformation similar to the one observed in the crystal structures.

There are two binding sites for monovalent cations near the active site. Especially the one near Asp21 is highly occupied in some simulations.

The D87E mutation causes His85 to spend more time in the active site. The T62A mutation brings Switch I into the tRNA binding site.

OP – 8

Seeing Biological Macromolecules in Action: From Ensemble to Single Molecule**Namik Akkilic¹, Fenna van der Grient², Thijs Aartsma², Frans Leermakers³, Wiebe de Vos¹**
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We use single-molecule fluorescence spectroscopy to monitor the electron transfer reactions in redox proteins that are not only crucial for many physiological functions but also contribute to applications in biomolecular electronics and biosensing. Herein, fluorescent labeling with Cy5 was used for the detection of the redox state of azurin based on excited state energy transfer (FRET) from the attached Cy5 to the protein redox center. The fluorescence intensity of a single azurin molecule shows an "on" and "off" switching as a function of time which can be externally controlled using 2 sensitive methods: (i) Chemically-induced (1) and (ii) Electrochemically-induced switch (2, 3). To conclude, we were able to make a quantitative assessment of the heterogeneity of the reaction kinetics and redox thermodynamics, for the first time, for individual azurin molecules, either immobilized covalently on a passive surface (method 1) or hydrophobically on gold electrode (method 2).

Secondly, we design smart polymer architectures that are covalently attached by one end to a substrate. We show that the fluorescence intensity of a single protein molecule shows a sharp and fast on-off switching behavior, controlled by the solution pH. We aim to extend these systems to create well-defined smart polymer brush films to be used in biosensors, enzymatic catalysis and in membrane technology.

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OP – 9

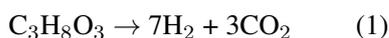
Renewable H₂ Production via Aqueous-Phase Reforming of Biomass-Derived Oxygenates

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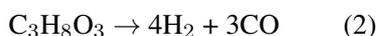
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Glycerol is a particularly attractive biomass-derived oxygenate, given its ready availability and strong potential to become a primary building block in future biorefinery schemes. It is formed in significant amounts as a by-product during biodiesel production and efficient catalytic processes that convert glycerol into value-added products are highly desired. Glycerol can be converted into hydrogen by aqueous phase reforming (APR) according to the following reaction:



as a result of both reforming (2) and water-gas shift (3) reactions which take place under typical APR conditions:



The production of hydrogen by aqueous phase reforming over supported metal catalysts comes with significant challenges with regards to selectivity. Indeed, the products CO₂ and H₂ are unstable at low temperatures and readily give alkanes and water by Fischer-Tropsch and methanation reactions. Therefore, hydrogen selectivity plays a role of utmost importance in catalyst development for APR of oxygenated hydrocarbons. Here, an efficient PtCu bimetallic catalyst system supported on mixed oxides derived from calcination of hydrotalcites is presented [1]. This new bimetallic catalyst system showed an improved hydrogen selectivity, as the formation of undesired alkanes such as methane, is significantly suppressed.

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OP – 10

Blue Energy-Ion Exchange Membranes for Reverse Electrodialysis**Enver Guler**

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Reverse electrodialysis (RED) or blue energy is a non-polluting, sustainable technology for generating power from the mixing of solutions with different salinity, i.e. seawater and river water. A concentrated salt solution (e.g. seawater) and a diluted salt solution (e.g. river water) are brought into contact through an alternating series of polymeric anion exchange membranes (AEM) and cation exchange membranes (CEM), which are either selective for anions or cations. Currently available ion exchange membranes are not optimized for RED, while successful RED operation notably depends on the used ion exchange membranes. In the current work, we designed such ion exchange membranes and for the first time, we show the performance of tailor-made membranes in RED. More specifically we focus on the development of anion exchange membranes (AEMs) as these are much more complex to prepare. Here we propose a safe and more environmentally friendly method and used halogenated polyethers such as polyepichlorohydrin (PECH) as starting material. A tertiary diamine (1,4-diazabicyclo[2.2.2]octane, DABCO) was used to introduce the ion exchange groups by amination and for simultaneous cross-linking of the polymer membrane. Area resistances of the series of membranes ranged from 0.82 to 2.05 $\Omega\cdot\text{cm}^2$ and permselectivities from 87 to 90%. For the first time we showed that tailor-made ion exchange membranes can be applied in RED. Depending on the properties and especially the membrane thickness, application of these membranes in RED resulted in a high power density of 1.27 W/m^2 , which exceeds the power output obtained with the commercially available AMX membranes. This shows the potential of the design of ion exchange membranes for a viable Blue Energy process.

OP – 11

Molecular Imprinting: From Biology to Chemistry

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Hybrid architectures which combine a MIP with an immobilized 'affinity ligand' or a biocatalyst sum up the advantages of both components. In this talk, hybrid architectures combining a layer of a molecularly imprinted electropolymer with a mini-enzyme or a self-assembled monolayer will be presented.

(i) Microperoxidase-11 (MP-11) catalyzed oxidation of the drug aminopyrine on a product imprinted sublayer: The peroxide dependent conversion of the analyte aminopyrine takes place in the MP-11 containing layer on top of a product-imprinted electropolymer on the indicator electrode. The hierarchical architecture resulted in the elimination of interfering signals for ascorbic acid and uric acid.

An advantage of the new hierarchical structure is the separation of MIP formation by electropolymerization and immobilization of the catalyst. In this way it was for the first time possible to integrate an enzyme with a MIP layer in a sensor configuration. This combination has the potential to be transferred to other enzymes, e.g. P450, opening the way to clinically important analytes.

(ii) Epitope-imprinted poly-scopoletin layer for binding of the C-terminal peptide and cytochrome c (cyt c): The MIP binds both the target peptide and the parent protein almost eight times stronger than the non-imprinted polymer with affinities in the lower micromolar range. Exchange of only one amino acid in the peptide decreases the binding by a factor of five.

(iii) MUA-poly-scopoletin MIP for cytochrome c: Cyt c bound to the MIP covered gold electrode exhibits direct electron transfer with a redox potential and rate constant typical for the native protein. The MIP cover layer suppresses the displacement of the target protein by BSA or myoglobin. The combination of protein imprinted polymers with an efficient electron transfer is a new concept for characterizing electro-active proteins such as cyt c. The competition with other proteins shows that the MIP binds its target cyt c preferentially and that molecular shape and the charge of protein determine the binding of interfering proteins.

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POSTER PRESENTATIONS

PP-1

Production of Melamine Formaldehyde Resin having Low Curing Temperature for Textile Substrate

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Melamine-formaldehyde resin, any of a class of synthetic resins obtained generally by chemical combination of melamine and formaldehyde. A complex, interlinked polymer that cures to a clear, hard, chemically resistant resin, melamine formaldehyde is employed in plywood and particleboard adhesives, laminated countertops and tabletops, dishwasher-safe tableware, and automotive surface coatings.

Melamine-formaldehyde resins are also used for a variety of textile applications such as improving wrinkle resistance in cotton and cotton-synthetic blends, providing mildew resistance and water repellence, dyeing fixative for disperse dyes, carrying pigment and fire retardant binder, reducing the shrinkage of cellulosic fibers, imparting permanent press characteristics to cotton - polyester blends, improving the stiffness or resiliency of synthetic fabrics.

A new melamine formaldehyde resin was synthesized by the condensation reaction of melamine, urea and formaldehyde with alcohols in the presence of acid catalysts in two step reaction mechanism. It has a low curing temperature, physical and chemical stable product for textile industry. The effects of reaction parameters (temperature, acidity, and water content) on resin characteristics were monitored to specify the best synthesis conditions and properties.

PP-2

Electronic Nature of Pyrene-Aromatic Amino Acid Complexes**Nursel Acar , Armagan Kinal**

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Photoinduced electron transfer systems are used in optical applications. The photonic energy which is harvested by an antenna is transformed into ground state chemistry utilizing photoinduced electron transfer or photochemical bond reorganization (1). Amino acids can possess weak van der Waals and hydrogen bonds, wide transparency ranges in the visible regions and zwitterions which are very important in materials science (2). In order to optimize the efficiency of optical devices, it is an advantage to understand completely the physical behaviour of compounds.

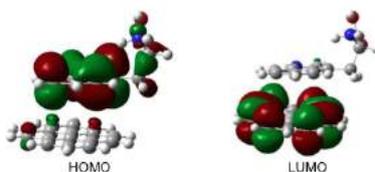


Figure-1. Molecular orbitals of Py-Trp system in vacuum of lowest excited singlet states

We have studied electronic structure and optical excitation of pyrene (Py) with aromatic amino acids in vacuum and in water using DFT and TD-DFT calculations. The density functional theory (DFT) computations have been performed at ω B97XD/6-311++G(d,p) level using Gaussian 09 program (3).

Pyrene was chosen as molecular antenna and aromatic amino acids were chosen as electron donors. Our results show that more stable complexes are formed in vacuum. Tryptophan (Trp) complexes are the most stable among all optimized complexes. Significant geometrical changes have been observed for the optimized complexes between gas phase and water. Pyrene-amino acid interactions via π - π stacking promote the photoinduced transfer reactions. Calculated HOMO-LUMO energies confirm that charge-transfer occurs between the molecules. The most significant charge transfer is observed for Trp complexes between HOMO and LUMO. It is concluded that the lowering of highest occupied orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap (3.78 eV) appears to be cause of its enhanced charge transfer.

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PP-3

New Type Thienyl Pyrrole Derivative and its Electrochromic Device Application

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In this study, new type 2,5-di(2-thienyl)pyrrole derivative namely N-(2,5-di(thiophen-2-yl)-1H-pyrrol-1-yl)-4-(vinylloxy)benzamide (TPV) have been synthesized via reaction of 1,4-di(2-thienyl)-1,4-butanedione and N-(aminomethyl)-4-(vinylloxy)benzamide. P(TPV) is stable and it has lowest band gap and better long-term stability compared with other thienyl pyrrole derivatives. Therefore, electrochemical and optical properties of P(TPV) was investigated and dual-type complementary colored polymer electrochromic device based on P(TPV) and P(EDOT) was constructed in sandwich configuration. Spectroelectrochemical studies of the device revealed that the oxidized state shows blue color whereas it shows light orange for the reduced state. Maximum contrast ($\Delta\%T$) and switching time of the device were measured as 13% and 1.0 s for 460 nm and 43% and 1.0 s for 625 nm.

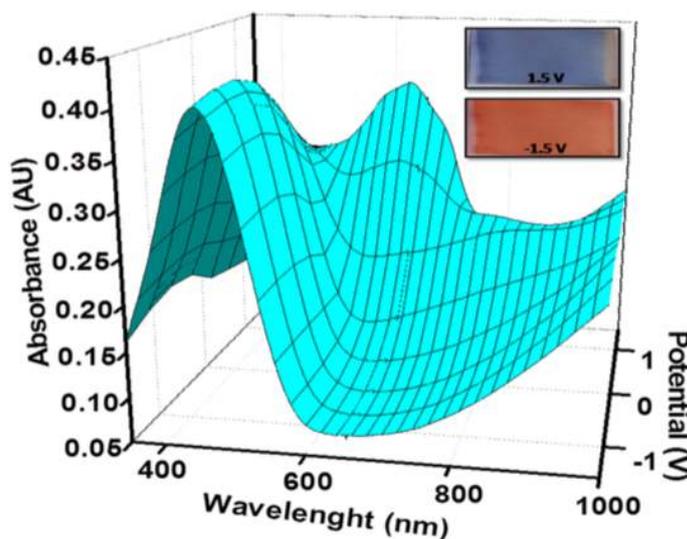


Figure: Spectroelectrochemistry of the P(TPV)/P(EDOT) device

Acknowledgement

We are gratefully thanks to the TUBITAK (project number: 111T074)

PP-4

Comparative Study of Ozonation and Catalytic Ozonation of Humic Acid

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Natural organic matter (NOM) is a complex mixture of organic compounds present in all fresh waters, particularly surface waters. NOM consists of a range of different compounds, from largely aliphatic to highly colored aromatics. Some of this organic matter is negatively charged consisting of a wide variety of chemical compositions and molecular sizes. Humic acid (HA), a major hydrophobic fraction of dissolved NOM (DOM). HA consists of anionic macromolecules having a wide range of molecular weights. These macromolecules are comprised of both aromatic and aliphatic components with primarily carboxylic (60-90%) and phenolic functional groups in aquatic environments.

Catalytic ozonation with metal oxides, as an alternative technique to ozonation alone to improve the decomposition of recalcitrant organic pollutants in water treatment, has received increasing attention in recent years. The mechanism of this technique can be ascribed to catalytically enhanced hydroxyl radical generation from aqueous ozone, formation of metal-pollutant complexes which react fast with molecular ozone, or simultaneous adsorption of both pollutants and ozone on catalyst surfaces.

In this study ozonation and catalytic ozonation of humic acid with iron oxide coated zeolite were comparatively investigated in terms of dissolved organic carbon (DOC) that specify organic matter, UV₂₅₄ reduction, SUVA (Specific Ultraviolet Absorbance at 254 nm) and Color₄₃₆. The ozonation and catalytic ozonation experiments were performed at HA concentration of 30 mg/L and pH 6.5. It was obtained in ozonation experiments that, DOC removal was 21.4%, 26.9 and 29.9% at oxidation time of 60 min when ozone concentration was 10 mg/L, 15 mg/L and 20 mg/L respectively. Also it was obtained that UV₂₅₄ and SUVA₂₅₄ removal efficiencies were 72.8%, 82.1% and 85.3% and 65.4%, 75.5% and 79.1% respectively when ozone concentration was 10 mg/L, 15 mg/L and 20 mg/L. Color₄₃₆ removal was 93.0%, 99.2% and 100% at ozone concentrations of 10 mg/L, 15 mg/L and 20 mg/L respectively.

In the catalytic ozonation experiments, it was obtained that DOC removal was 62.0%, 63.4 and 66.4% at oxidation time of 60 min when ozone concentration was 10 mg/L, 15 mg/L and 20 mg/L respectively. Also it was obtained that UV₂₅₄ and SUVA₂₅₄ removal efficiencies were 95.8%, 96.3% and 97.5% and 88.9%, 90.0% and 92.4% respectively when ozone concentration was 10 mg/L, 15 mg/L and 20 mg/L. The Color₄₃₆ was completely removed at all ozone concentrations. The results indicated that in comparison to ozonation alone, catalytic ozonation with iron oxide coated zeolite increased the DOC, UV₂₅₄ and SUVA₂₅₄ removal. The catalytic ozonation enhanced the destruction of the aromatic and UV-absorbing structures compared with ozonation alone. Increasing ozone concentrations did not increase removal efficiencies significantly in the catalytic ozonation processes.

PP-5

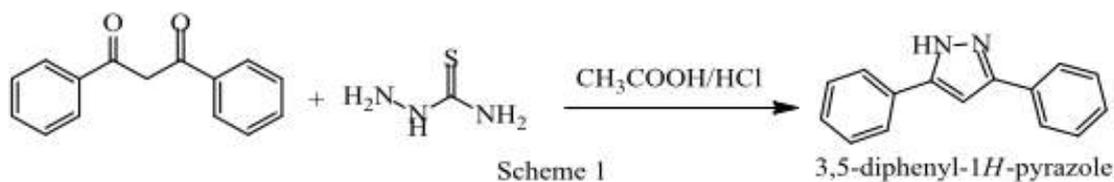
Structural analysis of 3,5-diphenyl-1H-pyrazole obtained by acid catalyze reaction

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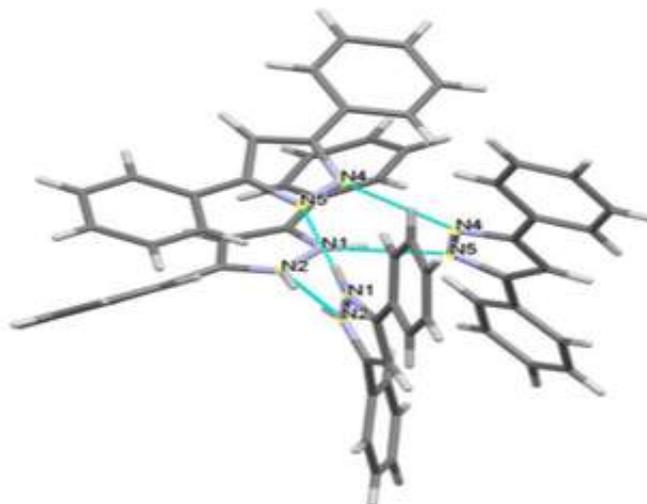
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The 3,5-diphenyl-1H-pyrazole have been prepared by acid catalyze reaction with dibenzoylmethane and thiosemicarbazide in good yield (85-93%)(Scheme 1).



The structure of the 3,5-diphenyl-1H-pyrazole was identified by a single crystal X-ray diffraction (Scheme 2), ¹H-¹³C-NMR and FT-IR analysis.



Scheme 2

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Ali, Sh. Shaukat; Ashraf, C. M.; Younas, M.; Ehsan, A. Pakistan Journal of Scientific and Industrial Research, 1993 , vol. 36, 12 p. 502 – 510.

PP-6

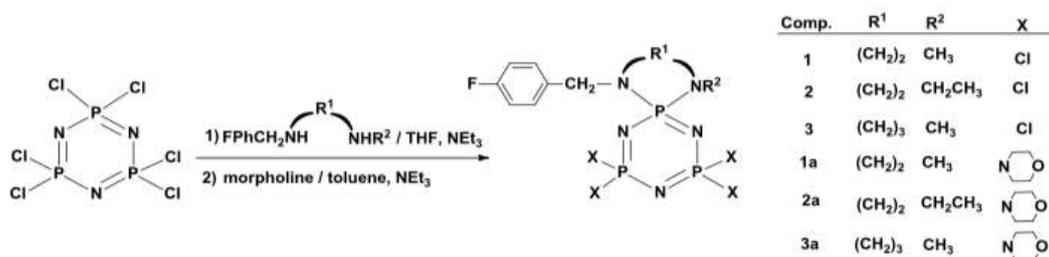
Syntheses and Spectroscopic Properties of Tetrakis(morpholino)-mono(4-fluorobenzyl)-spiro-phosphazenes

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The hexachlorocyclotriphosphazene, $N_3P_3Cl_6$, is the best known of inorganic heterocyclic ring systems, which can be converted to a large variety of cyclotriphosphazene derivatives through chloride replacement reactions. In the last decade, there has been a considerable amount of interest in the syntheses of spirocyclic phosphazenes in general and in the determination of the stereogenic properties of chiral cyclophosphazenes in particular. Aminocyclotriphosphazene derivatives in particular have attracted a great deal of attention for their potential as anti-cancer agents[1,2].



In this study, the condensation reactions of $N_3P_3Cl_6$ with NN-donor type diamines have been investigated. The reactions of $N_3P_3Cl_6$ with the diamines produce partly substituted mono(4-fluorobenzyl) spiro phosphazene derivatives (1-3). These compounds reacted with excess morpholino in toluene to give the corresponding new fully substituted morpholino phosphazenes (1a-3a). The structures of all the compounds have been examined by FTIR; ¹H, ¹³C and ³¹P-NMR, HMBC, MS and elemental analyses.

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PP-7

Synthesis and Characterization of Novel PEPPSI Pd-NHC Complexes

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N-Heterocyclic carbenes (NHCs) which are stable singlet carbenes are mostly prepared via deprotonation of the corresponding azolium salts. Since the first report by Ofele in 1968 [1], NHCs have much attention [2]. They are generally considered as analogues of phosphine ligands because of their good s-donating but weak p- accepting ability.

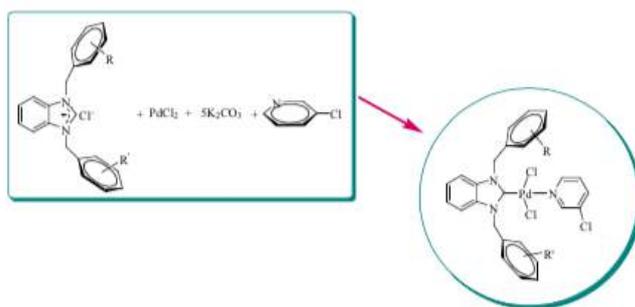


Figure: Synthesis of novel PEPPSI Pd-NHC complexes using benzimidazolium salts.

As a result, the structures of synthesized novel carben complexes were verified by using ¹H NMR, ¹³C NMR, FT-IR and elemental analysis techniques.

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Acknowledgements

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PP-8

Synthesis and Characterization of a Novel Amino Acid Schiff Base

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Schiff bases are the compounds containing azomethin group (-HC=N-). They are condensation products of ketones or aldehydes with primary amines. Formation of Schiff base generally takes place under acid or base catalysis or with heat. Schiff-bases are considered as a very important class of organic compounds and have a wide application in many biological aspects, proteins, visual pigments, enzymatic aldolization and decarboxylation reactions[1]. Moreover, some Schiff-bases were exhibits antibiotic, antiviral and antitumor agents because of their specific structure[2].

Amino acids are essential building of many biological molecules and play key roles in several neurochemical response mechanisms, such as memory, appetite control and pain transmission[3]. Phenylalanine is essential to many functions and is one of the few amino acids that can directly affect brain chemistry by crossing the blood brain barrier[4].

In this study, a new Schiff base compound derived from the condensation reaction of L- phenylalanine ester with Furfural have been synthesized. The Schiff base compound are characterized by FT-IR, ¹H and ¹³C NMR spectroscopy. Thermogravimetric analysis (TG) was carried out on a Perkin-Elmer Diamond TG- DTA thermal analyzer.

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PP-9

Inhibition of *Pseudomonas aeruginosa* Acyl Homoserine Lactone Synthase LasR Protein by *In silico* Methods

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Introduction: In natural and industrial water supplies, biofilm formation occurs. One of the bacterial genus normally found in drinking water is *Pseudomonas*. *Pseudomonas aeruginosa* is an opportunistic pathogen causes many serious infections such as cystic fibrosis via biofilm formation. Biofilms have been of considerable interest in the context of food hygiene. Bacterial biofilm and several virulence factors are demonstrated to be regulated by Quorum Sensing (QS) mechanism. QS is the communication mechanism whereby an individual microorganism synthesizes small and diffusible signal molecules that are able to be detected by surrounding organisms. There is a need for organic and healthy natural resources in the case of inhibiting this bacterial communication; hereby bacterial biofilm formation. Lichens are able to synthesize numerous specific 'secondary metabolites' that have various effects. Thus, lichens are thought to be the candidates of these natural resources. *In silico* (computer-based molecular simulations) methods as molecular docking are recently used in order to save time and cost; to generate preliminary data for further studies. Molecular docking, is a procedure that estimates non-covalent binding interactions of 3D structural macromolecules; proteins and small ligands as candidate drug molecules. Therefore, the objective of this study is *in silico* inhibition of acyl homoserine lactone synthase LasR protein of *P. aeruginosa* QS system with lichen secondary metabolites.

Materials and Methods: In this study, a 3D ligand library consisting of 607 secondary metabolite molecules and azithromycin as control, docked to AHL synthase LasR protein with Molegro Virtual Docker.

Results: Results are evaluated according to Rerank Score. 3 out of 607 ligand molecules exhibited higher Rerank scores on the active sites of LasR than azithromycin control antibiotic.

Discussion & Conclusion: The data obtained from this study could be used for further studies in the inhibition of the bacterial biofilm formation caused by *P. aeruginosa*, with the support of *in vitro* and *in vivo* researches.

Acknowledgement

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PP-10

Solvent effect on computational investigation of Polyaromatic Hydrocarbon- Porphyrin Complexes

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The electron donor-acceptor (EDA) complex plays an important role not only in energy and electron transfer processes in the excited state but also in the ion-pair formation process in the ground state. These processes correlate strongly with the molecular devices at the atomic and molecule levels. Hence, the structure and electronic states of EDA complexes have received much attention from both experimental and theoretical points of view [1]. Properties of dimeric porphyrins and the photoprocesses occurring in them are widely studied in order to understand pigment complex characteristics in photosynthetic reaction centers and to develop principles of model photosystems mimicking the biological photosynthetic apparatus [2]. Nitrogen containing porphyrin molecules and PAH can constitute donor-acceptor complexes as a result of their π -electronic systems.

In this study, the charge-transfer complexes between donor-acceptor molecules are examined by using of quantum chemical methods. Porphyrin and PAHs (pyrene and hydroxypyrene) complexes were investigated to determine minimum energy geometries by using Density Functional Theory (DFT/ ω B97X-D). Time-Dependent Density Functional Theory (TD-DFT/ B3LYP6-311++G(d,p)) has been used to investigate electronic transitions in the studied systems. The HOMO-LUMO transition indicates an electron transfer from pyrene derivatives to porphyrin ring, the lowest HOMO-LUMO energy gap is calculated as 2,62 eV.

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PP-11

**Solid Phase Extraction of Trace Metals in Environmental Samples
using BTAMB-loaded Amberlite XAD-16 and Determination by
FAAS**

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Application of 2-(2-benzothiazolylazo)-5-dimethyl aminobenzoic acid (BTAMB) coated Amberlite XAD-16, for preconcentration of Cu(II), Cd(II),Zn(II), Ni (II),Fe(II), Co (II) and Mn(II) by SPE and determination by FAAS was studied. The metals were desorbed with 2 mol L⁻¹ . The t_{1/2} values for sorption of metal ions were 2.4, 3.0, 2.8, 2.6, 4.0 ,2.9 and 4.1 min. Respectively for Cu(II), Cd(II),Zn(II), Ni (II),Fe(II), Co (II) and Mn(II). The effect of diverse ions the determination of the previously named metals were studied.Simultaneous enrichment of the seven metals was accomplished, and the method was applied for use in the determination of trace metal ions in environmental samples.

PP-12

Globe Artichoke Pullulanase Immobilization on PEG-Chitosan Beads

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Enzymes are astonishing natural protein catalysts often achieving rate enhancement factors of 10^{17} . Enzymes have the ability to catalyse reactions under very mild conditions with a very high degree of substrate specificity, thus decreasing the formation of by-products. The specificity of enzymes and their ability to catalyse reactions make them appealing for many applications in industrial fields. Pullulanase (EC 3.2.1.41) is an enzyme whose primary specificity is to hydrolyse the (1→6) α -D-glucosidic linkages in pullulan and amylopectin. This enzyme improves the saccharification of starch to produce glucose, maltose and malto-oligosaccharides together with glucoamylase, beta-amylase or α -amylase. The utilization of pullulanase is essential for efficient processing of starch in food industries.

The term 'immobilized enzymes' refers to enzymes physically confined or localized in a certain defined region of space with retention of their catalytic activities and which can be used repeatedly and continuously. In addition to a more convenient handling of enzyme preparations, the two main targeted benefits are easy separation of the enzyme from the product, and reuse of the enzyme. Easy separation of the enzyme from the product simplifies enzyme applications and supports a reliable and efficient reaction technology. On the other hand, reuse of enzymes provides cost advantages which are often an essential prerequisite for establishing an enzyme-catalysed process in the first place.

In this work, *globe artichoke* leaf pullulanase was immobilized by adsorption method on polyethylene glycolated (PEG) chitosan beads. PEG 6000 was preferred as a support due to its beneficial advantage of increased water solubility and limited toxicity. The immobilization yield was found to be %80.83. Immobilized pullulanases optimum pH, optimum temperature, K_m and V_{max} values were 8, 45°C, 0.1280 mg/mL and 7.8554U/mL, respectively. After storage at 4°C for 7 weeks, the residual activity of immobilized pullulanase declined to below 49.13% of initial activity. Immobilized enzyme showed 38.43% activity after 15 times re-use.

PP-13

A Systems-Based Metabolic Modeling Approach of Microbial Levan Production

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Levan is a bioactive fructan type polymer that is mainly associated with high-value applications. In commercialization of microbial biopolymers, economic hurdles need to be overcome, especially for very expensive biopolymers like levan. *Halomonas smyrnensis* AAD^T is a halophilic bacterium that can efficiently produce levan from sucrose via levan-sucrase activity. A systems-based metabolic modeling approach constitutes an important step towards understanding the interplay between metabolism and levan biosynthesis in *H. smyrnensis* AAD6^T and further enhances its metabolic performance for industrial application. As a significant step towards this goal, the first comprehensive genome-scale metabolic network of *Chromohalobacter salexigens* DSM3043, which is considered as model organism for halophilic bacteria, has been reconstructed based on its genome annotation, physiological and biochemical information. Subsequently, this network was recruited, and refined via integration of the available biochemical, physiological and phenotypic features of *H. smyrnensis* AAD6^T. The generic metabolic model was then systematically analyzed in silico using constraints-based simulations. To elucidate the relationship between levan biosynthesis and other metabolic processes, an enzyme-graph representation of the metabolic network and a graph decomposition technique were employed. Using the concept of control effective fluxes, significant links between several metabolic processes and levan biosynthesis were estimated. The major finding was the elucidation of the stimulatory effect of mannitol on levan biosynthesis, which was further verified experimentally. The optimal concentration of 30 g/L mannitol supplemented to the 50 g/L sucrose-based medium resulted in 2-fold increase in levan production in parallel to increased sucrose hydrolysis rate, accumulated extracellular glucose, and decreased fructose uptake rate.

