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ABSTRACT BOOK

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Tubba Jawad

ORAL PRESENTATIONS

Applications of Laser Techniques in Environmental Analysis

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Various laser techniques like LIBS (Laser Induced Breakdon Spectroscopy), LIDAR, laser induced fluorescence and Raman laser spectrsocpy are frequently employed as diagnostic methods in soil, water, food, and environmrntal analysis. One of the severe problems for the environmentologists is the chracterization and quantification of aerosols suspended in the atmosphere. The sources emitting these aerosols include oceans, wind, volcanic eruptions, plants and different anthropogenic means like cement plants mega construction projects. The chemical nature of particles depends on the processes from where they have been originated. So far these aerosols which may contain heavy metals and VOCs is the least understood aspect of the climate system. Aerosols with all their physical and chemical characteristics have a decisive influence on climate. More recent research suggests that particles smaller than 2.5 μm are more harmful to human health. In addition to primary aerosols, secondary particles are also formed as a result of chemical reactions between VOCs, NOx and ammonia in the atmosphere. With traditional analytical techniques it is highly difficult to understand the exact nature of chemical reactions occuring in higher troposphere and lower stratosphere zones especially in Antarctic regions. Modern laser techniques are ideal for mmonitoring Air Quality w.r.t. detection, characterization and quantification of aerosols in that area. Laser based techniques for continuous PM monitoring are usually complex, costly, time consuming and do not provide real-time measurements. However Micro Laser Induced Breakdown Spectroscopy (LIBS), provided an innovative method with an optical design and multi-elemental scanning imaging, for the characterization of PM collected from Antarctica.

Our research group performed valuable experimentation in Antarctic region in last summer for the characterization of atmospheric aerosols by using different analytical techniques, especially Calibration-Free LIBS (CF-LIBS). A laser-induced fluorescence (LIF) system was optimized using a solution of Micrococcus luteus in ethanol/water 50% (v/v) to obtain spectra in the gas phase of bioaerosols. Experimental designs such as Plackett–Burman and factorial design were applied to analyze the PM. The fluorescence spectra was treated chemometrically by principal component analysis, linear discriminant analysis and hierarchical cluster analysis to classify the microorganisms according to family, morphology and gram. The best results were obtained using LDA. The method was applied to air samples and the LIF results allowed to characterize bioaerosols with adequate reliability. The usefulness of the technique was demonstrated by the identification of a variety of bacteria.

Preparing Global Citizens for a Sustainable Future: Systems Thinking in Chemistry Education

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Chemistry is the central science. However, research indicates that current methods of chemistry teaching and learning do not always prepare students to understand and address the complex global challenges that they will encounter in their lives, such as climate change, energy for our future, food security, and planetary sustainability.

Systemsthinking is an approach for examining and addressing complex behaviors and phenomena from a more holistic perspective. It has recently been suggested that a systems thinking approach can not only help students learn chemistry content meaningfully, but to develop the knowledge and skills they need to take informed action to address these global challenges.

This presentation will explore how systems thinking might apply to chemistry education. Goals that will be addressed are:

- What a systems thinking approach looks like in chemistry education, its essential characteristics and the benefits of its use.

- How a systems thinking approach extends and differs from context-based approaches to chemistry teaching and learning. This approach motivates students to learn science, promotes their ability to see connections between chemistry and their everyday world and promotes long-term retention of knowledge.

- How a systems thinking approach can prepare students to become global citizens capable of taking informed action to support planetary sustainability.

This presentation will introduce the essential characteristics of a systems thinking approach in chemistry education through an example that is appropriate for a general chemistry course as well as discuss why a systems thinking approach can prepare students to be global citizens that support a sustainable future.

Safety/Security of Chemicals: A Perspective from Australia

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The Royal Australian Chemical Institute (RACI) is the professional association for chemists and chemical educators in Australia. The association for chemical industries is Chemistry Australia, still referred to by its earlier name, the Plastics and Chemical Industries Association, Pacia. The state of chemistry in Australia is reviewed every ten years by the Australian Academy of Science (https://www.science.org.au), looking at the current situation in education, research and industry. Opportunities and threats are identified and potential strategies considered

The RACI has recently celebrated its Centenary. During those 100 years, the Institute has developed a range of specialist groups called Divisions (e.g. analytical and environmental chemistry; health, safety and environment), a national organisation involving eight branches located in each of the States of Australia as well as other specific interest groups such as career development, a mentoring programme, women in chemistry. A full listing is on the RACI website https://www.raci.org.au/. The Institute publishes a national magazine, Chemistry in Australia, six times per year and delivers several National Awards for its members. The RACI has developed and promotes a Code of Ethics.

Chemistry Australia (https://chemistryaustralia.org.au/) represents the $40 billion chemistry industry in Australia, whose sectors employ over 60,000 people. As noted on their website: member companies range from small family-owned companies through to multinational enterprises, positioned widely across the industrial landscape. Through Chemistry Australia (and its predecessor Pacia) many Australian chemistry companies have signed on to the Responsible Care program https://www.icca-chem.org/responsible-care/ which commits chemical manufacturers to pursue an ethic of safe chemicals management and performance excellence. Australia was the third country to adopt this program that now extends to more than 65 countries and continues to grow in its global footprint. A desired outcome is to ensure the company's social license to operate, enhancing public confidence and trust through safe management of chemicals throughout their lifecycle. Analytical chemistry is critical in this regard.

The global network is the International Council of Chemical Associations (https://www.icca-chem.org/responsible-care/) ICCA has publicly committed to help implement the Chemical Weapons Convention CWC, administered by the Organisation for the Prohibition of Chemical Weapons (OPCW) https://www.opcw.org/ . Australian chemical industry worked closely with the RACI to support the development of the CWC, an initiative of science diplomacy. The OPCW recently developed a set of guidelines for an ethics code for chemists that were used by the American Chemical in a series of regional workshops (e.g. Kuala Lumpur, April 2016) and develop the global chemists code of ethics (GCCE: https://www.acs.org/.../regional/eventsglobal/global-chemists-code-of-ethics.html). In practice, codes of ethics are complemented by codes of practice in an industry and by the national laws in

place following the country's acceding to the CWC. Matters of continuing concern include dual-use technologies and the convergence of chemical and biological weapons.

The presentation will highlight aspects of these chemical safety/security issues.

Spatial-temporally resolved bioorthogonal decaging in living cells

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A universal method for spatial-temporal control of molecular activity under living settings, particularly in a gain-of-function fashion, is crucial to understanding how diverse cellular processes are organized in space and time. Although the rapidly emerging bioorthogonal cleavage chemistry has shown the potential in manipulating biological processes with either spatial or temporal specificity, a general approach for precisely coordinated spatial-temporal activation of various molecules under living conditions is still challenging. We herein envision that the bioorthogonal photocatalysis may hold the potential for precise spatial-temporal manipulations, with the spatial and temporal resolutions achieved by pre-targeting of catalysts and photo-irradiation, respectively. Systematic survey of the photocatalysts has led to the identification of $Ir(ppy)_2bpy$ type complexes for rapid rescue of azidoaryl-caged molecules by visible light with high efficiency in living cells. We demonstrated the generality of this system by *in situ* decaging of fluorophores, prodrugs, biotin, proximity reactive molecules, amino acid side-chains as well as intact proteins in desired intracellular and extracellular spaces. By antibody-mediated pre-targeting of the photocatalyst onto cell surface, we realized tumor cell-selective prodrug activation, cell tagging as well as membrane microdomain proteomic profiling controlled by external light. Furthermore, we identified a mitochondria-targeting iridium complex which allowed the on-demand fluorophore activation as well as uncaging of reactive intermediates for subcellular proteomic profiling in mitochondria. Our study offers a general platform for spatial-temporal manipulations with programmable modularity and diverse utilities, which further unleash the power of bioorthogonal cleavage chemistry in living systems.

Adding value to unused electroplating wastewater for Zn2Cr-layered double hydroxide (LDH) for pyrophosphate removal

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This work incorporated technological values into Zn_2Cr-layered double hydroxide (LDH), synthesized from unused resources, for removal of pyrophosphate (PP) in electroplating wastewater. To adopt a resource recovery for the remediation of the aquatic environment, the Zn_2Cr-LDH was fabricated by co-precipitation from concentrated metals of plating waste that remained as industrial by-products from metal finishing processes. To examine its applicability for water treatment, batch experiments were conducted at optimum M^{+2}/M^{3+}, pH, reaction time, and temperature. To understand the adsorption mechanisms of the PP by the adsorbent, the Zn_2Cr-LDH was characterized using Brunauer-Emmett-Teller (BET), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy/energy dispersive X-ray spectroscopy (SEM/EDS), transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS) analyses before and after adsorption treatment. An almost complete PP removal was attained by the Zn_2Cr-LDH at optimized conditions: 50 mg/L of PP, 1 g/L of adsorbent, pH 6, and 6 h of reaction. Ion exchange controlled the PP removal by the adsorbent at acidic conditions. The PP removal well fitted a pseudo-second-order kinetics and/or the Langmuir isotherm model with 79 mg/g of PP adsorption capacity. The spent Zn_2Cr-LDH was regenerated with NaOH with 86% of efficiency for the first cycle. The treated effluents could comply with the discharge limit of <1 mg/L. Overall, the use of the Zn_2Cr-LDH as a low-cost adsorbent for wastewater treatment has contributed to national policy that promotes a zero-waste approach for a circular economy (CE) through a resource recovery paradigm.

Recent Studies on Catalysis and Quorum Sensing

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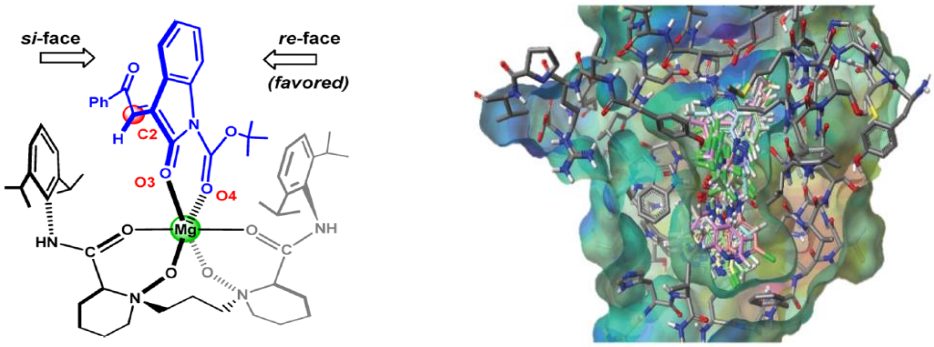
We have been working on the understanding of the chemical reaction mechanism and design of various small molecules acting on interesting systems. The first part of this talk is our recent research on the role of catalysts in organic and inorganic transformations. The formation of new bonds to the carbon atom is widely used in organic synthesis to introduce new functional group(s) to the parent compound. Due to the stability of chemical bonds in the parent compound, such reactions require high energy. It is, therefore, not feasible in ordinary conditions. To promote these reactions, many methodologies, reaction conditions (temperature, pressure, solvent, etc.) change, and introduction of catalyst were developed and applied in bench chemistry. One of the widely studied methodologies is to find a proper catalyst that can promote the reactions. The reactions we have studied include the Michael addition reaction, condensation of two alcohols, hydroarylation of α,*β*-unsaturated alkenes, and cleavage of biomass molecules. From this work, we understand the role of catalysts (see Figure 1a). First, the catalyst plays an important role in organizing reactant molecules in a proper orientation. Second, the reaction mechanism changed to a multi-step reaction, unlike the uncatalyzed reaction. Third, the activation barrier for the rate-determining step is lowered considerably compared to those of uncatalyzed ones. The second part of this talk is the design of *de novo* ligands based on *in-silico* modeling. Bacteria commonly sense and react to their environment through two-component systems (TCSs) that rapidly convert external stimuli into internal changes in gene expression. These systems are typically composed of a transmembrane sensor module, the receptor histidine protein kinase (HPK), and a cytoplasmic transcription factor, the response regulator (RR). Stimulus perception leads to activation of the receptor, which in turn affects the regulatory activity of the associated RR. There is, however, one important class of TCSs with known ligands, namely the quorum-sensing autoinduction systems, which regulate their target genes in response to population density. By activating a signal transduction substance (known as an autoinducer or quormone) with a low molecular mass, regulator protein, and sensor kinase, bacteria can sense the presence of other bacteria and thereby perform cell-cell communication to express specific genes. In this process, the concentration of the signal transduction substance is directly proportional to the number of bacteria, and the sensing of a critical level of a signal transduction substance is referred to as “quorum sensing (QS),” a mechanism wherein the cells begin to reveal themselves. The cell density-dependent increase of signal concentration is sensed by receptors, and the receptor-related regulators trigger the expression of target genes. QS is involved in controlling a wide range of biological functions, To examine the binding energies of the newly synthesized QS inhibitor candidates, molecular modeling studies were performed on the inhibitor-TraR, -LasR interactions using SYBYL packages. FlexX dockings of the inhibitors were carried out (see Figure 1b). Of all possible docking poses, the structures that fitted most

properly into the signal binding pocket were selected, and their docking scores were calculated. The docking score was calculated using the modified Böhm scoring function which includes entropic, hydrogen bonding, ionic, aromatic, and lipophilic terms. It is believed that modeling studies can provide insight into the binding poses and affinity of ligand compounds and help in the design of new inhibitors, at least until a better method that offers a full and easy prediction of the tertiary structure of the ligand-receptor binding can be developed.



(a) **(b)**

Figure 1 (a) Stereoselective addition reaction. (b) Docking of 20 ligands to the binding pocket.

Tacticity-dependent cross-plane thermal conductivity in molecularlyelectrostatically engineered amorphous polymers

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The low thermal conductivity of polymers impedes heat dissipation in plastic products and often limits their functionality and reliability. Extended polymer chain conformation (*i.e.*, planar zigzag) has widely been found to enhance heat transfer in both a single polymer chain and bulk polymers. Here, we show that the tacticity of polymers (poly(acrylic acid) (PAA) and poly(methacrylic acid) (PMAA)) significantly affects the thermal conductivity of ionized polymers, in which the extended chain conformation is induced by electrostatic repulsion. Depending on their tacticity, polymers with similar degrees of ionization were observed to have significantly different thermal conductivities, as high as 1.14 W $m^{-1}{\cdot}K^{-1}$ in ionized atactic PAA and 0.69 W $m^{-1}{\cdot}K^{-1}$ in ionized syndiotactic PMAA, but only 0.55 W $m^{-1}{\cdot}K^{-1}$ in ionized isotactic PAA and 0.48 W $m^{-1}{\cdot}K^{-1}$ in ionized isotactic PMAA. The elastic modulus, degree of ionized carboxyl groups, and viscosity data suggest that the size and spatial arrangement of side groups, which influence the conformation of the polymer chain, affect the thermal conductivity of polymers.

Programmable late-stage C–H bond functionalization enabled by integration of enzymes with chemocatalysis

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New chemo- and biocatalytic methodology is important for the future sustainable synthesis of essential molecules. Transition metal catalysis enables the late-stage C–H functionalization of some complex molecular scaffolds, providing rapid routes to valuable products, although this is largely dependent on the availability of electronically or sterically predisposed C–H bonds for selective metalation, leaving certain regioselectivities inaccessible. Unlike metal chemocatalysis, enzymes can catalyze C–H bond functionalization, discriminating between near-identical, non-activated C–H bonds, delivering products with exquisite regioselectivity. However, enzymes typically provide access to fewer functionalities than more divergent chemocatalysis. This work describes programmable, regioselective C–H bond functionalization methodologies for the installation of versatile nitrile, amide and carboxylic acid moieties through integration of halogenase enzymes with palladium-catalyzed cyanation and subsequent incorporation of nitrile hydratase or nitrilase enzymes. Using two- or three-component chemobiocatalytic systems, the regioselective synthesis of complex target molecules, including pharmaceuticals, can be achieved in a one-pot process operable on a gram scale.

Nano-space confined strategy towards 2D Hybrid Structures for Energy Storage Applications

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Two-dimensional (2D) layered metal dichalcogenides (LMDs) with semiconducting character have been attracting increasing attention in both fundamental studies and various applications. In the case of electrode material design for energy storage, integrating metal dichalcogenides with other conductive phases such as nanocarbons has been widely recognized as an efficient way to simultaneously achieve good electrochemical activity and conductivity. However, controllable synthesis of such composite electrode materials with well-defined structure and efficient interfacial contact is still challenging. In this work, we developed a nanospace-confined strategy to realize an effective combination of nanocarbons and other 2D LMDs, such as SnS_2, TiS_2. A new class of LMD nanosheets with distinct growth orientations on the surfaces of reduced graphene oxide and carbon nanotubes have been developed. MXene derived 2D metal sulfide/nitride nanostructures have been also demonstrated. The resultant composites present enhanced electrochemical performance in energy storage applications such as Na-ion, Al-ion or Li-S batteries.

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

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

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. The results of our finding will be presented.

Computational Techniques in Quantum Chemistry: Alternative Approach To Physical Measurements

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Matter is composed of microscopic particles, electrons and nuclei. These particles make atoms and atoms are bonded through electrons constitute different types of matter. The knowledge of microscopic particles is crucial in the understanding of the chemistry of materials. Classical particles are governed by Newtonian mechanics and microscopic particles by quantum mechanics, where unlike macroscopic particles with absolute reality, quantum reality changes with the observer. The emerging computing technologies have further boosted the need of quantum chemistry in the understanding of the electronic basis of physical properties of materials. In this article some computational results will be provided to confirm the effectiveness of DFT calculations in the structural, electronic and magnetic properties of selected compounds.

Boron Oxide a Novel Sensor of NH_3 and CH_2O

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Center for Computational Materials Science, University of Malakand, Chakdara, Pakistan
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DFT computations are used for the adsorption of different gases like NH3, CO, CO_2, CH_2O, PH_3, H_2S, H_2O, SO_2, NO, NO_2, HCN, CH_4, $COCl_2$, N_2O, NF_3, NCl_3, O_3 and H_2 onto porous hexagonal boron oxide monolayer (ph-BOL) to explore its potentials for gas sensing. The negative adsorption energies (-1.00 to -10.13 kcal/mol) demonstrates that the adsorption of various gas molecules over the ph-BOL monolayer is energetically favorable and exothermic process. The highest decrease in energy of HOMO-LUMO gap occurred in NH_3@ph-BOL (1.671 eV) and CH_2O@ph-BOL (1.875 eV) reflecting selectivity and sensitivity of ph-BOL toward NH_3 and CH_2O among studied analytes. The non-covalent interaction and reduced density gradient analysis for NH_3@ph-BOL and CH_2O@ph-BOL suggests that the formation of green isosurface between analytes and ph-BOL cavity indicate the role of van der Waal interaction in stabilizing complexes. This is confirmed by the atom in molecules analysis which shows that electron density values for the non-covalent interactions are in the range of van der Waal interactions. The electron density difference and natural bond orbital analyses reveals that significant charge shifting occurs between the analytes and ph-BOL monolayer. The SAPT0 energy components values are well agreed with the interaction energies. The recovery time of sensor for NH_3 and CH_2O molecules is estimated to be 1.6×10^{-6} s and 8.1×10^{-7} s, respectively, suggesting the rapid regeneration of sensor at room temperature. Thus, ph-BOL monolayer is a potent candidate for NH_3 and CH_2O gas sensing/detection for future experimental-validation.

