Two Day International Conference on

Recent Advances in Interdisciplinary Natural Sciences

27th–28th January 2022

Organized by

Department of Chemistry

Govt. College Women University, Faisalabad

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University of Alto, Finland

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Dr. Muhammad Shahid (Department of Chemistry, University of Agriculture, Faisalabad)

Dr. Asim Mansha (Department of Chemistry, GC University, Faisalabad)

Conference Program, 27-th January 2022, Day-I

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Inauguration **Jinnah Auditorium, GCWUF** **9:00-10:00 am PST**		
09:00-10:00am	Inauguration, Recitation from the Holy Quran by Ms Hafiza Hafsa Naat-e-Rasool e Maqbool by Ms Hira Rafique Remarks by Prof. Dr Imran Asghar, International Chair, Aalto University, Finland Vote of Thanks by Dr. Zill-i-Huma Nazli, National Chair Remarks by Chief Guest, Prof Dr Iqrar Ahmad Khan, Vice Chancellor, University of Agriculture. Faisalabad. Word of wisdom by Patron in Chief, Prof Dr Robina Farooq, Vice Chancellor GCWUF Distribution of Shields/Certificates	
Plenary Lecture Jinnah Auditorium, GCWUF 10:00-11:00 am PST		
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12:10-12:25 pm PST	Samina Jam Nazeer Ahmad, Department of Botany, University of Agriculture Faisalabad, Pakistan. Efficacy of Azadirecta indica fabricated zinc nanomaterial for the management of Rhopalosiphum pedi L. (*Hemiptera: Aphididae)*	30
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12:40-12:55 pm PST	Dr Sameera Shafi, Department of Chemistry, The Islamia University of Bahawalpur, Bahawalnagar campus. Synthesis of Silica Aerogel/Glass Fiber Composites with Improved Insulation and Mechanical Performance	32
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Chair: Prof. Dr Amir Jamil, Department of Biochemistry. University of Agriculture, Faisalabad. Co-Chair: Dr. Muhammad Anjum Zia, Department of Biochemistry. University of Agriculture, Faisalabad. Session Convener: Dr Sadia Nazir, GC Women University Faisalabad.		
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05:10-05:25 pm PST	Faisal Nadeem. Department of Chemistry, Kohat University of Science & Technology, Kohat. Effective Antiplasmodial Activities of Synthesized Iron oxide Nanoparticles using Extract of Nephrolepis Exaltata	95

Plenary Lecture

NATURAL PRODUCTS AS INSPIRATION FOR NEW CHEMISTRY IN ANTIBACTERIAL AND MATERIALS SCIENCE

Moloney G. Mark

Department of Chemistry, University of Oxford, Chemistry Research Laboratory, Mansfield Road, Oxford OX1 3TA, United Kingdom

mark.moloney@chem.ox.ac.uk

Abstract:

Natural products can provide inspiration for applied synthetic chemistry. This lecture describes how natural products have proved to be valuable starting points for the development of a completely novel class of antibacterial agents, and for the development of stable carbene precursors which have found application as surface modifying agents for a wide range of materials. The lecture will illustrate that the application of synthetic organic chemistry has an important role to play in the development of new technology which impacts on biology and materials science

Plenary Lecture

Hemicelluloses as Drug Delivery Materials

Iqbal.Saeed Muhammad

Department of Chemistry, Forman Christian College. Lahore.
saeediqbal@fccollege.edu.pk

Abstract

Hemicellulose is the second most abundant, renewable, non-toxic, and biodegradable hetero-polysaccharide after cellulose in plants consisting of different saccharide units [1]. The versatile physical and chemical properties of hemicelluloses make them a promising material for pharmaceutical and biomedicine applications [2, 3]. One of the most promising applications of hemicelluloses is their use in drug delivery systems [4 – 9]. Such systems can afford sustained, pulsatile and targeted drug deliveries. The objectives to be achieved from a delivery system are: i) to enhance bioavailability, ii) enhance efficacy and iii) minimize adverse effects. This talk will present an overview of the underlying principles and state of art relating to drug delivery.

Poster Session

Human Lung Cancer Targeted Cytotoxicity, Nuclear Condensation, and Mitochondrial Membrane Potential of Nepeta Paulsenii, A Perennial Herb

Hanif Aqsa, Tanwir Samina*, Ahmed Nazeer Jam, Hameed Mansoor, Mustafa Ghulam

Department of Botany, University of Agriculture Faisalabad, Pakistan

*saminatanveer414243@gmail.com

Abstract:

Nepeta is a genus of largest family Lamiaceae containing 300 species. It is widely distributed in different regions of Asia, Africa, America, and India. Amongst different plant families known for their therapeutic and medicinal values, Genus Nepeta of Lamiaceae (Mint family) remains relatively important. Hence, phytochemicals of nepeta paulsenii were extracted from different parts of the plant, like leaves, flowers, stem, and roots by using different solvents (water, methanol, ethyl acetate) obtaining 12 fractions. Each of the dried extract material was subjected to the Infrared spectroscopy (FT-IR) and Gas Chromatography-Mass Spectrometry (GC-MS) to assess possible identification of chemical constituents. The anticancer potential of each fraction were assessed trough MTT assay, Cell viability assay, and Nuclear Condensation. The cytotoxic potential of the Nepeta paulsenii was determined by the cytotoxicity which was based on the detection of lactate dehydrogenase (LDH) released from dead cells because of cytotoxicity. Effect of the extract on nuclear chromatin condensation in human lung cancer (A549) cells was quantified by fluorescence microscopy using Hoechst 33258 stain. Nuclear condensation and cytoplasm shrinkage was examined under a fluorescent microscope. Cells with bright colored, condensed or fragmented nuclei were considered apoptotic. The number of cells with apoptotic morphology was counted in randomly selected microscopic fields per well. Detection of the changes in mitochondrial membrane potential in A549 cells after the treatment with the extract was assessed by the retention of rhodamine 123. All assays were performed in triplicate and the final data was reported as mean ± SD. Various concentrations of Nepeta extracts were analyzed and then half-maximal inhibitory concentration (IC50) values for all the experiments were calculated by linear regression analysis (LRA).

Keywords: Nepeta Paulsenii, Lung Cancer, Isolation, Characterization

Silver loaded alumina (Ag-Al2O3): An effective visible light active photo catalyst for aqueous phase degradation of methylene blue dye

Ayesha Rafiq; Tooba Jabeen; Muhammad Saeed*

Department of Chemistry, Government College University Faisalabad, Pakistan

*msaeed@gcuf.edu.pk

Abstract:

Visible light induced photo catalytic degradation of dyes is an inviting approach in wastewater treatment techniques. In this study, silver loaded alumina (Ag-Al2O3) is used as catalyst for aqueous phase photo degradation of methylene under visible irradiation. Ag nanoparticles were immobilized on Al2O3 by facile green methods using leaves aqueous extract of Azadirachta indica. Advanced characterization techniques like particle size distribution, XRD, TGA, EDX and SEM were used for characterization of as prepared Ag-Al2O3 particles. The prepared Ag-Al2O3 was tested as catalyst for degradation of methylene blue under visible irradiation. Ag-Al2O3 showed improved photo catalytic performance for the degradation of methylene blue dye in aqueous medium. Effect of various parameters on catalytic activity were investigated. Curve Expert computer program was used for kinetics analyses of the data according to Eley-Rideal and Langmuir-Hinshelwood mechanism. A 100 mgL-1 solution (50 mL) completely degraded in 120 minutes of reaction duration at 50°C over 0.1g of Ag-Al2O3 as catalyst.

Keywords: Al_2O_3; Azadirachta indica; Methylene blue; Langmuir-Hinshelwood; Eley-Rideal

Aquatic Pollution of Microplastics and its Effects on Wildlife

Munir Asma[1], Naseer Rehana[1*], Zada Laiq [3]

Department of Chemistry, Government College Women University Faisalabad, Pakistan

[1]asmach994@gmail.com

Abstract:

Plastics are widely used in the packaging process due to their durability, hydrophobicity, low molecular weight, and cost-effectiveness. Plastics have a very slow degradation ability and most plastic products take up to 450 years to degrade completely. When plastic is exposed to UV radiation and wind abrasion, the plastic disintegrates into smaller particles (microplastics) and persists in the environment. The size of microplastics is less than 5 mm, and even various methods for wastewater treatment are unable to filter these small particles. Microplastics lead to the rivers and sea through drainage, rainfall, and streams. The numerous sources of microplastics in the oceans and their negative effects on marine animals are discussed here. The tiny size of these plastic particles renders them conveniently available for ingestion by a diversity of marine habitats, inflicting detrimental consequences on their health. Microplastics' ability to absorb several hazardous hydrophobic pollutants from the surrounding environment distributes these contaminants into the food chain in an indirect manner. As a result, new laws and guidelines must be created to address the major issue of microplastic contamination in the marine ecosystem. To minimize future risks, it is critical to stop producing it and replace it with environmentally suitable alternatives.

Keywords: Microplastics, wastewater, degradation, ecosystem, contamination

Effect of Reactive Group Chemistry on Printing Properties of Newly Synthesized Reactive Dyes Applied on Cellulosic Fabric

Siddiqua Habibah Umme *, Ali Shaukat, Nawaz Bhatti Haq, Yasir Madiha

Department of Chemistry,University of Agriculture Faisalabad, Pakistan

u.habibah5@gmail.com

Abstract:

Cellulosic fabric is a distinguishing printing substrate throughout the world in the textile industry. We have studied the effect of reactive group chemistry (nature, number, and position) on the printing properties of cellulosic fabric by newly synthesized six reactive dyes (D-1 to D-6) containing 2, 4, 6 trichloro- 1, 3, 5 triazine and 2[(4-Aminophenyl) sulfonyl] ethyl hydrogen sulfate functional groups. Effect of printing parameters including temperature, urea, and alkali on the physicochemical printing properties (fixation, color yield, and penetration) of dyes was explored and delineated. Results demonstrated that dyes with additional reactive groups and more linear and planar structures (D-6) revealed boosted printing properties. Colorimetric properties of printed samples were examined through spectraflash spectrophotometer which displayed superb color buildup. UPF of the printed samples was excellent to very good. Excellent colorfastness and presence of sulphonate groups entitled these reactive dyes commercially viable for urea free printing of cellulosic fabric.

Keywords: Printing properties; heterofunctional; fixation; penetration

EPIDEMIOLOGY OF IRON DEFICIENCY ANEMIA IN WOMEN OF REPRODUCTIVE AGE GROUP - A GLOBAL PERSPECTIVE

Momin Abdul[1]

National University of Medical Sciences (NUMS), Rawalpindi, Pakistan

abdul.momin@numspak.edu.pk

Abstract:

According to the estimations of the World Health Organization, approximately 50% of all pregnant women all around the world suffer from iron deficiency anemia (Aikawa et al. 2006; McLean et al. 2009). The World Health Organization furthermore reveals that around 56% of the pregnant women residing in developing countries are anemic. On the other hand, the prevalence of anemia among pregnant women in developed and/or industrialized countries has been found to be as 18%. It has been estimated that amongst non-pregnant women, the prevalence of anemia is 29% worldwide, whereas this figure increases to 38% for pregnant women. In terms of numbers, these prevalence percentages equate to 496 million non-pregnant women while 32 million pregnant women. For children, the equivalent number has been estimated to be 273 million. In case of severe anemia, the figures reveal that the condition is even more alarming. 50% non-pregnant women and 60% pregnant women across the globe have been approximated to be suffering from severe anemia (Peña-Rosas et al. 2014). In terms of prevalence of anemia, Asian continent is affected the most as 50% of all anemic women in the world live in the Indian sub-continent. Out of these women, 88% develop anemia through the course of pregnancy. National Nutrition Survey of Pakistan, 2018-19 revealed that 41.7% women of reproductive age group are anemic while 18.2% of these women are iron deficient. Thus, iron deficiency anemia is a serious threat to women belonging to the reproductive age group worldwide.

Keywords: Iron deficiency anemia; Women of reproductive age group; National Nutrition Survey; Pakistan

Nonwoven Hygiene Material: Sanitary Pads

Arshad Uzma, Yasmin Farah, Shafiq Nusrat*

Department of Chemistry, Government College Women University Faisalabad, Pakistan

*drnusratshafiq@gcwuf.edu.pk

Abstract:

This poster mainly emphasis on the chemistry of highly engineered composites and polymers. Concern is raised about environmental consequences, biodegradability and sustainability of polymeric material used in the production of sanitary pads.

Keywords: nonwoven hygiene material (NHMs), sanitary pads, polymers

Novel Phenolic Compounds As Potential Therapeutic Candidates Against SARS-Cov-2, Using Quantum Chemistry, Molecular Docking And Dynamic Studies

Rehman-ur-Shafiq[1], BiBi Shamsa[1*], Zia Maimoona

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

shafiq.urrehman@uaf.edu.pk; shamsa.shafiq@uaf.edu.pk

Abstract:

Anticancer drug delivery is now becoming a challenging approach for researchers as it allows controlled drug delivery near cancerous cells with minimized generic collection and avoiding secondary side effects. Hence in this work, the applications of nanostructures as anticancer drug delivery carriers are widely investigated to target cancerous tissues. Based on DFT calculations, we have investigated transition metal-doped boron nitride nanostructure as a drug delivery agent for Gemcitabine drug utilizing B3LYP/6-31G (d, p) level of theory. In this research, adsorption energy and electronic parameters of Gemcitabine drug on interaction with metal-doped BN nanostructures have been studied. It has been observed that metal doping significantly enhances the drug delivery properties of BN nanostructures. Among investigated nanostructures, Ni-BN has been found as the most prominent nanostructure to transport Gemcitabine drug with the elevated value of adsorption energy in the both gas phase (-45.79) and water media (-32.46). The interaction between Gemcitabine drug and BN nanostructures is confirmed through frontier molecular orbitals and stabilization energy analyses. The fractional charge transfer, MEP, NCI, and NBO analyses exposed the charge transfer from drug molecule to BN nanostructures. Transition density maps and UV-VIS spectra were also plotted to investigate the excited state properties of designed complexes. Thusly, the present study provides an in-depth interaction mechanism of Gemcitabine drug with BN which reveals that metal-doped BN nanostructures can be a favorable drug delivery vehicle for Gemcitabine anticancer drug.

Keywords: SARS-CoV-2, Phenolic compounds, Molecular docking, Molecular dynamics, ADMET.

Interaction of Victoria Blue dye in anionic and cationic micellar media: Spectroscopic Study

Noor Sadia[1], Naz Iram, Taj Babar Muhammad

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

[1]sadiaa613@gmail.com

Abstract:

The interactional study of a tri phenyl methane-based cationic dye Victoria Blue B (VBB) in the micellar media of various surfactants is presented in this manuscript. We herein are reporting the interactional study of the cationic dye in the presence of ionic surfactants [Sodium Dodecyl Sulphate (SDS); Sodium Docusate (SD) and Cetyltrimethylammonium Bromide (CTAB)] in aqueous media**.** The measurements at various micellar concentrations of surfactants were accomplished by UV-Vis absorption spectroscopy. The quantitative measure of interaction of the dye with surfactants in terms of partition constant (Kc), partition coefficient (Kx), binding coefficient (Kb), and their corresponding Gibb's free energy of partition (ΔGp), binding (ΔGb) were assessed from that spectroscopic data. The presence of anionic surfactant caused a greater red-shift in UV–Vis absorption of the dye and indicated their strong interactions as compared to cationic surfactant.

Keywords: Absorption spectroscopy, Micellization, Partitioning coefficient, Solubilization; Surfactants; Victoria Blue-B

Serum: Wonderful Skincare Product

Yasmin Farah, Arshad Uzma, Shafiq Nusrat*

Department of Chemistry, Government College Women University Faisalabad, Pakistan

*drnusratshafiq@gcwuf.edu.pk

Abstract:

A serum is an amazing skincare product which is used before moisturizing but after cleansing with intent to deliver an elevated concentration of potent ingredients (i.e., vitamins, moisturizing agents and antioxidants) to skin. Serums possess the capability to penetrate the deep layers of the skin,that makes them an effective tool to focus specific skin concerns, such as acne, wrinkles, brightness, or hydration.

