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18TH INTERNATIONAL & 30TH NATIONAL CHEMISTRY CONFERENCE ON RECENT TRENDS IN CHEMISTRY

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ABSTRACT BOOK

Jointly Organized by
Department of Chemistry, SSC
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Innovation & Commercialization
UMT Lahore – Pakistan
&
The Chemical Society of Pakistan

WELCOME TO CCUMT-2019

On behalf of the organizing committee, we are pleased to announce that 18th International and 30th National Conference on Recent Trends in Chemistry is going to be held from November 27 to 29, 2019 in LAHORE – PAKISTAN. The Conference aims to provide an atmosphere for colleagues from all over the world to share expertise, to exchange new ideas, to discuss challenging issues that describe significant advances in the following areas and dimensions of Chemistry; Organic, Inorganic, Physical, Analytical, Environmental, Natural Product, Material, Nano, Nuclear, Biological, Nutritional, Agricultural, Electro, Industrial, Polymer, Textile and Computational Chemistry. Over the last 50 years, the discoveries in the chemical sciences and the application of these inventions have been targeted at the development of technology and the prosperity of mankind that ensured the high quality of life away from environmental destructions for a sustainable future.

Initially, at the first place we are thankful to University of Management and Technology, which have supported the organizing of the conference at all levels. Without the great devotion of our faculty and administrative staff of the university, it would simply have been impossible to organize this esteemed event. The organizers of CCUMT 2019 are also indebted to Pakistan Academy of Sciences, Higher Education Commission and The Chemical Society of Pakistan for their utmost support in planning and executing the whole program.

We are very grateful that almost 300 participants from different cities and countries attend the conference. We wish you all a very pleasant and inspiring time in Lahore, with many fruitful discussions and opportunities for new contacts that will be of importance for the future of our field.

Best regards,

Dr. Sammia Shahid

Conference Chair

Organizing Committee of CCUMT-2019

Department of Chemistry, University of Management and Technology, Lahore.

Ch Jamil Anwar | Sammia Shahid | Ayesha Mohy ud Din | Sohail Nadeem

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Table of Content

ORAL PRESENTATIONS

POSTER PRESENTATION

ORAL PRESENTATIONS

Exciting Discoveries at the Interface of Chemistry and Biology

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Phytochemical constituents are highly evolved, specific, and effective gene products. Their diverse structural and stereochemical characteristics make them valuable templates for exploring novel molecular diversity. Nature has been the first source of cure for diseases and discomforts which have led to the foundation of many empirical therapeutic interventions, majority of these have emerged from a plethora of terrestrial resources. Today, natural products and their derivatives represents over 50% of all drugs in clinical uses and derived from diverse sources such as marine organisms, microorganisms, insects, and even animals. Natural products are thus playing a key role in global healthcare and economy.

Anti-infection drug discovery and development is unfortunately receiving lesser attention and funding in global healthcare R&D. Many pharmaceutical conglomerates have either closed down or down-sized their anti-infection drug discovery programs. Similarly fewer researchers are engaged in academic institutions in this field. This has created an alarming situation which needs urgent action to avoid the menace of pre-antibiotic era. In this lecture, examples of our studies, focusing on the discovery of potential anti-infective leads from nature will be presented.

Multidrug resistance is a challenging problem for the health care sector and is very common in familiar pathogens, such as vancomycin-resistant Enterococci and Staphylococcus aureus. Exposure and inappropriate use of the antibiotics is the major cause of MDR, both in developed and developing regions. Our study, focusing on the discovery of natural and synthetic compounds, active against multidrug resistant bacteria Staphylococcus aureus, and Pseudomonas aeruginosa have resulted in the identification of several novel and potent inhibitors of MDR Staphylococcus aureus (EMRSA-17, EMRSA-16, MRSA-252, and Pak clinical isolates) from natural sources. Resistance-reversal studies at molecular level were carried out by employing flow cytometric, microscopic, and spectroscopic techniques. Synergistic and partial synergistic

effects of these compounds, in combination with antibiotics, were investigated. This work has so far resulted in the identification of several novel "helper molecules", which can increase the efficacy of existing antibiotics to over 1000-fold in some cases.

Breast cancer is the most common cancer in women worldwide, with nearly 1.7 million new cases diagnosed in 2014 (second most common cancer overall). This represents about 12% of all new cancer cases and 25% of all cancers in women. Incident rates vary from 19.3 per 100,000 women in Eastern Africa to 89.7 per 100,000 women in Western Europe. In most of the developing regions the incidence rates are below 40 per 100,000. It has been reported in 2015 as the most prevalent cancer in women. Approximately one-third of all breast cancer patients and two-thirds of postmenopausal breast cancer patients have hormone-dependent (estogen-dependant) breast cancers, which express estrogen receptors and require estrogen for tumor growth. Aromatase inhibitors are currently being tested as primary preventing therapy in large randomized trials. While only a few chemotherapies such as exemestane and tamoxifen are in clinical practices for the inhibition of aromatase function. Therefore, there is a need to identify new structural analogues of available drugs and evaluated their anticancer potential. In this, study, we have synthesized the new derivatives of existing aromatase inhibiting drugs including exemestane, formestane, testolactone, mibolerone, boldenone, indomethacin, levonorgestrel, through biotransformation and evaluate their potential against aromatase enzyme. The new analogues of the drugs were found to be moderate to potent inhibotrs of aromatase enzyme as compared to standard drugs letrazole, and exemestane. During this presentation, underlying philosophy and approach of our research on cost-effective discovery of lead molecules from nature will be discussed.

Community-based/STEM Experiential Learning: Is it STEAM?

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This presentation will focus on four examples of community-based/STEM experiential learning strategies that have been successfully used to train our STEM workforce. The four areas include the National Science Foundation (NSF) Innovation Corps geared towards the K-12 grade level public school sector. The second are focuses on undergraduate STEM college students using the retention strategies found in the Creative Scientific Inquiry Experiences (CSIE) model. The third area will describe our efforts in online chemistry courses for nonscience majors. The fourth area folds in the needed soft skills for our students to be successful and is based on the very successful international BOOST workshops through the American Chemical Society with help from a grant from the US Department of State.

The Selenium Compounds with Antioxidant Properties

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Selenium is an essential trace element with physiological nonenzymatic antioxidant properties. Selenium is a structural component of several enzymes with physiological antioxidant properties, including glutathione peroxidase and thioredoxine that catalyse chemistry essential to the protection of biomolecules against oxidative stress and free radical damage. It is, however toxic above little concentration which is required for health. Selenium is incorporated into proteins as selenocysteine, the 21st amino acid. Despite the high toxicity of many selenium compounds, organic derivatives of selenium have been synthesized as anticancer, and for other medicinal applications, as well as biologically active substances exhibiting antiviral, antibacterial, antihypertensive, and fungicidal properties. The biochemistry and pharmacology of selenium is of intense current interest. The selenoprotein glutathione peroxidase may protect the thyroid gland from oxidative damage due to any excess hydrogen peroxide produced during thyroid hormone synthesis. Overt hypothyroidism is associated with dyslipidemia, hypertension, and an increased risk of cardiovascular disease. Selenium plays a major role in thyroxine (T4) conversion to triiodothyronine (T3). In recent years several inorganic or organic forms of selenium have been studied as possible cancer chemo preventive agents. In most of studies, the external selenium was given to experimental animals as selenite form. Selenium could prevent damage to the unsaturated fatty acid of sub cellular membranes by lipid peroxidation induced by free radicals. They have been found to inhibit or delay the process of carcinogenesis induced by chemical carcinogens. The concept that selenium-containing molecules may be better nucleophilic (and, therefore, antioxidants) than classical antioxidants have led to the design of synthetic organoselenium compounds. Thus, new approaches for the synthesis of selenium heterocycles by using more stable, less toxic, and easily accessible selenium reagents are of great interest. As a result, seleniumcontaining heterocycles are of increasing interest because of their chemical properties and biological activities. Recently, there has been a great deal of studies carried out on selenium metabolism.

Some Work of Phytochemistry and Biology of the Medicinal Plant, *Schefflera Leucantha R.Vig.*

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Schefflera leucantha R.Vig, previously published by the synonym, Schefflera kwangsiensis Merr. ex Li (Araliaceae), is the major ingredient of the drug “HanTaoYe Tablet” used for the treatment of trigeminal neuralgia, sciatica, rheumatalgia, and headache for more than thirty years in China. For searching the molecular basis and therapeutic potencial of S. leucantha, the aerial parts were proceeded for phytochemistry research. Consequently, ninety-four compounds were obtained from ethanolic extract S. leucantha, and their structures were determined by spectroscopic analysis and chemical methods. Among them, there are sixty-seven triterpenoids and saponins, the structures of which can be classified into three types: oleanane, lupane, and ursane, and sugar chains of the triterpenoid saponins are located at C-3 or C-28 of the aglycone. There are also ten sesquiterpenes and nor sesquiterpenes, four lignans, and thirteen other compounds. Fifty-five compounds were new and published gradually in the past six years. Eighty-six compounds were bioassayed for their hepatoprotective activities against D-galactosamine induced toxicity in HL-7702 cells, using bicyclol as the positive control, thirty-eight triterpenoid saponins, six sesquiterpenes and nor sesquiterpenes and five other compounds exhibited moderate hepatoprotective activities. Besides, a new lupane saponin, schekwanglupaside C (Sch C) was demonstrated as a potent SERCA activator (EC 50 = 1.20

μM). Given the pivotal role of SERCA in the progression of neuropathic pain and neurodegenerative diseases, Sch C represents a new drug lead compound to develop the treatment of neuropathic pain and Alzheimer disease. Furthermore, a simple and accurate analytical method was developed for simultaneous and quantitative analysis of six triterpenoid saponins in S. leucantha via highperformance liquid chromatography (HPLC) with mass spectrometry (MS). This analytical method has great potential to be a novel tool to qualify S. leucantha.

Smog Engulfing Lahore in Coming Years

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Smog is a noxious mixture of air pollutants including fine particulate matter from dust and soot, toxic gases like oxides of sulfur and nitrogen, volatile organic compounds and ozone. It is an extreme form of air pollution. Usually it results from heavy traffic in urban areas, soot from industries especially foundries, brick kilns and fires to burn agriculture waste. It can be categorized as industrial smog and photochemical smog. A number of factors such as local climate, topography, population, plantation, road, air and rail traffic, industry and other smoke causing sources and sky scrappers in the city play a vital role in smog formation and its persistence. Smog causes a number of respiratory problems especially in infants and people already suffering from chest diseases. London Smog in 1952 killed more than 4000 persons just in five days. With the rapid expansion of industry, multiple growths of vehicles on roads and increase in population, smog is engulfing a number of cities in the South Asian region of the globe including Beijing, Delhi and Lahore.

Lahore, which used to be a pollution free city till middle of the last century, has now become one of the top ten most polluted cities in the world. For last few years this city is experiencing mild smog attacks in winter months. Unfortunately, Lahore possesses all the factors favoring smog including population, vehicles on the roads, industrial units, brick kilns, railway station, air traffic and construction projects. The situation is alarming at present but could be out of control if proper measures would not be taken in time.

Extraction and Determination of Endocrine Disrupting Chemicals in Samples of Environmental Importance

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Endocrine Disruptors are chemicals that may interfere with the body's endocrine system and produce adverse developmental, reproductive, neurological, and immune effects in both humans and wildlife. A wide range of substances, both natural and man-made, are thought to cause endocrine disruption, including pharmaceuticals, dioxin and dioxin-like compounds, polychlorinated biphenyls, DDT and other pesticides, plasticizers like Bisphenol A. Endocrine disruptors may be found in many everyday products– including plastic bottles, metal food cans, detergents, flame retardants, food, toys, cosmetics, etc.

The analysis of endocrine disrupting chemicals is important because they cause adverse effects at concentration as low as 1 ng/L. level. Its determination is very challenging as EDCs are chemically very heterogeneous and may be present in trace quantities. Therefore, sample clean-up and pre-concentration of the sample is necessary before analysis. For this reason, its extraction from samples of environmental concern play dual role of clean up and preconcentration

A wide range of extractants both magnetic and nonmagnetic, unmodified, modified, have been synthesized, characterized and used for the efficient extraction followed by determination of endocrine disrupter chemicals in samples of environmental importance at trace and ultrarace levels.

Smart Polymer Microgels Loaded With Silver Nanoparticles for Catalytic Applications

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Synthesis and characterization of smart polymer microgels have gained a lot of attention in last decade due to their potential applications in various fields including nanotechnology and catalysis.1-4. In this study, silver nanoparticles with diameter of 10±5 nm were fabricated in microgels with different morphologies. The homogeneous microgels were engineered by a single step process of free radical emulsion polymerization while core-shell microgels were obtained by two step method. Silver nanoparticles were loaded into shell region of the microgel system by carrying out the reduction reaction of silver ions pre-loaded inside the sieves of polymer network. Both pure and hybrid microgels were characterized by UV-Visible spectroscopy, Fourier transform infra-red spectroscopy and transmission electron microscopy. Catalytic potential of the engineered hybrid microgels was investigated by carrying out the reduction of various nitroarenes and organic dyes in aqueous medium in the presence of the hybrid system. Effect of numerous reaction parameters including catalyst concentration, sodium borohydride concentration and substrate concentration on the value of apparent rate constant of reduction of the substrate was also studied. Catalytic reduction was found to be occurred according to the Langmuir-Hinshelwood mechanism. Catalytic system was found to be recyclable and may be used for other organic transformations.

X-Ray Crystallography in the Determination of Hydrogen Bonding in Molecular Structures

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X-ray crystallography is one of the most powerful methods to determine the molecular structures of crystalline materials in the solid state. The amplitudes of X-rays diffracted by the crystal are measured very precisely on diffractometers equipped with liquid nitrogen cryostat for cooling the crystals to 100 K during data collection and their probable phases are calculated mathematically. Further calculations lead to a complete picture of the molecule. From the X-ray diffraction data, the positions of individual atoms, the distances between atoms, bond angles, molecular conformations and absolute configurations are determined with high precision. The data also provide intermolecular, intramolecular and packing interactions between molecules in the solid state.

H-bonding plays a unique role in chemistry and material science. The formation of hydrogen bonds in crystals leads to characteristic one-, two- and three-dimensional patterns, which may be defined and utilized in predicting crystal packing or in designing crystals with predetermined structural properties. The areas in which H-bond may be utilized and the types of hydrogen bonding in molecular structures will be discussed.

Supramolecular Macrocycles and Evaluation of Their Drug Delivery Potential

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Macrocycles has been the subject of great interest due to its unique topology, binding sites and high selectivity towards analytes due to geometrically controlled cavity. A series of macrocycles bearing electron acceptors and electron-donor groups with high pH-sensing behavior were synthesized in good yields. The structures of all macrcycles and their precursors were established through 1D and 2D NMR spectroscopy, mass spectrometry, FT-IR, UV-visible spectroscopy and elemental analysis. Fluorescence-enhancement and quenching behavior of the macrocycles and their pre-cursors were utilized for the detection and distinction of environmentally important analytes in the drinking water resources of Karachi in one hand and biological matrix on the other hand. UV-Visible spectrophotometric titrations, cyclic volatmmetry were effectively used for on-off changes experienced upon binding of analytes with macrocycles. Analysis of the crystal structures of the macrocycles revealed their preference for well-preorganized bent-sheet conformations, both as free receptors and their complexes with anions.

Investigating Ectonucleotidase Inhibition Activities of Sulfonamide Based Aromatic/Heterocyclic Compounds

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Ectonucleotidase enzymes are metal dependent enzymes, they are the key regulators of purinergic signalling, and are responsible for hydrolysis of a wide range of extracellular nucleotides and nucleosides, and occasionally other phosphate containing substrates (such as phosphate mono- and di-esters etc). The Ectonucleotidase enzymes are divided into four categories, i) Ecto-Nucleoside Triphosphate Diphosphohydrolases (E-NTPDases), ii) Ecto-Nucleotide Pyrophosphatase/Phosphodiesterases (E-NPPs), iii) Alkaline Phosphatases (APs) and iv) Ecto-5'-Nucleotidase (e5NT). Once released, these extracellular nucleotides and nucleosides are recognized on their respective cell receptors and are important cell signaling molecules that are responsible for modulating a number of (patho)physiological responses. Selectively turning on or off these cell signals has immense therapeutic potential, hence the quest for selective small molecules as modulators (antagonist and agonists) of these ectonucleotidases. We have synthesized a number of sulfonamide containing compounds and evaluated their potential as inhibitors of ectonucleotidases. A number of compounds were identified as highly potent and even selective inhibitors of ectonucleotidases. Molecular docking studies further rationalized the binding site interactions, giving clues for the development of even more selective and potent inhibitors

New Class of Highly Potent Cytolysins for Antibody Drugs Conjugates

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Natural products are still the main source of structural versatility leading to un-expected biological activities helping mankind to fight against diseases. Tubulin binding agents have shown a vital role in current cancer therapy. Taxol is one of the leading compound used for cancer treatment in the last many decades. In 2000, Reichenbach and HÃfle discovered peptide-like compounds from Myxobectrea strains1 with potent cytostatic anti-tumor activity against a wide variety of cancer cell lines (ovarian, breast, prostate, colon, lung, and leukemia) as seen in the NCI-60 cell line panel.1,2 Moreover, they are equally potent in different MDR phenotype cell lines.2 The structure of these peptides is distantly related to marine alkaloid Dolastatin.3 The mode of action of these tubulin binders (tubulysins) resembles that of the vinblastine or vincristine.2,3 Total synthesis of tubulysins was hindered due to fragile N,O-actal side chain. Our structure-activity studies revealed that the side chain can be replaced without losing activity. We achieved g-scale synthesis of a number of derivatives with subnanomolar range activity (low nM â€“ pM). As tubulysins are not selective for cancer cells only so the drug development was not possible till the idea of targeted drug delivery gets appreciation by the FDA approval of first ADC based tubulin binder in August 2011 (AdcetrisÂ®).4 We have explored the possibility of using humanized anti-FAP antibody conjugated to a novel cytolysin which showed a remarkable 100% tumor growth inhibition.

Synthesis of Novel Lead Molecules as Urease Inhibitors

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Urease (urea amidohydrolase EC 3.5.1.5), the only Ni-containing metalloenzyme in eukaryotes, is widespread in nature, and found in a variety of plants, algae, fungi, and bacteria. It catalyzes the hydrolysis of urea to ammonia (NH3) and carbon dioxide (CO2). Liberation of ammonia increases pH significantly and allows the bacteria to survive during colonization. During Helicobactor pylori (H. pylori) infection, the increase of stomach pH is considered as a root cause of pathologies of gastric ulcers. Therefore, it is a common notion that ureases are involved directly in the pathogenesis of several diseases such as peptic and gastric ulcer, pyelonephritis, urolithiasis, ammonia and hepatic encephalopathy, hepatic coma and urinary catheter encrustation. The gastric and peptic ulcers, sometimes may lead to cancer. Hyperactivity of urease brings out considerable economic and environmental tribulations by releasing abnormally large quantity of ammonia into the atmosphere in the process of urea fertilization. To date, only acetohydroxamic acid, has been clinically used for the treatment of urinary tract infections by urease inhibition. In the current situation, the increasing resistance of bacterial pathogens to common antibiotics is the alarming situation for researchers working in this field. Therefore, it is foremost task to develop the novel classes of molecules that specifically target urease as enzyme inhibitors. Our research group has successfully identified a range of lead molecules for the inhibition of urease enzyme.

Evaluation of Nanoparticles, Prepared by using Extracts of *Trillium Govanianum Andangelica Glauca*

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The present study investigates green synthesis, characterization and biological evaluation of nano-particles prepared using extracts of Trillium govanianum and Angelica glauca. Gold and silver nano-particles (AuNPs and AgNPs) were synthesized from the methanol, ethanol and water extracts of T. govanianum and methanol and water extract of A. glauca by mixing 0.1 mM AuCl3and AgNO3solutions with plant extract at 1:10 and 1:9 ratios respectively. The color change from colorless to yellow in case of AgNPs, while in case of AuNPs from colorless to dark purple indicated the synthesis of the nanoparticles. The synthesis of both types of nanoparticles was further confirmed by UV-vis spectro-photometer in the required ranges. The AuNPs subjected to temperature stress demonstrated that these nano-particles were stable from 24°C to 39°C and beyond these temperatures were un-stable. Regarding the salt (NaCl) and pH stresses, AuNPs were more stable in mili-molar concentration of the salt than in molar concentrations and more stable at neutral pH than at basic and acidic pH. The results were further analyzed by FT-IR, XRD, SEM and AFM. It was inferred that alkenes and aliphatic amines were responsible for the synthesis of AuNPs (FT-IR).The crystallite size calculated was in the range of 8.87-15nm for various AgNPs of T. govanianum and A. glauca, cubic in nature (XRD). All the AuNPs synthesized were in nano-regime (AFM, SEM). The AgNPs were more stable in 25°C to 45°C and became unstable at higher temperatures. Like AuNPs, they were also more stable at mili-molar concentrations of the salt (NaCl) than in molar concentrations. AgNPs were more stable at neutral to slightly basic pH and were unstable at higher basic and acidic pH stresses. Mainly, aromatic amines were responsible for the synthesis of AgNPs (FT-IR). The crystallite size calculated was in the range of 9.99-11.99 nm for various AgNPs of T. govanianum and A.glauca, cubic in nature (XRD) and was in nano-regime (AFM). The rhizomes of T. govanianum and roots of A. glauca extracted with different organic solvents showed considerable antibacterial activity against various pathogenic bacterial strains. The rhizomes of T. govanianum extracted with different organic solvents showed better antibacterial activity than and roots of A. glauca extracts. The most susceptible bacteria in case T. govanianum were Pseudomonas aeruginosa (80-85%) followed by Staphylococcus aureus (60-66%) and the most resistance bacterium was Escherichia coli. While in case of A. glauca most susceptible bacteria were Pseudomonas aeruginosa (78-80%) followed by Xanthomonas compestris (66-69%) and

the most resistance bacterium was Klebsiella pneumonia. The various AgNPs and AuNPs of T. govanianum and A. glauca showed efficient antibacterial potential against the tested bacterial strains. In case of AgNPs of T. govanianum the most susceptible bacteria were E.coli (89.22 %) and X. compestris (83.87)and the most resistance bacterium was K. pneumonia, while in case AgNPs of A. glauca most susceptible bacteria P. aeruginosa (54-56 %) and most resistance bacterium were S. aureusandX. compestris. Similarly, in case of AuNPs of T. govanianum the most susceptible bacteria were P. aeruginosa (81-85 %) and K. pneumonia (62-65%) and the most resistance bacterium was B. subtilis, while in case AuNPs of A. glauca most susceptible bacteria were P. aeruginosa (60-66 %) and E. coli (73-66) and most resistance bacterium was K. pneumonia.

The rhizomes of T. govanianum and roots of A. glauca extracted with different organic solvents showed antifungal activity against the tested fungal strains. The most susceptible fungus in case of T. govanianum was Candida albicans (55-59%) and the most resistance was Rhizopus, while in case of A. glauca most susceptible fungus was Candida albicans (65-68%) and the most resistance fungus was Phacelomyces. The plant extracts showed maximum antifungal activity only against Candida albicans while the Au and Ag nanoparticles exhibited maximum activity against Candida albicans and Alternaria respectively, the most resistance fungus in the case AgNPs was A. niger and AuNPs was Alternaria,. All the extracted samples of the rhizomes and roots showed antioxidant activity, however, crude methanolic extract of both plants exhibited better antioxidant activity than the other extracts. The A. glauca root extracts showed better antioxidant activity than T. govanianum rhizomes. AuNPs showed better antioxidant activity than AgNPs. Regarding phytotoxity, in case of T. govanianum chloroform was the best solvent and highly toxic to Lemna minor. Similarly in case of A. glauca, maximum phytotoxity to Lemna minor was revealed by butanol and hexane. The plant showed insecticidal activity against Tribolium castaneu and S. oryzae. The qualitative analysis of the stems and roots extracts revealed the presence of different bioactive compounds such as alkaloids, flavonoids, sterols and tannins.

Impact of Industrial Processing on the Recovery and Composition of Canola Oil and Deodorized Distillate

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Edible oil is Pakistan's largest import item after petroleum products; resultantly vast foreign exchange is being spent every year. Pakistan is the fourth largest edible oil importing. Among vegetable oil Canola crop, being high oil contents and productivity has the potential to a bridge the gap between local production and consumption. Crude canola oil is refined in order to remove undesirable minor compounds that make this oil unusable in food products. However, refining can also cause the removal of desirable health promoting minor components from the oil. Industrial process creates significant amounts of undesirable by-products. However, the most important by-product of edible p refining is the deodorizer distillate (DD) obtained in the last step of refining called deodorization stage.

Aim of present study was to evaluate quality of collected sets of canola oil containing crude, neutralized, bleached, deodorized and deodorizer distillates (DD) form edible oil processing industry. Physiochemical properties such as moisture, color, free fatty acid (FFA), peroxide value (PV), saponification value (SV), iodine value (IV), unsaponifiable matter and soap content were evaluated in the collected sets.

Results of the present study indicated that high amount of natural valuable components such as sterols, tocopherols and fatty acid were present in the DD which could be used in various applications. High contents of FFA contents of deodorized distillate indicated that it could be used a potential source of biodiesel production.

Kinetics of the Thermal Decomposition of Polypropylene over LZ-Y52 Molecular Sieve

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The present work demonstrates the decomposition kinetics of polypropylene in the presence of molecular sieve LZ-Y52. The pyrolysis was performed at different heating rates in the temperature range 30â€“600 oC in inert atmosphere. The kinetics parameters were calculated applying Ozawa Flynn Wall, Tang Wanjun and Coats-Redfern (modified) methods. Based on activation energy all the three methods agree well. Moreover, pyrolysis was performed at 350-390 Â°C in a pyrolysis chamber and the conditions were optimized for maximum oil production. 10% catalyst amount, temperature 370 oC, nitrogen flow rate 16 mL/min and reaction time 60 minutes were the optimum conditions used during experimental work. The products collected were analyzed by gas chromatography/mass spectrometry. In case of thermal degradation, no oil was obtained; however, thermo-catalytic degradation resulted in more than 40% of the oil at 370 oC for 1 hour. Fuel properties of the oil obtained were determined which agree well with standard parameters and therefore, have potential applications replacing fuel oil.

Comprehensive Metabolomics Approach for the Standardization of Medicinal Plants and their Formulations through Advanced Mass Spectrometry Tools

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Plant metabolites can act as drugs for the treatment of a variety of diseases due to their unique skeletal features. A large number of plant metabolites are used as drugs for the treatment of many diseases. The structural diversity of these plant metabolites formed by complex enzymatically controlled pathways is still not fully explored. Moreover, to preserve the medicinally important endemic and non-endemic plant species and their sustainability, the quantity of plant material has been limited to the analytical level. Therefore, sensitive and high-throughput dereplication methods are required for better, unambiguous and high-throughput analysis of natural products in complex mixtures.

This talk will focus on the high-throughput dereplication strategy for the unambiguous identification of different classes of natural product through LC-ESI-MS/MS in the plant extract and their herbal formulations using an integrated approach which includes several confirmatory steps such as exact masses measurement, diagnostic fragment ions, databases search, and isotopic pattern [1-2]. Based on above mentioned integrated approach, we have recently investigated a different classes of natural products including withanolides (steroidal lactones) [3], pregnane-type steroidal alkaloids [4] and Buxus steroidal alkaloids [5, 6] and indentified them in the extract of Withania somnifera, Sarcococca coriacea and Buxus papillosa, respectively, by using electrospray ionization quadropole time-of-flight mass spectrometry (ESI-QTOF-MS/MS) and LC-QQQ-MS analysis. Moreover, the fragmentation pathways and characteristic fragments of a new triterpenoid [7] and some diterpenoids [8] by using ESI-QqTOF-MS/MS will also be presented.

Consequences of Oral Cancer Due to Toxic Elementin Smokless Tobacco Products

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In Pakistan, oral cancer ranks 2nd in all malignancies among both males and females, with the highest reported incidence in the world. The direct Smokeless tobacco products are linked with cancers of the cheek, gum, and inner surface of the lips. Many epidemiologic studies addressing the risk of. Smokeless tobacco products use for cancers of the oral cavity and adjacent sites are being reviewed. In south Asian countries including India and Pakistan tobacco is used liberally for smoking or chewing purpose irrespective of age, sex and economic status either for pleasure or to satisfy addiction. In Pakistan, consumption of gutkha, mainpuri and snuff is most prevalent amongst laborers, driver and young workers, who may be unknowingly harming their health through increased exposure to carcinogenic compounds in addition to toxic elements. The consumption of tobacco products and number of smokers have been increasing steadily world over. The use of smokeless tobacco is limited to some areas in all continents, and it can be used orally or nasally. Generally, chewing of smokeless tobacco products were found to be closely associated with the occurrence of oral cancer and other problems in adolescents and adults especially in Asia. The incidence of oral submucous fibrosis is common, especially in the youngsters who consume In south Asian countries including India and Pakistan tobacco is used liberally for smoking or chewing purpose irrespective of age, sex and economic status either for pleasure or to satisfy addiction. In Pakistan, consumption of gutkha, mainpuri and snuff is most prevalent amongst laborers, driver and young workers, who may be unknowingly harming their health through increased exposure to carcinogenic compounds in addition to toxic elements. The consumption of tobacco products and number of smokers have been increasing steadily world over. The use of smokeless tobacco is limited to some areas in all continents, and it can be used orally or nasally. Generally, chewing of smokeless tobacco products were found to be closely associated with the occurrence of oral cancer and other problems in adolescents and adults. The incidence of oral submucous fibrosis is common, especially in the youngsters who consume SLT products, even after a short period of use. In Pakistan, oral cancer ranks 2nd in all malignancies among both males and females, with the highest reported incidence in the world. The direct Smokeless tobacco products are linked with cancers of the cheek, gum, and inner surface of the lips. Many epidemiologic studies addressing the risk of. Smokeless tobacco products use for cancers of the oral cavity and adjacent sites are being reviewed. The importance of smokeless

tobacco chewing can lead mainly to inflammation of oral cavity. The total and artificial saliva extracted toxic elements, arsenic, cadmium, nickel and lead in smokeless tobacco products.

Synthesis and Characterization of Zinc Oxide Nanoparticles Hybrid with Humic Acid and Its Applications

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Naturally occurring macromolecular humic acid (HA) have gained interest in the chemical, biological and medicine industry owing to their unique behavior, i.e., strong adsorptive and non-toxic nature. In the present research work, the functionalization of organic (HA) with inorganic (ZnO) hybrid nanoparticles was investigated. Humic acid was extracted from agriculture soil by IHSS method and white ZnO nanoparticles were rapidly synthesized from Zn(CH3CO2)2 solution using KOH by precipitation method. Different spectroscopic and analytical techniques UV-Vis, FTIR, XRD and SEM were applied for characterization. The spectral data proved the successful isolation and formation of HA, ZnONPs and hybrid ZnONPs-HA. The XRD pattern indicated the humic acid semi crystalline and ZnONPs crystalline in nature. The crystal size was calculated from the XRD patterns by applying Schererâ€™s formula. The SEM results showed that the diameters of ZnO NPs were in the range of 10 Âµm and spherical shaped hybrid ZnONPs-HA found 1.0 Âµm. The comparison of spectral data of HA, ZnONPs and ZnONPs-HA vividly showed that the coating of HA on ZnONPs has been done and confirmed successful synthesis of hybrid ZnONPs-HA and their application to the plant seeds improved the germination, root and plant growth.

Characterization of Humic Acid Induced Silver Nanoparticles and Their Applications

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Synthesis of silver nanoparticles (AgNPs) with biological properties is of vast significance in the development of scientifically valuable products. In the present study, we adopted simple, nontoxic, eco-friendly method for synthesis of Humic acid from goat muck, used a traditional farming formulating agent and synthesis of AgNPs, Silver NPs were mixed with Humic acid (1:100 mg), water was added to prepare the solution then subjected for the biological activities of Ag-HA induced NP. The nanometallic dispersion was characterized by absorbance measuring 430 nm. Scanning electron microscopyâ€“energy-dispersive spectroscopy and X-ray diffraction analysis confirmed the presence AgNPs and showed the morphology and size of Ag-HA induced NPs. Fourier transform infrared spectroscopy analysis revealed that proteins in the humic acid were involved in the reduction and capping of AgNPs. The antibacterial activity of synthesized and HA induced AgNPs was also examined. The synthesized AgNPs (1â€“4 mM) extensively reduced the growth rate of antibiotic resistant bacteria such as B.Subtitis, S.Anueens, E. Coli, Psedomonas, according to the increasing concentration of AgNPs and Ag-HA induced NPs. However no any significant effect was observed for the gram +ve as well as for the gram â€“ve bacteria in Ag-HA induced NPs.

Study on simultaneous Removal Properties of Layered Double Hydroxide Composite for Cationic and Anionic dyes from Aqueous Solution

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Due to rapidly increasing water pollution by organic dyes, it is necessary to make wastewater suitable for dumping into running water bodies. To clean the wastewater at suitable levels; there is need to develop materials compatible with conditions with that of industrial effluents and should be able to remove most of organic dyes. In this study, a composite of Layered Double Hydroxide (LDH) and hydrothermal carbons (HTCs) were prepared and tested to be used as general-purpose adsorbent for simultaneous removal of cationic and anionic dyes (i.e. methylene blue, methyl orange and reactive yellow). The layered double hydroxide was synthesized by using co-precipitation method using nitrates of Al, Zn and Co while HTCs were synthesized by hydrothermal carbonization. Their composites in different ratios (i.e. 0.5: LDH, 1.0: LDH, 1.5: LDH, 2.0: LDH) also synthesized by co-precipitation method and characterized using FTIR, PXRD, SEM, and BET. Adsorptive study of dyes with various composites were studied using UV-Visible spectrophotometer. It was found that surface functional groups on composites were -OH, NO3, M-O bonds, whereas peaks from HTCs were not prominent in composites which shows dominated character of LDH in composites. LDH are crystalline material but crystalline nature decreases on addition of HTCs. Surface roughness increases while particle size and mesoporosity of composite decreases with HTCs content. Composite with 2.0 g content of HTCs does not show any mesoporosity. Initial experiments show good adsorption of dyes (i.e. MB, MO and RY) onto composite with 2.0 g HTCs which was selected for further experiments and Adsorptive removal was optimized by multivariate technique using response surface methodology (RSM). The optimized value of MB,MO and RY under RSM, such as Amount of adsorbents was found to be (312 mg, 257 mg, 278 mg), Contact time (67 min, 65 min,63 min),Volume (10 mL,31 mL, 30 mL) and Concentration (45 mg/L, 55 mg/L, 56 mg/L). Under such optimized conditions dye removal is 100 %.