Synthesis of Novel Drug Candidates 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 (NH_3) and carbon dioxide (CO_2). Liberation of ammonia increases pH significantly and allows the bacteria to survive during colonization. During Helicobacter 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. Interesting results our research on urease inhibitors would be presented.

Supramolecular Nanocarriers for Drug Delivery

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Macrocycles based nanocarriers 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.

Role of Capping Agent for the Colorimetric and Fluorescent Sensing of Different Materials Using Metal Nanoparticles

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The selection of capping agent depends on the method of synthesis, nature of nanoparticles (NPs), and type of the compounds to be analyzed. Therefore, different types of capping agents such as surfactants, drugs, amino acids, fatty acids, and polymers are used to increase stability of NPs, avoid aggregation, keep NPs away from one another, thereby achieving desired morphology as well as the size of NPs. Recently, the fabrication of NPs has been extensively carried out using synthetic chemical routes in a wide range of materials. In this review, a comprehensive assessment of the colorimetric and fluorescent sensing of metal nanoparticles using different capped agents, such as surfactants, drugs, amino acids, fatty acids, and polymers has been summarized for the present and future strategies. For the synthesis of metal nanoparticles, different methods, metals, and a variety of capping agents are used to obtain new properties and explore opportunities for innovative applications. Capping agents perform their significant role as stabilizers to avoid the over-growth and coagulation of nanoparticles. Capping agents play an essential role in the colorimetric and fluorescent sensing of metal nanoparticles for particular analytes.

Functional Nanomaterials – Tuning the Size and Surface Chemistry for Applications in Catalysis, Biomedical and Environmental Sciences

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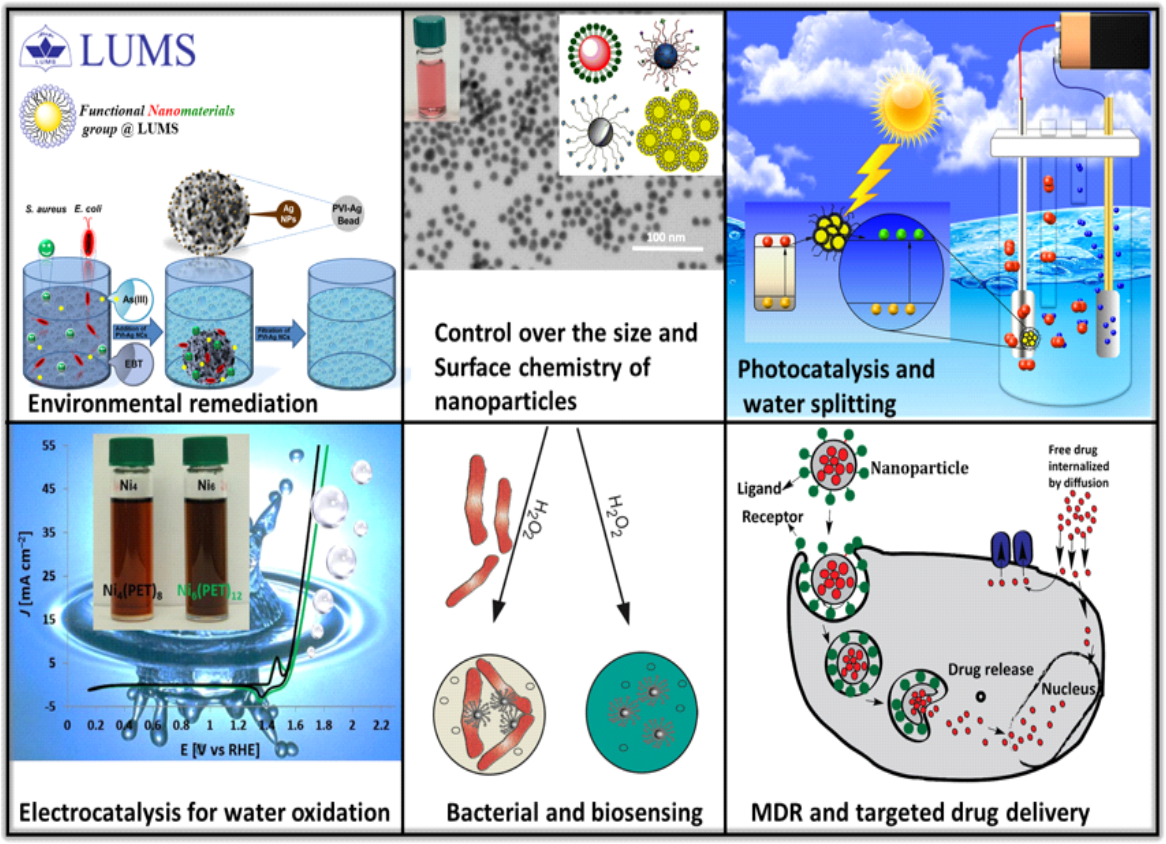
The unique chemical and physical properties of nanoscale materials have triggered much scientific interest to evaluate their potential applications in biomedical sciences, energy technologies, agriculture, environment, catalysis and industry etc. The chemical and physical properties of metal/ metal oxide nanoparticles can generally 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 nanocomposites in biomedical sciences i.e., bio-sensing (especially bacterial detection), bio-imaging, drug delivery, killing drug resistant bacteria, environmental remediation (water purification) and renewable energy technologies (mainly H_2 production and storage and electrode materials for batteries). This talk would, therefore, be an overview of our interdisciplinary research activities of Functional Nanomaterials Group at LUMS to synthesize customized inorganic/organic nanoparticles with tunable size and surface chemistry, and their composites having unique chemical and physical properties, and subsequent applications in biomedical sciences, environment, catalysis and renewable energy technologies.


LUMS
Functional Nanomaterials group @ LUMS
S. aureus
E. coli
Ag NPs
PVI-Ag Bead
As(III)
EBT
Environmental remediation
100 nm
Control over the size and Surface chemistry of nanoparticles
Photocatalysis and water splitting
Ni4
Ni6
Ni4(PET)8
Ni6(PET)12
J [mA cm-2]
E [V vs RHE]
Electrocatalysis for water oxidation
H2O2
H2O2
Bacterial and biosensing
Nanoparticle
Ligand
Receptor
Free drug internalized by diffusion
Drug release
Nucleus
MDR and targeted drug delivery

Molecular Dynamics Simulations: A Powerful Tool to Understand Medicinal Chemistry

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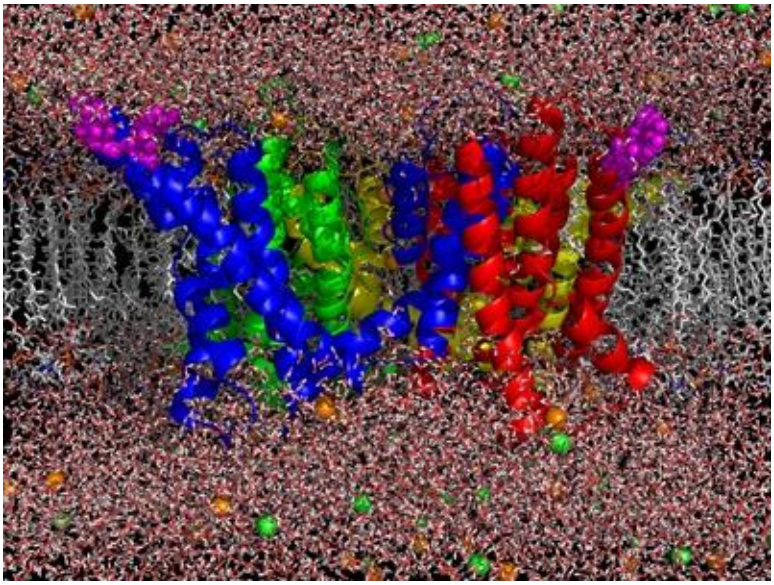
Molecular dynamics (MD) simulations allow researchers to investigate the behavior of desired biological targets at ever-decreasing costs with ever-increasing precision. Among other computational tools, molecular dynamic (MD) simulations have been rising in popularity in the past decade. Advancements in technology and bio-computational techniques made it possible to simulate even larger proteins that can now be used as supporting evidence for experimental findings, for elucidating protein mechanisms, and validating protein crystal structures. Unrelated to experimental data, these simulations can also serve to investigate larger scale processes like protein sorting, protein-membrane interactions, and more. In this talk, the history as well as the state-of-the-art methodologies in protein simulations will be presented. By using our ongoing projects, an emphasis will be put on how to set up and utilize MD simulation to understand medicinal chemistry related projects. An overview of the available tools for protein simulation along with its current limitations will also be discussed.



Initial Setup for Molecular Dynamics Simulation of Membrane Protein

Phytochemical Investigations on *Arisaema jacquemontii* Blume

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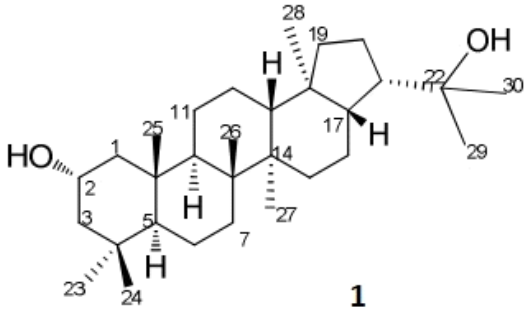
Arisaema jacquemontii Blume is known for its use in the folk medicine system to combating various ailments (1). The anticancer activity of the plant was reported from our laboratory in 1992 (2). Other researchers have also reported the presence of some chemical constituents in the plant (3-5). The extracts of the plant have shown a broad spectrum of biological activities including the cytotoxic activity. Continuing our investigations, we have detected a number of hitherto unknown compounds in the plant. The activity directed fractionation of the methanol extract of the plant have also resulted in the isolation of a crystalline compound. The structure of the compound was determined as the triterpenoid, 2-hydroxy diplopterol (**1)** on the basis of spectroscopic techniques including the 2D-NMR experiments (6,7). The triterpenoid also showed activity in the cytotoxicity assays and exhibited the IC_{50} value of 22 μM against the K 562 cell line.



1

Combining untargeted and targeted metabolomics approaches for the standardization of polyherbal formulations using advanced mass spectrometric tools

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Polyherbal formulations are an integral part of various indigenous medicinal systems such as Traditional Chinese Medicine (TCM) and Ayurveda. The presence of a very large number of compounds makes the quality control of polyherbal formulations very difficult. Many studies on the standardization of herbal medicines focus only on either HPLC-based fingerprinting or on the quantification of a few major peaks. However, environmental factors such as temperature, humidity, and soil can affect the amounts of secondary metabolites in a plant, which in-turn can lead to variations in the batch-to-batch quality of herbal medicines. It is therefore important to focus on the complete picture rather than a few specific compounds. Such knowledge can only be generated through a comprehensive metabolomics analysis that can convert analytical data into useful biological knowledge. Metabolomics data obtained through comprehensive and reliable methods for fingerprinting, profiling and quantification of active natural products can be used to study global metabolite composition, taxonomy, stress response, interaction of plant with the environment, drug lead discovery and for the study of mode of action of an herbal drug

We have developed several strategies for the dereplication of natural products in single and polyherbal formulations by advanced mass spectrometry tools [ref]. The strategy is based on five major steps: the collection of plant samples from different locations to observe the effects of environmental variables; LC-ESI-MS/MS-based untargeted metabolite profiling of the plant samples to identify marker compounds using extensive chemometric analysis of the obtained data; the identification of marker compounds in polyherbal products; the isolation, purification and characterization of the marker compounds; and MRM-based quantitative analysis of the isolated marker compounds using LC-ESI-MS/MS. Using this strategy, we identified a large number of compounds in plant extracts. Chemical fingerprinting of the plant led to the identification of characteristic peaks that are used to confirm the presence in complex polyherbal formulations. Moreover, marker compounds were isolated, purified and quantified in various herbal formulations containing respective plants. These methods demonstrate a comprehensive strategy based on untargeted and targeted metabolite analysis that can be used for the standardization of complex polyherbal formulations. Details will be discussed in the presentation.

Co-Crystallization of Bioactive Compounds- A Crystal Engineering Approach towards Enhanced Biological Activities

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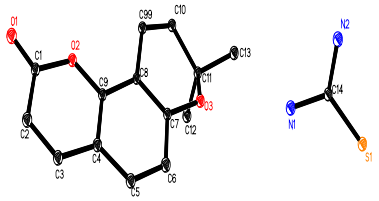
Co-crystals are crystalline structures made up of two or more components in a definite stoichiometric ratio linked through non-covalent interactions in same crystal lattice. They differ in their biological and physiochemical properties from their components. They have wide applications in drug designing and in analysis of active pharmaceutical ingredients (APIs). The US-FDA approval for co-crystals to be considered as drug intermediates has opened new vistas, both in pharmaceutical and academic research sector. Present lecture will cover the results of structural modification of antileishmanial natural product and commercially available drugs by using co-crystallization.

The co-crystals of anti-leishmainal natural product, sesselin (1) and an anti-cancer drugs exemestane (2) and nandrolone were synthesized by using neat grinding followed by liquid assisted grinding and solution methods and their anti-leishmainal and anti-cancer activities were evaluated and promising results were obtained.

Single-crystal X-ray diffraction techniques were used to establish the structure of co-crystal and non-covalent interactions responsible for the stability of co-crystal.



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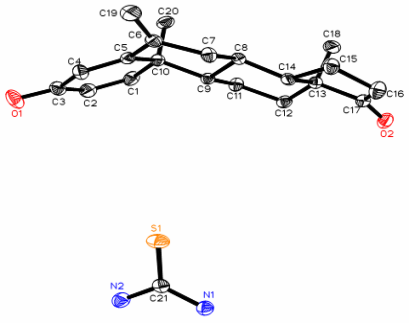

2

Metal-Organic Frameworks for Renewable Energy Applications

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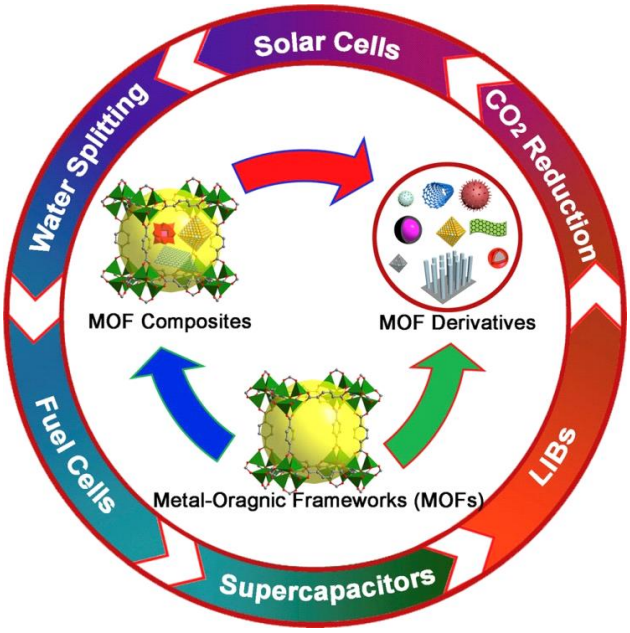
Metal-organic frameworks (MOFs) have attracted great interest because of their unique porous structures, synthetic advantages, organic-inorganic hybrid nature, and versatile applications. Recently, the applications of MOFs in energy fields such as fuel storage, photo-induced hydrogen evolution, fuel cells, batteries, and supercapacitors have experienced a new surge of interest in both the chemistry and materials science communities. Research on the various applications of MOFs has shown that they are promising porous materials for energy storage and conversion technologies. Furthermore, MOFs have been used as support substrates to accommodate metals, metal oxides, semiconductors, and complexes and have been used as sacrificial materials for the generation of various nanostructures for energy applications. Here, we present the highlights of renewable energy applications based on MOFs, their composites and derivatives.



Estd. 1990

Exposure of toxic elements via cosmetic products

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Cosmetics have been an essential part of personal care products since the ages. It is now used in common routine by every strata of populaces. The daily use of cosmetics is common to beautify the human body and skin especially of women. These products include lipsticks, creams, face powders, face lotions, lip, hair, and eye makeup. A large variety of coloring agents are used in these products, which mainly contains organic and inorganic pigments. Heavy metals such as cadmium, chromium and lead have been reported in these pigments which are the integral part of face powders, lipsticks, eyeshadow. Toxic metals are also used as a coloring agent in blushes and eye shadows. The compounds of Cd produce a broad range of colors like cadmium sulfide and cadmium selenide are used to give the yellow and dark orange color to the cosmetic products. Immensely uses of mercury compounds in skin lightening creams. The chromium oxide in addition to cadmium sulfide, forms light green color. Metals present in coloring pigments could be one of the factors to cause skin damages. Contact dermatitis is actually caused by Ni exposure, however trace quantities of other toxic metals may sensitize the immune system activate any allergy owing to combined effect. The cosmetics companies are not obliged to report on this kind of impurities and so consumers have no way of knowing about their own risk.

Green Extraction for Effcetive Recovery of Funtional Components/Plant Bioactives

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Plants are recognized as a vital source of a wide array of high-value components so called secondary metabolites with potential functional food and therapeutic benefits. Owing to diverse structural features, levels of concentration and biological activities, the extraction of functional bioactives from different plant materials is a challenging task. Conventional organic solvent extraction (COSE), which mostly involve the use of volatile organic solvents (VOSs), are usually employed for the recovery of plant bioactives. Nevertheless, there are serious concerns from the industry and consumers on the use of COSE method, esespecially, with regard to process safety and quality of end-use products. In recent years, there is growing demand from functional food and nutraceutical industry for healthier and purified natural extracts. In this context, green extractions have emerged as a viable eco-friendly alternative to COSE for recovery of safer natural bioactive extracts. This lecture mainly focuses on the usefulness and applications of green extractions such as microwave-, ultrasound-, and enzyme-assisted extractions, bio-solvent extraction, pressurized hot water extraction (PHWE), supercritical fluid extraction (SFE) and plant milking technology for effective recovery of safer bioactive extracts from plant materials with ultimate objective to explore their potential uses for d nutra-pharmaceutical applications.

Metal oxides nanostructure based ultra-sensitive, non-enzymatic electrochemical sensors for targeted environmental and pharmaceutical applications

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The widespread intensification of hazardous pollutants in the environment and the massive use of pharmaceuticals turned the modern researchers to fabricate the sensitive cost-effective sensors for the quantification of environmental pollutants and drugs in pharmaceutical preparations. In order to enhance the sensitive and selectivity of electrochemical sensors, we have made an effort to fabricate different metal oxide nanostructured based sensors such as copper oxide (CuO), nickel oxide (NiO) and cobalt oxide (Co_3O_4). To confirm the crystallinity, nanometric size, functionalities, phase structure and elemental composition, the as prepared metal oxide nanostructures were directed for characterization through different analytical techniques e.g. FTIR, SEM, AFM, EDS, and XRD. All these characterization tools confirmed the successful synthesis of metal oxide nanostructures with excellent phase purity, crystalline nature and nanoscale texture. The successfully fabricated nanostructures were applied as modified electrochemical sensors for the determination of environmental toxins such as 2,4,6 trichlorophenol (2,4,6-TCP), endosulfan and drugs e.g. tramadol and ascorbic acid in pharmaceutical formulations. Different modes of electrochemical instrument were tested to evaluate the sensitive and conductive nature of sensors such as cyclic voltammetry (CV), differential pulse voltammetry (DPV) and electrochemical impedance spectroscopy (EIS). All the fabricated nanostructures based electrochemical sensors exhibited excellent linear dynamic range, high sensitivity, selectivity, and low limit of detection for the selected analytes. The efficiency of prepared sensors was tested in different real samples as water, vegetable samples and pharmaceutical formulations. The percent recoveries of prepared sensors were observed in acceptable range which greatly signifies the effectiveness of modified sensors for the determination of analytes.