Keywords: serum, skincare, vitamins, moisturizers

Synthesis, Characterization, Docking Study and Anti-Cancer Evaluation of Novel 5-Fluorouracil Derivatives Against Hct-116 Colorectal Cell Lines

Jubeen Farhat*; Ijaz Sana; Sultan Misbah; Niazi Khan Bilal Muhammad, Jubeen Ishrat,

Huma-Nazli -i-Zill

Department of Chemistry, Government College Women University Faisalabad, Pakistan

*dr.farhatjubeen@gcwuf.edu.pk

Abstract:

To synthesize 5-Fluorouracil (**5**-FU) co-crystals with four different amino acids (Glycine, Leucine, Alanine **and** Tryptophane**)** dimers coformers via a co-crystallization protocol with an objective to enhance its antitumor effectiveness and cell-target specificity**.** The solution method was employed in the formation of four **5**-FU co-crystals with (2,**5** Diketopiperazine, 3,6-Dimethyl-2,**5**-Piperazinedione, 3,6-bis-2-methylpropyl piperazine-2,5dione, cyclic dioxopiperazine-L-tryptophane). Co-crystal development was supported by the FTIR and PXRD. Via FTIR, the main peaks of concern in the of **5**-FU spectrum, frequency (v) of N-H (3416 cm-1) and of carbonyl group (1671 cm-1), were significantly shifted in all the spectra of co-crystal exhibitingthe replacement as well as the development of already existing interactions with new ones. The new solid crystals were characterized by PXRD, distinctive peak of **5**-FU at 2θ = 28.48o was noticeably shifted in the co-crystal's graphs, not just in position but also Full Width at Half Maximum (FWHM) and intensity values. MTT assay was implemented by varying the concentrations of the drug from 0.78 to 200 μg mL−1**.** Somewhat different results against two cell line of the efficacy of 5FU (API) and co-crystals were examined. However, amongst all the new solids co-crystal forms, 5-FU-Luecine dimer and **5**-FU Tryptophane dimer co-crystals obtained via solution protocol shown to be the most efficient cell proliferation inhibitor against Colonic Cancer cell line at all concentrations.5FU Alanine dimer, **5**-FU-Luecine dimer and **5**-FU Tryptophane dimer indicated the most effectiveness at all concentrations against MCF 7 (Breast Cancer**)** cell line. Using the MOE (Molecular Operating Environment) software molecular docking and structural analysis of the interactions between the protein and **5**'-fluorouracil was done**.** Docking studies using the GOLD (Genetic Optimization for Ligand Docking**)** software were used to investigate the potential anti-cancer activities of the novel co-crystals against a colorectal **a**nd breast cancer target proteins (Thymidylate synthase (PDB ID:1HVY), protein kinase (PDB ID: 2X18) and C-myc. (PDB ID: 6G6K). Docking results indicated that new solid forms have promising anti-cancer effectiveness as compared to 5FU alone. After the effective synthesis **of these** cocrystals and consequent enhancement of cancer cells growth inhibition capability of **5**-FU**,** these new co-crystals can further than be assessed for in **vivo** examinations and membrane crossing abilities in future.

Keywords: 5-Fluorouracil**,** Co-crystals**,** Amino acids dimers, PXRD, FTIR, Molecular Docking**,** MTT assay**,** anticancer effectiveness

ADSORPTION PROCESS OPTIMIZATION FOR REMOVAL OF SELECTED DYES FROM POLLUTED WATER USING GRAPHENE OXIDE/CELLULOSE BASED COMPOSITE

Shafi Humaira, Nazir Sadia*

Department of Chemistry, Government College Women University Faisalabad, Pakistan

dr.sadianazir@gcwuf.edu.pk

Abstract:

Graphene oxide/cellulose composite was used for removal of reactive red 2 (RR2) and malachite green (MG)dyes from waste water using adsorption method. Extent of removal of selected dyes reactive red 2 (RR2) and malachite green (MG) by using graphene oxide-cellulose composite were estimated by UV-Vis spectroscopy. Different parameter affecting batch adsorption like pH, initial dye concentration, time and temperature were optimized to get maximum removal**.** Composite show maximum absorption for reactive red 2 (RR2) and malachite green (MG) dyes at pH 9 and 10 respectively. Kinetics, equilibrium and thermodynamics of the adsorption process were studied. Pseudo-second order was best fitted for prediction of kinetic study of both dyes**.** Among isotherms, the Langmuir isotherm well defined the sorption process **of** dyes onto composite**.** Thermodynamic parameters calculated values such as ΔG°, ΔH° and ΔS° showed the studied method is exothermic and spontaneous. All the data was statistically analyzed by ± S.D and regression analysis**.** Characterization of synthesized composite was done using Fourier Transform Infrared spectroscopy (FTIR). The whole study proved that selected composite has good removal potential for reactive red 2 and malachite green dyes containing wastewater.

Keywords: Graphene oxide, Cellulose, Adsorption, Malachite green, Reactive red 2, Optimization.

Optimizing cellulose-chitosan based composite for adsorption of ciprofloxacin from aqueous solution: Experimental and theoretical studies

Kinza[a*], Kausar Abida [a]

Department of Chemistry, Government College Women University Faisalabad, Pakistan

[a*]kinzaafzal838@gmail.com

Abstract:

In the present work dynamic adsorption of the pharmaceutical compounds such as ciprofloxacin from aqueous media was investigated by using cost effective adsorbent based on cellulose derived from waste paper. Cellulose nanocrystals (CNC) were synthesized, which were further utilized for synthesis of CNC/ chitosan adsorbent. The adsorbent was subjected to adsorb ciprofloxacin at different pH (2-12). Maximum adsorption capacity (67.89mg/g) was found at pH-7, for ciprofloxacin with CNC/ chitosan composite. Different parameters affecting batch adsorption like pH, temperature, initial drug concentration and time for CNC/ chitosan film to obtain maximum adsorption for the ciprofloxacin. Pseudo-second order is best fitted to adsorption data. Freundlich, Halsey and Dubinin-Radushkevich isotherm are most suited and optimum to determine the nature of adsorbent to adsorb ciprofloxacin. Calculated values of thermodynamic parameters i.e. ΔG°, ΔH° and ΔS° showed that adsorption process is exothermic and spontaneous. Confirmation of interaction between composite and ciprofloxacin was studied through DFT method. Characterization of ciprofloxacin onto CNC/chitosan composite has been studied by Particle size and Fourier transform infrared spectroscopy (FTIR).

Keywords: Cellulose, Chitosan, Ciprofloxacin, Adsorption, Isotherm, Kinetic

Inhibitory Potential of fruit wastes against the Biosynthesis of

Aflatoxins by Aspergillus Species in Wheat Grains.

Naseer Rehana[1], Munir Asma[2]

[1,2]*Department of Chemistry, Government College Women University, Faisalabad, Pakistan*

rehanan735@gmail.com

Abstract:

Plant material have wide application in agriculture to enhance shelf life and are better substituents than synthetic preservative. The current study was aimed to investigate Inhibitory potential of Citrus peel and Pomegranate peel powder against the growth and production of aflatoxins by *Aspergillus flavus* and *Aspergillus parasiticus* in wheat grains. Wheat grains with 21 % moisture level were Inoculated with spores of mould and stored with powdered peels (20% w/w) at 30℃ for seven months. Production of aflatoxins was estimated by HPLC at different time interval showed that maximum level of aflatoxin B1 accumulation by *Aspergillus flavus* and *Aspergillus parasiticus* in control samples was 123.24 ng/g and 98.65 ng/g. Pomegranate peel fully inhibit the aflatoxin B1 synthesis by *Aspergillus flavus* for 5 month and for 4 month by *Aspergillus parasiticus* while Citrus peel fully inhibit aflatoxin B1 synthesis for one month by *Aspergillus flavus* and *Aspergillus parasiticus.* However, Pomegranate peel fully inhibit synthesis of B2 ,G1 and G2 for 4 month and Citrus peel showed similar inhibitory effect for 1 months at same storage conditions. Studies showed that both fruit-wastes considerably inhibit aflatoxin production in wheat for long-term storage.

Keywords: Aflatoxins, *Aspergillus flavus,* wheat, fruit wastes, *Aspergillus parasiticus*

Session-I

Nano-Chemistry & Nano-Technology Applications

Invited Talk

Nanotechnology an emerging area for biosensors; defining key roles of nanomaterials in construct of biosensors

Hayat Akhtar[1]

Interdisciplinary Research Centre in Biomedical Materials (IRCBM), COMSATS University, Islamabad, Lahore Campus, 54000, Pakistan

akhtarhayat@cuilahore.edu.pk

Abstract:

The recent years have witnessed a major influence of nanotechnology in the field of biosensors. The integration of nanomaterials in the construction of biosensors is aimed to achieve better analytical figures of merit in terms of limit of detection, linear range, assays stability, low production cost, etc. Nanomaterials can play a variety of roles in the development of responsive, easy-to-use, and field portable biosensors. In this line, significant research efforts have been made towards exploration and synthesis of various types of nanomaterials for subsequent use in the fabrication of biosensors. Nanomaterials can act as an immobilization support, signal generating probe, signal amplifier, signal quencher, mediator and artificial enzyme label…etc. The present work will define the key roles of nanomaterials and relate the nano-based features to the analytical performance of the biosensor design. A critically analysis and level of success for each design will be discussed with emphasis on the future directions.

Meanwhile, as nanomaterials have become more widely accepted nanostructures entities, the risk of their release into the environment and resulting effects on ecosystem health is becoming a growing issue that must be addressed. The research on nanotoxicology will also be considered in the present work. Understanding the relationship between biosafety and nanomaterials is a crucial aspect of the future research.

In vitro screening of locally available herbal extracts and essential oils for their activity against fungus Malassezia furfur

Abrar Shazia[*a], Rafi Rida [a], Kiran Shumaila [a] , Rashid Rimsha [a]

Department of Applied Chemistry, Government College University, Faisalabad, Pakistan

Abstract:

Malassezia spp. are lipophilic yeasts that cause various skin diseases such as pityriasis versicolor, seborrheic/atopic dermatitis, and dandruff. The medications used to treat this fungal infection are based on older azole drugs, which have a number of side effects. The aim of this study is to assess the activity of different spices and herbs such as Cinnamon (Cinnamomum verum), Clove (Syzygium aromaticum), Hemp (Cannabis sativa), Lemongrass (Cymbopogon) and Moringa (Moringa oleifera) against dandruff causing fungus Malassezia furfur (M. furfur). All the extracts and oils were evaluated for their anti Malassezia activity by disc diffusion method. All the herbal extracts and essential oils exhibited antifungal activity against M. furfur when compared with standard Ketoconazole (32.2 ± 0.4 mm). Methanolic extract of moringa exhibited maximum activity 30.5 ± 0.4 mm. Antifungal activities were also shown by methanol extract of cinnamon i.e. 28.8 ± 0.9 mm, ethanol extract of clove 28.5 ± 0.5 mm, and lemongrass essential oil i.e. 28.2 ± 0.15mm. These findings suggest that the above mentioned essential oils and extracts can be applied as anti-dandruff agent in different skin care formulations. Proper use of herbs for the disease of dandruff will largely minimize the harmful effects and irritation potential caused by antifungal drugs.

Efficacy of Azadirecta indica fabricated zinc nanomaterial for the management of Rhopalosiphum pedi L. (Hemiptera: Aphididae)

Jam Samina[1]

Department of Botany, University of Agriculture Faisalabad, Pakistan

saminatmalik@yahoo.com

Abstract:

Rhopalosiphum pedi L is an important pest, damaging cereal crops globally. Due to the attack of this major pest, wheat cultivars could not meet the yield potential in many countries including Pakistan. It sucks the cell sap through its stylet, injects the toxic saliva, and also transmits the pathogens in the host plant. Short life cycle and frequent development of biotype is the main problem for the management of this pest. The main objective of this study was to check the effectiveness of Azadirecta indica synthesized zinc nanoparticles against R. pedi L. The trial was conducted in the semi-field condition with four levels of zinc nanoparticles and water as control treatment. Nanoparticles were sprayed in three doses 50, 100, 150 and 200 ppm of 50 ml. Results revealed that zinc nanoparticles significantly suppress the aphid populations. Variable suppression of R. pedi L. was observed at different concentrations. But no significant difference was observed between the two highest concentrations i.e., 150 and 200 ppm (89.87% and 92.25% mortality). Moreover, LD50 of nanoparticles was found to be 95.028 ppm with the slop 2.670. It can be thought that this study could be the first report which demonstrated that zinc nanoparticles could be used in R. pedi L. control. Additionally, this study could be highly helpful for the researcher to develop effective IPM strategies.

Keywords: Wheat aphid; zinc nanoparticles; IPM; Nan-pesticide

Green synthesis of magnesium oxide nanoparticles using Azadirachta indica leaves for mitigation of Reactive Red 195 dye

Kiran Shumaila[1]

Department of Applied Chemistry, Government College University, Faisalabad, Pakistan

shumaila.asimch@gmail.com

Abstract:

The synthetic dyes are being used in various applied fields. Their discharge is polluting our environment badly. The effluents having synthetic dyes are dangerous for eco-system. Bio-sorption is a low-cost and active mode for abolition of noxious dyes from the environment. Nanotechnology, in the present age is an evolving field to construct biomaterials of desired nano shape and size. Awareness of sustainable, low-toxic and greener attitude is increasing rapidly leading to green synthesis of nano-particles. Our research work was focused to synthesize eco-friendly Magnesium oxides nanoparticles (NPs) using the aqueous leaf extracts of neem *(Azadirachta indica*). Then synthesized nanoparticles were characterized by SEM and XRD analyses. Then the characterized nanoparticles were optimized for the remediation of Reactive Red 195 dye. All the results were recorded for spectral analyses. All the data were analyzed statistically. The currently synthesized magnesium oxide nanoparticles via a greener approach could be applied for the elimination of other toxic dyes as well.

Keywords: green synthesis, magnesium oxide nanoparticles, nanotechnology, reactive red 195 dye, remediation

Synthesis of Silica Aerogel/Glass Fiber Composites with Improved Insulation and Mechanical Performance

Shafi Sameera

Department of Chemistry, The Islamia University of Bahawalpur, Bahawalnagar Campus

Abstract:

Silica aerogel is a kind of amorphous mesoporous material with high specific surface area, low density, and high porosity, and is the best thermal insulation material to date. It has broad applications, such as in the thermal insulation material, sound insulation, dust removal, optics, catalysis, chromatographic separation, and drug delivery system. However, the mechanical properties of the silica aerogel are poor due to its highly porous structure, making it hard to use directly. In our study, a new strategy was proposed to improve the mechanical properties of the composite without deteriorating its thermal insulation property. Given the problems of existing big void space in the composite of silica aerogel/glass fiber and the weak combination between them, and long drying period, the composite was prepared by using an acid-base catalyzed sol-gel and supercritical CO_2 drying method, and characterized and analyzed by SEM, TEM, BET, FTIR, constant thermal analyzer, mechanical compressing tester, etc. The effects of adding silica gel and gas-phase silica on the properties of the composites were studied. The mechanisms of improving the performance of the composite were explored. The main results and conclusions are as follows:

The effects of adding 200-450 mesh size silica gel on the properties of the silica aerogel/glass fiber composite were investigated. Different amount of adding silica gel from 1%, 3%, 5%, 7% and 9% were examined. Results showed that the thermal conductivity of the composites decreased first and then increased with an increasing further amount. With adding 5 wt. % of silica gel, the thermal conductivity of the composite were reduced greatly at room temperature (25℃). SEM images showed that the added silica gel filled the void spaces between the glass fiber and silica aerogel, acted as a bridge between them through the Si-O-Si network. The added silica gel not only provides a skeleton structure for the aerogel but also enhances the strength of the composite. Moreover, it reduced thermal conductivity by the reduction of the route ways of heat transportation via decreasing the spaces between the fibers largely. The results provide a new strategy for improving the performances of the thermal insulating and mechanical strength of the composites.