FTIR Characterization of Residual Oil Recovered from Spent Bleaching Clay during Storage

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Edible oils and fats are important constituents of our diet, which provide energy and act as a carrier of fat soluble vitamins. When oil is extracted from oilseeds, itâ€™s known as crude oil. This oil cannot be used directly for cooking purpose because it contains undesirable components such as pigments, free fatty acids, metals, gums, waxes, phospholipids and odoriferous materials. These components must be removed from oil to get a stable product with a bland taste. Physical and chemical refining processes are carried out for purification of crude vegetable oils and these includes degumming, neutralization, bleaching and deodorization. Spent bleaching clay (SBC) is a waste material produced as part of the refining process (bleaching) in the vegetable oil industry. This waste material contains 20 to 40 % oil by weight and dumped in landfills without any treatment. Current study was carried out to check the quality of oil present in SBC and its FTIR characterization during 40 days of storage.

Design, Synthesis, Structural and Biological Studies of New bis((5-aryl-1,3,4-oxadiazole-2-yl)thio)Alkanes and Isatin Based Hydrazides

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A new series of bis((5-aryl-1,3,4-oxadiazol-2-yl)thio)alkanes have been synthesized via nucleophilic substitution reaction of dihaloalkanes with respective 1,3,4-oxadiazole-2-thiols and similarly different isatin based hydrazides were synthesized by the condensation of N-alkylisatin with carboxylic acid hydrazides. Fully characterized molecular structures were further studied by single-crystal X-ray diffraction. Density functional theory calculations at B3LYP/6-31+G(d) level of theory were performed for comparison of X-ray geometric parameters, molecular electrostatic potential (MEP) and frontier molecular orbital analyses of synthesized compounds. MEP analysis revealed that these compounds are nucleophilic in nature. Moreover, the non-covalent interactions have been characterized using the NCIplot index. Frontier molecular orbitals (FMOs) analysis was performed for evaluation of kinetic stability. All synthesized compounds were screened in vitro for different biological assays.

Single Source Synthesis and Characterization of Nanostructured Material, Thin Films And Hybrid Composite Materials for Variety of Applications

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The potential applications of semiconducting nano-structured crystalline material and their thin films in optoelectronic devices are strongly dependent on their unique properties and geometrical configuration. Therefore efforts are being focused to develop an effective method for thin films production that guarantees uniform structural, compositional, electronic and optical properties. Fabrication of nanostructured metal sulfide through the single source precursors for the deposition of thin films involves either sophisticated technology or use of hazardous chemicals. This presentation highlights synthetic strategy for the synthesis of single source molecular precursors that are capable of delivering all the elements of interest bonded in one structure so that the desired metal sulfide films can be deposited onto the target substrate. We, therefore, report the design, synthesis and characterization of a series of specifically tailored new single source molecular precursors for the deposition of metal, metal sulfide and iron sulfide thin films on glass and silica substrate using aerosol assisted chemical vapor deposition (AACVD) for their technological applications. The field Emission Scan Electron Spectroscopy (SEM), X-Ray diffraction spectroscopy (XRD) , Transmission Electron Microscopy (TEM) , Atomic Force Microscopy (AFM) are used for the determination of surface morphology and phase purity and geometrical configuration.

Steric Effect in the Design of New Ligand for Transition Metal Catalysis

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Cross-coupling reactions have fashioned extensive applicability and functional group tolerance. This is due to the advent in highly specialized ligand development. However, the cross-coupling reaction faces serious selectivity complications in a more complex system. The solution for most of these problems still exists in fine-tuning of the structure and electronic nature of the ligand. The desirable development in the catalyst stability and robustness, high reactivity and modification the electronic nature for a precise sweet spot may result in higher reactivity. For instance, a variety of ligands are available which could be used for efficient C-N coupling reactions. The most promising results have been demonstrated by diamine-based ligands. The promising examples include diols, 1,10-phenanthroline, neocuproine, thiophene-2-carboxylate, o-hydroxy biphenyl, substituted phenols, and natural amino acids. Thiophene-2-carboxylic acid and amino acids have a special place due to their ready availability. There is still a void that needs to be filled for a universal ligand that catalyzed a variety of reaction. Considering the tremendous coordination power of pyridine/picolinic acid and its suitability as a ligand for Goldberg and Ullmann reactions, we synthesized and screened a variety of picolinic acid-and pybox based ligand in standard C-X and C-C bond formation. The steric and electronic nature have been studied for a variety of reactants to showcase the substrate scope, functional group tolerance and electronic nature of the reacting partners.

Simultaneous Removal of Acidic dyes from Aqueous Solution by Picea smithiana Sawdust

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Mixture of dyes are usually discharged in in the effluents of many industries. This study presents the biosorption characteristics of sawdust of Picea smithiana for the simultaneous removal of mixture of dyes, Acid brown 349 and Acid black 234, from aqueous solutions. Effect of different parameters i.e., pH, contact time, temperature biosorbent and sorbate dose was studied. Sorption capacity of saw dust was 4.7, 4.3 mg/g for both the dyes respectively at pH 1, biosorbent dose 0.4 g and Contact time of 40 min was observed for ABR349 and AB234. The process followed various adsorption isotherms like Langmuir, Freundlich and Dubinin-Radushkevich models. Kinetics of biosorption data followed the Pseudo-second order mechanism. The intraparticle diffusion and film diffusion are the rate controlling process. Thermodynamics of dyes biosorption showed the exothermic (?H = -18, -11 KJ/mole) and spontaneous (?G = -8.6, -7.8 KJ/mole) nature of process for ABR349 and AB234 respectively. The used sawdust can be recycled many times with good efficiency. The results showed that saw dust could be used as a potential source and promising biomass for the removal of mixture of dyes from aqueous solutions.

Essential Trace Elemental Levels (Zinc, Iron and Copper) In the Biological Samples of Smoker Referent and Pulmonary Tuberculosis Patients

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Tuberculosis is one of the major causes of illnesses and deaths throughout world particularly in Asia. Smoking is linked with tuberculosis recurrence and its mortality and may influence bacteriological conversion, clinical symptoms and treatment outcome. The aim of current study was to estimate association among essential trace elements {zinc (Zn), iron (Fe) and copper (Cu)} in human biological samples particularly blood, serum, scalp hair, saliva, sputum, and nasal fluid of smoking and nonsmoking pulmonary tuberculosis patients (n=165, age ranged 16-65 years) residents of Hyderabad, Pakistan. The biological samples of age matched healthy controls were chosen as referents of both genders (n=171) for the comparison purpose. The human biological samples were wet digested in microwave oven by 65% HNO3 and 30% H2O2 with (2:1) ratio. The concentrations of elements in acid digested samples were determined by atomic absorption spectrometry. The average zinc and iron concentration was lower, while level of copper was higher in the biological samples of pulmonary Tuberculosis patients as compared to referent subjects (p < .001). It was also concluded as a result of Zn and Fe deficiency combined with high contact of copper due to smoking of tobacco can be synergistic with the risk factors related with pulmonary tuberculosis.

Sequential Assessment of Cd, Fe, Pb and Zn in Sugar Industry Products in Sindh, Pakistan and Their Intake Risk from Sugar in the Workers

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The aim of the current case study is to sequentially assess the cadmium (Cd), iron (Fe), lead (Pb) and zinc (Zn) in different products (raw juice, bagasse, mud cake, refined sugar, and molasses) and effluents of selected sugar industry nearby Hyderabad, Sindh, Pakistan. Meanwhile, daily intake and toxic risk assessment of Cd, Fe, Pb and Zn from refined sugar by the families of the workers belong to different age group (2-5, 6-15, 16-30, and 31-50 years) of selected sugar industry were also estimated. The highest contents of Fe, Cd, Pb, and Zn were quantified in molasses followed by mud cake, and bagasse whilst raw juice and refined sugar have the least amount of these elements. However, effluent samples of sugar industry have trace levels of studied elements might be due to the strong association of these elements with bagasse, mud cake and molasses, separated during the different processing steps of the sugar industry. The estimated daily intake of Fe and Zn from sugar in studied age groups of families of sugar industry workers were adequate and within the recommended dietary allowance by the Food and Nutrition Board. Whereas, weekly intake of Cd and Pb from sugar by studied subjects were 2 to 5 time lower than the WHO the provisional tolerable weekly intake levels for Cd and Pb from foodstuff. Toxic risk assessment revealed that the studied subjects were not at risk of Cd and Pb toxicity by the consumption of sugar of selected sugar industry. However, the possible carcinogenicity of Cd may be possible from sugar of the studied sugar industry.

Fabrication of Metal Nanoparticles Immobilized Fertilizer as Efficient Growth Regulator for Selected Vegetables

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Metallic Nanostructures (NCs) has been emerging as a new type of efficient materials. NCs are ultrafine particles whose dimensions are in the range between 1 and 100 nm. Due to their physical and chemical properties, nonmaterial is being studied for their use in several different fields of science and engineering. Increase in the context of sustainability, applying innovative nanotechnology in agriculture (including fertilizer development) is regarded as one of the promising approaches to significantly crop production and feed the world’s rapidly-growing population. Applications of diverse conventional fertilizers at high rates and for a long period in the agricultural sector have caused serious environmental issues globally. For example, heavy uses of nitrogen (N) and phosphorus (P) fertilizers have become the major anthropogenic factors exacerbating world-wide eutrophication problems in surface freshwater bodies and coastal ecosystems and even effecting peopleâ€™s daily life. We have synthesized Fe2O3, TiO2 immobilized fertilizer as growth regulator via reported procedure and characterized by different analytical instruments. After the successful synthesis and characterization Fe2O3 and TiO2 nanoparticles as growth regulator for coriander and chili plant the effect of time, dose and temperature on biomass and fruit production was monitored weakly basis. Simultaneously the conventional fertilizers (DAP, natural biomass and Urea) were also used to evaluate the effect of nanoparticles, It was concluded after complete growth and fruit production the TiO2 nanoparticles, NPK immobilized TiO2 and Fe2O3 and Biomass has shown better growth in shorter time as compared with conventional fertilizer (Urea and DAP).

Electrical Communication of Redox Enzymes with Electrodes: Routes towards Biosensors and Biofuel Cells

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Bioelectronics deals with integration of biomolecules with electronic elements to form functional devices. In bioelectronics, the biomolecule can be enzymes, organelles, antigen/antibodies, DNA or living cells, which can be integrated with electrical units to yield energy e.g. biofuel cells. Enzyme based bioelectronics could be biosensors or biofuel cells.

An enzymatic biofuel cells (EBFC) is a specific type of fuel cell, which uses biocatalysts i.e. enzymes especially redox enzymes, instead of metal catalysts, to convert energy stored within chemicals into electrical energy. Most of the (EBFCs) include anodes that oxidize the fuel substrates and cathodes that reduce the O2. In contrast to traditional fuel cells, the introduction of enzymes enables the operation of the cell under mild conditions and utilization of renewable, chemicals as fuels. In addition, if the enzymes are immobilized on the surface of the anode and cathode electrodes, the need for other components required for conventional fuel cells, such as a protective case and membrane are eliminated due to the specificity of the enzyme reactions at the respective electrodes and it is possible to assemble membraneless, noncompartmentalized biofuel cells. Biofuel cells design aims to maximize electron transfer at the two compartments, anode and cathode, in order to produce electric power for electronic devices. EBFCs can be build from low cost components, active in mild conditions (e.g. room temperature and near neutral pH) and are often included in green energy technology. In amperometric EBFCs, the biorecognition element is an oxidoreductase that is able to oxidize/reduce the analyte and transfers the corresponding electrons to the electrode. EBFCs could play a role in nice applications, including miniaturized detecting devices, electronic devices; self powered sensors and portable electronics.

Titania Supported Silver Strontium Nanoparticles for Photocatalytic H_2 Generation From Water Splitting Reactions

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In this study we have discussed a new approach to enhance the photocatalytic activity of TiO2 based-material i.e. Palladium/strontium nanoparticles (Pd/Sr-NPs@TiO2) for H2 generation from alcohol water mixture. The Pd/Sr-NPs are in-situ developed on the surface of TiO2(P25) using chemical reduction method. H2 evolution experiments were monitored at online GC equipped with TCD. The impact of Pd and Sr nanoparticles in the photocatalytic reactions are further declared. We observed that Sr in the form of SrO promotes electron transfer from the TiO2 (i.e. semiconductor) surface to Pd nanoparticles by enhancing premier Fermi level of the TiO2 support. To obtain morphology and structural information, the as-synthesized Ag/Sr-NPs@TiO2 composites were characterized using UV–Vis DRS, XRD, PL, TEM, and XPS techniques, based upon which the mechanistic insights are discussed.

Development in Nanoparticles Research for Applications in Biomedical Sciences, Environment & Renewable Energy Technologies

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The unique chemical and physical properties of nanoscale materials have triggered great scientific interest to explore their potential applications in many fields. The chemical and physical properties of metal/ metal oxide nanoparticles can be tuned by controlling their size, shape and surface chemistry. In this regard, we have developed several reproducible protocols to prepare functionalized metal/metal oxide nanoparticles from subnanometer to over 100 nm in aqueous/organic media with a decent control over their size, shape, and surface chemistry. Many of these metal nanoparticles have been used as building blocks to design/synthesize new nanostructured materials using template-based and template-less strategies. The functionalized metal/metal oxide nanoparticles/nanoclusters possess interesting optical, recognition and catalytic/bio-catalytic properties and currently we are focusing on the applications of these nanoparticles and their composites in biomedical sciences i.e., bio-sensing (especially bacterial detection), bio-imaging, drug delivery, environmental remediation and renewable energy technologies (mainly water splitting). This talk would, therefore, be an overview of our interdisciplinary research activities of Functional Nanomaterials Group at LUMS to synthesize customized inorganic/organic nanoparticles and their composites having unique chemical and physical properties, and subsequent applications in biomedical sciences, environment and renewable energy technologies.

Formulation of Nanobiomaterials and Their Sustained Release Profile with Polymeric Metal Nanoparticles

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We have formulated nano antibiotics, anticancer and antimalarial drugs with different polymers and metals for their sustained and targeted release. Nano-antibiotics having lesser adverse effects and greater efficacy at the targeted site are needed to be developed. Biodegradable and biocompatible polymer was used in combination with metal nanoparticles, which contributes its magnetic characteristics to the nano-drugs. The nanoparticles produced could be used as carriers for releasing at the targeted site.

Ciprofloxacin antibiotic is from the group of flouroquinolone and used to treat the infections like bone and joint, intra-abdominal, diarrhea, respiratory tract, skin, and urinary tract etc. Diethylaminoethyl cellulose was used at the nano scale level in the form of nanocapsules and nanospheres by the modified solvent evaporation method. Ciprofloxacin loaded polymeric nanoparticles established the sustain release characteristics when their dissolution profile was generated for more than 8 hours and their stability of dosage form was also confirmed. Antibacterial activity was studied against diversity of clinically significant Gram positive bacteria and pathogenic Gram negative bacteria and superior antibacterial activity was observed as compared to commercially available drug.

Chloramphenicol is an antibiotic which is being used for the treatment of a number of bacterial infections (typhoid fever, cholera, eye and ear infections etc.). Biodegradable and biocompatible polymer such as diethylaminoethyl-cellulose was used in combination with iron, which contributes its magnetic characteristics to the nanocomposite and is suitable for sustained and/or prolonged drug delivery. Antibacterial activity of chloramphenicol-loaded nanocomposite was found more extensive than the commercially available chloramphenicol (0.5 %) eye drops and showed a maximum of drug entrapment efficiency (DEE) in 48 h exhibiting sustained release of drug. Chloramphenicol has poor bioavailability when given orally due to its poor solubility in the gastrointestinal tract and its early degradation, which can be enhanced by giving Chloramphenicol loaded polymeric-iron nano-drug.

Formulation, characterization, interpretation and in-vitro drug release of methotrexate loaded with polymeric Zinc nanoparticles (anticancer drug) as well as polymeric iron nano-chloroquine phosphate (anti-malarial drug) will also be highlighted.

Functionalization of Native Adsorbent for Enhanced Bisphenol A Adsorption: Column Study

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The aim of present study was to explore the biosorption efficiency of peanut husk (PH) for the removal of bisphenol A (BPA) from simulated waste water. As it is carcinogenic, mutagenic and nervous system disturber, its removal is essential from environment. In this research work, synthesis, characterization and BPA adsorption properties of peanut husk (PH) and its biocomposite were investigated. Physical characterization of native and synthesized biocomposite was performed using Fourier transform infra-red (FT-IR), X-ray diffraction (XRD) and Scanning electron microscope (SEM). In column mode, different parameters like flow rate, bed height and BPA concentration were investigated. Maximum pesticide removal in continuous study was 7.39 mg/g at 4 cm bed height and 45 mg/L initial pesticide concentration. Different mathematical models like Thomas model and Bed Depth Service Time (BDST) model were used to analyze the adsorption rate. Based on the data of present investigation, this work suggests that PH and its biocompatible biocomposite are efficient and environment-friendly to adsorb Bisphenol A. Keywords: BPA; Biosorption capacity; Kinetics; Peanut Husk; BDST; Column study

Nanoscale Functional Materials for Catalysis, Synthetic Fuels and for Chemical Energy Conversion

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Nanoscale materials are becoming increasingly significant for many important applications in industry, for essential catalytic processes and for chemical energy conversion schemes [1,2]. In this pursuit, developing robust and high activity electrocatalytic materials for water oxidation and CO2 conversion, and their synergistic interfacing with competent light-harvesting modules is very important to progress the construction of solar to fuel conversion system [3]. During last 10 years, we have exploited various functional nanoscale materials for catalytic water splitting, CO2 reduction, and recently for biomass catalysis and solar energy conversion [3,4]. We implemented several molecular, inorganic nanomaterials and metal-oxides displaying great potential to be used in electrocatalysis [4,5]. Their effective interfacing with semiconductor photo-responsive materials and/or CO2 reduction systems can provide a potential scheme to make renewable energy supplies [6,7]. Further we are also exploring catalysis for biomass conversion into chemicals and synthetic fuels opening new ventures for chemicals and energy conversion.

Dyeing of Nylon Woven Fabric with Natural Dye Extracted from *Dalbergia Sisso*

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Textile wet processing is considered to be the most polluting industry due to the use of toxic and hazardous dyes and chemicals which not only affect the human but also the aquatic life. For sustainable approach, the researchers are motivated to work on natural dyes and its optimization in dyeing to replace synthetic dyes. Despite having non-toxic nature, these natural dyes also have other functional properties such as anti-bacterial, anti-inflammatory and UV protection. In this research work, natural dye was extracted from Dalbergia sisso leaves to dye 100% nylon 6,6 plain woven fabric. The effect of different parameters such as pH, temperature and concentration of dye on K/S value was studied using spectrophotometer. Colorfastness to washing was increased with increase in temperature containing value of 4-5 whereas color fastness to light showed poor to fair results. The color fastness to dry and wet crocking also showed promising results. The K/S (shade depth) value was increased with increasing temperature and concentration showing maximum value of 13.2.

Impact of Seasonal Variations on Chemical Composition and Biological Activities of Essential Oil from *Cymbopogen citratus* Indigenous to Pakistan

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Essential oils, owing the excellent biological activities have gained huge importance in drugs, skin care products and other medicinal applications. The aim of this study was to investigate the chemical composition and biological activities including antioxidant, antibacterial and antifungal activities of Cymbopogen citratus essential oil and their dependence upon seasonal variations. The chemical composition of essential oils was determined by GC-MS analysis followed by the investigation of physical characteristics such as refractive index and density. Antioxidant activities were assessed by following assays like total phenolics, total flavonoids, reducing power, DPPH radical scavenging ability and bleaching of ÃŸ-carotene-linoleic acid system. Both antibacterial and antifungal activities of essential oils were evaluated by disc diffusion method and Resazurin microtitre-plate assay test by measuring zone of inhibition in mm and minimum inhibitory concentration, respectively. The hydro-distilled essential oil contents ranged from 1.82 % to 1.93% in summer and autumn, with abundant constituents, geranial (51.70% and 47.7%), followed by neral (38.8% and 34.1%), ÃŸ-myrcene (3.90% and 7.10%) and geraniol (3.0% and 2.9%), respectively. The investigated essential oils exhibited good antioxidant, antibacterial and antifungal activities. The results of antimicrobial assays showed that all tested microorganisms were affected. Both the antimicrobial and antioxidant activities of oils varied significantly (p< 0.05) among seasonal variations. Essential oil from aerial parts in autumn season showed better activities as compared to those of summer.

Hybrid Organic-Inorganic Materials (SiO_2/Al_2O_3/C/SiPy+Cl) for Electrochemical Sensing Of Nitrite in Food and Water

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The SiO2/Al2O3/C (C= graphite) has been synthesized through the sol-gel processing technique and used as a support material. On silica surface the reactive species are the silanol, ºSi-OH, groups and functionalized with 3-n propylpyridinium silsesquioxane chloride functional groups. The material compactness and topography were confirmed by SEM, TEM images which show that there is no phase segregation at the magnification applied. The chemical homogeneity of the materials was confirmed by EDX mapping. The degree of functionalization was confirmed through 13NMR, and 29Si NMR. The conductivity of the materials was evaluated through electrochemical Impedance Spectroscopy (EIS) and voltammetry techniques. The sensor was fabricated by the surface modification of the glassy carbon electrode with the SiO2/Al2O3/C/SiPy+Cl materials and tested as an electrochemical sensor for NO2- detection. The detection limit, linear response range, and sensitivity are 0.02 µM, 0.25 to 6.25 mM, and 80 µA•µM cm−2, respectively. The response timé of the electrode is less than 1 s in the presence of 50 µM of nitrite. The sensor showed chemically stability, high sensitivity and is not interfered with by other electroactive molecules present in water and food samples. The repeatability of this sensor was evaluated as 1.9% (RSD; for n = 10 at a 40 µM nitrite level.

Synthesis of Self-terminated Aliphatic Polyamide Dendrimers and Dendron

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Aliphatic poly (amido amine) dendrimers and dendron have been synthesized. Poly (amido amine) dendrimers were synthesized either by convergent, divergent or both. Poly (amido amine) dendrimers were synthesized with piperazine core to generation five azide [G5N3(PPZ)] Polyamide dendrons were synthesized to generation three [G3(COOMe)NH2]. All the aliphatic poly (amido amine) dendrimer and dendrons were synthesized by two step reactions i.e. amidation followed by reduction. Each dendrimer growth was done by converting azide to amine followed by amidation. The present work is carried out to improve the existing methodology for the peptide bond formation using activated acid and amine, find the minimum steps for the iterative growth of dendrimers, study the effect of central core in dendrimer growth, compare the efficiency of divergent, convergent and combined convergent-divergent methodology. The synthesis of aliphatic poly (amido amine) dendrimer, ([G4NH2 (PPZ)] / 1 g scale reaction) is the major achievement of this work. These self-terminated polyamide dendrimers are enzymatically and hydrolytically stable and exhibit antimicrobial activity. Thus, these nanoscales construct open new avenues for biomedical applications. Fig. Structure of G4(PPZ)NH2

Rescent Advances in Indole Heterocycles

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Rescent Advances in indole Heterocycles the heterocyclic compounds constitute a larger class of organic compounds in that there may be a variation in the heteroatom(s) and the size of the ring system. Each heteroatom and the type of ring system have its own impact on the biological activity of a heterocycle. So by tailoring a compound with desired ring size and the choice of heteroatom (or a combination of more than one heteroatom) may lead to construction of a wide range of compounds attractive for pharmaceutical research Indoles represent one of the most well known classes of medicinally important organic compounds called the benzofused N-heterocycles. Indoles have been found to exhibit a broad spectrum of biological activities ranging from tranquillizers1 to their utility as anti-HIV agents2. Indoles have applications not only in pharmaceutical industry but these find uses as dyes3, chelating ligands and precursors which majorly contribute as metal complex catalysts for organic synthesis and metal complex drugs for stable and sustained drug release in biological system4. The presented work reflects our studies towards the synthesis of a variety of indole heterocycles.

Potential of Agricultural Wastes for the Production of Alginic Acid by Solid State Fermentation

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Alginic acid, an industrially important biopolymer is commercially extracted from farmed brown seaweeds. Owing to variation in composition of alginate isolated from different species, there is rising interest in bacterial alginate. Pakistan meets the industrial demand of alginate by importing it from developed countries. The present study was designed to assess the potential of different agro-industrial wastes like wheat bran, rice polishing, corn cob, corn stover and rice husk for alginate production by Azotobacter vinelandii through solid state fermentation. Optimization of basal media composition and various physical parameters was also done. Maximum yield of alginate (76 mg/ g) was achieved by fermentation of wheat bran at substrate water ratio of 10:36 after 72 hours of incubation time with 2mL volume of inoculum at pH 7.0 and 300C. Addition of different optimum levels of ionic salts i.e. 0.05% CaCl2 and 0.025% MgSO4. 7H2O raised the yield whereas KH2PO4 and NaCl reduced the yield of alginate. Among different nitrogen sources tested, corn steep liquor (0.25%) showed significantly higher yield of alginate (88 mg/g). Alginate produced was found to be 98% pure by HPLC method. The results indicated that alginate can be efficiently produced through solid state fermentation by utilizing cheap agricultural wastes as the substrate.

Analytical Characterization of Stones in Ornamental Architectural Elements of the Ancient Historic Buildings

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The diagnostic studies of heritage materials through the applied chemistry for the materialâ€™s identification and the better understanding of the degradation phenomenon in the last decade provided the major solutions to the several challenges faced by the conservation and restoration treatments all over the world. In Pakistan, the heritage is rapidly deteriorating due to the incomplete information and lack of understanding of the historic materials behavior over the years that left the significant gaps and is the root cause of the present scenario in conservation works. Mughal monumental and ornamental architecture, conservation and restoration requires the complete diagnosis of the original materials for the selection of the correct materials and innovative methodology to fill these gaps. This paper is focused on the analytical characterization of stones mainly used in the ornamental architectural elements of Mughal architecture in Lahore. The collected samples were initially studied with optical microscopy and X-ray powder diffraction which was further supplemented by scanning electron microscopy-energy dispersive spectroscopy. The chemical compositions were further elaborated with X-ray fluorescence and inductively coupled plasma atomic emission spectroscopy to measure the major elemental content in addition to trace elemental analysis. The obtained results paved the path for the selection of the materials, restoration methodology and highlighted the degradation processes for future conservation treatments.

Discrimination of Mungbean Cultivars Based on Minor Saccharides Composition By HPLC Coupled with Multivariate Statistical Analysis

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It is a strong desire of the end user to know about the food under their consumprtion. Food profiling using advanced analytical techniques combined with multivariate statistical analysis has recently been very useful in order to understand various food characteristics. The present study reports the potential use of HPLC coupled with principle component analysis (PCA) and partial least squares discriminant analysis (PLSDA), for differentiation of approved mungbean variety from the promising lines based on minor saccharides profiles. A total of 48 mungbean samples from one approved variety and seven promising lines were analyzed for minor saccharides using HPLC and multivariate statistical analysis. PCA showed a clear separation among the samples. PLSDA was conducted to extract the variables that were responsible for the separation of mungbean approved variety from the lines. Maltoheptaose, maltohexaose, maltopentaose, maltotretraose, maltitol, maltose, mannitole, betaine varied significantly while stachyose, raffinose, sucrose, lectitol, dulcitol, xylitol, galactose showed non-significant differences. The study highlights metabolic variation among mungbean variety and lines for minor saccharides profiles and its usefulness for consumers to choose for their desired variety or line as well as for breeders to look into the genetic factors responsible for this variation.

Extraction, Encapsulation and Characterization of *Tribulus Terrestris* Extract and Its Biological Applications

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Tribulus terrestris (family Zygophyllaceae), commonly known as puncture vine, has been used for a long time in the Asia for treatment of various kinds of diseases. The objective of the present study was to investigate the anticancer activity of Tribulus terrestris extracts. In this investigation moderate extraction approach was developed and leave and seeds extracts were encapsulated to protect and intact the efficacy of medicinal extract for better and viable applications. Tribulus terrestris extract was prepared using microwave assisted extraction method. Crude extract and encapsulated extracts were analyzed by GC-MS and HPLC for compositional attributes. Biological potential as anti-oxidant, anti-microbial and anti-cancer potential of Tribulus terrestris extracts were also be evaluated and compared using crude extract as well as encapsulated extract. Encapsulated Tribulus terrestris extract showed better biological application as anti-cancer, anti-oxidant and anti-microbial activities.

Lignocellulose Biomass: A Renewable and Sustainable Source for Generating Hydrochars and Activated Carbons for the Removal of Emerging Contaminants: Review of Recent Progress

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Emerging contaminants (EC & amprsquo's) are pollutants of growing concern. They are mainly organic compounds such as: pesticides, pharmaceuticals and personal care products, hormones, plasticizers, food additives, wood preservatives, laundry detergents, surfactants, disinfectants, flame retardants, and other organic compounds that were found recently in natural wastewater stream generated by human and industrial activities. The majority of ECs do not have standard regulations and could lead to lethal effects on human and aquatic life even at small concentrations. The conventional primary and secondary water treatment plants do not remove or degrade these toxic pollutants efficiently and hence need cost effective tertiary treatment method. Adsorption is one of the highly acclaimed techniques that has benefits such as ease of operation, good efficiency and economically more feasible. Among the adsorbents used for the removal of these unregulated compounds, lignocellulose based hydrochars and activated carbon from them have outperformed the existing commercially expensive materials. Hydrothermal method of preparing hydrochars is not only a cheap method but also environmentally friendly technique that reduces the emission of greenhouse gases and yield heavy metal free scaffold to prepare activated carbon in substantial yield. Thus, we have highlighted recent advances in different lignocellulose based hydrochars achieved through hydrothermal method followed by chemical activation for the removal of ECs. Their gaps associated with them have been highlighted and future recommendations are also proposed in this presentation to in order to widen the scope of these materials in green chemistry.

Synthesis and Optimisation of Tetrahydropyrimidines and 2-Hydroxypyrimidines as Novel Anti-Cancer Agents

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Pyrimidine nucleus has gained much attention of medicinal chemists due to its wide spread applications as antimicrobial, anticancer, antiviral, antibacterial and antioxidant agents. To explore pharmaceutical importance of tetrahydropyrimidines and 2-hydoxypyrimidine derivatives, a library of compounds (1-50) have been synthesized. Tetrahydropyrimidnes (1-25) have been synthesized by fusing urea, alkyl acetoacetate and a verity of substituted aldehydes in the presence of catalyst in solvent free condition at 80-90Â°C. 2-Hydroxypyrimidines (26-50) have been synthesized by oxidation of tetrahydropyrimidines (1-25) using, ceric ammonium nitrate (CAN). Synthesized compounds have also been investigated for their potential to act as anti-cancer agent and encouraging results have been discovered which will be discussed in presentation in detail.

Theoretical Study May Help us to Resolve the Mystery of Kinases Selectivity

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Kinome constitutes a substantial fraction of the human genome, with more than 518 unique genes. Among these kinases, the intracellular serine/threonine kinases provide essential nodes in the signalling pathway defining the intracellular communication. The functional relationship of these kinases in the regulation of growth and proliferation, intracellular signalling cascades, and cellular metabolism highlight the pleiotropic role of these proteins in different diseases. One of the eight hallmarks of cancer, sustained proliferation, is driven by the members of the kinase family including Aurora Kinases (AKB), and Casein Kinases (CK2). These kinases are involved not only in tumorigenesis, but their overexpression is also associated with poor prognosis. Herein, we report our efforts to understand the mechanism of inhibition of selected classes of AKB and CK2 inhibitors. In this connection, extensive Molecular Dynamics simulations studies was utilized to guide the synthesis of novel compounds with better understanding. Further, in the case of AKB, we have also carried out an extensive virtual screening campaign to evaluate the efficiency of available chemical space as AKB inhibitors. Furthermore, the â€˜Water Swapâ€™ and MMGB-SA calculations allowed us to access the binding energies of the ligand in a real-time dynamic system.

Probing Deep Eutectic Solvents in Organic Synthesis

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Deep eutectic solvents (DES) carries unique place in organic synthesis. A range of synthetic organic reactions have been catalysed in DES to develop eco-friendly chemistry by avoiding traditions volatile solvents. Moreover, thermal stability, non-volatility, recyclability and other many features of DES make them useful to do eco-friendly reactions. Typically, a deep eutectic solvent is the mixture of quaternary ammonium salt and hydrogen bond donor species such as urea, diethyl glycol, thiourea, ethanol etc. With such unique properties, we have also explores new DES melts to carry out different organic reactions include, Fisher indole synthesis, 1H-tetrazole, acridine formation via multicomponent reaction, pyrazole-5-carbonitriles, etc. The reactions have been optimized by using morpholine, piperidine and 1,4-diazabicyclo octane (DABCO) quaternary ammonium salts termed as ionic liquids with range of hydrogen bond donors. Moreover, the computational studies of new piperidinium and morpholinium based DES mixtures have also been carried to study the interaction between quaternary ammonium ionic salts/liquids and hydrogen bond donor species. The DES melts proved to be effective substitute of traditional volatile solvents to perform various types of organic reactions. Further studies are going on in our lab in the pursuance our interest in this field.