Rational Material Design for Ultrafast Rechargeable Organic Lithium-Ion Batteries

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It is very important to design the devices capable of fast charging and long life for commercial application. But fabrication of lithium-ion batteries with high power and energy density is quite challenging. In recent years, a lot of work has been done to improve the rate performance and life of LIBs. We believe that better understanding of the kinetics limitations for faster batteries can guide us to design materials for ultrafast long-life batteries. To prove this, we started exploring redox active conjugated microporous polymers as an electrode for LIBs. In these systems interconnected microporous network can facilitate faster diffusion of ions. Large surface area can make the deep buried active sites accessible on or near to surface and conductivity can be improved by making composite with suitable conductive media. Combining all these effects together we were able to develop a lithium-ion cell that can be charged as fast as 66C with significant capacity retention. Also, we found that cell can be charge and discharge for 3000 cycles without any capacity loss. Through carefully investigation we revealed that high surface area, porosity, and conductivity lead to energy storage process through surface or near surface pseudo capacitive energy storage mechanism which is usually found in supercapacitor and is faster than batteries. This study shows how we can transfer kinetically slow, diffusion controlled faradic reactions in batteries to faster pseudo capacitive reactions by rationally designing the materials. We expect that this will pave the way for high power batteries with high energy density.

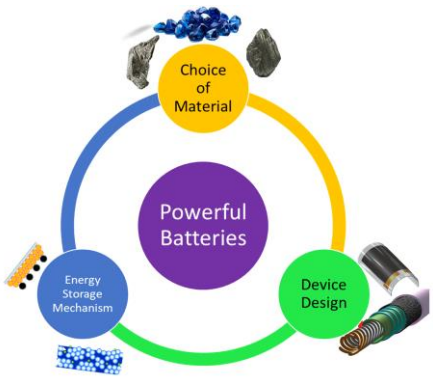

Figure 1: Important factors need to consider for high-power high-energy density batteries

Strategies for extraction of keratin from waste and its application for high-end products

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Sustainable consumption and production falls under UN sustainable development goal 12, which require environmentally sound management of chemicals and all wastes; and to reduce waste generation through prevention, reduction, recycling, and reuse. Leather industries produce huge solid keratinous waste and chromium contaminated wastewater. Keratin is considered an important raw material in variety of applications, for example wound healing fibers, composites, foams etc. This valuable raw material is abundantly available but locked in wool, feathers, hooves, horn, hairs and other hard and soft proteinous component of animals. Extraction methods of keratin have been studied including hydrolysis, reduction, sulfitolysis, enzymatic treatment, microbial treatment, ionic liquids for extraction. This presentation covers various extraction strategies and conversion techniques for high-end applications of keratin. A study where keratin sponges are obtained waste and tested to remove chromium from wastewater. Removal of chromium was optimized by multivariate method and procedure was applied for removal of chromium from synthetic and real tanning industry wastewater that showed 91% and 87.13% removal efficiency. Langmuir adsorption capacity of 270 mg/g was obtained. Desorption study showed that at pH 10 or above, sponge can be reused, and recovery of chromium is feasible. Sorption mechanism and continuous flow removal experiments were also carried out to understand the interaction and industrial viability of method. Overall finings support '*utilization of solid waste for treatment of liquid waste*' which would add into environmentally sustainable production in leather industry.

Synthesis, characterization and application of copper oxide nanoparticles coated with humic acid obtained from thar coal

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Nano particles possess great sorption ability, good mechanical properties and simple separability. Therefore magnetic CuONPs are increasingly prevalent these days are used as nano-sorbents not only in water treatment technologies but also in biomedical applications. In this study CuONPs were synthesized by co precipitation method and surface was coated with humic acid (HA) which was obtained from Thar coal by the method recommended by IHSS, then synthesized CuONPs were coated with HA. HA, CuONPs and coated CuO NPs-HA were characterized by UV-Visible, FTIR, Zeta potential and X- Ray diffraction. Finally the synthesized products applied for the elimination of organic pollutants from aqueous medium.

Design, Synthesis and Cytotoxic Effects of Curcuminoids on K562, MCF-7 and MDA-MB 231 Breast Cancer Cell Lines

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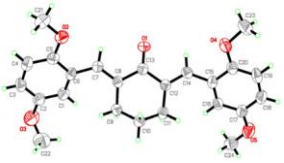
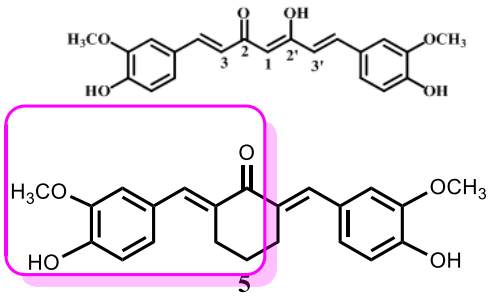
Curcumin is one of the leading compound extracted from the dry powder of *Curcuma longa* (Zingiberaceae family), which possess several pharmacological properties. However, *in vivo* administration exhibited limited applications in cancer therapies. Twenty-four curcumin derivatives were synthesized, comprising cyclohexanone **1-10**, acetone **11-17** and cyclopentanone **18-24** series. All the curcuminoids were synthesized by acid or base catalyzed Claisen Schmidt reactions in which the -diketone moiety of curcumin was modified with mono-ketone. These curcuminoids **1-24** were screened against HeLa, K562, MCF-7 (an estrogen-dependent) and MDA-MB-231 (an estrogen-independent) cancer cell lines. Among them, acetone series **11-17** were found to be more selective and potential cytotoxic agents. Compound **14** exhibited activity (IC_{50} = 3.02±1.20 and 1.52±0.60) against MCF-7 and MDA-MB-231 breast cancer cell lines. Among the cyclohexanone series, compound **4** exhibited potential cytotoxicity (IC_{50} = 11.04±2.80, 6.50±01.80, 8.70±3.10 and 2.30±1.60) against four proposed cancer cell lines, respectively. Curcuminoids with diferuloyl (4-hydroxy-3-methoxycinnamoyl) moiety with mono carbonyl group exhibited potential cytotoxic properties. The more recent SARs and structural insight will present in this coneference.





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IC_{50} = 6.70±3.10 and 2.30±1.60 µg/mL

Methods development and potential applications of graphene and metal oxides based nanocomposites

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Graphene has got a lot of attraction and is considered one of the most promising nanomaterials because of its exceptional properties and applications. Graphene oxide (GO) and reduced graphene oxide (rGO), derivative of graphene, are prepared from graphite by using variety of methods. GO and rGO are different from each other due to their C/O ratio, surface area, dispersibility, hydrophobicity, and electrical conductivity. Surface of GO and rGO is further modified with the doping of metal and metal oxides nanoparticles to further enhance their photocatalytic and biological activities.

The rGO, rare earth-transition metal oxides and their nanocomposites are prepared by using green synthesis and chemical methods for their applications in degradations of textiles pollutants, pesticides, organic pollutants, explosive materials etc. Other applications in hydrogenation reactions, slow release fertilizers, forensics, filtration and solar cells have also been studied.

We have successfully synthesized more than 60 nanocompostes with variety of metals, GO and rGO. Various factors e.g. change in precursors, pH, temperature, feed rate, surfactants, solvents, methods of preparation, concentration of precursors, were studied which change the efficiency of the nanocomposites.

The structural investigation, thermal stability, morphology, optical properties, and photocatalytic properties of synthesized samples were studied by using different characterization techniques i.e. Thermogravimetric analysis (TGA), *Differential scanning calorimetry* (*DSC*) Fourier transform-infrared spectroscopy (FTIR), Particle Size Analyzer (PSA), Powder X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Photoluminescence (PL) and Ultraviolet-Visible spectrophotometer (UV-VIS).

Emerging Aspects of Fly Ash based Active Zeolites and Zeolite synergized photocatalysts for Wastewater Treatment

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Fly ash as a particulate and leachate pollutant has been recognised as human carcinogen. Its dumping can be detrimental for soil fertility and ground water as well as financial liability. It can be utilized for the synthesis of value added materials like zeolites. In this work a variety of fly ashes from boiler plants of different industries were used for the synthesis of fly ash based active zeolites (FAAZ). Fly ash based zeolites and zeolite synergized photo-catalysts prepared by conventional and advanced curing techniques were characterized by state-of-the-art analytical techniques like; XRD, SEM, FTIR, ICP-OES, CEC and Raman spectroscopy and investigated for their wastewater treatment potential. It was observed that photo-catalyst assisted zeolite composites via recycling of fly ash waste for wastewater treatment is a positive move towards achieving a healthy environment and green technology.

A theoretical design of superalkali doped nanocages as high performance nonlinear optical materials

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Nonlinear optical (NLO) materials have surpassed a plethora of science and technology owing to their potential applications in optoelectronics. The effect of Li_4N and Li_4O doping on the structural, electronic and nonlinear optical properties of the $Al_{12}N_{12}$ nanocage has been investigated theoretically by using DFT simulations. The results reveal that superalkali doping has a significant impact on the $Al_{12}N_{12}$ nanocage. Interaction energies value up to -118.49 kcal mol^{-1} reflected that designed complexes are thermodynamically stable. Their HOMO-LUMO energy gap is reduced up to 50.75% in comparison to pristine $Al_{12}N_{12}$ nanocage. All isomers are electrides in nature and have diffuse excess electrons. These complexes possess deep ultraviolet transparency. Nonlinear optical response of superalkali doped $Al_{12}N_{12}$ is enhanced and the highest first hyperpolarizability of 5.7×10^4 au is obtained for $Li_4N@Al_{12}N_{12}$ isomer. The small transition energies (1.27–2.73 eV) and charge transfer from the superalkalis to the nanocage are responsible for the significant increase in the NLO response. The nature of intermolecular interactions between the superalkalis and $Al_{12}N_{12}$ nanocage is further investigated by using QTAIM and NCI analyses. The electrostatic contact between closed shells is dominating, according to QTAIM topological analysis. This research offers an insight into the design and fabrication of nonlinear optical materials with outstanding NLO properties for their remarkable applications in optoelectronics.

Development of glucose conjugated NIR fluorescent bioprobe for in vivo tumor targeting

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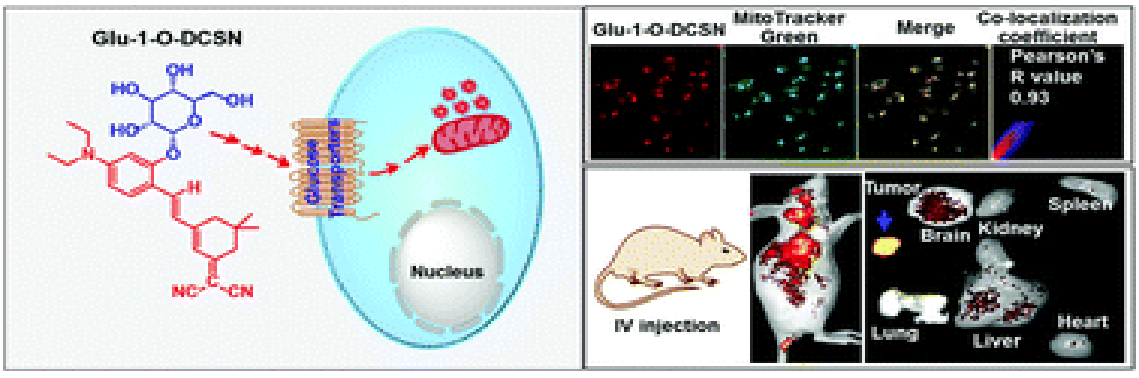
Fluorescent probes with high sensitivity, photostability, and operational efficacy are gaining popularity as bioimaging and disease detection tools. The majority of probes require UV light for stimulation, causing cell damage and processing issues. The current study looks into the synthesis of Glu-1-O-DSCN, a new red fluorescent bioprobe made by treating 2-(3, 5, 5-trimethylcyclohex-2-en-1-ylidene) malononitrile with 1-O-Glu-4-(diethylamino)-benzaldehyde. The C1-type D-glucose-conjugated fluorescent probe Glu-1-O-DSCN has been accomplished employing D-glucose. The C-1 type glucose conjugation is more appropriate than the C-6, C-2, and other positional isomers due to higher similarity to D-glucose and higher affinity for GLUTs. The bio-probe Glu-1-O-DCSN has been competitively phagocytized by cells in comparison to D-glucose through the phosphorylation pathway and showed good sensitivity and selectivity for mitochondrial organelle of cells. The Glu-1-O-DCSN expressed high fluorescence at 685nm, with λ_{ex} of 530 nm and offered stoke shift of 150 nm. The probe's quantum yield is moderate when compared to other AIE dyes and comparable to normal hydrophobic ACQ probes. The probe showed signal in malignant cells that lasted for 23 hours, while it was lost in non-cancerous cells after 1.5 hours. The considerable accumulation in tumor cells suggests that the Glu-1-O-DCSN probe could be used as a clinical tracer in intraoperative tumor-targeted imaging techniques for surgical navigation, as well as an indicator for anticancer medication screening and assessment.

Development of glucose conjugated NIR fluorescent bioprobe for in vivo tumor targeting
Ghulam Shabir and Aamer Saeed



Metal-Organic Frameworks towards N-doped carbon nanotubes: Energy Conversion and Storage Applications

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Carbon based materials have attracted much attraction in recent years due to their variety of applications in gas storage, as electrode material for super-capacitors and as a catalyst support for various electrocatalyst of energy related devices. We have recently explored that nitrogen rich carbon nanotubes (N-CNTs) could be synthesized via simple pyrolysis of Metal-Organic Frameworks (MOFs) under specific conditions. Not only this, but highly active metallic nanoparticles could also *insitu* embedded in these N-CNTs; which is otherwise difficult task to do. Once fabricated, these materials are very useful in variety of applications. We have found that cobalt oxide embedded N-CNTs can be utilized in energy related applications such as oxygen evolution reaction (OER), oxygen reduction reaction (ORR), and in battery applications. For instance, CoO_1-P_{1-x} /N-CNTS, CoO_1-P_{1-x} /N-CNTS, shows superior performance towards OER with an overpotential of 250 mV @ 20 $mAcm^{-2}$ and maximum current density of 180 $mAcm^{-2}$ in 1 M KOH solution.

Design, Synthesis and Structural Studies of some New Azoles as Important Biological Scaffolds

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A new series of 1,3,4 -oxadiazoles, 1,2,3-triazoles, pyrazoles and thiazoles have been synthesize and characterized by different spectroanalytical techniques.Fully characterized molecular structures were further studied by single-crystal X-ray diffraction where applicable. 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.

Basic Requirements Of A Kinetics Study

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There are three basic requirements of a kinetics experiment i.e., method of activation, suitable medium for reaction to proceed and method of detection. As far as activation is concerned, this can normally be carried out by thermal, chemical, photo activation and electric discharge. For a reaction to proceed, a suitable medium is required. The choice of the media depends upon the temperature at which the reaction is expected to take place and as such water bath, oil bath and salt bath are normally used for reactions in the temperature range from room to 750K. For higher temperature region special techniques like shock tube and flash photolysis are used. Once the reaction has initiated then there is a dire need to determine the kinetic parameters and mechanism of reaction and this can be followed by a using a suitable detection technique. The last step in the kinetics study is to interpret the experimental results and compare it with theoretical results using RRKM calculation. If the results coincide with each other, then our experimental observations are supported by theories, otherwise we have to seek explanation for the same. Moreover, the advantages and reliability of one system over the other are discussed.

Innovations in Chemical Science and Nanoscale Catalysis for Water Splitting and Synthetic Fuels

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

Use of whole cell enzymes as a green catalyst in the chemistry

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With the use of enzymes, one can omit the tedious blocking and deblocking steps that are common in enantioselective and regioselective organic synthesis. Thus, enzymes are considered to be more satisfactory catalysts than conventional chemical ones from economic and environmental points of view. Both isolated enzymes and whole cells have been used ; compared with isolated enzymes, whole cell catalysts can be much more readily and inexpensively prepared. Because enzymes in cells are protected from the external environment, they are generally more stable in the long-term than free enzymes. In current talk I will discussed the work done in our lab for isolation, identification and use of such whole cells for bioconversion of active compounds as well as for biodegradation of toxin studied. Among bioactive conversions, production of conjugated lipids like selective isomeric production of conjugated linoleic acid isomers using whole cells of *L. Plantarum* will be discussed with obtained results. Moreover role of whole cell for biodegradation of toxic compounds like phthalate esters, reluctant pesticides and petroleum hydrocarbons will be elaborated by outcome achieved using bacillus species isolated from soil.

Toxic elemental levels in whey milk of different cattle and human using an innovative digestion method based on a deep eutectic solvent: Risk assessment for children <6.0 month to 5 years

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In present study the toxic elements, arsenic (As), cadmium (Cd) and lead (Pb) were determined in whey of milk samples obtained from different cattle (cow, goat, buffalo, sheep, camel) and human of different areas of Sindh, Pakistan based on consuming groundwater and surface canal water. The whey of milk was separated by lowering the pH and centrifuges. The whey of milk samples was subjected to ultrasonic assisted digestion method using a deep eutectic solvent (DES) prepared by choline chloride–oxalic acid (ChCl–Ox) at different mole ratio. After different time and temperature, the contents of the tubes centrifuged to separate the upper layer and subjected to inductively coupled plasma optical emission spectrometry. The effects of different parameters on digestion efficiency of whey milk samples to determine the toxic elements including time and temperature of ultrasonic bath, mole ratio and volumes of DES were examined. The total levels of all selected toxic elements were also detected in milk samples of cattle and human, after acid digestion method. The validity of proposed method was carried out by a conventional acid digestion method of selected whey milk samples and spiked certified standards in real sample. At the optimum conditions, the limit of detection and quantification, and relative standard deviation (RSD %) were determined. The simplicity of the proposed experimental procedure, short analysis time, lack of using concentrated acids and oxidizing agents, as well as using inexpensive chemicals. The As, Cd and Pb contents in milk samples of cattle and human consumed contaminated ground water was found to be 2 to 3 folds higher than those values observed for milk samples of cattle consuming fresh surface water. The % of all three toxic elements were found in whey milk of all cattle corresponding to 24 to 50% of total contents of them. Based on concentrations of toxic metals; estimated daily intake (EDI), hazard quotient (HQ) and carcinogenic risk (CR) were calculated for <6 month to 5years old children.