Moreover, the preparation of the hydrophobic silica aerogel/glass fiber felt was studied by using tetraethylorthosilicate (TEOS) and methyltrimethoxysilane (MTMS) as co-precursors with adding silica gel. Results showed the lower thermal conductivity of the at room temperature when the ratio of TEOS: MTMS and silica gel addition were 1:1 and 5 %, respectively. The water contact angle and the density of the felt were 150°and 0.281g/cm3, respectively. The combination between the fiber and the aerogel of the felt was strong without a dust-release issue and had good thermal stability (664℃).

The effects of the amount of adding fumed silica (1%, 3%, 5%, 7%, 9%, and 12%） on the thermal insulation and mechanical properties of the composite were investigated too. SEM and TEM images showed that the fumed silica interconnected with the silica aerogel, and the big pores of the former reduced to the mesoporous and became a part similar to the latter, forming a mesoporous network. Therefore, the introduction of the fumed silica to the composite not only reinforced the -Si-O-Si- network on the surface of the fiber but also improved the pore structure. Thus, thermal insulation and mechanical performance were improved greatly. The research results provide a new method for the preparation of excellent thermal insulation materials.

Keywords: silica aerogel; glass fiber; silica gel; fumed silica; supercritical carbon dioxide

Silsesquioxanes-Based Nanolubricant Additives with High Thermal Stability, Superhydrophobicity, and Self-cleaning Properties

Ahmed Numan[1], Zhang Xianwei [2], Fahad Shah [3], Jamil Imran Muhammad [4], Aziz Tariq [5], E. Husamelden[6], Bittencourt Carla [7], Wan Jintao [8], Fan Hong [9]

[1]numan.bs922@outlook.com

Abstract:

Nanoadditives are promising materials for long-envisioned next-generation lubricants to achieve excellent tribological performance and thermal stability. Here, an instigative and novel approach has been scrutinized to facilely prepare the nanolubricant additive. For this purpose, three synthetic strategies were designed for i) preparation of uniform-sized poly(methyl silsesquioxane) (PMSQ) nanoparticles, ii) hydrosilylation of the long carbon chain of ethyl 10-undecenoate and iii) modification of PMSQ nanoparticles with hydrosilylation product through a condensation reaction, in order to obtain long-carbon-chain grafted nanohybrids. The morphology, composition, and properties of these nanohybrids were confirmed by 1H-NMR, FTIR, SEM, EDS, and TGA. The effects of different concentrations of unmodified and modified PMSQ nanoparticles on the tribological properties of silicone oil were discussed. In the comparison of unmodified PMSQ nanoparticles, the modified one performs very well to reduce the coefficient of friction and wear scar diameter at low concentration. The TGA results revealed the extraordinary thermal stability of these particles, as their weight loss was only 19% at 800 °C which is remarkably higher than other solid lubricant additives. In this research, we tried to fill the deficiency of thermally stable material in the field of heavy machinery and industry. In addition, the environment-friendly (fluorine-free), superhydrophobic and self-cleaning surface effect of modified PMSQ nanoparticles was also observed. These silsesquioxane-based nanohybrids having synergistic effects, advantageous scientific values, and promising application prospects are expected to be more useful with other longer carbon chains.

Keywords: Nanohybrids, Solid lubricant additive, Thermal stability, Hydrosilylation, Tribological performance, Self-cleaning

Synthesis and Characterization of Nano-Silicon Dioxide and Its Effects on Plants: A Review

Yasmin Farah [1], Sultana Sabiha [2], Shafiq Nusrat [1*], Arshad Uzma [1], Rashid Maryam [1], Parveen[1] Shagufta

Department of Chemistry, Government College Women University Faisalabad, Pakistan.

[1*]drnusratshafiq@gcwuf.edu.pk

Abstract:

Nanotechnology is a strenuously emerging area of science. The main reason of this intensive emergence of nanotechnology is immense expectations that have been placed on the accomplishments of nano-science in numerous sectors of society. Silica nanoparticles is considered the utmost admired nanomaterial as it has application in several fields, like wastewater treatment, food processing, environmental remediation, household and industrial applications, biosensor, disease identification, and biomedicine, etc. In agronomics, the utilization of Silicone dioxide nanoparticles as transporters in medicine delivery, or in take up and transformation of nutritive constituents and insecticide etc., has been considered specially. As, the impacts of Silica nanoparticles on herbage have been rarely investigated, so the intention of recent review article is to synopsize latest progress in research on the synthesis, characterization and the effects of Silica nanoparticles on plants.

Keywords: Nanotechnology, Silica nanoparticles, Silicon dioxide, Agronomics, biomedicine

Behaviour of FePc Molecules on the two-four fold Cu Facets

Rehman-ur-Ateeq[1], Zhang H .J[2], Kashif Ismail[3], Bao Shining[4]

Department of Physics, University of Agriculture, Faisalabad-Pakistan.

[1]ateeq215@hotmail.com

Abstract:

Organic molecular semiconductors have attracted tremendous attention in experimental and theoretical research due to their unique properties and widespread applications that range from biomedical through environment and information and communication to national security. In this scientific event, I will talk about the comparative study on the electronic and structural properties of iron phthalocyanine molecules on the two (four) Cu facets (Cu(110) and Cu(100)) which was carried out in the framework of density functional theory calculations. The strength of the molecule–substrate interactions is interpreted in terms of the lateral adsorption geometry and the site specific electronic structure of the molecule. In the case of FePc on a (100)-oriented copper surface, the benzopyrrole leg is found to be oriented at an angle of 9o or 3o from the [01-1] substrate direction. Further, an upward bend in the molecular plane ranging from 7o to 10o is also observed; giving an almost buckled shape to the molecule. This topological phase transformation from flat to almost buckled shape is attributed to the strong FePc-Cu(100) interaction. Interestingly, in the case of FePc on Cu(110), neither a bend nor a sizable rotation is observed. From the general knowledge of the principles of structural and electronic properties, it is concluded that FePc–Cu(100) interaction is relatively stronger than FePc–Cu(110) interaction, which is further evidenced by the charge transfer, work function changes, changes in the shape of the adsorbed molecular orbitals, and the orbital shifts. Furthermore, the density of states analysis shows that the valence band level shift is surface- and site-dependent.

Keywords: iron phthalocyanine; density functional theory; electronic and structural properties; copper

Session-II

Emerging Technologies in Environmental Sciences

Invited Talk

Designing of Organic Functional materials for optoelectronic applications

Javed Iqbal*

Department of Chemistry, University of Agriculture, Faisalabad, 38000, Pakistan.

Javed.Iqbal@uaf.edu.pk

Abstract:

Our research centralizes on modeling and DFT analysis of intended chromophores based on various cores to render them as economic competitors for solar cells. Substantial investigation on molecular levels of researched molecules is accomplished by pursuing computational DFT and TD-DFT simulations to probe photovoltaic characteristics. Different computational methods are used to analytically observe molecules for their simulated values of absorption maximum, frontier molecular orbitals **(FMOs),** ionization potential **(IP),** electron affinity **(EA),** light harvesting efficiency **(LHE),** quantum chemical parameters i.e. chemical potential ($\boldsymbol{\mu_0}$)**,** chemical hardness ($\boldsymbol{\eta}$), chemical softness (**S**), electronegativity ($\boldsymbol{\chi}$), and electrophilicity index (**ω**). Additionally, other geometric variables such as density of state **(DOS),** electrostatic potential **(ESP),** transition density matrix **(TDM),** binding energy **(E_b),** dipole moment **(μ),** reorganization energy **(RE),** and device performance **(V_{OC})** are enumerated**.** Results uttered that all our modeled molecules are preferential candidates for optoelectronic applications. Because of low RE values of electron mobility (λ_e) and hole mobility (λ_h) of designed chromophores, they exhibit magnified charge mobility. All designed chromophores depicted intensified metrics computationally, which is a convincing rationale for their possible experimental usage in developing solar cell technology.

Keywords: Density Functional theory; Organic Photovoltaics; Open circuit voltage; power conversion efficiency

Investigation of Catalytic Properties of Fish Scales Based Material.

Tullah Zakira [1]

Department of Chemistry, University of Wah

[1]fawad.ahmad@uow.edu.pk

Abstract:

In this research work, chlorpyrifos pesticide was successfully degraded using photocatalysis. A catalyst made from fish scales of fish species Labeo Rohita was prepared. Then photocatalyst i.e. ZnO/AC was prepared by loading zinc oxide on prepared catalyst from fish scales. The chemical composition, morphology and surface chemistry of photocatalyst were investigated by EDX, SEM and XRD. EDX characterization results showed successful loading of ZnO on AC surface. SEM results elaborated highly porous and large surface area of prepared AC. ZnO/AC is used as a novel approach in pesticide degradation techniques. The influence of dose, temperature, concentration, pH and contact time on the catalyst photocatalytic ability was investigated. The degradation capacity of catalyst was analyzed in comparison with raw fish scales of labeo rohita using UV-Vis Spectrophotometer at lambda max=290nm (i.e Chlorpyrifos wavelength of maximum absorption). ZnO/AC was able to 94% degradation of chlorpyrifos pesticide. The optimal conditions for 94% degradation ability for this catalyst was found to be 150 minutes under sunlight irradiation in basic conditions of pH>8 at 30°C with required catalyst dose of 100mg/L for concentration of pesticide solution reaching 10ppm.

Keywords: Photocatalysis, Activated Charcoal, Zinc Oxide, and Pesticides Degradation.

EXTRACTION OF CELLULOSE, LIGNIN AND THEIR APPLICATION IN COSMETIC INDUSTRY AND DYE REMOVAL

Iqbal Rahat [1], Sultan Misbah [1*]

Center of Applied Chemistry, School of Chemistry, University of the Punjab, Lahore

[1]rahatkhan122436@gmail.com

Abstract:

The study focused on the isolation of the two important macromolecules of plant, cellulose and lignin from agro waste. The extracted materials were evaluated for their potential applications in cosmetic industry and waste water treatment. Peanut shell was selected as the agro waste. The extraction of the cellulose was three-step process carried out by utilization of Sodium hydroxide followed by the reflux of two hours with nitric acid and ethanol. Third step was bleaching with Sodium hypochlorite. The results showed that about 42% cellulose was extracted from peanut shell waste. The extracted cellulose was converted into the cosmetic beads with the help of Sodium alginate. These beads were used in cosmetic products. On the other hand, extraction of the lignin was two-step process. The filtrate of cellulose extract was heated at temperature 75oC for one hour. Then it was acidified by 98% pure H2SO2. Lignin precipitates were separated and dried. These extracted materials were used to remove the different dyes from waste water. SEM, XRD, TGA and FTIR were used for the characterization of extracted cellulose and lignin. The finding demonstrated the potential of extracted cellulose and lignin for cosmetic applications and treatment of waste water.

Keywords: Agro-waste, cellulose, lignin, cosmetics, water treatment.

Patterns of Essential/Toxic Metals Distribution in the Blood of Diabetes Mellitus Patients in Comparison with Healthy Donors

Qayyum Abdul Muhammad[1]

Department of Chemistry, Division of Science & Technology, University of Education Lahore, Pakistan

hmaqayyum@ue.edu.pk

Abstract:

Diabetes mellitus is growing in prevalence worldwide. It is a serious disease which occurs when human body has difficulty in properly regulating the amount of glucose in your blood. This study was conducted to evaluate the essential/trace metals in the blood of diabetes mellitus patients in comparison with healthy donors. Selected essential/toxic metals (Fe, Ca, Zn, Cr, Cd, Se, Pb, V and Sr) were measured in the blood of diabetes mellitus patients and counter-part healthy donors by atomic absorption spectrometry employing nitric acidic acid-perchloric acid based wet digestion. The mean concentration of Cd, Pb, Fe and V were found to be significantly higher ($p < 0.05$) in the blood of diabetes mellitus patients compared with the healthy donor however significantly higher concentration of Zn, Se, Cr, and Ca were observed in the healthy donors. Most if the metal levels revealed higher dispersion and asymmetry in the blood of the patient than the healthy donors. The correlation study revealed significantly diverse relationship among the metals in the patients and healthy donors. Thee multivariate apportionment of the metals in the blood of the patients and healthy donors was also significantly different. The study evidenced considerably divergent variations in the metal levels in diabetes mellitus patients in comparison with healthy donors.

Keywords: Metals; Diabetes; Blood; AAS; Statistical Analysis; Pakistan

REMOVAL OF ORGANIC / INORGANIC POLLUTANTS FROM WASTE WATER THROUGH ACTIVATED CARBON PREPARED FROM APRICOT PITS

Ayman Ume [1], Sultan Misbah [1*]

Center of Applied Chemistry, School of Chemistry, University of the Punjab, Lahore

[1*]misbahsultan@ymail.com

Abstract:

Water is the most essential component of environment while world water resources are contaminated due to discharge of a large number of pollutants from industrial wastes. A number of pollutants such as dyes and hazardous metal ions present in industrial wastewater are discharged without any adequate treatment into water resources. These pollutants pose a serious risk to human and environmental health. Adsorption has found to be a useful and superior method for the treatment of wastewater due to its low-cost, high efficiency and easy operations. Moreover, the ability of this method to treat dyes, heavy metals and organic pollutants of waste water is appreciable. The aim of this work is to apply an activated carbon prepared from apricot stones as an adsorbent for removal of pollutants from water. Apricot pits are an abundant and inexpensive natural source in Pakistan. It was used to prepare the activated carbon by physiochemical activation with ortho-phosphoric acid as activating agent at 350oC to 450oC for 25 minutes and at 700oC for 13 minutes. While SEM, XRD, EDX, TGA and FTIR were used for the characterization. The adsorption process using activated carbon was carried out at neutral pH, ambient temperature and 0.2 grams of adsorbent dose. The initial concentration of heavy metals and dyes varied from 1000 to 5000 ppm. The adsorbent was able to remove the cationic and anionic dyes up to the concentration of 5000ppm. The heavy metals were removed completely where original was 50 ppm. Another pollutant i.e., phenol was also adsorbed and removed (around 60%). Hence, these findings suggested a prepared charcoal as a potential adsorbent for treatment of different pollutants.

Keywords: Activated carbons, Apricot pits, Wastewater pollutants

Effect of Economically Viable Chemical Stripping Treatment on Unevenness of Natural Dyed Cotton Fabric

Maria Khalid[1], Shaukat Ali[*1]

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

[1]mariakhalid1827@gmail.com

Abstract:

For getting great shading quality and high brilliancy of fabric with natural color, the job of coloring and chemical stripping can't be denied. Uneven coloring is one of the primary issue of textile industry for texture colored with natural color. This study was conducted to evaluate the color removal efficiency of the chemical stripping process for naturally dyed cotton fabric regarding economic and environmental effects. The chemical stripping process was carried out by caustic soda and hydrose. Pomegranate peel was used as a source of natural dye for the dyeing of cotton fabric. Pomegranate dyed cotton fabric was subjected to both stripping agents using alternative recipes. In these recipes, we studied the effects of stripping chemicals such as hydrose and caustic soda, the concentration of hydrose and caustic, process temperature on the stripping efficiency. To observe the efficacy of the stripping chemicals, we measured the strength (K/S value) of dyed and the stripped samples using a commercial spectrophotometer. It was seen from the obtained results, caustic soda shows the remarkable capability of color stripping/ dye removal of pomegranate dyed cotton fabric under optimized conditions and can thus be recommended for industrial application. Moreover, an optimized oxidative color stripping process was recommended for complete color stripping of the natural dye molecules from cotton fabric. The highest achieved final stripping percentage of cotton materials was 98.99% after oxidative stripping. The stripping efficacy of pre-mordanted cotton fibers was also evaluated. Tear and tensile strength and weight loss of stripped fabric were also calculated.