PP-14

Theoretical Investigations of Acetone - Diethyl Amine Binary Azeotrope Complex by DFT Method**Ibrahim Aydin , Ibrahim Narin**

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Diethyl amine and acetone make an azeotrope with the mole ratio of 4:3, respectively. Pure diethyl amine boils at 51°C, and pure acetone boils at 51°C while azeotrope boils at 47°C (at 733 mmHg) [1,2]. As the result of this azeotrope formation, some characteristic vibrational modes in FT-IR changes. The amount of these changes is an indication of the extend of interaction between two components and their orientation in unit structure of the cluster. This means there are weaker attraction forces between two molecules due to the azeotrope formation. In this study, we carried out experimental and theoretical study on structure of diethyl amine : acetone binary complex structure. ^1H and ^{13}C chemical shifts were calculated with Gauge Independent Atomic Orbitals (GIAO)[3] approach the DFT method and compared with tetramethylsilane (TMS) as the reference for chemical shielding. The harmonic vibrational frequencies and NMR calculations were calculated by Gaussian 09 program package[4]. The theoretical FT-IR and NMR spectra of the title molecule have been constructed.

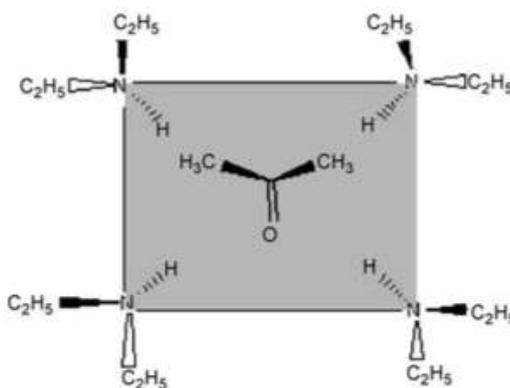


Figure: Proposed structure for unit-structure of azeotrope–diethyl amine acetone in one plain of structure[1]

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PP-15

Quantum chemical and vibrational spectroscopic study, conformational and HOMO–LUMO analysis of a flavonoid, Rutin, by DFT method

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Rutin (Vitamin P) is one of the phenolic compounds found in the invasive plant species and contributes to the antibacterial and antioxidant properties of plant [1]. Rutin is a flavonoid glycoside found in many plants [2]. Theoretical investigations of physical and chemical properties of flavonoids are important in order to disclose the relationship between the structure, properties and performance, and to help in the design and synthesis of new derivatives with improved properties [3].

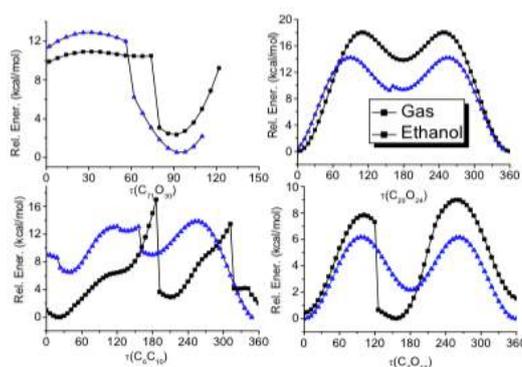


Figure: Potential energy surfaces of Rutin

The conformational analysis of the structure has been performed to find the most stable conformers in gas and ethanol phases. The vibrational band assignments of the most stable conformers in both phases have been made based on normal co-ordinate analysis. Natural Bond Orbital (NBO) analysis was performed to determine possible hydrogen bonds. The methods of DFT were employed by using Gaussian 09 programme [4]. The vibrational analysis was performed through VEDA4 programme [5] to elucidate the experimental vibrational frequencies.

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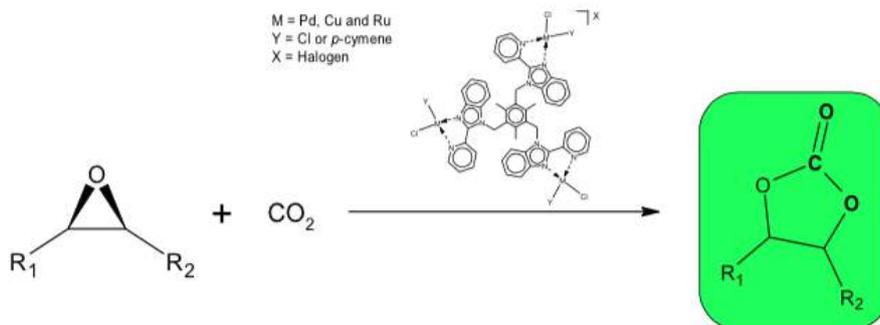
PP-16

Conversion of Carbon dioxide into Organic products in the presence of tri NN type as Catalysts

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Carbon dioxide is one of the green house gases, which lead to the global warming. Carbon dioxide is an attractive C1 building block in organic synthesis as it is highly functional, abundant, inexpensive, nontoxic, and nonflammable.[1] On the other hand, the conversion of carbon dioxide to the corresponding useful chemicals require high reaction temperature and pressure since it is thermodynamically and kinetically stable molecule. These restrictions can be overcome by means of catalyst application. Cyclic carbonates are used as polar aprotic solvents in cleaning, cosmetics and personal care products, as electrolytes in lithium secondary batteries, as precursors for the formation of polycarbonates, and as intermediates in the production of pharmaceuticals and fine chemicals. The conversion of CO₂ such this type of products using catalysts were investigated by us in previous study.[2]



In this study, novel tri-NN type ligand systems were synthesized by using 2-(2-pyridyl)benzimidazole. The metal complexes were easily obtained with the reaction of this ligand and related metal (palladium, copper and ruthenium) salts. The structures of these compounds were characterized by ¹H and ¹³C-NMR spectroscopy, FT-IR, elemental analysis and melting point measurement methods. The conversion of carbon dioxide (CO₂) into cyclic carbonates in the presence of synthesized metal complexes were used as catalysts.

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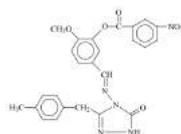
PP-17

Spectroscopic properties of 3-benzyl-4-[3-(3-nitrobenzoxy)-4-methoxybenzylideneamino]-4,5-dihydro-1H-1,2,4-triazol-5-one molecule

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3-Benzyl-4-[3-(3-nitrobenzoxy)-4-methoxybenzylideneamino]-4,5-dihydro-1H-1,2,4-triazol-5-one were synthesized by the reaction of 3-benzyl-4-amino-4,5-dihydro-1H-1,2,4-triazol-5-one with 3-nitrobenzoxy-4-methoxybenzaldehyde [1]. The molecule has been optimized using B3LYP/631G (d,p) and HF/631G (d,p) basis set [2]. Starting from this optimized structure with ¹H-NMR and ¹³C-NMR and IR spectral data values according to GIAO [3] method was calculated using the method of Gaussian G09W program package in gas phase. Theoretically and experimentally values were plotted according to $\delta_{\text{calc}} = a + b \delta_{\text{exp}}$ Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program.



Theoretically calculated IR data are multiplied with appropriate adjustment factors and the data obtained according to HF and DFT method are formed using theoretical infrared spectrum. The identification of calculated IR data was used in veda4f program [4]. Experimentally and theoretically UV-vis values in ethanol were calculated and compared. Additionally, the HOMO-LUMO energy of the molecule obtained from both methods was described.

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PP-18

Influence of the use of sea sand on steel corrosion behaviour in concrete

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Corrosion of steel reinforcement is the most important cause of concrete structures damage. This phenomenon is most frequently induced by chloride ions penetration, leading to localised corrosion activity. Chloride ions are commonly found in construction materials and may originate from contamination of the water used in concrete production, from contaminated aggregates, or even from the external environment, as in the case of marine environments or de-icing salts.

In construction, the sea sand is often used for concrete production, while this aggregate may contains a significant content of chloride ions adsorbed on the surface of its grain, which causes an increase in their concentration in concrete. To highlight the effect of the use of sea sand on the corrosion behavior of reinforcement steel and consequently the durability of concrete structures, electrochemical tests were performed in solutions obtained after leaching the sand with tap water and with saturated $\text{Ca}(\text{OH})_2$ solution. This latter is an alkaline solution which simulates the concrete pore solution.

Initial results indicate that solutions obtained after leaching the sea sand, either with tap water or saturated $\text{Ca}(\text{OH})_2$ saturation, exhibit a significant corrosivity. However, the solution obtained after leaching with tap water is more aggressive due to its low pH value.

The aggressiveness of these two solutions shows the contribution of sea sand in increasing of chloride ions concentration in concrete and therefore in the development of reinforcement steel corrosion. Thus, the use of unwashed sea sand for concrete production is strongly discouraged.

PP-19

Release Studies of Rifampicin from Extremely Halophilic Archaeon Haloarcula 2TK2**C. Bakir¹, A. Attar², A. Ogan¹, S. Demir¹, S. Ugurlu¹, Emrah Cakmakci¹, O. Danis¹, M. Birbir¹**

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Archaeosomes are a novel kind of liposomes made up of archaeal polar lipids. In the present study we prepared a special lipid-based oral delivery system: large unilaminar vesicles (LUV's) obtained by the polar lipid fraction extracted from Haloarcula 2TK2 strain and examined its potential as an oral delivery vehicle for controlled release of rifampicin (RIF) as a model drug. Thermal analysis of polar lipids were performed by using differential scanning calorimetry (DSC). The images of the archaeosomes were taken by environmental scanning electron microscope. Zeta potentials were measured by photon correlation spectroscopy (PCS). Thermal analysis of polar lipids revealed no well-defined phase transition in the temperature range of 20 to 120°C. The surface of the drug loaded archaeosomes was negatively charged and zeta potential of RIF loaded archaeosomes was found to be -41 mV. The maximum loading of RIF was determined to be 21.50% and the maximum encapsulation and cumulative release of the drug was found as 80.0% and 52.44% respectively. RIF could be successfully entrapped in archaeosomes with reasonable drug-loading and desired vesicle specific characters. It was concluded that archaeosomes prepared from extremely halophilic archaeon were compatible for the development of stable and sustained release of RIF.

PP-20

Antioxidant / prooxidant effects of hydrophilic and lipophilic antioxidants on lipid peroxidation

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Lipid peroxidation in foods causes rancidity and nutritional deterioration, which can be delayed or inhibited by antioxidant compounds. Lipid oxidation measurement methods are usually concerned with absorption of oxygen, loss of initial substrates, generation of free radicals, and formation of primary and secondary oxidation products. If oxygen is passed through a linoleic acid (LA) emulsion by adding copper (II) salts, primary oxidation products (i.e. hydroperoxides) and secondary products (i.e. aldehydes or ketones) are formed [1-4]. The peroxidation of linoleic acid (LA) in the presence of either Cu(II) ions alone or Cu(II) ions combined with Trolox (TR), ascorbic acid (AA) and hydroquinone (HQ) as hydrophilic antioxidants, or with α -tocopherol (TocH), ascorbyl palmitate (AP) and tert-butyl hydroquinone (TBHQ), as their respective lipophilic analogues, was investigated in aerated and incubated emulsions at 37 °C and pH7. LA peroxidation induced by copper (II) was observed to follow pseudo-first-order kinetics with respect to the formation of hydroperoxides and aldehydes, which were monitored by ferric thiocyanate (Fe(III)-SCN) and thiobarbituric acid-reactive substances (TBARS) methods, respectively. With the exception of TocH at certain concentrations, the tested compounds showed antioxidant behaviour depending on their polarities. The results were evaluated in the light of structure?activity relationships and the polar paradox [4].

Acknowledgement

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PP-21

Inhibition Effect of Sulfonamide- Copper(II) Complex Against Carbonic Anhydrase I (hCAI) by Electrochemical Methods

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Heteroaromatic sulfonamides and their derivatives constitute an important group of carbonic anhydrase (CA) inhibitors. The inhibition of CAs enzyme by sulfonamide drugs finds clinical uses in the treatment of glaucoma, epilepsy and other disorders. Metal ions play an important role in biochemical properties of the sulfonamide based drugs and indicate a new applications in chemotherapeutic agents and lowering toxicity. Voltammetry ensures important information on the interactions of the ligands with the metal ions. Many of the most important biological processes are based on redox processes and there are many similarities between electrochemical and biological reactions concerning electron transfer mechanisms [1].

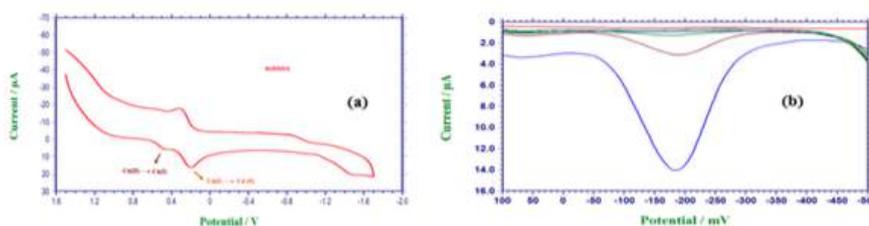


Fig. 1. (a) Cyclic voltammogram of sulfonamide- Cu(II) inhibitor
(b) Differential pulse voltammogram of PNF in the presence of sulfonamide- Cu(II) inhibitor

In this study, Cu(II) complex of heteroaromatic sulfonamide, 2-furaldehitmetilslfonilhidrazon was synthesized and characterized by spectroscopic methods. Electrochemical behavior of Cu(II) complex was investigated by cyclic voltammetry (CV) technique as inhibited in Fig. 1. The reduction peaks of Cu(II) complex were observed at 0.483 V and 0.199 assigned as $\text{Cu}^{II}/\text{Cu}^I$ and Cu^I/Cu^0 reduction process [2]. Also, inhibition effect of different concentrations of sulfonamide-Cu(II) complex (0.1–100 μM) on CAI was studied by differential pulse voltammetry (DPV). The enzyme activity was measured by reduction of the product (PNF) obtained from the enzymatic hydrolysis of PNFA with CAI. The DPV results showed that reduction peak current of PNF decreased with the increasing concentration of inhibitor.

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PP-22

Cooperativity Effect on Topologic Properties of H-bonded Molecular Clusters: $(\text{HNO}_3)(\text{CH}_3\text{OH})_2$ and $(\text{HNO}_3)(\text{H}_2\text{O})_2$ Ternary Systems**Hasan Ozsoy¹, F. Mine Balci², Nevin Uras-Aytemiz³**
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The aim of this study is to investigate the interaction of the hydrogen-bonded $\text{HNO}_3(\text{CH}_3\text{OH})_2$ and $(\text{HNO}_3)(\text{H}_2\text{O})_2$ ternary systems by using ab initio calculations. All calculations were performed by Gaussian 09 package program(1). The electron densities of the bond critical points for the clusters have been investigated by AIMALL package program(2). The results are discussed in terms of structure, energetic, topologic and spectroscopic perspectives.

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PP-23

Investigation of MOF/Polyimide Interactions in Mixed Matrix Membranes for CO₂ Separation

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The separation of CO₂ from industrially important gas mixtures like natural gas, syngas and flue gas is an enormously crucial issue in chemical industry. The new promising class of material is mixed-matrix membranes (MMMs) where polymer matrices are modified with metal organic frameworks (MOFs). The principle issue in these applications is the plasticization of the polymers at high partial pressures of CO₂, which leads to reduced membrane selectivity and unexpected transport properties at the polymer/MOF interfaces. In our molecular simulation study, we focused on the interfacial interactions of ZIF-8/Matrimid 5218MMM for CO₂/CH₄ separation. Polyimide was constructed using Accelrys Materials Studio 5.0 software and equilibrated by a series of Molecular Dynamics (MD) run using LAMMPS package. Polymer Consistent Force Field (PCFF) was used for simulations and density, Fractional Free Volume (FFV) and Glass Transition Temperature (T_g) of the polymers were compared with experimental values and the force-field was validated considering the agreement within these values. Monte Carlo (MC) and MD simulations were applied for estimating CO₂ and CH₄ sorption and diffusion in the polymers to validate the models. We obtained a 15% per weight ZIF-8 content in the mixed matrix. The same equilibration steps were applied to the mixed matrixes, and their sorption and diffusion characteristics were investigated via MC and MD simulations. Gas permeabilities up to 30 bar was estimated in order to investigate the plasticization of MMM's and subsequent changes at the polymer/ZIF-8 interfaces. Simulation results indicated that the interactions between the functional groups of the polymer and dangling ligands at the MOF surface may have significant contribution on the gas transport through the interface.

Acknowledgment

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PP-24

Determination of the Effect of Different Electrode Materials in Electrochemical Dye Removal Processes from Wastewater

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Dissolved or colloidal structure of coloured dyes is damaging to the environment. In recent years, colour removal studies have gained importance in order to control pollution and to minimize the damage. Coloured wastewaters are creating esthetical problems as well as damaging the ecological balance. Therefore, effective treatment of these wastewaters is needed to these type wastewaters to reuse.

Electro-coagulation (EC), which is known as a reliable and mainly cost-effective wastewater treatment process, is characterized by simple and easy-to-operate equipment, short operation time, none or negligible amount of chemicals and decreased amount of sludge. The flocs formed by EC are relatively large and contain less bound of water. They are also more stable and therefore amenable to filtration. Electrochemistry of industrial wastewater treatment brings new and interesting approaches. Electrochemical treatment is also needed no chemicals and use chemicals produces by chemical reactions carried out by the electrodes.

The aim of this presentation was to study the feasibility of the removal of dyes from aqueous solution by electro-coagulation. The process was examined using different electrode materials.

PP-25

Inhibitive Effect of Sodium Molybdate on the Pitting Corrosion Behaviour of Steel Reinforcements in Simulated Concrete Pore Solution

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Corrosion of reinforcement steel, induced by chlorides ions penetration, is the main cause of concrete structures damage. Because of its serious economic and social consequences, the protection against this phenomenon remains a major economic challenge. Thus, various methods to combat this problem have been proposed, among them the use of corrosion inhibitors has become a more attractive alternative due to its effectiveness, easily to implemented and low cost price.

The aim of this work is to study the inhibitive effect of sodium molybdate against pitting corrosion steel rebar in simulated concrete pore solution. The use of this mineral compound is justified by its non-toxicity.

The obtained results indicated that the addition of molybdate ions to the chlorinated solution decreases significantly the corrosion rate of steel by formation, on the steel surface, of passive film rich with phosphate which acts as physical barrier against chlorides ions. The optimal inhibition rate is given by phosphate ions concentration corresponding to $[\text{PO}_4^{3-}]/[\text{Cl}^-]$ equal to 0.5.

PP-26

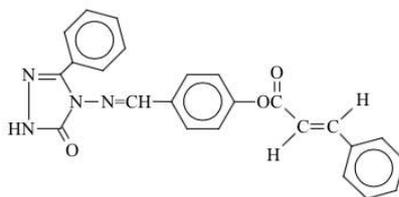
Synthesis and Gaussian calculations of 3-phenyl-4-(4-sinamoyloxybenzylideneamino)-4,5-dihydro-1h-1,2,4-triazol-5-one Molecule

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In this study, 3-phenyl-4-(4-cinnamoyloxybenzylideneamino)-4,5-dihydro-1H-1,2,4-triazol-5-one were synthesized by the reaction of 3-phenyl-4-amino-4,5-dihydro-1H-1,2,4-triazol-5-one with 4-sinamoyloxybenzaldehyde [1].

The molecule was optimized by using the B3LYP/631G (d) and HF/631G (d) basis sets [2,3]. Afterwards, $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W [2]. Experimental and theoretical values were inserted into the graphic according to equation of $\delta_{\text{exp}}=a+b \cdot \delta_{\text{calc}}$. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. Furthermore, molecule's theoretical bond lengths, bond angles, UV-Vis values, dipole moments, formal charges, HOMO-LUMO energies, total energy of the molecule, ionization potential, electron affinity and electronegativity for both methods were calculated.

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PP-27

Perylene Monolayer Protected Gold Nanorods

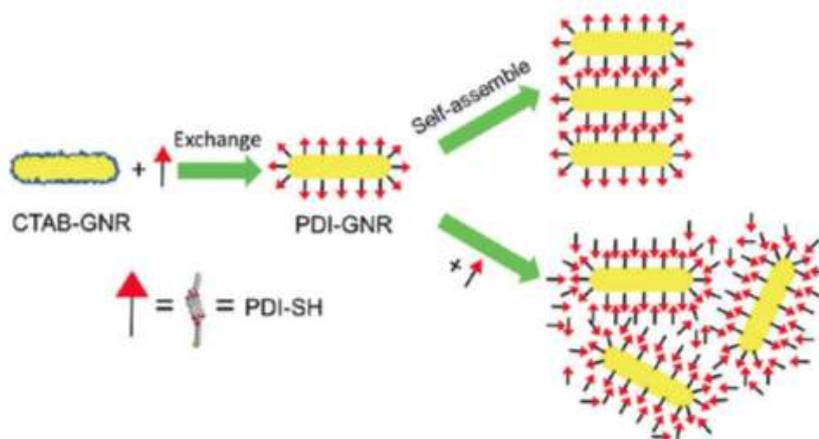
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We have synthesized organosoluble perylene monolayer protected gold nanorods and characterized with ¹HNMR, FT-IR, and differential scanning calorimetry experiments. The resulting gold nanorods encapsulated with perylene thiol molecules via strong covalent Au-S linkages showed unique optical and electronic properties compared to the initial free perylene molecules and gold nanorods. When attached on gold nanorods, the perylene chromophores did not exhibit any typical UV-vis absorption or fluorescence emission signal, originating from the charge transfer from gold nanorods to perylene chromophores. However, the missing signals reappeared upon the addition of iodine, which detached the perylene molecules from gold nanorods. The perylene thiol monolayer protected gold nanorods were able to aggregate. When drying from highly diluted solution, gold nanorods formed well-organized side by-side self-assembly arrays.



PP-28

The Effect of Different Anions Using Electrocoagulation Technique in Waste Water Treatment

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Waste water treatment is becoming significant importance day by day in terms of protecting natural environment. Especially, heavy metal pollution is one of the most serious environmental problem. Therefore, nowadays a lot of different waste water treatment technique can be used to remove of heavy metals from the waste water.

In present study, we examined to recovery of some heavy metals from synthetic waste water using electrocoagulation technique with aluminum electrodes. The effect of different anions to the recovery of metals were examined during the experiments. With this aim; different anions of Co, Ni and Cu metals' solutions were used in electrocoagulation cell.

PP-29

Investigation of Potential Genotoxic Activity of Asin Gulf in the Aegean Region

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This research examined the genotoxic activities associated with Asin Gulf in the Aegean Region. The potential genotoxicity was detected in the surface and deep water of determined gulf stations. The SOS Chromotest based on *Escherichia coli* PQ37 bacteria activities was used for the assessment of genotoxicity of the gulf. This assay utilized β -galactosidase activity, alkaline phosphatase activity, and four different solvent controls to generate reliable results when corrected induction factors (CIF) were used as quantitative measurements for the genotoxic activity of the gulf. The CIF values were obtained from a total of 12 different dilutions for potential genotoxic activities. The results of this study clearly indicates that the surface water and the deep water samples of the gulf have no hazardous impact in terms of potential genotoxicity on the off-shore fishery in the Asin Gulf.

PP-30

Syntheses and Structure of Acetylurea Complexes with Lanthanide Halides

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Lanthanide compounds attract attention of many researchers because of their variable applications [1,2]. Syntheses and structures of rare-earth complexes with the simplest ureide (acetylurea) are of interest, since the obtained data should help to predict structures and properties of complexes with more complicated ureides. Acetylurea $\text{CH}_3\text{CONHCONH}_2$ (AcUr) contains two carbonyl groups, one amide group, and one imide group, therefore, it can serve as a polydentate ligand.

In this work we present syntheses, IR spectroscopy, thermal and X-ray diffraction analyses of AcUr and its new complexes with lanthanide halides.

The AcUr complexes were synthesized by mixing lanthanide halides with AcUr in various molar ratios in water-ethanol medium. According to the results of chemical analyses, the complexes have the $\text{LaBr}_3 \cdot 2\text{AcUr} \cdot 5\text{H}_2\text{O}$ (I), $\text{PrBr}_3 \cdot 2\text{AcUr} \cdot 5\text{H}_2\text{O}$ (II), $\text{NdCl}_3 \cdot 2\text{AcUr} \cdot 5\text{H}_2\text{O}$ (III) and $\text{SmCl}_3 \cdot 2\text{AcUr} \cdot 5\text{H}_2\text{O}$ (IV) compositions. The shifts of the absorption bands in IR spectra of I–IV as compared to the spectra of free AcUr indicates that AcUr coordinates the rare-earth atoms through the oxygen atoms.

X-ray diffraction analysis shows that AcUr has a layered structure. In a crystalline state, the oxygen atoms of the AcUr molecules lie on the opposite sides of the line connecting two carbon atoms of the carbonyl groups. Structures I–IV are built of the $[\text{Ln}(\text{AcUr})_2(\text{H}_2\text{O})_5]^{3+}$ complex cations (coordination number 9) and uncoordinated halide ions. The coordination polyhedra are one-capped tetragonal antiprisms for compounds I and IV and three-capped trigonal prisms for II and III. The AcUr molecules are bidentate. On coordination, the acetylurea changes its conformation due to rotation around the C–N single bond. The angles between two OCN planes in the coordinated AcUr molecules are different, which can be due to electronic structures of the central atoms and sterical parameters of the complexes. The coordinated AcUr molecules are joined to the halide ions and water molecules of the adjacent complex cations by hydrogen bonds.

Thermal analysis shows that decomposition of complexes I–IV begins at 80– 82°C and proceeds in several steps.

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PP-31**Molecular Analyses of Lipid Transfer Gene Selected from Olive (*Olea europaea*) ESTs (Expressed Sequence Tags) Collection**

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According to the classification systems; the olive is a species in the Oleaceae family comprises 600 species in 24 genus. Previously, in our department two cDNA libraries were constructed from young olive leaves and fruits for generation of ESTs (Expressed Sequence Tags) which are useful for the discovery of novel genes and searching for the function of unknown genes and for the search the function of unknown genes. 3840 colonies which were randomly selected from the libraries were sequenced for obtained olive ESTs collection. The sequences were assembled in to contig with the Phred / Phrap, CAP3 programs and the putative functions of the genes were designated by gene homology based on BLAST and annotated using BLAST2GO program and BLAST analysis.

For this study, the presence of genes related to stress in EST collection, which prepared for the fruit and the olive leaves, were investigated. A major stress genes, lipid-transfer gene's sequence informations were found in EST's and contigs. This important stress gene, lipid transfer gene, was intended to clone. The purpose of gene cloning, full-length lipid-transfer gene was tried to obtain by using RACE (Rapid Amplification of cDNA Ends), is a method of molecular-based PCR (Polymerase Chain Reaction), by using specific primers to the 3' and 5' ends which was obtained from the sequence information of EST and the contig which are related to lipid transfer gene.

PP-32

Polymer-Dispersed Liquid Crystal Doped With Carbon Nanotubes

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Carbon nanotube (CNT) is a multifunctional nanomaterial that possesses excellent electrical, mechanical, thermal, and optical properties. Semiconducting CNTs have been utilized for the fabrication of nanotransistors and gas sensors with high selectivity. In addition; CNT-dispersed nematic liquid crystals (CNT-LCs) have drawn significant attention because of various interesting physical behaviors. As CNT particles are dispersed throughout an LC matrix, an aligned ensemble of LC and CNT molecules can be obtained because an LC orientational order can be imposed on CNTs. Moreover, CNT particles form conductive networks in CNT-LC materials, and the conductivity of a CNT-LC composite can be varied by changing the orientation of CNT-LCs. Therefore, it is possible to detect the concentrations of chemical and biological agents that change the orientation of LCs by measuring the conductivity of a CNT-LC material along a certain direction [1-2].

Recently, an approach based on polymer-dispersed liquid crystals (PDLCs) has been proposed to avoid the flow of LCs, to enhance the mechanical stability, and to simplify the fabrication process. PDLCs are composite materials in which LC molecules are generally trapped in a transparent polymer medium, forming micrometer scale LC droplets.