Role of Nano-Se Particles Supplemented Sunflower Meal Based Diet on Growth Performance, Nutrient Digestibility and Hematology of Cirrhinus Mrigala Fingerlings

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The research was conducted to estimate the effects of Se nanoparticles on growth performance, nutrient digestibility and hematology of C. mrigala fingerlings fed nano-Se particles supplemented sunflower meal based diets. The experiment was consisted on seven test diets on the basis of supplementation of nano Se graded levels (0, 0.5, 1, 1.5, 2, 2.5 and 3 mg/kg). Chromic oxide was added as an inert marker. Fingerlings were fed at the rate of 5% of their live wet weight. Maximum improvement in weight gain % (189) and the best FCR (1.58) was observed at test diet with 1 mg/kg supplementation of Se nanoparticles. Similarly maximum nutrient absorption (CP 72%, EE 73% and GE 67%) and hematological indices (RBCs 2.84 106 mm-3, WBCs 7.79 103 mm-3, PLT 66, Hb 8.5 g/100ml, PCV 25% and MCV 190fl) were also noted at 1 mg/kg supplementation of nano Se. It was concluded from the results of current study that supplementation of Se NPs (1 mg/kg) in sunflower meal based diet improves the growth performance, nutrient digestibility and hematology of C. mrigala fingerlings. Key words: Nano-Se particles, growth performance, nutrient digestibility, hematology and C. mrigala

Formulation, Quality Control, Biodistribution and Preliminary Clinical Application of 99mtc-5-Flurouracil Freeze Dried Kit

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5-flourouracil (5-FU) is commonly used as a chemotherapeutic agent against number of tumors and considered first line drug for the treatment of colorectal carcinoma; the worldâ€™s fourth highest common cancer. In this study the freeze dried cold kit of 99mTc-5-FU was formulated showing long enough shelf life stability for cancer diagnosis. Quality control analysis of labeling 5-FU with technetium-99m (99mTc) showed Ëœ98Â±0.02% radiolabeling efficiency. Biodistribution in rat model showed radiopharmaceutical is non-toxic and is freely excreted from kidney. Normal volunteerâ€™s scintigraphic study showed that 99mTc-5-FU is freely filtered from kidneys and showed no evidence of significant tracer uptake in any tissue of the body. No symptoms of side reaction or cytotoxicity were observed after several days of 99mTc-5-FU administration. Single photon emission computed tomography (SPECT) scintigraphic study of patients with biopsy proven colorectal carcinoma showed promising uptake of tracer agent in tumor cells and significant target to non-target ratio. The results indicates that 99mTc-5-FU freeze dried cold kit could be investigated as a potential SPECT imaging agent in colorectal carcinoma diagnosis and for other kinds of tumors in which 5-FU is advised as a chemotherapeutic agent.

Structural and Dielectric Properties of Aluminum Doped Cu-Ni Spinel Ferrites

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Sol-gel synthesizing procedure is employed to synthesize a novel variety Aluminum doped Copper-Nickel based spinel nano-ferrites having a representative formula of Cu0.7Ni0.3Fe2-xAlxO4 where (x = 0.0, 0.1, 0.2 and 0.3, 0.4). The structural analysis and required phase of these materials were performed by X-rays diffractometer (XRD) and Fourier Transform Infra-Red Spectroscopy (FTIR). The dielectric studies are also performed for the investigation of dielectric properties of these copper-nickel nanoferrites. The cubic spinel structure having a single phase fabrication is investigated by X- ray diffraction analysis (XRD) which resulted that the crystallinity of these materials fluctuate between the 30.04 nm to 28.38 nm and also confirmed when we increase the aluminum ion (Al+3) concentration the change must occur in lattice parameters (8.614 â€“8.604 Ã…). Fourier Transform Infra-Red Spectroscopy (FTIR) confirmed the representative peaks of metalâ€“oxygen oscillation in tetrahedral (460 â€“ 500 cm-1) and octahedral (380 â€“ 440 cm-1) sites respectively. A scientific work is performed on the dielectric analysis like dielectric constant, dielectric loss, tangent loss and quality factor and resulted that these properties depends on chemical composition and applied frequency from one MHz to three GHz at room temperature. The results of analysis and measurements also clarified that these are strong and promising candidates in high frequency purposes, high energy density super capacitor, high power microwaves absorbing, modern electronics, transformer core and memory storage devices

Study of Photocatalytic Performance and Antimicrobial Activity of Fe@ZnO/g-C3N4 Nanocomposites

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Discharge of industrial wastes and domestic effluents into the aquatic systems origins severe water pollution and this is one of the major environmental subjects craving immediate attention. Toxicity and colour of the organic pollutants are the crucial factors of the polluted water. Photocatalysis is one of the simplistic, green and environmental friendly technologies employed to degrade organic pollutants. ZnO is one of the acknowledged semiconductor photocatalysts because of its exceptional advantages, such as its low price, high photocatalytic activity, and nontoxicity. However, it has some serious drawbacks such as low charge separation efficiency, liability to photocorrosion, and poor visible light absorbance limited its widely commercial applications. The present work reports on the synthesis of a unique ternary nanocomposite of Fe@ZnO/g-C3N4 and its application as a photocatalyst for the degradation of methylene blue dye. The composite was synthesized by simple chemical co-precipitation method. The photocatalytic and antimicrobial activities of ZnO were tuned by Fe doping and composite formation with g-C3N4. Photocatalytic activity of the synthesized nanocomposites was checked against Methylene blue dye which was used as model dye. The synthesized nanocomposites showed enhanced photocatlytic activity as compared to undoped ZnO, Fe@ZnO, g-C3N4and g-C3N4 /ZnO. The antimicrobial activity of samples was checked against Gram positive and Gram negative bacteria. The antimicrobial ability of the nanocomposite was better than undoped ZnO, Fe@ZnO, g-C3N4and g-C3N4 /ZnO.

Synthesis and Characterization of Hydrogel Embedded with Cobalt Nanoparticles For Water Decontamination

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This work deals with the synthesis of poly (N-isopropylacrylammide-co-2-Acrylamido-2-methylpropane sulfonic acid) hydrogel, fabrication of cobalt nanoparticles in the prepared hydrogel and evaluation of catalytic potential of the as-prepared hydrogel-cobalt nanocomposite. The hydrogel was prepared by free radical polymerization and cobalt nanoparticles were prepared by in situ reduction of Co (II) ions inside the hydrogel network. The formation of hydrogel and presence of both the monomers in the obtained hydrogel was indicated by FTIR spectroscopic results. The prepared hydrogel was able absorb water as much as 63 times of its weight in dried water. The water absorption was found to follow the non-Fickian mechanism. The presence of cobalt in the hydrogel-cobalt nanocomposite was identified by ICP-OES analysis. The morphology of hydrogel and its composite with cobalt nanoparticles was studied by SEM. The shape and size of the cobalt nanoparticles fabricated in the hydrogel was assessed by TEM and it was found that the nanoparticles were almost spherical in shape and most them were having diameters around 25 nm. The thermal behaviour was studied via TGA and DSC which showed that both the hydrogel and its composite was thermally stable below 260 Â°C. The catalytic potential of the as-prepared hydrogel-cobalt nanocomposite was assessed in the reduction of 4-nitrophenol to 4-aminophenol. The effects of amount of catalyst, temperature and recycling on the rate of this catalytic reaction were studied. The maximum rate constant was found to be 4.67 min-1. The catalyst was also recycled and reused for five consecutive cycles

Targetted Functional Foods and Nutraceuticals to Cope with Malnutrition in Pakistan

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Functional Foods and Nutraceuticals have become an essential part of diet to cope with the increasing malnutrition problem. In Pakistan, there is a threatening increase in the malnutrition which can only be overcome by supplementing the food with the required macro- and micro-nutrients. New functional foods with hedonic demands as per regional requirements are being formulated and designed. Prepared functional foods and nutraceuticals are tested for the sensory evaluation, physico-chemical properties, antimicrobial analysis and stability parameters. These functional foods are with a targeted approach and will be a revolutionary benchmark in the Food Industry of Pakistan.

Nanocomposites

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In view of low cost material with fascinating applications, ZnO is being targeted in present work. The research regarding the use of ZnO in pure state discloses some limitations which vary in context to targeted applications. The limitations in use of ZnO as photocatalyst and as antimicrobial agent are also reported in literature. Various attempts are employed to remove these shortcomings but are not so successful till now. We are also going to address the factors which hindering the use of ZnO as photocatalyst and antimicrobial agent in pure state. We have addressed limitations by turning ZnO into a unique composite through transition of metal doping and unification with nonmetallic natured GCN. This composite is synthesized by using chemical route. The photocatalytic activity is studied against Methylene blue degradation which is well known textile dye. The antibacterial study is carried against Gram negative and Gram positive bacteria. The composite shows excellent bactericidal and photocatalytic activity as compared with ZnO/Cd doped ZnO and ZnO/GCN composites.

A Key Way of Solving the Severe Plastic Waste Problem: Pyrolysis and Kinetics

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Polymers wastes are major fraction of overall municipal solid waste, normally more than 11.8 %, whereas very small amount of polymer waste has been recycled i.e., 5.7 %. With small landfills existed for dumping of polymer waste each year, evolving suitable recycling techniques for polymeric waste is becoming progressively significant. The present study consists of two major parts, i. Pyrolysis, ii. Kinetics. In pyrolysis, decomposition of waste polymers was carried out in the presence and absence of catalyst in special furnace under inert condition. The pyrolysis products (liquid, gas and char) were collected in separate fraction and analyzed by various techniques i.e., GC/MS, FTIR etc. Main components in the liquid fraction were observed to be: 1,2-dimethyl benzene, ethyl benzene, diphenyl methane, 1,1- diphenyl ethylene and 1,2-diphenyl ethane. The oil properties determined by various techniques and then compared with the standard values. Whereas, the kinetic study is concerned, the waste polymers were analyzed by thermogravimetry at different heating rates under inert condition. The thermogravimetric data obtained was interpreted by using various kinetic models. All the kinetic parameters were calculated, and the most suitable model was investigated, which play key a role in industrial and engineering processes.

Durable Functional Textiles Using Nanomaterials

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Textile provides the most suitable surface for modification that could be achieved by application of various techniques. Along with conventional methods, nanotechnology offers the most prevailing and exciting opportunity for textiles to be multi-functional. Surface modification of textiles by metal oxide nanoparticles have opened new horizons for textile researchers due to the extravagant properties arising from their nanoscale dimensions. Though, the properties of nanoparticles change drastically due to their high surface area and high surface energy, but, their adhesion with textile substrate is still an issue. To overcome this problem researchers have been trying different techniques so that their durability could be enhanced. The functionalization of nanoparticles is one of the most recent techniques that have been tried in which chemical groups are grafted at the surface of nanoparticles. These chemical reactive groups such as cationic silanes could react with hydroxyl groups (-OH) at the surface of nanoparticles by chemical bonding. The functionalized nanoparticles could held with textile substrate by strong electrostatic force of attraction between positively charged nanoparticles and negatively charged cellulose providing the greater durability. Such modified textiles then provide functionality like antibacterial, superhydrophobicity, dye degradation, and ultraviolet protection upto the li

Removal of Anionic Dye from Water Using Novel Plant Based Silver Nano-Composites

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Water contamination is a topic of concern for addressing various environmental and health problems. Plant based silver nanocomposites were prepared and found very effective in water treatment against anionic dye. Further these composites showed very good antimicrobial potential against E.coli and salmonella sp. Batch mode removal of anionic dye (Alizarin Red S) from water was studied using Terminalia arjuna nuts. Various parameters like pH, adsorbent dose, temperature, time were optimized to further conduct the isothermal, kinetics and thermodynamic studies. Isothermal studies revealed that qmax value was (52.95 mg/g) following pseudo second order kinetics model. The process of anionic dye removal is spontaneous and exothermic in nature.

Synthesis, Biological Screening and Molecular Docking Studies of Multifaceted Sulfonamides Bearing 1,4-Benzodioxane-6-Amine Scaffold

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Sulfonamide has shown large number of pharmacological properties against different phenotypes of various disease models. The sulfamoyl and alkyl/aryl functionalities have been successfully introduced through a series of different methods in this present study. The parent compound N-(2,3-dihydrobenzo[1,4]dioxin-6-yl)propanesulfonamide was synthesized by the condensation reaction of 1,4-benzodioxane-6-amine with propyl sulfonyl chloride. IR, 1H-NMR and mass spectrometry techniques were used to confirm the structure of all the synthesized compounds. Then screening against various enzymes i.e. acetylcholinesterase, butyrylcholinesterase, lipoxygenase and a-glucosidase enzymes and bacterial strains were done. The synthesized compounds were found to be good inhibitors of lipoxygenase; whereas arylated compounds were found to be good antibacterial candidates. The interaction between inhibitors and target enzymes (cholinestrases and lipoxygenase) was computationally observed which correlated with the experimental results. The anti-inflammatory and antinociceptive activities of new compounds were evaluated with indomethacin and diclofenac sodium in experimental animal models respectively. COX-2 enzyme inhibition was evaluated with synthesized compounds through in vitro cyclooxygenase assays. Inhibition assays result revealed that compound 5d was the most potent compound.

Probing the Catalytic Activity of Pd Nano crystals Supported on Mica

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Catalyst mica supported Pd nanocubes were synthesized by depositing Pd nanoparticles on the surface of mica and used for catalyzing Heck reaction. Initially, the activity of Pd nano-cubes supported on mica was explored through probe reaction (oxidation reaction of benzyl alcohol). Probe reaction shows that Pdcubes /mica was an active catalyst for oxidation reaction. The prepared catalyst was characterized by sophisticated analytical techniques including Scanning electron microscope (SEM), Transmission electron microscope (TEM), X-ray diffraction (XRD) and Fourierr-Transform infrared spectroscopy (FTIR). The uniform distribution of nanocrystals on surface of mica was further confirmed with SEM and TEM images. The average size of the nanoparticles was 7-9 nm. The activity of the catalyst is checked in catalyzing Heck reaction of ethyl benzimidazole acetate and bromobenzene and the product phenyl benzimidazole acetate were obtained (90.3% yield). It was confirmed that Pd nanocrystals supported on mica exhibited very high catalytic efficiency towards Heck reaction.

Synthesis and Anticancer Evaluation of Oxadiazoles Based Acefylline Analogs

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Theophylline-7-acetic acid (acefylline) and its derivatives are pharmacologically active compounds and are generally recognized as bronchodilators for the treatment of respiratory diseases like acute asthma for over 70 years. To highlight their importance, synthesis of 2-((5-((1,3-dimethyl-2,6-dioxo-2,3-dihydro-1H-purin-7(6H)-yl)methyl)-1,3,4-oxadiazol-2-yl)thio)-N-arylacetamides is reported here. All the synthesized derivatives were structurally verified by FT-IR, 1H NMR, 13C NMR and were evaluated for their anti-cancer (using MTT assay) potential. N-(4-Chlorophenyl)-2-(5-((1,3-dimethyl-2,6-dioxo-2,3-dihydro-1H-purin-7(6H)-l)methyl)-1,3,4-oxadiazol-2-ylthio)acetamide was found to be most active having cell viability 53.58 Â± 1.28 using 100 Âµg/mL concentration of compound which was then in-silico modelled to describe the possible mechanistic insights for its anti-proliferative activity.

Synthesis and Anticancer Potential of Novel Ciprofloxacin Derivatives

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Ciprofloxacin, an antibiotic has been shown to have anti-proliferative and apoptotic activities in several cancer cell lines. Moreover, several reports have highlighted the interest of increasing the lipophilicity to improve the antitumor activity. These studies have led us to synthesize novel structural hybrids of ciprofloxacin linked with a variety of anilides. Antitumor activity of these derivatives were assessed against liver cell line (Huh-7) using MTT assay. Among the synthesized derivatives, methyl 1-cyclopropyl-6-fluoro-4-oxo-7-(4-(2-oxo-2-(phenylamino)ethyl)piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylate inhibited the growth of tumor cells by displaying 68.36% cell viability at 100 Âµg/mL concentration which was then in-silico modelled to delineate the potential mechanistic insights for its anti-proliferative activity. The PASS prediction indicated the topoisomerase II (TopII) as potential anticancer target of the compound. The induced fit docking revealed that this compound inhibits the TopII with superior binding affinity and forms stronger contacts with active siteâ€™s key residues responsible for DNA-TopII intercalation and catalytic inhibition consistent with its cytotoxic potential. Therefore, the representative compound can be considered as a potential lead for further optimization in the development of ciprofloxacin-derived anticancer drugs.

Synthesis Spectroscopic Characterization Biological Studies and Hypoglycemic Effect of New Organotin (IV) Complexes

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N-Phthalimido ÃŸ-amino acid derivatives and new series of di- and triorganotin(IV) complexes (1-12) have been designed and synthesized. All compounds are characterized by elemental analysis and bonding of these complexes was discussed in terms of their Infrared, Nuclear Magnetic Resonance (1H, 13C, 119SnNMR) and Mass spectroscopic studies. N-protection of ÃŸ-amino acids was verified by FTIR and the deprotonation of ligands was confirmed by the disappearance of ?(OH) at 3300-2600 cm-1.The results suggest that derivatives of ÃŸ-amino acids coordinate with tin(IV) compounds in various patterns. The triorganotin(IV) complexes verified monodentate coordination with tetrahedral geometry in solid form and bidentate co-ordination with trigonal bipyramidal geometry in solution form while diorganotin(IV) complexes exhibit bidentate co-ordination with trans-octahedral geometry as monomers and a unique view as dimers. All the compounds were tested in vitro for their antibacterial activity against two Gram-positive bacteria namely Staphylococcus aureus, Bacillus subtilis and two Gram-negative bacteria namely, Escherichia coli and Pseudomonas aeruginosa and in vitro antioxidant activities. The complexes are proved to be more reactive with respect to their corresponding ligands while the triorganotin(IV) complexes exhibited good activity as compared to diorganotin(IV) complexes. The compounds are also tested in vivo for their antidiabetic activities on five groups of Alloxan induced diabetic rabbits and were proved to be good hypoglycemic agents.

Influence of Corn Starch on Thermo-Mechanical Behaviour of Poly Vinyl Chloride Bioplastics

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The diverse and ubiquitous consumption of polymers, urge the necessity to make these materials easily available. However, the excessively used petrochemical based polymers such as; poly vinyl chloride (PVC) are non-biodegradable which is a motivation to modify it with ’green’ alternatives. In the present study, poly vinyl chloride (PVC, Mw= 48000 g-mol-1) has been incorporated with corn starch (CS) to synthesize a series of twenty five samples of bioplastics in addition to blank polymer samples. The films of five various thicknss (0.1mm, 0.2 mm, 0.3mm, 0.5mm and 1.0 mm) have been synthesized using insitu polymerization. Each sample of pure PVC film and bioplastic have been induced with different concentration of CS in the range of 1 to 5 wt.%. The synthesized samples were subjected to the structural characterization by using FTIR. TGA has demonstrated the three step degradation with the improved stability of 250Â°C. The 3% concentration of CS has shown the optimum storage modulus (E') of 1660 MPa from DMA and Tan d as 0.50. The swelling test performed using water has shown an induction of hydrophilicity in PVC up to 4%. Corn starch induced bioplastics can be a potential ecofriendly alternative of conventional polymers.

Green Biomass-Based Antioxidant for Increasing the Oxidative Stability of Lubricating Oil

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Lubricating oil suffer oxidative degradation during its service life in the engine, antioxidants are added to increase its stability towards oxidative degradation. In the current study the oxidative stability of mineral base oil (MBO) in the presence of methanolic extracts of rice husk and pine saw dust wood as antioxidants has been studied. The oxidation of lube oil was performed according to modified IP method, at 100 and 200 oC, respectively. The oxidative degradation of the lube oil was monitored by Rancimate method and FTIR analysis. Results indicated that in the presence of rice husk extract (RHE) the oxidative stability index (OSI) time of the MBO was increased from 36 to 68 h at oxidation temperature of 100 oC whereas from 30 to 84 h at oxidation temperature of 200 oC. Similarly, using Peak Area Increase (PAI) and Peak Height (PH) methods [ASTM 7214-07], the high oxidation stability of MBO additized with RHE was also quantified from the peak area and peak heights of the carbonyl (C=O) or olefin (C=C) bands in the FTIR spectra.

Synthesis, Spectroscopic and Biological Studies of Imide and Amide Derivatives of Para-aminohippuric Acid with Cyclic and Noncyclic Anhydrides

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A new series of N-alkylated imides were synthesized by simple two step method and amide by single step method from different cyclic and noncyclic anhydrides. In the first step cyclic anhydrides react with Para-aminohippuric acid to give the corresponding acid alkyl amides while in the 2nd step imides synthesis was carried out by dehydration process. The noncyclic anhydrides give amide by a single step only with additional production of corresponding carboxylic acid. The structural elucidation is being confirmed by spectroscopic techniques such as FTIR, 1HNMR, 13CNMR and mass spectral data. The products were tested for their antibacterial and antifungal activities.

Comparative Study of Anticancer Effect of Potentized Homeopathic Drug, *Lycopodium Clavatum*

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The kinetics of the reduction of dicyanobis(phenanthroline)iron(III); [FeIII(phen)2(CN)2]+ by iodide ion was studied in different volume fractions of the aqueous-dioxane co-solvent mixture(s). The reaction was performed at 0.06 M ionic strength and 287 Â± 0.5 K under the pseudo-first order condition, which was maintained by fixing the concentration ratio of [FeIII(phen)2(CN)2]+ << I-. The data were collected through UV-Visible double-beam spectrophotometer by using UVProbe 2.42 software. The linear fits of integrated rate equation(s) helped to determine the order(s) of complex reaction and the rate constants. This complex mechanism whilst undergoing completion was noticed to passing two stages that involved reactants and intermediates. The first stage was noted to undergo zeroth-order kinetics with respect to [FeIII(phen)2(CN)2]+ and first order with respect to iodide ion. In the second stage, a fractional (0.5) order was observed with respect to [FeIII(phen)2(CN)2]+ and first order with respect to iodide ion. The reaction followed an overall first and fractional (1.5) order in the first and the second phase, respectively in each proportion of the co-solvent mixture. The effects of various factors that include ionic strength, protons, and dielectric constant were studied on the rate constant in each phase of the reaction and a rate law was proposed.

Hepta & penta coordinated potentially bioactive Organotin (IV) complexes; Synthesis, crystal structure, cyclic voltammetry & DNA binding studies

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Five novel organotin(IV) complexes with general formula R_2SnL, where R= Me (**1**), n-Bu (**2**), t-Bu (**3**), Ph (**4**), Oct (**5**) derivatives of N'-(3-ethoxy-2hydroxybenzylidene)-2-phenylacetohydrazide (H_2L), have been synthesized and characterized. Crystallographic data of **1**, **3** showed that these compounds are mononuclear in which Sn atom is in distorted trigonal bipyramidal geometry where complex **3** is homobimetallic with each Sn atom in pentagonal bipyramidal environment. The Cyclic voltammetric and UV-Vis spectroscopic data for DNA binding studies with SS-DNA of synthesized compounds suggested an intercalative mode of interaction. Viscosity measurement data also support the intercalative mode of interaction for the synthesized compounds with DNA. Binding constants for Organotin(IV) complexes are of order **3>4>1>2>5** at 310 K. Complex **3** shows strongest interaction with DNA. All compounds were active against different pathogenic bacteria however the dimethyl and dibutyltin(IV) complexes showed highest antibacterial activity against *Staphylococcus aureus* and *Bacillus subtillis*.

Synthesis of Cuprous Oxide and Cupric Oxide Nano Particles and Evaluation of Their Photo Catalytic Activity

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In this study, cuprous oxide and Cupric oxide nanoparticles were synthesized using CuCl2.2H2O as a precursor through chemical reduction method. The synthesized Cu2O and CuO nanoparticles were characterized by UV-Visible spectroscopy, FT-IR spectroscopy, X-ray diffraction (XRD) and Scanning electron microscopy (SEM). Further, these synthesized oxides of copper have been employed for photocatalytic degradation of Congo red using sunlight. The various factors that can influence the catalytic efficiency of the nanoparticles including catalyst concentration, time duration and pH of solution have also been investigated. Both of these synthesized oxides of copper proved worthy towards the said photocatalytic reaction. Cu2O nanoparticles showed maximum catalytic efficiency of 90% at a time of 3 hours exposure to sunlight while CuO nanoparticles showed a maximum catalytic efficiency of 54% at a time of 2 hours exposure towards degradation of Congo red.

Controlled Delivery of Drug from pH Sensitive Chitosan PEG Blend Using 1, 4 Diaminobutane as a Cross Linker

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The main deficiency in the conventional drug release system is their lack of site specificity and inability to release the drug in a controlled manner and not to maintain its concentration effectively. As a consequence of which only a diminutive amount of the administered drug is consumed by the body while the rest is excreted out and cause unavoidable side effects. The novel 1,4 diaminobutane crosslinked hydrogels based on eco-friendly biodegradable chitosan/PEG were prepared by blending to develop pH sensitive hydrogels and achieved its hydrophilicity and target specificity for controlled release of drug. The crosslinker amount was varied to analyze its effect on the hydrogel properties and was characterized using FTIR, SEM, TGA, swelling studies (water, buffer and ionic solution) and in-vitro release of Cefexime. The swelling behavior in water showed that compared to the controlled hydrogel, the crosslinked hydrogels revealed more swelling and an increase in swelling with further increase in the amount of crosslinker was observed. The hydrogels showed low swelling at basic and neutral pH while maximum swelling was observed at acidic media. The hydrogel showed antimicrobial activity antimicrobial activity The drug was released in controlled fashion for 120minutes. This pH response made these hydrogels an ideal candidate for injectable controlled release system.

Synthesis and Characterization of Benzothiazine Hybrid Molecules by Multicomponent Reactions

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Multicompenent reactions is an efficient tool for the synthesis of a wide range of heterocyclic moieties. During our research work, we used this tool for the synthesis of benzothiazine hybrids with pyran to get pyranobenzothiazine. These compounds were well characterized by spectroscopic techniques like NMR and XRD. In addition, we isolated the crystal of bis-adduct from this reaction which led us the synthesis of a new series of bis-adducts as well.The precursor, benzothiazine was prepared starting with methyl anthranilate, its mesylation and followed by N-benzylation. The cyclization to precursor benzothiazine was carried out in sodium hydride suspension in DMF. The compounds found their application as antidiabetic agents.

Removal of Hazardous Dye Methyl Violet and Malachite Green Using Metal Impregnated Photocatalyst under Visible Light through Sonophotocatalytic Degradation

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To increase the performance of ZnO from UV to visible light, ZnO nanoparticles were impregnated with copper (Cu) using wet impregnation method. The synthesized impregnated nanoparticles were characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM) and Energy dispersive X-ray analysis (EDX).The extent of sonophotocatalytic degradation was high as compared to photocatalytic and sonocatalytic. The effects of the copper impregnated ZnO (Cu-ZnO) catalyst on the degradation of two textile dyes were investigated using the parameters like pH, catalyst dose, amount of enhancer, radicle scavenger and initial dye concentration. The addition of enhancer (H2O2) improved the degradation efficiency from 35% to 95% at pH 10. At optimum conditions, maximum degradation of dyes were 100% in 20 min using sonophotacatalytic degradation as compared to photocatalytic degradation the degradation efficiency was 95-98% in 60 min. With the addition of carbonate, sulphate and chloride as radicle scavengers, the degradation efficiency decreased from 100% to 92%, 94% and 92% with 0.025 M concentration of each scavenger, respectively. The degradation efficiency decreased only 5% after repeated use of Cu-ZnO catalyst. Therefore, Cu-ZnO nanoparticles can be used as a promising sonophotocatalyst for degradation of textile dyes with excellent reusability potential.

Stereoselective Modification of Dydrogesterone by using Microbial Transformation in Green Friendly Environment

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Microbial transformation is one of the well-known methods to obtain biologically active compounds in which microorganisms act as chemical reagents. The vast amount of work in this area has been stimulated by the medicinal importance of steroids, and the desire to develop new drugs with new or improved pharmacological properties. Various kinds of steroid modifications, such as hydroxylation, epoxidation, dehydrogenation, oxidation, reduction, hydrolysis and acetylation are now routinely performed on industrial level using a wide variety of microorganisms. Many of these reactions can not be achieved by means of conventional chemical synthesis. Through microbial reactions, many novel intermediates for the synthesis of new steroid pharmaceuticals have become available. Dydrogesterone (1) is a synthetic hormone, similar to the naturally occurring sex hormone, progesterone. It is a familiar drug, used to treat premenstrual syndrome, infertility and endometriosis. Incubation of dydrogesterone (1) with Gibberella fujikuroi has afforded various metabolites using standard two-stage fermentation protocol with interesting biological activities. Structures of these metabolites were deduced through modern spectroscopic techniques.

Application of FT-IR Spectroscopy for Rapid Quality Control Oil and Fat Processing Industries

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Simple, cost-effective and environment friendly methods could be used for the quantification of different parameters using Fourier Transform Infrared (FT-IR) spectroscopy for rapid quality control analysis. The results of our study revealed that the FT-IR spectroscopy could be effectively used for rapid determination of moisture, free fatty acids (FFAs), iodine value (IV), peroxide value (PV), saponification values (SV) and fatty acid composition of oils and fats. The investigated samples covered a wide range including extracted oil, during processing at different stages, final products, by-products and modified products. In most of the cases there is need of any toxic solvent or chemical. Once the calibration is developed, results could be obtained within few minutes. Therefore, instead of using classical titration methods which are time consuming and need a lot of chemicals, FT-IR spectroscopy is better choice.

Anti-Corrosion Application of Polyaniline Based Polymer

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This study reports the synthesis of nanoparticle sized polyaniline by a low cost and solvent free method. The polyaniline was doped with hydrochloric acid (HCl) in different molar concentrations and was characterized by Ultraviolet-Visible (UV-Vis), Fourier-Transform Infrared (FTIR), Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA) and Scanning Electron Microscopy (SEM). The electrical conductivity of the polymer was measured. It was found that electrical conductivity of the platinized PANI was increased from 8 to 79 S/cm with 2 M doped PANI. The anticorrosion potential of the polymer has been exploited.

Pyrazolyl Triazoles as Potent and Selective Inhibitors of Tissue Non-Specific Alkaline Phosphatase: A Therapeutic Target against Vascular Calcification

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Cardiovascular diseases (CVDs) are a cause of deaths for 17.9 million people every year. Vascular calcification (VC) has long been a major area of interest in cardiovascular medicine. VC is a pathological phenomenon causing vascular stiffening and can lead to heart failure owing to up-regulation of Alkaline phosphatase particularly, tissue-nonspecific alkaline phosphatase (TNAP) in the vasculature. Therefore the selective inhibition of TNAP may serve as a useful therapeutic strategy againstVC. In this study, we have designed and explored a series of novel pyrazolyl triazoles as potent and selective inhibitors of TNAP. The structures of the newly synthesized triazolyl-pyrazoles were established by readily available spectroscopic methods (FTIR, 1H and 13CNMR) and mass spectrometry. The biological screening against h-TNAP, h-IAP, h-NPP1 and h-NPP3 showed that compound 10q emerged as a highly potent and selective inhibitor against h-TNAP with an IC50 value of 0.16 Â± 0.01 ÂµM with 127-fold increased inhibition as compared to levamisole. To identify the putative binding modes inside the active pocket molecular docking analysis of all the selective and potent inhibitors was performed. MD simulations were also conducted to substantiate the reliability of docked poses. The newly discovered inhibitors are believed to represent valuable lead structures against VC.

Bioactivity Guided Isolation of Active Compounds from *Cannabis Sativa* Essential Oil

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Cannabis sativa essential oil and fractions were evaluated for its antioxidant, fungicidal, bactericidal and cytotoxic properties. Maximum 0.035% extraction yield was obtained at 110Â°C.Caryophyllene, trans-a-bergamotene, humulene and cis-ÃŸ-farnesene in different percentages were the major components of more than 29constituents identified in each essential oil of C.sativa GCâ€“MS analysis. Fractionation was performed by using vacuum fractionation method. Total phenolic contents were found to be 13.42- 13.83 and 11.24-14.68mg GAE/ml, total flavonoid contents were 14.12-14.22 and 10.78-15.39 mgCE/ml for C.sativa essential oil and fractions respectively. Antioxidant activity was assessed by scavenging of DPPHâ€¢ which was 20.55-26.26% for E.oil and maximum 37.77% for F1 of 110Â°C E.oil. Maximum inhibition of linoleic acid peroxidation was showed by F4, 25.67% of 130Â°C extracted E.oil. Maximum antibacterial 19.33mm, 19.67mm, 19.82mm zone of inhibition and antifungal activity 20.15mm, 22.13mm, 22.26mm zone of inhibition was showed by F1, F5 and F4 of 110Â°C,120Â°C and 130Â°C extracted essential oil of C. sativa respectively. Maximum brine shrimp cytotoxicity 20ppm and 25ppm showed by F1 and essential oil collected at 110Â°C. IC50 data of antitumor potential showed the maximum activity 40.22Âµl/ml of fraction 4 of 130Â°C extracted essential oil increased with increasing concentration.

Microwave Assisted Sol-Gel Synthesis of Iron Oxide Thin Films and Role of Aluminum Doping

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Three important crystallographic phases of iron oxide include maghemite (a-Fe_2O_3), hematite (a-Fe_2O_3) and magnetite (Fe_3O_4). Among these iron oxide phases, maghemite and magnetite are of particular importance due to their magnetic moment. Electronic and magnetic properties of iron oxide thin films can enhanced/tuned using doping strategies. Aluminum doped iron oxide thin films were prepared using microwave assisted sol-gel route with fixed microwave power of 720W and dopant concentration of 0%, 2%, 4%, 6%, 8% and 10%. XRD results confirm presence of maghemite phase in undoped thin films of iron oxide. With increase of 0% to 4% in dopant concentration from maghemite state of iron oxide persists. However, intensity of peaks of diffraction decreases. Decrease in intensity of diffraction peak indicates that dopant atoms occupy the vacancies on the cationic sublattice. As dopant atoms occupy the space available on the cationic sublattice transition from maghemite to magnetite phase was observed at high dopant concentration of 6%. With further increment in carrier concentration to 8% diffraction peak intensity increases exhibiting strengthening and increased crystallinity of the films. Higher dopant concentration of 10% resulted decrease in crystallite of the films.