Keywords: Reductive stripping; Oxidative stripping; Mordanting; Fabric quality; Tear and Tensile strength; weight loss

Solubilization and Micellar Enhanced Ultrafiltration for the removal of single and multiple pollutants in single cell by polymeric membranes

Yusaf Amnah[1]

Department of Chemistry, Government College University Faisalabad, Pakistan

[1]amnahyousaf581@yahoo.com

Abstract:

Micellar enhanced ultrafiltration (MEUF) has proved itself to be a potentially attractive tool to remove contaminants from waste water. This work is focused on the solubilization of Rhodamine B (cationic dye). The extent of solubilization has been, quantitatively, calculated using data of differential spectroscopy, in term of partition coefficient Kx and Gibbs energy of partition, ΔGp. It has been observed that mixed micellar media has better solubilization capacity than micellar solution of individual surfactants. Individual and multiple MEUF studies of Dye (Rhodamine B) has been carried out, so a combination of the dye with the metal ion (Co+2 Cobalt (II) have also been studied. Single dye as well as metal/dye removal efficiency has been assessed in terms of rejection percentage and permeate flux, using cellulose membrane of 10,000 molecular weight cut off (MWCO). The effects of various factors i.e. ionic strength, concentration of surfactants, concentration of electrolyte, pH, operating pressure and rotations per minute (RPM) has been observed. The maximum rejection has been observed and overall, it has been observed that the rejection coefficient is higher at higher concentration of surfactants and electrolyte and at lower values of pH, RPM and transmembrane pressure.

Keywords: Mixed micellization, SDS, SO, partition coefficient, solubilization, Surfactants, removal, Transmembrane Pressure, Rejection Percentage, Permeate Flux, Electrolyte, RPM, pH.

IONIC FLOCCULATION FOR REMOVAL OF POLLUTANTS FROM SYNTHETIC WASTE WATER

Usman Muhammad [1]*, Sultana Hamadia [2]

Department of Chemistry, Government College University, Faisalabad, Pakistan

musman@gcuf.edu.pk

Abstract:

This work reports the surfactant-based removal of reactive yellow 160 (RY-160) from synthetic waste water. Micellar enhanced flocculation technique was applied and optimized for the said purpose. The mixture of anionic surfactants, obtained from a bio-degradable source (base soap), has been found to have great potential to solubilize dye molecules. The polyvalent salts are able to flocculate the micelles and help in their subsequent removal. The removal of dye was analyzed by the use of a UV/Visible spectrophotometer. Different factors such as the effect of change inncentration, pH, temperature, contact time, and electrolyte were studied to evaluate the adsorption characteristics and removal efficiency of the process. The data obtained was further used to study the mechanism of adsorption with the help of various models e.g., Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich (D-R). The kinetic parameters were also calculated by employing pseudo-1st and pseudo-2nd order kinetic models. Furthermore, thermodynamic calculations were performed to determine the change in Gibb's free energy (ΔGo), enthalpy (ΔHo), and entropy (ΔSo). The results make it evident that the micellar flocculation-based adsorptive removal is an excellent and sustainable approach for the treatment of wastewater.

Keywords: Surfactants, flocculation, adsorption, isotherm, thermodynamics

Synthesis and Characterization Co-Doped-ZnO and Evaluation of its Photocatalytic Activity towards Photodegradation of Methyl Orange

Saeed Muhammad[1]

Department of Chemistry, Government College University Faisalabad, Pakistan

msaeed@gcuf.edu.pk

Abstract:

Photocatalytic treatment of organic compounds containing wastewater has gained significant attention in recent years. Generally, metal oxides have been reported as catalyst under ultraviolet light for treatment of organic compounds containing wastewater. It is important to develop an effective visible-light-driven catalyst for the eradication of aqueous phase organic pollutants. This study reports the visible light and CoO-ZnO assisted enhanced photodegradation of methyl orange as model pollutant. The composites including 5% CoO-ZnO, 10% CoO-ZnO and 15% CoO-ZnO were prepared and characterized by advanced techniques. The prepared catalysts were characterized by advanced techniques including XRD, DR-UV-Vis, PL, TPD and PEC. The prepared composites were tested as catalysts for degradation of dyes pollutants using methyl orange as model pollutant. It was found that CoO-ZnO loaded with 10% Co can remove the 100 mg/L methyl orange from water with 93% photocatalytic efficiency. Figure 1 shows the activity of various catalysts. The catalytic efficiency of CoO-ZnO loaded with 10% CoO was further explored in terms of various parameters including the concentration of dye, temperature, pH of solution, catalyst dosage and catalyst recycling. Figure 1 Comparison of catalytic efficiency of different catalysts.

Keywords: CoO-ZnO; Characterization; Methyl orange; Photodegradation

Session-III

Frontiers in Nutrition: Food Chemistry

Invited Talk

Recent Trends for Extraction of High-Value Biaoctives /Functional Components

Farooq Anwar
Institute of Chemistry, University of Sargodha, Sargodha- Pakistan
fqanwar@yahoo.com

Abstract:
Plants have always served as a vital source towards fulfilling the food, fuel, shelter and folk medicinal needs of human beings. On the other hand, they provide major portion of the world's molecular oxygen and are the basis of most beautiful ecologies on this earth. Most importantly, plants are recognized as a richest source of a wide array of high-value components / functional compounds with multiple biological activities and medicinal benefits. In fact, extraction of functional components from various plant materials with diverse structural features and polarity is a challenging task. Some conventionally employed methods such as maceration, decoction, infusion, percolation, Soxhelt extraction and hydro-distillation and are quite effective for recovery and extraction of bioactive components from plant materials. Nevertheless, such conventional techniques have certain limitations with regard to environmental pollution and process safety as well as quality of the end-use extracts/natural products. In line with the new developments in the area of optimal nutrition, coupled with growing demand from nutraceutical and food industry, there is greater need for the use of alternative green extraction for yielding safer and non-denatured plant extracts. This lecture, in particular, is framed to highlight the usefulness and applications of some innovative green technologies such as ultrasound-, microwave-, and enzyme-assisted extractions, supercritical fluid extraction (SFE), sub-critical water extraction and plant milking technology etc. for efficient extraction of safer bioactive extracts/functional extracts with potential uses in nutra-pharmaceutical and food sector.

Invited Talk

Mycotoxins: **Human-Animal-Environment Interface.**

Muhammad Kashif Saleemi[1*], Muhammad Imran[1], Muhammad Noman Naseem[1], Aisha Khatoon[1], Shafia Tehseen Gul[1], Muhammad Yousaf[2], Farhat Jubeen[3],
[1]*Department of Pathology, University of Agriculture, Faisalabad, Pakistan.*
*drkashif313@gmail.com

Abstract:
Fungal contamination of crops and production of toxic secondary metabolites (mycotoxins) are the inevitable issues throughout the world, mainly in the developing countries. These mycotoxins associated with adverse effects on poultry, animals, humans and crops, result in health issues and economic losses. Mycotoxins is second most important issue faced by the global poultry industry after high prices of feed. The major mycotoxins that have agro-economic importance are aflatoxins, fumonisins, ochratoxins, zearalenone and trichothecenes. These toxins are produced by different types of moulds that contaminate crops under favourable conditions and become the part of animal and human diet. Several studies have described their hepatotoxic, nephrotoxic, carcinogenic, immunosuppressive, toxigenic and mutagenic characteristics, and most mycotoxins represent a considerable risk to animal and human life. Compound stomach animals show some resistance against mycotoxicosis as compared to monogastric animals due to capability of rumen microbiota to degrade mycotoxins. The adverse effects of mycotoxins in humans include hepatocellular carcinoma, Reye's syndrome, Balkan endemic nephropathy (BEN), immunosuppression, abdominal pain, neural tube defects, infertility and retarded growth in children. This abstract describes different types of mycotoxins and their adverse effects on poultry, animal species and humans by keeping in mind the One-Health aspect.

Keywords: Mycotoxins, Moulds, Pathology, Humans, Animals.

Aflatoxin exploration in basmati brown rice collected from various locations of Lahore, Pakistan

Zahra Naseem[1], Saeed Khalid Muhammad [2]

Food and Biotechnology Research Centre,PCSIR Laboratories Complex, Lahore Pakistan

drnaseemzahra@gmail.com

Abstract:

Different fungal species like *Aspergillus parasiticus* and *Aspergillus flavus* produce secondary metabolites named "Aflatoxins". Aflatoxins are declared as potent carcinogen. Aflatoxins are prevalent and may contaminate various food commodities making those poisonous and toxic. In current study basmati brown rice samples were analyzed for aflatoxin contamination by ELISA (Enzyme linked immune-sorbent assay). The basmati brown rice samples (n=50) were collected for the analysis of aflatoxins from different shops of Lahore, Pakistan. The study was conducted during the year 2019-2020. The samples collection was done in summer (n=25) from April-September and in winter (n=25) from October-March. A miserable condition of the basmati brown rice was observed due to high concentrations of aflatoxin contamination. Total Aflatoxins were detected in 88% and 80% samples of brown rice collected in summer and winter seasons correspondingly. 60% samples collected in summer and 44% samples collected in winter were found exceeding permissible levels. Aflatoxin contamination in basmati brown samples was found maximum in summer as high temperature and high humidity is favorable for aflatoxin growth. The highest concentration in sample collected in summer was 49.60±0.45µg/kg and in winter was 25.07±0.04 µg/kg i.e. beyond permissible levels (10µg/kg for total aflatoxins) according to European Union. The terrible results are alarming as aflatoxins are very dangerous to human health and may be too fatal. It is direly needed to implement quality management practices like quality assurance, quality control and regular monitoring. These should be strictly implemented by all rice producers and exporters in order to reduce aflatoxin infectivity in basmati brown rice samples in Pakistan.

Keywords: Aflatoxins, ELISA, Brown rice, Quality assurance, Lahore

EXTRACTION OF KERATIN FROM CHICKEN FEATHERS AND ITS APPLICATION IN COSMETIC.

Sajjad Bakhtawar [1], Sultan Misbah [*]

Center of Applied Chemistry, School of Chemistry, University of the Punjab, Lahore

hamdiakamran@gmail.com

Abstract:

This research work was performed for the extraction of keratin from chicken feathers. Protein is not only an important ingredient for the maintenance of various body structures but also has wide applications in medical and cosmetics fields. Chicken feathers are a rich source of keratin. In this study, chicken feathers were treated with various reducing agents such as Ascorbic acid, sodium borohydride, thiourea and sodium sulphide in order to check the efficiency of reducing agents. Sodium sulphide proved to be the best and most efficient with high yield of keratin. Then, precipitation of protein with the help of ammonium sulphate was carried out. In order to purify, this precipitated protein was washed several times with water and then it was dissolved in sodium hydroxide solution. FTIR and UV were used for characterization of extracted keratin. The analysis by FTIR confirmed the presence of carboxylic acid and amino groups in the protein solution. The analysis by UV showed peak at 280nm that confirmed the presence of keratin. This keratin was used in preparation of a shampoo. The UV, FTIR and various physical tests were carried out for the comparison of shampoo with and without keratin. Shampoo with keratin showed an absorbance at 280nm in UV light which was absent in shampoo without keratin. Some other parameters such as pH, foam difference, color and consistency differences were also noted which led to the conclusion that shampoo with keratin was better than shampoo without keratin.

Keywords: Keratin, shampoo, reducing agents.

Effect of Pre-Biotics & Iron Fortificants on Production of Short-Chain Fatty Acids In Iron Deficient Female Sprague Dawley Rats

Momin Abul[1]

National University of Medical Sciences (NUMS), Rawalpindi-Pakistan

[1]abdul.momin@numspak.edu.pk

Abstract:

Among the leading public health issues worldwide is the problem of iron deficiency, which is considered to be the most prevalence micronutrient deficiency globally. The primary objective of the current research was to determine if pre-biotics and iron fortificants can enhance the production of short chain fatty acids in iron deficient female Sprague Dawley rats. For the purpose of the current research, n = 126 female Sprague Dawley rats were obtained from the National Institute of Health, Islamabad. They were initially divided into two control and sixteen treatment groups, acclimatized with the environment for one week and were given a routine diet. Iron deficiency was then induced using CCl4, following which a prebiotic and iron fortified diet was prepared to be given to rats for the trial of 90 days. Two iron fortificants including Ferrous sulphate and Sodium Iron EDTA and two prebiotics namely Inulin and Galacto-oligosaccharides were used at different dosages during the experiment. Fecal samples were obtained from the rats at baseline, 30th, 60th and 90th days of the trial and short chain fatty acids (Acetic acid, Butyric acid and Propionic acid) were determined using the technique of GC (Gas Chromatography). Similarly, pH of the fecal contents was directly measured using pH meter. The results of the study showed that concentrations of Acetic acid, Butyric acid and Propionic acid steadily increased during the trials. Also, pH of the fecal contents was gradually decreased indicating increased production of Short-chain fatty acids. Our study concluded that pre-biotics and iron fortificants enhanced the production of short-chain fatty acids and decreased the pH of fecal contents. This characteristic of pre-biotics can further be exploited to tackle the menace of iron deficiency, as increased production of short-chain fatty acids leads to enhanced iron absorption.

Keywords: Iron Deficiency; Pre-biotics; Iron fortificants; Short chain fatty acids; pH

Synthesis, structural characterization, biological efficiency and antioxidant studies of 2-thiophenemerhylamine based Schiff bases and their Fe(ll), Co(ll), Ni(ll) and Cu(ll) complexes

Saleem Maryam, Ali Ghulam Kulsoom

Department of Chemistry, Government College University Faisalabad, Pakistan

Kulsoom@gcuf.edu.pk

Abstract:

Synthesis, structural characterization, biological efficiency and antioxidant studies of 2-thiophenemethylamine based Schiff bases and their Fe(II), Co(II), Ni(II) and Cu(II) complexes Maryam Saleem| Dr Kulsoom Ghulam Ali*| Mehwish Ashraf | Dr.Bushra Parveen Abstract In this study, eight novel complexes comprising divalent Co (II), Fe (II), Ni (II) and Cu (II) with imine based ligands derived from 2-thiophenemethylamine with 2-hydroxy-3-methoxybenzaldehyde and 2-Hdroxy-1-naphthaldehyde have been synthesized. All the ligands and their newly synthesized complexes were checked for melting point, solubility, elemental analysis and molar conductance. These compounds were also characterized with spectroscopic techniques such as 1H NMR, FTIR, UV–Vis spectroscopy and powder XRD. Elemental analysis data showed that the prepared complexes have stoichiometric ratio consistent with (metal: ligand) ratio of (1:2). Molar conductance data revealed the non-electrolytic nature of ligand (HL) and its metal (II) complexes. UV-Vis electronic spectral data of the metal (II) complexes revealed formation of complexes by charge transfer transitions. FT-IR study confirmed the bidentate (N, O) donor nature of the ligand (HL). It showed that the metal (II) ions are coordinated to ligand via phenolic oxygen and azomethine nitrogen atom. Spectral data suggested an octahedral geometry for all the complexes and the general formula [ML2].2H2O (M (II) = Cu2+, Co2+, Ni2+, Fe2+] was proposed for them, where L represents deprotonated Schiff base. Powder XRD study was carried out to determine the grain size of ligand and its metal complexes. Significantly, these metal-imine complexes showed strong and efficient antimicrobial activities against various gram-positive (B. subtilis and S. aureus), gram-negative (E. coli and P. multocida) bacteria, and four strains of fungi (A. niger, A. flavus R. solani, and C. albicans). The complexes showed better antibacterial activity and antifungal activity as compared to ligand (HL). Hemolytic activity of Schiff base and the synthesized complexes was also found out against the human red blood cells by. Hemolytic activity of the ligand and complexes was compared against standard PBS (Negative control) and Triton X-100 (Positive control). Moreover, the antioxidant activity was measured on the basis of the radical scavenging effect of 1, 1-diphenyl-2-picryl-hydrazyl (DPPH) activity. All complexes exhibited efficient antioxidant activity.