Applications of FTIR spectroscopy in Oils and fats analysis

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In the last few decades, Fourier transform infrared (FTIR) spectroscopy has shown great potential in food analysis due to its simplicity and easy to use the technique. Oils and fats are important food components of daily life. The quality and safety of oils and fats pose a major concern for consumers and food producers. In this talk, recent developments of chemometrics in FTIR applications to the oils and fats quality parameters will be discussed such as moisture, iodine value, free fatty acid, peroxide value, CD and CT, FAC, TFA, classification, adulteration, oxidation stability, etc.

Structural tuning of non-fullerene acceptors and small molecule donors to get their high estimated power conversion efficiency for high performance organic solar cell. A quantum chemical analysis

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The designed molecules were estimated for their structural, optical, electronic and photovoltaic properties using density functional theory method MPW1PW91/6-31G (d, p). The simulated results of all the modelled molecules comparative to the reference molecules lie in the range of efficient solar cell light harvesting unfused non-fullerene acceptors. In addition, they were successfully tested for their solution processability and their interface with donor material PBDBT was made to calculate fill factor and open circuit voltage. In all modelled molecules, BDCl2F-DS has highest value of open-circuit voltage (1.71 eV) and fill factor (92.25%). PCE estimation of modelled molecules was incurred by assuming a similar value of short circuit current from the reported work of reference molecules. The extraordinary PCE values (in the range of 27.36 % to 33.76 %) were estimated for these modelled unfused non-fullerene molecules which is fruitful theoretical work for the experimental scientists to advance the investigation of unfused non-fullerene acceptors.

Ionic Liquids as Designer Solvents for Green Processing of Agricultural Waste

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Ionic liquids (melting point <100 °C) are designer solvents constituting organic moiety as well as ionic interactions in the same molecule, that is responsible for their unique 'solvating' properties. They can efficiently be used to dissolve biopolymeric components of lignocellulosic agricultural waste that cannot be dissolved in traditional solvents. We have developed a method to process agricultural waste using ionic liquids to produce a variety of carbon constrained biofuels, fine platform chemicals and food grade sugars. The process is highly green, economic and eco-safe as we are using waste as raw material, biodegradable, biocompatible and highly recyclable ionic liquids as well as ambient processing conditions. Our main highlighted products are 5-hydroxymethylfurfural (5-HMF), 5-ethoxymethylfurfural (5-EMF), food-grade glucose, carboxymethylcellulose (CMC) and vanillin.

Synthesis and Molecular Docking Studies of Some Bioactive Sulfonamides Incorporating bromoacetamide Moiety

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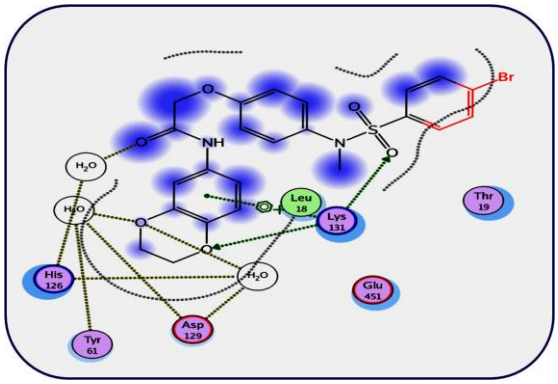
This study explores the effect of the structural changes of novel sulfonamide and their behavior toward enzyme inhibition and antifungal activities. Novel sulfonamide derivatives were developed by reacting 1,4-benzodioxane-6-amine with ethane sulfonyl chloride, this compound on treatment with various alkyl/aralkyl halides, in aprotic solvent and basic conditions resulted in the formation of *N*-alkyl substituted derivatives. The structures elucidations were ascertained with spectral and elemental analysis. The prepared sulfonamides were subjected to in-vitro enzymatic and antifungal activities which have shown that prepared compounds exhibited excellent antifungal and better lipoxygenase activities. Structure activity relationship was ascertained by introducing different alkyl group derivatives at p-position which showed electron withdrawing group have a profound effect on the biological activity. In addition, computationally docked studies of the compounds showed significant interaction with AChE, LOX and BChE active sites, verified by experimental data.



MOFs for Water Purification

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Heavy metals especially lead (Pb) and mercury (Hg) are recognized as most emerging pollutants in underground water and are major threat to public health around the world. Major challenge to mitigate water pollution is construction of effective materials containing a host of deceivingly accessible high-density and high-level efficiency. Herein, we have synthesized two metal-organic frameworks (MOFs) with efficient porosity showing the right combination of structures. Representatively, ZIF-8 and ZIF-67 were designed by reacting Zn, Co salts with 2- methyl imidazole showing superior efficacy in removing Pb and Hg (1978.63 & 1436.11 mg/g respectively) from water. These adsorbents displayed high distribution values permitting them to quickly reduce concentration level of $Pb2^{+}$, Hg2 + below permissible limit (Pb = 0 – 15 µ g/L, Hg = 1 – 10 µ g/L). EDX, FTIR analysis revealed that Pb2 + , Hg2 + bound through weak interactions. Results presented here have shown extraordinary potential with high environmental remediation performance having 99.5% and 98.1% removal efficiency for lead & mercury respectively. Results revealed that adsorbents have same organic linker that identifies same morphology required for adsorption. The difference in adsorption capacity and porosity (ZIF-8 = 937 & 1370 m2/g, ZIF-67 = 1289 & 1889 m2/g) are deliberately caused due to presence of metal atoms having different electronic distribution, as cobalt in ZIF-67 and in case of ZIF-8 zinc metal.

Role of Pyridine as enzyme inhibitors

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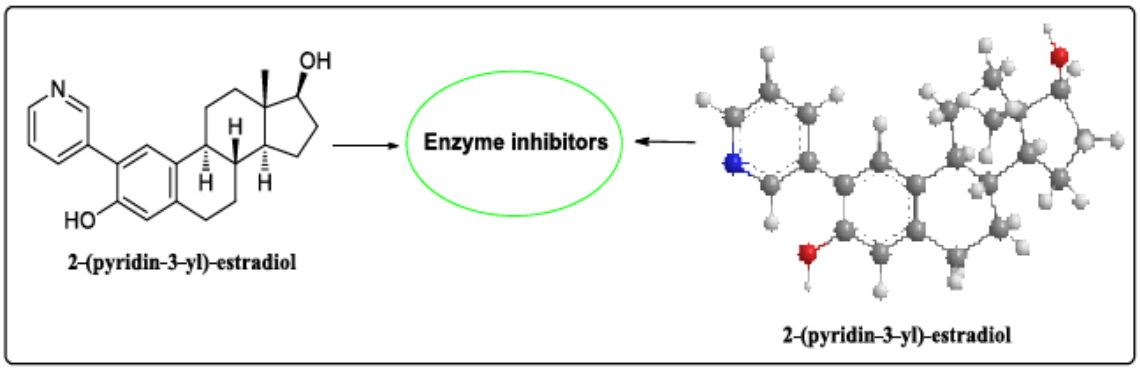
Research teams are investigating new approaches for the synthesis of alternative scaffolds to be used as promising chemotherapeutics. In advancement of this, replacing of benzene ring with a pyridine ring-tagged sulfonamide moiety. A new class of functionalized benzothiazole and benzimidazole-based pyridine incorporating sulfonamide moieties are came into being the clinical trial of imidazole-type inhibitors an orally active inhibitor.

An inhibitor could modulate the bioactivation of procarcinogens while reducing drug resistance. Inhibition of enzymes such as cytochrome P450 1B1 (CYP1B1) is a promising therapeutic strategy. 2-(pyridin-3-yl)-estradiol is the best inhibitor reported until now. A major point of consideration is that the position of the nitrogen atom in the aromatic ring has little influence while the position of the pyridine ring plays a key role and difference between the oxidized and reduced form on their inhibition potency is not much important for the synthesized derivatives until now. Actually, the pyridine ring interacts with the heme group through a nitrogen−iron bond. Moreover, we found that the pyridinyl moiety promotes an ideal orientation to perform pi-stacking interactions. Promising results with the pyridinyl moiety opens the door for the development of a new generation of inhibitors.



Infection imaging potential evaluation of Technetium-99m labeled Antimicrobial Agent

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The aim of this study was to evaluate the Technetium-99m labeled antimicrobial agent, livofloxacin. Livofloxacin is known for its broad spectrum antibacterial affect and well known for in quite good pharmaceutical efficacy. This property was exploited for labeling with gamma emitter radionuclide, Technetium-99m to diagnose deep seated bacterial infections. The development of Technetium-99m labeled livofloxacin was carried out at room temperature and mild reaction conditions. The labeling efficiency was recorded >95% and the complex was found quite stable in injection solvent and fresh blood serum for 6 and 4 hours, respectively. The biodistribution study in normal and S. aureus infected rabbit model showed satisfactory results. No unwanted accumulation was noted in the body. The infected muscle to normal muscle ratio was found 3.6 which is comparable to FDA approved infection imaging agent, Infecton®. In conclusion, the Technetium-99m labeled livofloxacin is quite good candidate for infection imaging which could be tested further to start clinical trials?

Development of Glucose Conjugated NIR Fluorescent Bioprobe for In Vivo Tumor Targeting

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Fluorescent probes having high sensitivity, high photostability and high operational efficacy are emerging as powerful tools in bio-imaging and disease diagnosis. Most of probes require ultraviolet light for their excitation which creates cells damaging and processing problems. The present investigation deals with the synthesis of new red fluorescent bioprobe Glu-1-O-DSCN which has been accomplished by treatment of 2-(3,5,5-trimethylcyclohex-2-en-1-ylidene)malononitrile with 1-O-Glu-4-(diethylamino)-benzaldehyde. D-Glucose has been xploited to achieve C1-type D-glucose-conjugated fluorescent probes Glu-1-O-DSCN. The C-1 type conjugation of glucose is more apropos as compared to C6, C2 and other positional isomers because the C-1 type glucose-conjugated probes show superiority with higher similarity to Dglucose and higher affinity for GLUTs and unnecessity of glucose depletion for monitoring glucose uptake in live cells. The bio-probe Glu-1-O-DCSN showed high sensitivity and selectivity for mitochondrial part of cells and were competitively phagocytized by cells with respect to Dglucose through phosphorylation pathway. The Glu-1-O-DCSN probe exhibited high fluorescence at 685nm with excitation wavelength of 530 nm demonstrating stoke shift value of 150 nm. The quantum yield of the probe is moderate as compared to the general AIE type dyes and is close to that of regular hydrophobic ACQ probes. The probe displayed signal in cancerous cells and maintained it for 23h while its signals was diminished within 1.5h in non-cancerous cells. The significant accumulation in the tumor cells promises various applications of Glu-1-O-DCSN probe, as an indicator for anticancer drug screening and assessment, and a clinical tracer in intraoperative tumor-targeted imaging approaches for surgical navigation.

Synthesis of carbohydrazones as promising alpha-glucosidase inhibitors for treatment of Diabetes Mellitus

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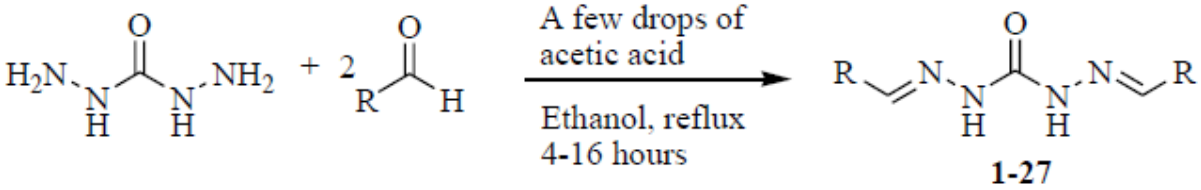
Diabetes Mellitus is a chronic disorder in which the body does not produce enough or respond normally to insulin, resultingly, causing blood sugar (glucose) levels to be abnormally high. It is the most common disease worldwide. According to an estimate, global diabetes prevalence will be increased to about 10.2% (578 million people) by 20230. Therefore, scientists are constantly looking for inexpensive and safe therapies to control diabetes mellitus. *Alpha*-glucosidase is an exoenzyme which is responsible for hydrolysis of starch to simple sugars and located in the brush border surface of small intestinal cells. In human beings, the enzyme helps in digestion of carbohydrates and starches to produce glucose for intestinal absorption which ultimately leads to increase level of blood glucose (hyperglycemic condition). Therefore, inhibitors of this enzyme are important for treatment of hyperglycemic condition in patients of type II diabetes mellitus. We have synthesized carbohydrazones (**1-27**) by refluxing carbohydrazide and a variety of substituted aldehydes in the presence of ethanol and acetic acid. Synthesized compounds (**1-27**) have been purified and characterized by mass spectrometry and NMR spectroscopic techniques. In addition, all synthesized compounds have furnished good CHN analysis. All synthesized compounds have also been evaluated for their potential as alpha glucosidase inhibitors and study have identified interesting lead molecules having alpha-glucosidase inhibition potential even better than the standard acarbose. The talk will highlight synthesis and bioactivity study of carbohydrazones.



Scheme: Synthesis of carbohydrazones (**1-27**).

Environmental Deterioration of Historic Ornamented Façade of Chauburji, Lahore Pakistan

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The environmental deterioration is an alarming phenomenon that is destroying the historic structures assemblage of hidden past around the globe. The multi-analytical and nondestructive techniques over the last decade aided in the identification of deterioration products of historic materials and developed the diagnostic procedures for better understanding of the components along with their transformations over the years. The selected heritage site of Chauburgi is one of the Mughal monuments constructed during the reign of Emperor Shah Jahan as a gateway to a large garden built on Chahar-Bagh concept. This paper is particularly focused on the glazed tiles ornamentation, one of the distinct symbolic features of Mughal decorative arts. The glazed tile ornamentation which is known for the tangled geometric expression with minute detailing reflected the refined artistic taste of the builders. The rapid deterioration due to the environmental conditions (natural and anthropogenic) displaying ruthless behavior needs a systematic thorough investigation for reduction in the process. The obtained samples were studied through the optical microscopy and X-ray powder diffraction as the first step in sequential process of diagnostic investigation. The major and trace elemental analysis were also carried out to understand the transformations of historic materials along with the texture analysis through scanning electron microscopy-energy dispersive spectroscopy. The generated results unveiled the causes and impacts of environmental deterioration necessary for the understanding of the deterioration phenomenon and products. The future restoration plans based on these results would save this historic site for the next generations.

Green synthesized silver activated Copper oxide nanocomposite for photocatalytic degradation of Methylene blue

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Ag decorated CuO nanoparticles (Ag-CuO), an efficient photocatalyst was synthesized by sol-gel method. Capparis decidua plant extract was used as natural reducing and stabilizing agent. Surface decoration of nanoparticles by Ag were studied by SEM. XRD suggests monoclinic crystalline structure for CuO and also gave clue for successful Ag doping. Particle size and effect of Ag doping on particle size were sighted by HRTEM images. EDX spectra were used to study purity of nanocomposites. Cu-O bond formation was confirmed by FT-IR spectra. Superior catalytic activity of Ag-CuO was explored by methylene blue (MB) degradation from aqueous solution. Various amounts of Ag were doped to investigate the structural morphologies and applications deeply. Experimental conditions such as pH, catalyst dose, analyte initial concentration, contact time were optimized. Degradation mechanism and enhancement of catalytic properties with Ag doping were deeply studied and explained.

CTAB-assisted development of hierarchical flower-like multimorphology magnesium oxide for phosphate removal from the aqueous phase

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In this work, a series of hierarchical flower-like magnesium oxide (MgO) adsorbents were fabricated in a cetyltrimethylammonium bromide (CTAB) assisted solvothermal route using hexamethylenetetramine (HMTA) as a precipitating agent. Effects of CTAB feeding amount on the structure, morphology, pore structure, and corresponding adsorption behavior were investigated. The hierarchical gardenias flower-like MgO demonstrated a surface area of 336.54 m_2g^{-1} at a minimum ratio of the CTAB/Mg^{2+} in the reaction system. The hierarchical MgO phosphate removal capacity was found to be 265.11 mg g_{-1}, which followed the pseudo-second-order and Freundlich isotherm model obtained from the large surface area and appropriate pore size. The value of n also suggesting the feasible nature of phosphate adsorption under the examined conditions. Indeed, this CTAB assisted hydrothermal method can provide a new understanding to tune the desired properties of a material by merely adjusting the reaction parameters (Fig. 1).

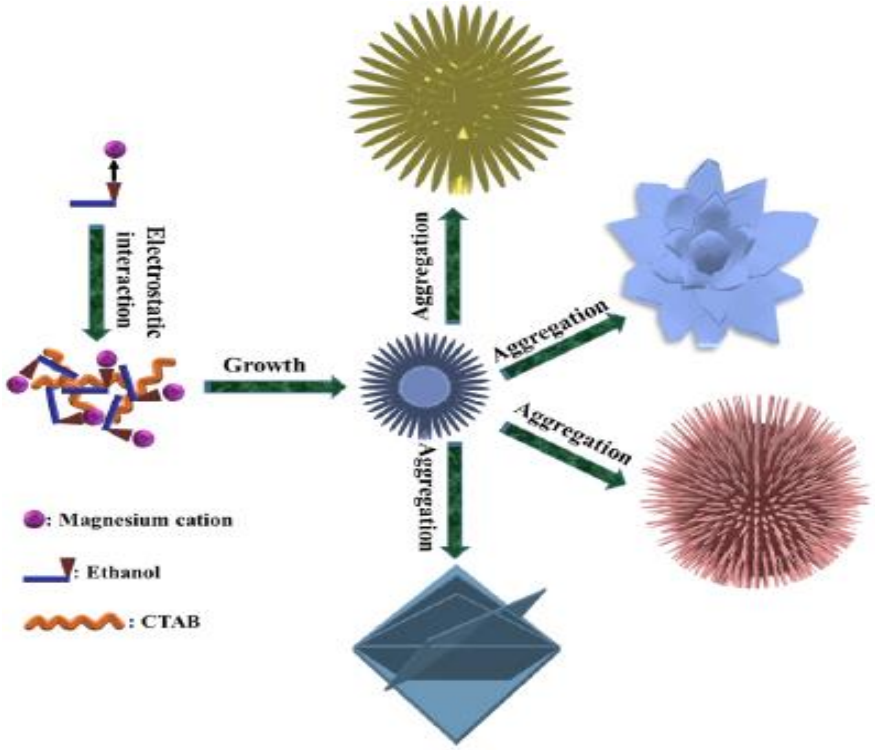

Fig. 1 Development of hierarchical MgO flowers using the CTAB-assisted hydrothermal route

Plant mediated synthesis of MnO-GO-Ag nanocomposite and its potentized anti-inflammatory and antioxidant activities

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In this work we reported the plant mediated synthesis of MnO-GO-Ag nanocomposite and its potentized anti-inflammatory and antioxidant activity. The plant used in this work is Fagonia arabica a medicinal herb. Manganese oxide and silver nanoparticles were fabricated by using green synthesis approach. Graphene oxide was synthesized by hydrothermal method and hummer's method with some modifications. The synthesized nanocomposite were characterized by SEM, XRD, EDX and UV-Visible spectroscopy. According to SEM analysis the composite showed bipyrimidal morphology with reduced agglomeration. XRD analysis provide information about crystallographic data, crystallinity and particle size. XRD spectra obtained is in a strong agreement for the formation of desired product. Elemental analysis was confirmed by EDX. Presence of C, O, Ag and Mn confirmed the formation of our desired nanocomposite (MnO-GO-Ag nanocomposite). Anti-inflammatory and antioxidant activity was evaluated both for the sample (MnO-GO-Ag) and standard by UV-Visible spectroscopy. The synthesized nanocomposite showed more % inhibition of about 34.15 and 81.71 at the concentration of 0.1 and 0.5 mg/ml while standard has a % inhibition value 10.98 and 35.37 at similar concentration. In the same way MnO-GO-Ag nanocomposite showed high % scavenging and lower value of IC50 as compared to standard (ascorbic acid). Lower the value of IC50 higher is the efficiency of nanocomposite for anti-inflammatory and antioxidant activity.