In this work, a new material design that uses a hybrid material of PDLCs and CNTs (CNT-PDLC) for detecting gas such as acetone, chloroform and dichloromethane was proposed.

CNT-PDLC film was made from a mixture of 20 wt% LC, 77.5 wt% poly (methyl methacrylate) (PMMA) and 2.5 wt% CNT materials and characterized by differential scanning calorimetry (DSC) and polarized optical microscopy (POM).

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PP-33

Investigation of thermodynamic and surface characterisation of 4-[4-(2-methylbutoxy)benzoyloxy]benzoic acid thermotropic liquid crystal by inverse gas chromatography

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The inverse gas chromatography (IGC) technique is widely applied to study of surface energies and the physicochemical properties of individual substances and mixtures by the analysis of quantities characterizing the chromatographic retention behaviour of known volatile liquids and gases [1].

In this study, IGC method was used to obtain surface properties of the thermotropic liquid crystalline (LC) material, 4-[4-(2-methylbutoxy)benzoyloxy]benzoic acid (MBBB). The retentions of several organic solvents on the LC derived from benzoic acid were measured in the temperature range from 308,2 K to 333,2 K by IGC. The dispersive component of the surface free energy, γ_s^D of studied adsorbent surface was estimated using retention times of different nonpolar organics in the infinite dilution region. Thermodynamic parameters of adsorption (free energy, ΔG_A^S , enthalpy, ΔH_A^S and entropy, ΔS_A^S), dispersive components of the surface energies, γ_A^S and the acid, K_A and base, K_D constants for the MBBB liquid crystal were calculated. The obtained results proved that IGC is an efficient and successful technique for the characterization of adsorption properties and acid-base quantity of these kinds of materials.

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PP-34

Thermodynamic Behavior of the Protonation and Cu(II) Complexation of L-Ornithine and L-Lysine

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Determination of the formation constants and the other thermodynamic quantities of metal complexes of biologically important substances (bioligands) like L-ornithine (Orn; component of urea cycle in terrestrial vertebrates) and L-lysine (Lys; an essential amino acid for humans) would provide useful information about the metabolism of them. In the recent decades, considerable studies have been carried out on the complex formations between transition metal ions and amino acids or drugs [1,2].

In this study, formation constants of the complexes of Cu(II) with Orn and Lys and pK_{as} of them were determined potentiometrically (3) at 5.0, 20.0 and 35.0 °C and $I = 0.10 \text{ mol L}^{-1}$ (NaClO_4). $\Delta_f G^\circ$, $\Delta_f H^\circ$ and $\Delta_f S^\circ$ were determined for protonation and for Cu(II) complexations of these ligands. The results is tried to explain according to hard and soft acids and bases rule[1,2,4-6]. Protonation of all $-\text{NH}_2$ groups are found to be exothermic for H – Orn and H – Lys systems. Driven force is both of $\Delta_f H^\circ$ and $\Delta_f S^\circ$ in these reactions. pK_O (pK_{COOH}) of Orn can not be determined under the experimental condition of this work. pK_O of Lys increase with increasing temperature; driven force is $\Delta_f S^\circ$ alone in this protonation. $\Delta_f H^\circ$ of both 1:1 and 1:2 Cu–Orn complexations are found to be negative. Contribution of $\Delta_f H^\circ$ and $\Delta_f S^\circ$ to $\Delta_f G^\circ$ are expected to be ca. equal 4-6. $\Delta_f H^\circ$ of 1:1 Cu–Lys complexation are found to be positive (driven force is 100% $\Delta_f S^\circ$). Occurring both enthalpic and entropic stabilization together for Cu–Orn, Cu–Orn₂ and furthermore entropic stabilization for Cu–Lys complexations implies that O atom of $-\text{COO}^-$ group is participated more effectively in formation of these complexes [2,5,6]. They may be included Cu–N bond or bonds also, but their strength should be weaker than that of Cu–O bonds.

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PP-35

Analysis of Thermal Properties of PP/PET Blends with Artificial Neural Networks

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Artificial neural networks (ANN) are computer systems that developed to produce new information as the human brain does and to create new information automatically. In recent years, ANN was implemented especially to the difficult and complex areas and generally succesful results were taken. The aim of this study was to related to between artifcial neural networks (ANN) and diferential scanning analysis method (DSC).

In this study Polyethylene terephthalate (PET) were used for the modification of PP that were aimed at improving the mechanical and thermal properties. Thermal properties of the blended PP/PET were changed by the influence of PET .Thermal phase transitions of polymers were analysed by diferential scanning analysis method (DSC) method. Also kinetic parameters of blends were investigated and phase transitions were observed of PP/PET polymers blends (Pure PP, PP+%10PET, PP+%20PET, PP+%30PET, PP+%40PET, PP+%50PET, PP+%60PET).

Then as an alternative method artifical neural network is used to compare experimental results .Additionally a computer model based on, three-layered multilayer perception (MLP) feed-forward neural network architecture is used and trained with the error back propagation algorithm were used for the stimulation and prediction of thermal properties of PP/PET blends. The ANN predicted outputs were compared and verified against the experimental date. The results show that there is good agreement between predicted and the actual values. It also demonstrates that ANN approach can be effective to reduce cost and time of the experimental work.

Acknowledgement

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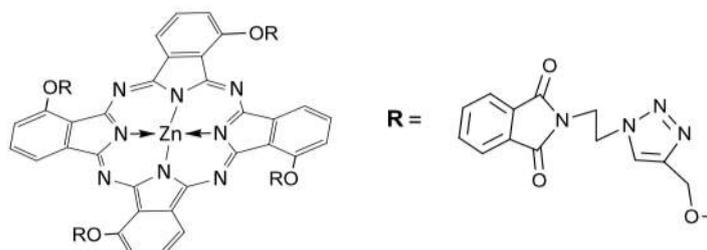
PP-36

Synthesis and Characterization of Nonperipheral Zinc phthalocyanine bearing Phthalimide units via 'click' chemistry**Ahmet Cetinkaya , Bahadır Keskin**

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Phthalocyanines have attracted considerable interest for many decades because of their remarkable thermal stability, chemical resistance, strong colors and negligible vapor pressure at room temperature[1]. This class of compounds exhibits a wide range of qualities in the area of dyes and photoconducting agents in photocopying devices, chemical sensors, electrochromism agents, electrocatalyst, liquid crystals, optical limiting and nonlinear optics [2].



The best known click reaction is the copper-catalyzed Huisgen 1,3-dipolar cycloaddition between azides and terminal alkynes and refers to biological syntheses that assemble small units together with high yields and very simple processes [3]. We described herein, the synthesis and characterization of novel non-peripheral Zn(II) phthalocyanine derivatives which contain tetra-substituted 1,2,3 triazole and phthalimide units on each benzo group. ZnPcs structures were characterized by FT-IR, TLC, UV-Vis, ¹H NMR and MALDI-TOFF spectroscopy techniques .

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PP-37

Synthesis, characterization, spectroscopic properties, molecular structure, and theoretical calculation of 3-chloro-N-(4-sulfamoylphenethyl) propanamide

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The derivatives of sulfonamide are very important because of their varied structures and biological activities [1-3]. Due to the wide variety of the biological and biochemical importance of the sulfonamides, the study of sulfonamides crystal structure and other physical, chemical and biochemical studies has become interesting field in research for a long time [4]. In this study, the derivative of sulfonamide, 3-chloro-N-(4-sulfamoylphenethyl) propanamide, was synthesized (Figure 1). The structures of title compounds were identified by elemental analysis, FT IR, ¹H NMR, ¹³C NMR, Mass Spectra and X-Ray diffraction method. The geometrical parameters, vibrational frequencies, 1H and 13C chemical shifts, and UV-vis absorption spectra of the title compound were also calculated by DFT-B3LYP levels with the 6-311++G(d,p) basis set. In order to compare the theoretical results with the experimental values, R-squared, correlation coefficient, root mean square error (RMSE), maximum difference and standard error are used. The results obtained using the DFT-B3LYP levels with the 6-311++G(d,p) basis set showed an excellent agreement between the experimental and calculated values. Finally, theoretical calculations of title compound contribute to a better understanding of the experimental spectra.

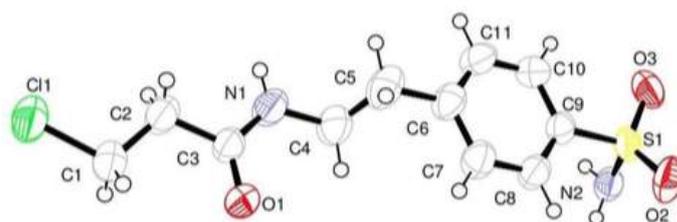


Figure: The molecular structure of the title compound

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PP-38

Assessing the Ligand-protein Binding Modes with Computational Tools

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Designing small molecules with desirable binding affinity and biological activity is one of the major goals in computational biology.[1-4] Molecular docking, is one of the most popular methods used to identify the orientations of molecules into the active site of a target protein structure.[2,3] An important goal of computational medicinal chemistry is to develop methods that accurately can estimate the free energy of binding, ΔG_{bind} , which allows to predict the binding strength of any drug candidate without synthesizing it. Computational methods that combine molecular mechanics energy and implicit solvation models, such as Molecular Mechanics/Poisson–Boltzmann Surface Area (MM/PBSA) and Molecular Mechanics/Generalized Born Surface Area (MM/GBSA), have been widely used in free energy calculations.[1-3] The inhibition of phosphodiesterase (PDE) enzymes, which are responsible for the breakdown of adenosine 3',5'-monophosphate (cAMP) will be investigated.[5] The potentially clinical benefits of PDEIV inhibition require to design novel inhibitors for PDEIV enzyme with less side effects than known potent PDEIV inhibitors. For this purpose, we will consider the results of our previous work where we used pharmacophore modeling and docking process for the PDEIV-B enzyme to propose candidate inhibitors.[6] For PDEIV-ligand complex, the PDEIV selective inhibitor rolipram, whose X-ray structure is co-crystallized with PDEIV (pdb code: 1RO6) will be used. The experimental binding free energies of rolipram ($\Delta G_{exp} = -49.66$ kJ/mol) and 'Syntex 3' (-53.97 kJ/mol) and a few other ligands that are known from the experimental IC_{50} results of Dal Piaz et al.[7] will be tested for PDBIV (1RO6) and its complex. Then, the same procedure will be repeated for the complexes with ligands proposed in our earlier work[7] and the knowledge of calculating binding Gibbs Free energies will be extended to further studies.

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PP-39

STEREODYNAMICS PROPERTIES OF $O^+ + H_2 \rightarrow OH^+ + H$ REACTION

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A great amount of information about reaction mechanisms and stereodynamics properties of reactions is obtained by studying how the reaction cross-section depends on the initial excitation of reactants/products. In order to understand, the stereodynamics these reactions, it is important to study not only general properties, but also the vector properties and initial states. In this work, the effect of projection of rotational quantum number have been investigated and reaction cross section have been calculated for the reaction of $O^+ + H_2 \rightarrow OH^+ + H$ by using a wavepacket method. The H_2 reagent is initially considered in the ro-vibrational states of $v=0, j=2$. The integral cross section decrease with increasing collision energy as expected an exothermic barrierless reaction.

Acknowledgements

This work has received financial support from the Scientific and Technological Research Council of TURKEY (TUBITAK) through project no. TBAG-112T827. We also acknowledge CSIC for a travelling grant I-LINK0775.

PP-40

Synthesis and Characterization of Novel Photoinitiators from Alkyl α -Hydroxymethacrylates

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Photopolymerization has been the subject of growing interest in polymer science and technology due to a wide range of application areas in coatings, adhesives, inks, printing plates, dental materials and microelectronics. Photoinitiators, which produce radicals upon absorption of light to initiate polymerization of monomers play an important role in these processes. There are some requirements for photoinitiators; high absorptivity, good solubility, high quantum yield, high reactivity, low odor, low toxicity, no yellowing and good storage stability. Small molecular weight commercial photoinitiators do not exhibit all of these properties. Therefore, in recent years, the development of monomeric and polymeric photoinitiators which do, has become an important issue.

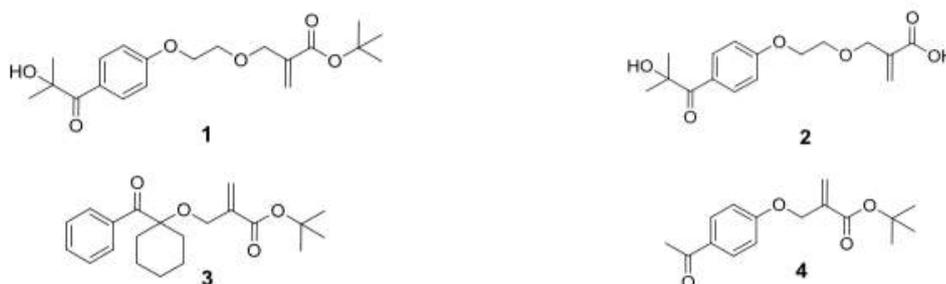


Figure: Structures of synthesized novel photoinitiators.

In this study, four novel methacrylates with one side-chain photoinitiating moiety have been synthesized and their photoinitiating abilities were investigated. Synthesis of photoinitiators involved reactions of tert-butyl α -bromomethacrylate with Irgacure 2959, Irgacure 184 and 4-hydroxyacetophenone to give monomers 1, 3 and 4 respectively; and cleavage of tert-butyl ester groups of monomer 1 with trifluoroacetic acid for conversion to monomer 2. In order to evaluate their photoinitiating activities and compare with the commercial ones, photopolymerization using photo-DSC and UV absorbance studies were done. Also the electronic absorption spectra for the compounds were calculated with the TD-DFT at B3LYP/6-31+G(d) level using Gaussian09 program.

PP-41

Enantioselective Hydrolysis of Dihydrobenzofuranone Derivatives with Chemoenzymatic Reactions

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Dihydrofuranone and benzofuranone compounds are presences extensively in natural products. Benzofuranone derivatives exposes important biological activities such as antiulcer, antioxidant, antidepressant, antibacterial, antifungal, antiinflammatori, antibiotic, anticancer, antinociceptive, antimalarial, anti-HIV 1, antileichmanial, anticholinesterase, preferential cytotoxic activity, anti-angiogenesis agent and in addition to being radiotracer as a probe for PET/SPECT to detect of β -amyloid (Ab) plaques in the brain of patients with Alzheimer's disease (AD).The furan skeletons are privileged scaffolds in medicinal chemistry, and they have been widely found in natural products and therapeutic agents. Chiral synthesis and enantiomerically pure products of precursor and intermediate drugs such as α -hydroxy ketones and benzofuran derivates represents promising important positive effects on human health in drug industry.

Chiral α -hydroxy ketones are also important structural units in many biologically active natural products. Chiral α -hydroxy ketones are important biological compounds since they have important activities such as antibiotic, antibacterial, antifungal, antinociceptive, antidepressant, antiviral and therapeutic effects on many diseases such as infection, allergy, tumefaction, rheumatoid arthritis and cancer.

In this study, robust synthesised drug precursor compounds planned to obtain in high enantiomeric purity, yield and selectivity with biotechnological and chemical methods by using lipase enzymes. For this purpose, first we synthesised 6,7-dihidro-6-metilbenzofuran-4(5H)-one derivate, then acylated 6,7-dihidro-6-metilbenzofuran-4(5H)-one into 4,5,6,7-tetrahydro-6-methyl-4-oxobenzofuran-5-yl acetate by manganese (III) acetate-mediated acetoxylation, and followed by the lipase enzyme-mediated kinetic resolution of α -acetoxy enone provides acetoxy and hydroxy derivatives in good yields and high enantiomeric excesses.

PP-42

Detection of Nitroaromatic Explosives Based on Fluorescence Quenching of Silafluorene Containing Polymers: A TD-DFT Study

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The detection of the explosive materials continues to attract attention. Detection based on fluorescence quenching of conjugated photoluminescent polymers is a promising technology to be developed.[1] The use of conjugated photoluminescent polymers allows the detection of explosives by means of signal gain or loss in response to interactions with analytes. Silafluorenes are silicon-containing π -conjugated systems to be used as chemical sensors for explosive detection because of their improved optoelectronic properties. They are highly sensitive to explosives containing nitroaromatics. It has been proposed that Lewis acid-base interactions between the nitro groups of these explosives and the silicon center helps explosive binding in these polymers.[2] We have shown that two types of interactions, π - π stacking and Lewis acid-base, promote the binding of analytes to polymers.[3] The fluorescence quenching mechanism to detect various explosives containing nitro groups with the use of silafluorene-containing oligomers is analysed using TD-DFT techniques.[4]

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PP-43

A Computational Approach to Effect of Pi-Pi Interaction on The tacticity of Bulky Methacrylate Polymers

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Inherent tacticity in bulky methacrylates are investigated by quantum chemical calculations to understand contribution of pi-pi interaction on polymer tacticity. Controlling tacticity is desired due to it has effect on physical properties of polymer products such as melting point, solubility, density, crystallinity and mechanical strength. Geometries and conformer distributions of monomers and oligomeric propagating radicals are calculated to study the impact of pi-stacking interactions on the preferences for meso versus isotactic propagation. Correlating with the previous experimental studies by Satoh and Kamigaito (1), we have demonstrated that, whilst pi-stacking interactions in aryl methacrylates are significant, the extent to which they influence the tacticity depends on their bulkiness and associated helical tendency. We have also provided an explanation for their solvent dependence in terms of the disruption of pi-stacking conformations by the formation of inclusion complexes.

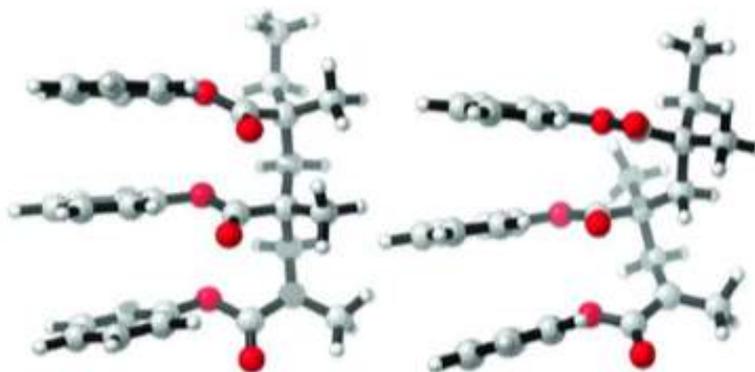


Figure: Trimeric growing chains of PhMA

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PP-44

**The crystal and molecular structure of
(E)-2-(((4-iodophenyl)imino)methyl)-4-nitrophenol molecule**

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The crystal structure of (E)-2-(((4-iodophenyl)imino)methyl)-4-nitrophenol ($C_{13}H_9IN_2O_3$), was characterized by IR and XRD technique. The molecule crystallizes in orthorhombic space group $Pna2_1$ and the unit cell parameters of the title compound are $a=12.8153(4)$ Å, $b=24.4520(9)$ Å, $c=4.1464(1)$ Å and $Z=4$. The molecule has halogen atom and the iodine atom links to molecule at meta position. The molecule has intramolecular O–H...N hydrogen bond and this hydrogen bond creates S(6) motif at graph set notation. In addition to crystallographic structure of the molecule, the optimized geometry of the molecule has been created density functional theory (DFT/B3LYP) method with LanL2DZ basis set. The obtained values theoretically were compared with the experimental values.

PP-45

Conformational Changes of Bcl-xL upon Deamidation of Asparagine Residues Monitored by MD Simulations

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Bcl-xL is an apoptosis regulating protein belonging to the Bcl-2 family. Opposite to the most of the other Bcl-2 family members, Bcl-xL inhibits apoptosis by blocking the pro-apoptotic activity of BH3-domain-only proteins [1]. Recently, Deverman and co-workers have reported that deamidation at the asparagine residues of Bcl-xL turns the protein inactive and consequently, makes the cell more susceptible to apoptosis [2]. The evidences suggest that deamidations have modulating effects on the activity of Bcl-xL but the mechanism lays behind these effects is still unclear. In this study, we aimed to investigate the conformational changes of Bcl-xL after deamidation of Asp 52 and Asp 66 residues in order to gain more insight on the activity changes of the protein upon deamidation. Bcl-xL is bound to mitochondrial membrane, and therefore, we performed MD simulations inside a lipid bilayer to have a more biologically relevant environment. Simulations were repeated for the N52DN66D deamidated form of the protein and the structural details in the conformational changes with deamidations were monitored. RMSD values for 10 ns simulations of native and deamidated forms of the protein were calculated as 0.43 nm and 0.48 nm, respectively. Thus, this suggests that conformation of the protein is not changing in significant amount towards a probable membrane embedded structure. On the contrary, it preserves the water exposed conformation and tends to interact with water molecules. The snapshots of the simulations also showed that bilayer is not stable and become thinner around the protein. This suggests that protein is highly hydrophilic exposed and tends to interact with water, consequently disrupts bilayer structure. With the light of this observation, future studies will be focused on MD simulations of Bcl-xL bound to the membrane at the C-terminal instead of embedding the whole molecule into the bilayer.

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PP-46

Synthesis and Mesogenic Properties of The Trisiloxane-terminated Salicylaldimine Liquid Crystal

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Salicylaldimines and their derivatives have special interest due to their structure-property relationships. These compounds exhibit mono- or polymorphism depending on the type of terminal groups such as alkyl or alkyloxy chain, perfluorinated chain and oligosiloxane unit [1]. The addition of oligosiloxane units to calamitic mesogen has been shown to promote lamellar organization and smectic phases. The tendency of siloxane and alkyl side chain has been caused segregation of into the sublayers. The polysiloxane unit has been supposed to enhance the thermal stability and has been lower the phase transition temperatures in the mesogenic materials [2]. In this study, new trisiloxane-terminated salicylaldimine mesogen compound was synthesized and its liquid crystal behaviours was studied. Characterization of the trisiloxane-terminated salicylaldimine mesogen **SiLC** which has dodecyloxy alkyl side chain was performed by using spectroscopic methods (UV-Vis, FT-IR, ¹H-NMR, ¹³C-NMR, ²⁹Si-NMR, MS) and elemental analysis. The thermal behaviour of this the trisiloxane-terminated salicylaldimine mesogen **SiLC** was studied by polarizing optical microscopy (POM) and differential scanning calorimetry (DSC). The effect of trisiloxane unit for mesogenic properties was investigated and trisiloxane unit was caused a change in mesogenic properties.

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PP-47**A sensitive molecular imprinted surface plasmon resonance nanosensor for determination of lovastatin in rice**

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Lovastatin (LOV) is a mycotoxin with highly toxic, mutagenic, teratogenic and carcinogenic properties, which has been found as a natural contaminant in commercial red yeast rice. A novel and sensitive molecular imprinted based on surface plasmon resonance (SPR) biosensor was developed for selective determination of LOV in rice. Firstly, the modification of gold surface of SPR chip was performed by allylmercaptane. Then, LOV-imprinted poly(2-hydroxyethyl methacrylate–methacryloylamidoglutamic acid) [p(HEMAGA)] nanofilm was generated on the allylmercaptane modified gold surface. The unmodified and imprinted surfaces were characterized by fourier transform infrared (FTIR) spectroscopy, ellipsometry and contact angle measurements. The developed method was validated according to the ICH guideline. The developed molecular imprinted nanosensor was applied to red yeast rice sample for the determination of CIT. In addition, isotherm models were applied to data to explain adsorption process.

PP-48**Monitoring the Removal Efficiency of the Herbicide Aclonifen by Soil Bacteria**

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In this study, laboratory campaigns were done to determine the removal efficiency of aclonifen (Chekic 600, 2-chloro-6-nitro-3-phenoxyaniline, $C_{12}H_9ClN_2O_3$). This compound is widely used during weed activity in Thrace Region and Anatolia in order to protect grain and cereal cultivation. Bacteria isolated from these lands were used in this study. Monitoring were mostly conducted by chemical oxygen demand (COD) experiments. Additionally, during the outset of the experiments, turbidity and bacteria population determination was conducted. Isolation of bacteria from the soils, where aclonifen was applied, were made through seeding to standard plate count agar. Bacteria acquired from this isolation procedure were identified by 16s RNA gene technique. Herbicide including liquid of 100 ml was prepared and bacteria culture was included in this liquid. This mixture was held in a shaker having standard temperature of 20 °C. This study took 5 days at aerobic condition. Daily culture sample was taken and COD analysis was made within this culture. According to the achieved COD results, highest removal efficiencies and lowest removal efficiencies were occurred by *Bacillus simplex* and *Micrococcus luteus*, respectively. Additionally, above experiments were done by the isolated bacterial culture (*Bacillus simplex*, *Bacillus muralis*, *Micrococcus luteus*, *Micrococcus yuannesis*, *Bacillus megaterium*), in parallel. The amount of pesticide active ingredients removed per unit time were determined from the curve equations of the graphs which were formed by the correlation of COD results and time. Experimental studies were completed by adding the analysis of turbidity and bacteria population for the aim of determining the beginning time of digestion in terms of COD and monitoring of the process.

PP-49

The Synthesis and Electro-optic Investigation of Biphenyl-3,4'-diol Derived Banana-shaped Compound with (S)-3,7-Dimethyloctyloxy Chain

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Banana-shaped liquid crystals are one of the active subfield of research in both mesogenic materials and supramolecular chemistry. Since the discovery of electro- optic switching in the mesophase of this new kind of fascinating materials in the mid- 1990s, interest in such nonconventional mesogens increased remarkably. As a result, a large number of bent-core compounds have been synthesized with various combinations of structural fragments up until now in order to realize relationships between molecular structure and the formation of banana phases [1,2].

Banana-shaped molecules generally consist of five or more aromatic rings, in which rod-like units are attached to the central bent unit such as typically a 1,3- disubstituted benzene ring, a 2,6-disubstituted pyridine ring, a 2,7-disubstituted naphthalene unit or a 1,3-disubstituted biphenyl unit, The type and length of the terminal chain of the bent-core also plays an important role in determining the phase structure. Also, branching of the chains is of great importance to low transition temperatures [3].

In this study, Biphenyl-3,4'-diol derived bent-core compound with (S)-3,7- dimethyloctyloxy chain attached to on one of the wings and n-dodecyloxy chain at the other end have been synthesized and characterized. The structure of the compound was characterized using classical spectroscopic methods (1H-NMR, 13C-NMR and IR). The liquid crystalline properties of the compound with branched chain was investigated by differential scanning calorimetry, optical polarizing microscopy and electro-optic methods. The high effect of alkoxy terminal chain on mesomorphic and electro-optic properties of the new biphenyl based bent-core mesogen is discussed by the comparison of the biphenyl based mesogenic compounds carrying (S)-3,7- dimethyloctyloxy chain at one terminus reported by us previously [4].

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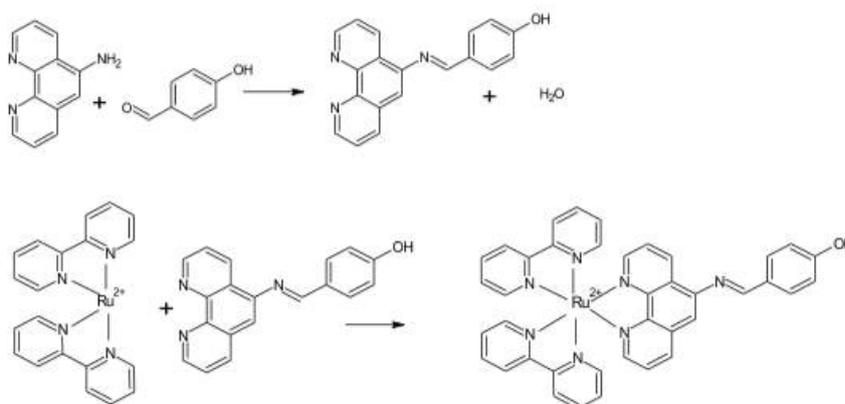
PP-50

Synthesis, Characterization and Fluorescence Properties of a Schiff Base Derivative and its Ru(II) Complex

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Schiff base derivatives and metal complexes are widely applicable in inorganic, biological, analytical chemistry, food industry, dye industry, and catalysis [1,3]. We report to the synthesis and characterization of a new phenanthroline derivative Schiff base and its Ru(II) complex. The structures of the ligand and its complex have been characterized by elemental analysis, FTIR, ^1H NMR, ESI-MS, electronic and fluorescence spectra. Fluorescence studies show that the values of the fluorescent Ru(II) complex increase the more movement of electrons on the structure than the ligand. This new complex can have promising application in new technology such as field of organic light emitting device.