Keywords: Schiff base, antimicribual activity, powder Xrd, spectroscopy, antioxidant potency

CARBON-BASED NANOMATERIALS FOR ADVANCED FLEXIBLE LITHIUM-ION BATTERIES

Ashraf Nawal and Zhixiang W*

CAS Key Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, University of Chinese Academy of Sciences, China

*weizx@nanoctr.cn

Abstract:

Carbon-based nanomaterials hold a promising future for a new generation of flexible Li-ion batteries. Our research group has developed bottom-up approaches to assemble such nano- engineered electrode materials with novel electrochemical properties. Various nanostructured carbon-based materials such as carbon nanotubes (CNTs), graphene and their composites, have shown potential prospects to tailor composition and fabrication of flexible electrodes. In part, we are focused on the design, synthesis, characterization, and application of redox-active organic electrode materials for the Li-ion batteries. While they offer superior versatility, tunable theoretical charge-storage capacity, multiple electron-transfer reactions, long cycling stability, relatively less structural degradation during charging-discharging process, and low cost, they also suffer from various drawbacks, such as; high dissolution in organic electrolytes (in case of small organic molecules), poor rate performance, low electrical/ionic conductivity, etc. This talk will discuss the charge storage mechanism of organic electrode materials which enables fast flexible batteries with high practical energy density, cover some of the strategies to improve these challenges of low conductivity and poor stability, and propose their potential solutions by tweaking the electrode composition using nanomaterials like CNTs and graphene. In addition, some key parameters for the design of flexible batteries will also be highlighted, followed by an overview of some recent contributions of our research group in this direction.

Keywords: carbon-based nanomaterials, lithium-ion batteries, flexible electrodes, CNTs, graphene

Plenary Lecture

Materials and the Functionalized Chemistry for Biomolecules Analysis in Diagnostics

Haq-ul-Najam M.

Institute of Chemical Sciences, Bahauddin Zakariya University, Multan, Pakistan

najamulhaq@bzu.edu.pk

Abstract:

The material science offers diverse range of materials in micro- and nano-sizes. The characteristics vary between the types of materials. Multiple applications are therefore designed based on unique properties. Health is the top beneficiary of materials, particularly the nanomaterials. This lecture is focused on the health side of applications which involve extensive work on complex biofluids. Any information from biofluid can be made available if the biomolecules are brought to their individual levels or at least separated on basis of their classes. These pretreatments prior to specific detections use materials in general and functionalized materials in particular. The functionalization's bring specific functionalities onto the materials for the targeted separations of classes of biomolecules and more specifically, the signaling biomolecules representing a diseased process, helping in earlier diagnosis. The evolved strategies are designed in triangular form; material, targeted biomolecules and sample preparation protocol. The biomolecules cannot be detected from biofluids without the prior desalting of the samples. Functionalized materials play role in this regard through unprecedented combinations of hydrophilic and hydrophobic characteristics. The modern Omics Sciences are utilizing materials for meeting the modern needs of structural properties of biomolecules. The nanomaterials-based methodologies are fabricated particularly in the field of proteomics and metabolomics. The strategies are highly selective, specific and sensitive. The detection of enriched biomolecules is made with mass spectrometry to the extent of sequences. The materials employed encompass carbon-based, polymeric, cellulose and metal oxides. The nanomaterials are also fabricated to be used in sensing of signaling molecules. The designed nanomaterials and their functionalizations can pre-concentrate the targeted biomolecules from range of bio-samples like non-fat milk, egg yolk, human serum and HeLa cell extract.

Session-I

Natural & Synthetic Medicinal and Pharmaceutical Sciences

Invited Talk

Nutraceutical, prospects and challenges

Qaiser Naeem Muhammad

College of Pharmacy, University of Sargodha, Sargodha-Pakistan

naeem.qaisar@uos.edu.pk

Abstract:

Nutraceuticals have received considerable interest due to potential nutritional, safety and therapeutic effects. Recent studies have shown promising results for these compounds in various complications. Many nutraceuticals and naturally occurring compounds that have been investigated and reported in various studies revealed that these products are extremely active, have profound effect on cell metabolism and often have little adverse effect. It is natural that people's focus is shifting to a positive approach for prevention of diseases to stay healthy. Despite widespread consumption, nutraceuticals are found to have been contaminated with heavy metals, and others do not contain the expected quantities of active ingredients. In general, supplements are not needed except in cases of established deficiencies, and excess of some nutrients can increase cancer rates. This study also discusses the public health concerns associated with use of nutraceuticals and suggests directions for the establishment of scientific criteria for health claims for nutraceutical, especially in relation to the increasing global economy. Consumers, government, industry and academia all need to be involved in an international understanding, based on science and ethics, for health claims for functional foods, including those of phytochemical origin

Single Cell Protein (SCP): A comprehensive review

Walait Manam[1]

University of Central Punjab Lahore, Pakistan

[1]manam.walait@ucp.edu.pk

Abstract:

Protein is high energy molecule, humans and animals use single cell protein as a protein source, single cell protein are dry dead cells of microorganisms. Microorganisms for example bacteria, fungi and yeast are used as s protein source and are generally declared safe. Microorganisms (amino acids, biomass) or the protein source use microbial growth culture components which are inexpensive and can be used for the source of energy to grow and as a source of carbon. Single cell protein strains have wide range of properties such as it can be used to eradicate pathogenic microorganisms from animals and humans gut by producing enzymes, metabolites with the antimicrobial activities or by the competition with the available nutrient source, single cell protein is also used as food or feed supplements. The global demand for high quality protein rich food has increased because the population of the world is increasing rapidly day by day. Single cell protein shear with the capacity to develop the cell wall degrading enzymes and metabolites with the antimicrobial activity could play significant role to meet the needs of protein in the progressing world. To meet the need of protein in the progressing world farming of boilers and layers is playing huge role. Anyhow, the specific boundaries that need additional care are high nucleic acid content, complex cell wall, intolerable color and flavor and high contamination rate.

Keywords: Single cell protein. Protein, mechanism of production; nutritional benefits

Potential of silver against human colon cancer: (synthesis, characterization and crystal structures of xylyl (Ortho, meta, & Para) linked bis-benzimidazolium salts and Ag(I)-NHC complexes: In vitroanticancer studies)

Iqbal Adnan[1], Haque A. Rosenani[2]

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

[1]adnan.iqbal@uaf.edu.pk

Abstract:

Background Since the first successful synthesis of Ag(I)-N-heterocyclic carbene complex in 1993, this class of compounds has been extensively used for transmetallation reactions where the direct synthesis using other metal ions was either difficult or impossible. Initially, silver(I)-NHC complexes were tested for their catalytic potential but could not get fame because of lower potential compare to other competent compounds in this field; however, these compounds proved to have vital antimicrobial activities. These encouraging biomedical applications further convinced researchers to test these compounds against cancer. The current work has been carried out with this aim. Results N-ipropylbenzimidazole was synthesized by reaction of benzimidazole with ipropyl bromide. The subsequent treatment of the resulting N-alkylbenzimidazole with ortho/meta/para-(bromomethylene) benzene afforded corresponding bis-benzimidazolium bromides (5-7). The counter anion (Br-) of each salt was replaced by hexaflourophosphate (PF6-) for the ease of handling and further purification (8-10). Each salt (Ligand), in halide form, was further allowed to react with Ag2O with stirring at room temperature for a period of two days to synthesize dinuclear Ag(I)-NHC complexes (11-13). All synthesized compounds were characterized by spectroscopic techniques and microanalysis. Molecular structures of compounds 5, 9 & 10 were established through single crystal x-ray diffraction technique. All the compounds were assessed for their anti-proliferation test on human colorectal cancer cell line (HCT 116). Results showed that the ligands (5-10) showed mild to negligible cytotoxicity on HCT 116 cells whereas respective silver complexes (11-13) exhibited dose dependent cytotoxicity towards the colon cancer cells with IC50 ranges between 9.7 to 44.5 μM. Interestingly, the complex 13 having para-xylyl spacer was found the most active (IC50 9.7 μM) that verifies our previously reported results. Conclusions All the bis-benzimidazolium salts (8-10) were found inactive whereas after bonding with silver cations, the Ag(I)-NHC complexes (11-13) showed a dose dependent cytotoxic activity. This proved that silver practice an important role in death of cancer cells. Also, the N-alkyl/aryl substitutions and ortho/metal/para xylyl units regulate the cytotoxicity.

Keywords: Synthesis, Organometallic, Silver-NHC, Complexes

Green synthesis of Organoselenium Compounds, their DFT Studies, Biological Potential, and study of their 3D interaction with protein molecules by Molecular Modelling

Abbasi Mahvish , Yaqoob Munazzah, Saleem Shahzaib Rehman, V Nazari Mansoureh, Iqbal Javed, Iqbal Adnan Muhammad *

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

*adnan.iqbal@uaf.edu.pk

Abstract:

N-heterocyclic carbenes (NHCs) are the most eminent group of organic chemistry, because of their stability which is caused by the inductive effect, mesomeric effect, steric protection, and also aromatic character. It also acts as a good sigma donor due to the presence of a nitrogen atom and pi character due to the presence of a double bond. These legendary properties of NHCs make more stable transition metal ions in the catalytic pathways. Due to the versatility of the NHCs ligand, it is used for multi-purposes such as antioxidant agents, anticancer agents, catalysts, especially in organic conversions and medicine. In the current research, the compounds were studied through computational chemistry via the Density Functional Theory method by using the basis set of 6-31G and functional of B3LYP. Compounds were designed through Gauss view 5.0 and run at Gaussian 09 and these organoselenium compounds and their respective salts were synthesized as their synthesis is the dire need of time due to their refined properties. After the synthesis of desired compounds, characterization was done through UV-visible, FT-IR, carbon, and proton NMR spectroscopies. The synthesized compounds were then tested against their biological potential as an antioxidant and anticancer agent. Moreover, Molecular modelling of compounds was done, it was found that among all other compounds MC1 shows strong bonding with proteins.

Keywords: N-heterocyclic, sigma donation., organocatalysis, exigency

Synthesis of ethyl esters of 2-hydroxypyrimidines as pharmaceutical agents

Iqbal Sarosh[1]

Department of Applied Chemistry, Government College University Faisalabad, Pakistan

[1]sarosh.iqbal@yahoo.com

Abstract:

Drug discovery and development is essential for cures from diseases and its success depends on combined efforts of chemical and biological research. Therefore, synthesis of novel compounds and their evaluation as pharmaceutical agents is need of time. In current era, cancer is second leading causes of death in humans worldwide so, many scientists are struggling for development of improved anticancer therapies. We have synthesized ethyl esters of 2-hydroxypyrimidine derivatives (16-30) in two step reaction sequence. Firstly, ethyl ester of dihydropyrimid-2-one (1-15) have been synthesized via fusion of ethyl acetoacetate, different aldehydes, and urea in the presence of catalyst (copper nitrate) then corresponding ethyl ester of 2-hydroxypyrimidine derivatives (16-30) have been synthesized via oxidation of synthesized compounds (1-15) using ceric ammonium nitrate. Synthesized compounds (1-30) have been purified and characterized by mass spectrometry and NMR spectroscopic techniques. In addition, all synthesized compounds have furnished good CHN analysis. All synthesized compounds have also been evaluated for their potential as anticancer agent and study have identified interesting lead molecules having potential for further study. The talk will highlight synthesis and bioactivity study of 2-hydroxypyrimidine derivatives.

Keywords: 2-hydroxypyrimidine , anti-cancer, catalyst, oxidation, ceric ammonium nitrate

Design and synthesis 1,2,4-triazole-3-thiol analogues to evaluate their angiogenesis response

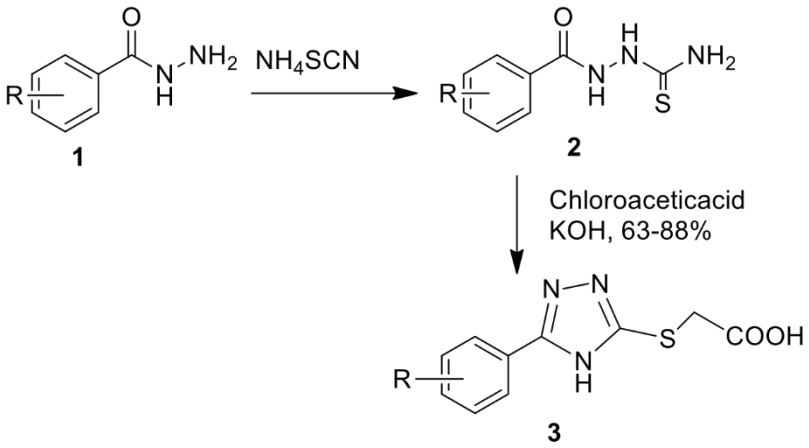
Khan ZULFIQAR ALI [1*]

[1]*Department of Chemistry, Government College University, Faisalabad, 38000, Pakistan.*

zulfiqarchem@gmail.com

Abstract:

There are angiogenic factors that promote trigger tumor angiogenesis unsolicited angiogenesis, and accelerates proliferation of endothelial cells during cancer metastasis. Thymidine phophorylase (TP) enzyme is over-expressed in solid tumors, and its inhibition is a prime method in cancer research and therapy to make potent antitumor agents. The presence of Thymidine phophorylase (TP) in cancer cells activates human endothelial cell migration and invasion by the secretion of several angiogenic factors. A series of 1,2,4-triazoles were synthesized and characterized UV-visible, FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopic techniques. Further, angiogenic response of compounds **3** have been evaluated using the chick chorionic allantoic membrane (CAM) protocol. Therefore, structure activity relationship (SAR) and molecular docking studies of selected triazole derivatives **3** to regulate main binding interactions were discussed. The synthesized analogues **3** interacted with active site residues of thymidine phosphorylase enzyme through hydrogen bonding, thiolate and π-π stacking interactions revealed by docking studies.



Scheme 1 Synthesis of compound type **3**.

Keywords: Angiogenesis, Thymidine phosphorylase inhibitors, 1,2,4-Triazoles, SAR, Docking

Structure-Based Designing, Solvent Less Synthesis of 1, 2, 3, 4-Tetrahydropyrimidine-5-carboxylate Derivatives: A Combined In Vitro and In Silico Screening Approach

Arshad Uzma[1], Ahmed Sibtain [2]*, Shafiq Nusrat [1]*, Ahmad Zaheer [3], Hassan Aqsa [1], Akhtar Naseem [4], Parveen Shagufta [1] and Mehmood Tahir [5]

Department of Chemistry, Government College Women University Faisalabad, Pakistan

[1*]dr.nusratshafiq@gcwuf.edu.pk

Abstract:

In this study, small molecules possessing tetra-hydro-pyrimidine derivatives have been synthesized having halogenated benzyl derivatives and carboxylate linkage. As previously reported, FDA approved halogenated pyrimidine derivatives prompted us to synthesize novel compounds in order to evaluate their biological potential. Methodology: Eight pyrimidine derivatives have been synthesized from ethyl acetoacetate, secondary amine, aromatic benzaldehyde by adding catalytic amount of CuCl2·2H2O via solvent less Grindstone multicomponent reagent method. Molecular structure reactivity and virtual screening were performed to check their biological efficacy as an anti-oxidant, anti-cancer and anti-diabetic agent. These studies were supported by in vitro analysis and QSAR studies. Results: After combined experimental and virtual screening 5c, 5g and 5e could serve as lead compounds, having low IC50 and high binding affinity.