Bacterial Exopolysaccharides: Screening, Optimization for Economical Production and Characterization

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Bacterial exopolysaccharides (EPS) are exceptional polymers comprised of a variety of monosaccharides and other substituents, such as acyl-containing functional entities. The unique structural and multifunctional characteristics make EPS a complex group of polymers with high research and applied interests, however, costly production of EPS remains a challenge. In this context, herein, a cost-effective production with optimal EPS yield was achieved using mango seeds powder as a substrate with waste to value theme. Initially, three locally isolated bacterial strains, i.e., Macrococcus brunensis (M. brunensis), Staphylococcus aureus (S. aureus), and Streptococcus thermophilus (S. thermophilus) were screened, and EPS yield was optimized for different submerged fermentation periods, i.e., 48, 72, 96, 120 and 144 hours. The bacterial culture (M. brunensis) fermented for 120 h yielded highest EPS (14.56 g/L) with 97.8 % total carbohydrate contents. EPS yield was further optimized using response surface methodology (RSM) under central composite design (CCD). After RSM-assisted optimization, the highest EPS yield (30.93 g/L) was achieved with 85.94 % total carbohydrates and a complete absence of proteins. The optimally yielded fraction was subjected to high-performance liquid chromatography (HPLC) for compositional analysis, Fourier transform infrared spectroscopy (FTIR) for functional group analysis and scanning electron microscopy (SEM) for morphological analysis. HPLC profile revealed heterogenous carbohydrate composition with glucose, galactose, and fructose as predominating monomers. FTIR confirmed the presence of alcohol, carbonyl and amid functional groups and glycosidic linkages. SEM images revealed less porous flakes like topography. In conclusion, the economical EPS production, along with unique structural and multifunctional characteristics, can confer beneficial effects and may be useful for different industrial and biotechnological sectors.

A Voltammetric Method for the Determination of Nitrite by Using a Multiwalled Carbon Nanotube Paste Electrode Modified With Chitosan-Functionalized Silver Nanoparticles

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A cyclic voltammetric method is described for the determination of nitrite by using a multiwalled carbon nanotube paste electrode (MWCNT) that was modified with chitosan-functionalized silver nanoparticles (Chit-AgNPs). The AgNPs were prepared by one step procedure using chitosan as stabilizing agent. The resulting modified AgNPs were drop-coated onto the electrode. By combining the advantages of chitosan, AgNPs (in the form of Chit-AgNPs) and MWCNT, the assay exhibits a remarkable improvement in the cyclic voltammetric response towards the oxidation of nitrite at a typical peak potential of 0.811 V (vs. SCE) in buffer of pH 4.0. The accumulation of nitrite on the electrode also was achieved, and this further enhances the analytical sensitivity. Under optimized conditions, the oxidation peak current increases linearly in the 100 nM to 50 ÂµM nitrite concentration range, and the detection limit is 30 nM. The method showed high selectivity for nitrite even in the presence of other potentially interfering ions. A cyclic voltammetric method is described for the determination of nitrite by using a multiwalled carbon nanotube paste electrode (MWCNT) that was modified with chitosan-functionalized silver nanoparticles (Chit-AgNPs). The AgNPs were prepared by one step procedure using chitosan as stabilizing agent. The resulting modified AgNPs were drop-coated onto the electrode. By combining the advantages of chitosan, AgNPs (in the form of Chit-AgNPs) and MWCNT, the assay exhibits a remarkable improvement in the cyclic voltammetric response towards the oxidation of nitrite at a typical peak potential of 0.811 V (vs. SCE) in buffer of pH 4.0. The accumulation of nitrite on the electrode also was achieved, and this further enhances the analytical sensitivity. Under optimized conditions, the oxidation peak current increases linearly in the 100 nM to 50 ÂµM nitrite concentration range, and the detection limit is 30 nM. The method showed high selectivity for nitrite even in the presence of other potentially interfering ions.

The Study of Ionic Interactions of Monovalent Electrolytes in Aqueous Polyvinyl Alcohol and Polyacrylamide by Conductance Method

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The electrical conductance (?), molar conductance (?m), and limiting molar conductance (?mo) of NaCl and KCl in different compositions (0.1, 0.5, and 1.0 % w/v) of aqueous PVOH and PAAM were determined at temperatures from 298 to 318 K with a difference of 5 K. The concentration of NaCl and KCl was from 2.0 to 10.0 x 10-3 mol.dm-3. The electrical conductance of KCl was higher than NaCl. The electrical conductance increased with the concentration of NaCl and KCl while a reverse trend was observed for the molar conductance. The electrical conductance and molar conductance increased with the increase of temperature and concentration of polymer in the solvent. The change in conductive properties of NaCl and KCl in aqueous PVOH and PAAM was used to evaluate the fundamental changes inside the solution at the molecular level. The degree of dissociation and dissociation constant decreased with the increase of temperature due to the exothermic nature of the dissociation of NaCl and KCl. The ion-ion and ion-solvent interactions were evaluated by the Debye-Huckel relation. The ion-ion interaction (A) decreased while the ion-solvent interaction (B) increased with the increase of temperature. The thermodynamic parameters for the dissociation of NaCl and KCl were also determined to understand the energetics and spontaneity of the process. The results are explained in terms of electrostatic interactions, structural effects, and energetics of the processes involved.

Fluorescence Quenching of the Probes L-Tryptophan and Indole by Anions in Aqueous System

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Fluorescent probes (L-Tryptophan and indole) quenching by anions were explored in aqueous system. Fluorescence quenching of both the probes by SO_4^(2-) are shown in Figure 1 below. L-Tryptophan (B) Indole The anions used included NO_3^-, Cl-, SO_4^(2-). Indole quenching by all the studied anions were lower than quenching of L-Tryptophan by all the anions. Quenching data was successfully adjusted with Stern-Volmer equation. Fitting with the Stern-Volmer equation resulted in the Stern-Volmer constant. Higher Stern-Volmer constant was observed for NO_3^- while lower was found for SO_4^(2-). Stern-Volmer constant gives us the information regarding the sensitivity of the method. So the method was more sensitive for NO_3^- , then for Cl- and was found least sensitive for SO_4^(2-). LOD and LOQ in case of L-Tryptophan quenching by anions varied between 4.08×10-5 and 4.56×10-4 mol L-1, while in case of indole quenching varied between 3.87×10-5 and 6.59×10-4 mol L-1 respectively.The studied method shows good reproducibility for the determination of anions. The method could be very effective for the determination of anions.

Extraction of Bioactive Compounds from *Mentha Arvensis L* using Green Extraction Media

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In present study, deep eutectic solvent was synthesized by combining the choline chloride and glycerol and used for the extraction of bioactive contents from M. arvensis L. using maceration and ultrasound assisted extraction (UAE) techniques. The optimization of extraction parameters and their interactive influence was evaluated by response surface methodology (RSM). The highest extraction yield of total phenolic contents (TPC) 117 mg GAE/g, total flavonoids contents (TFC) 80 mg QE/g and 2, 2-diphenyl-1- picrylhydrazyl (DPPH) radical inhibition 94% was assessed with deep eutectic solvent through UAE. The antibacterial activity of extracts was evaluated against Staphylococcus aureus and Escherichia coli and antifungal assay was performed against Fusarium solani and Aspergillus niger by well diffusion method. The eutectic solvent showed significant antibacterial and antifungal activity against these strains with UAE using Rifampicin and Terbinafine standards respectively. Chrysin, p-coumaric acid, naringenin, scopoletin, phenylpyruvic acid, pinocembrin, hesperidin, carnosic acid and caffeic acid were main bioactive components of Mentha arvensis L. characterized by LC-ESI-MS.

MICE-PES: An Algorithm for Accurate Conformational Analysis and its Implementation to Natural Products

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Secondary metabolites play a key role in the chemical industry. Thus, careful determination of their structure is critical for their synthesis and investigation of pharmacological properties. A lot of these secondary metabolites are structurally flexible and can co-exist in many different conformations which makes it challenging to determine their relative configuration experimentally.

Computational chemistry has played a vital role in absolute structure determination of complex and conformationally flexible secondary metabolites by computing their theoretical NMR, ultraviolet, infra-red, and CD spectra, etc. based on a careful conformational analysis. Currently available conformational analysis tools utilize different molecular mechanics methods and generate a large number of possible conformers and are not general-purpose, thus compromising accuracy.

In this work, MICE-PES (Method for the Incremental Construction and Exploration of the Potential Energy Surface) is presented which is a software tool to perform a conformational analysis with the help of high level quantum chemical calculations by building the molecule incrementally from its smallest possible analogue whose conformational degrees of freedom are very well separated than the rest of the molecule. The validation of this method has been done by benchmarking it against 3-epixestoaminol whose absolute configuration is well known. MICE-PES, after its validation on 3-epixestoaminol, was used to assign the relative stereochemistry of a secondary metabolite (meroterphenol C) whose configuration was not determined with the experimental techniques.

Facile Synthesis of Novel Anti-inflammatory Oxazoles in DES

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Deep Eutectic Solvent has appealed considerable attention as new chemical strategy for organic synthesis [1,2]. Synthesis of novel heterocyclic compounds having versatile biological activities and medicinal applications is an ever-attracting area of research for synthetic chemists [3]. Two series of disubstituted oxazoles were prepared in high yield (70-80%) via DES facilitated reaction of N substituted Tetrahydrocarbazole and dinitrotetrahydrocarbazole with different ketones. DESs was proved as efficient, green and reusable solvent as well as catalyst for fabrication of oxazoles. Further all the innovative compounds were evaluated for their in vitro anti-inflammatory screening and compared to the standard drug. Structure elucidations of the accomplished compounds were achieved with FTIR, MS, and 1H NMR spectroscopic methods.

Role of polymorphic gene expression and Pharmacokinetics in response of direct acting antiviral drug therapy for HCV in Pakistan

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HCV is the major cause of death for decades in Pakistan and one-third populationsâ€™ lives with this disease. There are many antiviral drugs available in market for eradication of viral load from the patients but no validation system exists for these drugs here in Pakistan. Materials and methods: Total 100 HCV patients were selected for this study and there blood and urine samples were taken for pharmacokinetics of antivirals (sofosbuvir, simeprevir, daclatasvir and ribavirin). Genetic polymorphism near IL 28B and IL 10R gene was examined for each patient and its effect on treatment response was assessed. Results: Pharmacokinetics including AUC for sofosbuvir, GS 331007, simeprevir, daclatasvir and ribavirin were 1036Â±212, 16300Â±401, 23750Â±201, 10834Â±405 and 13100Â±103 respectively, average Cmax (ng/ml) were 746Â±261 1676Â±361, 2021Â±221, 640Â±102, 792Â±92 respectively, average Tmax(h) were 1.30Â±0.61, 3.30Â±0.91, 6.0Â±0.3, 2.3Â±0.4 and 1.8Â±0.2 respectively, Urinary excretion rate was 85.31% sofosbuvir, 0.90% simeprevir, 93.90% daclatasvir and 30.19% ribavirin. The presence of T allele near IL 28B gene and G allele near IL 10R gene indicates delayed response. Conclusion: Treatment success rate was based on polymorphic gene expression of the patients so response to antiviral treatment in patients with CHC, suggesting broader study in this regard.

Nanoformulation of *Allium Cepa* Crude Extract and Evaluation of its Bioactivities

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In this study nanosuspension technology was used to enhance the therapeutic potential of Allium cepa peels extract by improving its dissolution rate. Nanoprecipitation approach being simple and reproducible was used for the preparation of nanosuspension using sodium lauryl sulphate as a stabilizer. Particle size, polydispersity index and zeta potential of prepared nanosuspension was measured by using dynamic light scattering technique. DPPH assay was used for determining the antioxidant activity of crude extract and the prepared nanosuspension, whereas, disc diffusion method was used for determining the antimicrobial potential. The in vitro hemolytic and thrombolytic activities of prepared nanosuspension were determined to evaluate any toxic effect related to nanosuspension. The formulated nanosuspension of A. cepa showed means particle size of 275.5 nm with PDI value of 0.415 and zeta potential value of -48 mV respectively. Comparative evaluation of bioactivities of crude extract and nanosuspension illustrated superior antioxidant, antimicrobial, and thrombolytic potential of A. cepa nanosuspension. However, reverse trend was noted in hemolytic activity in which nanosuspension showed lower hemolytic activity toward human erythrocytes as compared to crude extract of A. cepa. Overall results showed that nanosuspension technology can prove to be a better approach to enhance the therapeutic potential of herbal extracts.

Metal Organic Framework Based Catalysts: Nano-Engineering Enhanced the Electrocatalytic Performance

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Metal organic frameworks have been recognized as emerging class of porous materials with high surface area. Easy tuning of MOFs makes them versatile for electrocatalytic applications. MOFs derived catalysts stand out as a renowned applicant for hydrogen/oxygen evolution reaction (HER/OER) and oxygen reduction reaction (ORR). In this study, we have rationally planned a series of MOFs based hierarchical nanostructures and tested for electrocatalytic performance of HER, OER, and ORR. The controlled pyrolysis of MOFs directly grown on layered double hydroxides (LDH) can produce different catalysts with hierarchical nanostructures such as metal nanoparticles on metal oxide sheets, carbon nanotututubes grown on metal oxides and carbon nanosheets on metal oxides. It is observed that carbon nanotubes vertically grown on metal oxide nanosheets have enhanced electrocatalytic performance due to its unique structure.

Green Synthesis of Highly Fe-doped ZnO Nanoparticles by Environmentally-Friendly Solution Plasma Process

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Diluted magnetic semiconductors (DMSs) have the advantage of exhibiting both ferromagnetic and semiconducting properties in a single material by substitution of transition-metal (TM)/rare-earth ions. Among DMSs, TM-doped ZnO is a promising candidate considering its chemical and thermal stability with a wide band gap. Among TMs, Fe ions are preferred because of their large effective magnetic moments. Herein, we report a one-step synthesis of highly Fe-doped ZnO nanoparticles (NPs) by a solution plasma process (SPP) using FeCl2 and FeCl3 as precursors without any addition of chemicals. Fe- doping levels in Zn1-xFexO NPs can be tuned by changing the Fe-precursor concentration and plasma discharging time. We achieved high doping content (x) of up to 0.46 within 30 min, which is difficult to achieve using traditional solution-based synthesis approaches. All Zn1-xFexO NPs exhibit ferromagnetic behavior but the magnitude is strongly dependent on Fe2+ to Fe3+ ionsâ€™ ratio (optimal ratio of Fe2+:Fe3+ was ~3:7), which can be explained by the dominance/competition between the ferromagnetic and antiferromagnetic exchange interactions. SPP has a great potential as an alternative strategy for the synthesis of highly Fe-doped ZnO NPs, which can be expanded to the synthesis of other doped metal-oxide nanostructures for a broad range of research applications.

Optimization and Validation of Reverse Phase- High Performance Liquid-Chromatographic Method for Determination of Thiacloprid in Fruits and Vegetables

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Thiacloprid (THI) insecticide belongs to family Neonicotinoids that are widely used against pestiferous substance to enhance crop yield and food production. Thiacloprid marketed under the trade name Calypso (Syngenta, Pakistan), recommended concentration of 0.5 mg/plant was sprayed on selected fruits (guava and citrus) and vegetables (cauliflower, tomato, and okra). Fruit and vegetable samples were harvested at different time intervals (0, 1, 7, 14, 21, 28 days) after foliar application. Samples were extracted using salting out Liquid Liquid extraction for recovery of THI. Meanwhile, Reverse-Phase High-Performance Liquid Chromatography (RP-HPLC) based method was also optimized and validated for the standard THI over concentration range 0-100 Âµg/mL. Recovery of standard THI was found within range of 78.33-92.00 % at an acceptable repeatability (RSDr) 1.81-4.30 % and reproducibility (RSDR) 1.08-4.74%. The limit of detection (LOD) and Limit of Quantification (LOQ) were found to be 0.03 and 0.05 Âµg/mL, respectively. The real time analysis investigated the presence of THI in selected fruits and vegetables exceeding maximum residual limits (MRL) established by Codex Alimentarius Commission during the first week of foliar spray. The present study provides an expedient, reliable, and sensitive method to analyze THI and its metabolites in fruits and vegetables.

Rational Synthesis of Beta Amino Acids and Their Metal Complexes: In Vitro Antiviral, Antibacterial and Antifungal Activity

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The microbes cause a variety of life threatening infections in humans and poultry. Since the chemotherapeutic agents available for these microbes like viruses, bacteria and fungi are either low in quality or limited in efficiency. Thus it is necessary for the development of new and more effective antimicrobial agents. Herein, a series of ÃŸ-amino acids like as 3-amino butanoic acid (A), 3-amino-3-(2-nitrophenyl) propanoic acid (C), 3-amino-3-(4-nitrophenyl) propanoic acid (E), 3-amino-3-2, 4, 6-tri chloro phenyl propanoic acid (F), 3-amino-3-(3-nitrophenyl) propanoic acid (G), 3-amino-3-(4-hydroxy phenyl) propanoic acid (H), 3-amino-3-(naphthalene-2-yl) propanoic acid (I), 3-amino-3-(phenyl) propanoic acid (J), 3-amino-3-(2-methoxy phenyl) propanoic acid (K) were synthesized by using different aldehydes and further used for the synthesis of metal complexes. The â€“OH and â€“NH groups give unique singlet peaks at 4.6 ppm, 2-4 ppm and 1-5 ppm in 1HNMR spectra as characteristics peaks of zwitter ion and resonating structure of carboxylic group in ÃŸ-amino acids respectively. The metal complexes of ÃŸ-amino acids were confirmed by FTIR data which showed increased C=O peaks value due to the participation of carboxylic group in complexation. In vitro investigations of compounds showed remarkable results against new castle disease virus (NDV), infectious bronchitis virus (IBV) and influenza (H9N9) viruses. The compounds exhibited maximum inhibition activity against investigated three strains (NDV, IBV and H9N9 viruses). All the compounds showed maximum inhibition activity against H9N9 except K7, which showed maximum activity against IBV only. In the field of poultry, this study would be considered as the revolutionary step against these viruses.

Performance of MOFs based Materials: Adsorptive Removal of Tetracycline, Ciprofloxacin, Nitroimidazole and Sulfachloropyradazine from Water

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The increasing concerns on toxicity of antibiotics in water require a prompt action to establish an efficient waste water treatment process for their removal. Herein, we have summarized recent research for the efficient removal of selective antibiotics (Tetracycline, Ciprofloxacin, Nitroimidazole and Sulfonamides) by using Metal-Organic Frameworks (MOFs) and their derived composite materials. Due to high surface area, open metal sites, void spaces, easy tuning of the shape, size and bridging ligands; MOFs are the respectable materials for adsorption of antibiotics. These MOFs adsorb antibiotics through hydrogen bonding, p-p interactions, covalent bond formation between MOF and antibiotics, electrostatic interaction and P-complexation. Furthermore, the factors such as contact time, pH, initial concentration of antibiotics, ionic strength and adsorbent dose are well-documented for adsorption of antibiotics by MOFs.

Zno Nanorods as an Efficient Adsorbent for Removing Cr (VI) From Aqueous Media

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ZnO nanorods were manufactured by using Zinc nitrate hexahydrate as a zinc precursor and Triton-x 100 as a capping agent via hydrothermal process. These nanorods provide work for as an adsorbent for removing Cr (VI) from water. Characterization of ZnO nanorods was done by UV-visible spectroscopy (UV), Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), and energy dispersive X-Ray spectroscopy (EDX). Adosrption mechanism was evaluated by various factors including kinetics, isotherms, and thermodynamics. Studies revealed highest absorption capacity of 250 mg/g for Cr (VI) at adsorbent dosage of 0.055 g/L and pH 2.0 under stirring for 30 min. Pseudo-second-order kinetic model and Langmuir isotherm explicated well adsorption pathway. While thermodynamics proposed adsorption was endothermic and spontaneous in nature. Taking into consideration, ZnO nanorods efficiently used for removing Cr (VI) from aqueous medium and also widen their role in removal of other heavy metal.

Synthesis, Spectroscopic Characterization of Biologically Active Azo-Compounds and their Metal Complexes

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The expansion of novel and extra operative antibiotic proxies are essential for human health. Here, we have produced a new series of azo-compounds including, (5,5-dimethyl-2-[(E)-phenyldiazenyl]cyclohexane-1,3-dione (DMPDCDO), 5,5-dimethyl2-[(E)-(2-methylphenyl) diazenyl]-5,5-dimethylcyclohexane-1,3-dione (DMMPDCDO), 5,5-dimethyl-2-[(E)-(4-ethylphenyl) diazenyl]cyclohexane- 1,3-dione (DMEPDCDO), and 5,5-dimetyl-2-[(E)-(4-methylphenyl) diazenyl]-5,5-dimethylcyclohexane-1,3-dione (DMPDACDO) were successfully synthesized via diazo-coupling of substituted amine's diazonium salts with dimedone at 0-5℃. Then azo compounds were further utilized for the synthesis of metals complexes with Zn 2+, Mn 2+, Ni 2+, Co 2+ etc. The purification of the synthesized ligands along with the metal complexes was known by TLC technique.Moreover, 1 HNMR, FTIR, and Mass spectrometric systems were successfully utilized to confirm the synthesis of ligands as well as metal complexes. The FTIR results distinctly confirmed synthesis by a characteristic (distinct) peak of (-N=N-) in 1500-1400 cm -1 range, while the C=O peak in 1740-1530 cm -1 range. The metal complex syntheses were confirmed by lowering the carbonyl functional group frequency owing to the metal carbonyl interaction. The 1 HNMR results confirmed synthesis by vanishing -NH group peak at chemical shift value in of 4.05-4.07 ppm range. The Mass spectrometric study confirmed the synthesis due the presence of clear molecular ion peaks, base peaks and the ion fragments pattern. Biological activities were also performed. Results have shown that synthesized compounds and their metal complexes are good to moderate antibacterial and antifungal agents against americane and fluconazole respectively.

Sonochemical Synthesized NiO Nanoparticles as Adsorbent for Lead sequestration

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NiO nanoparticles were fabricated through sonochemical itinerary in accompany of cetyl trimethylammonium bromide (CTAB) as surfactant and NiSO4.6H2O as precursor of Ni. UV-visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), and energy dispersive X-Ray analysis (EDX) were characterizing techniques. Adsorption parameters as amount of adsorbent, solution pH, time duration, and temperature were considered and preferred for isothermal modeling. Best fitted model was found to be Langmuir isotherm model depicting highest adsorption capability of 166 mg/g. Kinetics data pursued pseudo-second-order rate equation and thermodynamics suggested endothermic temperament of the procedure. In view of this, NiO nanoparticles can be taking up as adsorbent for heavy metals sequestration from aqueous media.

Kinetic Study of Enzyme Assisted Extraction of Essential Oil from Citrus Peel

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Energy-based extraction techniques (such as thermal, heating, microwave, and ultrasound assisted extraction) which not only associated with limited recovery rates but also causes detrimental effects on the quality of essential oil. In present study, an enzymatic maceration step was performed prior to hydro-distillation by Clevenger type apparatus. Orange peels were crushed manually, pretreated with ViscozymeÂ®L and hydro distilled using only distilled water. The essential oil obtained was analyzed for antioxidant activity using TEAC, LIPAC and RSC as the major biological tests applied. GC-MS characterization of the product confirmed the presence of D-limonene as one of the major compounds establishing the product as a valuable entity. Four parameters studied (Enz C, L/S ratio, incubation time and temperature) and optimization of the process carried out using Rotatable Central Composite Design .RCCD proved the reliability of the model giving an R2 value of 0.9893.The best conditions to carry out the process concluded were 5ml Enz C,1.8 L/S ratio ,incubation at 48? for 4.2 hours. Kinetic study established that all experimental treatments yield better results in lesser maximum recovery time than the control.

Structure-Based Design of Potential BRDT Inhibitors: Synthesis and Characterization of Indanone and Isoindolinone Analogues

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Epigenetics is the study of cellular and physiological trait variations that are not caused by changes in the DNA sequence. Histone modifications are important in regulating gene expression in eukaryotes. In histone modifications, acetylation is one of the best characterized and is generally associated with active genes. Bromodomains recognize the acetyl lysine residues. These are the readers of post-translational modifications which are strucÂ¬turally diverse proteins than contain one or more effector modules that recognize covalent modifications of proteins and DNA. Proteins that contain bromodomains are involved in the regulation of transcriptional programs and have a key role in the development of several aggressive types of cancer A library of 5-aminoindanone and 5-aminoisoindolinone analogues were designed to develop bromodomain (BRDT) Inhibitors. For that purpose computational docking studies were performed for designed compounds against the human BRDT (PDB: ID 4FLP). All the designed compounds stabilized the protein by making crucial hydrogen bonding interaction with Asn109 through carbonyl oxygen of indanone and isoindolinone. Synthesis of amides and sulfonamides of indanone and isoindolinone was achieved by reaction with various acid chlorides and benzene sulfonyl chlorides respectively. Synthesized analogues were screened for biochemical assay in dynamic scanning flourometry (DSF). It was found that most of the analogues were positive shifters i.e. stabilizing the protein. Binding affinities (Kd) of the analogues were determined by using protein observed fluorinated NMR (proF NMR) and inhibitory activities were found from Fluorescence polarization (FP) analysis in terms of Ki and IC50 values. All the synthesized compounds were characterized by available spectroscopic techniques like FTIR, 1H NMR, 13C NMR, Mass spectrometry.

Graphene Ferrites and its Applications

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Graphene oxide was synthesized by modified Hummerâ€™s method and by reducing the GO along with formation of magnetite in it, the rGO/ Fe3O4/Prussian blue nanocomposites were synthesized. Graphene oxide (GO) has been considered widely as a prominent precursor and a starting material for the synthesis of this processable material. The characterization was done to confirm the formation of nanocomposites. The results obtained from the characterization techniques mentioned above is also explained. FTIR results confirmed the formation of sample. The noise of different waves can be detected by this nanocomposite. Due to high electric conductivity and magnetic permeability, it is good for detection in the frequency range of 1-18GHz and for EMI shielding. Different concentrations of GO were used in different nanocomposites. Comparison was done to check the effect of concentration and changing in bands position. The detection of different noise wave can be detected by nano composites through their highly beneficial properties of electrical conductivity, magnetic permeability and permittivity. There are many composites which are highly responsive on E.M waves. Different types of composites have conductive and magnetic properties and have microstructure which can be prepared and characterized. Our material is best for the detection of 1-18 GHz frequency range and best for EMI shielding due to its electric and magnetic properties.

A Voltammetric Determination of Lead and Antimony for GSR (Gun Shot Residue) Application

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Lead and Antimony, two major constituents of GSR (gunshot residue) are studied for simultaneous determination at trace level. Anodic stripping cyclic voltammetry is employed for identification and quantification of these two metals in aqueous solution. Effect of different working parameters, such as nitrogen purging, stirring, deposition potential, deposition time, scan rate, supporting electrolyte, pH, and analyte concentration on their current response are studied.

Oxidative Deformation of Aniline, a Polymer Study

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Polymers are being part of many researches because of their vast range of structures and variety. They had been extensively used in many ways such as capacitors, gas sensors, electrodes, hardening and covering material. Polyaniline is among the many polymers that are being analyzed for conducting properties. This article refers to the synthesis of polyaniline as a conducting polymer. The easiest and time effective procedure of polyaniline has been proposed in this research. Polyaniline has been synthesized by redox process with APS (ammoium persulfate) at room temperature. The synthesized polyaniline has high environmental stability, high yield, and stability with multiple compounds. It can be shaped into different structures, can be used as a coating or covering agent. The synthesized polyaniline was characterized for conducting properties.

Preparation of Nanophotonic Structures and their Applications

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It has been a challenging issue to develop an efficient, scalable and viable method for the production of stable nanophotonic structures. In this paper, we have proposed magnetron sputtering technique based route to prepare blackbody character nanophotonic structures for stray light reduction, thermal regulation and solar energy applications. The suggested technique is free of any masking methodology, substrate independent (insulating, conducting, amorphous, crystalline, rigid or flexible) and can easily be up scaled, endorsing good adhesion and corrosion resistance. Refractory metals based nanophotonic structures afford unique features to deploy incident photons of light at subwavelength scale and withstand in adverse environments. Vertically aligned uniform nanostructures of TiAlN black absorbing coatings have successfully been grown on different kinds of substrates. An average wideband (with wavelengths from 200-2500 nm) absorption of 89 % was attained from single absorbing coating, and was improved to 95 % after depositing thin anti-reflection coatings. This absorption is higher than any refractory metals based absorbing coatings. Moreover, robust stability is an exceptional character of our wideband super absorbers. The proposed growth process would offer new platform to design, formulate and integrate nanophotonic structures.

Assessment of Antibacterial and Radical Scavenging Activities of phenolic compounds extracted from *Ziziphus Mauritiana (Lam)*

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This is the first time to study the antimicrobial and antioxidant activities of extracted free and bound phenolic compounds from areal parts of Ziziphus mauritiana plant. The antibacterial activities of phenolic compounds were evaluated against two bacteria, i.e. Escherichia coli and Staphylococcus aureus. Phenolic compounds were detected using RP-HPLC-DAD system. Seventeen phenolic compounds were identified including 10 phenolic acids; 7 flavonoids (3 known flavonoids as naringin, rutin and naringenin; 4 unknown were identified by comparison with those in the literature). The results from ultrasonic base hydrolysis revealed the p-coumaric, ferulic, 4-hydroxy-3,5-dimethoxybenzoic, 3,4-dihydroxy-cinnamic and sinapinic acids while sonication extraction method showed vanillate, sinapinic, 4-hydroxy-3,5-dimethoxybenzoic and chlorogenic acids as main constituents. Furthermore, radical scavenging activity was found greater in leaves and stem; while total flavonoids are higher in flowers and total tannins in leaves. Z. mauritiana stem, leaves and flowers extracts observed to be efficient against E. coli and S. aureus.

Fabrication of Efficient Calixarene Based Silver Nanoparticles as Bioactive Agent

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Due to increase in infectious diseases, researchers are trying to synthesize effective, less toxic and inexpensive antimicrobial agents. After development of Nanotechnology, silver nanoparticles have been proved as potential antimicrobial agents. Therefore, in present study, Calixâ€“AgNPs (4) were synthesized and characterized with UV-Visible spectroscopy, FT-IR, SEM and XRD. Synthesized Calix[4]aren derivative (3) and Calix-AgNPs (4) were explored for antimicrobial activity against two bacteria (G+ve S. areus, and Gâ€“ve E.coli) and fungi (R. stolonifer) using solution of silver nitrate salt as reference. For antimicrobial study five dilutions (10, 5, 2.5, 1.25 and 0.62 Âµg/mL) of each compound were prepared. Finally it was revealed that Calix-AgNPs are efficient antimicrobial agents as compared to Calix[4]aren derivative (3) and silver salt. All of five dilutions of Calix-AgNPs showed bioactivity, and MIC was observed at 0.62 Âµg/mL against selected microorganisms.

Synthesis of Particles Originating from Silica Monolith with Improved Chromatographic Performance in Liquid Chromatography

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Partially porous silica monolith materials have been synthesized using the modified sole gel procedure with sophisticated control in formulation, heating steps and overall protocol. The resultant silica monolith materials have pore size of about 350 Ã. ith particle size within the range of 1Âµm. The diversity in the shape made it easy to fabricate a delicate architecture during packing leading to monolith like morphology of the stationary phase. The Effect of pore size is of critical importance since large pore size silica monolith material result in increased mass transfer kinetics and hence high separation efficiency and improved chromatographic performance. Very high separation efficiency (N value~180,000 plates/m) was obtained out of the column of current study where the pore size was 350Ã… in comparison to the stationary phase comprising of 200 Ã… when evaluated in HPLC system using a mobile phase of 60/40 (v/v) % acetonitrile/water with a flow rate of 25 ÂµL/min. the column of current study was also capable of fast HPLC analysis.

The Prevalence of Respiratory Illnesses among the Workers of Crushing Industry in Pakistan: A Cross Sectional Study

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Respiratory illnesses are considered to be the main burden of work-related diseases in Pakistan which occurs mostly in the form of cardiovascular diseases, occupational asthma, COPD, neurotoxicity, different types of cancers, hearing loss due to noise, psychological and skin disorders. The major contributors of these illnesses are dusty occupations. The crushing industries are the backbone of construction sector and provide employment to almost 0.5 million people. The lack of literature on respiratory illnesses shaped the rationale of the present study. A cross-sectional survey was conducted in a large crushing unit located in the province of Punjab. The main survey encompasses questionnaire and few measurements including chest expansion measurement and peak flow obstruction. Apart from direct exposure to crushing dust, different factors like sociodemographic, tobacco use, indoor air quality and occupational health and safety components were analyzed to find out the risk association of any respiratory illness. The bivariate and multivariate analysis were done in SPSS. The result discussed four main types of respiratory illnesses. The prevalence of diseases was reported in percentage such as chronic bronchitis, chronic asthma, chronic rhino sinusitis, peak flow obstruction and any other form of respiratory illness as 15, 20, 24, 42 and 53% respectively. The significant predictors were occupation category in the industry, job duration of 25 years or more and working hours more than 36 hours a week. Among different socio-demographic variables, lower education level, rural residence and use of non LPG fuels were strongly associated with higher risks. Another important predictor was the use of tobacco (cigarette or any other form) which was significantly associated with chronic asthma [OR 2.79], chronic bronchitis [OR 5.38], and peak flow obstruction [OR 5.38]. Poor compliance with OHS practices was significantly associated with higher occurrence of various diseases. Compliance with OHS measures with training and awareness can be a short-term solution. But for a holistic approach, changes in living standards and linking of socioeconomic inequalities are needed.