**Acknowledgement**

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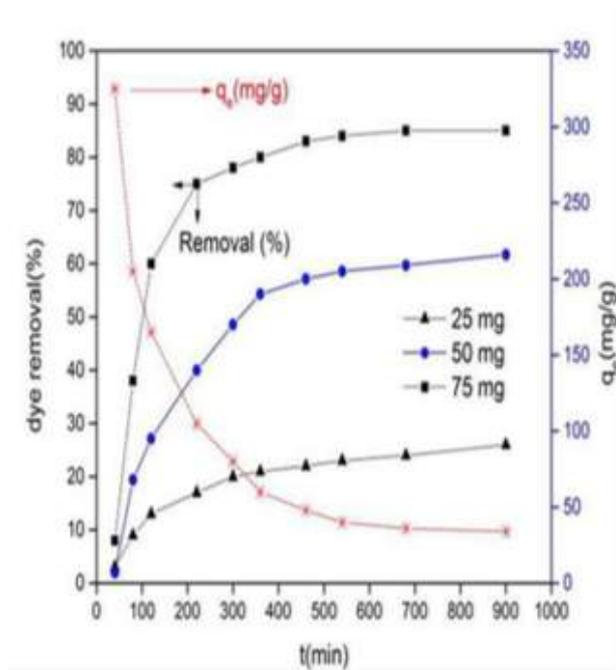
PP-51

Preparation of Chitosan-Starch Hydrogel for Efficient Removal of Multi-Azo Dye from Aqueous Solution

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Chitosan-starch hydrogel (CSH) was prepared in the presence of glutaraldehyde and employed to adsorb direct red 80 (DR80) dye from aqueous solution. The effects of various operation parameters examined, CSH adsorption capacity (309.15 mg/g) was determined, and the experimental results were fitted to different mechanistic equations. The mean adsorption energy ($E = 13.3\text{--}14.9 \text{ kJmol}^{-1}$) demonstrated that DR80 adsorption is mainly chemisorption in nature. The isotherm results were finally analysed using different error functions. The temperature dependence data demonstrated that the adsorption process was spontaneous and endothermic due to the ΔG° and ΔH° values obtained. Boyd model confirmed that intraparticle diffusion was the limiting step for DR80 uptake.



PP-52

Thermal Kinetic Investigation of PVAc/Calcinated Sepiolite Nanocomposites

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Nanocomposite technology has been portrayed as the next great frontier of materials science, because by using minimal addition levels (<10 wt.%), nanoclays exaggerate mechanical, thermal, dimensional and barrier performance features importantly[1]. The process of the thermal stability examination is searching for an indication of material's ability to keep a particular physical, chemical, mechanical or biological feature above a certain level after confession to high temperatures and/or enlarged periods of time. The knowledge of temperature-dependent behaviour of the properties considered has an great number of applications in the area of e.g. chemicals, energetic materials, biopharmaceutics, vaccines, polymers, etc. Thermogravimetry (TG) may be one of the most popular thermal analysis techniques. And the reaction is performed under a linear temperature program in the most of reported TG studies. [2]. According to the TGA data, the kinetic parameters of thermal decomposition of material such as apparent activation energy (E_a), pre- exponential factor (A), apparent reaction order (n) and rate constant (k) can be calculated using various kinetic models such as Friedman [3][4], Kissinger [5], Coats- Redfern [6][7], Flynn-Wall-Ozawa [8] and Horowitz-Metzger [9] methods. In this work, nanocomposites were synthesized with solution intercalation method. PVAc and sepiolite/calcinated sepiolite were selected as matrix and filling material, respectively. Sepiolite was calcinated at 150, 400, 600 and 900 °C. Detailed kinetic analyses of the nanocomposites have been performed using thermogravimetric analysis (TG), to analyze their thermal behavior at different heating rates in the nitrogen atmosphere. Kinetic parameters of nanocomposites degradation are calculated by Friedman, Ozawa-Wall-Flynn and Coats-Redfern methods.

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PP-53

Synthesis and Characterization of Poly(caprolactone)-g-polystyrene-g-poly(D,L-lactid) graft copolymers using ROP and ATRP

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One-pot synthesis of graft copolymers by ring-opening polymerization and atom transfer polymerization using brominated poly(caprolactone) (PCL-Br), D,L-lactid and styrene is reported. Graft copolymers having structures of poly(caprolactone)-g-polystyrene-g-poly(D,L-lactid) were synthesized from PCL-Br, having bromide group in end chain by the combination of atom transfer radical polymerization of styrene and ring-opening polymerization of D,L-lactid in one-step. Principal parameters, such as monomer concentration, initiator concentration, and polymerization time, which effect the one-pot polymerization reactions were evaluated. The obtained graft copolymers were characterized by ¹H NMR spectroscopy, gel permeation chromatography, thermal gravimetric analysis and differential scanning calorimetry techniques.

No	PCL-Br (g)	LA (g)	Styrene (g)	Yield (g)	Yield %	Graft copolymer (%wt)*		
						PCL	PLA	PSty
PCLSty	0.5	-	1.39	0.39	20.63	9.42	-	90.58
PCLLa-Sty-1	1.0	1.0	1.18	2.14	67.30	27.13	31.54	41.32
PCLLa-Sty-2	1.0	1.0	1.39	2.66	78.47	31.90	16.54	51.85
PCLLa-Sty-3	1.0	1.0	2.08	3.48	85.30	28.85	6.06	65.10
PCLLa-Sty-4	1.0	1.0	2.78	4.32	90.38	20.20	4.84	74.95

* calculated ¹H NMR

Table 1. One-pot synthesis of graft copolymers at 120 °C for 24 h. Effect of styrene amount on copolymerization. Catalyst:(kalay(II)-eti hegzanoat/Monomer:1/100). [M0]:[I0]:[Cu(I)Cl]:[PMDETA]:[88/100/150/200]:[1]:[1]:[3]

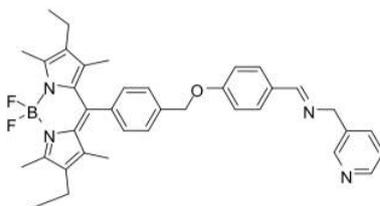
PP-54

The Fluorescent Pb (II) Chemosensor of Based On Bodipy-Pyridine

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The using of fluorescent sensors is an attractive study for the detection of metal ions due to high selectivity and easy applicability in most science areas as medicine. If an appropriate functional group attached to any position of the fluorescent compound, useful fluorescent sensors could be obtained. The photophysical mechanism of sensor operation can show to the different citation of the binding groups for same receptor. The fluorescent compounds with antenna type were developed for the increase of selectivity and the molecules capable of their transferring energy in itself. Bodipy's as a photo-active material have a big potential for laser dyes due to their superior fluorescence property and energy transfer capability. Moreover, Bodipy is the most important of the compound classes which realized energy transfer through-space and through-bond and itself laser behavior. So, a lot of Bodipy derivatives not just substituted owing to its new origin and up-to-date. In this study, a Bodipy derivative was preferred as the fluorescent antenna groups due to their increasing popularity in recent years [1-3].



In this study, a novel molecule based on Bodipy-pyridine was designed. The absorption, emission and excitation properties of the chemosensor were investigated in presence of several metal ions. The results show that the prepared Bodipy-pyridine may use as a selective fluorescent chemosensor for Pb (II) ion. After the complexation with lead ion, the fluorescence intensity of Bodipy-pyridine was significantly quenched and the wavelength slightly shifted to red by increase concentration.

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PP-55

Potential carbon sources for the denitrification of nitrate contaminated groundwater

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Nitrate pollution of ground and surface water resources has become a major problem worldwide. High nitrate levels in drinking water may cause to higher risks of methaemoglobinaemia in infants and cancer (WHO, 1999). A nitrate limit of 50 mg NO₃ L⁻¹ in drinking water supplies was set by of the World Health Organization (WHO) and European Union (Drinking Water Directive 98/83/EC; WHO, 2004). The Nitrate Directive requires the implementation of relevant measures for the reduction of nitrate concentration in groundwater. New treatment strategies have emerged for in-situ nitrate removal from groundwater contaminated by point sources. The groundwater treatment relies on the 'high science low technology' principle, which enables more economical and practical solutions. The removal of nitrate from groundwater by the heterotrophic denitrification process was the major objective of the present study. For this purpose two dominant organic wastes, tea factory waste and hazelnut husk, were used as potential carbon sources to stimulate nitrate removal in low cost permeable reactive barrier (PRB) systems. Leaching and batch experiments were carried out to determine the dissolution level and the degree of denitrification process. The denitrifying bacteria was detected by targeting *nirS* and *nirK* genes in bacteria using quantitative PCR. Both organic substrates enabled the reduction of nitrate (NO₃⁻) to nitrogen (N) gases. However, the percentage of organic substrate was found to have great influence on the nitrate removal efficiency. Evaluation of C/N ratios revealed that both carbon abundant and absent conditions were observed within the study. At carbon abundant conditions, dissimilatory NO₃⁻ reduction to NO₄⁺ (DNRA) may be counterproductive process in this denitrification study.

PP-56

Development of Solid Dosage Formulation that has non-steroidal anti-inflammatory Effect and Evaluation of Quality Parameters**Ozgul Gungor Culcu , Inci Arisan**

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Objectives: The aim of this study is to develop a stable generic tablet formulation of Aceclofenac that has non-steroidal anti-inflammatory effect and evaluate quality parameters and performed analytical test results.

Materials & Methods: Aceclofenac (Suyash Laboratories Limited), Microcrystalline cellulose (JRS Pharma), Croscarmellose sodium (Vivasol) (JRS Pharma), Povidon K-30 (BASF), Glyceryl distearate (Type I) (Gattefosse), Ethanol (JT Baker), Advantia Prime (ISP) has been supplied. CartrexTM 100 mg Film Coated Tablet (Almirall Prodesfarma) has been used as a reference product. Although the composition of the product have been inspired by CartrexTM 100 mg Film Coated Tablet as the reference tablet product, the final composition of the product is decided on the basis of the results obtained from the trial formulations. Based on different characteristics of raw materials, final formulations, it has been decided the trial in accordance with product features. Developed product contains same excipients with reference product. Three different batches of tablets each containing 100 mg of aceclofenac have been formulated and evaluated for optimization of dissolution. The active ingredient of the formulation Aceclofenac which has a tendency to adhesion and formed about 50% of the formulation has been found not appropriate for the direct compression method. For this reason, wet granulation technique has been chosen. As a result of the dissolution and evaluation of pharmacokinetic data, we decided to be used in pH 6.8 Phosphate buffer for dissolution study of Aceclofenac 100 mg Film Coated Tablet. The scale-up batches in decided formulation have been manufactured and followed the stability in 40 °C ± 2 °C / % 75 RH ± % 5 RH for 6 months.

Conclusion: All analytical and stability study results are supported that the quality parameters of developed formulation is significantly similar with the reference product and Aceclofenac 100 mg Tablet is a stable, generic, pharmaceutical product.

PP-57**Determination of Dopamine by Overoxidized Nanofiber Structure Polypyrrole Modified Pencil Graphite Electrode****Hurmus Gursu , Yucel Sahin**

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Dopamine is a kind of the catecholamine neurotransmitter in the central nervous system that plays an important role regulation and control of cognitive enhancement. As a result of neuronal damage low levels of dopamine cause Parkinson's disease, high level of dopamine cause Schizophrenia. Imbalance in dopamine synthesis leads to neurological disorders such as Huntington's disease, HIV infection, sleep, eating disorders and drug addiction as well. Besides these features, drugs containing catecholamines hypertension, bronchial asthma, organic heart disease and heart surgery when considering the use of such drugs in the area, one of the determination of dopamine is an important issue for neuroscience.

Nowadays, chromatographic, electrophoretic, spectroscopic, and hybrid systems are used for the determination of dopamine. These methods are more expensive than electrochemical methods, greater need for consumables and specialized personnel are needed. Dopamine is an electroactive substance that allows determination of more sensitive, faster and cheaper electroanalytical method.

Within the scope of this work, over-oxidized nanofiber polypyrrole film using as a sensor for the determination of dopamine was investigated for the first time in the literature. Existing electrochemical applications increase the costs of measuring by using expensive electrodes such as gold, platinum, diamond, etc.. In this work, carbon-based pencil graphite electrode was modified to dopamine with nanofiber conductive polymer that has a large surface area. Later, disposable sensor was designed by changing the surface charge of the polymer with excessive oxidation process for increasing the selectivity of dopamine.

PP-58

**Nickel(II)-triphenylphosphine complex with
5-Bromo-2-hydroxyacetophenone thiosemicarbazone**

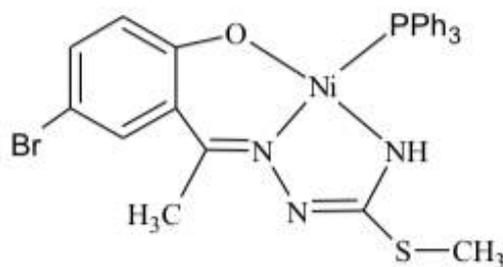
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Thiosemicarbazones have a wide range of biological activities. The presence of nitrogen and sulfur donor atoms in the ligands may be responsible for their potential biological activity. The importance of metal ions in biological systems is well established.[1-3] Nowadays metal based drugs have gained importance and become the burning topics in the experimental oncology.

One of the most interesting features of metal-coordinated systems is the concerted spatial arrangement of the ligands around the metal ion.[4]

The reaction of 5-Bromo-2-hydroxyacetophenone-S-methyl-thiosemicarbazone with $[\text{Ni}(\text{PPh}_3)_2\text{Cl}_2]$ has given solid complex corresponding to the general formula $[\text{Ni}(\text{L})\text{PPh}_3]$. The complex is formed from an *ONN* donor set of the thiosemicarbazone and the P atom of triphenylphosphine in a square planar structure. These mixed- ligand complexes have been characterized by elemental analysis, IR, UV-Vis and ^1H spectroscopies. The structure of $[\text{NiL}(\text{PPh}_3)]$ was determined by single crystal X-ray diffraction.



$[\text{NiL}(\text{PPh}_3)]$

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PP-59

Synthesis, Characterization, Spectroscopic Properties, Theoretical Calculation and Electrochemical Studies of Butanesulfonylhydrazones

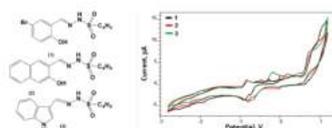
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Hydrazones are important compounds for drug design, as possible ligands for metal complexes, organocatalysis and also for the syntheses of heterocyclic compounds. Many of the physiologically active hydrazones have applications in the treatment of illness like tuberculosis, leprosy and mental damage. For this reason, the electrochemical behaviour of the hydrazones may be very helpful for their efficient uses. The enlightening of the electroreduction mechanism can serve as models for the biological pathway of the hydrazones, because their activities depend on reductive processes in the body [1]. Due to the widespread usage of the hydrazones in drug industry, the redox properties of these compounds are thought to be useful to understand the metabolic fate of the drug containing hydrazones or pharmacological activities [2]. Electrochemical reduction (EC) mechanism contributes to the suggestion of the biochemical behavior of the hydrazones [3].



In this study, three butane sulfonylhydrazone derivatives; 5-bromo salicylaldehydebutanesulfonylhydrazone (1), 2-hydroxy-1-naphthaldehydebutanesulfonylhydrazone (2), indole-3-carboxaldehyde butanesulfonylhydrazone (3) have been synthesized and characterized by using elemental analysis, ¹H-¹³C NMR, IR spectra. Gaussian 09 software was used to obtain the most stable conformation of the compounds based on DFT/B3LYP/6-311G (d,p) method. The electrochemical behaviors of butane sulfonylhydrazones (1-3) were evaluated by cyclic voltammetry (CV) as shown in Figure. Electrochemical reduction mechanism of compound 1-3 was also proposed that butanesulfonylhydrazones follow EC mechanism by semireversible electron transfer steps.

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PP-60

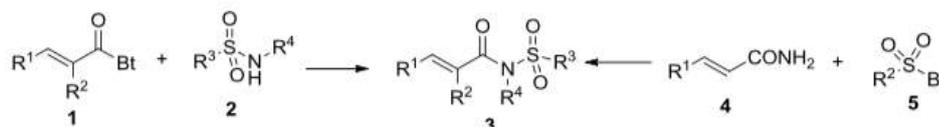
Theoretical Calculations of Some New N-(α , β -Unsaturated acyl)sulfonamides and Investigation On Correlations With Those Experimental Values

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In this study, certain theoretical properties of some N-(α , β -Unsaturated acyl)sulphonamides (3) and reactants; Sulfonamides(2) with N-(α , β -unsaturated acyl) benzotriazoles(1) and α , β -unsaturated carboxamides(4) with sulfonylbenzotriazoles(5) (Table 1), calculated in Gaussian09 program [1] using DFT method at B3LYP/6-311+G(d,p) and B3LYP/6-311++G(d,p) level of theory.

The theoretical data at two different levels was compared with each other then that of certain experimental results [2]



Molecule	IUPAC Name	Substituents		
		R ¹	R ²	R ³
3a	4-Methyl-N-[(E)-3-phenyl-2-propenoyl]benzenesulfonamide	Ph	H	Tol
3b	N-[(E)-3-(2-Furyl)-2-propenoyl]-4-methylbenzenesulfonamide	Furyl	H	Tol
3c	4-Methyl-N-[(E)-3-(2-thienyl)-2-propenoyl]benzenesulfonamide	Thienyl	H	Tol
3d	N-[(E)-3-Phenyl-2-propenoyl]methanesulfonamide	Ph	H	Methyl

Table 1. IUPAC Nomenclature of the Studied Molecules

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PP-61**QSAR's for the Degradation Reactions of Organophosphorous Compounds by DFT**

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Organophosphorous compounds constitute an important class of pesticides. Since they have high volatility, they are of great environmental interest. They cause severe health problems. In recent years, due to their carcinogenicity and mutagenicity, kinetic studies on their removal from air and water have gained a considerable interest [1,2]. These compounds are released into the environment and due to their physicochemical properties; they can disperse in various environmental media, provoking serious health problems. Therefore, there is a need for certain molecular descriptors to predict the reactivity of OPs.

Quantum-chemical descriptors have become quite popular recently and are widely used to the reliability and accuracy, as well as capability to characterize electronic properties of the molecules. In this study, the structures of 21 organophosphorous pesticides were investigated theoretically with the intention of finding certain molecular descriptors to predict the degradation potency for both gas and aqueous phases. Conformational analyses and geometry optimizations of all the structures were performed to determine the most stable structures. Modeling of the molecules was performed with DFT at B3LYP/6-31G* level. The solvation effects were computed using COSMO as the solvation model. The electronic energies, electron densities , molecular charge distributions of the molecules and the DFT reactivity descriptors such as chemical hardness, softness, electronegativity, Fukui functions for all the molecules were calculated.

In this study, quantitative structure activity relationships, (QSAR's) expressing the degradation rate constants in terms of the DFT descriptors were derived by using multiple linear regression for 21 organophosphorous compounds. The correlations between the experimental degradation rates and the calculated descriptors were examined. The properties used were chosen by taking the electrophilic nature of the degradation reactions. As a result, the molecular descriptors that describe the molecular reactivity in oxidative degradation reactions of OPs were determined.

Acknowledgements

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PP-62

Comparison of Exo-biopolymer production by *Pleurotus* spp.

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Basidiomycetes, namely white rot fungi from the genera *Pleurotus* have reached a high commercial importance due to their nutritional or medicinal properties. Recently, many bioactive compounds isolated from basidiomycetes fungi have been reported to possess various bioactivities. Exo- biopolymer (EBP) is one of the most important bioactive compounds isolated from fungal sources and has been found to have some potential pharmaceutical applications, such as antitumor, antioxidant, hypoglycemic, anti-radiation, hypolipidemic and hypoglycemic, and antifatigue activities and other biological activities. EBPs are biomaterials used on a variety of applications in chemistry, food, cosmetic, pharmaceuticals industries, biomedical and medicine and having biofilm formation, emulsion stabilization, gelling agents, foam stabilization and antitumor agents properties, their low toxicity, ecological acceptability. EBPs formed of glucose units which are connected by glycoside bonds can be found in the structure of heteropolysaccharides or homopolysaccharides as straight or branched. In most cases, the molecular weight variations and sugar compositions of EBPs are dependent to culture medium composition and different physical conditions provided during fermentation. This study aims EBP production by three white rot fungi *Pleurotus* spp. (*P. djamor* (Rumph. Ex Fr.) Boedijn (MCC15), *P. sajor caju* (Fr.) Singer (MCC2), and *P. eryngii* (DC.) Gillet (MCC58)) in submerged culture fermentation (SmF). The composition of medium was as follows in (g/L): glucose, 10; NH₄NO₃, 0.724; KH₂PO₄, 1.0; MgSO₄.7H₂O, 1.0; KCl, 0.5; yeast extract, 0.5; FeSO₄.7H₂O, 0.001; ZnSO₄.7H₂O, 0.0028; CaCl₂.2H₂O, 0.033; peptone, 10. The pH of media was adjusted to 6 and the inoculated flasks were incubated on the rotary shaker at 150 rpm and 25°C. The produced EBP was precipitated with cold absolute ethanol. Throughout the EBP production, levels of protein by Bradford method, reducing sugar by DNS method and nitrogen by phenol hypochlorite method of medium and isolated EBP were investigated. Additionally, total carbohydrate (by phenol-sulphuric acid method) of isolated EBP was determined. Our results indicated that the lowest EBP production was deduced with *P. djamor* while the highest EBP production was with *P. eryngii*. The maximum EBP productions by *P. sajor caju* and *P. djamor* were achieved on 5th and 3rd of incubation as 4.24 mg/mL and 3 mg/mL, respectively. The highest EBP production by *P. eryngii* was determined on 6th day of incubation as 8 mg/mL. Total carbohydrate and nitrogen content of EPB were determined as 657.42 µg/mg and 302.4 µg/mg, respectively. Limited C and N levels of medium were arrived after 4th and 10th days of incubation, respectively in *P. eryngii* culture. To sum up, in this study, *P. eringii* rise to prominence for EBP production potential of investigated three *Pleurotus* spp. in SmF. In literature studies, produced EBP by *P. eringii* was found to have high antioxidant and antitumor activity. These properties enable use of the EBP in biomedical, medicine and pharmacology areas.

PP-63

Photocatalytic Reactor Configuration Effect to Humic acid Removal by TiO₂ Nanoparticles

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Natural organic matter (NOM) is a complex and abundant heterogeneous aggregate of organic compounds originated from plant and animal degradation products in the water environment. Due to their undesirable color causing aesthetic problems, forming complexes with metal ions and many organics and interacts with aqueous free chlorine, leading to the formation of disinfection by-products, the removal of humic acids from drinking water supplies has been an important concern. The presence of DBPs in drinking water is a major issue for water utilities and public health authorities. Besides the conventional treatment processes, the application of advanced oxidation techniques is considered as an effective tool for the elimination of humic acids from natural waters. Recently, photocatalytic oxidation using TiO₂ nanoparticles has gained more attention as an advanced water treatment technology. Those reactive species which created from water when UV light is absorbed by the TiO₂ layer are subsequently used to degrade the organic pollutants or microorganisms. Suspension or slurry type reactors have been reported to be efficient due to the large surface area of catalyst available for reaction and the efficient mass transfer within such systems. This study investigated that humic acid degradation in two different type of reactors (Horizontal and Vertical) in which TiO₂ were used in the slurry form. The results were evaluated in terms of the parameters that are specific to organic matter content such as dissolved organic carbon (DOC), UV₂₅₄, VIS₄₀₀ and specific UV absorbance at 254 nm (SUVA) and also formation potential of Trihalomethanes (THMs) with species according to dosages (0.1 g L⁻¹ and 0.5 g L⁻¹) of Degussa P-25 TiO₂. UV₂₅₄ and VIS₄₀₀ were analyzed by using spectrophotometer. DOC measurements were performed by non-purgeable organic carbon by TOC analyzer. Formation potential concentrations of THMs were determined according to EPA method by using Gas Chromatograph with electron capture detector. UV₂₅₄ implies reduction of aromaticity and had high removal for 86% with 0.5 g L⁻¹ in horizontal reactor comparing to vertical reactor (63%) within 1 hour reaction time. Total THMs in the horizontal and vertical reactor were reduced to 80% and 85%, respectively, after photocatalytic oxidation at 0.1 g L⁻¹ TiO₂ dosage.

PP-64**Synthesis and Characterization of Calcined Sepiolite/Poly(methyl methacrylate) Nanocomposites**

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Polymer nanocomposite researches are related to fundamental structure/property relationships, manufacturing techniques, and applications of polymer nanocomposite materials [1]. Poly (methyl methacrylate) is one of the most important polymers, which are used in different industry areas. In this study, poly(methyl methacrylate)(PMMA) nanocomposites containing the calcinated sepiolite samples of different temperature were prepared by melt blending method. The characterization of nanocomposites was made by XRD, AFM, FTIR-ATR, DTA/TG, DSC and optic contact angle instruments. XRD measurements showed that sepiolite samples homogenously dispersed at nanometer scale in PMMA matrix. The thermogravimetric and differential scanning calorimeter analyses showed that the thermal stability and the glass transition temperature (T_g) of PMMA matrix shifted to higher temperature with increasing sepiolite content.

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PP-65**The Effect of Chiral Moiety on Mesophase Behavior of Bent-Core Mesogens Derived from 4-Cyanoresorcinol****Hande Karabuga , Hale Ocak , Belkis Bilgin-Eran**

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Bent-core mesogens have gained particular interest in the field of liquid crystal research due to their ability to form new mesophases with unusual properties. The mesophase behaviour of compounds with bent-core structure is much more strongly influenced from the structural modifications than calamitic liquid crystals [1].

There are several studies on five-ring bent-core mesogens in which the central phenyl ring was substituted at different positions by polar groups. It is well-known that cyano group at 4-position of the bent unit play an important role in the emergence of mesogeneity. Besides, the directions of the ester linking groups between the aromatic rings can lead to quite different mesophases having some unusual properties [1-3].

The effect of a cyano substituent on the mesomorphic behaviour also depends on the type of the terminal groups. For example, chiral moieties in the terminal positions of rod-like wings can yield the polar smectic phases as well as blue phases which are of significant interest for the display applications [3].

In this study, bent-core compounds derived from 4-Cyanoresorcinol unit with two terephthalate based rod-like wings terminated by 3,7-Dimethyloctyloxy chains have been synthesized to investigate the effect of molecular chirality on mesomorphism. The target compounds have been characterized by spectroscopic methods (IR, ¹H-NMR, ¹³C-NMR). Liquid crystalline properties have been investigated by polarization microscopy, differential scanning calorimetry and electro-optical methods.

Acknowledgment

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PP-66**Preparation of Pantoprazole loaded sodium alginate-chitosan beads using Fe₃O₄ nanoparticles for controlled release**

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In recent years, there has been increased interest in the field of controlled release of drugs from polymeric devices has attracted many researchers. These studies have been performed to reduce side effects and the amount of the drug necessary to cause the same therapeutic effect in patients and to increase the pharmacological effect.

The purpose of this study was to prepare pantoprazole covered by alginate and chitosan as microcarriers designed like magnetic core-shell beads. Pantoprazole was used as model drug. Primarily, pantoprazole in various concentrations was prepared and mixed with iron oxide nanoparticles coated by sodium alginate followed by coating with a thin layer of chitosan Shell. The pantoprazole release experiments have been performed in the external magnetic field. The swelling behaviour of the samples were first examined. The equilibrium of the swelling was obtained in 60 mins at 37°C and in 90 min at 25°C. The drug release experiments will be performed in distilled water and phosphate buffer solutions in the asidic (pH 2,4) and basic (pH 7,4) medium at two different temperatures (25°C, 37°C). During the drug releasing experiments UV-Spectrophotometer is used in order to determine the concentrations of the pharmaceutical ingredients in the solutions at 295 nm.

The release profiles were analyzed by a rapid initial release followed by a slower release. The greatest swelling occurred in buffer solution at pH 4.2 and the less swelling occurred at pH 7.4. The hydrogels were not very stable in basic solution.