Keywords: pyrimidine; solvent less; in silico; in vitro; QSAR; DFT; MTT; molecular docking

Theoretical calculation of Selenium N-heterocyclic carbene compounds through DFT studies: Synthesis, characterization and biological potential

Yaqoob Munazzah[1], Iqbal Javed[1*], Iqbal Adnan Muhammad[1]

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

[1]adnan.iqbal@uaf.edu.pk

Abstract:

N-heterocyclic carbene (NHC) is one of the significant class of compounds in organometallic chemistry. Strong sigma donating property and weak pi-accepting property of NHC makes it prominent so that they can interact with metals to form the stable organometallic complex. These ligand compounds have the capability to release the metal in the form of ions slowly and at a sustainable rate at any site in the biological system. Selenium is also a very active element having highly demanding applications like an antioxidant agent and is a necessary trace element for the human body. In the current research work, two new imidazolium salts (as pre ligands) and respective selenium-NHC compounds have been designed and computed theoretically before the synthesis of active compounds among the designed compounds. Compounds, namely ML1, ML2, MC1, and MC2, on the basis of imidazole units were designed and computed for different properties, absorption spectra, dipole moment, theoretically estimated biological potentials, and frontier molecular orbitals, by calculating the HOMO/LUMO energy orbitals via Density functional theory method. The density functional method was applied using Gaussian 09 software and the Gauss view 5.0 program. Analysis of compounds was done at B3LYP level by using 6-31G (d) level of DFT (Density Functional Theory). Theoretical calculation showed that compounds are highly biologically active, as their synthesis is exigency of the time so these compounds were synthesized. Synthesized compounds were characterized by UV-visible, FT-IR, carbon, and proton NMR spectroscopies. Antioxidant and anticancer properties of compounds were calculated and their characteristics were compared with the characteristics of imidazole present in the literature and results were the almost same as calculated by the theoretical method.

Keywords: N-heterocyclic, sigma donation, dipole moment, exigency

Osteogenic and antibacterial copper doped mesoporous bioactive glass nanoparticles: invitro cyclophosphamide delivery to the U2OS cancer cell line.

Shoaib Muhammad [*1], Rahman ur Saif Muhammad [2], Ali Bahadur[3]

Department of Chemistry, Government Graduate College Samanabad Faisalabad, Pakistan

relyables@gmail.com

Abstract:

In this study copper doped mesoporous bioactive glass nanoparticles (Cu-MBG NPs) were prepared by employing cetyltrimethylammonium bromide (CTAB) as a soft internal template. These multifunctional NPs were evaluated for antibacterial and osteogenic potential and drug delivery. Hydroxycarbonate apatite formation was evaluated by immersing the as-synthesized NPs in simulated body fluid (SBF) and confirmed by FTIR and XRD analysis.Osteogenic ability was further confirmed by biomarkers such as alkaline phosphatase (ALP)activity and osteocalcin (OC) assay. Size, shape, morphology, and elemental analysis weredetermined scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy-dispersive x-ray (EDX). Surface area and pore size were determined by BET and BJH method. Size, surface area, and pore size were determined to be 60 ± 5 nm, 313 m 2 /g, and 10.74 nm. Cyclophosphamide (Cpa); an anti-cancer drug was loaded by taking different initial loading concentrations (2-10 mg/mL). For all these loading concentration cumulative Cpa released in SBF was found to be in the range of 65-89% over the period of two weeks. MTT assay indicated no significant cytotoxicity in normal human fibroblast (NHFB) cells. Cpa loaded Cu-MBG NPs inhibited the U2OS cancer cell viability at all concentrations. Thus, a safe biomaterial was developed which is biocompatible, non-cytotoxic, anti-bacterial, and has the potential of drug delivery, bone-repair and regeneration.

Keywords: bioactive glass; bone regeneration; sustained release; histopathology;

Cyclophosphamide

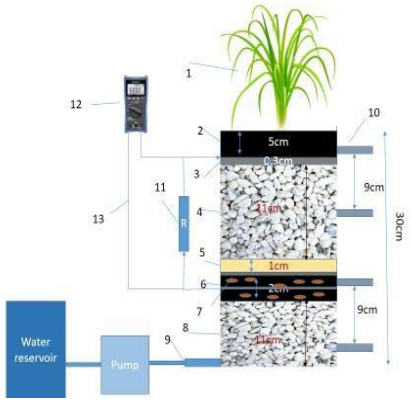
Study of Selected Sulfonamide Removal Efficiency in Constructed Wetlands Coupled with Microbial Fuel Cell Model System

Jubeen Farhat[1], Nazir Alina[1*], Farooq Robina[2]

Department of Chemistry, Government College Women University Faisalabad, Pakistan

***Alinanazir379@gmail.com**

Graphical abstract:



Schematic diagram of CW-MFC (1) *cymbopogon nardus,* (2) GAC cathode, (3) stainless steel mesh, (4) gravel middle layer, (5) glass wool, (6) GAC anode, (7) bacterial strain, (8) gravel bottom layer (9) influent, (10) effluent sampling ports (11) resistance (12) digital multimeter, (13) copper wires

Abstract:

The presence of antibiotic residues in waste water are posing lethality to food crops and human health, there is an urgent need to treat waste water. Constructed wetlands coupled with microbial fuel cell (CW-MFC) is considered as the most promising installation for the treatment of waste water. This study aimed to investigate the removal of Co-trimoxazole (CMX) along with its general co-existing pollutant i.e biological oxygen demand (BOD) and generation of green electricity with low hydraulic retention time (HRT) and open circuit mode. The results indicated that the effluent from configuration 1 (gravel based) had lower (CMX) concentration because of having greater electrode absorption capacity for (CMX) and exhibited best removal performance. The removal percentage was 92.58% at HRT of 3d when the influent conc. was 4mg/L. CW-MFC1 showed the best BOD removal (39%) irrespective of the increasing influent antibiotic concentration. Pure strain of *Geobactor sulfereducens*, acclimatized with anaerobic sludge stimulate the bio-film development. Maximum voltage of 1200 mV observed for CW-MFC1. Electricity generation characteristic were also found to be effected with HRT.

Key words: Co-trimoxazole, Constructed wetlands microbial fuel cell, Acclimatization, Hydraulic retention time, Open circuit mode, Green power production

Session II

Smart & Sustainable Development in Materials Manufacturing and Energy

Invited Talk

Recent Innovations in Nanoscale Catalysis for Water Splitting and Synthetic Fuels

Joya S. Khurram*

IUM, Madinah and King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

* khurram.joya@gmail.com

Abstract:

With the advent on innovative science, chemical research and technology, nanoscale materials can be engineered and programmed to perform specified function at macro level applications. The innovation in chemical science, nanomaterials, catalysis, and electrochemical processes for Water Splitting has a lead now for solar and chemical energy conversion. These systems can be implemented as surface immobilization along with thin-films for catalytic processes, sensing applications and for energy conversion schemes. We have invented, discovered and developed specialized methods, and exploited various thin-film nanoscale materials for catalytic water splitting, CO_2 reduction, and recently for electrochemical sensing, biomass catalysis and solar energy conversion. Now we implement and developing new methods for making advanced electro functional nanomaterials and nanoclusters derived from thin-films molecular assemblies, inorganic nanomaterials and metal-oxides displaying great potential to be used in high performance water splitting catalysis and for chemical energy conversion and storage schemes. In this discussion we also highlight the challenges in chemical energy conversion and the possible way forward.

Invited Talk

PLASTIC POLLUTION AND BIO-PLASTIC MATERIALS

Hussain ZH[1], Din MI[2], Siddique N[2]
1Centre for Applied Chemistry, School of Chemistry, University of the Punjab, Pakistan
2 Centre for Physical Chemistry, School of Chemistry, University of the Punjab, Pakistan
zaib.chem@pu.edu.pk

Abstract:

Increasing demand for plastic has caused a relative increase in all kinds of plastic materials whether they are used for domestic or commercial purposes. Use of such conventional petroleum based plastic materials has caused resource, environmental and waste management problems mainly due to their non-biodegradability, non-recyclability and liberation of poisonous pollutants. This study focuses on the replacement of synthetic plastics with biodegradable plastics to facilitate the environment and climate. Biodegradable plastics based on annually renewable agricultural and biomass feedstock were synthesized. Cellulosic biopolymer was utilized as raw material for synthesis of biodegradable plastic. Simple solution casting method was employed to synthesize plastic films. Calculated ratio of raw material, along with plasticizer and other additives, was added. To have minimum effect on biodegradability, bio-plasticizers and bio-additives were considered. Cellulosic based films are moisture sensitive which cause variation in mechanical properties and thermal stability hence restricting further use of the films. To reduce the hydrophilic character of these cellulosic based films and enhance their mechanical properties, fillers were added. Structural characterization was carried out using UV-Vis and FT-IR analysis. Parameters such as solubility, water resistance and biodegradability were tested hence confirming that the composites were biodegradable. Solubility and water absorption were controlled by increasing the amount of filler. The development of such bio-plastic materials will help to conserve non-renewable sources, save energy, reduce environmental pollution and contribute towards soil remediation.

Keywords: plastic pollution, bio-plastics, biomass, solubility, biodegradability

Invited Talk

Interdisciplinary Research in the Textile Circular Economy

Majeed Hammad *

Department of Chemistry, University of Management and Technology, Iqbal Campus, Sialkot, Pakistan

*dyeing@gmail.com

Abstract:

The textile industry is converging on a textile circular economy to reduce the impact of climate change. This segment is trying to save water to avoid scarcity and energy in processing. Climate change is a worldwide thought-provoking concern that is at the primacy of the whole world. All industrial segments are trying to opt for the best way out which can lessen the influence of climate change. In Pakistan, most of the industries especially textile export oriented are changing their mentality and production system to save water and energy. Sustainable crops productions to avoid the use of herbicides, pesticides, etc. to give organic and green raw material for textile industry to manufacture sustainable and environment-friendly textile goods. Enzymatic or safer chemical products usage in textile production is mandatory for them to fulfil the different certifications audit like REACH, ZHDC, GOTS, Oeko Tex Standard 100, Blue Sign, Higg Index etc. The textile waste water and material is getting recycled, reused to reproduce the best products to diminish trash on our planet with reduction in carbon footprint. Synthetic plastic polymer is replaced by biodegradable polymers which are less dangerous for the environment. Artificial intelligence and other latest tools are also helping to give smart solutions to all types of industries to save the environment. Climate change and the temperature rise is serious issue and the international business community is trying to follow the race to zero targets to avoid more determinantal effects. In short, all science disciplines are involved in textile circular economy latest concept to meet the challenges.

Keywords: Textile, Circular Economy, Climate Change; Industry; Water; Temperature

Simulating the Effects of Construction Materials in Different Climate Zones of Pakistan for the Design of Zero-Energy Buildings

University of Central Punjab, Lahore- Pakistan

Maryam Zuha[1] and Ehsan Sarwar Muhammad[1*]

[1*]sarwar.ehsan@ucp.edu.pk

Abstract:

Building energy performance and energy-saving design strategies leads to a sustainable and low-carbon society. Environmentally friendly building designs while maintaining comfort and optimal thermal conditions in architectural form, discourse energy efficiency problem. Assessment of building energy performance while designing has a great influence on energy expenditure. During the last decade, the emerging trend of using computational algorithms for designing and assessing architectural forms is a valuable tool to explore design potential and evaluate cost-optimal and energy-efficient solutions. In this paper, we have simulated energy-saving and energy-efficient building designs using integrated energy simulations with renewable energy sources. Beopt-building energy optimization software and Polysun are used to design buildings and estimate, evaluate and optimize the energy used under real conditions. We design and compare residential building energy performance in different weather conditions using different materials. As a result of software simulation, there is a remarkable difference between the energy demand of a standard home and our proposed home. The total energy performance index of the house goes from 94.6 to 67.6 percent.

Keywords: zero-energy building, construction materials, climate-zones

Experimentally determined Photophyical and computational studies of 7-Hydroxycoumarin

Mansha Asim [1], Asim Sadia [2], Fatima Sana [3]

Department of Chemistry, Government College University, Faisalabad- Pakistan

[1]mansha.asim@gmail.com

Abstract:

7-Hydroxycoumarin's FT-IR solid phase spectra were observed at 4000-400 cm-1. The spectra were analyzed in aspects of significant approaches. By using the B3LYP level with 3-21G, 6-31G, and 6-311++ G (d, p) basic sets, DFT was used to optimize the structure of the compound and its structural properties. The molecular properties were also determined by the HF/3-21G level. The bond lengths and bond angles were obtained by the computational study of the optimized geometry. The vibrational frequencies were determined in all these approaches, which were then matched to experimental frequencies, yielding an excellent agreement between measured and estimated frequency ranges. The UV-visible spectrum of 7HC was obtained and the electronic characteristics HOMO and LUMO energies were monitored by the time-dependent TD-DFT method. The spectral behavior of 7-Hydroxycoumarin was studied using fluorescence spectroscopy in a wide range of polar and non-polar solvents. There was Solvatochromism in both the fluorescence and absorption spectra. The structural properties, energies, IR intensities, absorption wavelengths, and harmonic vibrational frequencies were compared with the obtainable experimental information of the molecule.

Keywords: Photophysics, Computational Chemistry

Gemcitabine-Based Anticancer Drug with Metal-Doped BN24 As A Drug Delivery Carrier: Density Functional Theory

Bibi Shamsa[1], Rehman -UR – Shafiq[1*], Khalid Laryeb[1*]

Department of Chemistry, University of Agriculture Faisalabad, Pakistan

[1]shamsa.shafiq@uaf.edu.pk

Abstract:

Anticancer drug delivery is now becoming a challenging approach for researchers as it allows controlled drug delivery near cancerous cells with minimized generic collection and avoiding secondary side effects. Hence in this work, the applications of nanostructures as anticancer drug delivery carriers are widely investigated to target cancerous tissues. Based on DFT calculations, we have investigated transition metal-doped boron nitride nanostructure as a drug delivery agent for Gemcitabine drug utilizing B3LYP/6-31G (d, p) level of theory. In this research, adsorption energy and electronic parameters of Gemcitabine drug on interaction with metal-doped BN nanostructures have been studied. It has been observed that metal doping significantly enhances the drug delivery properties of BN nanostructures. Among investigated nanostructures, Ni-BN has been found as the most prominent nanostructure to transport Gemcitabine drug with the elevated value of adsorption energy in the both gas phase (-45.79) and water media (-32.46). The interaction between Gemcitabine drug and BN nanostructures is confirmed through frontier molecular orbitals and stabilization energy analyses. The fractional charge transfer, MEP, NCI, and NBO analyses exposed the charge transfer from drug molecule to BN nanostructures. Transition density maps and UV-VIS spectra were also plotted to investigate the excited state properties of designed complexes. Thusly, the present study provides an in-depth interaction mechanism of Gemcitabine drug with BN which reveals that metal-doped BN nanostructures can be a favorable drug delivery vehicle for Gemcitabine anticancer drug.

Keywords: Density Functional theory, Boron nitride nanostructures, Drug delivery, Gemcitabine anticancer drug, Adsorption, Metal Doping.

Chromium Doped Lanthanum Cerates: Synthesis, Characterization and Hydrazine Electrocatalysis

Poshmal Sumreen

Department of Chemistry, Quaid-e-Azam University, Islamabad, Pakistan

Abstract:

The current research was focused on synthesis of lanthanum cerate and doped lanthanum cerate by simple co-precipitation method. B-site doping was done by transition metal element chromium (x = 0.02-0.10) to enhance their conductive and electrocatalytic properties towards hydrazine oxidation and as electrode material in SOFC. The electrocatalytic facility in hydrazine oxidation is manifested in two of the electrochemical output parameters: the lower onset potential and the higher peak current response. The robustness of the envisioned scheme of using lanthanum cerates perovskite (LaCeO3; LCO) in combination with doped compositions provides better electrochemical results for hydrazine electrocatalysis as compared to the use of costly metallic or alloy nanomaterials. Effect of B-site doping in lanthanum cerates was studied and the resulting chemistry for the hydrazine electrocatalysis. Series of LaCe1–xCrxO3 (LCMO; M = Cr3+) nanopowders were synthesized and tested electrochemically by using cyclic voltammetry and impedance analysis for hydrazine oxidation in the presence of 0.1 M phosphate buffer solution using LaCe1-xCrxO3 modified glassy carbon electrode at ambient conditions. An obvious correspondence was detected between the electrocatalytic activity and the morphological, structural properties of perovskite ceramic powders.