Green Synthesis of Silver Nanoparticles for Potential Antibacterial Applications

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The research in the field of nanotechnology is developing fastly due to the broad spectrum applications of nano materilas. Many of these nano materials find important applications in the field of medical sciences. The research and development of potential bactericidal/fungicidal pharmaceuticals is the utmost requirement of the time to protect present and coming human generations from infectious diseases. Among metal based bactericidal agents, silver nano particles (AgNPs) possess potential bactericidal properties. Chemical as well as green synthetic approaches could be used to synthesize these particles. However the green synthesis method is preferable due to associated benefits. Here, we present AgNPs synthesis using Populus ciliata leaves extract. The characterization was carried out with different techniques. The XRD results indicated the crystalline purity of the NPs. TEM studies revealed spherical shaped nano particles with average size (4 nm). The small sized NPs are ideal for good bactericidal activities. The bactericidal potential of these NPs was tested against selected gram positive (Staphylococcus epidermidis and Streptococcus pyogenes) and gram negative bacteria (Klebsiella pneumoniae, Serratia marcescens, and Pseudomonas pseudoalcaligenes). The small sized AgNPs have shown significant antibacterial activities.

Zinc Oxide Nanocomposites Using Various Types of Berries: Synthesis, Characterization and Applications

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Green synthesis of nanocomposite is a simple, cheap, and eco-friendly alternative to physical and chemical synthesizing techniques. In this study, ZnO nanocomposites were prepared using three fruit extracts. The synthesized ZnO nanocomposites were characterized by Scanning electron microscope, UV/VIS spectrophotometer, Fourier transform infrared spectroscopy, and X-Ray Diffraction techniques. The X-ray diffraction patterns verified the crystalline nature of the produced nanocomposites as well as their size in the range of 10-80nm. FTIR analysis confirmed the existence of several functional groups in synthesized ZnO nanocomposites. The UV absorption peaks of Elaeagnus umbellata thumb (ZnO-EUT) nanocomposite at 340nm, Rubus idaeus L.(ZnO-Ri) nanocomposite at 360nm, and Rubus fruticosus L.(ZnO-Rf) nanocomposite at 360nm are observed. The shape, particle size, and morphology of ZnO nanocomposites are assessed by using SEM. Nanocomposites were analyzed for their antimicrobial activity and found to be effective against three tested phytopathogens. The antimicrobial activity of ZnO nanocomposites showed good results against Escherichia coli (341), Staphylococcus aureus(345B), and Pseudomonas aeruginosa (5994 NLF). This study presents a simple and inexpensive green strategy for synthesizing zinc oxide nanocomposites with effective antibacterial activity.

Tumor homing and pro-apoptotic hybrid peptide-based novel self-assembled nanoparticles as multimodal imaging probe for cancer diagnosis and therapy

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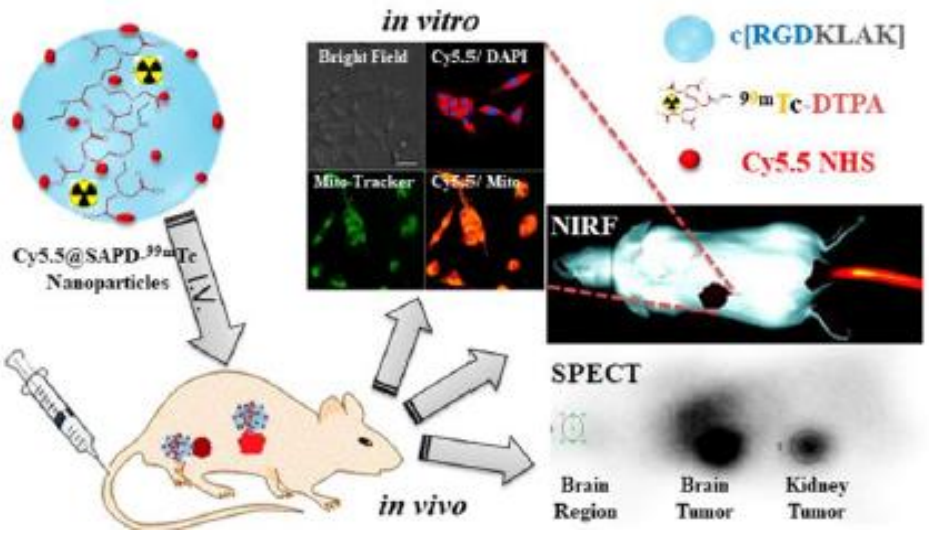
Dual-Targeting drug delivery technique serves as a “guided missile” to enhance the efficient targeting of the drug towards cancer cell’s vasculature. In the past two decades, the drugs fabrication strategy has been developed by hybridization of integrin-receptor targeting ligands, peptides, proteins, and aptamers. The goal of the presented research was the design of novel short-chain cyclic peptide having RGD-coupled KLAK motifs, which were further transformed into self-assembled spherical nanoparticles. The RGD tripeptide serves as tumor-homing motif whilst KALK sequence as mitochondrial apoptosis-inducing motif. This novel peptide nanoprobe was further modified using Cy5.5 NHS as near infrared fluorescence dye as well as ^{99m}Tc-DTPA as gamma-emitting radionuclide via covalent bond to show multimodal imaging functionality. These nanoparticles were showed improved cellular internalization, in vitro cytotoxicity, and apoptosis-inducing applications in U87MG cells. Moreover, this probe showed promising enhancement for $\alpha_v\beta_3$-integrin receptor binding efficiency against U87MG cells, excellent dual-imaging potentials, and improved apoptosis-inducing features. Surprisingly, the in vivo investigations in tumor-bearing mice models highlighted the profound dual-imaging as well as therapeutic efficacy of this newly developed hybrid peptide-based nanoparticles. This research study may serve as an excellent approach for the development of multimodal imaging probes for the diagnosis of cancer while minimizing the drawback of individual techniques.



Novel designed dual-targeting peptide-based self-assembled nanoparticles conjugated with Cy5.5 dye (NIRF-dye) and Technetium-99m (γ-emitting radionuclide) for multimodal imaging of glioblastoma multiforme as well as efficient therapeutic agent

Electrochemical determination of some important anions using modified and unmodified multiwalled carbon nanotubes paste electrodes

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The determination of anions such as sulphide, nitrite and iodide are essential for both environmental and biological significance. For this purpose, a sensitive and simple cyclic voltammetric (CV) assay using multiwalled carbon nanotubes paste electrode (MWCNTPE) has been proposed for the direct detection of sulphide. Sulphide exhibited a distinct oxidation peak at about 0.56V in NaCl as a suitable supporting electrolyte. The oxidation peak current values were found to increase in a linear way as the concentration of sulphide increased in the range from 1×10^{-7} to 3×10^{-5} M (R^2 = 0.9985). The detection limit was 4×10^{-8} M. The proposed method exhibited high selectivity towards the oxidation of sulphide than other competing anions.

A CV method has also been investigated for the determination of nitrite by using a MWCNTPE modified with chitosan-functionalized silver nanoparticles. By combining the advantages of chitosan, AgNPs and MWCNT, the assay exhibited a remarkable improvement in the cyclic voltammetric response towards the oxidation of nitrite. The oxidation peak current increased linearly in the range from100 nM to 50 μM for nitrite concentration and the detection limit was found to be 30 nM.

In another work, a MWCNTPE was modified with cuprite (Cu_2O) to develop a new voltammetric method for the detection of iodide. The effect of pH, accumulation time etc. of the method was investigated. A good linear correlation between peak current and iodide concentration was achieved in the concentration range from 1×10^{-8} – 1×10^{-4} M with a LOD of 4×10^{-9} M. The proposed assay showed high efficiency in the determination of iodide in urine samples.

Anion exchange removal of arsenic by calcined and uncalcined samples of $Fe(OH)_3$

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The adsorption study of arsenate on to iron hydroxide was conducted in terms of the effect of arsenic concentration, ionic strength of background electrolyte, calcination of adsorbent and pH of the system. Adsorption of arsenate was maximum in the lower pH range and decreases with the increase in initial pH of the system. Thermal treatment drastically reduces both the surface area as well as the sorption capacity of iron hydroxide towards the arsenate removal from solution in the order: iron hydroxide (uncalcined) > iron hydroxide (300C) > iron hydroxide (550°C) > iron hydroxide (750C). Desorption of arsenate was found to be maximum at pH 12. It was concluded that the freshly prepared iron hydroxide behaves as a promising material for the anion exchange adsorption of arsenate from aqueous electrolyte solution.

Novel Moldable Hard Tissue Implants with High Hydroxyapatite Loading

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Hard tissue implants are used to fill and speed up healing of bony defects caused by orthopedic injuries, infections, tumors, and osteonecrosis. Hydroxyapatite (HA) is a gold standard bioactive regenerative ceramic. Many pre-mixing steps are required before it can be employed on defective site during surgery. In this work the moldable hard tissue regenerative implants are prepared by using HA and polymeric carrier to achieve ease of handling. Polyalkylene oxides i.e. PEG, PAA, PEO, PPG, p123, F127, and Polyoxamers are safe and cost-effective polymers that are part of a variety of FDA-approved products for internal consumption are explored. To achieve the necessary moldability, type and amount of polyalkylene oxides as well as their ratio to HA were optimized. Finally, desired osteoconductivity and mold ability of bone graft substitutes were achieved by loading of 70% HA into PEG. Different characterization data such as FTIR, SEM and XRD confirmed that bioactive ceramic reinforcement was incorporated and evenly distributed within the polymeric matrix. Cell viability studies elucidated that the moldable graft is expected to have no negative effect on the biological environment. Evaluation of the mechanical behavior of the moldable bone graft confirmed the easy mobility and an expected ease of use for the surgeon whilst treating a bony defect site hence fulfilling the initial objectives of the reported study. Prepared moldable grafts are potential candidates for effective regeneration of bone defects, dry sockets, implant site development, periodontal defects, coronal flaws, extraction site repair, implant dehiscence defects, sinus left defects, and localized mild ridge defect.

Metabolic Profiling Of Macrophomina Phaseolina

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Microorganisms are a huge source of structurally diverse and pharmacologically important molecules. Solid phase culture of Macrophomina phaseolina was studied for its chemical profile and biological potential. The crude methanolic extract of the culture exhibited moderate to good antioxidant, leishmanicidal, anti-bacterial and anti-fungal activities. GC-MS analysis of the semi-pure fractions obtained from the crude extract showed the presence of about 35 metabolites in different yields. Preparative column chromatography led to the isolation of a pure compounds, among which one was structurally characterized as 1,5-dimethyl citrate (1). The chemical structure of the purified compound was established with the help of 1D- and 2D-NMR spectroscopy and mass spectrometry.

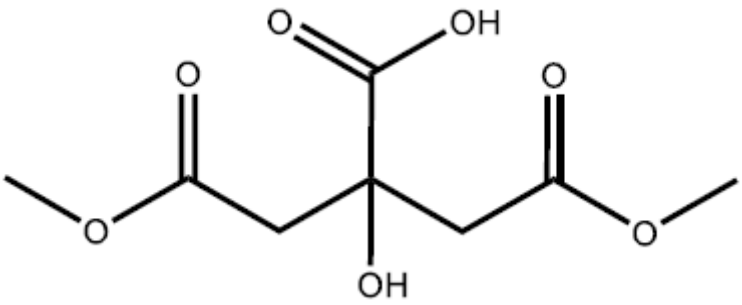

Fig: Structure of 1,5-dimethyl citrate (1)

Functionalized Libraries of Nitrogen Containing Heteroaromatic Scaffolds for Urease Inhibition

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The resistance towards the numerous physiological disorders ascribed to ureolytic enzyme (urease) is still a challenge due to inefficient and unsafe administration of drugs. For instance, Urease (EC 3.5.1.5), a heteropolymeric nickel-containing enzyme from the amidohydrolases and phosphotriesterases family are responsible for the rapid hydrolysis of urea into ammonia and carbon dioxide thus a leading cause of increased ammonia level. In short, the higher level of ammonia is devastating and leads to numerous health issues such as gastrointestinal (peptic ulcer, gastric cancer, duodenal ulcers) and urinary tract (catheter encrustation, kidney stone formation, hepatic coma, encephalopathy, and pyelonephritis) infections. In this aspect, the burgeoning of potential inhibitors of urease could be considered as promising therapy to overcome such challenging issues and capable of treating disorders emerged as a result of pathogenic activities of microorganisms. The current presentation is focusing on the development of new libraries of diverse nitrogen containing heteroaromatic scaffolds as urease inhibitors.

Synthesis, Characterization, Anti-Cancer and Anti Inflammatory activities of 3, 5 Disubstituted Thiadiazine-2-thiones

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In view of developing potent bioactive compounds, a series of Tetrahydro-2H-1, 3, 5-Thiadiazine-2-Thiones were synthesized in good yield. The structures of all the compounds were characterized using H-NMR C-NMR and mass spectrometer. The synthesized compounds were screened for anticancer activity against HeLa cell line and nitric oxide (NO) inhibition. Most of tested compounds showed good anticancer activity while compound 3, 5, 6 and 9 were found to be the most potent inhibitor of HeLa cells with IC50 values of <1 µg/mL. All the screened compounds were found to be the potent inhibitor of NO with an IC50 value ranges between <0.1 to 3.8 µg/mL. It was found that the substitutes at N-3 and N-5 position in 1, 3, 5-thiadiazine-2-thione nucleus played a vital role in the anticancer and anti-inflammatory potential of the title compounds. More active title compounds might be obtained via further structural modification.

Long term impact of wastewater irrigation on potentially toxic elements in crops

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Metal contamination of vegetables and fodder crops as a consequence of wastewater irrigation is the most important concern today. The cultivation and consumption of crops irrigated with wastewater is the principal factor contributing potential risks to human health. Therefore, insight into the assessment of heavy metals in crops grown with wastewater irrigated soil is a matter of time. For this purpose, vegetable and fodder crop samples grown in wastewater irrigated areas were collected and analyzed for heavy metals (lead, cadmium, and nickel). The results showed that heavy metal concentration in wastewater irrigated soil and wastewater were varied from crop to crop and region to region. Furthermore, the degree of contamination, metal pollution index, and transfer factor was also varied. Among the metals, maximum contamination of Pb and Cd was observed compared to Ni. However, frequent monitoring of wastewater treatment may be required to prevent the buildup of heavy metals in the food chain.

Synthesis and characterization of PEG-based composites for drug loading and controlledrelease studies: a step towards preparation of new materials for tablets

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The development of new materials for the controlled release of drugs is always under investigation. Polyethylene glycol (PEG) is a non-ionic, hydrophilic polymer, with high swelling behavior that can be linked with other molecules through covalent bond and apply in various fields. The use of PEG-based materials in making drug delivery system is of prime importance because of their biocompatible and biodegradable nature. Water soluble-based core-shell particles (CSP) provide an efficient material for drug loading. In the present study, we successfully fabricated a composite material consisting of core-shell particles incorporated into the PEGDA-700 matrix. The mixture of CS and PEGDA was prepared by physico-mechanical process and converted into a hydrogel composite by the initiation reaction under N2 atmosphere. The composite hydrogels were characterized by UV, FTIR, TGA, SEM, XRD and EDX and then utilized for drug loading and controlled release studies using ciprofloxacin as a model drug. The obtained results revealed that the synthesized PEG-based composite hydrogel can be used as a potential material in tablet development and other drug delivery systems.

Study of the effect of RAFT agents on the characteristics of butyl methacrylamide and poly(2-acrylamido-2-methyl-1-propanesulfonic acid) based core-shell particles

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The reversible addition-fragmentation chain transfer (RAFT) agents are widely used for controlling the polymerization reaction and obtaining polymers with a low polydispersity index. The use of RAFT agents in the preparation of core-shell particles has also been reported previously. However, their role in controlling the final characteristics of water soluble polymers and their core-shell materials was not been evaluated. Hence, in the present study, we decided to check the effect of two types of RAFT agents on the final characteristics of the final properties of the water-soluble polymer poly(2-acrylamido-2-methylpropane sulfonic acid) (PAMPS) and their PAMPS@butyl methacrylate (BMA) core-shell particles. The final properties of the PAMPS and the obtained core-shell particles were examined by different analytical techniques including SEM, FTIR, EDX, TGA and XRD analyses. The study revealed a clear effect of RAFT agents on some of the properties of the PAMPS and PAMP@BMA while other properties were not affected much.

Natural and Synthetic Polymeric membranes for desalination by reverse osmosis

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To overcome the rising issue of water scarcity, desalination is a smart alternative to utilize the available sources. In this study, a series of polymeric membranes were synthesized by blending polyurethane with alginate (0.2, 0.4, 0.6, 0.8 and 1.0%). The structural, morphological and thermal aspects of the membranes were examined by Fourier transform infrared (FTIR) spectroscopy, scanning electron microscopy (SEM), atomic force microscopy (AFM) and thermal gravimetric analysis (TGA), respectively. Performance evaluation (salt rejection and flux) was assessed through reverse osmosis technique. The FTIR spectra of membranes confirmed an extensive hydrogen bonding around 3350cm-1. Both, SEM and AFM analyses supported a progressively rising surface roughness of blend membranes. The hydrophilicity, crosslinking density and thermal stability of blend membranes was improved with an increase in alginate content. The capability of salt (NaCl & MgCl2) rejection was improved with alginate addition upto 0.8% but declined slightly at 1.0%. In addition, the rejection of divalent was better than monovalent ions. The blend membranes ascertained an effective chlorine resistivity which might be considered a response of hydrogen bonding among individual moieties. The antibacterial activity was also upgraded with the addition of alginate as the membranes became more hydrophilic. Hence, this study can trail an efficient approach to develop the blend membranes with tunable properties for water desalination.