Preparation of Mixed Oxide of Mn and Ce as Photocatalyst for Degradation of Profenofos from Aqueous Solution

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The present study was focused to the preparation of CeO2-MnOx by Co-precipitation method and characterization of prepared CeO2-MnOx was performed using X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), Scanning electron microscope (SEM) and Energy dispersive X-rays (EDX). The prepared CeO2-MnOx mixture was utilized for the degradation of profenofos under the influence of various operational parameters such as time of reaction, dose of catalyst, initial concentration of profenofos, pH of the solution and temperature. The results showed that degradation of profenofos was depend upon the solution pH and maximal degradation was achieved at pH 7. The degradation study was revealed that % degradation of profenofos increased with the progress of catalyst dose as well as temperature. The degradation studies were fitted into Arrhenius equation to calculate the activation energy and it was found to be 9.02 KJmol-1. Kinetics of the degradation of profenofos was also studied.

A Computational Approach for Structural Properties of 2-Methoxy-1, 4-Naphthoquinone

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The molecular structure of the 2-Methoxy-1, 4-Naphthoquinone (MNQ) has been analyzed computationally to identify its applications in the field of chemical and biological sciences. Most of the theoretical calculations have been performed for MNQ employing DFT and TD-DFT approaches with 6-311++G basis set. A comparison of IR spectra computed in four different solvents i.e. water, DMSO, acetone and ethanol as well as in gas phase was made using intensified vibrational analysis of MNQ. The experimental FTIR spectrum has been assisting the computed IR spectra. Fundamental vibrational modes have been assigned and analyzed using experimental as well as quantum mechanical data. Hartree-Fock method and DFT analysis have been employed for computing Raman spectra utilizing 6-31+G as well as 6-311++G bases set. The complete information on geometrical properties has been collected in the gas phase in addition to four other solvents by means of B3LYP and MP2 techniques, while energies, ground state transitions (HOMO-LUMO energies), and absorption spectra were calculated by DFT/6-311++G. NBO characterization at DFT/B3LYP/6-311++G described important interactions which are supposed to occur in this compound. Dipole moment, Mulliken charge distribution, Natural population analysis and thermodynamic parameters have been calculated as well. Molecular electrostatic potential (MESP) calculations have also been run to investigate the reactivity of title compound.

Remarkable Catalytic Degradation of Arsenic by Magnetite Iron oxide Nanoparticles using Inductively Coupled Plasma- Mass Spectroscopy

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More than seven Lac people are diagnosed with arsenic-related diseases and 100 million humans are endangered by arsenic-contaminated water sources, particularly in Asia. In this study we reported the greener, smaller size and stable synthesis of Iron Nanoparticles (Fe3O4 NPs) using L-Cysteine having pH (10) which are magnetite in nature and their catalytic application behave as an efficient catalyst f the removal of arsenic from the water in a very short time. These particles were characterized by different characterization techniques including Transmission electron microscopy (TEM), Energy dispersive spectroscopy (EDS) and Ultraviolet-Visible spectroscopy (UV-Vis). The size of Fe3O4 NPs were in range of 5-30nm, they were spherical in shape and the spectrum was observed between 300-700nm wavelength. Arsenic solution of 0.5mg/L (500Âµg/L) was prepared using arsenic standard solution by VWR chemicals, Belgium. For application study using Inductively Coupled Plasma- Mass Spectroscopy (ICP-MS) of PerkinElmer to check the reduction of arsenic concentration levels by L-Cysteine functionalized magnetite iron nanoparticles. The results obtained from ICP-MS shows 89-90% reduction in arsenic levels with the presence of iron nanoparticles (Fe3O4 NPs) act as an excellent ultrafast catalyst to remove the arsenic contamination from the water rapidly.

Highly Efficient and Size Tunable Synthesis of Indium Phosphide Based Quantum Dots

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We proposed in detail the core growth temperature (CGT) over a wide temperature range from 90-240oC, concentration of precursors and waiting time for the synthesis of highly efficient and color tunable InP(Zn)ZnS alloy-core/shell quantum dots (QDs). CGT has very important role for the controlling of the nucleation and growth process in a particular temperature. The photo-luminscence (PL) quantum yield (QY) values of InP(Zn)ZnS alloycore/shell QDs decreased as CGT was increased from 90, 130, 170, 200 and 240oC were found at 75, 66, 35, 29 and 18%, respectively. Moreover, PL full width at half maximum (FWHM) was raised at 63 nm, 75, 77, 88, 96 nm from 90 to 240oC. We have optimized that CGT of 90Â°C is best for PL QY (75%) and FWHM (63 nm) as compared to others. PL emission and UV-visible absorption peaks were shifted to a longer wavelength (red shift) from 508 to 621nm through 90 to 240oC. The synthesized QDs were characterized by UV-visible spectrophotometer, FT-IR spectroscopy, XRD, TEM and PL, respectively. The developed QDs will be more effective for scientific, reliable and producible applications for sensors development, photo-catalytic, electronic devices, optoelectronics, LED, biological imaging and so on

Organolead Halide Perovskite Solar Cells: Potentials, Challenges, Structural, Optical and Electrical Properties of Perovskite Materials

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Perovskites are very interesting, various group of matter, exhibiting great change of useful properties defined via their composition. Recent advancements in the area of perovskite photovoltaics have drained wide attention of scientific community, mostly because of unexpected light absorbing properties exhibited via these organometallic halides. Organolead halide perovskite materials have a combination of wonderful optoelectronic properties, such as steep optical absorption edge and high absorption coefficients, long charge carrier distribution lengths and eras. Perovskite solar cells based on organometal halides represent an emerging photovoltaic technology. Perovskite solar cells stem from dye-sensitized solar cells. In a liquid-based dye-sensitized solar cell structure, the adsorption of methylammonium lead halide perovskite on a nanocrystalline TiO2 surface produces a photocurrent with a power conversion efficiency (PCE) of around 3â€“4%, as first discovered in 2009. The PCE was doubled after 2 years by optimizing the perovskite coating conditions. One of the key advantages of perovskites have is their capability to be processed from solutions at comparatively low temperatures. The ultra-long hole/electron diffusion lengths, high mobilities, high absorption coefficients, and the tunable band gap of organolead halide perovskite resources build the study on perovskite solar cells to progress quickly. The efficiency of perovskite solar cells (PSCs) above 18% were obtained in various device structures. This paper in a few words describes main structural, optical and electrical properties of perovskite materials, as well as the most accepted solution processing techniques. Over the extent of only three years, reported photoconversion efficiencies of such devices went from 3.8% to over 19% .The arrangement of high efficiency, low cost and supplementary (non-PV) applications provides great potential for commercialization. Performance and applications of perovskite solar cells often associate with their device structures. Key Words: Organolead halide perovskite materials, efficiency of perovskite solar cells (PSCs).

Selection of Suitable Micellar Media to Remove Reactive Dyes from Aqueous Solution

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This manuscript reports the improved solubilization capacity of mixed micellar media for reactive dyes. The solubilization of anionic reactive dyes i.e Reactive red 195 (RR-195) and reactive blue 221(RB-221) has been studied in micellar media of a cationic surfactant, Cetyltrimethyl ammonium bromide (CTAB) in absence and presence of a nonionic surfactant Triton X-100 (TX-100) using UV/visible spectroscopy and electrical conductivity. UV/Visible spectroscopy is helpful to evaluate the degree of solubilization in term of partition coefficient (Kx), Gibbs energy of partition (?Gp), binding constant (Kb) and Gibbs energy of binding (?Gb). The electrical conductivity has been employed to detect critical micelle concentration (CMC) and to calculate thermodynamic parameters such as Gibbs energy (?Gm), enthalpy (?Hm) and entropy of micellization (?Sm) of surfactants in the presence of said dyes. The values of said parameters reveal that solubilization is spontaneous process favored by enthalpy and entropy. It has been observed that mixed micellar media of CTAB and TX-100 has higher solubilization capacity than that of CTAB alone. Increase in concentration of TX-100 has increasing effect on solubilizing power of CTAB. It is concluded that solubilization is exothermic, spontaneous and enthalpy driven process.

Desulfurization

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Desulfurization of model oil was investigated by adsorption over Zn and ZnO supported on Hydroxyapatite (HA) and activated carbon (AC) . The adsorbents were characterized by XRD,Ft-IR, TGA and SEM. Adsorption experiments were carried out in batch mode under mild conditipns. Results indicated that % desulfurization attained using Zn/AC, ZnO/AC, Zn/HA and ZnO/HA was 95.77, 95.62 and 94.4 respectively. The estimation of adsorptive capacity of Zn/AC, ZnO/AC, Zn/HA and ZnO/HA was analysed to maximize the desulfurization efficiency.

Synthesis of Modifiable p(Methacrylic Acid-Co-Acrylonitrile) Microgel Fabricated With Metal Nanoparticles for Simultaneous Catalytic Reduction of Multiple Water Pollutants

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We synthesized poly(methacrylic acid-co-acrylonitrile) hydrogel in the form of spherical microparticles. The hydrophilicity of the hydrogel was enhanced by converting nitrile groups into amidoxime groups. The amidoximated microparticles of hydrogel were used as substrates for in situ synthesis of copper and cobalt nanoparticles. The prepared substrate microparticles of hydrogel and their corresponding metal nanocomposites were characterized by SEM, TEM, TGA and AAS. Catalytic reduction of nitro aromatic pollutants like 2-nitrophenol (2-NP) and 4-nitrophenol (4-NP) and organic dyes with both the cationic and anionic character such as eosin Y (EY), methylene blue (MB) and methyl Orange (MO) was carried out to investigate the catalytic potential of the prepared catalysts. The simultaneous reduction of oppositely charged dyes and a nitrophenol was also studied. The catalyst containing copper nanoparticles showed better catalytic activity than that containing cobalt nanoparticles, however, the recycling results were in opposite trend.

Functional Modification of Selected Beta Lactam Antibiotic in Search of More Useful Antibiotic Agents

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A series of Thiadiazine-2-thiones were synthesized by the reaction of various primary amines with carbon disulfide, potassium hydroxide followed by addition of formaldehyde, cefaclor and cefadroxal in phosphate buffer medium. The determination of these compounds was elucidated by spectral methods (IR, NMR and Mass spectra). The antimicrobial potential of these compounds was also investigated against different bacterial strain including; Streptococci, staphylococci and fungal strain including; Aspergillus nigerall, all these compounds showed significant activity. Their structure activity relationship showed that position 3 and 5 substituents have a key role against leishmanicidal activity. The antimicrobial activities of these compounds were screen against some bacteria and fungi.

Importance of Marine Sponges as Potential Sources of Antiplasmodial Compounds

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Marine life has a diverse structure consisting of about 30 million species spread out over 70% of the earth surface. Only a limited number of bioactive natural products are known from this highly rich source of unlimited compounds. Marine organisms are thus expected to become a source of novel bioactive compounds that can ultimately help in the development of new drugs. Sponges belonging to Hyrtios and Coscinoderma genera are important sources of marine natural products. Most recent work on these sponges have led to isolation of antiplasmodial compounds from two species of the aforementioned genera.

Synergistic Effect of Silane Crosslinker (APTEOS) On Gelatin and PVA Blend for Packaging Applications

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The practice of traditional packaging material causes severe environmental issues that need to be addressed. We have designed biodegradable hydrogels which are perfect for packaging applications. Solution casting method was used to prepare hydrogels using PVA and gelatin cross-linked by 3-aminopropyl triethoxysilane (APTEOS). Two different kinds of hydrogels were formulated; one with cross-linker and the other without cross-linker. The structural characterization and morphology of the developed hydrogels were achieved by FTIR, SEM and TGA. Porous surface of the developed hydrogel was confirmed by SEM analysis. Shift in the intensities of the peaks of the developed hydrogels was confirmed by FTIR spectra. Mechanical properties of the films were checked by tensile test. The swelling tests were performed in water. Soil burial test evaluated the biodegradability of developed hydrogels. All the developed hydrogels showed good tensile strength and biodegradable properties. Biodegradability decreases and tensile strength increases with the increase in the amount of cross-linker. Therefore, these APTEOS cross-linked hydrogels are suitable and useful candidates in packaging field.

Synthesis, Structural Characterization and Biological Studies of Silver(I) Complexes

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The emergence of microbeâ€™s resistant antibiotics against bacterial infections is a worldwide problem that provoked the development of novel antimicrobial agents. Silver metal and silver salts has been utilized as antimicrobial agents for thousands of years. Due to its antimicrobial activity, silver(I) complexes provide a versatile platform for drug design and are captivating parts of bioinorganic chemistry [1-2]. Mixed ligand silver complexes have been reported in the literature and shown promising activity against microorganisms [3-9]. Here in, we synthesized silver(I) complexes and evaluated for their potential antimicrobial activity with much lower toxicity to human cells. We synthesized, characterized a series of three new silver(I) complexes that contain bisphosphine and dithiocarbamate (DTC) ligands. The structures of new complexes were characterized using spectroscopic and analytical techniques. Single crystal studies revealed that the geometry of two complexes is binuclear and one complex is one-dimensional (1D) polymer, respectively. All the complexes were further tested for their antimicrobial activities.

New Picolylamine Template Organo-Catalyst for Enantioselective Aldol Reactions

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Aldol reaction is known to be carbon-carbon bond connecting reactions since decades. Aldol reactions can be used for variety of pharmaceutical applications. Different organo catalysts could be used for the enantioselective Aldol reactions. The picolyl amine based catalysts were designed and prepared from commercially available acetyl pyridine and these catalysts were screened for enantioselective aldol reaction. Tetralone were best choice as aldol donor and it was treated with variety of aldehydes to make different aldol Products with mediocre to high ee.

Modified Graphene Based Zinc Ferrite for the Degradation of Methylene Blue

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Present study describes a novel eco-friendly method for the synthesis of rGo/ZnFe2O4 (GZF) as an adsorbent and photo-catalyst for the removal of Methylene blue from aqueous solution. Graphene Oxide was used as precursor and FeCl3.6H2O and ZnSO4 has been anchored on its frame work through in situ reaction using EtOH as green solvent with normal temperature range. Insertion of Fe and Zn ions will impart magnetic character and through Fenton type reaction will help in degradation. The synthesized GZF will be easy to reuse and recover bearing magnetic character. The material has been characterized by XRD and FT-IR spectroscopy which indicates that the Go has been reduced to rGO and all characteristics indices in XRD confirm the formation of GZF. Similarly SEM and TEM study revealed an excellent surface morphology of the GZF. Evaluating the process at different pH value indicates that at pH 4 and 10 both adsorption and degradation takes place respectively, while at neutral pH i.e.7, only adsorption is predominant process. The composite exhibits excellent degradation of 82 and 90 % at pH 4 and 10 respectively while at neutral pH it shows 85% adsorption only. The synthesized GZF has excellent regeneration ability and remain efficient in degradation of Mb for six cycles. Key Words: Graphene Oxide, Zinc Ferrite, Methylene Blue, Degradation

Treatment of Cadmium Contaminated Water Using Chemically Modified Amberlite XAD-2

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This study reports two step synthesis of a new resin i.e. Trifloro Acetyl Acetone (TFAA)-XAD (X) resin via Schiffâ€™s base reaction. Synthesized resin was used to treat cadmium contaminated water. Before application to the real water system a method for removal was optimized using Design of Experiment (DoE). A face centred composite design (CCD) predicted 97.0% removal at pH 10, other optimum parameters were, concentration of Cd(II) ion 10 mg l-1; Sorbent amount 82.0mg; shaking speed 200 RPM and shaking time 63 min. Predicted removal was found to be in good agreement with experimental removal. Equilibrium data was good fit to Langmuir, Freundlich and D-R isotherms with a correlation coefficient (R2) of0.98, 0.97 and 0.98, respectively.

Fabrication of a Highly Effective Electrochemical Urea Sensing Platform

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Our investigation involves the successful functionalization of a glassy carbon electrode (GCE) with amine groups (−NH 2) was carried out, to produce aminated GCE. The aminated GCE could be effectively used to detect current changes during the urease-catalyzed decomposition of urea. The silk fibroin (SF) scaffolds were employed to place urease near the surface of the aminated GCE (Urs/SF/aminated GCE). The prepared electrode was employed for electrochemical urea sensing via cyclic voltammetry and amperometry techniques. The fabricated sensing platform displayed rapid detection response (~1 min) and a very high sensitivity (112.3 μA mM -1 cm -2) with a linear correlation (0.3-8.4 mM) between current and urea concentrations. The analogous sensing responses obtained using replaceable SF scaffold discs (generated and functionalized in the same batch) in the Urs/SF/aminated GCE assure the suitability of the present platform for application in portable urea sensing devices.

Turn-on Fluorescent Probe for Highly Selective Discrimination of Hypochlorite from Oxidants in Aqueous Media

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A fluorescent probe based on cabazole moiety was synthesized and found to be selectively fluorescent (λ = 440 nm) for hypochlorite. The synthesized probe is highly selective for hypochlorite even in the presence of other interfering strong oxidants. The probe was also found to be useful for quantifying the presence of oxidant (ClO^-) for different sources of water. Mechanism involved was elucidated by different techniques i.e. NMR, HRMS, cyclic voltammetry. The mechanism was also confirmed by DFT calculations.

In-Silico Estimation of Inhibition Potential of Phytochemicals against Zika Virus

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Zika virus (ZIKV) is related to other viruses in spreading many diseases e.g. microcephaly small heads in neurological diseases. The virus has been reported in Africa since 2015 but no vaccination or treatment is developed yet. ZIKV consist of 10 proteins that play significant part in virus simulation. Inhibitory effect detection of ZIKV was calculated against three structural proteins 1-Envelop protein, 2- capsid protein and 3-precursor protein and seven non-structural proteins 1-NS1, 2-NS2A, 3-NS2B, 4-NS4A, 5-NS4B 6-NS3, 7-NS5. In this study NS3 helicase and NS5 polymerase RdRp were used to explain the information about biological target in life cycle. The crystal structure of NS3, NS5 were retrieved from PDB and phytochemicals were also selected from medicinal plants. In-silico theoretical comparison of antibacterial activity and antifungal activity of concerned medicinal plants was also carried out. Almost 200 phytochemicals were studied. Thirty compounds were tested for inhibitory action by docking method and density functional theory and they showed good result. These compounds depicted highest affinity and reactivity as inhibitor against NS5, NS3 protein target. HOMO-LUMO energy gap was calculated by docked phytochemicals output in DFT. Pharmacological properties like drug potential, solubility, GI absorption, BBB penetration, toxicity and carcinogenicity of compounds were determined by ADME server. Therefore in-silico studies can help in selection of phytochemicals used for inhibitor against replication of RNA for drug discovery. Key word: Zika virus, NS proteins, Phytochemicals, Inhibitor and Computational analysis.

Synthesis and Characterization of Cerium(III) based Metal Organic Frame Works

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Metal organic frame works (MOFs) were synthesized using citric acid as a green linker while oxalic acid was used as co-ligand. While cerium metal ion was used as metal node. Effect of variation of mole ratios of citric acid and oxalic acid was checked on morphology of two MOFs namely 1 and 4. The formation of synthesized MOFs was confirmed by FT- IR spectroscopy, carbon hydrogen nitrogen analyzer technique (CHN), Powder X-Ray Diffraction (PXRD) and Scanning electron microscopy (SEM). The preliminary confirmation for successful formation of synthesized MOFs was obtained from FT-IR spectroscopy where the absence of peaks at 1720 cm-1 indicated that the carboxylate group is no more present in free form. While, presence of peaks in the range of 1610-1550 cm-1 were attributed to the association of COO- with Lanthanide metal ion. PXRD studies revealed that although the MOFs were obtained in powder form, still they were crystalline in nature. Their morphological studies were performed using SEM and it was unveiled that obtained MOFs were grown in different morphologies when mole ratios of the ligands and lanthanide metal ions were varied. The MOFs were produced in good yield. Further work is under way with the same ligands and metal systems to find effect of using different solvents and variation of temperature on morphological forms of MOFs. More over scale up synthesis of the synthesized MOFs is also underway so that MOFs in gram levels could be produced which might be employed for potential applications in near future.

De-Contamination of a Drinking Water Contaminant Using Batch Mode

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A batch mode strategy was used for the de-contamination of arsenic from drinking water. The interaction between iron and silicon was used for this purpose in a mixed system. This mixed system was characterized using different techniques and then was compared with the individual oxides system. Evaluation of the effectiveness of the mixed system as compared to the individual oxide system was carried out at different batch mode conditions. Effect of phase changes at elevated thermal treatment of the mixed system was also studied to understand the effect of phase changes on the de-contamination of the contaminant. The mixed system of oxides proved to be effective for the de-contamination of arsenic from the drinking water.

Green Synthesis of Silver Nanoparticles Using Green, Brown and Red Seaweeds

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Synthesis of silver nanoparticles was done by the reduction of silver metal using seaweeds. Three species of seaweeds, each belonging to green, brown and red classes were used. The study has led to show the potential of Seaweeds with reference to the presence of certain functional moiety, which are involved in the bio reduction and stabilization of silver nanoparticles (AgNPs). Absorption peaks were observed in the range of 400 nm â€“ 450 nm using UV-Visible Spectrophotometer. The intensity of color increased after incubation period. It was observed that incubation period for the synthesis of silver nanoparticles using brown and red seaweeds was 48h while with the green seaweeds was 98h. Silver nanoparticles were further characterized by using Scanning Electron Microscopy and Fourier Transform Infrared technique. Stability of AgNPs was observed at different concentration of silver. This synthesis is environmental friendly. No toxic reagent was used. Silver Nanoparticles formed by this method has potential to be used in the drug manufacturing, biomedical devices, water purification, microbial activity and agricultural purposes.

Study of Trace Metals Imbalances in the Scalp Hair of Stomach Cancer Patients with Different Types and Stages

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Stomach cancer is among the most common forms of cancers and diet as well as environmental factors play important roles in its malignancy. This study was conducted to evaluate the trace metals contents in the scalp hair of stomach cancer patients and healthy donors to investigate probable relationship between metals imbalances and cancer. The samples were digested in HNO3-HClO4 mixture and the metals were quantified by flame atomic absorption spectrophotometry. Mean concentrations of Pb and Cr were found to be significantly higher in the patients than controls, while average levels of Fe, Mn and Cd were considerably elevated in the controls. The correlation pattern of metals in the patients manifested significantly divergent mutual relationships compared with the controls. Multivariate analyses showed appreciably diverse apportionment of the metals in the patients and healthy donors. Variations in the metal levels were also observed for various types (adenocarcinoma and gastrointestinal stromal tumour) as well as stages (I, II, III & IV) of stomach cancer patients. Most of the metals revealed noticeable disparities in their levels based on gender, habitat, dietary habit and smoking habit of patients and controls. Accordingly, the essential/toxic metals exhibited significant imbalance due to pathogenesis of stomach among the patients.

Synthesis of Novel Oxadiazole Based Structural Hybrids of Ibuprofen with Low Ulcerogenic Effect

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Ibuprofen is used for treatment of chronic painful and other inflammatory conditions. But unfortunately, it has some side effects like gastrointestinal side effects include gastric ulcer. It is proved from literature that â€“COOH moiety of Ibuprofen is responsible for GI toxicity. So we have designed scheme for derivatization of free â€“COOH group of Ibuprofen for improving their safety profile. We have derivatize â€“COOH group of NSAIDs with various five membered heterocycles like oxadiazole and triazole nucleus along with different functionalities like acetamide and propanamide. Oxadiazole and triazole molecules worked in two ways i.e masking the acidic group of drugs, so decreasing the side effect of acidity and improving anti-inflammatory activities. The H groups of oxadiazoles/triazoles was further replaced with different active groups like acetamides and propaneamide. The resulting biomolecules have different functionalities together in one structure. After successful synthesis, compounds were screened for their biological activities like anti-inflammatory, antibacterial, antiplatelytic and anticonvulsant activities compared with parent drug both in vivo and in vitro and good results were obtained. These heteroarylcarboxamide derivatives with improved properties could be an interesting alternative to classical anti-inflammatory drugs.

Recent Trends of Suzuki Miyaura Cross Coupling Reaction of Heterocyclic Compounds

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In Suzuki Cross Coupling Palladium catalyst, boronic acid and organo-halide compounds couples to form carbon-carbon bond. The Suzuki Cross-Coupling was the subject of many research studies because it was used in synthesis of many biologically and pharmaceutically active heterocyclic compounds. In synthesizing heterocyclic derivatives Suzuki cross-coupling is used for development of carbon-carbon bond. It has advantages over other reactions because its reagents are stable, its handling is easy and the by-products can be separated easily

Green Alternative to the Synthetic Ionic Surfactants

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Surfactants are widely used in a number of different industries and for other household purposes. Synthetic surfactants with a number of applications also contain toxic aspects of health and environment and cannot be neglected. For that purpose, a biodegradable environmental friendly and safe for human use surfactants are highly needed. The natural surfactant is suitable alternatives for that matter. The natural plant material was selected and tested for surfactant properties. The natural surfactants showed great ability to form ion pair with different dyes. The extracted saponins were found to be more efficient than synthetic surfactants. The Natural surfactant has lower CMC values and thus efficient in detergent qualities. The changes in the conductivity of the dye-surfactant solution were observed at different temperatures. The natural surfactant found to be a good replacement of two synthetic surfactants. The extracted natural surfactants were tested for their biodegradability and found positive results. The end biodegradable products were Cunninghamella blakesleeana, Phanerochaete chrysosporium, Cunninghamella echinulate types of fungus. The findings of the work showed that the proposed natural surfactants were not just efficient in working, but cheap and environmental friendly as well.

One Pot Synthesis of Metal-Metal Sulphide Supported Over Carbon Nanofibers for Oxygen Evolution Reaction

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The development of efficient and low-cost electrocatalysts of non-precious materials for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) is crucial for the successful application of water splitting technologies. Herein, we reported the successful synthesis of bi-metallic (FeCo) and tri-metallic (FeCoNi) electrocatalysts and their sulphides supported over carbon nanofibers (CNFs). The facile method consisted of the simple electrospinning of the precursor blend solution consisting of metal salts and polyvinylpyrrolidone (PVP) and polyvinylacrylonitrile (PAN) polymers. The obtained nanofibers were then carbonized at 600 - 800 °C in a tube furnace under argon flow. The samples were characterized by scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD) and nitrogen adsorption-desorption using Brunauer–Emmett–Teller (BET) method. The nanoparticles were crystalline in nature and uniformly distributed over the CNF surfaces. The fabricated FeCo and FeCoNi electrocatalysts and their sulphides over CNF exhibited excellent OER activity in 1 M KOH with low overpotential and enhanced current densities.

Human Health Risk Associated with Polychlorinated Biphenyl

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Polychlorinated biphenyls (PCBs) are synthetic organochlorine compounds, that were widely used past but their production was banned in many countries because of the bioaccumulation in the body. Many industries in Pakistan end up producing “Persistent Organic pollutants” and their residues ends up in the food we eat. PCBs are metabolized by cytochrome P450 in mammals. PCBs can be transported through the placenta to the fetus about 30% of their amount in plasma of mother. These fat soluble substances can influence visual system development, oro-motor behavior, intelligent quotient and down-regulation in gene expression of retinal photoreceptor cell development in infants of women exposed to PCBs. Infants of such women are low birth weight, who are at life time risk for several complications. Exposure to the moderate doses of PCB can cause alterations in 1) communication abilities, 2) action choice and 3) social behavior. Iron metabolism and iron homeostasis can be affected by them. Some non-human & human studies show that PCBs may disturb menstrual cycle. It can increase the risk of cancer, diabetes, cardiovascular and liver diseases. Because of their knowledge of the toxic effects of is growing faster than the level of environmental decrease, PCBs are still dangerous pollutants.

Ultrasound Assisted Extraction by Optimizing Different Parameters Using Statistical Design, Degradation Rates and Identification by High-Performance Liquid Chromatography-Electrospray Ionization-Mass Spectrometry

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Rapid ultrasound Assisted extraction of anthocyanins (ACNs) from brinjal peel was investigated by statistical designs: Placket Burman Design (PBD) and Face-Centered Central Composite Designs (FCCCD). Three potential factors were studied by PBD including extraction time, temperature and solid to liquid ratio. After selection of significant factors, a FCCCD was set up with two controllable factors (Temperature and time) along with response (ACN's yield). The maximum ACN's yield (1399.7µg/g) was achieved at 40°C and 30 min extraction time. In addition various mathematical models were fitted to observe data in order to attain the adequate regression model and the results exhibited that quadratic model with F-value 36.67 was significant. There was only a 0.04% error in model could occur due to noise. Additionally degradation rates of anthocyanin pigments was also examined at variable temperature range (10, 25, 40, 55°C) along with luminescent light and dark conditions for several days. Thus conclusive results have shown that the extraction temperature 10-25°C in absence of light enhance the anthocyanin pigments stability. Furthermore, detailed characterization of individual ACNs such as Dp3Ga, Cy3G, Cy3xylGGa and Pg3acetylG was done by LC-ESI-MS analysis. Keywords: PBD, FCCCD, anthocyanins, ultrasound Assisted extraction and LC-ESI-MS.

Bioagents – The Major Sources to Clean the Environment

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

Synthesis of New Arylsulfonylspiroimidazolidindiones as Aldose Reductase Inhibitors and Their Effect on Stimulation of Insulin Release

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A novel class of spiroimidazolidine-2′,4′-diones substituted with aryl sulfonyl group at different positions was designed and synthesized. The target compounds were evaluated for their potential to release insulin from MIN6 cell line derived from in-vivo immortalized insulin-secreting pancreatic cells. Some of the compounds exhibited high potency. Compound 2d and 3f exhibited excellent insulin release activity from MIN6 cells when compared with standard drug, tolbutamide. Some of these compounds had a potent inhibitory activity for human recombinant aldose reductase (ALR2), an enzyme which converts glucose into sorbitol and plays a key role in development of complications arising from diabetes, such as retinopathy, nephropathy, neuropathy and cataract formation. Against human recombinant ALR2, compounds 2a, 3a-d, and 3f-h displayed effective inhibition activities. The results were augmented by the ability of the compounds to prevent sorbitol accumulation in the isolated rat lenses, sciatic nerves and erythrocytes. Some of the compounds were found to possess excellent dual activity, hence they may be promising candidates to modify and evaluate their dual action, i.e., insulin release to combat diabetes and ALR2 inhibition to prevent/treat diabetic complications. The compounds were also found to possess good antioxidant efficacy. Furthermore, most of the compounds lack toxicity as determined on human embryonic kidney cell lines 293 (HEK293).

Development of Pheromone Traps to Capture Date Palm Pests in Sindh

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Development of Pheromone Traps to Capture Date Palm Pests in Sindh Ranjhan Junejo a, Shahabuddin Memona, Muhammad Usman Sharb aNational Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro-76080-Pakistan bEntomology Section, Agricultural University Tandojam, Sindh, Pakistan Abstract Date palm is affected by number of insect pests such as red palm weevil, lesser date moth, termites, date scales, mealy bugs and mites. Among all the insect pests; red palm weevil (Rhynchophorus ferrugineus L.) is a serious problem to date palm trees, which causes 10-20% loss in production to different varieties of dates. The red palm weevil very dangerous insect pest, which attacks date palm trees during the process of suckers removal and destroys it. The red palm weevil mostly attacks the soft parts of the date palm plant. Due to its attack, date production have been reduced up to 10 tons per hectare. The use of trapping systems certainly provides an efficient techniques to be included in any integrated pest management program (IPM) to control the red palm weevil, by means of reducing its population. Therefore, in this study, pheromone traps have been implied at the date palm orchards of khairpur Mirs' Sindh. Keywords: Red palm weevil, Date Palm, IPM, Kairomone, Pheromone, Traps. Acknowledgement: We are thankful to SAGP-CARDF (Sindh agricultural growth program –Competitive agricultural research development fund and the National Centre of Excellence in Analytical Chemistry, University of Sindh Jamshoro for the financial as well as technical support for this work.

Sonication Assisted Extraction of Propolis; A Step towards Sustainability

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Propolis is a honeybee's resinous material of high value, collected from tree buds and plant. Traditionally, propolis has been used for its medicinal and antioxidant properties [1]. Polyphenols present in propolis are responsible for biological and pharmacological properties [2]. In this research different methods for the extraction of propolis were compared, where ultrasonication techniques was found best in terms of yield and time. The extract was analyzed through GC-MS and chemical methods. All extracts and fractions were screened for their antioxidant and anti-inflammatory activities.

Synthesis And Characterization of Anti-Static Charge Properties of Polyaniline Based Nano-Composites

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Polyaniline and its composites were prepared with metal doped nanoparticles, in order to minimize surface energy of nanoparticles process was conducted in ice chilled environment. This technique reduced coagulation of particles even after process of polymerization. Manganese doped zinc sulfide (Mn doped ZnS), TiO_2, Co doped SnO_2 (Cobalt doped tin oxide) and carbon particles were used as templates with aniline to form composites. Resulting products were characterized by SEM, FTIR, XRD and capacitor discharging techniques. Discharging of 220µF capacitor was conducted with all above mentioned composites and discharging time was recorded. Carbon-polyaniline and Mn doped ZnS polyaniline composites discharging time was very fast whereas Co doped SnO_2 and TiO_2 polyaniline composites were proven insulators and capacitor did not discharge. Metal particles were in size between 1µm to 10µm. antistatic charge ability of carbon-PANI, Mn doped ZnS - polyaniline was appreciable whereas TiO_2 and Co doped SnO_2 proven good insulators. Discharging time of 4.6KΩ resister was also recorded for a reference. Composites were placed in circuit by replacing resister. Current of the circuit was dropped from 0.1A to 0.01A in case of conducting composites when they were placed in ammonia environment. These composites can also be used in gas sensing devices.