Keywords: Perovskite, Hydrazine oxidation, SOFC, Electrocatalysis

Synthesis of lignite/ZnO hybrid material for removal of some toxic metal ions from water

Arooj Maria[1], Manzoor Hassan[2], Arshad Asfia[3]

Department of Chemistry, Government College University Faisalabad, Pakistan

[1]drkiranaftab@gcuf.edu.pk

Abstract:

Lignite based ZnO hybrid material was synthesized and screened for the sorption efficiency of lead and nickel from aqueous solution. The removal of toxic metals lead and nickel from water had been widely investigated using various sorbents, but still seems crucial for bringing the process to a successful application stage. This investigation describes the use of lignite based ZnO composites for removal of lead and nickel from aqueous solution in a batch system under different experimental conditions. The highest Pb(II) and Ni(II) sorption (31.7 ± 1.7 mg/g, 84.2 ± 2.2 mg/g) were observed at 100 µg/ml initial lead and nickel concentration. Sorption data were well defined by Langmuir isotherm and pseudo-second order. The FTIR, SEM and XRD techniques were used for characterization of lignite/ZnO composites. High Ni (II) uptake selectivity by lignite based ZnO hybrid proved it to be an efficient, economic and ecofriendly material especially for nickel removal from solutions.

Keywords: Hybrid material, nickel, lead, water, remediation

EXCESS ENERGY EVALUTION BASED ON PERFORMANCE RATIO FOR LARGE-SCALE SOLAR PROJECT (LSSP)

JAMIL Irfan [1, 4*], LUCHENG Hong [1], MUBASHIR Syed Hassan [2], BAKAR Abu Muhammad [3], JAMIL Rehan [4]

[1]*School of Electrical Engineering, Southeast University, China*

[2]*School of Electrical and Electronic Engineering, North China Electric Power University, China*

[3]*Department of Electrical and Information Engineering, Tianjin University, China*

[4]*TBEA Xinjiang SunOasis Co., Ltd*

*irfan.edu.cn@gmail.com

Abstract:

This study presents an industrial technique to analysis the excess energy (EE) of large-scale solar plants (LSSPs) using a novel performance ratio (PR) formula model based on energy production. The PR is a main quality indicator that can be used as a performance metric when solar power plants are interconnected to the national grid to ensure that energy is guaranteed and that the plant is running at a high degree of efficiency. The PR then reveals the true face of the plant's efficiency because the effective incident global irradiation (GlobInc) value is never available, and it has no stable value over the year. The proposed PR formula model is used to calculate the proper performance guarantee for the grid-connected 100MWdc-LSSP at Pakistan's Quaid-e-Azam Solar Park (QASP). The primary goal of this research is to introduce a PR formula based on energy production to achieve the excess energy of the LSSP projects. Based on 1-year on-site plant data FY (2020–2021), the plant's performance energy inputs, including production, irradiance, and PR, are evaluated to determine the final excess energy of QASP. Through the theoretical calculations, the excess energy of the 100MW QASP is computed at 1,504.32 MWh, PR of 75.64%, and the system fed 8% higher PR than the target PR of 74.94%, a difference of 0.7%. Thus, additional production of 165,588.58 MWh and bonus energy of 300,864.87 USD are produced.

Keywords: Performance Ratio, Energy Production, Excess Energy, Bonus Energy, QASP.

Session III

Rational Drug Designing and Discovery

Invited Talk

Mathematical Modeling of Infectious Diseases Dynamics

Rafiq Muhammad

Department of Mathematics Faculty of Sciences, University of Central Punjab Lahore, Pakistan

m.rafiq@ucp.edu.pk

Abstract:

Mathematical models play a significant role to analyze and control infectious diseases in a population. These models provide conceptual insights such as thresholds and basic reproduction numbers for various infectious diseases. Some very important theories are built and tested, some quantitative speculations are made and some specific questions are answered with the help of mathematical models. This leads to a better strategy for overcoming the transmission of infectious diseases.

Key Words: Mathematical Model, Infectious Diseases, Basic Reproduction Number, Numerical Simulations

Invited Talk

Natural Product are untapped source of bioactives against the consortium bacterial biofilm

Shahid Muhammad, Rehman Tjammal, Fatima Hina

Department of Biochemistry, University of Agriculture, Faisalabad, Pakistan

mshahiduaf@yahoo.com

Abstract:

Sinusitis is microbial loaded infection of the membranes lining the paranasal sinus. It is one of the most frequently disease diagnosed in the USA population. Biofilm formation by sinusitis microbes with special reference to bacteria in human is one of the major problems. Microbes present in the biofilm are highly resistant to antibiotics and scientists are looking for medicinal plants as potent biofilm agents. An attempt was conducted on the medicinal plants to develop a product to explore the untapped source of bioactives by using different biological activities. The current study was aimed to develop a natural product (namely SinuCure) against sinusitis from five plant (Green cardamom, Garlic, Ginger, Cinnamon, Cumin) extracts. Product exhibited higher antioxidant activities with minimum hemolytic activity, while the highest anti-inflammatory activity was shown by this product. Increased thrombolytic activity was also observed in case of ethanol extract. Antibacterial activity of ethanolic extract was remarkable followed by water extract against sinus isolates and consortium from human volunteer. MIC was also recorded for tested bacterial strains and consortium. Ames assay and DNA damage protection assay was also performed, and results revealed that these extracts are non-mutagenic as well as non-toxic. Water decoction was also tested on human volunteer having sinusitis problem. SinuCure product drains sinusitis quickly and patient feels comfortable within 6 hours. Results of this study have shown that (polyherbal drug) product developed have high antioxidants, lowest toxicological and remarkable antibacterial and biofilm inhibition activity. This product is safe to use as its toxicological and biological profile is very good.

Isolation and characterization of novel serine protease inhibitors for the treatment of microbial infections

Shahzad Asif[1], Kamal Shagufta[2], Rehma Saima[3], Bibi Ismat[4] and Rehman Kanwal[5]

Department of Chemistry, Government College University Faisalabad, Pakistan

[2]shaguftakamal@gcuf.edu.pk

Abstract:

Peptides play an important role as mediators of key biological functions. Their unique properties, in terms of efficacy, selectivity, specificity and low toxicity, make them particularly attractive as therapeutic. In this study, different varieties of plants will be collected from the different regions of Faisalabad distt. Peptides were extracted from selected plant species and purified by different chromatographic methods. Different techniques like UV-VIS, FTIR were used for the characterization of extracted bioactive peptides. The antimicrobial activity revealed that the 2mg/ml dilution showed best results. The MIC of the biological peptides were 0.39mg/ml, 0.781mg/ml, 1.562mg/ml, 3.12mg/ml, 1.562mg/ml and 3.12mg/ml. The values of MBC ranged from between 1.06 to 4.682 which showed that some peptides were bacteriostatic and some were bactericidal. The antioxidant activity was checked with 2, 2-diphenyl-1picryl hydrazyl and the samples showed results from 10% to 68% but sample 4 showed 68.35% and sample 6 showed 45.56% activity. The results of average log reduction of viable cell count in time kill assay indicated that E.coli and Bacillus thurigenesis are the most susceptible species. The present study has involved the high-throughput screening, protein structure prediction methods, protein–ligand docking, to make a better drug against serine protease of virus.

Keywords: Peptides; Log kill assay; bacteriostatic; MBC

Phytochemical and Biological analysis of Moringa olifera based on its broad-spectrum applications in pharmaceutics

Naz Nida[1*], Parveen Shagufta[1], Shafiq Nusrat[2], Khan Maryam[3], Arshad Uzma[4], Yasmeen Farah[5], Riaz Rabia[6]

Department of Chemistry, Government College Women University Faisalabad, Pakistan

[1]shaguftaparveen@gcwuf.edu.pk

Abstract:

Moringa olifera is well known plant due to its notorious, medicinal and pharmaceutical values worldwide. Due to its significant uses, this plant has been utilized as food, forage, nutraceuticals, tincture, teas, extracts etc. to cure a large number of diseases from ancient times when human being was in struggle for survival. Form a decade, researchers and chemists were attracted in investigation of Moringa olifera for its phytochemical and biological actions. Purpose of present study is to provide a detailed review covering all aspects related to pharmaceutical, cosmetics, food etc., all its secondary metabolites, biological activities in a single form to readers and researchers.

Keywords: Moringa Olifera, phytochemical analysis, secondary metabolites

SCALE UP SYNTHESIS OF MONODISPERSED AND STABLE ZnO NANOPARTICLES AND THEIR POTENTIAL APPLICATIONS

Din Imran Muhammad[1]

School of Chemistry, University of the Punjab, Lahore, Pakistan

[1]imran.chem@pu.edu.pk

Abstract:

Nanotechnology acknowledged as the study of the particle ranges in size that is 1-100nm having one dimension. Currently, most of the available techniques are environmentally harmful, costly, and ineffective with respect to the resources and energy use. Objective: There are several factors that greatly affect the quantity and quality of the synthesized nanoparticle, also affect their application and characterization. These factors include the method used for synthesis, temperature, time, pH, pressure, particle size, environment, and salt concentration. Synthesis of nanoparticles can be done by using the extract of plant. Green synthesis of the nanoparticles is environmental friendly, non-toxic and safer reagents. Methodology: Syzygium cumini leaves have variety of metabolites such as phenolic compounds, reducing sugars and others, these metabolites behave as reducing agent for the synthesized metal NPs. Color of zinc nitrate solution change by the addition of extract showed the synthesis of MNPs. Results: The characterization done by using various techniques such as Ultraviolet-Visible spectrophotometry and Fourier transform infrared spectrometry. Spectroscopic methods confirmed the formation of ZnO nanoparticles. Fourier transform infrared technique is used for the functional group analysis. Significance & conclusion: As an application the Zinc Oxide nanoparticles were employed as photo-catalyst for methylene blue degradation dye, also act as a catalyst for 4-nitrophenol degradation for water purification.

Keywords: Catalytic Pyrolysis; Nanotechnology; Photocatalyst

Zinc(ll), Cadmium(ll), Mercury(ll) and Iron(ll) complexes derived from 2-((ortho-tolylimino)methyl) phenol Schiff base ligand: Synthesis, Spectral Characterization and Antimicrobial studies

Kanwal Attia, Ashraf Rizwan, Parveen Bushra [*a], Tariq Haider Noman, Ali Ghulam Kulsoom

Department of Chemistry, Government College University, Faisalabad, Pakistan

[*a]bushraparveen@gcuf.edu.pk

Abstract:

Schiff base was prepared by the reaction of o-toluidine with 2-hydroxybenzaldehyde. A series of new complexes [C28H24HgN2O2] (1), [C28H24CdN2O2] (2), [C28H24ZnN2O2] (3), [C28H24FeN2O2] (4), [C14H12ZnNO] (5), [C14H12HgNO] (6) were prepared by the Schiff base ligand 2-((o-tolylimino)methyl)phenol [HL]. The ligand and newly synthesized complexes were characterized by analytical and spectroscopic techniques including 1H-NMR, elemental analysis, FT-IR, and UV-Visible studies. The FT-IR results confirmed the bidentate binding of the ligand involving phenolic oxygen and azomethine nitrogen. Elemental analyses and NMR spectral data of the ligand and their metal complexes agree with their proposed structures. The magnetic moments and electronic spectral data suggested that metal complexes 2 - 4 have an octahedral geometry while distorted tetrahedral for complex (1) and (6). Molar conductivity results showed that these synthesized complexes were non-electrolyte in nature. The XRD studies revealed the nanocrystalline behavior for the complexes. The synthesized ligands, along with their metal complexes, were screened for their invitro antibacterial activity against Gram-negative (Escherichia coli and Pseudomonas aeruginosa) and Gram-positive (Bacillus subtilis and Staphylococcus aureus) bacterial strains and for in vitro antifungal activity against (Candida albicans, Aspergillus flavus). The results of these studies show the metal chelats to be more antibacterial/antifungal against one or more species as compared with the Schiff base ligand.

Keywords: Transition metal compounds, spectral characterization, Antimicrobial Studies, Schiff base, XRD tw

A systematic review on: Microbial degradation of Bisphenol A by Bacterial strains and Toxicological evaluation in rats

Munir Asma[1], Salah Ali Muhammad [2]

Department of Chemistry, Government College Women University, Faisalabad, Pakistan

[1]asmach994@gmail.com

Abstract:

Bisphenol A (BPA; 2, 2,-bis (hydroxyphenyl) propane) is an organic compound is made up of two phenol rings joined by methyl bridge, with two methyl functional groups attached to the bridge. It is a compound that is widely used and present in polycarbonate plastic manufacture and epoxy resins for several years. This compound is present abundantly in beverage containers baby bottles, plastic food products, food cans coatings, dental secants, and medical devices. People of different ages were observed to be unavoidably exposed to BPA in daily life. BPA was also detected in different samples of the environment such as water, sewage, dust, indoor and outdoor air. In several studies, it was reported that BPA was observed in human amitotic fluid, breast milk, human placenta, cord blood, and fetal liver. However, exposure to BPA induces serious environmental pollution and causes adverse effects on human and animal health. The adverse effects of BPA are associated with several diseases such as diabetes, neurobehavioral, abnormal karyotypes, inflammatory cytokine dysregulation, and mitochondrial-mediated apoptosis in hepatic tissue. Therefore, the aim of this review is to consider scientific attempts to control the hazardous effects of BPA. Biodegradation of BPA by using different bacillus strains would be a safer and efficient way of controlling and removing this compound. Acute and chronic toxicity studies should also be considered to evaluate different toxicological effects of BPA and how the biodegraded BPA give its effects.

Keywords: Bisphenol A, hazardous, biodegradation, bacterial strains, toxicity, epoxy resins

Risk assessment of **Liver Carcinoma Associated** with **AFB1 Exposure** from **Consumed Edile Cooking Oil Food Products** in **Faisalabad Punjab**, **Pakistan**

Jubeen Farhat [1], Zahra Nida, Nazli Huma-i-Zill, Saleemi Kashif Muhammad

Department of Chemistry, Government College Women University Faisalabd, Pakistasn

[1]**dr.farhatjubeen@gcwuf.edu.pk**

Abstract:

Contamination of edible vegetable oils with aflatoxins is a worldwide problem due to the harmful effects of AFs on human health and cooking oils are the main source for fungal growth particularly storage fungi (sp. Aspergillus).The purpose of this paper was to retrieve all data available on AFB1 in edible cooking oil used in fried food from Faisalabad **(**Pakistan**)** to assess the risk of cancer due to AFB1 exposure through fried food using the EFSA's Margin of Exposure (MOE) and FAO/ WHO's quantitative liver cancer risk approaches**,** respectively. One hundred samples of different cooking oils (Canola, Sunflower and Soybean oil**)** were collected from various food points/restaurants of**,** Faisalabad **(**Pakistan**)** and studied for AFs contamination using Mycosep 226 columns and HPLC-FLD, 89% cooking oil samples were AFs as well **as** AFB1 positive with 65% exhibiting AFs content above the permissible limits. Higher level of AFB1 and AFs were observed in canola oil than soybean and sunflower oil**.** Approximately 71% (ranges 54.4-281.1 µg/kg) of the samples of canola oil were contaminated with AFs levels that exceed the permissible limits suggested by the European Commission regulations (20 µg/kg)**.** The MOE values calculated from the intake of canola oil samples used in fried foods from Faisalabad **(**Pakistan**)** were substantially lower than the other oils (sunflower, soybean oils), indicating that risk control is possible. Besides that, canola oil showed higher risk of liver cancer cases associated with AFB1 exposure (17.13 per 100,000 males over 35 years) and (10.93 per 100,000 females over 35 years) than soyabean and sunflower oil**.** Health risk assessment revealed that both males and females over the age of 35 are at substantial risk of liver cancer by using a quantitative liver cancer approach. The novelty of this study lies in the factthatnosuchstudyisreportedrelatedto liver cancer risk assessment associated with AFB1 exposure from consu med edible cooking oil in Faisalabad, Pakistan. Therefore, a national plan to address this issue is recommended, as well as regulatory authorities' strict inspection of edible oil products**.**

Keywords: AFB1**,** AFs, HPLC, dietary intake, MOE, quantitative liver cancer**,** risk assessment**,** Faisalabad**.**

Novel Synthesis of Biogenic Nanoparticles using Desert plant and Its Dye Degradation Investigations

Hassan Warda *, Nisa Un Fakhar

Department of Chemistry, The women University, Multan, Pakistan

Abstract:

The capacities and potential of biogenic nanomaterials of low cost desert plant for the removal of basic hazardous dye from its aqueous solution were investigated. Different techniques were used for the characterization of nanomaterials including UV, FTIR, SEM-EDX and elemental analysis. The influence of different parameters on the sorption process was studied using the batch process to determine the equilibrium sorption capacity of the synthesized nanomaterials. The equilibrium sorption capacity of the material increased with increasing the initial dye concentration. The extent of dye removal decreased with increase in the temperature. Kinetic parameters and sorption isotherm models were studied for determination of kinetic rate and maximum sorption capacity. The negative values of ΔGo and ΔHo indicated the spontaneous, feasible and exothermic nature of the sorption process. The studies indicated that synthesized nano composites were very attractive material for removing the selected dye from dyed effluents than many of those reported in the literature.