PP-67

Chemical Composition of *Eremurus spectabilis* Leaves

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Eremurus spectabilis (Serish) belongs to the family of Liliaceae and geographically distributed in the region of South Asia and Central Asia, including Iran, West Pakistan, Afghanistan, Iraq, Turkey, Palestine, Lebanon, Syria and Caucasus.(1) It is distributed in the provinces of Erzurum, Sivas, Yozgat, Bitlis, Kars, Agri, Erzincan, Van, Artvin and Ardahan of Turkey. The leaves of *Eremurus spectabilis* are edible and used in folk medicine to treat some ailments such as hemorrhoids and diabetics and also used as anti dysuria, antihypertensive, eczema, fungal infection, ocular pain and rheumatism.(2)

According to studies of antioxidant and antimicrobial activities, *Eremurus spectabilis* young leaves have beneficial effects on DPPH radical-scavenging ability and may thus protect against oxidative damage.(2) It's roots accumulate high levels of fructans during their growth. Also, it has been applied as glue for industrial application. Fructans are an important product of the industry of prebiotics. In addition to its interesting nutritional and health benefit properties, fructans are also used in food formulations for its techno-functional properties such as fat substitute, bulk agent and water retention.(1)

The aim of this project is to determine the chemical composition of *Eremurus spectabilis* leaves. In our study, 5 compounds were isolated from %90 methanol extract. The structure of compounds 1 and 2 were identified as sucrose and as isoorientin, using 1D and 2D NMR spectroscopic methods and literature data (3-6). Compounds 3, 4 and 5 were under investigation. Compounds 1 and 2 were isolated from the *E. spectabilis* leaves for the first time.

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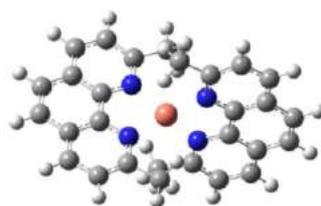
PP-68

Investigation of Reactions of Some Antioxidants Molecules with Radicals using DFT Methods

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Oxidation is a chemical reaction that transfers electrons or hydrogen from a substance to an oxidizing agent, which can produce chain reaction starting free radicals causing damage or death to the cells. Antioxidants terminate these chain reactions by removing free radical intermediates, and inhibit other oxidation reactions. ABTS, DPPH, FRAP and CUPRAC are frequently used by the food industry and agricultural researchers to measure the antioxidant capacities of foods. In this assay ABTS is converted to its radical cation by addition of sodium per sulfate. This radical cation is blue in color and absorbs light at 734 nm [1]. The ABTS radical cation is reactive towards most antioxidants including phenolics, thiols and Vitamin C. DPPH has two major applications, both in laboratory research: one is a monitor of chemical reactions involving radicals, most notably it is a common antioxidant assay [2]. FRAP, is often used to measure the antioxidant capacity of foods, beverages and nutritional supplements containing polyphenols. CUPRAC method should be advantageous over the ferric reducing antioxidant power (FRAP) method because the redox chemistry of copper (II)-as opposed to that of ferric ion- involves faster kinetics. In this study, we used gallic acid, epicatechin, resveratrol, kaemferol, hydroxytyrosol as antioxidant compounds and ABTS, DPPH, CUPRAC, FRAP, linolenic acid as the radical components. Reaction energies of the studied antioxidants with radicals are calculated by the density functional theory (DFT) using B3LYP functional at 6-31g(d) level. By comparing reaction energies suitable radicals for the each antioxidants have been identified.

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PP-69

**Dispersive Surface Energy and Acid-Base Constants of
Thiazolidinone Derivative:
3-(6-Methyl-2-pyridyl)-2-(2-thienyl)-1,3-thiazolidin-4-one**

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Inverse gas chromatography at infinite dilution was used for the first time to determine the adsorption properties and acid-base contributions to the surface energy of thiazolidin-4-ones bearing heteroaryl substituents: 3-(6-Methyl-2-pyridyl)-2-(2-thienyl)-1,3-thiazolidin-4-one (MPTT). The retentions of nonpolar solvents such as n-hexane, n-heptane, n-octane, n-nonane, n-decane and other acidic, basic and amphoteric probes such as tetrahydrofurane, dichloromethane, chloroform, acetone and ethyl acetate used without further purification on MPTT was measured in the temperature ranges from 303 to 333 K by inverse gas chromatography (IGC). The dispersive component of the surface energy, γ_s^D of studied adsorbent surface was estimated using retention times of different nonpolar organics in the infinite dilution region. Thermodynamic parameters of adsorption (free energy, ΔG_A^S , enthalpy, ΔH_A^S and entropy, ΔS_A^S), dispersive components of the surface energies, γ_s^D Fowkes and Dorris-Gray approaches and the acid, K_A and base, K_D constants for the 3-(6-Methyl-2-pyridyl)-2-(2-thienyl)-1,3-thiazolidin-4-one was calculated.

PP-70

The Effect of Different Terminal Chains on the Mesomorphism of Chiral Rod-Shaped Molecules

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Liquid Crystals (LCs) which possess the fluid properties of liquids as well as the anisotropic properties of crystals are the one of fascinating states of matter. Among the subclasses of liquid crystals, chiral mesophases such as SmC* have attracted considerable interest due to their ferroelectric or antiferroelectric properties for potential use in display and light shutter devices [1, 2].

Conventional calamitic (rod-shaped) molecules which consist of a rigid aromatic core and two paraffinic side-chains generally exhibit smectic phases due to the difference in conformational rigidity between aromatic and paraffinic segments. The amphiphilicity can be constituted in the design of the rod-shaped molecules by using hydrophilic and lipophilic segments, fluorocarbon and hydrocarbon segments or siloxane and hydrocarbon segments, etc. [3]. The occurrence of smectic mesophases is strongly influenced by the amphiphilicity which is combined in terminal positions of rod-shaped molecule. For example; incorporating fluorinated chains into calamitic liquid crystals leads to a significant stabilization of smectic mesophases in comparison to their hydrocarbon analogues due to the incompatibility of fluorocarbon segment with aromatic and aliphatic hydrocarbons [4].

In this study, we have synthesized and characterized biphenyl based new rod-shaped mesogens terminated by chiral moiety and different units such as olefinic, semifluorinated or siloxane groups in order to study the impact of microsegregation and the chirality on the mesomorphic properties. The mesomorphic properties of the new compounds have been investigated by differential scanning calorimetry, optical polarizing microscopy and electro-optic methods. The new chiral rod-shaped molecules exhibit a variety of enantiotropic chiral smectic phases in a broad mesomorphic range. The introduction of semifluorinated segment as well as siloxane units to the terminals leads to a significant stabilisation of smectic phases. The transition temperatures of rod-shaped mesogens incorporating a fluorocarbon chain significantly become higher than those of alkoxy and olefine terminated analogues whereas the siloxane derivative exhibits lower temperatures than alkoxy and olefine terminated analogues.

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PP-71

Spectrofluorimetric Determination of Cilazapril in Pure and Pharmaceutical Preparations

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A selective and sensitive spectrofluorimetric method was developed and validated for the determination of cilazapril in pure and pharmaceutical preparations. The proposed method is based on derivatization using 1-dimethylaminonaphthalene-5- sulphonyl chloride (dansyl chloride) as fluorogenic agent and measuring the fluorescence of the products at emission wavelengths of 503 nm after excitation at 374 nm. The method was validated for linearity, limit of detection, limit of quantification, precision, accuracy, recovery. The limits of detection were calculated to be 7.49 ng/mL and 22.49 ng/mL respectively. The proposed method was applied to study of cilazapril in pure and pharmaceutical preparations.

PP-72**Antioxidant activity of *Cirsium bulgaricum* DC. leaf extracts****Ayca Karasakal**

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Cirsium bulgaricum DC. (Asteraceae) is a plant species grows in Derekoy, Kirklareli. This work aims to measure the antioxidant capacities of *Cirsium bulgaricum* DC. In this study, The leaves of *Cirsium bulgaricum* DC. have been investigated for their antioxidant activity/capacity. Leaf extracts were extracted by % 80 methanol and acetone. Two different methods (CUPRAC and DMPD) were used for determination. The 80% methanol and acetone extracts showed 0,005-6,16 mmol/g (TR, CT, EC, RT, QR, NG) in CUPRAC methods. According to DMPD methods, inhibition effect were showed 2.3% for 80% methanol and 4.6% for acetone.

PP-73

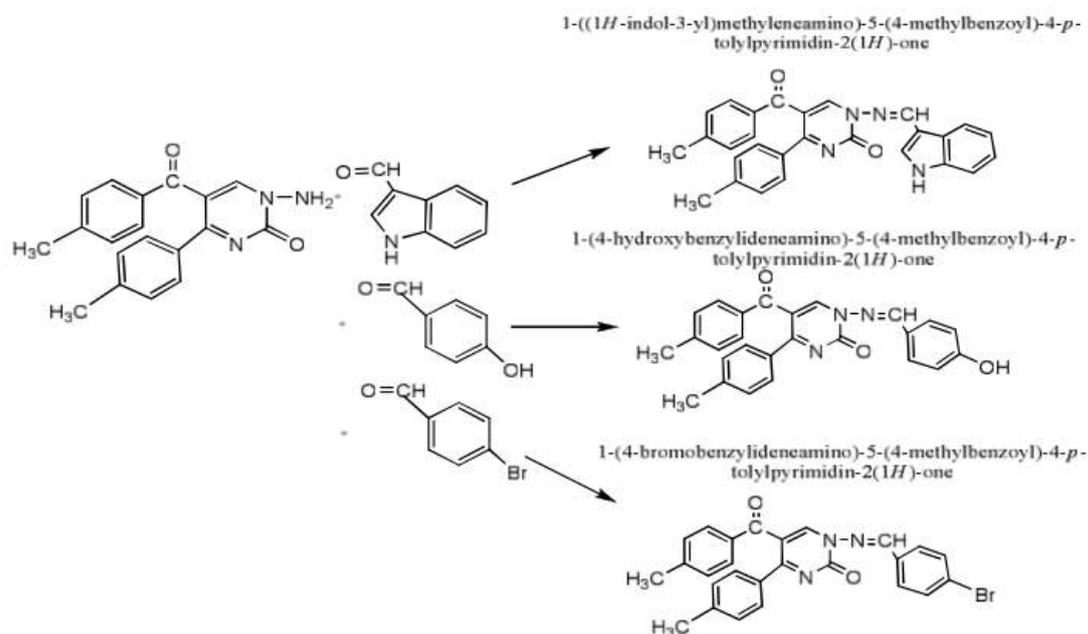
Synthesis, Structural Characterization and Catalytic Activity of Some Schiff Bases

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We presented the synthesis of some novel schiff bases in this study. For this, 1- amino-5-(4-methylbenzoyl)-4-p-tolylpyrimidin-2(1H)-one as a starting material was synthesised to produce 1-((1H-indol-3-yl)methyleneamino)-5-(4-methylbenzoyl)-4-p- tolylpyrimidin-2(1H)-one,1-(4-hydroxybenzilideneamino)-5-(4-methylbenzoyl)-4-p- tolylpyrimidin-2(1H)-one and 1-(4-bromobenzilideneamino)-5-(4-methylbenzoyl)-4-p- tolylpyrimidin-2(1H)-one. The structures of these new compounds were characterised by the FT-IR, ^{13}C NMR, ^1H NMR elementary analyses techniques. Also we studied for catalytic activities in Suzuki-Myyaura cross coupling reactions in aquaus media.Schematic representation of the synthesis route of the compounds shown in scheme 1.

Scheme 1. Schematic representation of the synthesis route of the compounds



PP-74**Adsorption Parameters of Different Organic Dyes on the Synthetic Resin XAD-7**

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Pollutants that are emitted into the water streams as the end products of industrial processes threaten the human health. Some of these pollutants are dyes and pigments used in many diverse industries. These pollutants not only make the wastewaters toxic but also prevent the recycle and reuse of water. Dyes that are not directly toxic yield a very intense color even in minor concentrations and prevent light going through the water and reach the aquatic life (Chatterjee et. al., 2007). In recent years as the need of clean water resources increased and 'green' applications gained importance, many methods to rid the waters from these harmful substances have been designed and used. Adsorption is one of the widely researched methods.

Natural or synthetic materials can be used as adsorbents (Ahmed et. al., 2000; Dogan et. al., 2009). Synthetic resins are polymer based, nontoxic, chemically inert, modifiable, regenerable materials that can be stored at room conditions for many years. Adsorbent resins may also be used for adsorption of neutral substances as opposed to ion-exchange resins.

In this study, the adsorption of Brilliant Green (BG), Aniline Blue (AB), Congo Red (CR) and Rhodamine B (RB) dyes on Amberlite XAD-7 was investigated using a batch system. The Langmuir and Freundlich adsorption isotherms were plotted to find out the adsorption capacities. Also the optimum operational parameters such as temperature, initial dye concentration, adsorbent dosage were determined. Using the data obtained from the experiments conducted at different temperatures, the thermodynamical parameters for the adsorption process were calculated.

Acknowledgement

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PP-75

A New Method for Calculation of Molecular Hardness

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The chemical hardness introduced by Pearson in 1960s is an extremely useful theoretical descriptor. This concept has been associated with many scientific issues along with Hard and Soft Acid-Base Theory (HSAB) and Principle of Maximum Hardness (PMH) that there is chemical hardness concept on the basis. Also today, chemical hardness concept takes places in content of many experimental and theoretical studies. In the present report, a new molecular hardness (η_M) equation to calculate chemical hardness of functional groups and molecules was derived utilizing the relationship with charge of the electronic energy for atoms, Density Functional Theory and Datta's global hardness equalization principle. The reliability of the new equation was proved by comparison with experimental data and the results of Datta's geometric mean equation for molecular hardness and molecular hardness values that were obtained in the present work. The new equation will provide the opportunity to calculate the molecular hardness from first ionization energies (IE_1), first electron affinities (EA_1) and second ionization energies (IE_2) of atoms in the molecules. The new equation is presented as follows

$$\eta_M = \frac{\left[\sum_{i=1}^P \left(\frac{IE_{1_i} - EA_{1_i}}{IE_{2_i} - 2IE_{1_i} + EA_{1_i}} \right) + (N - P) \left(\frac{IE_1(H) - EA_1(H)}{IE_1(H) - 2EA_1(H)} \right) \right] + q_M}{\sum_{i=1}^P \left(\frac{1}{IE_{2_i} - 2IE_{1_i} + EA_{1_i}} \right) + \left(\frac{N - P}{IE_1(H) - 2EA_1(H)} \right)}$$

In this equation, N represents total number of atoms in the molecule, P is number of atoms different from hydrogen and (N-P) is number of hydrogen atoms in the molecule. q_M is charge of molecule or functional group.

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PP-76

Crystal structure, linkage isomerizations, spectroscopic investigations and DFT/TD-DFT studies of palladium(II) complex containing acetyl hydrazone oxime

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Oximes and hydrazones are interesting compounds because of their wide application in medicine, industry and analytical chemistry. These compounds are used as analytical reagents for the detection and determination of some metal ions [1,2]. Thus oximes and hydrazones and their metal complexes have been widely studied. In recent years, much attention has been given to theoretical studies on oximes, hydrazones and their complexes. Experimental studies of oximes, hydrazones and metal-oximes have been matched by theoretical calculations.



Figure 1. Molecular structure and optimized geometries of five different linkage isomers of [Pd(hipeahH)₂]

A new palladium(II) complex, [Pd(hipeahH)₂], where hipeahH = acetyl hydrazone oxime, [(1E,2E)-2-(hydroxyimino)-1-phenylethylidene]acetohydrazone, has been prepared and studied by IR, UV-vis and X-ray crystallography. The complex was crystallized in the triclinic system (P-1) with the unit cell parameters of $a = 8.8819(7)$, $b = 10.2597(8)$, $c = 12.0191(9)$ Å, $\alpha = 81.656(6)^\circ$, $\beta = 87.583(6)^\circ$ and $\gamma = 77.367(6)^\circ$. X-ray diffraction analysis of the [Pd(hipeahH)₂] shows that have a 1:2 metal:ligand ratio, the hydrazone and oxime protons of different ligands are lost and this result in the coordination of the ligands with five- and six-membered chelates (Fig. 1). In addition, the five isomer structures were suggested for palladium(II) complexes. The molecular geometry and vibrational frequencies of the five suggested complexes in the ground state have been calculated using the density functional method (B3LYP) with the LANL2DZ basis set. The calculated results show that the optimized geometry can well reproduce the crystal structure, and the theoretical vibrational frequencies show good agreement with experimental values. The absorption spectra of ligand and its complexes in EtOH have been modeled by time-dependent density functional theory (TD-DFT) using a hybrid functional, B3LYP, as well as the LanL2DZ basis set.

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PP-77

Effect of Polymer Matrice on Biodegradability LDPE/Starch Films and PLA/Starch Films

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Durability is the property that make plastics ideal for many applications such as packaging, building materials and commodities. However, increasing consumption of these materials can lead to waste disposal problems, as these materials are not readily biodegradable because of their resistance to microbial degradation. One way to reduce plastic waste is to design new materials that are susceptible to chemical, photochemical or biological processes, so that degradation will occur over a shorter period [1]. To achieve this susceptibility, resistant plastics could be blended with natural polymers (e.g., starch, cellulose or chitosan) or synthetic polymers containing ester, hydroxyl or ether groups that are prone to hydrolytic cleavage by microorganisms [2-4].

In this study, potato starch was blended with film-grade poly(lactic acid) and low density polyethylene pellets at ratios of 90:10, 80:20 and 70:30 and extruded into thin films in a co-rotating twin screw extruder. Before extrusion process, potato starch was mixed with glycerol to increase compatibility of hydrophilic starch with hydrophobic PLA and LDPE matrice. Thermal, morphological and mechanical properties of blends were determined by differential scanning calorimetry, scanning electron microscope and stres-strain tests, respectively. Moreover, biodegradability of blends were investigated by water absorption, soil burial and bacterial strength tests. According to analyse results, in the presence of a synthetic polymer derived from renewable sources, degradation period declined prominently.

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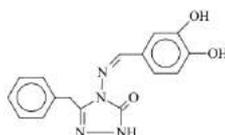
PP-78

**The Investigation of Spectroscopic Properties of
3-benzyl-4-(3,4-dihydroxybenzylidenamino)-4,5-
dihydro-1H-1,2,4-triazol-5-one using B3LYP and HF Basis Set**

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The compound was optimized by using the B3LYP/631G (d, p) and HF/631G (d, p) basis sets [1,2]. $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09W [2]. Experimental and theoretical values were inserted into the graphic according to equation of $\delta_{\text{exp}} = a + b \cdot \delta_{\text{calc}}$. The standard error values were found via Sigma Plot program with regression coefficient of a and b constants. IR absorption frequencies of analyzed molecule were calculated by two methods. The veda4f program was used in defining IR data, which were calculated theoretically [3]. The experimental and the obtained theoretical values were compared and found by regression analyses that are accurate. Furthermore, experimentally and theoretically UV-vis values in ethanol were calculated and compared. Experimental spectroscopic data of 3-benzyl-4-(3,4-dihydroxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one molecule have been described in the literature [4].



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PP-79

Performance of PM6-DH2 and PM7 Methods on Determination of Hydrogen Storage Capacity of Small B₂₄N₂₄ Nanocage

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Tremendous amounts of fossil fuels are being consumed every passing minute by the world's population without thinking their environmental impact. Using this huge amount of fossil fuels causes global warming. Therefore, scientists have been seeking for alternative, clean, renewable energy resources instead of fossil fuels. Hydrogen energy is one of these desired resources. Due to being an environment-friendly energy source, hydrogen fuel has attracted great attention both scientific and industrial communities for its potential use in vehicles, portable power application, etc. [1-3]. Many hydrogen storage materials such as carbon based materials, metal hydrides, metal-organic frameworks and organic polymers have been investigated both experimentally and computationally. Shortly after their discovery, boron- nitride nanotubes BNNTs were tested as new material for hydrogen storage. These studies resulted in that boron nitride nanotubes could store up to 2.6 wt% hydrogen at room temperature and also their hydrogen capability was better than carbon nanotubes [4].

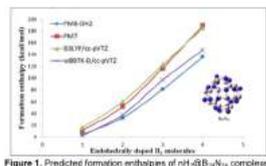


Figure 1. Predicted formation enthalpies of nH₂@B₂₄N₂₄ complexes

In this study, we present endohedral hydrogen storage capacity of the B₂₄N₂₄ nanocage structure determined by the semi empirical PM6-DH2 and PM7 methods that can deal with interactions between non-bonded molecules and also the performance of these methods against more reliable DFT methods such as wB97X-D that accounts for dispersion interactions among non-bonded structures. The predicted formation enthalpies of endohedrally doped H₂ - B₂₄N₂₄ nanocage complexes (nH₂@B₂₄N₂₄) by the semi empirical PM6-DH2 method are in almost perfect agreement with wB97X-D/cc-pVTZ level results while the formation enthalpies of these complexes predicted by PM7 is slightly higher than the DFT predicted energies. As a result, this study reveals that PM6-DH2 can be used to calculate endohedral hydrogen storage capacities of larger BN nanocages with the accuracy of higher level DFT methods in enormously short (compared to DFT methods) computational times.

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PP-80

A QM/MM Investigation of the GTP Hydrolysis in Elongation Factor-Tu (EF-Tu)

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Accuracy of protein synthesis is achieved with the help of a number of translational factors. During elongation cycle; Elongation factor Tu (EF-Tu) is responsible of delivering the aminoacyl-tRNA to the ribosome as part of a ternary complex with GTP. GTP hydrolysis is crucial for the activity of the protein since EF-Tu can bind tRNA when bound to GTP, and releases tRNA when GTP is hydrolyzed to GDP. Cognate codon-anticodon pairing triggers GTP hydrolysis, leading to drastic conformational changes in the protein and EF-Tu loses its affinity towards the aminoacyl-tRNA and ribosome. As a GTPase superfamily member, EF-Tu regulates and ensures that the correct aa-tRNA is left in the ribosome.

With homology to other GTPase superfamily members, GTP hydrolysis mechanism of EF-Tu was analysed mainly by focusing on the roles of Histidine 85 (His85) and Arginine 57 (Arg57) (*T. aquaticus* numbering). Three different models were designed: one with His85 in the active site, one with Arg57 in the active site and one where both His85 and Arg57 are outside of the active site. Our QM/MM calculations indicate that the presence of Arg57 or His85 in the active site decreases the activation energy, demonstrating that these residues have catalytic roles.

GTP hydrolysis reactions are a type of phosphate hydrolysis reactions which are very common in biological systems. Phosphate hydrolysis reactions are supposed to proceed by an associative or dissociative path. To identify the type of mechanism, different model structures representing the associative or dissociative path of GTP hydrolysis have been optimised and the energy values have been compared. All optimised transition structures have associative character. For the models studied, we observe that the energy increases at the points where the dissociative path is supposed to occur. The assistance of a second water molecule on the reaction was also analysed. The assistance of a second water molecule to the proton transfer does not have any catalytic effect.

PP-81

Biological activities of *Sideritis Montana* and DFT investigation of major components

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Medicinal plants contain chemical constituents which exhibit antioxidant properties. Antioxidants are viewed as compounds that protect cells against oxidative stress, which might cause cell damage. *Sideritis*, which are members of the Lamiaceae family, have significant antioxidant capacities. *Sideritis L.* is approximately 150 species of annual and perennial plants and 39 species are endemic in Turkey[1]. These species are known to have pharmacological, antiinflammatory, antimicrobial and antioxidant activities [2, 3, 4].

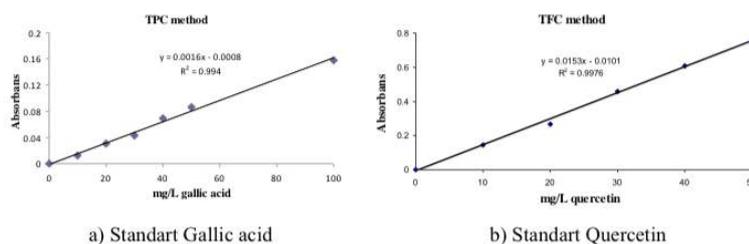


Figure. Calibration curves of the standards

In this study, it was aimed to determine total phenolic compounds, total flavonoid and radical scavenging activities of methanolic extracts of *S. Montana* and the major components of *Sideritis montana*, chlorogenic acid and apigenin, were calculated in terms of the bond cleavage and radical formation mechanisms of these phenolic antioxidant species. The calculations for studied compounds have been carried out by DFT/B3LYP methods using Gaussian 09 programme[5].

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PP-82

Synthesis and Characterization of Al-Pillared Montmorillonite/Poly(methyl methacrylate) Nanocomposites

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Many clay is used as a filler in the nanocomposite synthesis. However, the use of pillared clay is quite limited. The pillaring process imparts various unique physicochemical properties to these clay materials, including large specific surface areas, increased surface acidity and good thermal stability [1]. In this study, Alpillared-montmorillonite/poly(methyl methacrylate) nanocomposites were synthesized with solvent blending method using acetone, chloroform, toluene and THF. The effect of solvent and pillared clay content on the structural and thermal properties of PMMA nanocomposites was investigated. Characterization of nanocomposites was performed with XRD, TEM, FTIR-ATR, DTA/TG and DSC. The morphologies of nanocomposites and dispersion of montmorillonite into PMMA were examined by XRD and TEM. Images showed that pillared clay dispersed at nanometer scale in polymer matrix. The thermogravimetric analysis showed that with increasing montmorillonite content the thermal stability and the glass transition temperature (T_g) of polymer matrix shifted to higher temperature. This characterization procedures were assigned that pillared clay as a filler could used in the nanocomposite preparation.

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PP-83

Preparation of Interpenetrating Polymer Network Microspheres of Poly(Vinyl Alcohol) and Carboxymethyl Cellulose for Controlled Release of Ketorolac Tromethamine

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In this study, we aimed to product of pH sensitive microspheres for controlled release of nonsteroidal anti-inflammatory drug ketorolac tromethamine (KT). For this purpose, interpenetrating polymer network (IPN) microspheres of poly(vinyl alcohol) (PVA)/sodium carboxymethyl cellulose (NaCMC) were prepared based on different formulations using glutaraldehyde (GA) (0.66 M) and hydrochloric acid (HCl) (3%, v/v) as crosslinker. The prepared microspheres were characterized by fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), differential scanning calorimetry (DSC) and X-ray diffraction (X-RD). Preparation condition of the microspheres was optimized by considering the percentage entrapment efficiency and swelling capacity of microspheres and their release data. Effects of ratio of PVA and NaCMC, exposure time to GA and drug/polymer ratio on the release of KT were discussed at three pH values (1.2, 6.8 and 7.4) for 6 h. The release of KT increased with the increasing NaCMC/PVA (w/w) ratio and decreasing drug/polymer ratio. At the end of 6 h, the highest release of KT was found to be 99.6% for the 1/1 NaCMC/PVA (w/w) ratio and 1/8 drug/polymer ratio. The swelling measurements of the microspheres supported the release results. Release kinetics was described by Fickian and non-Fickian approaches.this study, we aimed to product of pH sensitive microspheres for controlled release of nonsteroidal anti- inflammatory drug ketorolac tromethamine (KT). For this purpose, interpenetrating polymer network (IPN) microspheres of poly(vinyl alcohol) (PVA)/sodium carboxymethyl cellulose (NaCMC) were prepared based on different formulations using glutaraldehyde (GA) (0.66 M) and hydrochloric acid (HCl) (3%, v/v) as crosslinker. The prepared microspheres were characterized by fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), differential scanning calorimetry (DSC) and X-ray diffraction (X-RD). Preparation condition of the microspheres was optimized by considering the percentage entrapment efficiency and swelling capacity of microspheres and their release data. Effects of ratio of PVA and NaCMC, exposure time to GA and drug/polymer ratio on the release of KT were discussed at three pH values (1.2, 6.8 and 7.4) for 6 h. The release of KT increased with the increasing NaCMC/PVA (w/w) ratio and decreasing drug/polymer ratio. At the end of 6 h, the highest release of KT was found to be 99.6% for the 1/1 NaCMC/PVA (w/w) ratio and 1/8 drug/polymer ratio. The swelling measurements of the microspheres supported the release results.

PP-84**Preparation of Zinc-Phthalocyanine Modified Polypyrrole Nanofiber Electrode**

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Phthalocyanines (Pcs) show very important properties in modern technology with applications in fields including: as solar cell, chemical sensors, dyes and pigments, non-linear optics and, liquid crystals, gas sensors, catalysts, semiconductors, light emitting diodes, optical data storage, photodynamic therapy. For such applications, the solubility of phthalocyanines in organic solvents and water is very important [1,2].

Metallophthalocyanines are especially important in this respect because of their rich redox behavior, the ability to use almost any metallic and some nonmetallic elements in the central cavity, their easy modification by substituting the ring, and chemical stability [2]. On the other hand, it has been demonstrated that phthalocyanines are easily adsorbed very strongly on the graphite electrodes and that is possible to examine their electrochemical and catalytic properties on the electrode surface [3].

In this study, the polypyrrole and polypyrrole nanofiber films were prepared by electrochemical method on pencil graphite electrode. The zinc-phthalocyanine was adsorbed on the surface of the polymer electrodes. The electrochemical performance of the modified electrodes as sensor were investigated by differential pulse voltammetric method.