3-Diethylaminopropylamine (DEAPA) Hardener Based PDLC Films Technology

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Polymer Dispersed Liquid Crystal (PDLC) film is a kind of novel material in liquid crystal displays (LCDs). It offers several advantages over the conventional LCD materials, such as simple manufacturing process, no polarizers, and no viewing angle problem, unnecessary for the strict control of the space between substrates and easy to fabricate large-area display. To optimize the electro-optical (E-O) properties, much research has been done on adjusting the interaction between LC and polymer matrix. In the current research, the effects of polymer networks containing amine (-NH_2) group on the E-O properties of thin films were studied to use the 3-Diethylaminopropylamine (DEAPA) hardener. The smart films were fabricated by the polymerization induced phase separation (PIPS) method with heat curing monomers/LC/hardener mixtures. Scanning electron microscopy (SEM) was used to observe the structure of the polymer network, LCD Parameters Tester was used to measure the E-O properties of the films. It was demonstrated that the heat curing monomers with -NH_2 group affect the structure of the polymer network remarkably. Especially, the crosslinking density of the polymer network containing this group tended to increase with increasing the content of the curing monomers with -NH_2 group in the thermally curable monomers in epoxy monomers/LC/hardener mixtures. Meanwhile, the tendency for the crosslinking density to decrease with increasing the temperature of curing the mixtures became smaller. The E-O properties of the smart thin films could be optimized with the following properties: The threshold voltage is about 18.0V, the saturation voltage is smaller than 47.0V and the contrast is about 250. Meanwhile, the thermal curable and E-O stabilities of films remain well. Moreover, this film is an Innovative way to curb the spread of viral diseases challenge and it is offering hygienic alternatives for curtains and blinds, which can harbor pathogens.

Green nanoconjugates of silver and seaweeds for antibacterial studies

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Seaweeds extracts were used to reduce silver metal, resulting in a greener synthesis of silver nanoconjugates. Three different seaweed species from the green, brown, and red groups were chosen. The findings revealed that the potential of seaweeds in terms of the existence of functional moiety involved in the bio reduction and stability of silver nanoparticles (AgNPs). The absorption peaks of these nanoconjugates were measured using a UV-Visible spectrophotometer in the 400–450 nm range. After the incubation period, the color intensity rose and the incubation period for the creation of silver nanoparticles utilizing brown and red seaweeds was 48 hours, whereas the incubation period for green seaweeds observed 98 hours. Scanning electron microscopy (SEM) and the Fourier transform infrared (FTIR) technique were used to further analyze silver nanoconjugates. The stability of AgNPs was verified at various silver concentrations. Silver nanoconjugates were evaluated for antibacterial studies. Which demonstrated effective results against S. aureus and E. coli, both species can cause food poisoning. This is an environmental friendly synthesis and there were no hazardous steps involved. This silver nanoconjugates have the potential to be used in medication development, medicinal devices, water purification, microbial activities, and agriculture applications.

Brassica campestris leaves extract mediated green synthesis of metals nanoparticles

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In this study leaves of *Brassica Compestris* plant were collected for synthesis of Fe and Cu nanoparticles from garden of Shah Abdul Latif University Khairpur. NPs were synthesized from plant leaves extract in aqueous medium by green method. The formation of NPs occured at room temperature. The results recorded from several spectroscopic techniques FTIR, ZP, SEM and XRD supports the bio synthesis and characterization of Fe and Cu NPs. The appearance of sharp peaks between 500-600 cm^{-1} in FTIR spectra confirmed the synthesis of NPs. XRD technique depicted the size of NPs about 25-35nm, calculated by Debye Scherer equation, which indicate a high surface area to volume ratio of the NPs. SEM shows the spherical shape and porous structure of stable NPs. Zeta potential (ZP) values +25 mV overall charge of NPs indicates the good stability of NPs. Finally the synthesized NPs showed potent anti microbacterial activity conducted against water borne pathogens (*S. aureus, E. calis*, *E. coli* , *Pseudomonas SB*) using agar well -diffusion method.

Production and biodegradation potential of lipase isolated from Penicillium fellutanum

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Microbial lipases take up a place of eminence among biocatalysts due to their ability to catalyze extensive reactions in aqueous and non aqueous media. In the present study, *Penicillium fellutanum* lipase was characterized and exhibited good characteristics as it was stable over wide range of pH having optimum pH 8.5 and an optimum temperature of 45 ºC with activation energy of 66.37 kJmol^{-1}. The kinetic studies revealed that the K_m and V_{max} for pNPP hydrolysis by *P. fellutanum* lipase were 0.75 mM and 83.33 µmol mL^{-1}min^{-1} respectively. The Gibbs free energy was found to decrease with an increase in temperature and the enthalpy of thermal unfolding of the transition state (ΔH^*) was nearly same up to 54 °C while a very slight decrease was observed at 61 °C. The entropy (ΔS^*) of the enzyme demonstrated an increasing fashion with increasing temperature up to 54 °C but it was dropped again at 61 °C. Mn^{2+}, Pb^{2+} and Ca^{2+} were proved better activators when effect of metal ions on lipase activity was taken into account. It also exhibited good stability when incubated with different organic solvents while in the presence of urea, lipase activity was declined. After characterization, lipase was used to degrade poly (ε-caprolactone) and 66 % weight loss was observed which proved that *P. fellutanum* lipase can be used for the degradation of polyesters. Different process parameters were also optimized for maximum biodegradation of PCL. FTIR, DSC and SEM studies confirmed the weight loss measurements.

Silver Nanoparticles Incorporated Composite Microparticles For Catalytic Degradation Of p-nitrophenol

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This study addresses the effective assembly of silver nanoparticles followed by facile and singlestep in situ chemical reduction method in an already prepared polystyrene-poly (N-isopropyl methacrylamide-acrylic acid) core/shell microgels. Different techniques like UV-Visible spectroscopy, Fourier transform infrared spectroscopy, dynamic light scattering and transmission electron microscopic analysis were used to confirm the formation, size and morphology of silver nanoparticles inside the microgel particles. It was investigated that due to the presence of silver nanoparticles in the thin layered shell of core/shell polymer system, p-nitrophenol was reduced into p-aminophenol in feasible time period with high rate of reaction. The synthesized composite microparticles showed change in the value of apparent rate constant by varying the reaction parameters such as concentration of $NaBH_4$, p-nitrophenol, catalyst and temperature of the medium. Temperature dependent values of rate constant for catalytic reduction of p-nitrophenol reveals the thermally tunable activity of composite microparticles due to incorporated Nisopropylmethacrylamide co-monomer. Depending upon the temperature of the medium the value of apparent rate constant was found between 0.0141- 0.0356 s^{-1}. As the enthalpy of activation ($\Delta H^* = 17{,}334.69$ $jmol^{-1}$) and the entropy of activation ($\Delta S^* = 37{,}105.4$ $jmol^{-1}K^{-1}$) have positive values which suggests that the formation of activated complex is endothermic and entropy driven. The synthesized composite microparticles were found to be easily recoverable and their catalytic activity was also maintained up to four cycles

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Fabrication and characterization of cadmium sulfide nanowires on Anodized Aluminum Oxide templates

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Cadmium sulfide nanowires have unique electrical and optical properties and applications. To obtain cadmium sulfide nanowires with regular and good aspect ratios, they were be synthesized by template synthesis method. Porous anodized aluminum oxide is the most promising template with regular hexagonal shapes. Their aspect ratio was controlled by controlling the anodization voltage and temperature of the electrolyte. In this research, comparatively low purity aluminum was used to prepare nanotemplates at 5-6°C in 1M phosphoric acid and cadmium sulfide was deposited electrochemically using a co-solution of thiourea, cadmium acetate, and ammonium acetate. pH was maintained at 11 in a heat bath at 75°C with the help of an aqueous ammonia solution. Both porous anodized alumina and cadmium sulfide nanowires were characterized using XRD, TEM, and SEM. Nanowires obtained were in the form of bunches with a reasonably high aspect ratio. It was concluded good quality nanomaterials can be obtained by controlling reaction parameters even by using commercial grade aluminum templates.

Density Functional Theory Simulations of NbS_2 Monolayer as Efficient Cathode Material for Mg Ion Batteries

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Nowadays, magnesium ion batteries (MIBs) gained much attention due to its high energy density, low cost and toxicity as compared to lithium ion batteries. In this study we explored NbS_2 as cathode material for MIBs using DFT. Two different sites for Mg ion storage over NbS_2 are explored i.e. at center of hexagonal ring (site-1) and at top of three sulfur atoms (site-2). The adsorption energies reveals that the Mg most stably stored over site-1 having larger adsorption energy value (-3.15 eV). The charge transfer shows that charge transferred from the Mg atom to the S atoms. Band structure evince that the band gap reduced after the Mg ion adsorption, represent that the conductance enhanced. Theoretical capacity reveals that the NbS_2 stored twelve Mg ions with negative adsorption energies and with capacity value of 311.68 mAh/g. The voltage analysis shows that the NbS_2 has positive value of voltage which depicts that the material can store more Mg ions. The Mg ion diffusion analysis indicates that the Mg ion is a fast migration behavior due to smaller energy barrier 0.14 eV. The obtained results demonstrates that the NbS_2 can be used a promising cathode material in MIBs in real applications.

Density Functional Theory Analysis of Adsorption of Small Gas Molecules over Ru-anchored Black Phosphorene

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Using density functional study (DFT) simulations, electronic properties, and systematic adsorption of small toxic gases (CO, CO_2, NO, NO_2, H_2S, SO_2, and NH_3) onto bare and Ru-anchored black phoshorene (BP) is studied. The charge transfer, adsorption distances, adsorption energies, and density of states of these toxic gases on bare and as well on Ru anchored BP is systematically considered in this work. Our investigation shows that anchoring of Ru metal over the BP is quietly strong and having higher energy of formation (E_f = -6.66 eV). The charge transfer and electron density difference study proofs the stronger adsorption of small gases onto the Ru-decorated BP. Besides, the results indicates that the Ru-supported BP effectively capture the small gases having higher negative adsorption energies (-0.28 eV to -2.34 eV), and is most effective for capturing of NO and NO_2 for bare as well for Ru doped due to large adsorption energies of -2.344 and -2.133 eV, respectively. Moreover, the analysis for electronic band structure indicates that band gap of Ru@BP significantly changed after the adsorption of small gases which encourages the stronger sensing behavior of Ru@BP. Thus, our studies shows that Ru supported BP is the foremost candidate for sensing of NOx and can play a vital role in reducing pollution.

Structural tuning of non-fullerene acceptors and small molecule donors to get their high estimated power conversion efficiency for high performance organic solar cell. A quantum chemical analysis

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The designed molecules were estimated for their structural, optical, electronic and photovoltaic properties using density functional theory method MPW1PW91/6-31G (d, p). The simulated results of all the modelled molecules comparative to the reference molecules lie in the range of efficient solar cell light harvesting unfused non-fullerene acceptors. In addition, they were successfully tested for their solution processability and their interface with donor material PBDBT was made to calculate fill factor and open circuit voltage. In all modelled molecules, BDCl2F-DS has highest value of open-circuit voltage (1.71 eV) and fill factor (92.25%). PCE estimation of modelled molecules was incurred by assuming a similar value of short circuit current from the reported work of reference molecules. The extraordinary PCE values (in the range of 27.36 % to 33.76 %) were estimated for these modelled unfused non-fullerene molecules which is fruitful theoretical work for the experimental scientists to advance the investigation of unfused non-fullerene acceptors.

Cycling performance degradation of Ni-rich layered NCM materials in full-cells: Effect of elevated temperature

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Lithium-ion batteries (LIBs) have dominated portable electronics and they are now opening potential applications in electric vehicles (EVs) and grid energy storage markets. For EVs, driving range anxiety is one of the main concerns for customers that requires development of high energy density LIBs. In this regard, Ni-rich layered cathode materials (LiNi1−x−yCoxMnyO2) with excellent electrochemical performance under harsh conditions are in urgent demand owing to their high capacity (over 200 mAh g−1) and relatively high working voltage (3.8 V). In this work, we evaluated the capacity fading of NCM85/Graphite full-cell at elevated temperature. A systematic failure analysis confirmed that it is the cathode material where elevated temperature causes structural degradation due to the formation of microcracks, decomposition of the electrolyte and increase in resistance.

Molecular interactions of organophosphate pesticides in colloidal solutions in terms of Thermo-acoustic and DFT studies

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Recently, use of agrochemicals, most importantly pesticides have experienced an enormous upsurge as a consequence of continuously increasing demand of enhanced crop production. Excessive exposure of pesticides causes genetic disorders and several other diseases (Cancer, chronic obstructive pulmonary disease, infertility). In present study, thermo-acoustic method was aimed to study binding and transport behavior of organophosphate pesticides in aqueous and colloidal solutions containing ionic surfactants micelles (micelles are being used as mimic structures for cell membrane to study biological system/process). Experiment was carries out at different temperatures (293.15K–313.15K). Different volumetric and acoustic parameters were calculated. Positive values of apparent molar volume ($V\phi$) increased with increasing pesticide concentration in aqueous solutions are indicative of strong associative molecular interactions in solutions. While in presence of ionic micelles, comparatively greater magnitude of $V\phi$ values for aqueous pesticide solutions showed that pesticide molecules get solvated in hydrophobic core of micelles. When pesticide molecules enter into body, get solvated in cell membrane and a very small number of pesticides could get to approach blood for binding with different biomolecules affecting their nature and functions. These molecular interactions could explain controlling the toxicity level in human being exposed to pesticides in natural way.

Environment Friendly Sr2xBixCoRuO6 ($0 \leq x \leq 0.8$) Double Perovskite Oxide Materials for High-Temperature Thermoelectric Application

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A series of Sr2-xBixCoRuO6 ($0 \leq x \leq 0.8$) double perovskites have been synthesized in air by a traditional solid state chemistry method at 1200 ºC. Powder X-ray diffraction data (x = 0.0, 0.2, 0.4, 0.6 and 0.8) show that all the samples are phase pure and adopt monclinic crystal structure with space group I2/c. Scanning electron micrographs (SEM) show uniform distribution of micron size particles in all samples. Energy dispersive spectroscopy microanalysis (EDS) confirms the chemical homogeneity and elemental compositions of all samples. Thermogravimetric analysis (TGA) suggests the formation of oxygen vacancies in all the Sr2-xBixCoRuO6 materials. Magnetic measurements on vibrating sample magnetometer (VSM) indicate an antiferromagnetic ordering below Neel temperature TN = 70 K in most of the oxide samples. However, the x = 0.2 sample shows ferromagnetic domains characterized by a Curie temperature of TC = 280 K.

Synthesis, characterization, and resolution of X-ray photoelectron spectra of tetrachloroferrate based ionic liquids

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A series of ionic liquids based on tetrachloroferrate anions with methyl and benzyl substituents cations have been synthesized. They have been characterized by using $_{1}H$, $_{13}C$ NMR, Raman, ESI-MS spectroscopy, and AAS along with single crystal XRD for their structural elucidation. In addition, the chemical state and composition of all the elements present in these involatile synthetic products have been determined by using ultra-high vacuum X-ray photoelectron spectrometry (XPS). For the element carbon in different ionic liquids, it has been very difficult to interpret the complex spectra because of an eclectic mix of its chemical states in ionic liquids and subsequently obscuring the significant information due to ambiguity in the signal identity. Herein we report XPS peak fitting models for C *1s* spectra with methyl and benzyl substituents to provide accurate binding energies for carbon photoemissions and exact information of elemental chemical composition of synthesized ionic liquids. Notably, the chemical and physical properties of ionic liquids such as non-volatility, ionic conductivity and magnetism augment the substantial progress in peak fitting and XPS data interpretation. Effective magnetic moment and ionic conductivities values of synthesized ionic liquids have also been determined to appraise their potential applications in catalysis, synthesis, and magnetic separation.

Biodegradable thin films for advanced applications

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Grafting of cellulose using acrylic acid, methyl methacrylate and 2-Ethyl hexyl acrylate has been achieved through free radical polymerization using Ammonium persulphate as a free radical facilitator along with Leutensol-100 as an emulsifier. The grafted cellulose was made composite using carbon nanoparticles, obtained from carbon soot of millet. Grafted cellulose and its carbon nanocomposites were characterized by Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), tensile strength, electrical conductivity and biodegradation. Soil burial test revealed the biodegradation of cellulose grafted terpolymer nanocomposite. The controlled biodegradation of this composite may have potential applications be used in various applications in advanced materials.

Enhanced static and dynamic nonlinear optical responses of face specific superalkali based alkaline earthide complexes of Janus all-cis-1,2,3,4,5,6-hexafluorocyclohexane

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Designing of nonlinear optical materials (NLO) is an area of immense scientific investigation for their optoelectronic applications. Experimental synthesis of a Janus face C6H6F6 (all-cis-1,2,3,4,5,6-hexafluorocyclohexane)has urged the scientists to design novel NLO materials. Superalkali and alkaline earth metal doping at both faces of C6H6F6 has been carried out by using DFT simulations. As a result, stable superalkali based alkaline earthide complexes (M3O+-1-M' (M'=Be,Mg,Ca &M=Li,Na,K)) have been observed. The alkaline earthide nature of complexes is confirmed by NBO analysis. The high interaction energies up to -115.51 kcal mol-1show that these complexes are thermodynamically stable. The NCI and QTAIM analyses have confirmed the non-covalent interactions. The results of absorption analysis reflect that these complexes are transparent in UV region. The linear and nonlinear optical properties of the designed complexes are remarkably high and the highest first hyperpolarizability is up to 5.2×106 au. Their EOPE coefficients and SHG coefficients are also computed at 1064 nm and 532 nm. Second hyperpolarizabilities of the designed complexes are up to 5.7×108 au. The quadratic nonlinear refractive indices are computed and maximum value is up to 2.3×10-7 au. These findings show that the designed complexes can be used to rationally design stable and high-performance NLO materials.

Constituents of liver oil obtained from a dead *Rhincodon typus* (whale shark)

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Post-mortem lipid analysis of liver oil from a whale shark exploiting GC-MS, and confirmation through RI has resulted in identification of 62 constituents. 26 FAs identified comprises ~81% by composition. These included 11 SFAs, 9 MUFAs, and 6 PUFAs. 13 FAs have also been justified from dietary preferences, specially the C16 and C17 FAs. Collectively palmitic acid, oleic acid, palmitoleic acid, elaidic acid, stearic acid, myristic acid, and gondoic acid constituted 2/3rd of the oil composition. 25 Constituents, originating from degradation but accounting ~13%, included 18 FAlds, 2 FAlcs, 2 ketones, and 3 oxygenated FAs. The degradation pathways of LCFAs, MUFAs, and PUFAs to produce 25 degraded metabolites have been discussed. Since whale shark is a filter feeder, the constituents reported from primary producers of marine food web were found dominating. 33 identified metabolites were correlated with the preferred dietary preys of whale shark. Majority of these were overlapping with FAs and their degraded products. 2 marine pollutants were also identified in minute % composition. The concentration profile of the different constituents e.g., malondialdehyde, peroxides, FAld, ketones and FAlc has led to conclude that the animal was already dead at least four days before the liver oil was sampled.

Synthesis, Characterization, and Dyes Degradation activity of *Solanum pseudocapsicum* Mediated Metal (Ag, Ni, Pd) Nanoparticles

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Solanum pseudocapsicum (family Solanaceae) is a nightshade specie containing a high content of phosphorous and nitrogen having a significant cytotoxic, hepatoprotective, and anti-tumor properties. The present study highlights the synthesis of metal (Ag, Ni, Pd) nanoparticles of *S. pseudocapsicum* (SPNPs) under the conditions of stirring, heating and stirring, incubation, and sunlight. The results depicted that stable nanoparticles are produced in the ratios ranging from 1:2 to 1:15. The synthesized nanoparticles exhibited significant reducing/degradation property against methyl orange, methylene blue, Rhodamine B, nitrophenols (*ortho*-nitrophenol, *para*-nitrophenol) and several food colours such as deep green, bright red, and zarda yellow. Hence, the subject SPNPs might be helpful in the removal of industrial unfixed dyes from contaminated water.