Session-IV

Online

Invited Talk

An Antiaging Molecule: The Cellular Energy Sensor 'NAD+'

Selamoglu Zeliha[1]

Department of Medical Biology, Faculty of Medicine, Nigde Ömer Halisdemir University, Nigde, Turkey

[1]*zselamoglu@ohu.edu.tr*

Abstract:

Nicotinamide adenine dinucleotide (NAD+) has essential functions in metabolism. In metabolism, NAD+ is involved in redox reactions, carrying electrons from one reaction to another, therefore, found in two forms in cells. NAD+ is an oxidizing agent and it accepts electrons from other molecules and becomes reduced. The balance between the oxidized and reduced forms of NAD is called the NAD+/NADH ratio. This ratio is an important component of what is called the redox state of a cell, a measurement that reflects both the metabolic activities and the health of cells. NAD+ and its related derivatives are major coenzymes in various enzymatic reactions, such as oxidoreductases and dehydrogenases in living cells. NAD+ is also involved in fundamental metabolic processes including glycolysis, the citric acid cycle, and mitochondrial oxidative phosphorylation leading to energy production. NAD+ has been shown to be the key substrate for poly(ADP-ribosyl)polymerases, NAD+ glycohydrolases, and histone deacetylases known as sirtuins. These enzymes have been termed 'NAD+' consumers, and are involved in modulation of DNA repair, maintenance of intracellular calcium homeostasis and immunological roles, and epigenetically modulated gene expression. Nowadays, the researchers focus on the metabolism of NAD+ is used by the body as area of intense researches on unravelling the secrets of our cellular '*energy sensor*' NAD+ for promoting healthy ageing. As a result, researches in the last two decades have shown that NAD+ is more than a mere regulator of metabolism, but rather may play a key role in the ageing process.

Keywords: NAD+, Cellular Energy Sensor, Coenzyme, Anti-ageing, Metabolism.

Invited Talk

Two-Dimensional Covalent Organic Framework Membranes for Water Purification

Khan Ali Nazi

Wuhan Textile University, Wuhan, China

niaz2mn@hotmail.com

Abstract:

Water scarcity has become a big challenge in the modern world due to the exponential increase in population, urbanization and health awareness. Distillation is one of the widely used method to purify water, but it is an energy extensive method relying on burning fossil fuel which in turn pollutes the environment. Membrane technology is an alternative to distillation which requires a much lower energy profile. Indeed, reverse osmosis membranes for desalination have gained an enormous amount of share in the water purification in the last few decades. However, the performance of these membranes is extremely low (1 L m^{-2} h^{-1} bar^{-1}). Therefore, new materials and methods are required to obtain a higher water purification rate to fulfill the evolving water demand. Covalent Organic Framework (COFs) are emerging polymeric materials with some distinct properties such as high crystallinity, ordered pores and high porosity. Due to these properties, COFs have attracted enormous research interest in water purification field. However, COFs are generally synthesized as polycrystalline powders which are difficult to translate to defect-free membranes. In this presentation, some representative works based on COF membranes will be presented. Focus will be laid on the intelligent design of new methods such as solid-vapor interfacial polymerization, monomer exchange in-situ polymerization to develop defect-free COF membranes. The speaker will focus on the results from these publications such as permeance of 411 L m^{-2} h^{-1} bar^{-1} compared to 1 L m^{-2} h^{-1} bar^{-1} for the commercial membranes, which is the highest reported for COF membranes. The speaker will talk about the first ever report using monomer exchange strategy to report defect-free COF membranes. The work presented here has global impact and has been cited in many top journals.

Keywords: nanofiltration, desalination, covalent organic frameworks, thin films, interfacial polymerization

Invited Talk

Synthesis of highly efficient $MA_xFA_{1-x}PbI_3$ perovskite films from an aqueous halide-free lead precursor for high-performance perovskite solar cells

Adnan Muhammad[1]

Graduate School of Energy Science and Technology, Chungnam National University, Republic of Korea

[1]adnan5750@gmail.com

Abstract:

All sequential-dip-coating deposition of mixed organic cationic $MA_xFA_{1-x}PbI_3$ perovskite films from an aqueous non-halide lead precursor solution was effectively developed. Efficient crystal phase and surface morphologies of $MA_xFA_{1-x}PbI_3$ perovskite films were successfully realized by varying MAI/FAI molar ratios in precursor solution over as-prepared $Pb(NO_3)_2$ layer. The various grain sizes and boundaries as well as cubical lumps of $MA_xFA_{1-x}PbI_3$ perovskite crystal were also modulated after annealing at 120 °C of produced $MA_xFA_{1-x}PbI_3$ perovskite films formed with suitable concentrations of MAI and FAI solution. Interestingly, all-dip-coating-treated $MA_xFA_{1-x}PbI_3$ perovskite layers have no presence of d-$FAPbI_3$ perovskites, even at low MAI insertion into the FAI solution. Efficient device performances and improved stability with a power conversion efficiency of 14.1% in perovskite solar cell devices with the all-dip-coating processed $MA_{0.5}FA_{0.5}PbI_3$ perovskite layers realized by incorporating $Pb(NO_3)_2$ layers into MAI/FAI (1/1 molar ratio) solution.

Keywords: Dip-coating, Non-halide precursor, aqueous precursor, Perovskite solar cells

Invited Talk

Effect of different therapeutic agents in COVID-19 patients admitted in High Dependency Unit (HDU).

Waheed Yasir[1]

Foundation University Medical College, Foundation University Islamabad, Pakistan.

[1]yasir_waheed_199@hotmail.com

Abstract:

COVID-19 has affected all the countries of world with over 335 million cases and 5.5 million deaths. Pakistan is currently experiencing 5th wave of COVID-19 with over 29,000 deaths. Fauji Foundation Hospital, Rawalpindi, is a large, tertiary care hospital, which established COVID-19 High Dependency Unit (HDU) at the start of pandemic. Our HDU is fully equipped with all the necessary advanced facilities, all investigational therapies and availability of investigational pharmacological agents for management of severe to critical Covid-19 patients admitting in HDU. In this study we analyzed the effect of Plasmapheresis, Anti-coagulants, Steroids and Remdesivir used in HDU for the treatment of COVID-19 patients.

Patients administered with anticoagulants showed a survival rate of 74.5% compared with 38.3% survival in non-anticoagulant group. Patients are treated with three different doses of steroids in HDU. Patient group which received Dexamethasone 6 mg / day showed best results with only 3% mortality rate, high median time from hospital admission to death and lowest dependence on respiratory support after 10 days of steroid administration. Plasmapheresis did not showed any improvement in the survival rate of patients. Patients with different co-morbidities showed high mortality rate in HDU. Remdesivir administered to dialysis patients, improved the survival rate.

Anticoagulants, Steroids and Remdesivir improved the survival rate of patients admitted in HDU of a tertiary care hospital in Pakistan.

Keywords: COVID-19, Steroids, Remdesivir, Anticoagulants.

Invited Talk

Recent advancements in the application of Nanotechnology in Textiles

Sharjeel Abid[1*]

[1]Department of Textile Engineering, School of Engineering and Technology, National Textile University, Pakistan.

Sharjeel.abid@ntu.edu.pk

Abstract:

With the recent advancements in nanotechnology, its applications have penetrated all scientific fields, including the world of textiles. Nanomaterials embedded into textile substrates can induce stain/water repellence, wrinkle-free effect, anti-static surface, and antimicrobial effects to fibers without compromising their comfort and flexibility. Nanomaterials also offer a more comprehensive application potential to create connected garments that can sense and respond to external stimuli via electrical, color, or physiological signals. Bioactive nano textiles have been engineered with advanced biomaterials to facilitate a healing response in the body. The biomedical structures with advanced nano-features are sophisticated devices for cardiovascular, neurovascular, orthopedics, and general surgery applications. This talk highlights some of the important recent advancements in the application of nanotechnology in textile substrates with specific end outcomes.

Case Study Surveillance of sensitization and adverse health effects assessment by low molecular weight organic acid anhydrides exposure in the Site Area Kotri, Jamshoro, Pakistan.

Qureshi Tahira [2*] & Qureshi Sumera [1]

Department of Plant Pathology,Faculty of Crop Protection,Sindh Agriculture University,Tandojam,Sindh.

Government College University Hyderabad, 71000, Sindh, Pakistan

qureshitahira@gmail.com

Abstract

The major aim of this present study was to explore the exposure-response effects of harmful chemicals organic acid anhydrides (OAAs) frequently used in polymer and different industries including chemical (n=50), paint(n=70), plastic(n=30), dye(n=50) and Pharmaceuticals (n=50) compared with control (n=150) of same age groups (20-60yrs). The Serum total protein, serum Albumin and Hemoglobin levels were evaluated clinically. The demographic study of all of worker groups (n=250) was done by questionnaire, medical history and habitual addictions were also obtained. The comparison of serum total protein showed no significant difference ($p>0.05$), However, the serum albumin of plastic industry ($p>0.01$) and dye industry ($p>0.05$) workers found below the normal range. The Haemoglobin was significantly decreased ($p>0.05$) among all of worker groups than control (non-exposed) may revealed the prevalence of anemia. This suggests that changes in serum protein after exposure to anhydrides may play the key role behind the pathogenesis of allergy and hypersensitivity among workers, SITE Area, Kotri.

Keywords: *harmful;serum albumin;anemia;allergy;anhydrides.*

Extraction of phenolic compounds from Iraqi Coriandrum Sativum L. and loaded on copolymeric hydrogels and examine there as drug delivery system and antioxidant

Sadoun Ali Ula[1], Shakir Zainab, Ali-Aland and Haddad Mahmood Athir[1*]

Department of Chemistry College of Science, University of Basrah

[1]alula3li95@gmail.com,[1*]athir.haddad@uobasrah.edu.iq

Abstract:

The phenolic extracts for leaves and stems (L+S) parts and leaves (L) part of Iraqi Coriandrum Sativum L. and their total phenols, total tannins and total flavonoids are described. Three copolymeric hydrogels prepared and loaded with phenolic extract 4 (U1-U3). The HPLC results show three phenolic compounds, while the GC-Mass results show one phenolic compound and four non-phenolic compounds. Gained results showed that there are significant ($P < 0.05$) variations in total phenols (9.822 ± 0.634–4.015 ± 0.118 mg GAE/g DW), total flavonoids (8.112 ± 0.115–2.811 ± 0.371 mg QE/g DW) and total condensed tannin (4.245 ± 0.276–1.135 ± 0.091 mg QE/g DW) contents for all phenolic extracts. The swelling rate for (U1-U3) in distilled water, the SGF, and the SIF was estimated. The maximum swelling was observed in copolymeric hydrogels at pH 6.9 in distilled water. The IC50 values of radical scavenging activity of the phenolic extracts 4, 8 and phenolic extract 4 released from copolymeric hydrogels (U1-U3) show varied significantly ($P < 0.05$). Our results indicated that Iraqi Coriandrum Sativum L. could constitute a rich and novel source of natural antioxidants. When it loaded on, copolymeric hydrogels could be used as a drug delivery system.

Keywords: Iraqi Coriandrum Sativum L., phenolic extracts, copolymeric hydrogels, drug delivery system, antioxidant

Structural and morphological properties of Graphene oxide nanocomposite (r-GO/$La_{1-x}Co_xCr_{1-y}Fe_yO_3$) for the removal to toxic and carcinogenic industrial pollutant

Bibi Ismat[1*], Nazeer Zarish[1]

Institute of Chemistry, the Islamia University of Bahawalpur, Pakistan

[1]Drismat@iub.edu.pk

Abstract:

Cobalt and iron co-doped La1-xCoxCr1-yFeyO3 (x, y = 0.24) and undoped $LaCrO_3$ perovskite nanomaterials were synthesized using micro-emulsion route and the La1-xCoxCr1−yFeyO3 composite was prepared with 5% reduced-graphene oxide (r-GO) using ultra-sonication process. The morphological, structural and thermal properties were investigated by Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Raman Spectroscopy, Thermogravimetric Analysis (TGA) and Fourier Transform Infrared Spectroscopy (FTIR) techniques. The effect of Co, Fe doping and r-GO on the conductivity of the synthesized samples was investigated by current-voltage (I-V) analysis. The perovskite structure was orthorhombic with particle size in 21.24 to 31.58 nm range. The EDX spectra of doped La1-xCoxCr1-yFeyO3 and La1-xCoxCr1-y FeyO3/r-GO nanocomposite shows the clear characteristic peaks of La, Co, Cr, Fe, O and La, Co, Cr, Fe, C and Crystal violet (CV) dye was selected for evaluation of photocatalytic activity (PCA) of the prepared materials under visible light irradiation. La1-x CoxCr1-yFeyO3/r-GO showed remarkably higher PCA as compared to pristine LaCrO3 and La1-xCoxCr1-yFeyO3. The r-GO composite degraded 89.08% of CV within 100 min irradiation under visible light. This valuable enhancement in PCA was due to the structural features of La1-xCoxCr1-yFeyO3/r-GO nanocomposite. In view of promising PCA, the composite has potential for the catalytic degradation of dyes in effluents using sunlight irradiation.

Effective Antiplasmodial Activities of Synthesized Iron oxide Nanoparticles using extract Of Nephrolepis Exaltata

Ahamd Ijaz [1], Nadeem Faisal

Department of Chemistry, Kohat University of Science and Technology Kohat, Pakistan

[1]drijaz_chem@yahoo.com

Abstract:

The synthesis of metal nanoparticles using biological systems is an expanding research area due to the potential applications in nanomedicines. The green synthesis of iron oxide nanoparticles (FeO-NPs) is convenient and extracellular method which is less expensive and environmentally safe. In the present study the iron oxide nanoparticles were successfully synthesized through a simple green route, where FeCl3. 6H2O used as precursor and the plant extract of Nephrolepis exaltata as reducing as well as capping agent. The obtained nanoparticles were characterized by different techniques. The iron oxide nanoparticles surface plasmon resonance peak showed maximum absorption at 294 nm in colloidal solution. The FT-IR (Fourier transform infrared-spectroscopy) studies was used to identify different photoactive biomolecules -OH, C-H, C-C, and CO, responsible for the reduction of FeCl3 to FeO-NPs. X-ray diffraction (XRD) showed the particle size, which was 16 nm and crystallinity of nanoparticles. Scanning electron microscopy (SEM) was used to recognize the spherical image of nanoparticles and the elemental composition was confirmed by an energy dispersive X-ray spectrometer (EDX). The anti plasmodial activity of these nanoparticles was studies against Plasmodium parasites. The parasitic property was analyzed by Parasite inhibitory values,that were 23±0.3 at concentration of 25 µg/mL, 55±0.6, 71±0.9 and 89±1.3 at 50, 75 and 100 µg/mL. The important outcome of the study was to the development of value-added products from medicinal plants of Pakistan for biomedical and nanotechnology-based industries

Keywords: Iron Nanoparticles, Plant Nephrolepis Exaltata ,Characterization,AntiPlasmodial Activity.