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PP-85

Kinetic, Isotherm and Thermodynamic Studies of Cadmium Adsorption on Zeolite

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Many toxic heavy metals have been discharged into the environment as industrial wastes, causing serious soil and water pollution, and they become a severe public health problem. Due to their extreme toxicity, metal ions are nowadays among the most important pollutants both in surface water and in groundwater. Since levels of metals in the environment have increased because of industrial pollution, the elimination of such ions from water is essential to protect public health.

Cadmium is a toxic heavy metal of significant environmental and occupational concern. It has been released to the environment through the combustion of fossil fuels, metal production, application of phosphate fertilizers, electroplating, and the manufacturing of batteries, pigments, and screens. This heavy metal has resulted in serious contamination of both soil and water. Cadmium (Cd) has been classified as a human carcinogen and teratogen impacting lungs, kidneys, liver and reproductive organs. The World Health Organization (WHO) has set a maximum guideline concentration of 0.003mgL^{-1} for Cd in drinking water. Given pervasive cadmium contamination and the low drinking water guideline, there is considerable interest in the development of techniques to remove cadmium from contaminated water.

There are several methods available for the removal of cadmium and other heavy metals from wastewater, which include precipitation, flotation, ion exchange, membrane-related process, electrochemical techniques, biological processes and adsorption. The selection of the wastewater treatment methods is based on the concentration of the waste and the cost of treatments. Adsorption process is economic and it is a feasible alternative for removing low concentrations of cadmium. The main disadvantage of adsorption processes is the high cost of the adsorbents. Therefore, it is important to search for inexpensive adsorbents that may be used in the wastewater treatments.

The purpose of this work was to determine the adsorption behavior of cadmium by natural zeolite. Batch experiments are carried out for kinetic studies on the removal of Cd from aqueous solutions. The influence of various contributing parameters such as pH, adsorbent concentration, contact time, and initial Cd concentration and temperature is investigated. Three adsorption isotherm models (Langmuir, Freundlich, and Temkin equation) are used to study the fit of the experimental equilibrium data obtained in the study, and several kinetic models are used to evaluate the mechanism of adsorption.

PP-86

The Design Of The Dual Fluorescent Ag (I) Sensor of Based On Bodipy Using Click Chemistry

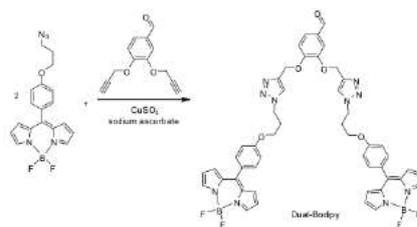
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Since their discovery and particularly over the past two decades, Bodipy derivatives (4,4- difluoro-4-bora-3a,4a-diaza-s-indacene, boron dipyrromethene) have emerged as a fascinating class of dyes with excellent performance and stability, thus finding applications in sensing, labelling, light- harvesting and photodynamic therapy [1]. The Huisgen alkyne?azide cycloaddition reaction (CuAAC) [2] has attracted considerable attention, and is usually regarded as the most widely applied of the 'click' reactions. In recent years, azido-cyclizing form click reaction has been frequently used to construct ligands with cation chelating ability. This facile reaction has been applied to the assembly of sensor constructs [3-4]. Ag (I) has moderate coordination ability, making it quite difficult to be discriminated from other chemically similar heavy metal ions. While a lot of sensor literatures for several metal ions, the design and synthesis of a selective and sensitive fluorescent chemosensor for Ag (I), preferably a ratiometric one, is still highly desirable to date [5].

In this study, a dual novel molecule based on Bodipy was prepared. After the characterization processes, [MS, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$, elemental analysis], the absorption, emission and excitation spectra of this molecule were investigated in presence of several metal ions. The results show that the synthesized dual Bodipy may use as a selective fluorescence sensor for Ag (I) metal. After the complexation with silver ions, the fluorescence intensity of Bodipy is significantly quenched and the wavelength slightly shifted to red by increase concentration.



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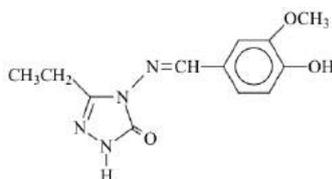
PP-87

Gaussian Calculations of 3-ethyl-4-(3-methoxy-4-hydroxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one Molecule

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In this study, 3-ethyl-4-(3-methoxy-4-hydroxybenzylidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one compound [1] was optimized by using the B3LYP/6311G (d,p) and HF/6311G (d,p) basis sets [2, 3]. ¹H-NMR and ¹³C-NMR spectral data were obtained theoretically by using this optimizing structure. The experimental and the obtained theoretical values were compared and found by regression analysis that are accurate. Theoretically calculated IR data are multiplied with appropriate adjustment factors and the data obtained according to HF and DFT method are formed using theoretical infrared spectrum. The identification of calculated IR data was used in veda4f program [4]. Furthermore, molecule's theoretical bond lengths, bond angles, dipole moments, Mulliken charges, HOMO-LUMO energies and total energy of the molecule for both methods were calculated.



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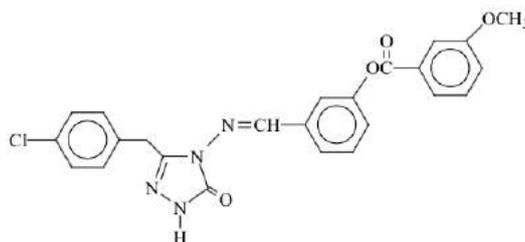
PP-88

A Study on Theoretical and Experimental Spectroscopic Properties of New 3-(p-chlorobenzyl)-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one

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3-(p-Chlorobenzyl)-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one molecule was optimized by using the B3LYP/6-311G (d) and HF/6-311G (d) basis sets [1, 2]. ¹H-NMR and ¹³C-NMR isotropic shift values were calculated by the method of GIAO using the program package Gaussian G09 [2]. Experimental and theoretical values were inserted into the graphic according to equation of $\delta_{\text{exp}}=a+b \cdot \delta_{\text{calc}}$. The standard error values were found via SigmaPlot program with regression coefficient of a and b constants. IR absorption frequencies of analysed molecule were calculated by two methods. Then, they were compared with experimental data, which are shown to be accurate. Infrared spectrum were composed by using the data obtained from both methods. The veda4f program, was used in defining IR data, which were calculated theoretically [3]. Additionally, this compound was found bond angles, bond lengths, the HOMO-LUMO energy and mulliken charges by using the B3LYP/6-311G (d) and HF/6-311G (d) basis sets.



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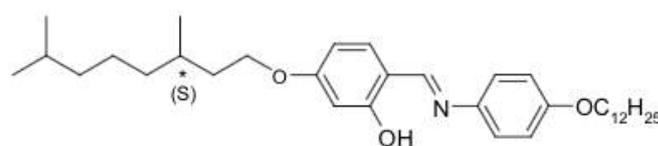
**Surface Lewis acid?base properties of
5-((S)-3,7-Dimethyloctyloxy)-2-[[[4-(dodecyloxy)phenyl]imino]methyl]phenol Liquid Crystal
measured by inverse gas chromatography**

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Liquid crystals (LCs) which have attracted much interest for many years due to their use in numerous applications such as display devices, optical and thermal sensors and stationary phases in chromatographic columns are soft materials that are considered as the fourth state of matter between a solid and a liquid. Acid–base forces are known to contribute significantly to surface interactions in composite systems. Surface Lewis acid–base properties of many liquid crystals were measured by some researchers with inverse gas chromatography (IGC) in the recent years. In this work, the surface properties of a new chiral salicylaldimine-based liquid crystal which is shown in Fig.1 were determined by IGC method. Five n-alkanes (n-C6, n-C7, n-C8, n-C9 and n-C10) were used as apolar probes to characterize the surface dispersive free energy. The retentions of tetrahydrofuran (THF), dichloromethane (DCM), chloroform (TCM), acetone (Ace), toluene (T) and diethyl ether (DEE) on LC were measured at temperatures between 303 and 323 K. And then surface Lewis acid?base constants, K_a and K_b of the liquid crystal were determined.



Cr 53 SmC* 92 Iso

Fig.1. The chemical structure and phase transition temperatures chiral salicylaldimine-based liquid crystal

PP-90

Kinetic Analysis of Lactate Dehydrogenase from *Theileria annulata*

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Theileria annulata is a protozoan parasite that causes an important disease theileriosis which has significant effects on mortality and morbidity in livestock. Recent studies have been reported antibiotic resistances against disease. Therefore new approaches are needed to fight against this disease. In our previous studies, gene encoding lactate dehydrogenase enzyme (LDH) was cloned and the recombinant protein expressed in *E. coli* BL21 (DE3) cells. Then enzyme was purified by affinity chromatography. In this study, protein was purified by affinity chromatography. Purity of protein was evaluated by SDS-PAGE. *Theileria annulata* LDH have been obtained with 95% purity. Specific activity of enzyme was calculated to be 8,23 U/ml and enzyme unit per 1 mg protein was calculated to be 168 U/mg. This pure protein was then used to determine the kinetic parameters of the enzyme for the first time in the literature. In kinetic analyses; pyruvate was used as a substrate, NADH was used as cofactor and Tris-KCl was used as a buffer for enzyme. Steady-state kinetic parameters of the pure enzyme was calculated by choosing substrate inhibition module in Graphpad Prism 6.0. Then kinetic characterization was carried out at pH 7,5 and 25 °C. K_m , k_{cat} , k_{cat}/K_m , was found to be 0.1324 mM, 44,55 s⁻¹, 3,3693x10⁵ mM⁻¹s⁻¹ respectively. K_i value was calculated as 4,295 mM due to substrate inhibition of enzyme. These results could be used in further drug design studies.

PP-91

Syntheses, Crystal Structures, Spectroscopic and Stereogenic Properties, Antituberculosis, Antimicrobial and Cytotoxic Activities and DNA Interactions of Ansa-Spiro-Ansa Cyclotetraphosphazenes

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The cyclophosphazenes are an important family of inorganic heterocyclic ring systems constituting a regular and homologous series[1]. Although there is plenty of work on the reactions of cyclophosphazenes with monodentate ligands in the literature, the studies with the multidentate ligands are very limited[2].



A number of novel ansa-spiro-ansa (asa) cyclotetraphosphazenes was prepared. The structures of the compounds were verified by MS, FTIR, ¹H, ¹³C and ³¹P NMR, HSQC and HMBC techniques. The crystal structures of some of the phosphazene derivatives were determined by X-ray crystallography. The 1,4-dioxaspiro[4,5]decaphosphazene was analyzed by the changes in the ³¹P NMR spectrum on addition of the chiral solvating agent (CSA) to investigate its stereogenic properties. All of the compounds were screened for antibacterial activities against G(+) and G(-) bacteria, and for antifungal activities against yeast strains. The interactions of the phosphazenes with plasmid DNA and the evaluations for cytotoxic activity against MCF-7 breast cancer cell lines were investigated. The piperidine substituted phosphazenes were found to be more effective than Cisplatin against MCF-7 breast cancer cell lines at lower concentrations.

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PP-92

Separation of Acetone/Water Mixtures through Poly(vinyl alcohol)-graft- Acrylonitrile/2-Hydroxyethyl Methacrylate-ZnO Membranes by Vapour Permeation with and without Temperature Difference**Merve Olukman , Oya Sanli**

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Pervaporation (PV) is a separation process considered as an attractive alternative to conventional techniques for the separation of aqueous organic mixtures and organic liquid mixtures having azeotropic points and similar physical and chemical properties [1]. However, with the PV method, polymer membranes become swollen or shrunk since the feed solutions are directly in contact with the polymer membrane, and so the original functionalities of membranes, designed chemically and physically, are sometimes impaired by the swelling or shrinking of the membranes. Therefore, Urugami and coworkers proposed a vapour permeation (VP) method having the advantages of PV but not its disadvantages [2-5].

In this study ZnO nanoparticles were synthesized in poly(vinyl alcohol)-graft-acrylonitrile/2-hydroxyethyl methacrylate (PVA-g-AN/HEMA) membranes and used in the separation of acetone/water mixtures using VP and temperature difference vapour permeation (TDVP) methods. PVA-g-AN/HEMA-ZnO nanocomposite membranes were characterized by Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM) and differential scanning calorimetry (DSC). The effects of the feed composition (0-100 wt. %), operating temperature (30°C-50°C) and membrane surrounding temperature (0°C-30°C) on the permeation rate and separation factor of the acetone/water mixtures were studied. The permeation rates in VP were higher than those in TDVP, while the separation factors were lower. PVA-g-AN/HEMA-ZnO nanocomposite membranes gave permeation rates of 0.14-0.02 kg/m²h and separation factors of 53-2175 depending on the operation conditions and the method.

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PP-93

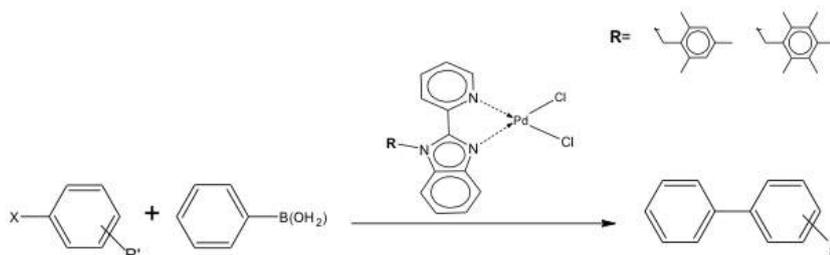
Pd-MONO NN Catalyzed Suzuki C-C Coupling Reaction

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Palladium-catalyzed cross-coupling reactions are powerful synthetic tools for carbon-carbon bond formation, which plays a very important role in the synthesis of natural products, pharmaceuticals, and functional polymer materials [1-2]. Hence the Suzuki-Miyaura cross-coupling reaction is one of the most widely used methods for the construction of biaryl compounds, owing to the stability and low toxicity of the organoboranes relative to other organometallic reagents [3-4].



In this study, the mono-NN type palladium complexes of mesityl and pentamethyl benzyl substituted 2-(2-pyridyl)benzimidazole were synthesized. The structures of these compounds were characterized by ^1H and ^{13}C -NMR spectroscopy, FT-IR, elemental analysis and melting point measurement methods. The synthesized palladium complexes were tested as catalysts for the Suzuki coupling reactions to give the biaryl compounds. After determining the best catalyst system, the optimization studies were carried out by changing various parameters such as temperature, time, aryl halide and base.

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PP-94**Ab initio intermolecular potential energy surfaces for the He-H₂ and Ne-H₂ molecules**

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The interaction potential energy surface (PES) of He-H₂ and Ne-H₂ is of great importance for quantum chemistry, as the simplest test case for interactions between a molecule and a closed-shell atom. It is also required for a detailed understanding of certain astrophysical processes, namely collisional excitation and dissociation of H₂ in molecular clouds, at densities too low to be accessible experimentally.

In this study we have sought to accurately determine the He-H₂ and Ne-H₂ potential surface including an accurate representation of the energy change by using a systematic approach to the modeling of the interaction. The potential energy surfaces were calculated by *ab initio* calculations at CCSD(T)/aug-cc-pVTZ level. The study covers a range of $R = 2.0$ [U+FFFD]o $R = 10.0$ Å for the He-H₂ and Ne-H₂ separation and $r = 0.3$ Å to $r = 1$ Å for the H-H separation using molecular orientations of $\theta = 0^\circ, 45^\circ, \text{ and } 90^\circ$. Additional computations at intermolecular distance R , varies in the range of 2-10 Å and different angular orientations were selected by changing the angle θ in the steps of 10° . The present study has shown that considerable computational effort is required to accurately model the van der Waals interaction of even a simple system such as He-H₂ and Ne-H₂ by *ab-initio* calculations.

Acknowledgement

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PP-95**Kinetic modelling for the binary sorption of LR-G and LG-B onto sepiolite modified with decyltrimethyl ammonium cation**

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Sepiolite (SEP) is a natural clay mineral ($Mg_4SiO_6O_{15}(OH)_2 \cdot 6H_2O$) with fibrous morphology and intracrystalline channels.[1] It is one of the most abundant locally available clay mineral in Turkey with estimated above 100 Mt reserves.[2] In this study, modified SEP samples SEP-C10 was prepared using decyltrimethylammonium (DTMA⁺) cation.

The sample was characterized using DRIFT technique and used as adsorbents for removing textile dyes from aqueous solutions. Adsorption behavior of Lanaset Green B (LGB) and Lanaset Red G (LRG) in single- and binary component solutions depending on time was studied at 298 K.

The kinetic data obtained from 0.1 mM dye solutions were analyzed using the pseudo-second-order equation based on chemisorption and Vermeulen approximation based on the homogeneous surface diffusion model (HSDM). Conformation of the pseudo-second-order model with the experimental data suggests that electrostatic interactions between negatively charged dye molecules and positively charged admicelles are important in adsorption process.

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PP-96**Effect of solvent polarities on electronic properties of pyrene derivatives****Humeyra Orucu¹, Nursel Acar²**

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A series of pyrene derivatives with different asymmetrical substituents has been theoretically studied using the density functional theory (DFT) with the hybrid B3LYP exchange correlation function and the split valence 6-311G++(d,p) basis set. The ground state absorption spectral bands, vertical excitation energies, oscillator strengths, molecular orbitals, and intramolecular charge transfer properties of the asymmetrical pyrene derivatives were performed by time dependent density functional theory (TDDFT) calculations. Electronic properties and HOMO–LUMO energy gaps have been analyzed and compared using electron donor and electron acceptor substituents in gas phase and in solution. The results are pointed out that absorption maxima of $\text{PyC}_6\text{H}_5\text{NH}_2$ correspond to the electron transition between frontier orbitals such as transition from HOMO to LUMO. The HOMO is located over the aniline group and pyrene, the HOMO \rightarrow LUMO transition implies an electron density transfer to pyrene from the aniline group. The lowering of the HOMO–LUMO energy gap (3.08 eV for $\text{PyC}_6\text{H}_5\text{NH}_2$) value has substituent effect on the intramolecular charge transfer.

PP-97

Investigation of the Topoisomerase-targeted Anti-cancer Drug Molecules: Ab-initio and Molecular Dynamics Study

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Many enzyme proteins that bind DNA at and ahead of the replication fork affect large DNA fragments, and do actual mechanical work using the energy of binding and/or hydrolysis of nucleotides. These proteins are known as the ‘motor proteins’. One such family of proteins, that cut one or both strands of DNA and therefore bring changes in the topology of DNA, is called topoisomerases (shortly topos). They are ubiquitous enzymes which are essential for the cellular regulation of DNA supercoiling caused by processes such as replication, transcription, and recombination. These enzymes also adjust the steady state level of DNA supercoiling in order to facilitate protein-DNA interactions. Because of their crucial roles in DNA replication, topoisomerases are the focus of many cancer research, as they are the sole target for several families of anti-cancer drugs that are typically medium size organic molecules (e.g. camptothecin family).

Topo-I forms a single-strand break in DNA, remaining covalently linked to the 3'-phosphate through a tyrosyl residue. This intermediate is commonly referred to as a ‘cleavable complex’. Under physiological conditions, Topo-I catalyses the religation of the broken strand. Camptothecins are the prototypical agents belonging to a class of antitumor drugs known as Topo-I poisons, because they have Topo-I as a unique target. The drug specifically inhibits the religation step, thus preventing release of DNA [1]. Currently, topotecan (Hy-camptin) is one of the camptothecin derivatives in the clinical use. It has shown tremendous promise as solid tumor drug [2].

In this project, the aim is to combine both electronic level static calculations (quantum chemical data based on the time-independent Schrödinger equation) and time dependent data obtained at the atomic level (molecular dynamical calculations), and use them together to gain more understanding about DNA motor protein interactions.

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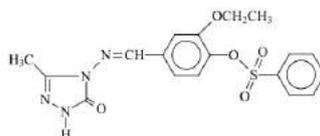
PP-98

The Investigation of Novel 3-methyl-4-(3-ethoxy-4-benzenesulfonyloxybenzilidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one with GAUSSIAN 09W Program

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3-Methyl-4-(3-ethoxy-4-benzenesulfonyloxybenzilidenamino)-4,5-dihydro-1H-1,2,4-triazol-5-one was synthesized by the reaction of 3-methyl-4-amino-4,5-dihydro-1H-1,2,4-triazol-5-one with 3-ethoxy-4-benzenesulfonyloxybenzaldehyd. The compound has been optimized using B3LYP/631G(d, p) and HF/631G(d, p) basis set [1]. Starting from this optimized structure with $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ spectral data values according to GIAO method was calculated using the method of Gaussian G09W program package in gas phase [2]. Theoretically and experimentally values were plotted according to $\delta_{\text{exp}} = a \cdot \delta_{\text{calc}} + b$, Eq. a and b constants regression coefficients with a standard error values were found using the Sigma Plot program. In the theoretical part of study also, Theoretically calculated IR datas of synthesized new compound was calculated in gas phase by using of 631G(d) basis sets of B3LYP and HF methods and are multiplied with appropriate adjustment factors and the data obtained according to B3LYP and HF methods are formed using theoretical infrared spectrum. The identification of calculated IR data was used in veda4f program [3]. Additionally, the molecule was found dipole moments, the HOMO–LUMO energy and total energy of the molecule with from both methods.

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PP-99

Construction and Comparison of EST (Expressed Sequence Tags) Library for Expressed Genes in Normal and Tumoral Mammary Gland Tissue of the Terrier Dog

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Mammary gland tumor is the main tumor in the dog that frequently concurred. Approximately %50 of the neoplastic cases in female dogs are the mammary gland tumors. Data on genes that are involved in tumorigenesis and mechanism of tumor development are insufficient. Comparative studies have been conducted in order to see if tumorigenesis studies in dog could be a model for human mammary gland tumors.

In this study, mammary tissue samples were collected from both normal mammary tissue of a healthy Terrier dog and neoplastic mammary tissue of a sick dog. From the tissues, total RNA and mRNA were isolated for construction of two different cDNA libraries. Total 2304 colonies which are randomly selected from the two libraries were sequenced for developing a dog mammary gland ESTs collection. Phred/Phrap, BEAP and CAP3 programmes were used for bioinformatic analysis. Putative functions of all unique sequences were designed by gene homology based on BLAST. Genes of the human and dog are compared and investigated the effect of these genes on mammary pathogenesis with BLAST method. The results of this study are very valuable resource for functional genome studies of the dogs.

PP-100

The Oxidation of Phenylalanine by Transition Metal Ions Studied by Quantum Mechanical Calculations

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The aim of this study is to focus on the mechanism of the oxidative catabolism of phenylalanine (the simplest aromatic amino acid) by first-row transition metals, in particular cobalt, using quantum mechanical tools. All the ground and transition state structures are optimized using the density functional method M06-2X/cc-pVDZ level of theory. Also, additional calculations have been carried out using M06 to check similar methods. All the optimizations have been performed using the SMD solvent model and explicit solvent molecules are added where necessary. Although the in vitro decomposition of amino acids has been considered in various studies in the literature, the mechanism and intermediates formed during the reaction are not very clear. The reactions use oxidizing agents such as diperiodatocuprate(III) in alkaline medium, or manganese(III) and its hydroxide form ($Mn(OH)^{2+}$) in sulfuric acid medium [1, 2]. But the reaction of cobalt(III) with phenylalanine was not studied. However recently, a couple of works for profiling the transcriptomic data of the yeast *Saccharomyces cerevisiae* when exposed to transition metals, such as cobalt and nickel were done by Cakar and co-workers [3, 4]. According to their results, the cobalt-resistant mutants had a tendency to reduce the amount of aromatic amino acids, suggesting that cobalt(III), but not other metals, reacts specifically with aromatic amino acids, yielding harmful products. In this study, it has been shown that cobalt(III) ions are powerful oxidizing agents against aromatic amino acids. Our study has revealed several pathways of the decomposition reaction of zwitterionic phenylalanine at neutral pH and the effect of the cobalt(III) ion on the decomposition reaction. It was shown that the oxidation of phenylalanine by a cobalt(III) ion results in decarboxylation and deprotonation of phenylalanine. The presence of the aromatic ring facilitates the redox reaction. We believe that the lower activation free energy of this pathway, which involves the interaction between carboxylate and side chain, explains why cobalt reacts preferentially with aromatic amino acids. Then, oxidation by a second cobalt(III) in concert with the nucleophilic addition of a OH^- ion leads to a pathway that yields phenyl acetaldehyde. Also, a different pathway may proceed through oxidation by two more cobalt(III) ions and yield phenylacetamide. But this pathway has a higher activation free energy. Another possible decomposition pathway yielding phenylpyruvate also requires a considerably high reaction activation free energy. The reactions of iron(III) and nickel(III) with phenylalanine have also been investigated. It has been found that these two transition metal ions are not considered as better oxidizing agents than cobalt ions.

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PP-101

Interaction of Gluconate Derivatives with Magnetite (Fe_3O_4) Surface in α -D- glucose coated iron oxide nanoparticles: A DFT study

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Pharmacologically active anticancer drugs reach to tumor tissue with low specificity and they have dose-dependent toxicity in chemotherapy applications. Classical drug administration routes are oral and intravenous. Orally taken tablets or capsules result in irregular pharmacokinetic due to the metabolic pathways and they frequently damage healthy tissues due to low specificity. Nowadays, after the developments in nanotechnology, it is possible reduce these harmful side effects by using nano particular drug delivery systems [1,2]. When α -D-glucose coated iron oxide (magnetite) nanoparticles are loaded with anticancer drug (e.g. doxorubicin), this drug loaded iron oxide nano particles can be directed to tumor tissues via an external magnetic field by mostly eliminating the side effects of classical oral treatment [3-5].

In the present study, we have computationally investigated the thermodynamics and characteristics of the interactions between gluconate derivatives and Fe_3O_4 surface in α -D-glucose coated iron oxide nano particles. Since this system is enormously large for quantum chemical calculations, we used $[\text{Fe}_{10}\text{O}_{12}]^{2+}$ surface as the model system to mimic the characteristics of glucose coated iron oxide surface. Approaches of several gluconate derivatives to the model $[\text{Fe}_{10}\text{O}_{12}]^{2+}$ surface were computationally studied at DFT-M06-2X/LANL2DZ level. The results of M06-2X calculations indicated that gluconate and its derivatives spontaneously bind to the surface and they form strong chemical bonds after exothermic reactions. Gluconate and molecule A have a four-dentate bonding character with the iron oxide surface. Molecule B has a five-dentate bonding character with the iron oxide surface (Fig.1).

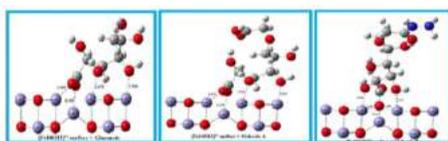


Fig. 1 M06-2X/LANL2DZ optimized structures of gluconate derivatives with the $[\text{Fe}_{10}\text{O}_{12}]^{2+}$ surface

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PP-102

Immobilization of *Hypocrea jecorina* β -Galactosidase onto Chitosan Beads

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Enzymes are biocatalysts that promote the rate of reaction, without itself consumed in the reaction and can be used repeatedly for many times as long as they remain active. Enzymes generally work at mild conditions of pH, temperature, and pressure in comparison to chemical catalyst that requires extreme conditions to promote the rate of reactions. Because of these qualities, enzymes reduce manufacturing costs as well as make the process energy saving. The enzyme β -galactosidase (3.2.1.23) is classified as a hydrolase, with transferase capacity for galactosil groups, catalyzing the hydrolysis of the terminal residue β -galactopyranosil from lactose (Gal β 1 4Glc) to form a mixture of glucose and galactose. The enzyme hydrolysis of lactose is an important biotechnological process, especially for lactose intolerant people and for recycling or reusing of whey. The enzymatic activity of β -galactosidase is important both from nutritional and technological aspects. β -Galactosidases can be found in nature, distributed among plants, animal organs as well as in large amount of microorganisms, such as filamentary fungi, bacteria and yeasts.

For industrial applications, enzyme immobilization is required to facilitate the continuous and long-term processing and reuse of the biocatalyst. Industrial enzymes have been immobilized by adsorption, entrapment, microencapsulation and covalent attachment on various insoluble carriers. The influence of immobilization on catalytic activity depends on the type and structure of enzyme, physical and chemical structure of the carriers, activity methods and specific conditions of the assay. Chitosan is the deacetylated product of chitin and it appears to be economically attractive because chitin is the second most abundant biopolymer available in nature after cellulose. As an ideal support for enzyme immobilization, chitosan offers a unique set of characteristics: biocompatibility, biodegradability to harmless products, non-toxicity, physiological inertness, antibacterial properties, hydrophilicity, and remarkable affinity to proteins.