Sonochemical synthesized NiO nanoparticles as adsorbent for Lead sequestration

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NiO nanoparticles were fabricated through sonochemical itinerary in accompany of cetyl trimethylammonium bromide (CTAB) as surfactant and NiSO4.6H2O as precursor of Ni. UV-visible spectroscopy, Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), and energy dispersive X-Ray analysis (EDX) were characterizing techniques. Adsorption parameters as amount of adsorbent, solution pH, time duration, and temperature were considered and preferred for isothermal modeling. Best fitted model was found to be Langmuir isotherm model depicting highest adsorption capability of 166 mg/g. Kinetics data pursued pseudo-second-order rate equation and thermodynamics suggested endothermic temperament of the procedure. In view of this, NiO nanoparticles can be taking up as adsorbent for heavy metals sequestration from aqueous media.

A Field Assessment Soil Quality and Toxic Metals in Saline Soil

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There are about a billion hectares of salt-affected land worldwide, which may be resource opportunities for halotechnologies, such as halophyte crops, which grow better under high salinities. Chemical characteristics of soil are adversely affected by salinity because it results in increased heavy metals ion concentrations. Halophytic plants are of special interest because these plants are naturally present in environments. This study evaluated the potential of 4 plant species growing on saline contaminated sites areas of the Hyderabad. Plantâ€™s root, shoot and the soil samples were collected and analyzed for selected metal concentration values. To evaluate the potential of plant species for phytoremediation: Bio concentration Factor (BCF), and translocation Factor (Tf) were calculated. The concentration of Cd in surrounding and adjoining soils varied from 52-76.5 and 12-33.1 mg/kg, Cr from 3.68-20.6 and 4.26-18.4 mg/kg and Pb from 11.2-14.5 and 3.30-8.57 mg/kg, respectively. The concentration of Cd in plant root varied from 13.9-29.9, in shoot 6.74-32.9 mg/kg, Cr in root varied from 1.35-6.20, in shoot 1.51-7.71 mg/kg, and Pb in root from 3.24-9.38 in shoot from 3.25-6.81 mg/kg, respectively. It was also noted that several evaluated plant showed bio concentration factor (BCF) greater than one for accumulated metals i.e. Cd in Tamarix aphylla (1.194), Typha domingensis (2.588) and Phragmites (2.849) was noted. On the other hand, Pb in Typha domingensis (1.596) and (1.628) was shown in Table. Furthermore, greater than one translocation factor (TF) for Cd in Alhagi maurorum, Tamarix aphylla and Phragmites, for Cr in Salvadora persica and for Pb in Salvadora persica and Typha domingensis showed strong evidence for phytoextraction and in situ remediation potential of these plants. The results of this study can be used for management and decontamination of soils with heavy metals using plant species having phytoremediation potential/characteristics

Tailor-made Biopolymer Nanocomposites for Biomedical Applications

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Biopolymer clay nanocomposites are exceedingly desirable materials, mostly due to their applications in a variety of fields such as fuel and solar cells, ionics, electronics, environment, mechanics, optics and temporary packing items [1,2,3]. New biopolymers based nanocomposites were prepared from neutral guar gum by adopting a simple and environmental friendly intercalation method. All synthesized compounds are characterized by FTIR, and thermal methods of analysis TGA/DTA.

Spectroscopic and Conductometric Analysis of Molecular Interactions of Polysaccharide in Colloidal Solutions

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Interaction between saccharin and ionic surfactants; sodium dodecyl sulfate (SDS) and cetyl trimethyl ammonium bromide (CTAB) has been studied at different temperature ranges from 293.15K to 318.15K conductometrically. The effect of saccharin on the critical micellar concentration of surfactants has been studied by various concentrations of saccharin. Micellization and thermodynamic parameters such as degree of ionization (α) and counter ion binding (β), Gibbs free energy (ΔGm), enthalpy (ΔHm) and entropy (ΔSm) have been calculated. Results showed that CMC of amphiphiles in the presence of saccharin increases more than in aqueous medium. For further support to conductometric study, spectroscopic data has also been reported which showed that with the increase in the concentration of surfactant the absorbance increases. It is also confirmed by the differential spectroscopy that the spectrum of saccharine also changes in the presence of SDS and CTAB. The partition co-efficient (KX) and interaction parameter (θ) for SDS and CTAB have also been determined using spectroscopic data.

Cell Free Culture Broth of Pseudomonas Aeruginosa Being an Enormous Source of Biodispersant for Ecofriendly Dyeing of Polyester

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In last few decades, conventional chemical dispersants had extensively been used in textile processing due to their availability and low cost. But now due to awareness about their toxicity and environmental threats, researchers are in search of ecofriendly alternative dispersants like biosurfactants that are more specific in action as compared to chemical dispersants, even under extreme conditions. Nevertheless, biosurfactants had not been competitive with chemical surfactants on the base of economics. It had been observed that the major cost on the production of biosurfactant had been on downstream recovery followed by product purification. Therefore, in the present study we used as-collected cell free culture broth (CFCB) of Pseudomonas aeruginosa grown on crude soybean oil in minimal media as indigenous source of rhamnolipid surfactant as dispersion media for anionic dyeing of polyester fabric. Herein, the performance of CFCB has been compared with some of nonionic, anionic, and cationic surfactants with different concentrations of azo disperse 73 at 130oC temperature for 30 min. After reduction clearing, the sample of best choice against tensile, fastness, color depth and shade evenness properties was proceeded for advance characterizations i.e. surface resistivity, scanning electron microscope, x-ray diffraction, and diffraction scanning calorimeter.

Bio-Electrochemical Conversion of CO_2 into Biofuels and Treatment of Oily Wastewater

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Decrement in natural resources and increased environmental pollution has heightened up the demand for the production of fuels i.e. biologically synthesized, renewable in operation, with the least possible energy and chemical consumption. Electrocoagulation, a process that has been employed for the production and then conversion of CO2 into alcohols, carboxylic acids and somewhat esters i.e. valuable energy producing biofuels. The source of CO2 that has been utilized was synthetic oily wastewater, in order to get it converted into long chain hydrocarbons also, as those biofuels are considerable more these days. Aluminum was used as a sacrificial anode for the generation of coagulants naturally into the electrokinetic system. The experimental design was established using stainless steel and aluminum electrodes along with the recyclization of used engine oil so as to reduce the cause of oil spills and refineries pollution. Clean water was extracted after physical and electrochemical treatment given to the wastewater with 89% removal of COD, 64% reduction in the size of unwanted and hazardous flocs. The production of carboxylic acid with long chains has been investigated prior by the help of FT-IR of the sludge and later confirmed by the results of GC-MS. Linolenic esters in organic phase and acids of that group in the polar phase were reported.

Development of Deep Eutectic Green Solvent Micro Extraction Method for Trace Analysis of Nicolsamide

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In present study a very sensitive and easy spectrophotometric method was proposed for trace analysis of Nicolsamide base on its liquid phase micro extraction using deep eutectic solvents (DES) prior to its quantification. DES system of phenol and choline chloride 2:1 was selected among different DES systems like Cholinchloride(ChCl) + Malonic acid, Cholinchloride + Glycerol, Cholinchloride + ethylene glycerol with different ratio. Analyte give maximum absorption at 378 nm. This method was found more effective at pH 10.0. Optimum volume for THF and DES was optimized which was 300 and 400µL, respectively. Validation of method was investigated with percent recovery 99.26% with RSD value < 2%. Inter assay precision was 0.51% and Intermediate precision was 0.0323%. Method was found linear from 0.0048 to 0.048µg/ml. The proposed method is comparable to British pharmacopeia with more easier and simple procedure. The proposed method was tested for Nicolsamide analysis in different pharmaceutical products and waste products. This proposed method was also compared with other methods of lab practice.

Fabrication, Characterization and Applications of Novel Low Cost Dicarbonyl Reflective Coatings

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Increasing global warming and decreasing natural resources is the most urgent issue at the moment. There is a clamant necessity to dissipate surplus heat into heat basins like clear sky. Daytime radiant cooling is a passive cooling method by which a surface provides reflectance of sunlight and radiates the heat to outer space without any energy input in the heat budget of the earth. Various reflective coatings are formulated, characterized and tested for radiative cooling and emittance of solar radiations in an atmospheric transparency window. Various coatings showed diverse temperature difference with different reflectance percentage like Mg11(HPO3)8(OH)6 Coating with 5o difference and 68% reflectance percentage(%R), banana stalk coating with 7o difference and 79%R, banana stalk & CaCO3 coating with 10o difference, TiO2 and dicarbonyl polymer coating with 14o difference and 84%R.A noticeable temperature difference of 16o was observed with low emissivity glass and dicarbonyl polymers coating along with metallic layer (silver) with 96%R in the range of 300nm-1100nm and this coating proved to be a promising one among others for its use as passive radiative cooling material. FTIR, PXRD and SEM results further highlighted the effectivity of the coating. To best of our knowledge, our newly formulated coatings are with highest thermal gradient and lowest in cost so far.

Functional Nano Materials for Water Splitting Catalysis and Energy Conversion Applications

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Water splitting is an emerging field for production of hydrogen based fuels having zero emissions. However, discovery of efficient electrocatalytic system in this regard is still a challenge. Here, we disclosed highly efficient thin film electrocatalysts prepared via time effective and cost effective strategies. Regarding this, thin film catalyst having high electroactive sites are shown to facially propel kinetically sluggish OER. We further anticipate to align transparent catalytic films with photo electrochemical as well as photocatalytic assemblages.

POSTER PRESENTATION

Evaluation and Comparison of Antioxidant Activity in Different Types of Citrus Peels Collected From Local Market of Lahore and Dera Ghazi Khan

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Citrus peels are extensively useful as source of natural antioxidant. Their main and active components which have numerous remedial characteristics and display anti-oxidant, anti-bacterial and anticancer activities. The present study showed the comparison of antioxidant potential in citrus peels samples collected from local market of Lahore and Dera Ghazi Khan. Lemon has highest antioxidant potential as compared to other samples of citrus peels. Antioxidant potential relative to the standard ascorbic acids solutions was formulated. Hence it is concluded that all the citrus peels samples have antioxidant potential in each solvent like water, n-hexane and Ethyl Acetate but lemon peels are significantly more beneficial and safe for diseases.

Electrochemical Degradation of Sunset Yellow Dye

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The wastewater containing dyes is considered as the very pinnacle of poisonous compounds of water toxins discharged into the environment. This work investigated the electrochemical degradation of a food dye, Sunset Yellow. The influence of different parameters such as pH, current density and different electrolytes were critically examined. The electrochemical degradation of dye was investigated at Ti/Ru0.3Ti0.7O2 electrodes in the presence of 0.1M NaCl electrolyte solution in a batch electrochemical reactor. Experimental parameters were operated at 200ppm/400mL of sunset yellow dye concentration, 5-40mA/cm2 current density, at room temperature in 8 minutes electrolysis time. Sunset Yellow decolorization increased by increasing pH and density upto 5 and 20mA/cm2 respectively, so it was considered as the optimum pH and current density for the dye degradation. Also maximum degradation was obtained when NaCl solution was used as the electrolytic solution. Depending on the electrochemical reaction conditions, Sunset Yellow dye decolorization was obtained upto 100%. The electrochemical degradation is an effective technique for removal of sunset yellow dye from industrial effluent.

Removal of Eriochrome Black T Dye by Using Surface Modified Bentonite

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The present study deals with the surface modification of bentonite with a cationic surfactant (CTAB) and a non-ionic surfactant triton X-100 to enhance its adsorption ability. The FTIR results confirmed the attachment of the surfactants to the surface of bentonite. The prepared materials were used to remove eriochrome black T dye from aqueous solutions. Different parameters like effect of time, effect of concentration and effect of pH were studied to observe the percentage removal of the dye. It was found that the efficiency of CTAB-bentonite was maximum at pH 6, (about 98% removal of dye was observed), while triton X-100 bentonite showed maximum adsorption at 12 pH (96% dye removal). The efficiency of modified clays was far superior than unmodified clay indicating the effectiveness of the process. Keywords: Bentonite, CTAB, Triton X-100, Eriochrome black T, Adsorption

Preparation of Novel Arsenic Imprinted Polymer for the Selective Extraction As(III) Toxic Ions from the Aqueous Environment

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In this study, we prepare synthetic arsenic imprinted polymer (As-IP) by simple precipitation polymerization method by using 4-vinylpyridine and 2-hydroxtethyl methacrylate as ligand and functional monomer use for the selective elimination of arsenic (As3+) from the aqueous environment. To achieve maximum sorption capacity several factors i.e. pH, agitation time, shaking speed, and sorbent dose were optimized. This prepared polymer was characterized by using SEM, EDX and FT-IR. Adsorption isotherm and kinetic data of As3+ fallow the Langmuir isotherm and pseudo-second-order kinetic model. The maximum sorption capacity of As-IP is 106.3mg/g. The limit of detection (LOD), and limit of quantification (LOQ) was found to be 0.87 and 2.9Âµg/L. The adsorption efficiency of As3+ ions by using As-IP from real water samples is approximately 99% which shows that As-IP has good sorption capability and highly selective for the extraction of arsenic ions.

Synthesis of Novel and Economical Solar Light Responsive Bismuth Doped Titania (Bi-Tio2) Through a Facile So-Gel Technique

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The present study is focused on the synthesis of novel and economical solar light responsive bismuth doped titania (Bi-TiO2) through a facile so-gel technique. Interestingly, a high concentration of oxygen vacancies i.e 7% was reported for the first time in titania lattice, as can be revealed from X-ray photoelectron spectroscopy (XPS). The transmission electron microscopy (TEM) and high resolution TEM (HRTEM) images also supported the successful induction of Ti3+. Furthermore, the absorption band was shifted to solar region by significantly decreasing band gap but with enhanced charge carriers separation via introducing bismuth (Bi3+), oxygen vacancies and Ti3+ in the doped material as revealed by diffused reflectance spectroscopy (DRS). Energy dispersive X-ray spectroscopy (EDX), Fourier transform infrared spectroscopy (FTIR) and X-Ray diffraction (XRD) results revealed that Bi3+ has been successfully incorporated into the titania crystal lattice. Besides, the Brunauer-Emmett-Teller (BET) analysis showed mesoporous nature of the as-synthesized Bi-TiO2. Moreover, the solar light induced photocatalytic degradation of FLU by the as-synthesized Bi-TiO2 followed pseudo-first-order kinetics. The mechanistic investigation revealed that ?OH and SO4?- are dominant species involved in the degradation of FLU. In addition, the photocatalytic performance of the as-synthesized TBi5 material aided PMS under solar light irradiation for Milli-Q water (MW), tape water (TW) and synthetic wastewater (SWW) was 92, 82 and 70 % with kapp values of 0.096, 0.085 and 0.066 min-1, respectively. Besides, the degradation products (DPs) of FLU and their pathways were proposed accordingly, Furthermore, cyclic photocatalytic stability and ecotoxicity of the as-synthesized material was also evaluated.

Antileishmanial Activity of Three Different Species from Piperaceae Family

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The species of Piperaceae family are found almost all around the world. A large number of Piper species have been reported to possess anti-inflammatory, antinociceptive and antileishmanial activities. Nowadays we are depending mostly on synthetic drugs and consequently being resistant to these drugs gradually and we are compelled to use the fourth generation of antibiotics with severe adverse effects. This comparison study covers three species, Piper angustifolium, Piper claussenianum and Piper amalago. This study revealed that species of Piperaceae family are incredibly effective against many microorganisms and are being used as folk medicines for different diseases. The essential oil or plant extract was tested for antileishmanial activity using disc diffusion method and broth dilution assay. The comparison of this study will encourage the scientist to return their research to natural products as these natural medicines are safe, easily available and affordable as compared to synthetic drugs.

Synthesis of Pyrimidine Derivatives Using Isobutyl Acetoacetate and Evaluation of Their Pharmaceutical Importance

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In recent research, it has been noticed that ÃŸ-glucuronidase enzyme slows down the process of glucuronidation which leads to accumulation of toxic substances in living bodies and may cause colorectal cancer or other related diseases. So there is an urgent need to synthesize ÃŸ-glucuronidase inhibitors. Currently, we have synthesized pyrimidine derivatives in two steps. In first step, 1,2,3,4-tetrahydropyrimidne (1-10) were synthesized by fusing urea, isobutyl acetoacetate and a verity of substituted aldehydes using catalyst in solvent free condition. In second step, compounds 1,2,3,4-tetrahydropyrimidne (1-10) were oxidized to obtain 2-hydroxypyrimidines (11-20) by using, ceric ammonium nitrate (CAN). All synthesized compounds (1-20) have been evaluated for their beta- glucuronidase inhibition potential and the promising results have been found which will be discussed in poster in detail.

Comparison of Hepatoprotective Activity of Ocimum sanctum against paracetamol, Lead and CCl_4 induced hepatotoxicity

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Liver is the largest internal organ in the body that performs the normal metabolic homeostasis of the body as well as detoxification and excretion and environmental chemical. Herbal treatments are the most popular form of traditional medicine. Plants and natural products have been used traditionally worldwide for the prevention and treatment of liver disease. Leaves of Green tulsi (Ocimum sanctum) belonging to family Lamiaceae are used traditionally for their hepatoprotective effect. These compounds are likely to be used in remedies for stomach disorders, inflammation, antiseptic, anti-catarrhal, heart disease, various form of poisoning and malaria. This present study revealed that leave extract of Ocimum sanctum are incredibly effective against paracetamol, lead and CCl4 hepatic injury causing drugs. The AST, ALT and ALP (p<0.001) liver function test value showed the positive heptatoprotective effect of Ocimum Sancutum compared to standard silymarin. The comparison of this study gave the hepatoprotective activity of alcoholic leave extract and will encourage the researchers to research natural product as these natural medicines are safe, easily available as compared to synthetic drugs.

Comparative Study of Synthesis Techniques of $BaTiO_3$

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Dielectric barium titanate nanoparticles are essential to develop reliable microelectronic devices. BaTiO3 nanoparticles were developed by various synthesis methods seeking to compare and evaluate their crystal structure, size and homogeneity. Synthesis were carried out by six distinct synthesis method including polymeric precursor (pechini), electrochemical, hydrothermal, microwave-assisted hydrothermal, ultrasonic assisted and sol-precipitation route. The phase composition, functional groups and morphology of synthesized nanoparticles were characterized using XRD, FTIR, TEM and SEM. TEM indicated the morphology of barium titinate nanoparticles as a mono dispersed bowl like structure in size range of 15nm. XRD and FTIR revealed cubic structure of Ba TiO3. Pechini method showed the smaller particles than any other method about 15nm. By electrochemical synthesis and sol precipitation route nanoparticles of size 20nm were obtained. By ultrasonic method 18.18nm size of nanoparticles obtained. Size of about 16nm was obtained by microwave assisted hydrothermal synthesis as compared to hydrothermal synthesis where particle size of 60nm was obtained. All the synthesis methods were effective to synthesize crystalline BaTiO3 nanoparticle with size and structural characteristics. Thus the choice of the suitable method of synthesis will depend on the desired properties of the Ba TiO3 nanoparticles.

Comparative Study of Hepatoprotective Effect Solanum Xanthocarpum Leaf Extract

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Solanum xanthocarpum belongs to family Solanaceae, commonly found in Asia and used to treat cough, bronchial asthma and fever. Hepatoprotective activity of Solanum xanthocarpum on experimental rats were checked, whose livers were injured by CCl4 and paracetamol. Comparative study evaluated the hepatoprotective potential against acute liver damage in experimental rats. CCI4 (1ml/kg) induced hepatotoxicilty in five groups of rats. S. xanthocarpum leaves extract administrated in five groups of rats with dose ranges (100, 200mg/kg) and (100, 200, 400mg/kg) in infected rats for 14 days respectively. In another method, paracetamol induced toxicity in liver of rats and after S. xanthocarpum extract given in dose range (200,400mg/kg) along with silymarin in five group of rats. Hepatoprotective activity was checked by using biochemical parameters such as aspartate aminotransferase (AST), alanine aminotransferase (ALT) and alkaline phosphate (ALP) total bilirubin. Doses level inhibit toxicity and protect against liver injury. Comparative study of research papers demonstrate that S xanthocarpum significantly reduced the lipid peroxidation in the liver tissues and its antioxidant activity scavenged the free radicals and restore the activities of antioxidant enzymes GSH, SOD and catalase towards normal levels and proteins and bilirubin. Histopathology of liver tissues represent reduced inflammatory cells and hepatocellular necrosis.

Comparison of Pb-Free Cu Front Electrode Si-Based Solar Cell

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Improved materials can result in manufacturing silicon-based solar cells at lower cost. Photocurrent from the Si emitter in a typical silicon based solar cell is usually collected with a front-side Ag electrode, which is mostly fabricated with low cost screen printing and rapid thermal processing. However, this is not favorable because of two issues. One is high cost due to silver metal, another is the glass containing Pb which causes serious environmental pollution, it will be more desirable to take Pb out of the content of solar cells. We have compared different researches to established copper front electrode Si base solar cell, because Copper easily oxidize in air atmosphere. The comparison study explain copper front electrode Si base solar cell. Cu paste, designed for making low cost electrodes. These paste printed on screen printing method. This process gives products more environmentally friendly and long term stability of silico solar cells with copper front electrode. SEM imaging used to investigate the structure of the front electrode. TEM cross-section imaging used to investigate reactions close to the interface. EDS used to investigate the reduction. The cells with diffusion barrier donâ€™t show any degradation. Comparison of cell and module results indicate that fast degradation on hot plates at cell level gives a reasonable first estimate regarding cell degradation due to copper diffusion. The method given by Kraft was found best.

Extraction and Characterization of Pectin from Orange Peels

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Present study focused on the potential of citrus peel as a source of pectin. In order to increase profits for citrus orange growers and processors, citrus orange peels, a by-product of citrus orange processing, were investigated as a source of pectin. Pectin was extracted from orange peel powder using two different acids (citric acid and nitric acid) and at three different temperature, time and pH via (60Â°, 70Â° & 80 Â°C), (1.5, & 2.5 pH) respectively. Pectin yield extracted by using citric acid and nitric acid as reagents medium was varied from 22.5 % to 25.9% and 19.6% to 23.8% respectively. The best extraction condition by both the extraction reagents showed higher in yield by using citric acid at 80 Â°C and 1.5 pH. The degree of esterification of extracted pectin showed low Methoxyl pectin. The ash and moisture content of isolated pectin were also determined. Pectin is a natural product and it has long been used for its gel formation, thickening and stabilizing properties in a wide range of applications from food to the pharmaceutical and cosmetic industries.

Comparison of Hepatoprotective Effect of *Sida Cordata* (Family *Malvaceae*) Plant Extract on Rats

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Sida cordata (family Malvaceae) is native species of Brazilian north east known as Bala. The plant is distributed along with other species of this genus throughout the tropical and sub-tropical plains of India. The roots, leaves, stem, and seed are used in folk medicine as anti-inflammatory, anti-diabetic and hypoglycemic activity. This comparative study revealed that Sida cordata is incredibly effective against many diseases. The plant extract was tested for hepatoprotective activity using Soxhlet extraction apparatus and semi autoanalyzer were used for parameter testing. Earlier phytochemical studies have demonstrated the presence of fatty oils, steroids, resin, and potassium nitrate in plant. Toxicity studies and antidiabetic activity of methanol extract on roots were reported. The methanolic extract and aqueous extract showed that S. cordifolia showed incredible effect on glucose level and as well as on body weight. The comparison of this study will encourage the scientist to return their research to natural products as these natural medicines are safe, easily available and affordable as compared to synthetic drugs

Microwave-Induced Ecofriendly Synthesis of Isoxazolines in Aqueous Media

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The synthesis of organic molecules in water is a challenging task and continues to attract wide attention among synthetic chemists [1]. Isoxazolines are five-membered heterocyclic compounds that have gained much attention in medicinal chemistry due to vast biological profile [2]. In this work, new derivatives of isoxazolines were designed and synthesized via multi-component 1,3 dipolar cycloaddition reactions in aqueous medium under microwave conditions catalyzed by brÃ–nsted acid. These conditions provide green approach due to environmentally benign nature of the reaction. The results showed high yields in shorter reaction time which reveal efficiency, simplicity, easy work-up, achieved by this protocol. All prepared compounds were confirmed by spectroscopic techniques.

Comparative Study of Anticancer Effect of Potentized Homeopathic Drug, *Lycopodium Clavatum*

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Cancer is a disease that requires miscellaneous approaches of treatment. Cervical cancer is considered as third common type of cancer having few or no symptoms until it reaches to an advance stage. The famous treatments are chemotherapy and radiotherapy. Homeopathy is an alternative therapy. In the present paper comparative study of anticancer effect of Lycopodium clavatum was examined. Lycopodium clavatum commonly known as club moss is a member of Lycopodiacea family is of great importance and considered as an important constituent of traditional medicine used for treatment of various diseases. Crude ethanolic extract of the spores of Lycopodium clavatum have been shown to have anti-carcinogenic effect. Cells were exposed to either LC-5C or LC-15C and changes were analyzed by using different experimental assays. MTT assay was examined after exposure to LC-5C and LC-15C for the viability of HeLa cells. The proliferation of HeLa cells decreased with an increase in concentration of LC-5C and LC-15C. Apoptosis induction in cancer cells by highly diluted dynamized homeopathic remediesLC-5C and LC-15C shows their possible use as supportive medicine in cancer treatment. An overall analysis of results shows that Lycopodine considerably inhibit the growth of HeLa cells and thus have significant role in cancer therapy.

Isolation and Separation of Sesquiterpenoids Fromcannabis Sativa Essential Oil and Their Effects on Carbon-Tetrachloride Induced Liver Fibrosis Model in Rats

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Hepatoprotective activity of Cannabis sativa(Hemp) essential oil was studied using a carbon tetrachloride induced liver fibrosis model in rats. The hepatotoxicity produced by chronic carbon tetrachloride administration was found to be inhibited by Cannabis sativaessential oil with evidence of decreased levels of serum aspartate aminotransferase, alanine aminotransferase, alkaline phosphatase and bilirubin. Histopathological findings also suggest that Cannabis sativaessential oil prevents the development of chronic liver damage. The changes in body weights in the rats assigned to the study groups supported these biochemical and histopathological findings. The results of this study clearly indicate that Cannabis sativaessential oil has a potent hepatoprotective action against carbon tetrachloride-induced liver fibrosis in rats.

Synthesis of *Capsicum Annum L* capped Gold Nanoparticles and their Application in Sensor

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Owing to the importance of metallic nanoparticles, different research studies have been performed to synthesize these nanoparticles in several ways. One of the ways that paid great attention is the green synthesis method of nanoparticles or the ’’eco-friendly methods’’. The most common sources that have been used for green fabrication of nanoparticles are extracts of plants, leaves, fungi and microorganisms. Green synthetic methods are cheaper, environmentally sustainable, and can lead to the fabrication of Nano objects with controlled size and shape. In the present study, AuNPs were synthesized by using green bell pepper or Shimla Mirach extract as reducing as well as capping agent after mixing with aqueous HAuCl4 as precursor and NaOH used as accelerating agent to speed up the reaction. Synthesized gold nanoparticles were confirmed through the color change from yellow to ruby red. The optimization study included a range of parameters such as concentration of plant extract, sodium hydroxide, chloroauric acid and pH of solution in order to obtain blue shifted spectrum. The surface Plasmon resonance band was controlled at 519 nm. The synthesized gold nanoparticles were characterized by UV/Vis spectroscopy, FT-IR, AFM, ZPA and DLS to check the stability, morphology, crystallinity and size of nanoparticles. Synthesized nanoparticles were successfully applied as colorimetric sensor for detection of selected metal ion Fe2+. The linear range of Ferrous ion was 3.3-8 ppb based on increase in absorption intensity with R2 value of 0.987 using UV-Vis spectrophotometer. The sensor was successfully applied to real water samples regarding the detection of Fe2+.

Green Synthesis of Gold Nanoparticles and Their Detection of Metal Ion through Water Samples

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In present work, we have explored a simple, sensitive, rapid and highly practical colorimetric method has been proposed for detection of chromium ion by Ziziphous mauritiana capped gold nanoparticles (ZM-AuNPs). To achieve stable and small size nanoparticles parameters were optimized such as concentration of salt, concentration of extract, pH study (3-11), temperature (10-80 min) after optimization final stable particles were obtained at surface plasmon absorption band was centered at 524 nm with ruby red color. Synthesized gold nanoparticles were characterized via different sophisticated analytical techniques such as UV-Vis spectra, Transmission Electron microscopy (TEM), Atomic Force microscopy (AFM), Fourier Transform infrared spectroscopy (FT-IR), X-Ray Diffractrometry (XRD) in order to check morphology, size and crystalline nature of nanoparticles. The colorimetric sensing ability of ZM-AuNPs was investigated by addition of various metals ions such as Cu2+, Co2+, Mg2+, and Hg2+ etc. in aqueous medium. Among the tested metal ions, addition of Cr3+ showed appreciable red-shift in the SPR band from 524 nm to 580 nm and different color change of the AuNPs solution from red to purplish blue. Addition of other metal ions showed no noticeable color and spectral changes under similar conditions. This highly selective and sensitive sensor allowed for the direct assay of chromium ion shows the good correlation of coefficient value (R2) of 0.995 with limit of detection 8.21 nM and limit of quantification 27.3 nM respectively. Besides, selective detection of trace Cr (III) in aqueous solution in the presence of other transition metal ions has been achieved. Keywords: Gold nanoparticles Chromium, Real water Samples

Comparison of Nanofibrillated Cellulose and Copper Nanoparticles with their Antibacterial and Antimicrobial Activity

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In this study cellulose coated copper (Cu) nanoparticles were prepared. Morphology and structure of these nanocomposite films were characterized with thermogravimetric analysis (TGA), X-ray diffraction (XRD), atomic force microscopy (AFM), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). The regular crystallite size for Cu, assessed from both scanning electron microscopy (SEM) and X-ray diffraction (XRD), was of the order of 17.23 nm. Antimicrobial analysis manifest that up to 5-log microbial reduction results as one-week exposure of nonpathogenic E. coli DH5α to the nanocomposite films. Cellulose-templated Cu-NP material showed efficient Antibacterial properties, which were tested with Staphylococcus aureus (Gram positive) and Escherichia coli (Gram negative) bacterial strains. The diverse application of copper-based nanocomposites and hybrid materials outcomes in that copper nanoparticles and ions can be released into the atmosphere. Cu-nanoparticles coated Cellulose films can be considered as potential materials as they act as biocide in medical and related fields.

Selection of Suitable Stabilizer for the Preparation of Terminalia Arjuna Nanosuspension and Evaluation of its Dissolution Potential

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The study was intended to select a suitable stabilizer to formulate Terminalia arjuna nanosuspension with best physical stability and with minimum particle size to provide better dissolution potential. To select a suitable stabilizer for the optimum synthesis of nanosuspension, six different stabilizers namely PVA, PVP, HPMC, polysorbate 80, PEG-400 and SLS were screened. To formulate nanosuspensions, 0.25g plant extract, 1.0% stabilizer solution and antisolvent-to-solvent ratio of 10 was used. The parameters like physical stability, particle size, polydispersity index and zeta potential values of all the prepared nanosuspensions were determined. The dissolution potential of the best formulated nanosuspension was determined with respect to coarse extract. All the nanosuspensions of T. arjuna showed good physical stability when freshly prepared. The particle size of all the prepared nanosuspension was in the range of pharmaceutical nanosuspension except for HPMC which showed particle size of 724.1nm. The nanosuspension prepared by using polysorbate-80 showed overall good results with particle size of 124.1nm, PDI value of 0.253 and zeta potential of -27.6mV. The formulated nanosuspension showed 1.77-fold higher dissolution potential than the coarse extract which clearly illustrated that nanotechnology can be used as a promising approach to enhance the dissolution potential of herbal extracts.

Modification on the Pyrazolic Core to Synthesize Novel Diazolic Conjugates with Antioxidant Activity

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Pyrazole, belongs to the diazolic family of heterocycles, is one of the most significant pharmacophores which found in a variety of pharmacologically potent agents. Similarly, imidazole ring is another diazolic molecule which is the fundamental constituent of biologically important natural molecules (histidine, histamine, alkaloids) and of synthetic drugs as well. As literature revealed multifaceted therapeutic potentials of these organic motifs, hence, the present work was designed to synthesize imidazole-pyrazole conjugates which may have better synergistic biological activity effects. A convergent, one-pot multicomponent synthetic approach was adopted which conveniently lead to imidazolylpyrazole hybrids. The synthesized novel compounds 2(a-h) were evaluated by 1H NMR and mass spectroscopic data. Afterwards, these molecules were screened for their in vitro antioxidant potentials by DPPH assay. All of the derivatives have displayed moderate to good DPPH radical scavenging activity however nitro group substituted derivative 2a, with IC50 16.50Â±1.02, was found to be the most active antioxidant compound among the series.

Design and Performance Evaluation of Dye-Sensitized Solar Cells using Cu/rGO/TiO2 Nanoparticles

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Renewable energy resources play an important role in the global increase of energy demand. This research have been performed to enhance the efficiency of Plasmonic DSSCs by harvesting the maximum sunlight. In this research, a nanocomposite of rGO, Cu and TiO2 Nanoparticles have been used to fabricate the Plasmonic Dye sensitized solar cells (PDSSCâ€™s). Furthermore, simple DSSC with TiO2 and PDSSC with rGO/Cu/TiO2 have been synthesized by using the sol gel techniques. The rGO/Cu/TiO2 nanocomposite have enhance the efficiency of PDSSCs due to the Plasmonic effect. Different equipmentâ€™s such as EDX, scanning electron microscope (SEM) have been utilized for the analysis of samples. XRD and UV-Vis spectroscopy technique used for crystallite size and micro strain, texture orientation. Due to limited resources of fossil fuels it is necessary to find out other ways for utilization of renewable energy sources. Although DSSCs are widely used in solar energy applications the performance of these cells is low. Transformation of the electron is necessary to achieve high conversion efficiency. Efficiency can be increased by increasing optical absorption. Furthermore, higher efficiency can also be obtained by increasing electron injection by minimizing the large band difference between TiO2 layers.