Folate Conjugated Polyethylene Glycol Probe for Tumor-Targeted Drug Delivery of 5 Fluorouracil

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Introduction

Development of targeted drug delivery system is meant primarily to deliver anti-cancer drug at target tumor lesions present in specific tissues inside the body. Here, we present a carrier designed by the conjugation of folic acid (FA) with bis-amine polyethylene glycol (PEG) to deliver a potent anticancer drug (5-FU) at the tumor lesion.

Methods

FA was linked through amide bond with PEG and the resulting carrier (FA-PEG-NH2) was linked to 5-fluorouracil (5-FU) through methylene group to develop folate-polyethylene glycol conjugated of 5-fluorouracil (FA-PEG-5-FU). The resulting products were characterized through UV-Vis, 1HNMR, FTIR, and HPLC. In vitro drug release patterns were determined for 5-FU and FA-PEG-5-FU for ten days (240 h). In vitro cytotoxicity assays were performed in Vero cells and HeLa cancer cells to see the response of folate receptors (FR+) mediated transport of folate conjugate,. Antitumor activity was measured in tumor bearing mice models. The molecular docking was rationalized by molecular dynamics simulations.

Results

Characterization elucidated the formation of pure folate conjugate (FA-PEG-5-FU). In-vitro drug release pattern analysis showed matrix-controlled diffusion of the test drug. Conjugate molecule produced enhanced uptake in HeLa cells due to the FR+ affinity as compared to Vero cells. The tumor size of the test group mice (FA-PEG-5-FU) was considerably reduced after 15 days of treatment than standard group mice (5-FU). The molecular docking results elucidated the importance of Lys136, Trp138 and Trp140 by stabilizing the flexible loop flanking the active site.

Discussion

Bisamine-PEG serves a decent linker between 5-FU and FA and it does not affect the anti-cancer activity and FR+ affinity of 5-FU and FA. The slow release pattern of the prodrug illustrated that PEG is gradually degraded and discharged 5-FU; folate conjugate in HeLa cells showed higher anti-cancer activities than 5-FU and also exerts the powerful tumoricidal effect in-vivo. The molecular dynamic simulations provided comprehension on the resulting stabilizing interactions of 5-FU and PEG upon binding to folate receptor.

Conclusion

The data support FR-targeted FA probe usage for the delivery of small molecular weight anticancer drug at the tumor lesion in a sustained release patterns.

First theoretical insight into tuning the nonlinear optical response of 1N-atom functionalized corannulene by alkali metal doping

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Nonlinear optical (NLO) materials have attracted considerable attention of scientific society in recent years due to the wide range of uses they have in a variety of fields. This research aimed to theoretically model 1N-functionalized corannulene molecules doped with alkali metals (Li, Na, and K). The designed geometries, thermodynamic stability and nonlinear optical properties are all investigated using the DFT approach. The stabilities of designed complexes are exhibited by negative interaction energy values ranging from -11.23 to -31.13 kcal mole^{-1}. The $E_{(H-L)}$ gap is dramatically reduced, reaching up to 1.17 eV after doping. The computed first hyperpolarizability (β_o) of the designed compounds is determined to be 4.84×10^4 au, which is the highest value ever found for this surface. The charge transfer, kind of interaction, and fragment's participation in electronic properties are confirmed by the NBO, NCI, TDOS, and PDOS studies, respectively. The results of TD-DFT calculations demonstrate that these compounds are transparent in the ultraviolet area and almost all of their isomers exhibit maximum absorption in the visible region. This unique technique, which has comparatively greater static first hyperpolarizability values than previous reports on the corannulene surface, may offer up new opportunities for scientists to design novel NLO materials in the future.

Theoretical investigation of magnetic, electronic and optical properties of $YFeO_3$

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This work presents theoretical investigations of magnetic, electronic, and optical properties of YFeO3. Orthoferrites are essential due to their specific optoelectronic properties and are used in sensors, light spot measurements, and optical switches. We have conducted the theoretical investigations under density functional theory using a generalized gradient approximation and a GGA+U framework. Several magnetic configurations are studied to find the most appropriate one that could adequately describe a YFeO3 system. Various properties, including reflectivity, dielectric function, refractive index, absorption, and extinction coefficient, are calculated. The calculated properties are in good agreement with the experimental findings.

Bioactive Heteroleptic Bismuth(V) Complexes: Synthesis Structural Analysis and Antileishmanial Activity

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Lower toxic nature of bismuth compounds makes them an attractive choice as drug candidate for all the scientists working in the field of medicinal chemistry. We hereby propose bismuth compounds as least toxic alternative for the antimony compounds that are currently in use for the treatment of leishmaniasis.

In present research work the synthesis, structural chemistry, bioactivity, cytotoxicity and stability of heteroleptic triorganobismuth (V) complexes having general formula, $R_3Bi(OOCR')_2$ (**1**–**8**), where R = C_6H_5 (**1**–**4**) and *p*-$CH_3C_6H_4$ (5–**8**) has been studied in detail and a structure activity relationship has been developed. X-ray crystal analysis for selected complexes validates a distorted pentagonal bipyramidal geometry. Compound (**1**-**8**) has been tested for antileishmanial starins (*Leishmania tropica* KWH23) and their cytotoxicity has been checked against human *Lymphocytes.* The results suggested that some of these compounds are highly effective against the target species (*Leishmania tropica* KWH23) while being non-toxic towards the mammalian cells at levels even below 0.74 μgmL^{-1}, making them highly auspicious and ideal future drug candidate. A broad analytical approach has been followed to testify the stability for (**1**-**8**) in solid state as well as in solution and in leishmanial culture M199, ensuring them to be stable enough to exert a significant antileishmanial effect with moderate to significant results. Being least toxic and highly active against leishmania parasites these compounds emerge as promising drug candidate that can be administered orally.

Screening of trace and essential elements in the serum of esophagus cancer patients with different types and stages of Pakistani Population

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Esophageal cancer is a very deadly disease ranking 8th most common cancer in terms of incidence and the 6th highest in terms of mortality both in USA and around the world. A growing body of evidence indicated that changes in the concentrations of essential and toxic elements may affect/increase esophagus carcinoma risk. The aim of this study was to measure serum levels of essential and toxic elements (Fe, Ca, Na, K, Mg, Zn, Co, Sr, Pb, Li, Se, Sb, Cu, Mn, Ni, Cr, Ag, Cd, As and Hg) in patients with esophagus carcinoma and controls. Atomic absorption spectroscopy was used to determine serum concentrations of essential and toxic elements by employing nitric acid/perchloric acid–based wet digestion method. Average concentrations of Cu, Ni, Cr, Cd, Pb, As, Ag and Na were exhibited to be significantly higher in the serum of cancer patients than controls. The correlation coefficients among the elements in the patients revealed significantly dissimilar communal relationships than the controls counterparts. Multivariate methods demonstrated noticeably different apportionment between the elements in the cancerous patients and the controls. Significant disparities in the elemental concentrations were also noticed for esophagus cancer types (adenocarcinoma and squamous cell carcinoma) and stages (I, II, III, and IV) among the patients. Majority of the elements exposed perceptible disparities in their contents based on smoking habits, dietary habits, habitat and gender of the esophagus cancer patients and controls. Multivariate analysis of the essential and toxic elemental data explained significantly divergent apportionment in the serum of esophagus cancer patients when compared to controls.

Comparison Of Proximate Analysis And Elemental Composition Of Pakistani And Saudi Arabian Date Varieties

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In this study fourteen Pakistani date varieties and six Saudi date varieties examined to evaluate the proximate parameters and minerals of date palm varieties. The contents of moisture, ash, fat and fiber in date varieties of Pakistan were varied from 11 – 18, 1.3 – 2.9, 2.0 – 3.40, and 2.5 – 10 %, respectively. The Saudi date varieties have low contents of moisture, high contents of ash and fiber and comparable contents of fat as compared to Pakistani date varieties. Both Pakistani and Saudi date palm varieties are a good source of Ca, K, and Mg. The studied date varieties showed low contents of Na whilst higher in case of K in the studied date varieties. The fat contents observed to be lower in date varieties of both Saudi and Pakistan (< 3.50%) suggesting them a best fat controlling fruit for human. The kashu wari Pakistani (55.0 µg/g) and suqai Saudi (63.0 µg/g) varieties showed highest contents of Fe. Similarly, Mn levels were maximum in kupro (Pakistani) and kalmi (Saudi) date varieties. The maximum levels of Zn detected in Pakistan kashu wari date variety and sukkari in Saudi variety. The resulted analyses data showed the same trend of macro and micronutrients in both countries date palm varieties. The variations in macro and micronutrients in studied varieties (date palm) may be associated to the environmental and genomic factors such as the kinds of date varieties, soil filed, irrigation water, type of fertilizers (synthetic organic), applies pesticides, weathering, and the drying treatment approaches.

Synthesis of Mechanical and Thermally robust SEBS-g-MA/OMMT Nanocomposites

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Triblock copolymer, polystyrene-b-poly(ethylene-co-butylene)-b-polystyrene (SEBS-g-MA) derived nanocomposites have been prepared with improved thermal resistance. SEBS-g-MA/OMMT nanocomposites were prepared through solution intercalation methodology using chloroform as the supporting medium. Nanocomposites were investigated through fourier transform infrared (FTIR) spectroscopic analysis, and confirmed for structural changes upon addition of reinforcement to the polymeric matrix through transmission electron microscopy (TEM). Nanocomposite films were further studied for X-rays diffraction (XRD) and thermogravimetric analysis (TGA) analyses techniques. XRD spectra provided structural insight with confirmation of formation of nanocomposite as there was no sharp peak observed in spectrum. Thermal gravimetric analysis confirmed the decomposition temperature which was improved with increasing the clay content in the polymer matrix. Decomposition temperature has been noticed in the range of 418-448^{o}C for 2-10% OMMT content. Mechanical properties further confirmed homogeneous dispersion of clay platelets into the polymeric matrix, as improvement in tensile strength was observed. Maximum stress, strain, and modulus of elasticity was observed to be improved while addition of organically modified MMT.

Solar light driven C-TiO_2 based photocatalysts for enhanced activity towards Microbes and removal of Dye

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Solar-driven photocatalytic approach is an attractive, clean and effective way for decontamination of water. In this work, visible light activated nanophase TiO2 (tubes TNFs and flakes TNFs) and carbon doped TiO2 (C-TNTs and C-TNFs) were synthesized via facile hydrothermal route using different carbon source. Powder X-Ray diffraction (XRD), scanning electron microscopy (SEM), fourier transform infrared spectroscopy (FT-IR), and UV-visible spectrophotometer were used to characterize the synthesized nanocatalysts, critically disclosing anatase nature containing titanium-oxygen having flakes/platelets and tubes like morphology with ~ 32 nm in size respectively. The photocatalytic activity was characterized via degradation of methylene blue (MB) and bacterial inactivation of Escherichia coli (Gram-negative) and Staphylococcus aureus (Gram-positive). The experimental results showed that C-TNTs and C-TNFs significantly enhanced the photocatalytic activity when compared to bare TNTs and TNFs. It was found that RGO-TNFs nanocatalyst exhibited superior photocatalytic activity against photodegradation of MB (92.7 %) and antibacterial activity (85.6 %) under sunlight irradiation. In addition, RGO-TNFs have a good recycling ability and expected to be a promising candidate for photocatalytic applications under sunlight. Consequentially, higher activity of C-TNTs and C-TNFs nanocatalyst under sunlight irradiation for dye degradation and bacterial inactivation implies that hydrothermal synthesis allows for the preparation of efficient and low-cost carbon-doped photocatalysts for the photodegradation of wide range of environmental pollutants.

Synthesis and characterization of CoO-ZnO and evaluation of its photocatalytic activity for photodegradation of methyl orange

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Photocatalysis is one of the techniques used for the eradication of organic pollutants from wastewater. In this study, CoO-ZnO was tested as a photocatalyst for the degradation of methyl orange under irradiation of visible light. Co-ZnO loaded with 5%, 10%, and 15% CoO were prepared by precipitation method. The advanced techniques including X-Ray Diffraction (XRD), X-ray photoelectron spectroscopy (XPS), Diffuse Reflectance UV-visible (DR-UV-Vis) spectroscopy, Photoelectrochemical (PEC) measurements, Temperature Programmed Desorption (TPD), Photoluminescence (PL) and Fluorescence spectroscopy related to $OH^{\cdot}$ measurements were used for characterization of prepared CoO-ZnO. Experiments showed that 10% Co-ZnO was a highly efficient catalyst for the photodegradation of methyl orange as compared to ZnO. The enhanced photocatalytic activity of CoO-ZnO is attributed to the implantation of CoO which inhibits the electron-hole recombination. A 100 mg/L solution of methyl orange dye was completely degraded within 130 minutes. The reaction kinetics has been described in terms of the Eley-Rideal mechanism.

Construction of Zn-based 3D-dimensional MOF via sequential insertion technique, accompanied by SC-SC transformation

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Metal-organic frameworks are a fascinating class of porous functional materials assembled by combining metal nodes and organic linker with diverse applications. These are generally synthesized by one-pot solvothermal reactions. This technique is associated with some disadvantages when various linkers are involve such as linker stability, linker solubility, formation of other domains and competition between the linkers. Recently, more valid strategies like post synthetic modification (PSM) of MOFs have proved to be an effective in case this case. In the present study replacement of structure building linker and sequential insertion technique has been exploited in order to convert a two-dimensional MOF **(BUT-25)** to three dimensional MOFs (**BUT-26, 27**) with distinct topologies. For the first time bent/angular linker was used instead of linear linker for example bipyridine. The sequentially inserted linkers were dicarboxylates (2,5-thiophenedicarboxylic acid and isopthathalic acid) .The different angles between the arms of carboxylates may be the reason for two different and distinct topologies. All the MOFs were characterized by SC-XRD to elucidate their structures. The as-synthesized pxrd patterns matched well with simulated one. Further the efficiency of BUT-25 was checked for the detection of Fe^{3+} and $Cr_2O_7^{2-}$ ions in water. BUT-25 proved to be a highly sensitive and selective towards these ions and also act as colorimetric sensor.

Zinc-Magnesium Bimetallic Nanoparticles synthesis, characterization and Application as Catalyst and Fuel Additive

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Zinc-magnesium (Zn-Mg) bimetallic nanoparticles are manufactured via reflux assisted co-precipitation technique by using precursor salts of magnesium acetate and zinc acetate, solvent ethanol and reductant phenyl hydrazine. Energy dispersive X-ray spectroscopy is used to determine the chemical composition of product which turned out Mg_2Zn_{11} bimetallic nanoparticles. X-ray diffractometry confirmed presence of Mg_2Zn_{11} and gave its more detail via lattice parameters and structural model of product. The morphology and size of particles are analyzed by scanning electron microscopy. Synthesized product is employed for removal of organic compounds: 4-nitrobenzoic acid, 4-nitrophenol and reactive carbon black 5 dye. The catalyst is found to be more active towards 4-nitrobenzoic acid as compared to 4-nitrophenol and dye. Synthesized product is found to be an efficient catalyst towards nitroarenes substituted with electron withdrawing groups. Synthesized particles were also tested as fuel additive and proved highly efficient in it.

Design and Synthesis of Furan-Dicarboxylic Acid based Metal-Organic Frameworks and their structural diversity

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In the recent past vast research work have been carried out on Metal-Organic Frameworks due to their fascinating promising applications, but insufficient chemical stability deters some practical applications, where the stability is very important for real-life environment. For the MOF stability, the metal-ligand coordination stability pre-condition along with the orientations and configurations of ligand. It is believed that the rigid carboxy ligand provide stability to the framework. In this work we synthesized Cu-Fdc and Zn-Fdc MOF, both these MOFs showing unexpected stability by using a different metal in these two frameworks in the synthesis process. Both MOFs have been solvothermally synthesized and characterized by single-crystal X-ray diffraction (SXRD), powder X-ray diffraction (PXRD) and Brunauer-Emmett-Teller (BRT). More interestingly the Cu-MOF showing good stability and exhibiting BET surface area 300 m2/g while the Zn-MOF shows a negligible BET surface area, and suggested that the Zn-MOF may have collapsed during the degassing process while showing no surface adsorption. It is expected that the 2-D Cu-MOF may have some good applications in the detection/adsorption of water-based pollutants but it can be explored in the future experiments.

Synthesis, characterization and antibacterial studies of Schiff Base metal complexes derived from drug

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In the two-step production of Schiff base ligand and metal complexes, the antibiotic agent was utilised with appropriate ligand to metal molar ratio. FT-IR, 1H-NMR, 13C-NMR, Mass, Atomic absorption spectroscopy, Elemental analysis, UV-visible spectroscopy, Evans balance, and Conductivity were used to characterise the Schiff base ligand and metal complexes after synthesis. The newly synthesised ligand and transition metal complexes were evaluated against Gram positive and Gram negative bacteria. Metal complexes demonstrated stronger activity against reported pathogens when compared to free Schiff base ligand, according to the research.

Photosynthetic Microbial Fuel Cell as a Green Alternative Renewable Energy Approach for Sustainable Bioelectricity Production

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Development of new green alternative renewable energy approaches came into the limelight in the modern technological era to sustain future stability. The most important property of alternative energy resources should have their environmental compatibility and sustainable energy production. The Photosynthetic Microbial Fuel Cell (PMFC) is considered to be the best green alternative way to protect the environment and for the sustainable bioenrgy production. The PMFCs have a great potential to generate energy by switching of chemical energy present in waste material into Bioenergy by using photosynthetic microbes as biocatalyst. The main objective this research work to used double chamber mediator-less microbial fuel cell to convert the chemical energy store in the organic molecules present in the wastewater samples into electrical energy by a bioelectrochemical reaction by using blue green algae as photosynthetic microbes. The wastewater sample was subjected to aerobic fermentation in double chamber PMFC for 7 days by using blue green algae. The physical parameters such as pH, conductance, current density, voltage, power output and resistance were monitored for a week to observe changes due to metabolic activities of photophes. A maximum current and voltage of about 381 mV and 529 MA were obtained respectively. These results concluded that the adding cynobacteria to the domestic wastewater result in a valuable increased in electrical energy.

Kinetics of the thermal decomposition of peanut shells using termite mound as catalyst

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This study is focused on pyrolysis of peanut shells in the temperature range of 310-380 oC in presence and absence of termite mound as catalyst. The termite mound was characterized by EDX, XRF, SEM, SAA and XRD. The bio-oil obtained from peanut shells pyrolysis was analyzed by GC-MS. To know the kinetic parameters of the reaction, thermogravimetric analysis of peanut shells was carried out at heating rates of 3, 12, 20 and 30oCmin-1 with and without termite mound catalyst. TG/DTG of peanut shells revealed three steps degradation in temperature range of 25-800 oC. Calculations of kinetic parameters were done by using Ozawa Flynn Wall (OFW) and Kissinger method. Activation energy and frequency factor for non-catalyzed reaction were observed as 201.527 kJmol-1 and 6.775 x1022 min-1 respectively for Ozawa Flynn Wall while 124.71kJmol^{-1} and 7.515 x10^{10} min^{-1} for Kissinger method respectively. For catalyzed reaction activation energy and frequency factor were calculated as 134.0755 kJmol-1 and 5.4028x10^{13} min-1 for Ozawa Flynn Wall and 83.14 kJmol^{-1} and 3.7381x108 min^{-1}for Kissinger method respectively. The termite mound catalyst not only reduced degradation temperature and activation energy but also brought change in the composition of bio-oil i.e. in-case of non-catalytic pyrolysis the bio-oil was found to consist of C3-C24 compounds while in-case of catalytic pyrolysis it produced more components ranging from of C4 - C31 compounds.