This work aims to investigate the immobilization of the β -galactosidase onto chitosan beads and determine its properties such as the optimal operating pH and temperature, the thermal and storage stability of the enzyme, and the kinetic parameters K_m and V_{max} of the enzyme β -galactosidase from *Hypocrea jecorina* strain QM9414. According to the our results, the immobilization yield was found as 80%. The optimal pH for free enzyme activity was found to be 7.0 while the optimal pH for immobilized enzyme activity was found to be 8.0, while the optimal operating temperatures were 37 °C and 80 °C, respectively. The immobilized enzyme retained nearly 100% of its initial activity when it was stored at 4 °C for 30 days.

PP-103

A New Approach to Structure–Tacticity Relationships of Bulky Methacrylates

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Controlling the tacticity (stereochemistry) of a polymer is highly desirable because it influences its physical properties such as the melting point, solubility, density, crystallinity and mechanical strength (1). Experimental studies have demonstrated that methyl methacrylate (MMA) and other aliphatic methacrylic esters had a tendency to form syndiotactic rich polymers, presumably due to steric repulsion between the alpha-methyl groups and the ester groups(2). However, the syndiotactic preference decreases, rather than increases, as the ester side chain becomes more bulky, to the extent that some exceptionally bulky monomers form highly isotactic polymers. It has been suggested that these differing impacts of steric repulsions are due to changes in the chain structure as the size of the bulky groups increase. Theoretical calculations are performed to explore the origin of inherent tacticity in bulky methacrylates. Geometries and conformer distributions of monomers and oligomeric propagating radicals are calculated to study the impact of steric bulk interactions on the preferences for meso versus isotactic propagation. Our quantum chemical study has demonstrated a correlation between the preference for meso propagation and the steric bulk of the ester side chain, where the latter is measured as the volume of the side chain. We have also confirmed that syndiotactic methacrylates prefer linear chains, isotactic methacrylates prefer helical chains and the increasing isotactic preference with chain length can thus be understood in terms of the increasing helical tendency as substituents become more bulky.

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PP-104

The Stability Behavior of Poly(Maleic Anhydride-co-Vinyl Acetate)- Doxorubicine Polymer-Drug System in Simulated Body Fluids

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Modern advances in drug delivery are now predicated upon the rational design of polymers tailored for specific cargo and engineered to exert distinct biological functions. Polymers have played an integral role in the advancement of drug delivery technology by providing controlled release of therapeutic agents in constant doses over long periods, cyclic dosage, and tunable release of both hydrophilic and hydrophobic drugs. [1]

In this study, bioactive polymeric drug delivery system, MAVA/DX, was synthesized by the reaction of poly (maleic anhydride-co-vinyl acetate) (abbreviated as MAVA) copolymer and Doxorubicine (DX) active chemotherapeutic agent. At specific intervals, the stability behaviors of MAVA/DX system have been examined by Zeta Potential Analyzer and UV Spectrophotometer in different simulated body fluids such as daily fresh prepared SBF, PBS buffer and dextrose (5%) solutions. Zeta potential, mobility, conductivity and particle size of prepared polymer-drug system were determined by using the Zeta Potential Analyzer in different SBFs. Absorption and permeability of MAVA/DX, MAVA and DX were also determined by UV Spectrophotometer to check the stability of MAVA/DX, MAVA and DX solutions in SBFs.

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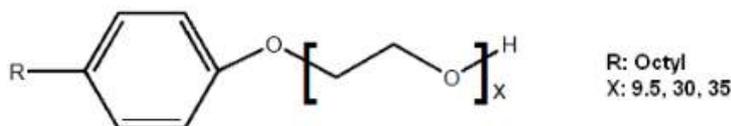
PP-105

Semicontinuous Emulsion Copolymerization with Triton X Series

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Nonionic surfactants, in general, composed of a polyethylene oxide chain to which a hydrophobic part is attached, have widespread industrial and technological applications [1]. Detergency, foaming, emulsification, and lubrication are just a few examples of processes in which these surfactants used [2].



The copolymerization of vinyl acetate (VAc) and butyl acrylate (BuA) in water semicontinuous emulsions made with the nonionic surfactant, Triton X, was studied as a function of ethylene oxide (EO, x) and their concentrations. The copolymerization of VAc and BuA was initiated by peroxide at proper temperature in order to improve the efficiency of droplet nucleation and maintain the stability of the emulsion. The effects of EO's in the surfactant structure and surfactant concentration on latex colloidal, adhesion, and film forming properties were investigated.

Acknowledgement

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PP-106

Moleccular Modelling of Enolase From *Trypanosoma cruzi* that Causes Chagas' Disease

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The protozoan parasite *Trypanosoma cruzi* causes Chagas' disease known as American trypanosomiasis. Chagas' disease is found to be common in Latin America, United States of America and has reached to dangerous level in Europe in recent years. According to World Health Organisation report in 2014, about 7 million to 8 million people is infected by *Trypanosoma cruzi* worldwide. Cardiovascular diseases are also found to be mostly related to vector-borne Chagas' disease. In the current fighting against the disease is applied either as treatment of the disease with benznidazole and nifurtimox drugs or vector is controlled as an effective prevention method. But, methods defined are not efficient to diminish Chagas' disease. Enolase is one of the key enzyme in the parasites metabolism and converts 2-phosphoglycerate (PGA) to phosphoenolpyruvate (PEP) in the glycolytic pathway. An enolase enzyme homology model was built by comparative modeling using MODELLER software. Modelled 3D structure was generated with experimentally defined structure of a homologous protein as a template using BLAST protein structure database. Secondly, for the purpose of evaluating the model quality was performed using ERRAT, PROSA and RAMPAGE web based programs. Besides, secondary structure of the protein, physical and chemical parameters were determined using SOPMA and ProtParam softwares. In summary, built homology model leads to further docking studies to find out potential inhibitors of *Trypanosoma cruzi* enolase to possibly combat the disease.

PP-107

Synthesis and Applications of Alkyldimethylamine Oxide Surfactant and its Carbon Distribution Analysis by HPLC**Ahmet Ozemre , Hande Savas , Ebru Toprak**

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Generally, detergents are used for removing soils from fabrics, dishes, human bodies, and other articles. So, it is very important to ensure mildness of such detergents in the fields of all household goods, since detergents are in direct contact with the human body [1].

Amine oxides constitute a class of substances that is used in various areas of chemistry [2]. Amine oxides come under the special class a surfactant known as amphoteric surfactants. The main reason behind that is, amine oxide changes from net cationic via zwitterionics to nonionics on going from low to high pH; which confirms it's amphoteric nature [3]. Amphoteric or zwitterionic surfactants contain both positive and negative charges in their hydrophilic polar heads that can change between anionic or nonionic character and the cationic character depending on the pH value [4-6]. Amphoteric surfactants have unique properties such as low toxicity, no significant effect of small change in temperature, high stability against electrolytes, acids, alkalis, hard water, and degradation by reducing or oxidizing agents [4-8].

In this study, we synthesized alkyldimethylamine oxide by oxidation of tertiary amines by hydrogen peroxide. The characterization of a surfactant's carbon distribution was performed by High Performance Liquid Chromatography. The effects of carbon distribution on the physical properties of the end-product were investigated in detail using various characterization methods.

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PP-108

Validated spectrofluorimetric method for the determination of famciclovir in in Pure and Pharmaceutical Preparations

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A sensitive spectrofluorimetric method was developed for the determination of famciclovir in in pure and pharmaceutical preparations. The method is based on the derivatization reaction of famciclovir with fluorescamine. The different experimental parameters that affect the fluorescence intensity were carefully studied, at once. The method was validated for linearity, limit of detection, limit of quantification, precision, accuracy, recovery, robustness. The assay was linear over the concentration range of 100 and 1000 ng/mL. The limits of detection and limit of quantification were calculated to be 51.13 ng/mL and 153.39 ng/mL. The proposed method was applied to study of famciclovir in pure and in pharmaceutical preparations.

PP-109

Experimental FT-IR, Laser-Raman and DFT spectroscopic analysis of 2,3,4,5,6-Pentafluoro-trans-cinnamic acid

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In this study, the experimental and theoretical vibrational frequencies of a newly synthesized 2,3,4,5,6-Pentafluoro-trans-cinnamic acid have been investigated. The experimental FT-IR ($4000-400\text{ cm}^{-1}$) and Laser-Raman spectra ($4000-100\text{ cm}^{-1}$) of the molecule in solid phase have been recorded. The theoretical vibrational frequencies and optimized geometric parameters (bond lengths and bond angles) have been calculated by using density functional theory (DFT/B3LYP: Becke, 3-parameter, Lee-Yang-Parr) and M06-2X (the highly parametrized, empirical exchange correlation function) quantum chemical methods with 6-311++G(d,p) basis set by Gaussian 03 software, for the first time. The assignments of the vibrational frequencies have been done by potential energy distribution (PED) analysis by using VEDA 4 software. The theoretical optimized geometric parameters and vibrational frequencies have been found to be in good agreement with the corresponding experimental data, and with the results in the literature. In addition, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies and the other related molecular energy values have been calculated and depicted.

PP-110

In silico Investigation of Anti-Biofilm Effects of the Lichen Secondary Metabolites on *Pseudomonas aeruginosa* Attractant – Repellent Mechanism

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Pseudomonas aeruginosa, one of the opportunistic bacteria, causes serious infections and diseases such as cystic fibrosis via biofilm formation. It is demonstrated that biofilm formation in bacteria is regulated by Quorum Sensing (QS) mechanism, which is a part of bacterial Two Component System (TCS). QS could be briefly described as the mechanism whereby an individual microorganism synthesizes small diffusible signal molecules that are perceived by surrounding organisms. The attractant-repellent mechanism, regulates bacterial attachment on surfaces, is also under the control of TCS. There is a need for novel, environment-friendly, less toxic and organic active substances, natural resources in the case of inhibiting bacterial quorum sensing mechanism, herewith biofilm formation. Lichens, the unique symbiotic organisms formed by association of fungi and algae, are able to synthesize numerous specific 'secondary metabolites' that have various effects such as antibacterial, antifungal, antitumoral, antiherbivore, allelopathic, etc. These organisms are used as ancient medicines and today their numerous effects have been scientifically proven. Thus, lichens are thought to be the candidates of these natural resources. *In silico* (computer-based molecular simulations) methods as molecular docking are recently used in order to save time and cost from expensive laboratory works and to generate preliminary data for further studies. Molecular docking, is a procedure that estimates non-covalent binding interactions of 3D structural macromolecules; proteins and small ligands as candidate drug molecules. Therefore, the objective of this study is *in silico* inhibition of proteins are responsible for the attractant – repellent mechanism in *P. aeruginosa* quorum sensing system. In this study, a 3D ligand library consisting of 607 secondary metabolite molecules and azithromycin as a control antibiotic of *P. aeruginosa*, docked to 6 proteins (a total of 22 active and potential binding sites) in attractant – repellent mechanism via Molegro Virtual Docker (MVD) software. Results are evaluated according to Rerank scoring system of MVD. 3 out of 607 ligand molecules exhibited higher Rerank scores on the active sites of these 6 proteins than azithromycin control antibiotic. As a conclusion; the data obtained from this study could be used for further studies in the inhibition of the bacterial biofilm formation caused by *P. aeruginosa*, with the support of *in vitro* and *in vivo* researches.

Acknowledgement

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PP-111

Investigation of Energetic and Mechanistic Pathways in the Rotation of a Nicked DNA

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Rotational degree of freedom of a nicked DNA molecule is important in many cellular processes and in DNA-protein interactions. The rotation of such a nicked DNA is especially crucial in the relaxation of supercoiled DNA by human topoisomerase I.

Therefore, the dynamic mechanism of a nicked DNA rotation about the its intact strand has been simulated using Molecular Dynamic (MD) method based on the force-field potentials. In order to see large scale movement of DNA atoms, we employ a novel technique known as the Half Quadratic Biased Molecular Dynamics (HQBMD). Rotations in both directions (clockwise and anti-clockwise, that correspond relaxation of negative and positive supercoils respectively) have been performed. Fifty different simulations have been carried out. As we rotate the downstream part of the DNA, we focused on the structural and energetic changes, especially in the nicked region of the DNA. The results we obtained have been compared with the literature studies on the canonic B-DNA.

As a result of a detail discussion on the data produced out of these fifty different simulations, we have proposed the most favorable axes for the rotation of a nicked DNA molecule. The proposed DNA rotations should yield new perspectives in the relaxation mechanism of a supercoiled DNA within the enzyme, as we found different axis of rotations for positive and negative supercoiled DNAs. Also, we propose here that although a single anti-clockwise DNA downstream rotation is enough to bring DNA to the canonical form, at least two clockwise DNA rotations are needed to bring DNA to its initial structure. The current study presents the first report of the data on a nicked DNA molecule while extensive literature studies exist for only intact DNA.

PP-112**Adsorption Properties of Acid Blue 113 onto Magnetic Polymer Microspheres****Sevgi Sozucecer , Ali Kara**

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Azo dyes, which contains azo group and aromatic group in their structure, are one of the most persistent contaminants present in industrial effluents. Besides, they are highly toxic and non-biodegradable. They accordingly have high biological oxygen demand loading. Acid dyes, which have anionic colored component, cause more problems than basic and disperse dyes since anions dissolve and retain in the soil solution due to their structural negative charge. Therefore, removal of the acid dyes is of capital importance. Adsorption is a highly effective technique to reduce the concentration of stable dyes. Although number of methods such as, filtration, electrodeposition, membrane systems, ion exchange systems are used in order to remove dyes from industrial waste water as conventional physicochemical and biological treatment methods, they are ineffective for the dye removal. In this study, Acid Blue 113 is chosen as a potential carcinogenic agent according to International Agency for Research on Cancer (IARC) reports. Magnetic poly (ethylene glycol dimethacrylate-N-vinyl pyrrolidone) is used as an adsorbent due to its excellent adsorption properties observed from our previous studies. The adsorption properties Acid Blue 113 onto the magnetic polymer microspheres are investigated by means of exploring the effect of pH, concentration, temperature to dye removal.

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PP-113

Sol–Gel Phase Transition Behavior of pH and Temperature Sensitive Block Copolymers

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Smart polymers with specific responses to various environmental stimuli, including temperature, pH and electric field, have been extensively investigated. In particular, temperature and pH sensitive hydrogels, consisting of hydrophobic and hydrophilic blocks, have attracted increasing attention for their biomedical applications, e.g. as a drug delivery system, for cell encapsulation and for tissue engineering. An injectable stimuli sensitive hydrogel with a lower sol–gel transition at around physiological temperature and pH enables a pharmaceutical formulation to be easily mixed in the sol state at low temperature and pH, which will then form a gel when injected by syringe at the target location, to work as a sustained delivery depot of the drug.

Triblock copolymer hydrogels can play important roles in the biodegradable in situ gel-forming controlled drug delivery system because they show sol-gel transition, they are compatible and non-toxicity and can release drugs over an extended period.

In this study, we prepared a kind of biodegradable and injectable methoxypoly(ethylene glycol)-block-poly(ϵ -caprolactone)-poly(β -aminoester) (mPEG- b-PCL-b-PBAE) hydrogel that undergoes sol–gel phase transition (due to the difference in the mPEG and PBAE molecular weight, hydrophobic/hydrophilic block ratio and copolymer concentration) by changing the temperature and pH. The gel forming properties of these copolymers were investigated by tube inverting method. The aqueous solution of the present triblock copolymer is a free-flowing sol at ambient temperature and becomes a gel at physiological temperature and pH. The structure–property relationship of the sol-gel transition, its in vitro degradation behavior and its in vitro drug release behavior are also investigated.

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PP-114

Photocatalytic Activity of Poly(2-aminofluorene) for Degradation of Methylene Blue Under UV Light**Recep Tas¹, Muzaffer Can²**

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In the recent years, conductive polymers with conjugated double-bond, has received much attention due to its metallic like conductivity. These conductive polymers possess a relatively narrow band gap and can enable an efficient separation of charge, which is important for photocatalytic application [1]. The use of organic dye compounds in the paper, textile, food, and other industries causes pollution of the environment because of their non-biodegradability and high toxicity [2,3]. Several techniques are used for removal of such hazardous contaminants from water. Photodegradation of organic pollutants by inorganic semiconductors, for example TiO₂ and ZnO, has attracted much interest in recent years [4].

In this study, Poly(2-aminofluorene) (AFP) have been synthesized in acetonitrile the chemical oxidative polymerization of 2-aminofluorene. Scanning electron microscopy, X-ray diffraction, FTIR spectra, UV–vis spectroscopy measurements were used to characterize the resulting AFP. Photoactivity of the Poly(2-aminofluorene) polymer was evaluated by monitoring the degradation of methyl blue (MB) in aqueous solution. The change in MB concentration was monitored by determining the UV–visible adsorption of 3.0 ml of sample taken from the solution every 15 min. The polymer photocatalysts have good photocatalytic stability and can be reused five times with only gradual loss of activity. Thus, AFP polymer are efficient photocatalytic materials for degrading contaminated colored wastewater for reuse in textile industries under mild conditions.

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PP-115

Isolation and characterization of bioactive compounds from *Albizia chevalieri* (Mimosoideae)

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The isolation and structural elucidation of some secondary metabolites from *Albizia chevalieri* is described. *Albizia* is a genus of about 150 species of mostly fast-growing subtropical and tropical trees and shrubs in the subfamily Mimosoideae. Triterpenoid saponins are commonly described in this genus. *Albizia chevalieri* is used in folk medicine as purgative, vermifuge and also remedy for coughs. A decoction of leaves is used in Nigeria for dysentery. There are also reports on the local use of the leaves extract for cancer treatment. The methanol root extract of *Albizia chevalieri* was managed to purify several compounds. Few of them were characterized on the basis of spectroscopic methods and mass spectrometry analysis, as well as by comparison of their physical and spectral data with those reported in the literature.

The aim is to further investigate the cytotoxic activity of extracts and some of isolated compounds.

PP-116

The Synthesis and Mesomorphic Properties of Rod-like Liquid Crystals Derived from Terephthalic Acid

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Liquid crystal research which involves the design, synthesis and characterisation of novel materials have received considerable scientific interest since 1970s due to their striking physical properties. Their electro-optic (EO) response in ferroelectric (FE) phases made them preferentially usable in display devices. Liquid crystals nowadays are the basis of numerous technical application such as displays in mobile telecommunication and computing devices [1].

Involvement of ester moieties, acid moieties, polar group substitutions, chiral centres and flexible end chains are proved as successful strategies for the design of LC molecules with better performance. Shape of an LC molecule is also known to influence the LC organisation with characteristic phase structure [2]. The molecular structures of LC materials actually used in these devices are mostly rigid rod-like molecules which are functionalized with one or two flexible hydrocarbon tails [1]. The influence of chemical moieties and their interaction need to be investigated in order to understand the relationship between the structure of an LC phase and the chemical structure. The application of supramolecular interactions such as hydrogen-bonding in rod-like liquid crystal molecules with acid moiety is of great importance to modify their physical properties such as melting and clearing temperatures, inducing new phases with the wide thermal range and forming a thermotropic mesogen [1-3].

In this study, rod-like liquid crystal molecules derived from terephthalic acid having different alkoxy chains or branched groups in the terminal position have been synthesized and characterized using classical spectroscopic methods (IR, ^1H -NMR, ^{13}C -NMR). The liquid crystalline properties of the compounds have been investigated by differential scanning calorimetry and optical polarizing microscopy.

Acknowledgment

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PP-117

The Synthesis and Mesomorphic Properties of Salicylideneimine-based Liquid Crystal Molecules

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Aromatic Schiff bases are one of the most important class of organic compounds and have broad interest for applications in biological functional materials, photochromic materials, polymer ultraviolet stabilizers, laser dyes, and molecular switches in logic and memory circuits [1]. Besides, Salicylidene derivatives have attracted considerable attention in view of its numerous potential applications due to their ability to exhibit liquid crystal properties.

Liquid crystalline (LC) materials represent a fascinating area in soft matter science, providing new supramolecular structures, phenomena and properties [2]. Liquid crystal molecules containing an azomethine group (Schiff bases) are one of the typical structure of calamitic liquid crystal molecules. It is remarkable that Salicylideneimine unit often show interesting polymorphism. This type of molecules can be used to create some new mesogens consist of different molecular geometry. An important structural modification can easily alter the thermal behavior. For example, salicylideneimine moiety as a linear rigid segment can be connected to each other or attached to the 1,3-positions of a central phenyl ring to form twin molecules or banana-shaped mesogens, respectively [3].

Herein we present the synthesis and mesomorphic characterization of salicylideneimine compounds with different chain lengths or branched groups in the terminal positions. Additionally, the effect of molecular chirality and the intramolecular hydrogen bonding on the mesophase behaviour of these calamitic compounds consists of a relatively thermally and hydrolytically stable salicylaldimine unit has been studied. Molecular structures of all the target compounds were confirmed by spectroscopic methods (IR, $^1\text{H-NMR}$, $^{13}\text{C-NMR}$). The liquid crystalline properties of the compounds were investigated by differential scanning calorimetry and optical polarizing microscopy.

Acknowledgment

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PP-118**Characteristics of Iron-Loaded TiO₂ Supported Montmorillonite Catalysts : B-Naphtol Degradation Under UV-A Irradiation****Duygu Tuncel , A. Neren Okte**

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The novel ternary photocatalysts were prepared by deposition of iron ions (Fe³⁺) on TiO₂ supported mntmorllonite (MMT). The synthesized catalysts were characterized by using X-ray diffraction (XRD), scanning electron microscopy with energy disperse X-ray analysis (SEM-EDX) and atomic force microscopy (AFM) techniques. XRD analysis revealed characteristic anatase reflections and supplied information about cyristalline sizes of TiO₂ nanoparticles. SEM and AFM images clearly exhibited the variatios of raw MMT after ion deposition and TiO₂ loading. Photocatalytic activities of the catalysts were examined under UV irradiation for the degradation of B-naphtol probe molecule. The supported catalysts showed better adsorption capacity due to the meso-transformation of the synthesis catalysts. Also, the mixed-valence existence of Fe was found to be efficient in electron transfer reactions improving the photocatalytic activities of the supported catalysts. The highest degradation percentages were achieved with the lowest iron content. Pseudo-first order kinetics was followed in the degradation runs.

PP-119

DFT Investigation of Tetra and Octa Substituted Zinc Phthalocyanine Derivatives in Photodynamic Therapy of Cancer

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Photodynamic therapy (PDT) is becoming widely accepted as a potential treatment for many forms of cancer. PDT involves three main components, a photosensitizing compound, visible light and molecular oxygen that in turn will become the prime component of selective tumour cell destruction. Zinc phthalocyanine derivatives have attracted a considerable amount of attention as second-generation photosensitizers for treatment of malignant tumors by photodynamic therapy (PDT) in the last decade [1]. Especially for the large molecules such as metallophthalocyanines, time- dependent density functional theory (TDDFT) is a very powerful tool for precisely calculation of excited state energies and many related response properties.

The density functional theory (DFT) and time-dependent density functional theory (TD-DFT) study of the ground and excited states of zinc phthalocyanine (ZnPc) derivatives have been carried out in order to determine ground and excited state structures and absorption and fluorescence spectra. The theoretical results present an accurate description of the UV-Vis and fluorescence spectra of tetra- and octa- Poly(oxyethylene) substituted zinc phthalocyanines in solvent, providing a very well agreement with the experimental data. The detailed explanations of the electronic excitations have been presented in terms of excitation energy and oscillator strength. Furthermore, extensive molecular orbital analyses have been conducted due to obtain clear depiction of the electronic structure and compute the changes in energy of different positions of the peripheral octa and tetra substituents. The detailed atomistic-level excited state DFT calculations of the zinc phthalocyanines bring some valuable directions in the rational designing of new metallo phthalocyanine compounds having photodynamic potential in cancer treatment as well as in the experimental synthesis. The results of photophysical and photochemical measurements indicates zinc phthalocyanines have a potential as photosensitizers in applications where singlet oxygen is required [2].

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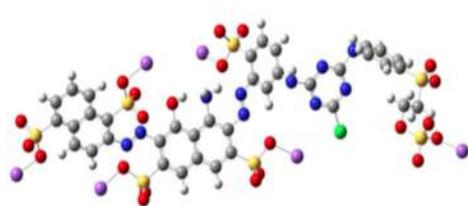
PP-120

The Use of DFT Descriptors for Prediction of the Photocatalytic Degradation Mechanisms of Reactive Blue 222 and Reactive Red 195

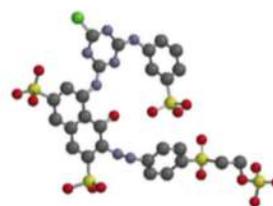
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Azo dyes are characterized by one or more ($-N=N-$) azo bonds attached to two aromatic rings combined with reactive groups making them hard to degrade. Reactive azo dyes are resistant to aerobic degradation and their degradation products are highly carcinogenic. Thus, TiO_2 photocatalysis is an alternative way to remove highly carcinogenic and toxic dyes from water and convert them to harmless compounds.



Reactive Blue 222



Reactive Red 195

This study deals with the prediction of photocatalytic degradation mechanisms of Reactive Blue 222 and Reactive Red 195 under UV light irradiation in the presence of TiO_2 . The Conceptual DFT was applied to the degradation reaction of the target molecule and reactivity descriptors were calculated by means of DFT/B3LYP/6-31G* level of theory. Eventually, the reactive sites of the molecule for OH radical attack were determined and the reaction mechanism was predicted by combining the results of the DFT calculations with the experimental FT-IR and GC-MS analyses.

Acknowledgement

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PP-121

Determination of the Inhibitory Effect of Some Coumarin Derivatives on *Bacteroides fragilis* D-LDH

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Cancer is one of the most leading causes of death worldwide. Cancer therapies have clear limitations and unfortunately projected as the primary cause of death in the future. Chemotherapy is one of the most significant methods used to treat cancer. Recent studies show that enterotoxigenic strain of *Bacteroides fragilis* is associated with colon cancer. It is an anaerobic bacteria that is found in the colon flora in human. D-lactate dehydrogenase in *Bacteroides fragilis* (BfD-LDH) is one of the key enzyme that catalyzes the oxidation of D-lactate to pyruvate and organises a major checkpoint of anaerobic glycolysis. In this study, the enzyme is targeted for potential drug design studies. Coumarins are inherently occurring phytochemicals in many plant species with a wide range of biological activities such as anti-inflammatory, antitumor, antiviral, antimicrobial, antidepressant, anticancer and anticoagulant effects. It has been shown that some hydrophobic compounds inhibit catalytic activities of D-lactate dehydrogenase (D-LDH) enzymes by binding covalently or non-covalently. Naturally occurring plant polyphenols are potent inhibitors of D-lactate dehydrogenase (D-LDH) activity. Coumarins are comprised of numerous naturally occurring polyphenolic benzo- α -pyrone compounds with important and diverse physiological activities. In this study, three coumarin derivatives C1; (3-(3,4-dihydroxyphenyl)-6,7-dimethoxycoumarin, C2; (3-(3,4-dimethoxyphenyl)-6,7-dihydroxycoumarin) and C3; (3-(3,4-dimethoxyphenyl)-6,7-dimethoxycoumarin) have been synthesized and confirmed on the basis of their spectral data in order to evaluate them as potential *Bacteroides fragilis* D-lactate dehydrogenase (BfD-LDH) inhibitors which could be used as chemotherapeutic agents in cancer therapy. They were examined for the first time for their inhibitory effect on *Bacteroides fragilis* D-lactate dehydrogenase (BfD-LDH), by using pyruvate as substrate. IC50 values for C1 and C2 were found as 9.05 and 2.28 μ M, respectively, while C3 showed no activity at 50 μ M concentration. For in silico analysis, chemicals were sketched and conformers were identified by ChemDraw v10 and MarvinSketch v6.2 programs. Docking of the coumarins were carried out using Molegro Virtual Docker and Glide Docking (Schrödinger-Small Molecule Discovery Suit 2014-3) programs. As a result of docking study, the chemicals bound to the active site residues where found. Our studies demonstrated that ortho dihydroxy coumarins were found to possess high inhibitory activity and o-hydroxyl groups at B ring of the 3-arylcoumarins is more effective than the A ring to inhibitory activity on BfD-LDH enzyme.