Maceration Mediated Extraction of Essential Oil from Hemp Leaves

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The essential oils (Eos) find their applications in food, chemical, perfume, medicine, and pharmaceutical industries. The EOs being present in plants are extracted by variety of extraction solvents using different techniques, however majority of these offer limited recovery rates because the extraction solvent may not be efficiently distributed over the sample matrix. The present research work was planned to apply the maceration power of least hazardous surfactant (Triton-x 100) to macerate Hemp (Cannabis sativa L.) leaves for the enhanced recovery of essential oils. For this purpose, the hemp leaves were treated with different concentration of Triton X-100 and NaCl under various liquid to solid ratio and time to extract essential oil by hydro-distillation. It was observed that hemp leaves when macerated with 1.0 % Triton X 100, 2.0 % NaCl at L/S of 8.0 and processed for 10 hours of hydro distillation offered 176 mL of essential oil. The extracted essential oil was analyzed for in-vitro antioxidant characteristics. It was observed that oil produced via maceration mediated hydro distillation contains constituents of high antioxidant activities.

Ionic Based Liquid Extraction for Essential Oils from Black Pepper

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Essential oils belong to the volatile class of plant bioactives used in food, fragrance, cosmetic, and pharmaceutical industries. A great deal of research has been devoted for the extraction of essential oils from plant sources. In present research, ionic liquids are used for extracting essential oil from black pepper. Black pepper collected from local market of Lahore, was ground to fine powder and processed via hydro distillation method using Clevenger tube. The extraction parameters like incubation time, ionic liquid composition (Quantity of Acetic acid (ml) and Glucose (ml)), and L/S ratio were varied, and optimum conditions were evaluated. Maximum yield (135-140 ml) was obtained by using this method corresponding to conditions: Acetic acid 25-35ml, Glucose 65-75ml, incubation time of 4-5h and L/S ratio of 5-6. All the reactions were carried out by taking 20g of black pepper powder, at 90oC and 150 rmp at hot plate. Essential oils were measured for their antioxidant activities by Trolox Equivalent Antioxidant capacity (TEAC) and Free radical scavenging Capacity.

Synthesis of Green Nanoparticles and Their Application for Colored Wastewater Remediation

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Industrial dyes are the major part of environmental pollution. The novelty of this work is the extract of three plants Fan palm (F.P), Dombiya willaichi (D.W) and Pyrus cumminies (P.C) were used as reducing agent to prepare Iron nanoparticles (F.P/FeO, D.W/FeO and P.C/FeO). To check the optimum conditions for the elimination of anionic dye from waste water various investigational constraints like pH, dose, contact time, initial dye concentration and temperature were studied. The utmost pH for reactive blue dye was detected in acidic value series 3, whereas 0.01/50mL biosorbent dose F.P/FeO, D.W/FeO and P.C/FeO found as utmost dose for removal of anionic dye. The preliminary concentration of dye in the range of 20-200 mg/L was measured as finest for gaining the highest exclusion of anionic dye by various kind of chosen biosorbents. The best removal was achieved at 200mg/L. The best temperature to get extreme subtraction of chosen anionic dyes were detected at 65ÂºC and lessening in biosorption ability of all bio sorbents was examined by the reduction in temperature. SEM and FTIR were used to characterize the nanoparticles which gave info about the morphology and functional groups on dyes.

Electronic, Magnetic, Thermoelectric and Elastic Properties of the Cubic Perovskite $YFeO_3$ by Using PBE-Sol Approximation

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The full potential linearized augmented plane wave (FP-LAPW) method used for first principles calculations of the electronic, magnetic, thermoelectric and elastic properties of the cubic perovskite YFeO3 by using PBE-sol approximation. The overlapping of highest valence and lowest conductive band gives zero energy band gaps which shows metallic nature of YFeO3. The spin moment of YFeO3 completely contribute to total magnetic moment while contribution of orbital moment is negligible. The total magnetic moment of YFeO3 is about 3 Bohr. Elastic coefficients use to measure the elastic parameters of Poissonâ€™s ratio, youngâ€™s modulus ratio, bulk modulus and shear module. It shows that YFeO3 is brittle, stiffer and covalent in nature .The YFeO3 See beck coefficient is negative at all temperature range. The figure of merit ZT in thermoelectric shows maximum value of 0.030 at room temperature.

Green Synthesis of Substituted Pyrazolines in Deep Eutectic Solvent

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Toxic chemicals and volatile organic solvents are one the major cause of pollution. The possible solution of these problems under lies the use of green solvents like Deep eutectic solvents as they are less volatile, inexpensive, biodegradable [1,2]. In this research, substituted pyrazolines derivatives have been synthesized in deep eutectic solvents. Efficient yield, less time-consuming reaction were obtained by employing deep eutectic solvents and target product were characterized by spectroscopy.

Silica Nanoparticle Polyurethane Membranes for Reverse Osmosis Applications

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Polyurethane (PU) is an exclusive class of polymers with special significance in membrane technology. In this work, a series of pure PU membranes were prepared and then doped with silica nanoparticles (SiNPs). The effect of doping of SiNPs (0.01â€“0.03 wt.%) was investigated in terms of structural, thermal, morphological, antibacterial and permeation properties of PU membranes. The FTIR spectral band at 944cm-1 confirmed the impregnation of SiNPs in PU matrix. The water content measurements revealed improved hydrophilic character of doped membranes. The SEM analyses exposed a uniform dispersion of SiNPs in PU matrix upto 0.02%, while aggregation was perceived at higher content. The PU membranes with highest SiNPs content (0.03%) showed highest thermal stablility. The systematic study of desalination demonstrated the RO capability of prepared membranes. The membrane with 0.02% loading of SiNPs supported for highest salt rejection and water flux at effective pressure of 20bar. Hence, these results recommend the PU membrane doped with 0.02% SiNPs as a promising candidate for reverse osmosis applications.

Synthesis and Characterization of Graphene Oxide Laminates for Separation of Toxic Pollutants from Wastewater

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Membrane technology has attracted an enormous attention for wide range of separation applications in energy and environmental areas due to its high efficiency, low cost and environmentally friendliness. Up to date, various materials have been explored for fabrication of separation membranes, however, could not get success due to several drawbacks associated with these membranes. Recently, graphene oxide (GO) a functional derivative of graphene has exhibit great potential to replace these materials due to its supreme properties such as two-dimensional structure, good chemical and mechanical stabilities, and high antifouling. Herein, we prepared GO-based lamellar membranes from GO and ginger (Zingiber officinale) plant extractive by using vacuum filtration method. The prepared membranes exhibited an excellent separation performance with 90% rejection for rhodamine B and methylene blue dyes with pure water permeability of 110 lm-2h-1bar-1. Further, these membranes are stable under aqueous environment for more than 10 days.

Fabrication of Highly Efficient Reduced Graphene Oxide-Based Nanocomposite Membranes for Water Purification

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With the increasing demand for clean water, filtration technology has been widely explored in wastewater treatment applications. Recently, graphene oxide (GO) is emerging as one of the most promising nanomaterial for water purification, desalination, and gas separation applications because of its unique properties such as large surface area, single layered structure, interesting functional groups, and high affinity for pollutants. Here, we report a unique class of reduced GO-based membranes with enlarged interlayer distance fabricated by using tyrosine/valine amino acids as reducing agent and cross-linker and polyethylene glycol as a binder. As-prepared membranes will be characterized by using Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscope (SEM) techniques. The membranes showed an outstanding separation efficiency for dyes such as rhodamine B (92%) and methylene blue (90%) with good water permeability. Further, membranes are stable under acidic and basic environments.

Chemical Composition and Bioactivity Studies of Tamarix Dioica Essential Oils

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The current study is based on two parts. In part-1, the essential oil of T. dioica flowers and leaves were isolated by hydrodistillation method and analyzed by GC-MS to determine their chemical composition. Results show that total 24 and 14 constituents were identified. Part-2 of this study is based on qualitative and quantitative evaluation of phenolic acids, total phenolic content, antioxidant potential and antimicrobial activity of various parts of T. dioica extracts. The base hydrolysis extraction method was applied for phenolic acids analysis followed by HPLC-DAD separation technique. Results revealed the gallic acid was found in higher quantity, i.e. 21.86 mg.gâ€“1 and 18.37 mg.gâ€“1 in leaves and flowers extracts, respectively; whereas, caffeic acid was found in higher amount (11.77 mg.gâ€“1) in stem. T. dioica leaves, stem and flowers extracts were used to determine the antibacterial activity by following the disc diffusion method. All the extracts of T. dioica showed good antibacterial activity against E. coli (G -ve) and S. aureus (G +ve). Total phenolic content (Folin-Ciocalteu assay) and antioxidant activity (DPPH assay) were also measured by using UV-Visible spectrophotometer at λmax of 765 nm and 517 nm, respectively.

Coenzyme Q10: Deficiency Determination in Different Stages of Oral Cancer Patients

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Coenzyme Q10 (CoQ10) is a nutrient like fat substance and normally found in the heart, liver, kidneys and pancreas malignant growth is the most well-known strong tumor analyzed in people and is increased with age. Along these lines, present research work is based on the assurance of CoQ10 by applying detailed strategy. HPLC-DAD was utilized for the evaluation of CoQ10 levels. Blood samples were collected from four phases of oral disease persistent (T-1 T-2, T-3 and T-4) from NIMRA clinic LUMHS, Jamshoro during 60 days. Results demonstrate that, CoQ10 in the patients of T-I arrange were found between 0.53-1.26 Âµg/mL and their age range from 42-58 years. While in T-II stage, CoQ10 was found in the range from 0.42-1.07Âµg/mL (age between 33-69 years). T-III phase of oral malignant growth patients show CoQ10 level as 0.17-0.67 Âµg/mL with various ages from 29-68years. T-IV phase of oral disease patients show CoQ10 level as 0.06-0.28 Âµg/mL with various ages from 22-69 years. The required range of CoQ10 is from 0.4-1.7 ug/mL. Control sound people have CoQ10 run from 1.47-1.67 Âµg/mL. In conclusion, as cancer stage increases the level of CoQ10 decreases may be due to the chemotherapy etc treatment of patients.

Self-assembly of Metal Nanoparticles by Base Hydrolyzed Extracts of Bioactive Phenolic Compounds from Wheat Flour and Their Applications

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The purpose of this work is to fabricate and evaluate synthesized metal nano-particles of bioactive phenolic compounds (BPCs) from wheat flour followed by base hydrolysis extraction. The extracted BPCs were identified by using HPLC-DAD. Results shows that about 16 BPCs were identified from which 7 were quantified while 9 were identified as unknown phenolic acid as Unk-1 to UnK-9. The known phenolic acids were identified by their retention time and Uv-spectra, however; unknown phenolic acids were identified by respected Uv-spectra and available literature. Ferulic acid was quantified as major phenolic compound (735.13mg/100g) as compare to remaining phenolic acids. The total phenolic compounds were quantified as (781.93mg/100g). The extracted phenolic compounds were further used for the synthesis of silver nanoparticle. The silver nanoparticle of BCs are prepared by self-assembly method with three variables, including silver nitrate concentration, silver metal to bioactive compounds mass ratio, and pH to obtained blue shifted spectra at 408 nm. The structure and properties of the nanoparticles will be studied by FTIR, SEM, XRD, and AFM. Average size of our synthesized AgNPs was calculated as 23 nm by AFM Analysis. These Nanoparticles of Ag will be applied for different purposes such as sensing, catalysis and others.

Oxidative Desulfurization of Model and Real Oil Using Air Oxidation System in the Presence of Transition Metals Supported on Montmorillonite Clay as Catalysts

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In petroleum sulfur compounds are undesirable, because of causing environmental pollution, corrosion problems and catalysts during processing, therefore sulfur compounds should be removed from the petroleum. The current desulfurization technology is hydrodesulfurization which is inadequate in term of economics and efficiency. Oxidative desulfurization is one of the efficient alternative approaches toward desulphurization of petroleum. In the current study, catalytic oxidative desulfurization of model and real oil samples was investigated using H2O2/formic acid and transition metal oxides/ supported on montmorillinite clay as catalysts. The catalysts were prepared in the laboratory and characterization by XRD, EDX and SEM analysis. The catalyst used included Fe2O3/MMT, NiO2/MMT and ZnO/MMT clay. The ODS of model oil was carried out with different catalyst under different temperatures and reaction times. The Fe2O3/MMT clay was found to be most effective catalyst in the current oxidation system, which reduced the sulfur content from 120 ppm to 49 ppm in model oil in 60 min and at 60 oC. Under these conditions the ODS of commercial oil sample was also studied. In case of gasoline, kerosene and diesel oil, the sulfur content was decrease from 25.3 mg/L to 11.7 mg/L,3296.6 mg/L to 2450 mg/L and 3800.53 to 14674.7 mg/L respectively. Key words: Oxidative desulfurization, catalytic desulfurization, pre-impregnated catalysts.

Synthesis and Anti-Inflamatory Profile of Structurally Diversified 3, 5 – Disubstituted – Tetrahydro –2h –1, 3, 5 –Thiadiazine–2–Thiones

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A series of 3, 5-disubstituted tetrahydro-2H-1, 3, 5-thiadiazine-2-thiones was synthesized by the reaction of various alkyl or aryl amines with potassium hydroxide, carbon disulfide, formaldehyde and different amino acids. These structures were elucidated by spectral methods (IR, NMR and Mass spectra). The synthesized compounds were evaluated for their anti-inflammatory potential. The antimicrobial potential of these compounds was also investigated against bacterial strain including; Escherichia coli and fungal strains including; Aspergillus niger all these compounds showed significant activity. Their structure activity relationship showed that substitution at N-3 and N-5 position play key role.

Synthesis of 3, 5–Disubstituted–Tetrahydro –2*h* –1,3,5–Thiadiazine–2– Thiones Derivatives and Their Metal Complexes in Search of Potential Bioactive Agents

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Thiadiazine-2-thiones derivatives was synthesized and these compounds have been prepared by the reaction of various alkyl/aryl primary amines with carbon disulfide, potassium hydroxide followed by addition of formaldehyde and different another primary amines in phosphate buffer medium. The synthesized compounds was transformed into organometallic complexes using Ni(II), Co(II), Cu(II), Zn(II), Fe(II) metal salts. The determination of these compounds was elucidated by spectral methods (IR, NMR and Mass spectra). Their structure activity relationship showed that position 3 and 5 substituents have a key role against leishmanicidal activity. The antimicrobial activities of these compounds were screen against some bacteria and fungi. Keywords: Thiadiazine thione derivatives, Biological activities.

Kinetic of the Pyrolysis of Pomegrante Peels in the Presence of Sulfonated-Derived Tea Waste-Heterogeneous Catalyst

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The present study is focused on the production of bio-oil from pomegranate peel using pyrolysis gas chromatography mass spectrometry. Experiments were carried out in a Pyrex vessel in presence/absence of a sulfonated-derived tea waste-heterogeneous catalyst under inert conditions in an indigenously made furnace in the temperature range 500-750K. The pyrolysis oil was collected and analyzed by GC-MS and FTIR. Fuel properties of the oil were determined and compared with commercial fuel.The results indicates that the pomegranate waste can be utilized as fuel if the oil obtained from it is properly upgraded to make it equivalent to commercial fuel. Furthermore, thermogravimetric analysis of pomegranates sample was conducted in inert atmosphere at heating rate of 5,10,15,20? /min in the temperature range of 30 to 600 in presence and absence of catalyst. Kinetic parameters were calculated applying Cost-Redfern and Ozawa Flynn Wall methods. The results confirmed that the catalyst used has not only decreased the degradation temperature but also resulted in reduction in activation energy of the pyrolysis reaction.

Solvent Free Synthesis of Asymmetrical Pyridine Derivatives

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The core nucleus of Pyridine is one of the imperative part of medicinal chemistry and used as AKT inhibitors [1,2]. Among organic ligands, asymmetrical pyridines have a significant place and are popular to serve as pincers in catalysis [3]. In this research, new asymmetrical pyridine analogues have been synthesized using aldehyde, ketones and ammonium acetate in solvent free conditions with good yield and short time. The structure confirmation was achieved by FTIR, 1HNMR and elemental analyses

Stereoselective Synthesis of Spiro-fused Pyrazolines

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Spiro-fused pyrazolines are nitrogen bearing heterocycles that offers feasibility to construct structurally relevant spiro analogues for the better exploration of potential biological properties particularly as anti-inflammatory agents [1,2]. In the present work,spiro-fused-pyrazolines were synthesized by 1,3-dipolar cycloaddition of aryldiene-chromanones and hydrazine derivatives with the help of microwave which results in dramatic reduction in reaction time and increased yield. The target compounds were characterized1H and 13C NMR spectroscopy and provide the stereochemistry was established by mechanistic insight.

Synthesis of chitosan zinc sulfide nanoparticles for the photocatalytic degradation of acid black 234 and acid brown 98

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The photocatalytic efficiency of chitosan zinc sulfide (CS-ZnS) nanoparticles have been evaluated using anionic carcinogenic azo dyes, Acid Black 234 and Acid Brown 98. Nanoparticles were successfully synthesized in the aqueous solution through co-precipitation method. The successful synthesis was validated by analyzing through FTIR spectroscopy. SEM evaluation showed that the average particle size obtained from SEM images is found out to be 40nm. The EDS analysis were used to interpret the composition of the nanoparticles. XRD analysis illustrated the crystallinity and hexagonal crystal structure of the CS-ZnS nanoparticles. The photocatalytic deterioration of dyes was assessed using UV lamp (254nm) as an irradiation source. The CS-ZnS nanoparticles showed 96% of discoloration at optimum conditions under UV lamp for Acid Black 234 in 100min and 84.4% for Acid Brown 98 in 165min. The degradation phenomena followed the first order kinetics. Therefore CS-ZnS nanoparticles are considered as a highly productive, cost effective and auspicious catalyst in degrading pollutants and are effectively used up to four cycles of degradation. Keywords: Photocatalysis, Acid Black 234, Acid Brown 98, Chitosan-zinc sulfide

Computational Chemistry

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OBJECTIVE: The aim of this pilot study is to retrieve structural information through theoretical methods and highlight I.R spectrophotometric confirmation of 2,4diBromo Aniline/benzene amine. METHODOLOGY: Density function theory approach with the assistance of computational simulating. In the next step its possible toxicity effects on human skin is calculated through QSAR (Quantitative structureâ€“activity relationship modelling) method. Four different types of cell lines are applied. Three different oral toxicity predictions, RESULTS: The aforementioned aniline is class 4 according to Globally Harmonised System. After obtain theoretical results, we will able to suggest that the mentioned molecule is not suitable for cosmetic and food items manufacturing. The I.R spectrogram of 1,2,4 tri substrate results are compiled in a comprehensive way to conform structure. CONCLUSION: The mentioned organic precursor molecule is not safe for humans use.

Synthesis of Thiadiazine-2-Thiones and Their Derivatives

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A series of Thiadiazine-2-thiones and their derivatives were synthesized by the reaction of various primary amines with carbon disulfide, potassium hydroxide, formaldehyde and different another primary amines. The determination of these compounds was elucidated by spectral methods (XRD, IR, NMR and Mass spectra). Their structure activity relationship showed that position 3 and 5 substituents have a key role against leishmanicidal activity. Besides anti-leishmenial activity these compounds also showed anti-inflammatory activity. The antimicrobial activities of these compounds were screening against some bacteria and fungi. Keywords: Thiadiazine thione derivatives, Biological activities.

Solar Photocatalytic Degradation of a Real Textile Wastewater using $CuCo_2O_4$ Nanocomposite

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Among the countless blessings water is the most precious gift of nature for creature. Among the various negative impacts regarding to the increase of population is the shortage of natural water resources. The industrial wastewater has become a leading source of water pollution due to diverse nature of pollutants present in the effluents which are hazardous and toxic. Present study is focused on the heterogeneous photocatalytic degradation of dye (Black RRC) by CuCo2O4 nanocomposite. Highly crystalline spinel CuCo2O4 nanocomposite over metal beads at 500 Â°C were grafted by spray pyrolysis method, confirmed by X-ray diffraction pattern, Fourier transform infrared spectroscopy, energy dispersive X-ray and scanning electron microscopy. The photocatalytic degradation efficiency of CuCo2O4 nanocomposite was evaluated by studying degradation and mineralization of dye Black RRC. Maximum photocatalytic degradtion (94%) of dye Black RRC using CuCo2O4 nanocomposite was achieved at neutral pH with in 180 minutes of exposure to sunlight. The independent variables such as irradition time, pH, concentration of H2O2 and conentration of dye Black RRC were optimized using response surface methodology for maximum degradaition of pollutant. Effective degradation of dye Black RRC through CuCo2O4 nanocomposite is confirmed by disappearance of characteristics UV peaks of dye Black RRC in the range of 595 nm wavelength after treatment with CuCo2O4 nanocomposite further confirmed effective degradation. After treatment % reduction in water quality parameters were COD (85%), BOD (80%) and TOC (80%) and textile effluents containing nonionic surfactants can be reused for industrial and agriculture purpose since the water quality parameters showed their values within the permissible limit.

Microwave Accelerated Synthesis of Thiazoles

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Energy conservation prevent pollution, thus one of the green chemistry pathway. Microwave assisted organic synthesis (MAOS) is one of the energy saving method that cost less amount of electricity. While conventional heating method is not only time consuming but also expensive. Thiazole derivatives have become significant in past few decades as they serve as a subunit for synthesis of new bioactive compounds. Inspired by these facts, aryl ketone and amide derivatives are deployed for synthesis of thiazole derivatives in microwave. It was observed that MAOS was better and rapid approach towards synthesis of target molecules as compare to conventional method. All compounds were characterized by FTIR, 1H NMR spectroscopy and elemental analyses.

Transition Metal-based Solid Support Catalyst: Application in N-Heterocyclic Compound Synthesis

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N-Heterocyclic compounds such as sulphonamides, indole, 1,4-dihydropyridines scaffolds etc. serve as core structure in the synthesis of new bioactive molecular entities. The potential therapeutic agents serve as drug molecule against bacterial infection, viral diseases, cancer, inflammation etc [1]. The project aim to to synthesize novel heterocycles containing sulphonamides, indole and 1,4-dihydropyridines moieties by using metal salts based solid support catalyst. Heterogenous catalyst systems attracts the chemists by providing green and efficient method for the synthesis of chemical libraries that exhibits potential biological activities [2]. Moreover, solid support catalyst aids in catalyst recovery and minimizing pollution. Elucidation of the structure of synthesized compounds by using analytical and spectroscopic techniques such as UV-Vis absorption, fluorescence, mass spectrometry and NMR spectroscopy. In addition, the synthesized functional molecules will be screened for their biological potential to find lead as potential drug candidates.

Synthesis of Metal Sulphide Nanomaterials and its applications

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Nanoparticles are particles that exist on a nanometre scale below 100 nm in at least one dimension. They can possess physical properties such as uniformity, conductance or special optical properties that make them desirable in material science and biology. Metal sulphides have been recognized as advanced materials for many applications including catalyst and sensor materials. Nanoparticles have significant potential for these applications due to their small size, high-surface area and low sintering temperatures. Recent years, a number of studies have been carried out to develop methods for synthesizing sulphide nanoparticle. Nano sized zinc sulfide, were successfully synthesized via a simple chemical hydrothermal method.

Synthesized nanoparticles were confirmed by different analytical technique like SEM, TEM, XRD, FTIR, and UV-VISIBLE Spectroscopy. To check the catalytic activity of particles were applied to degrade rhodamine B dye as model reaction. Rhodamine B (RhB) is widely used in industrial purposes, such as printing and dyeing in textile, paper, paints, leathers etc. However, the organic dyes will cause serious environmental and biological problems, even capable to induce irritation to the skin, eyes. Thus, the removal of dye from water is a great challenge and task. Therefore, synthesized nanoparticles were used for the degradation of Rhodamine B by economic, simple and environmental friendly method.

Comparison of Synthesis and Oxygen Sensing Properties of Zinc Oxide Nanorods

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This paper is a comparison of the synthesis of one-dimensional zinc oxide (ZnO) nanostructures and oxygen gas sensing properties are also studied due to the influence of their morphology. ZnO structures were synthesized through CVD, sol-gel and hydrothermal processes. Samples were structurally characterized through X-ray diffraction (XRD) as well as field emission SEM methods. This paper is offerings the unique ultraviolet (UV) irradiation supported nanostructured ZnO film for extraordinary oxygen sensing performance at low process temperature. The method used in current study delivers simplest yet high performance technique for the oxygen sensing in low process temperatures. ZnO nanorods sensing layer that is supported with UV radiation give 419% response in contrast the sensing layer in the absence of UV irradiation give only 74% response. On other hand, the vertically aligned ZnO nanorod arrays are grown hydrothermally as well as they are very favorable for production of the high performance and cost effective oxygen gas sensors.

Preparation and Applications of Solid Support Silica as Catalyst

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Organic Solvents were found to be hazardous due to their toxic and flammable nature since their discovery. Hence, there is a growing need for more environment safe techniques for the chemical transformations. For this purpose, highly efficient and eco-friendly solvent free approach comes up as a solution. In this research work, Bronsted acid impregnated with silica support catalysts were prepared conventionally and characterized. After structure confirmation of catalyst, metal-free solid support catalyzed synthesis of new Imidazole and pyrazoline analogues has been proficiently carried out with respect to yield and time. The target compounds were also validated with the help of FTIR and 1HNMR.

Desulfurization of Transportation Fuel

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Desulfurization of model oil using composites of Zn/hydroxyapatite and activated carbon Taj Muhammad, Waqas Ahmad Institute of Chemical Sciences, University of Peshawar, 25120, KPK, Pakistan Abstract In the present study, composites of Activated carbon (AC) and Zn impregnated on Hydroxyapatite (Zn/HAP) were prepared in different weight ratios, including 75:25, 50:50 and 25:75 % respectively. The composite materials were characterized by FTIR, XRD, EDX and SEM analysis. The composites were employed as catalyst and as adsorbent in separate and simultaneous oxidative and adsorptive desulfurization of model oil. Results indicated that, in case of sole adsorption and oxidation experiments maximum sulfur removal of 97 %, was attained with AC:Zn/HAP composites. The optimum conditions for maximum removal of sulfur in simultaneous desulfurization experiments was found at 45 Â°C in 60 minutes reaction time, 0.2 g composite dose. Keywords: Oxidative desulfurization (ODS); oxidation; hydroxyapatite; composites of activated carbon

Synthesis Of 3,5-disubstituted Tetrahydro-2H-1,3,5-Thiadiazine-2-Thiones their Antimicrobial and Anti-Inflamatory Activities.

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Herein, a series of biologically active thiadiazine-2-thione nucleus were synthesized by the reaction of three different primary amines with carbon disulfide, followed by cyclocondensation with formaldehyde and hydrazine in buffer medium. The synthesized THTT, were further functionally modified in search of potential bioactive nucleus. All the synthesized compounds were characterized with the help of spectroscopic techniques including FTIR, Hâ€™NMR and mass spectra. The synthesized compounds were investigated for antimicrobial and antioxidant activities and were found active. Keywords: Thiadiazine-2- thione derivatives, Biological activities.

Synthesis and Leishminacidal Potential Evaluvation of 5-(Arylideneamino)-3-(2-Alkyl/Aryl)-1, 3, 5-Thiadiazine-2-Thiones

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A series of 5-(Arylideneamino)-3-(2-Alkyl/Aryl)-1,3,5-Thiadiazine-2-thiones was synthesized. These compounds have been prepared by the reaction of thiadiazine-2-thiones with various aldehydes. The confirmation of these compounds was elucidated by spectral methods (IR, NMR and Mass spectra). All these compounds showed significant antileishmanial activity. Their structure activity relationship showed that N3 and N5 substituents have a key role against leishmanicidal activity.

Desulfurization and Demineralization of Pakistani Coal by Catalytic Air Assisted Performic Acid Oxidation System

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Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬Â¬ Huge reserves of coal are available all across the globe. Due to dwindling supply of petroleum and natural gas reserves coal is the immediate source of energy. Pakistan is home to the world seven largest reserves for coal, however most coals being low rank and rich in sulfur and mineral matter, these cannot be used for power generation and industrial uses. In this study we report the desulfurization and demineralization of Hangu coal by air oxidation system in the presence of co-oxidants and transition metals as catalyst. Coal was oxidized in slurry phase with continuous air bubbled in the presence of co-oxidants (H2O2 and HCOOH). The optimum conditions for maximum removal of sulfur and ash was found to be; temperature 60oC, oxidation time 30min, and H2O2+HCOOH volume (1+1) mL. Under optimized conditions, about 50% of total sulfur and 45% ash was removed from coal sample. In the presence of Fe and Cu catalysts pre-impregnated on coal sample the level of desulfurization and demineralization were increased to 80% and 70% respectively. The process can be scaled up for upgradation of coal for industrial and power generation purposes. This process can attract local industrialist for exploitation of our indigenous coal rather than importing foreign coal and hence a huge foreign exchange can be saved. Key words: Coal upgradation, oxidative desulfurization, deashing, air assisted oxidation, pre-impregnated catalysts.

Synthesis of Polymers for Improved Dielectric Properties

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Flexible PVC/BaTiO3 composites with different volume fractions upto 30% vol% were fabricated in the form of films from (1−2nm) by solution cast method. These composites were Characterize by different techniques such as Impedance analyzer (LCR meter), Fourier transform infrared (FTIR), scanning electron microscopy (SEM) and X-Ray Diffraction (xrd). The effects of different % composition of BaTiO3 ceramic on the morphology and microwave dielectric properties of flexible PVC/BaTiO3 composite films were investigated in detail. The Dielectric constant (εr) and dielectric loss (tanσ) increases and the product of quality factor decreases with increase in the volume fraction of BaTiO3 ceramic. In the present work the experimental results shows that BaTiO3 ceramic improves the dielectric and microwave dielectric properties of Polyvinyl chloride (PVC).

Comparative Study of Ligand- Free Suzuki-Miyaura Coupling Reactions

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The essential tool for the synthesis of C-C bond is the use of Suzuki-Miyaura cross coupling reactions, which is catalyzed by transition metals. The Palladium catalyst was the best among all in past, this catalyst provided green pathway for the fabrication of C-C bond. But now days the C-C bond is being formed by the use of Nickel as a catalyst. Nickel is cheaper than Pd. This catalyst is being used due to its abundance and easily availability. This catalyst has an advantage of being used again and again without loss. It is useful to synthesize poly-olefins, styrenes and biphenyls. The progress in the field of Suzuki-Miyaura cross-coupling reaction, especially with respect to ligand free catalyst is being discussed in studies. Magnificent amount of aryl boronic acid is obtained by cross-coupling of aryl halides with triflates at room temperature by using aqueous media.

Comparison of Supercritical Fluid Process in Nanoparticles Production and Applications

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In production process of pharmaceuticals, nano-particulate form active ingredients is highly desirable but the subsequent product is hard to handle and to apply. So, to overcome this, a novel process is supercritical fluid process used now as rapid expansion of supercritical solution (RESS). In this method supercritical solution having some dissolved constituents is quickly depressurized to ambient pressure through a nozzle. Upon expansion pressure rapidly drop and this high rate of super saturation leads to the precipitation of the dissolved material. Here this (RESS) employed for the production of olanzapine OLZ naoparticles and continuous nanonization of lonidamine by modified-RESS. It is also employed in applications of nano-particle coating to carrier particles. The comparison study of supercritical process gives significant results in the production and application of nanoparticles. Physical characterization of nanoparticles were done with SEM and other spectroscopy techniques. As this process improving the bioavailability of poorly water-soluble drugs for its future pharmaceutical applications.

Recycling of Tanneries Solid Waste for Insulation Products

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Leather industry has great importance in Pakistan due to the large production of leather. It is the second largest export industry as per ranking of Pakistan Bureau of Statistics. Disposing of solid waste is a major problem in leather industry. Skin trimmings, buffing dust, fleshing and chrome shavings are present in the solid waste. Chrome shavings are more dangerous due to the presence of carcinogenic element. Utilization of tanneries solid waste into useful products can solve many social problems. The sample of leather waste was collected from the tanneries of Kasur city. This waste was mixed with plaster of paris to make the insulation boards. Ten boards were developed by using different quantities of waste and plaster of paris. Different physico-chemical tests were applied on them and the board which has maximum thermal conductivity was selected for characterization. FTIR detected the amino groups which are present in proteins of solid waste. These boards can be used for ceiling of buildings. Key words: Tanneries waste, Insulation boards, Physico-chemical tests and Thermal conductivity.

Comparative Study of Synthesis of Silver Nanoparticles and Their Application

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For the synthesis of AgNPs, the development of an environmentally benign process is meant to be important part of current nanotechnology research. Several methods are available for the synthesis of AgNPs that include; Green synthesis using onion extract, synthesis by using leaf extract, Synthesis of AgNPs using Dioscorea bulbifera tuber extract. AgNPs synthesized by these methods were characterized by UV-visible absorption spectroscopy, TEM, high-resolution TEM, EDS, and XRD. By using onion extract, UV-Vis spectroscopy showed that the AgNPs absorption band was located at 397 nm in aqueous solution while it was at 424nm by using leaf extract. TEM and XRD determined the morphology of AgNPs that was spherical in shape having average diameter of 6nm by TEM and 5.3 to 10.2nm by XRD and was triangular and hexagonal according to method 3. According to method 3 the AgNPs were found to possess potent antibacterial activity against both Gram-negative and Gram-positive bacteria. The effect of synthesized NPs by onion extract on ascorbic acid signal was investigated by square wave voltammetry in method 1 and LOD of ascorbic acid was 0.1mM. Ascorbic acid and dopamine were determined by differential pulse voltammetric in method 2 and LOD was 0.085ÂµM for DA.