PP-122**A Java Program for Analysis of Nucleic Acid Sequences Towards Designing Microbial Diagnosis Kits****Osman Mutluhan Ugurel , Dilek Turgut-Balik**

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Bioinformatics analyses of peptide and nucleic acid sequences are essential for the long-term researches of most molecular approaches from nucleic acid-based microbe detection for public health to enzymes used in industrial processes. For researchers in academic studies, analysis and storage of these sequences with new identity numbers in research specific databases is a very important procedure because of Nevertheless sometimes identification can be wrong because of naming of species and gene product at genbank. But increasing biological datas complicate this procedure day by day. Huge data, software compatibility and complex data sets are the major challenges in this area. Considering that challenges, we have developed a program for analysing such nucleic acid sequences. The program is implemented in Java and is designed to set up a research specific database for nucleic acid sequences. It employs genbank format and assign identity numbers to sequences for species, subspecies and gene product. It can give a fasta file of identical genes for allingment tools and an excel list sorted by species id. This desktop tool has simple interface for user. By increasing biological datas, similar applications and research specific databases could be used to develop nucleic acid based microbial diagnosis kits.

Acknowledgement

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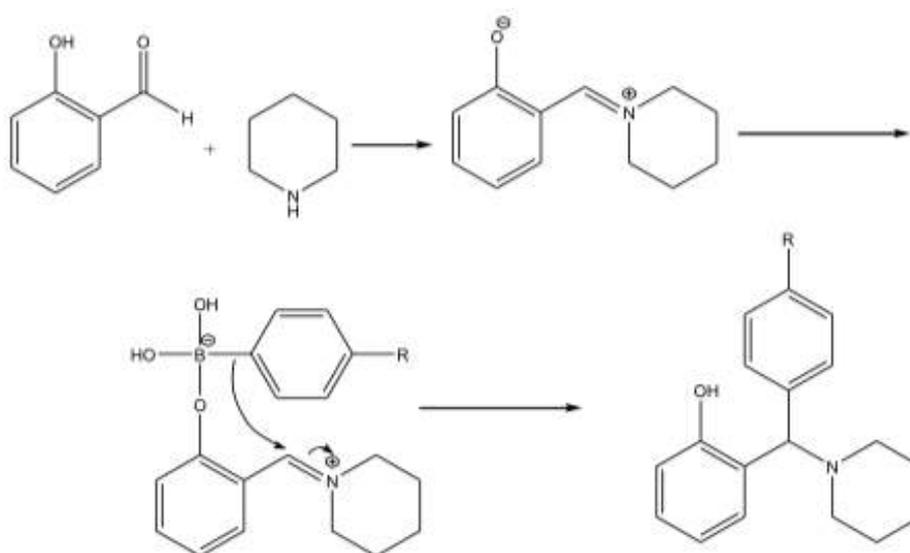
PP-123

Petasis Reaction of secondary amines with various boronic acids**Yeliz Ulas**

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Boronic acids were reacted with salicylaldehyde and secondary amines. The reaction with piperidine was provided Alkylaminophenols, which were characterized by NMR spectroscopy. Here in, Petasis reaction was carried out without catalyst. Electron donating substituents in phenyl group of boronic acid gave higher yields than the electron withdrawing substituents.



Scheme. The model petasis reaction between boronic acids, salicylaldehyde and piperidine

PP-124

Computational Bandgap Engineering of Designed EDOT Derivatives and Investigation of Their Physicochemical Properties

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Conducting polymers (CPs) are known as synthetic metals because they exhibit electric, electronic, magnetic and optical properties that are similar to those exhibited by metals and semiconductors. The discovery of high electrical conductivity in doped polyacetylene has stimulated an enormous amount of work towards the description of the electronic properties of conjugated organic polymers[1]. CPs continue to fascinate many scientists due to their potential applications in the development and the construction of new advanced materials such as sensors, photovoltaic devices, artificial muscles and displays. Over the last two decades, the quantum theory of polymers and design of efficient organic conducting polymers have witnessed a growing interest related to their appealing properties. 3,4- Ethylenedioxythiophene (EDOT) and its improved derivatives are certainly the most attractive organic conducting polymers due to both their good conductivity and stability properties[2]. These compounds are also known as competitors to other existing low band-gap polymers.

In this work, we deal with EDOT and its 3-substituted or 3,4-disubstituted analogues. Various electron donating and withdrawing groups (Cl, CN, CH₃, NH₂, OH, OCH₃) by the inductive and/or mesomeric effects were selected in order to detect the influence of these substituents on the EDOT ring system's physicochemical characteristics[3]. On that account, quantum chemical calculations were performed using the GAUSSIAN 09 package (Windows and UNIX versions) and visualization of computed structures were rendered by Chemcraft 1.7W. Geometry optimizations were carried out using ab-initio (HF/3-21G and MP2) and density functional theories (B3LYP/6-31G**, B3LYP/6-31+G**, B3LYP/6-31++G**). Molecular geometries (bond lengths, bond angles), highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO) energy levels, HOMO-LUMO energy gaps (ΔE), dipole moment (μ), polarizability (α), and Mulliken charges were calculated for all the optimized structures. The ionization potential (I), electron affinity (A), electrophilicity (ω), electronegativity (X), softness (S) and hardness (η) were also computed, respectively.



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PP-125

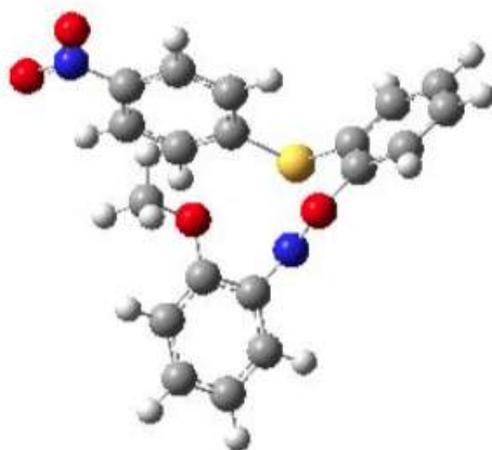
HIV-1 VIF-APOBEC3G Axis Inhibitor Characterization and DFT Modeling of the Surface

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We describe structure–activity relationship and optimization studies of RN-18, an HIV-1 Vif-APOBEC3G axis inhibitor. Chemotherapies that target inhibition of HIV-1 proteins, in particular HIV-1 protease and reverse transcriptase have been of immense help in prolonging the lives of patients with acquired immunodeficiency syndrome (AIDS). However, the high rate of HIV-1 replication has led to the emergence of drug-resistant strains that remain a major challenge in the field of anti-HIV chemotherapy. Considerable effort is being focused on understanding the structural basis of HIV-1 multidrug resistance (MDR) and to develop new inhibitors that are effective in HIV-1 MDR mutants. In this regard, we recently reported the discovery of small molecule inhibitors of HIV-1 viral infectivity factor (Vif) HIV-1 mainly infects CD4+ T lymphocytes in vivo; thus, if the infection is not controlled, the immune system becomes seriously weakened, and AIDS develops.



Calculations were carried out using the Density Functional Theory DFT/B3LYP/6-31G* levels by using COSMO as the solvation model. For this purpose, possible reactions was examined estimately using Gaussian 09 package software.

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PP-126

Flexibility analysis of communication pathways between distant functional sites on bacterial ribosome: Hints on new druggable sites

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Ribosome, a protein-RNA complex, is the molecular machine to synthesize proteins in all living cells. All stages of protein synthesis are controlled by various functional sites on the small and large subunits of the complex, which communicate allosterically as experimental data suggest [1,2]. Revealing communication pathways among distant functional sites on the bacterial ribosome is important both for understanding the functional mechanism of this molecular machine and for developing new antibacterial therapeutics targeting the signaling paths to block the transmission of information. Various studies point to the allosteric communication between the decoding center (DC), where the genetic information is decoded, and other distant functional sites such as the peptidyl transferase center (PTC) and the catalytic centers of elongation factors (EFs)[1,2]. In this study, the intact crystal structure of *Thermus Thermophilus* ribosome complexed with EF-Tu is investigated to clarify shortest signaling pathways between DC (residue A1492 on small subunit) and GTPase center of EF-Tu (residue GDP) and sarcin-ricin loop (residue G2661 on large subunit). For this purpose, *k*-shortest path algorithm³ is employed with an elastic network approach [4], describing the ribosome structure as a network of nodes linked by edges. In this representation, nodes are placed at alpha-carbon and phosphor atoms of residues, and length of edges between node pairs are calculated based on total atom-atom interactions. All pathways are analyzed in terms of phylogenetic conservation and structural flexibility. Results suggest distinct alternative signal transmission lines between these distant functional sites. Paths pass through the highly conserved intersubunit bridges B2a or B3, the entire SRL, antibiotic binding residues on ribosomal RNA, as well as the acetylated-tRNA, which was proposed to play a critical role in allosteric communication [5]. Calculated pathways may also give hints into new drug binding sites. Structural data for bacterial ribosome indicate that antibiotics usually target flexible residues, and hinder their ability to adopt distinct conformations during translation stages. Receptor flexibility is highly critical for allowing a ligand to bind, and flexibility of solvent accessible allosteric sites offer a wide range of possibilities for the drug design field [6]. Therefore, a flexibility analysis is carried along the signaling paths residues; besides the intersubunit bridge B3, the highly conserved, flexible and solvent exposed SRL seems to be an attractive site for designing new antibiotics.

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PP-127**Determining Possible Reaction Pathways of Pyridazine Molecule with OH radical****Alkan Gulsen , Yelda Yalcin Gurkan**

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Pyridazine is a widely used industrial solvent. In addition, its substituted derivatives are present in a great number of pesticides. Due to their harmful effects to living organisms, unpleasant smell, stability and solubility in water, pyridazine and its derivatives constitute an important class of water contaminants. There are many conventional methods to destroy such compounds, but each method has its shortcomings.

In this study, the kinetics of pyridazine and its hydroxy derivatives have been investigated theoretically. With the intention of predicting intermediates forming in the degradation reaction of pyridazine, geometry optimizations of the reactants and the transition state complexes have been performed with the semiempirical PM3, AM1, Hartree-Fock 3-21 ve Hartree-Fock 6-31G methods. Based on the results of the quantum mechanical calculations, the rate constants of all the possible reaction paths have been calculated by means of the Transition State theory.

Acknowledgements

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PP-128

Optimum pH Determination and Thermostability Analysis of Recombinant *Fusobacterium nucleatum* Enolase Enzyme

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Biological macromolecules including proteins, enzymes and nucleic acids have been used as a target on structure-based drug design studies. The target molecule is required to be analyzed for the drug design. *Fusobacterium nucleatum* enolase enzyme (*Fn*ENO) was identified as a target in this study. *F. nucleatum* is located on oral microbiome, responsible of infections on periodontal tissues in human. These infections generate periodontal diseases such as gingivitis and periodontitis. In addition, it has been known that this bacteria have developed resistance against several antibiotics. Enolase enzyme has a critical role in *F. nucleatum* metabolism, carries out the conversion reaction of 2-phosphoglyceric acid to phosphoenolpyruvate in glycolytic pathway. Therefore; the gene encoding enolase enzyme from *F. nucleatum* was expressed in *E.coli* (BL21)DE3 and the recombinant enzyme was purified for determination of effects of pH and temperature on the enzyme activity prior to further kinetic studies. The reaction was carried out in 50 mM Tris-HCl buffers at different pH (6,5-9,5). 1,5 mM 2- PGA was used as substrate and 1,5 mM MgCl₂ as cofactor for evaluating the effects of pH on the activity of enzyme. As the results; optimum pH was determined as 8,5. Then, thermostability analysis of *Fn*ENO were performed at different temperatures (60°C, 40°C, 30°C) for 15 minutes in reaction assay consists of 1,5 mM 2-PGA, 1,5 mM MgCl₂ and 50 mM Tris- HCl buffer, pH: 8.5. Significant variations on *Fn*ENO enzyme activities at different temperatures were not observed and the enzyme activity remained stable for 15 minutes at different temperatures. In conclusion; these biochemical parameters can be used in both kinetic analyses and further inhibitor studies towards structure-based drug design.

PP-129

Salt Effect on Poly(sulfonic acid diphenyl aniline)

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The polymers bearing both positive and negative charges, i.e. polyzwitterions, were investigated in order to use of drug delivery and especially gen transfer. It seems possible that these polymers can bind to the gen by means of their charges and they can release the gen after transportation if provided the required conditions such as, pH, salt concentration, etc. However, the aggregates of the aliphatic polyzwitterions are not so much stable and then decompose during transportation.

Poly (sulfonic acid diphenyl aniline) (PSDA) is a water soluble and more stable aromatic polyzwitterion since it bears both positive and negative charges. Therefore, it bears the potential for the use in controlled delivery of a gene or drug. In order to investigate the suitability of PSDA for this field, the zeta potential, hydrodynamic radius and ionic conductivity of the PSDA aggregates in aqueous solutions were measured as a function of pH, type of salt and salt concentration. SEM/STEM pictures of some samples were taken. It was found that PSDA can give some pH sensitive aggregates of which size and shape can change by salt type and concentration at very low pH values. It was concluded that PSDA can be used in drug and gen delivery systems and in preparing pH sensitive materials at very strong acidic media.

Acknowledgements

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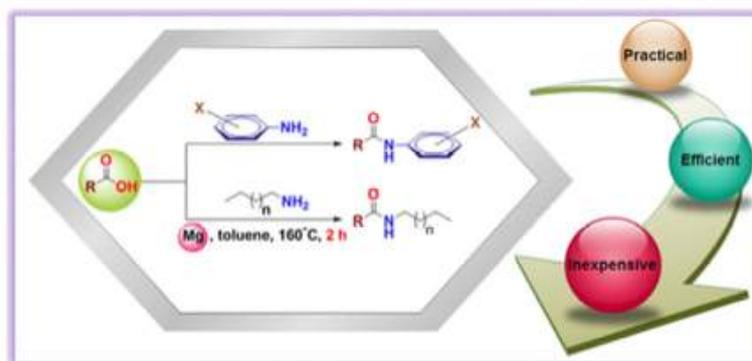
PP-130

Metallic magnesium an efficient catalyst toward N-aryl and N-alkyl substituted amides directly from aliphatic carboxylic acids

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Because of their biological and chemical significance, amides are important as biological active compounds, industrial products and precursors for variety of organic compounds. The preparation of amides directly from carboxylic acids is fairly difficult task. The most commonly used process for synthesizing amides in a laboratory scale is converting the carboxylic acids with special reagents into their more reactive acyl halide or anhydride derivatives and then to make interact these derivatives with amines. However, some reagents such thionyl chloride (SOCl_2) and dicyclohexylcarbodiimide (DCC) are moisture sensitive, toxic and require special reaction conditions. Therefore, alternative methods for the direct synthesis of amides have attracted considerable interest. But available methods have several disadvantages. For the conventional amide preparation method carboxylic acid is allowed to react with the amine at elevated temperatures. Especially for the preparation of anilides long reaction times at $180\text{--}200^\circ\text{C}$ is require and due to these excessive reaction conditions the final product is contaminated with dark coloured decomposition products. Also the by-products complicate isolation of amide from observed complex mixture and in most cases considerably reduces its yield. Because of all these disadvantages, alternative efficient and cheap method for direct conversion of aliphatic carboxylic acids into N-aryl and N-alkyl amides was developed. This simple method does not require any special coupling reagents for the conversion.



PP-131

Electron Paramagnetic Resonance of Cu^{2+} Ions in Pyridine-2,6-Dicarboxylato Complexes

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EPR studies on $[\text{Cu}(\text{H}_2\text{dpc})(\text{dpc})]\cdot\text{H}_2\text{O}$, Cu^{2+} -doped $[\text{Cd}_2(\text{dpc})_2(\text{H}_2\text{O})_6]\cdot 2(\text{H}_2\text{dpc})$ [H_2dpc : pyridine-2,6-dicarboxylato; dpc :pyridine-2,6-dyil bis complexes have been performed at ambient temperature in three mutually perpendicular planes. The principal values of g tensors were obtained. The studies revealed that the paramagnetic centers have rhombic symmetric g values. The calculated results of the Cu^{2+} -doped $[\text{Cd}_2(\text{dpc})_2(\text{H}_2\text{O})_6]\cdot 2(\text{H}_2\text{dpc})$ indicate that Cu^{2+} ion substitute with the Cd^{2+} ion in the host lattice. It is found that the ground state of the unpaired electrons in the $[\text{Cu}(\text{H}_2\text{dpc})(\text{dpc})]\cdot\text{H}_2\text{O}$ complex is dominantly $\text{dx}^2\text{-y}^2$ and unpaired electrons' life time is spent over this orbital. The optical absorption spectrum of $[\text{Cu}(\text{H}_2\text{dpc})(\text{dpc})]\cdot\text{H}_2\text{O}$ shows two bands, centered at 521 nm (19194 cm^{-1}) and 638 nm (15674 cm^{-1}) which confirms the rhombic symmetry. The molecular orbital bond coefficients of Cu^{2+} ion in d^9 state is also calculated by using EPR and optical absorption parameters.

PP-132

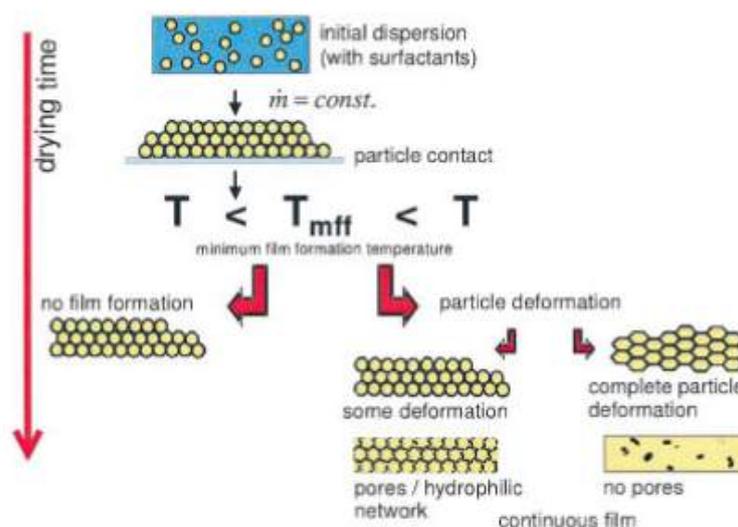
Paint Formulation Using Waterborne Latex and Film Formation Property

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Compared to solvent-based formulations, aqueous latex dispersions, aqueous polyurethane dispersions or alkyd emulsions are environmentally-friendly alternatives for coating and paint formulations. Acrylic latexes are widely used for paints mainly because of their good exterior durability, film clarity, stability under excess of UV, heat and alkalinity, and a good dirt pickup/crack resistance balance [1-2].



The copolymer latex of vinyl acetate and butyl acrylate in water semicontinuous emulsions made with the mixture of anionic and the nonionic surfactants. Water-borne paints were prepared by blending this latex and the mill base in a 250 mL lined tin. This blend was then stirred at low shear for 10 min. The paint was then filtered through a 125 μm nylon mesh. The effects of additives in paints on colloidal, adhesion, and film forming properties of water-based paint were investigated.

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PP-133

Extraction of Anthocyanines from fruits

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Anthocyanins are one of the main ingredients of the fruits and they are naturally colouring substances for fruits, vegetables and plants [1] and most of anthocyanins have been found in nature [2,3].

Anthocyanins are extracted from plants by using methanol containing small amounts of hydrochloric acid. In the present study, the ultrasonically assisted extraction has been established to extract anthocyanins from fruits of blueberry and cranberry. The factors affecting the extraction efficiency has been searched such as selection of solvent, ratio of solid/liquid, number of extraction and extraction time for both fruits. The optimum conditions for extraction were examined.

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PP-134**Comparison and Determination of Total Phenolic Content of Red Pepper Flakes in Maras Region**

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The interest in the consumption of pepper fruits (*Capsicum annum* L.) is, to a large extent, due to its content of bioactive compounds and their importance as dietary antioxidants. Phenolic compounds, especially phenolic acids and flavonoids, are considerably present in vegetables and fruits; thus they are an integral part of the human diet. Recently, they have received much attention since many epidemiological studies suggest that consumption of polyphenol-rich foods and beverages is associated with a reduced risk of cardiovascular diseases, stroke and certain forms of cancer [1]. These protective effects have partly been ascribed to the antioxidant properties especially of flavonoids. Kahramanmaras, which ranks 28th rank in Turkey in terms of agricultural potential, stands out with production and industry of 'Maras Pepper'.

In this study we aimed that phenolic compound of red pepper flakes in Maras province extracted and compared total phenolic content of this extract. Total phenolics of twenty red pepper flakes collected from Maras Province were analyzed spectrophotometrically using the modified Folin-Ciocalteu colorimetric method [2].

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PP-135

Preparation of Hierarchical Porous Polyester Composites via Emulsion Templating

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Hierarchical porous polymer composites have been synthesized by the cross-linking of the continuous phase of polyester/divinylbenzene (UPE/DVB) water-in-oil concentrated emulsion templates with the presence of conventional surface modified montmorillonite nanoclay. The effect of monomer composition, emulsifier concentration, and internal phase amount on the emulsion stability and the morphology of the resulting porous composites have been investigated. Furthermore, the degree of nanoclay loading on the mechanical and morphological properties of the resulting composites has been investigated. All the composites reinforced with nanoclay particles were found to have an improved mechanical strength comparing to bare polymer matrix. Moreover, the morphological features, namely surface area and cell diameter, were found to be altered dramatically with the amount of nanoclay loading.

PP-136

Microspherical PolyHIPE Composites**Funda Cira , E. Hilal Mert**

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The fabrication of open porous microspherical polyHIPE composites have been demonstrated by using water-in-oil-in-water (w/o/w) double emulsions. PolyHIPE particles were generated by the polymerization of individual high internal phase emulsion (HIPE) droplets in a secondary aqueous medium consisting of a surfactant (hydroxyl ethyl cellulose, HEC) and water-soluble initiator (potassium persulphate, KPS). HIPEs were prepared by dispersing the internal phase in the continuous phase. The aqueous solution of pullulan, a linear homopolysaccharide composed of α -1,6 and α -1,4 maltotriose units, was used as internal phase; while the mixture of glycidyl methacrylate (GMA), 1,3-butanediol dimethacrylate (BDDMA), a polymeric surfactant (Pluronic L121) and an oil-soluble initiator (2,2'-asobissobutyronitril, AIBN) was used as the continuous phase. The particle size distribution and morphological features, namely surface area and pore size of the resulting microspherical polyHIPEs have been investigated depending on the composition of the double emulsions. Further functionalization procedure has been carried out by using functional amine compounds for the modification of the resulting materials.

PP-137

Effect of pH and Temperature on the Adsorption of Textile Dye onto Nanotube

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Considering that food, cosmetics, paper, automotive, but most importantly, textile industry use pigments and dyes to color their products, then, wastewater discharges from these are worrisome. In the last few decades, adsorption has been proved to be a well-established and cheap pollutant removal process among other purification techniques. From the multitude of available adsorbents carbon nanotubes are one of the most popular for both liquid and gas purification due to their porous structure and large sorption capacities. Multi-walled carbon nanotubes was used as adsorbent for successful removal of Disperse Yellow 211 textile dye from aqueous solutions. The effects of pH, shaking time and temperature on adsorption capacity were studied. The experimental adsorption equilibrium data were compared with the Langmuir, Freundlich and Temkin isotherm models and the isotherm model parameters were determined. The obtained results suggest that the solution temperature and pH appears to be a key factor of the Disperse Yellow 211 adsorption process. Pseudo- first-order and pseudo-second-order equations were fitted to the kinetic data, and the rate constants were evaluated. The samples revealed relatively fast kinetics reaching equilibrium in around 90 min, which follow the second-order-rate equation, while adsorption unaffected by the pH of the solution.

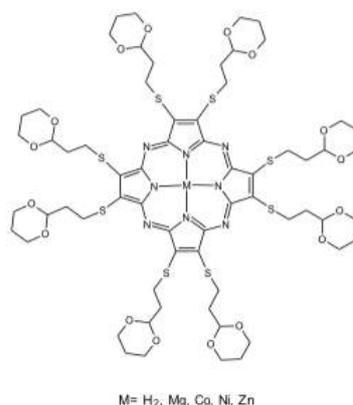
PP-138

Synthesis, characterization, spectral, aggregation and fluorescence properties of novel porphyrazines

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Porphyrazines, which are the latest in the discovery of tetrapyrrole-macrocycles among porphyrins and phthalocyanine, are now the subject of increasing importance and interest in their synthesis, properties and application [1-3]. Their applications involve diverse areas such as biomedical agents for diagnoses and therapy, precursors to new conducting materials, chemical sensors, ladder polymers and dyes [4]. In this work, the synthesis, characterization, photophysical and spectroscopic properties of the peripherally bulky 2-(ethyl)-1,3-dioxanethio substituted free-base, zinc, nickel, cobalt and magnesium porphyrazines are reported.



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PP-139

Synthesis, spectral and fluorescence properties of double-decker Lu(III) and Eu(III) phthalocyanines bearing peripherally octakis-[4-(thiophen-3-yl)-phenoxy] substituents

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Sandwich-type porphyrinato and/or phthalocyaninato complexes, in which two planar and parallel conjugated p-systems are held in close proximity by lanthanide metal cation between the two macro-tetrapyrrole rings, have been intensively studied over several decades in both fundamental academic and applied fields [1]. They are chemically robust and therefore have been used as dyes, pigments, catalysts for the removal of sulfur in oil, and more recently expanding in many fields such as xerography, optical discs, laser dyes, molecular metals, electro-catalysis, chemical sensors, magnetic materials, and photodynamic cancer therapy [2]. In this study, we report the synthesis and characterization, spectral and fluorescence properties of peripherally octakis-[4-(thiophen-3-yl)-phenoxy] substituted phthalocyaninato sandwich-type rare earth complexes. The new compounds have been characterized by elemental analysis, UV, FT-IR, ¹H-NMR spectroscopy and mass spectra.

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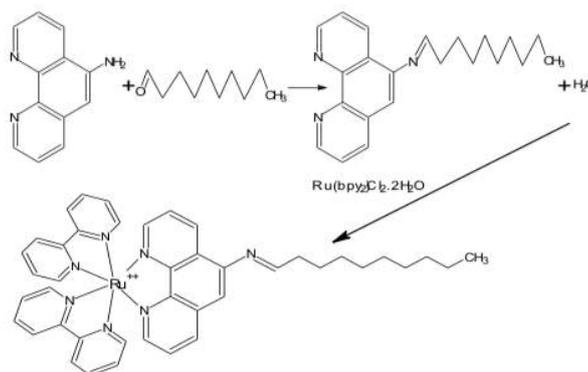
PP-140

The Easy Soluble 1,10-Phenanthroline Derivative of Schiff Base, its Ru(II) Complex and Fluorescence Properties

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Schiff bases are formed when any primary amine reacts with an aldehyde or a ketone under specific conditions. Structurally, a Schiff base is a nitrogen analogue of an aldehyde or ketone in which the carbonyl group (C=O) has been replaced by an imine group.[1,2] We report here the synthesis and characterization a new multi donor Schiff base derivative ligand, carrying N3 donor atoms, namely 5-decanaldehydeimino-1,10-phenanthroline (L), prepared from the condensation reaction of 5-amino-1,10-phenanthroline with decanal and its complex with Ru(II) was obtained.



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PP-141

Optimization of Low-Cost Culture Media for Microbial Levan Production

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Levan is a fructose homopolysaccharide that is produced by a variety of microorganisms in sucrose-based media. Due to its outstanding properties like high solubility in oil and water, strong adhesivity, good biocompatibility and film-forming ability, microbial levan find wide range of commercial applications in various fields such as food, feed, packaging, chemical, textile cosmetics and pharmaceutical industry, agriculture and medicine. In fact, a recent literature analysis on microbial exopolysaccharides attributed levan together with xanthan, curdlan and pullulan as the most promising polysaccharides for various industrial sectors hence levan has a high commercialization potential. Moreover, there is a growing body of interest in research associated with levan and its applications. It is microbially produced in Switzerland, Germany, England, China, Korea, Japan and USA using mesophiles at very high production costs. Hence development of novel microbial production processes for levan holds great industrial importance. Recently, halophilic bacterium *Halomonas smyrnensis* AAD6^T has been reported as a high-level levan producer extremophile for the first time by our research group. Extremophilic microorganisms provides great advantages for the development of novel and low-cost production processes for levan by eliminating the risk of contamination as well as the energy and time needed for sterilization. Using both conventional and systems based approaches, production yields in semi-chemical media were substantially improved. Considering the important effect of fermentation substrate on production costs, the sucrose containing sugary wastes of the University Dining Hall were used as a substitute for sucrose and improved the production yields with concomitant reduction in production costs. Further reduction in costs was achieved by replacing distilled water with tap water and using Natural Salt samples obtained from companies located in Erzincan.

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