Comparison of Synthesis of Manganese Oxide Nanoparticles by using Green, Chemical, and Physical Methods

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Synthesis of Manganese oxide nanoparticles by various approaches i.e. green, chemical and physical methods were compared. KMnO 4 , Mn (NO 3) 2 , MnSO 4 .H 2 O and MnCl 2 .4H 2 O were used as a precursor salt for synthesis. Different shapes and sizes were obtained via green, oxidation- precipitation, ultrasonic-hydrolyzation, sol-gel methods along with use of deep eutectic solvent. First method consists of using Justicia adhatoda and MnSO 4 .H 2 O. Nanoparticles were obtained by adding leaf extract solution to precursor solution. In second method, oxidation-precipitation method was used. Mn (NO 3) 2 solution was used into which citric and tartaric acid was added. In third method, MnCl 2 .4H 2 O and ethanol amine were used for synthesis purpose and functioned in ultrasonic field. In fourth method, eutectic solvent was used. KMnO 4 was added to solvent, then stirred, centrifuged, washed and dried to synthesize nanoparticles. In fifth method, nanoparticles were formed by using sol-gel method. In this, reaction between KMnO 4 and glycerol was very fast. Gel was formed. Synthesized nanoparticles were then characterized by different techniques i.e. XRD, SEM, TEM, FT-IR and HR-TEM. Nanoparticles with diameter of ranging between 5- 45 nm were obtained with different morphologies. Efficient synthesis was carried out by using green approach.

Comparison of Antioxidant Activity of Three Different Species of Genus

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Antioxidant capacity is an important parameter for nutritional health food characterization.This comparative study was designed to evaluate the antioxidant activity of three species of genus Mentha.These species were named as Mentha arvensis (Pudina), Mentha piperita (peppermint) and Mentha pulegium (pennyroyal mint). Pervious study shows that plants with their aromatic secondary metabolites have strong antioxidant activities. Phytochemical studies of these species have shown presence of components like terpenoids,flavonoids and alkaloids.The species of this genus are also well known for its antimicrobial and antibacterial activities.Antioxidant activities of these species are measured by DPPH, reducing power and ÃŸ-Carotene/linoleic acid assay method. Mentha arvenis shows strong activity with IC50Â¬~41Âµg/ml as compared to standard antioxidant ascorbic acid with IC~ 19Âµg/ml in ethanolic extract. Mentha piperita have excellent activity as compared to standard BHT (IC50~6.1Â± 0.3) with IC50~15.2 Â± 0.9 in chloroform extract. Mentha pulegium (IC50~95.14Â±0.03) have markable activity close standard BHA (IC50 ~96.46Â±0.17).This present study also shown that following genus Mentha species shows good efficiency against the oxidants like ROS/RNS causing carcinogen effects. .Overall, the comparative study suggest that the members of the genus Mentha used in this study possess exploitable antioxidant properties in vitro.

Synthesis and Characterization of Silver Nanoparticles from Waste Vegetable Extract and Their Antimicrobial Activity

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Nanoparticles as compared to bulk material have unique properties and potential application in different fields due to their distribution, size and morphology. The purpose of this study was the development of eco-friendly method which have several advantages such as recycling of waste material, ease of use and less use of hazardous chemicals over conventional method for synthesis of NPs using vegetable waste extract. Among metals silver has more attention because of its strong antimicrobial properties. The silver nanoparticles (AgNPs) produced by the addition of waste vegetable extract to AgNO3 solution at room temperature. The fabricated NPs were characterized by various techniques such as UV-Visible spectroscopy, Fourier transmission infrared spectroscopy (FTIR), X-ray diffraction (XRD) technique and Atomic force microscopy (AFM). The antibacterial activity of AgNPs against Staphylococcus aureus, Streptococcus pseudopneumoniae, Escherichia coli and Klebsiella pneumonia bacteria was analyzed. The results showed that AgNPs inhibit the growth of bacterial stains. The present work suggest a green method for the synthesis of AgNPs with good antibacterial and antioxidant efficacy.

Comparative Study of Antimalarial Activity of *Garcinia Mangostana Linn*. (Purple Mangosteen)

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Malaria is profoundly irresistible ailment that has been one of the common reason for human death. Enormous number of restorative plants have been recognized as potential antimalarial agent. Garcinia mangostana fruit pericarp has been utilized in customary prescription in a few Asian nations for a few reason including treatment of skin contaminations and wounds. The development and spread of mutidrug-safe Plasmodium flaciparum has turned out to be hazardous in under mining jungle fever control programs in the greater part of the world. Some parasites can endure the treatment for a more drawn out timeframe than expected. This rises the probability of an extraordinary endurance system not quite the same as an old style tranquilize opposition phenotype. The antimalarial action of G. mangostana Linn separate against Plasmodium berghi were evaluated utilizing cooperative energy brands green-I based measure than a suppressive test was performed to explore vivo antimalarial action. Current correlation demonstrates that G. mangostana Linn indicated feeble antimalarial action of the concentrate both in vitro and vivo and it could be because of impediment of ingestion of the dynamic compound. Protein includes in the glycolysis pathway might be the objectives for against malarial action of G. mangostana Linn.

Correction of Trace and Toxic Metals in Biological Samples of Stomach Disordered Patients Consuming Drinking Water of Different Areas of Sindh

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Correction of trace and toxic metals in biological samples of Stomach disordered patients consuming Drinking water of different areas of Sindh Sadaf parveen*, Hassan Imran Afridi, Tasneem gul kazi National center of excellence analytical chemistry Sindh university jamshoro Corresponding author: Sadaf parveen Email: Sadafgill19@gmail.com Drinking contaminated water is resulting in steep rise in renal ailments in Pakistan. In the last 20-25 years, many people of Sindh, Pakistan have suffered from chronic diseases that to serious studies to find out the relationship between drinking water and chronic diseases. The emissions of Cadmium into the environment are increasing, implying that more attention should be paid to Cadmium contamination and its impact on human health among all Stomach risk factors, such as Cd, are classi?ed as certain/probable carcinogens by the International Agency for Research on Cancer. The objective of this study was to examine the relationship between Trace and Toxic elements and Drinking water with related to risk of stomach disorder. The water samples were collected from different areas of Sindh, Pakistan. The Biological Samples of both genders, age ranged 20â€“35 and 36-55 years both male and Female, consuming different types of water, have or have not stomach disorders, were selected. The Zn concentration was determined in Biological Samples of study subjects and water by flame atomic absorption spectroscopy, whilst Cd level was determined by electro thermal atomic absorption spectroscopy. The Cd concentration in the scalp hair and Blood samples of stomach disorder patients consuming different types of drinking water was found to be higher while Zn level was lower as compare to referents subjects in both genders and also due to smoking habit. A relative risk and odd ratio were calculated; there lative risk had a strong negative association with incidence of stomach disorder, which depends on types of drinking water.

Development of Green Microextraction Method for the Preconcentration of Hg in Artificial Saliva Extracts of Chewing Tobacco Products

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In present study a novel method was developed for the determination of total mercury and its species in artificial saliva extracts (ASE) of chewing tobacco products (CTP). The ASE of CTP (mainpuri and gutkha) were subjected to dispersive liquid-liquid microextraction based on back extraction (DLLÂµE-BE) with the aid of ultrasound energy. The soluble inorganic specie of mercury (iHg) in ASE was complexed with 1-(2-pyridylazo)-2-naphthol (PAN) and extracted in ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate ([C4MIM][PF6]). The back-extraction of enriched Hg was carried out with the aid of L-cysteine prior to analysis at optimized condition of electrothermal atomic absorption spectrometry (ETAAS). For comparative purposes ICP-OES was also used. Factors affecting the extraction efficiency and complex formation were optimized. The accuracy of the total and inorganic mercury (iHg) was checked by analyzing CRM of tobacco and standard spiking method. The limit of detection (LOD) of iHg was found to be 0.17Âµg L-1 and the enrichment factor was obtained as 167. Microwave assisted acid digestion of CTP was carried out for the total Hg content. Whereas, the organic mercury was calculated after the subtraction of iHg from total mercury content in ASE of CTP.

Development of Green Microextraction Method for the Preconcentration of Hg in Artificial *Saliva* Extracts of Chewing Tobacco Products

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Synthetic preservatives for stored food have influenced the fungal management impressively for both nutritional and economical aspects. But collateral effects of these chemicals are alarming situation for human and animal health. These adverse effects can be complemented by green methods to prolong the shelf-life of processed products as well as stored cereals. In this regard, the in-vitro antifungal activity of Eucalyptus camaldulensis were assessed against two Fusarium species; F. graminearum and F. culmorum. The chemical profiling by Gas Chromatography-Mass Spectrometry revealed the presence of thirty-five components with the major portion contributed by Eucalyptol (53.73%), followed by a-Pinene (14.74%), Terpinolene (4.66%), L-4-terpineneol (1.94%) and (-)-Ledol (3.7%). In-vitro evaluation of antifungal capacity was done using poisoned food technique. 70% inhibition of mycelial growth were observed for F. culmorum at the concentration of 30Âµl/ml, while for F. graminearum the inhibition was 95% at 30Âµl/ml concentration. These findings confirm the fungicidal effects of volatiles derived from Eucalyptus camaldulensis and their potential role as substituent of synthetic preservatives.

Comparative Study of the Synthesis Methods of PbS Nanoparticles

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Synthesis of Nanoparticles has received immense importance because of its vast applications especially in the fabrication of nanodevices with magnetic properties, electric as well as optical properties. The extraordinary applications of PbS nanoparticles are due to the low band energy (0.4eV) and the higher excitation Bohr radius (18nm). This comparative study involves different methods used for the fabrication of PbS nanorods (Sonochemical, Hydrothermal, Solvothermal route and aqueous chemical methods). Characterization of PbS nanorods were done with the help of transmission electron microscopy (TEM), selected area electron diffraction pattern (SAED), energy-dispersive X-ray spectroscopy (EDX) Scanning electron microscope (SEM), and X-ray powder diffraction (XRD). This study finds that their specific concentration and reaction duration with surfactants plays a vital part in the synthesis of narrow shapes and high yields of PbS nanorods. The PbS nanorods produced by the Sono Chemical method were approximately 20-60 nm in diameter, by the hydrothermal method were approximately 20-50 nm in diameter and by Solvothermal had a diameter of 60-70 nm. PbS hollow nanospheres with a diameter of 80-250 nm were synthesized by a surfactant-assisted sono-chemical route. Based on size the hydrothermal and sonochemical methods were found to be best for Nanoparticle synthesis

Synthesis and Evaluation of Novel A-Substituted Chalcones with Potent Anticancer Activities

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Chalcones are medicinally important scaffold. Forty novel alpha-substituted chalcone derivatives were synthesized and biologically tested for antiproliferative activities against breast (HCC1954) and colorectal (HCT116) cancer cell lines and were found to induce G2/M cell cycle arrest. 2-Benzoyl-N-benzyl-3-(methoxyphenyl)acrylamide and 2-benzoyl-N-(4-chlorobenzyl)-3-(4-methoxyphenyl)acrylamide served as novel hits. These compounds stabilize p53 in a dose-dependent manner in HCT116 cells (24-hour treatment) and have ability to overcome multidrug resistance in MDR-1 overexpressing multidrug resistant cell lines. These compounds overcome multidrug resistance (MDR) by not being phosphoglycoprotein (Pgp) substrate. Therefore they can be further optimized for their MDR ability.

Study of the Effect of Micronized Nanoparticles on Agriculture

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Micronized nanoparticle technology is an emerging field. It has many potential application in agriculture. It has recently emerged as powerful tool for pest resistance, to increase shelf life, growth rate, and germination rate, retention of quality of agricultural products, soil remediation and the yield of product. All of these factors contribute toward an increased food production and realization of sustainability. A comparative study on decontamination of seeds, growth enhancement of plant and soil remediation using the CO2/ZnO nanoparticles. These nanoparticles were used as a spray on cabbage, tomato alexander, ice berg lettuce, pepper mix, and capsicum. It was observed that cabbage sprouting started on 2nd day after 48 hour while normal cabbage took 10-12 days. Ice berg lettuce sprouting starting on 5th day and tomato alexander sprouting starting on 6th day. It was concluded that the use of nanoparticles can enhance the growth germination rate, production rate and also can increase the shelf life of vegetables. Keywords: Micronized nanoparticles, Plant

Comparative Study of Different Synthesis Method of Chromium Oxide Nanoparticle

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The synthesis of Cr2O3 nanoparticles is the subject of a growing concern now a days. Cr2O3 nanoparticles can be mainly synthesized by three routes i.e. chemical route, physical route and biological route. Although, preparation of chromium oxide nanoparticles by chemical route is quick process and results in uniform sized nanoparticles but in this method toxic chemicals are used for the stabilizing and capping which leads to the creation of toxic environment. Physical method is usually expensive and involve complex experimental instrument for the fabrication of nanoparticles. Furthermore, the nanoparticles synthesized from chemical and physical methods are less used in medicines. In this study, it was observed that many biological systems have the capabilities of converting metal ions into metal nanoparticles by the reductive capacities of the proteins and metabolites present in these organisms. Syntheses of chromium oxide nanoparticles by biological methods are easy, cost-effective and environmental friendly. Their characterization was done by UV-VIS spectroscopy, SEM, TEM and FT-IR.

Synthesis of Poly (Vinylidene Fluoride) Based Nanocomposite Membranes for the Removal of Dyes

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In the present work polyvinylidene fluoride based nanocomposite membranes were fabricated which are used for the removal of dyes. The membranes were fabricated using phase inversion method with polyvinylidene fluoride as polymer matrix, nanodiamonds as nanofillers and lithium chloride as a pore former. The polyvinylidene fluoride, lithium chloride and nanodiamond composite were fabricated by changing the concentration of NDs from 0 wt% to 0.7 wt% resulted in five nanocomposite membranes i-e PLN0%, PLN0.1%, PLN0.3%, PLN0.5% and PLN 0.7%. Fabrication of composite membranes were confirmed by X-ray Diffraction, Fourier Transform Infrared spectroscopy and Thermo Gravimetric (TGA) analysis. The fabricated membranes were used for the removal of methylene blue and malachite green dye from water. Spectrophotometer was used for the determination of absorbance of methylene blue at 654nm and malachite green at 624nm. Different membrane properties including pure water flux, porosity shrinkage ratio, solvent content and fouling recovery ratio was also determined. The results showed that membranes with 0.5 wt % of NDs filler enhance membrane properties and showed high dye rejection. The results proved that that hydrophilicity of the membranes increased by increasing the nanodiamond (NDs) concentration. Results supported the applications of the PVDF/LiCl/NDs membranes for the removal of dyes.

Comparative Study of Zno Nanoparticles by Different Euphorbia Species

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ZnO nanoparticles synthesized by green synthesis by using different species of Euphorbia plant [1] Euphorbia Jatropa Latix, [2] Euphorbia Hirta L and [3] Euphorbia tirucalli with different photochemical, electrochemical, microwave and laser oblation methods. In ZnO nanoparticles synthesis plant extract acts as reducing agents and reduce the ions of ZnO nanoparticles. Plants extract concentration plays a very important role to control particle size and morphology. Green synthesis is very cheap and eco-friendly method for preparation of ZnO particles. Euphorbia Jatropa Latix is best extract among all plant extracts and play important role controlling particle side. Particles were hexagonal in nature and that is confirmed by SEM (scanning electron microscopy) and TEM (transmission electron microscopy). Characterization of ZnO particles takes place by FTIR, UV, PL, SEM and TEM. Atomic states were conform by XPS and purity of particles conformed by EDS. Scherrers formula were used to calculate the size of ZnO particles [3]. Optical properties of the reaction mixtures were analyzed by the UV-Visible double beam spectrophotometer [2]. In Euphorbia Jatropa Latex UV-Visible spectra average energy gap was 3.63eV [1]. Phosphorus was suitable WLED (white light emitting diode). ZnO particles have properties antimicrobial, antifungal, biosensing and naanoeletronics due to band gaps.

Study of the Impacts of Nanoparticles on Crops

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Various studies revealed that nanoparticles have remarkable effects in the field of agriculture. In agriculture, nanoparticles are widely used to enhance seed germination, inactivation of microorganisms and fungal spores. Hybrid seeds of celery, broccoli, china cabbage, capsicum and tomato were treated with CO2/ZnO nanoparticles. Nanoparticles and Nitrogen, Phosphorus and Potassium were sprayed on the treated ones while control with the simple water. Seed germination started in china cabbage and broccoli on the next day after sowing. While celery sprouted after nine days. Control capsicum germinated on third day and tomato had no affects. Further study is needed to check the yield, shelf-life, plant growth, stem growth, temperature, and humidity.

Comparison of Synthesis of Zno Thin Films by Sol Gel Technique for Biosensor Application

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Nano-scale metal oxide semiconductors are much in talk for their extraordinary applications and non-toxic properties. ZnO is famous due to its great gas sensitivity, high stability, high ratio of adsorption and low in cost. Toxic gases like H2, CO, NO2 are easily detected by ZnO. Among various ones, sol-gel method is selected due to its simple procedure, ability to operate at room temperature .Thin flims(68-94 nm diameter)were grown at temperature of 250Â°C using zinc acetate dehydrate and monoethanol amine. I-V characteristics of ZnO thin flims sensors were discussed. The comparison study reveals the different routes to synthesize ZnO thin flims. Predominantly sol-gel technique using zinc acetate dehydrate Zn(CH_3 COO)_2.2H_2 O, monoethanolamine (NH_2 CH_2 CH_2 OH) & 2-methoxyethanol is more effective because thin flims were grown at the annealing temperature of 250Â°C.

Utilization of Micronized Nanoparticles for Agriculture Applications

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Micronized nanotechnology is an innovative and emerging area of research. Micronized nanoparticles have been reported to show satisfactory results in agriculture, as it controls the germination rate of seed, improves yield of plant, pest resistance, decontamination of food, sanitation, microorganisms resistance and to control the shelf life of plants. In present study Seeds of cabbage, iceberg lettuce, tomato, pepper mix, broccoli, celery and china cabbage were treated with micronized nanoparticle. A 10 % solution of micronized particles was sprayed on sample group and control group was treated with tap water. After that effect of nanoparticles was examined. Sprouting of seeds was significant in treated group then the control group. There was a significant difference in the sprouting time of some vegetables as in the case of cabbage, it sprouted within 48 hours of seedling. The following parameters were checked during the experiment includes temperature, humidity, stem length and number of leaves. It was found that micronized nanotechnology has significantly increased the growth rate of crops under investigation.

Evaluation of Extraction Methods for the Recovery of Fat with Fatty Acid Composition from By-Products of Selected Ruminants

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Lipids extraction efficiency of popular methods was compared along with fatty acid composition (FAC) of selected ruminant (Cow, goat, lamb, and bull) by-products (Suet, Tongue, Pancreas). Four popular methods including Soxhlet (SOX), acid hydrolysis, Bligh & dyer (B&D) and Folch (FOL) were assessed. After methylation extracted lipids were analyzed by Gas chromatography for FAC. Data indicated that all selected methods were significantly (p<0.05) different from each other, particularly higher differences were noticed for low lipid containing products (Tongue, Pancreas) as well as their respective FAC. Based on Analysis of Variance and Principle component analysis, the effective method for lipid and FAC was the FOL method. The Soxhlet method was only effective for samples with high fat content i.e. suet, while B&D method gave comparatively low lipid content in analyzed samples. Hence based on the results, it is found that extraction methods suitability is largely depended on sample fat contents.

Quantitative Assessment of Azo-Dyes and Toxic Elements in Waste Water of Dying Industry and Their Environmental Impact

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Azo dyes are very important class of synthetic chemicals known as organic colorants commonly prepared by coupling of a diazonium compound with a phenol or an aromatic amine and have various industrial applications. Although some azo dyes are toxic in nature, these dye molecules are biologically inactive, but the living organisms can cleave the azo (N=N) groups, forming aromatic amines most of them are also toxic and even carcinogenic which affect the human health by direct contact or through the environment. Due to the toxicity of these dyes and their intermediates the European Parliament has recently approved the bane in 19th amendment for the use of twenty-two aromatic amines. Hence, the assessment of dyes from waste effluents has significant importance to the environment. The current study will be comprised of two aspects (i) Quantitative assessment of azo-dyes and toxic elements in natural water (ii) Toxic impact of selective azo-dyes and toxic elements on the workers of dye industries. For this purpose, four selective azo-ye (DB-38, RB-5, RB-19 and RR-45) are purchased from PCSIR complex Karachi. The quantification of azo-ye (DB-38, RB-5, RB-19 and RR-45) were performed by UV-Visible spectroscopic methods. Whereas, the contents of toxic metals (Cd, Cr, Pb and Ni) were determined by graphite furnace atomic absorption spectroscopy. These methods will be analytically validated by standard addition method and applied on the real industrial effluent samples.

Biosynthesis Of Copper Oxide Nanoparticles By Selected Microorganisms

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The yield of nanotechnology has generated great enthusiasm in recent years because of its expected impact on the energy, chemical, electronics and space industries and drug and gene delivery.Thus, the development of experimental procedures for the synthesis of nanoparticles of different chemical compositions, sizes/shapes and controlled monodispersity is essential for its advancement. As far as the synthesis of nanoparticlesis concerned, a number of chemical methods exist in the literature that uses toxic chemicals in the synthesis protocol, which raises great concern for environmental reasons. The utilization of biological systems has emerged as a novel method for the synthesis of nanoparticles. It is well known that many organisms, both unicellular and multi cellular, produce inorganic materials either intra-or extracellularly. This work presents utilization of microorganisms bacteria (bacillus thrungenisus) as a greener approach for the synthesis of copper nanoparticles with catalytic applications.

Impact of Deodorization Parameters on the Recovery and Composition of Deodorized Canola Oil and Its Deodorized Distillate

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Canola is a member of the Brassica family and has become one of the most important source of vegetable oil in the world. Crude canola oil is composed mainly of triacylglycerols but contains considerable amounts of desirable and undesirable minor components such as free fatty acids (FFA), monoacylglycerols, diacylglycerols, phospholipids, phytosterols, polyphenols, triterpene alcohols, tocopherols, tocotrienols, carotenes, chlorophylls, hydrocarbons (e.g. squalene), trace metal ions (e.g. iron, sulphur and copper), oxidation products, gums, waxes, pesticide residues and flavour compounds. Crude canola oil is refined in order to remove undesirable minor compounds that make this oil unusable in food products. The most important by-product of edible oil refining is the deodorizer distillate (DD) obtained in the deodorization stage. DD is considered as a waste material, but it is a rich source of naturally occurring bioactive and nutritive compounds that make it economically valued. The concentration of constituents present in deodorizer distillate depends on the type of refining process and operating conditions. During deodorization, volatile components are evaporated from liquid to gas and subsequently back to liquid via condensation. The aim of current research is to check impact of deodorization parameters on the recovery and composition of deodorized canola oil and it's DD.

Heavy Metal Analysis in Poultry Supplements by Solid Phase Extraction

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A new simple, selective, and economical preconcentration method was developed for the determination of Cd, Pb, and Ni in poultry antibiotics and supplements. The proposed preconcentration procedure is based on SPE using 8-hydroxyquinoline and Amberlite IRC-50 resin as complex and adsorbent, respectively. The determination was carried out by micro sample injection system (MIS) flame atomic absorption spectroscopy (FAAS).Several analytical parameters were examined, including pH, type of resin, amount of resin, type of eluent, eluent volume, flow rate, sample volume and interference of diverse ions. Under optimum experimental conditions, LODs and LOQs were 0.017and 0.055, 0.016 and 0.53, and 0.074 and 0.248 µg/L for Cd, Pb, and Ni, respectively, with RSDs < 2.50%. The accuracy of SPE-MIS-FAAS was successfully tested by the standard addition method, with obtained recoveries >99%. The proposed method was successfully applied for the determination of Cd, Pb, and Ni in poultry supplement and antibiotic samples.

Exploration of Potential Satmpk Inhibitor: A Molecular Dynamic Approach

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Bacterial infections are persistent and increasing threat to human health because of emerging resistance to presently used antibiotics. Thymidylate kinase (TMPK), a nucleotide kinase crucial for DNA synthesis in bacteria. TMK phosphorylating deoxythymidine monophosphate (dTMP) to deoxythymidine diphosphate (dTDP), therefore it is a potential antibacterial drug target. In this study we aimed to develop new chemical scaffold and understand their inhibitory mechanism within the binding pocket of thymidylate kinase. In this connection, sophisticated computational approaches were implemented to introduce new chemotypes for the inhibition of SaTMPK, we carried out an exhaustive virtual screening. For the initial screening, a selective pharmacophore model was developed using the shared features of the available crystallized ligands. It was followed by the virtual screening, which consists of molecular docking to identify the binding mode and the strength of intra-molecular contacts between proposed ligands and the residues spanning the active site of SaTMPK. The structure-based virtual screening brought forth four different four different chemical scaffolds; Quinazoline, Triazine, Triazole and Pyrimidine, which reflect the scaffold hopping ability of the protocol developed in the present study. The selected hits were subjected to molecular dynamics simulation, which provide detailed insight into the binding pattern of the proposed ligands.

Fabrication and Characterization of Cadmium Sulfide Nano Wires on Aluminum Oxide Templates

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Cadmium sulfide nanowires have unique electrical and optical properties and applications. They can synthesized by electrochemical deposition on porous anodized aluminium oxide template with regular hexagonal shapes. Their aspect ratio can be controlled by controlling the pores' depth and diameter which greatly depend on anodization voltage and temperature of the electrolyte. In this research, high purity aluminium was used to prepare nano templates at 5-6°C in 1M phosphoric acid and cadmium supplied was deposited electrochemically using a co-solution of thiourea, cadmium acetate and ammonium acetate. pH was maintained at 11 in heat bath at 75°C with the help of aqueous ammonia solution. Both porous anodized alumina and cadmium supplied Nanowires were characterized suing SEM. A good quality Nanowires were obtained in bunches with reasonably high aspect ratio.

Exploring the Mechanism of Selective Inhibition of EPAC2: An Interdisciplinary Approach

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Exchange Protein Activated by cAMP 2 (EPAC2), is a direct target of 3'−5'-cyclic adenosine monophosphate (cAMP) and is involved in cAMP-mediated signal transduction through activation of the Ras-like small GTPase Rap. EPAC signals play crucial roles in almost all diseases related to dysfunctional signalling pathways. Therefore, EPAC represents excellent drug target against various diseases as signal transduction component. To date, very few EPAC inhibitors are available; however, there is still a lack of isoform selective inhibitors due to off-target effects. Selectively inhibiting one isoform leads to work on allosteric site in EPAC2 that is distinct from the active site shared by EPAC variants. Here we present a site-directed approach, targeting specifically EPAC2 isoform. We emphasized to dig out the allosteric site by performing pharmacophore modeling, molecular docking, and molecular dynamics simulation. Primarily, commercially available databases NCI, Maybridge and ICCBS In-house database were screened against validated pharmacophore models. Molecules obtained were scrutinized by molecular docking to predict their binding affinities. In step wise screening four compounds were short listed for stability dynamics to get deep insight into their binding mechanism. Simultaneously, inhibitory activities of these compound were investigated to validate their effect on mice pancreatic islets. The results highlighted the potency of screened inhibitors that can contribute in designing of selective probes for EPAC2 associated pathologies.

Quality Characteristics and Oxidative Stability of Almonds oil During Storage

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Almonds, which belong to the Rosaceae family, are most important nut crops in the world. They can be used for human nutrition and health. Almonds are typically used as snack foods as well as ingredients in a variety of processed foods, especially in bakery and confectionery products. The fruit of this crop is highly valued for its dietetic, cosmetic and pharmaceutical properties. The high concentration of unsaturated fatty acids is demonstrated that the almond oil is highly susceptible towards oxidation reactions induced by various environmental factors such as humidity, temperature, light and oxygen content at storage atmosphere. The oxidative stability is an important indicator to determine oil quality and shelf life because low molecular-weight off-flavor compounds are produced during oxidation, which can make oil unacceptable to consumers for industrial use as a food ingredient. The objectives of our study is to monitor the oxidative stability of three different varieties of almonds (Australian, American and Irani) during storage at room temperature for 10 weeks and forced oxidation at 60□C by using UV- Visible spectrophotometer as well as conventional methods. In this regard the Almonds were subjected to quantify various parameters such as moisture, oil content, peroxide value (PV), p-anisidine value (p-AV), free fatty acids (FFA) and total oxidative value (TOTOX). Moisture content was observed 2.6%, 3.2% and 3.1% in Australian, American and Irani Almonds. While oil content was observed 43%, 44% and 47% in Australian, American and Irani Almonds. Current study shows that the oxidation influences the quality characteristics of Almond oil. Results showed that PV value increased from 7.65 to 10.0 meq/kg, 8.65 to 11.6 meq/kg and 8.66 to 11.3 meq/kg till 5 weeks then continuous decrease was observed between 9.30-7.41 meq/kg, 10.8 to 7.30 meq/kg and 9.80 to 6.80 meq/kg among 6-10 weeks in Australian, American and Irani almonds, respectively during storage. The FFA content was continuously increased from 0.66 to 1.05%, 0.39 to 0.95% and 0.37 to 0.77% during storage of Australian, American and Irani almonds, respectively. During 10 weeks of storage, p-AV value observed for Australian Almonds in between 4.23 to 7.81, American Almonds 4.33 to 9.32 and Irani Almonds 4.33 to 8.32, respectively. TOTOX value was observed in between 19.5 to 26.4, 18.9 to 32.9 and 17.9 to 32.0 for Australian, American and Irani Almonds during 10 weeks of oxidation process. FTIR study illustrated major effect on the CLNA band during oxidation. The most abundant fatty acid in almond oil Range was observed oleic acid (65–82%) followed by linoleic acid (16–28%). There

were also smaller amounts of palmitic (6–7%), stearic (1.7–2.7%) and palmitoleic (0.37–0.54%) acids.

2-Dimensional Metal Carboxylate Metal Organic Frameworks (Mofs) for the Adsorption of Different Dyes

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Metal organic frameworks are well known as coordination polymers. They use different metal ions and organic ligand and form the expanded framework. Their latent porous nature and smooth durability frame them for use in various fields. This study deals with the synthesis of Copper nitrate.trihydrate (Cu (NO3)2.3H2O) and Zinc nitrate.hexahydrate (Zn (NO3)2.6H2O) metal organic framework by using Terephthalic acid (BDC) as a ligand. A very common method Solvothermal method is used for this study. It requires N,N Dimethylformamide as a solvent ,temperature require is (80-85 ^{0}C) in a Teflon autoclave for 48hrs. The prepared MOFs will be further used for the adsorption of different dyes. The newly made metal organic frameworks are characterized by using UV-spectroscopy, Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD).

Enhancement of Shelf Life of Fruits by Immobilizing Gox on ZnO Nanoparticles

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Glucose oxidase is an oxidoreductase enzyme that catalyze the oxidation of glucose to gluconic acid. In this process H2O2 also produce in second phase. In this work glucose oxidase was produced by Aspergillus. niger in lab. Different concentrations of carbon source such as glucose ranges from 6-16 g (%, w/v), nitrogen source such as sodium nitrate ranges from 0.1-0.6 g (%, w/v) and calcium carbonate ranges from 1-2.25 g (%, w/v) were optimized. Growth medium conditions such pH ranges from 4.5-7, temperature ranges from 12-120 h were optimized. Size of inoculums ranges from 1-5% was optimized to increase production of GOD.When enzyme activity was measured by UV-Visible spectrophotometer, it was concluded that at 10% glucose (w/v), 0.2 % urea (w/v) and 1.75 CaCO3 (w/v) A. niger gave maximum enzyme activity after the incubation of 48 h. Zinc oxide nanoparticles were prepared from zinc nitrate hexahydrate and NaOH by using co-precipitation method. The UV-Visible analysis was observed. It was investigated ZnO-Nps showed the maximum absorbance at 370 nm. SEM image showed spherical shape nanoparticles. By plotting histogram 44 nm average size was observed. For immobilization, first surface of ZnO-Nps was modified by using L-cysteine HCl. After surface modification, GOx was immobilized with nanoparticles by using gluteraldehyde. From UV-Visible analysis, it was concluded that after immobilization enzyme activity was increased as compare to free enzyme. This solid bioconjugate was used in food application to increase the shelf life of fruits and vegetables.

Comparison of Anti-malarial Activity of *Gracinia mangostana* of Family Clusianeae

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High case fatality rate and resistance of malarial parasites developed against prevailing anti-malarial drugs has triggered the research in order to enhance the anti-malarial activities of various drug. Plants are an important source of medicines including anti-malarial drugs as in case of quinine and artemisinin. So various efforts are done in this context to increase the anti-malarial activities using plants. *Gracinia mangostana* L grows in tropical area of indonesia, where malaria is epidemic. Its general name is mangosteen and belongs to family clusiaceae. This plant is known to have anti-malarial activity as commonly used by the native patients of malaria. In this regard a comparative study on the anti-malarial activity of the rind, pericarp and husk of *Gracinia mangostana* was conducted. IC_{50} values of all the three methods were compared in order to identify the best inhibition of malarial parasitic growth. The pericarp gave the IC_{50} value of 3.7 to 20 µM whereas rind and husk gave the IC_{50} value of 0.41 to > 100 µg/mL and 0.2 ± 0.01 µM respectively. The study concluded that the rind showed the most efficient anti-malarial activity of the all and proved to be even better when used with artemisinin.

Knowledge is in many things and can have many different garbs and can have many different directions and dimensions but the knowledge that is gained by seeking the truth and knowledge that comes out of the pursuit of truth, unbiased, unprejudiced, based upon crystalline reasoning and logical understanding and rational thinking is the one that we care for and we should value. So knowledge is actually consisting of truth and nothing but truth.

(Dr Hasan Sohaib Murad)