A comparative study and photocatalytic activity of zinc encapsulated manganese ferrites under UV irradiation for methylene blue dye from aqueous solution

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Mostly dyes are used for preparation of different chemicals in many industries like rubber, leather, and paint, pharmaceutical and in textile also. But during process of industries, some portion of dyes remain unfixed and detach from fabric and wasted as effluent in water which may cause the serious health problems to plants and animals. However, dyes should be totally eliminated from water on immediate effects. Different methods have been reported for their removal, conventional methods may produce secondary by products which are also harmful, like adsorption, coagulation, precipitation methods. Advanced oxidation process are involved in degradation of these emerging pollutants using fenton chain mechanism. Semiconductor photocatalysts have been reported. Manganese ferrite nanoparticles have been reported in this article for degradation pf methylene blue dye under UV light. These ferrites have spinel structure, high coericivity, manetization and single domain used in industrial and biological process. $MnFe_2O_4$ have inverse spinel structure, where Mn^{2+} lies at tetrahedral (A) site & just 20% lies at octahedral (B) site. Where as, many properties like NEEL coupling scheme magnet & moment consistent with low resistivity are used. Mn ferrites actually show the extensive properties, like saturation and bulk magnetization from 80emu/g 20emu/g -70emu/g for nanoparticle ferrites respectively. The work deals with manganese ferrites and zinc encapsulated Mn ferrite via hydrothermal route and their application as dye degrading agents. The properties of prepared material was checked by employing various spectroscopic techniques like UV-Vis, FTIR, SEM and XRD. This work will be beneficial for future and helps in environmental remediation.

The Rational Design of Ni/ZnO/Al$_2$O3 Adsorbents for S-Zorb Desulfurization Activity

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In present work, different types of Ni/ZnO based Alumina materials with various ZnO to Al_2O_3 catalysts were synthesized using one step urea precipitation approach, and employed as adsorbents to measure the performance of reactive desulfurization utilizing model gasoline in a novel design reactor. The prepared mesoporous catalysts were examined through Nitrogen adsorption-desorption isotherms, Phase Analyser, transmittance electron microscopy (TEM), ultraviolet-visible diffuse-reflectance (UV-vis DRS) and X-ray Photoelectron (XPS). Results show that different morphology and Ni pressures doping and synthesis approach play a vital role on adsorbent's desulfurization performance. Among the investigated catalysts, 10%Ni/ZnO/ Al_2O_3 shows excellent RADS performance up to 96% conversion and immense sulphur adsorption capability of 86 mg S/g, that is 34% larger as compared to template-assisted adsorbents. Template-free approach could facilities the production and distribution of small sized ZnO particles along with large ratio of ZnO, by inhibiting the formation of inactive ZnAl2O4 verified with XRD, UV-vis, and Raman. On the other hand, the preparation approach of template-free method, as well as the appropriate Ni content can also provide more Ni0 active sites by decreasing the possibility of forming NiAl2O4 confirmed with XRD. Five cycle test upon regeneration shows a drop of a negligible amount (3%) in desulfurization activity demonstrating the structural stability of template-free prepared Ni/ZnO/Al_2O_3.

Pharmacophore modelling of Urease Inhibitors by In-Vitro, Kinetics and Molecular docking Approach

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The ureases are important class of enzyme which occur in jack beans, soybeans, and seeds of other plants. These are also found in some animal tissues and microorganisms which lived in the intestine of living organism. It is very harmful to mammals due to over production of ammonia. The sources of urease are different bacteria in mammals, which are found in the intestine of mammals like humans. Urease plays major role in the intensification of *H. pylori* poison. It catalyses the reaction in which, conversion of urea into carbon dioxide and ammonia occur. It has also ability to neutralize gastric acid and stop the infection of *H. pylori* which occurs at lower pH in the stomach of humans. The synthetic approaches towards the production of urease inhibitors give new way to control disorders associated with urease. Natural and synthetic clinical entities are major contributor to overcome the hyperactivity of the enzyme. The main purpose of this research is to determine the new inhibitors of urease and to check their mechanism of action. For this purpose, high-throughput mechanism is carried out which is based upon spectro-photometric assay procedure. The new inhibitors both natural and synthetic can be used for the treatment of number of diseases caused by the rapid action of urease enzyme.

Catalytic role of extended π-conjugation in the redox reactions of Fe(III)/(II) complexes

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Ferricyphen and ferricypyr may be feasible substitutes for the sensitizer in dye-sensitized solar cells due to their high reduction potential, stability, outer-sphere oxidant ability, and photosensitivity (DSSCs). Meanwhile, ferrocyanide might be used as a mediator in DSSCs instead of iodide. In this study, the redox capacity of competent prospective sensitizers to oxidize the likely mediator in water was compared. Each redox reaction proceeded through a complex kinetics at 0.06 M ionic strength, splitting into two phases, the first of which was zero order and the second of which was overall second order. UV-Vis spectral studies identified the relevant Fe(II)/(III) complexes as the reactions' products. The rate-resisting effects of decreasing pH and increasing ionic strength have negated the catalytic effect of lowering medium dielectric constant. Because of this pattern, which was seen for both reactions' rates, $[Fe^{II}(CN)_6^{4-}]_F$ and $[H_2Fe^{II}(CN)_6]^{2-}$ were predicted as the reactive species leading the rate-determining step. The kinetic and thermodynamic parameters of both processes were measured and compared. π-conjugation in 1,10-phenanthroline sped up the redox process by lowering the activation energy and enthalpy of activation, as well as demonstrating catalytic activity, as compared to the 2,2'-bipyridine system.

Forensic Discrimination Potential of inks using Analytical techniques and Chemometrics

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Investigation of inks is significant in dealing with fraud cases involving forensic questioned documents. Such cases of forgery where cheques, marriage papers, entry of birth and death etc. are questioned, are more pronounced in developing countries. Although, literature is available related to the analysis of inks using analytical techniques but data of discriminating potential (D.P) in terms of preference of anticipated techniques is not comprehensively present. In this research, inks of different colors from fountain pen, ballpoint pen and rubber stamp commercially used in Pakistan, have been investigated by Altered light sources, UV-Vis and FTIR Spectroscopy, TLC, and Gas Chromatography-Mass Spectrometry. Results have been calculated and compared in terms of discriminating power. Moreover, Statistical chemometric techniques has been used to improve the D.Ps. All sample pairs have been discriminated successfully by GC-MS, thus making this technique attractive for dealing fraud cases involving use of fountain pen inks. Among different colors of fountain pen inks, red is suggested to be used based on its DP value. Likewise, green ballpoint pen inks shows best D.P. compared to other colors. All analytical techniques used for studying green ballpoint pen ink showed similar value of D.P. therefore, green ballpoint ink is recommended to be used. High D.P for Black & red ballpoint pen inks was obtained using UV/vis spectroscopy but FTIR spectroscopy is used to discriminate blue ballpoint pen inks. Lowest D.P for blue and red ballpoint pen inks with TLC compared to UV/Vis and FTIR spectroscopy shows the least effectiveness of this technique for ballpoint pen inks. In contrast, TLC can discriminate the results for all colors of rubber stamp pad inks commercially available in Pakistani local markets to its best however, comparison of their D.P values obtained from different analytical techniques suggests the use of red stamp pad inks in dealing official matters.

Synthesis and evaluation of novel S-benzyl- and S-alkylphthalimideoxadiazole benzenesulfonamide hybrids as inhibitors of dengue virus protease

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Viral infections have become biggest threat to the humanity. Synthesis of effective drugs to treat viral infections has become the need of the time. Direct Acting Anti HIV and HCV drugs have been efficaciously established by targeting the viral proteases. Likewise, dengue virus (DENV) protease, which is comprised of NS2B and NS3pro proteins, can also be explored for finding new anti-dengue drugs. Here, we have established two alternate series of novel hybrids, namely S-alkylphthalimideoxadiazole-benzenesulfonamides (8a-j & 14a-f) and S-benzyloxadiazole-benzenesulfonamides (9a-c & 15a-e). To obtain first series of hybrids, the reaction of p-aminobenzoic acid (1) with 4-methyl and 4-trifluoromethylbenzene-sulfonyl chloride (2a-b) provided 4-{[(4-methylphenyl)sulfonyl]-amino}benzoic acid (3a) and 4-{[(4-trifluoromethylphenyl)sulfonyl]amino}benzoic acid (3b), respectively. The sequential esterification, hydrozinolysis and cyclizaation of carboxylic acid group of (3a-b) resulted 4-{[(4-methylphenyl)sulfonyl]amino}phenyl 1,3,4-oxadiazole-2-thiol (6a) and 4-{[(4-trifluoromethyl-phenyl)sulfonyl]amino}phenyl 1,3,4-oxadiazole-2-thiol (6b). The intermediate (6a-b) reacted with N-bromoalkyl substituted phthalimides (7`a-f) and trifluoromethylated benzyl chlorides (7a-c) to afford 8a-j & 9a-c in good yields. To access second series of hybrids, probenecid (10) was converted into 4-[(dipropylamino)sulfonyl]benzene 1,3,4-oxadiazole-2-thiol (13) and d similarly elaborated to sulfonamido-1,3,4-oxadiazole-2-thiols (13) which is then bifurcated to S-alkylphthalimide and S-benzyl 4-[(dipropylamino)sulfonyl]benzene 1,3,4-oxadiazole-2-thiol hybrids (14a-f) and (15a-e), respectively. Bioactivity screenings revealed that 8g and 8h are found to be the most potent inhibitors of DENV NS2B/NS3 protease among the synthesized analogs, possessing the IC50 values of 13.9 μM and 15.1 μM, respectively. Molecular docking studies anticipated the binding of the inhibitors at an allosteric site generated in the open conformation of DENV2 NS2B/NS3pro. All these inhibition findings establish that the synthesized novel S-benzyl- and S-alkylphthalimideoxadiazole-benzenesulfonamide hybrids possess a great potential for further antiviral drug development.

Synthesis, Functionalization and Biological Screening of 5-Hydroxyalkylated Thiadiazine – 2 – Thiones

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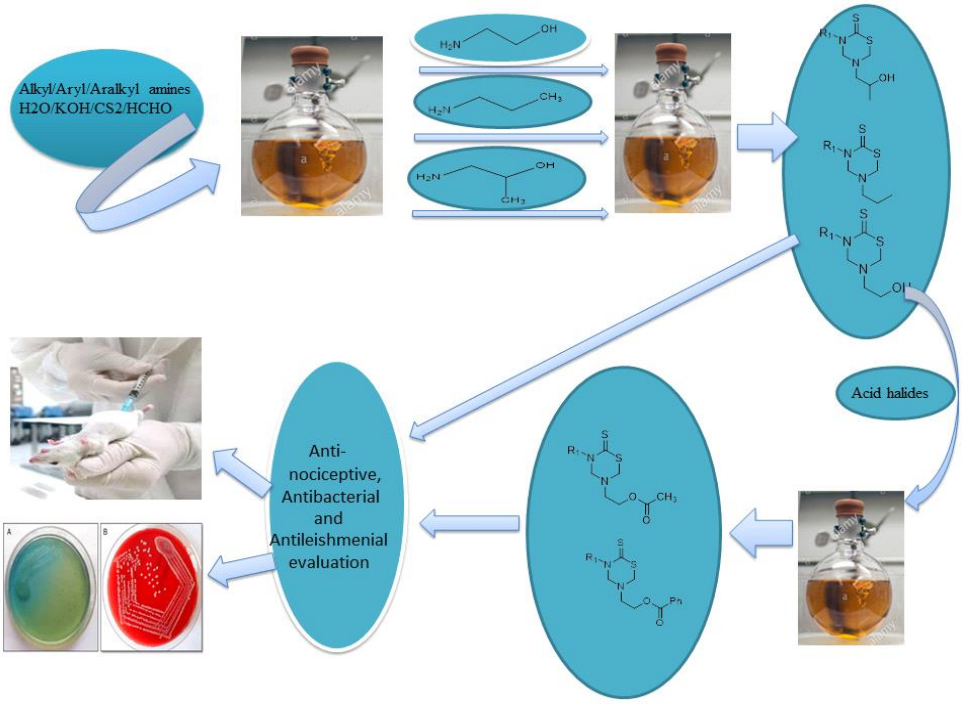
Synthesis of a series of tetrahydro-2*H*-1, 3, 5-thiadiazine-2-thiones (THTT) compounds were carried out by reacting of suitable primary amines including Alkyl /Aryl amines with CS_2 and KOH give rise diathiocarbamate salt which undergoes cyclocondensation with formaldehyde and selected primary amines (Hydroxyl amines). Esterification of selected tetrahydro-1, 3, 5-thiadiazine-2-thiones were conceded under ice cooling conditions by reacting with acetyl chloride and benzoyl chloride in pyridine for 2-3h. Different spectroscopic techniques such as IR, NMR and mass spectral data were used for structure determination. Anti-nociceptive, anti-microbial and anti-leishmanial evaluation of all the synthesized compounds were calculated.

Graphical Abstract



Antibacterial properties of binuclear Zn(II)-azomethine complexes derived from diaminodiphenylsulphide bridged spacer

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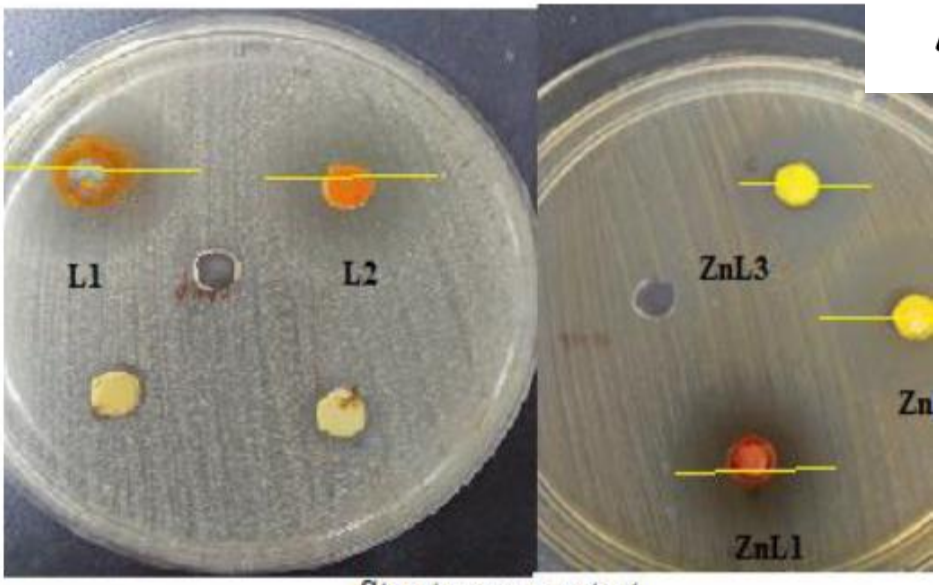
Antimicrobial resistance of microbes against treatment that once could cure, has inspired an urgent need for new drugs development**.** Accordingly, three binuclear Zn(II)-Schiff bases complexes ZnLa - ZnLc were prepared by direct reaction of the ligands La-Lc with Zn(II) ions in equimolar ratios bearing salicyldehydes with OH, NO_2 and Cl functional groups. The synthesized compounds ZnLa - ZnLc were evaulated against Gram positive (*Enterococcus faecalis NCIMB 13280, Streptococcus mutant ATCC 25175™ and Staphylococcus aureus ATCC 6538™)* and gram negative (*Escheria coli NCTC 12900, Salmonella typhi* and *Pseudomonas aeruginosa* ATCC 15442) bacterial strains, respectively, by agar well diffusion and broth microdilution techniques. The minimum inhibitory concentration (MIC90) values were calculated by microplate reader at 550 nm to optimum result. It was found that all the synthesized compounds showed promising antibacterial activity against the genus *Streptococcus mutant* followed *Staphylococcus aureus* and *Escheria coli.* Binuclear Zn(II) complexes had a superior antibacterial activity compared to their parent Schiff base ligands. In general, 3,4-dihydroxy derived Schiff bases alongwith their relevant complexes exhibited magnificent antibacterial activity and hence merits to be established as promising keystone for subsequent antimicrobial drug advancement.

N,N-bis-(3,4-dihydroxybenzaldehyde)-4,4-diaminodiphenylsulphide Zn(II) complex (ZnLa)

N,N-bis-(5-nitrosalicylidene)-4,4-diaminodiphenylsulphide Zn(II) complex (ZnLb)

N,N-bis-(5-chlorosalicylidene)-4,4-diaminodiphenylsulphide Zn(II) complex (ZnLc)

Antibacterial Activities



Streptococcus mutant

A mechanistic study of photodegradation of Moxifloxacin using Oxone activated by TiO_2 in presence of UV-LED

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The antibiotic Moxifloxacin (MOX) has been degraded using Oxone activated by TiO_2 under UV-LED lamps. The TiO_2/Oxone/UV LED process was followed with the addition of Oxone (0.025, 0.05, 0.1 and 0.2 mM) activated by TiO_2 doses 0.0125, 0.025, 0.05, 0.1 and 0.5 g/L. The degradation efficiency was monitored by HPLC having UV/Vis detector, C18 column (5µ, 4.6 x 250 mm^2) with the mixture of acetonitrile, ultrapure water and phosphoric acid (20%, 80% and 0.1% respectively) as mobile phase. The complete removal of MOX was observed at initial concentration of Moxifloxacin 10 ppm, 0.1 g/L TiO_2 and 0.1 mM Oxone with UV-LED exposure time of 12 minutes. The TOC analysis was performed to verify the treatment efficiency and 55% reduction in TOC was achieved after TiO_2/Oxone/UV-LED process. The parameters such as drug initial concentration, Oxone and TiO_2 dosages and pH of the solution were optimized and their effects on degradation were also noted. The pseudo-first order kinetics was observed for degradation. It was revealed from the mechanism of activation that and have played a key role in the degradation. The effect of pH ranging from 3.6-11 was observed to evaluate the degradation rate of Moxifloxacin. The pH 9.4 achieved the maximum degradation and believed to be the optimum pH. Liquid Chromatography coupled with Electrospray Ionization Mass Spectrometry (UPLC-ESI-MS) was used to identify the intermediates and radiolytic end-products. This work provides new insight into the development of the TiO_2/Oxone/UV-LED process for organic contaminant degradation as well as hospital waste management.

Asymmetric Synthesis of α–Trifluoromethylated Piperidines: Applications to the first asymmetric synthesis of Tfm_pipecolic acids and piperidine-based γ-aminoacids

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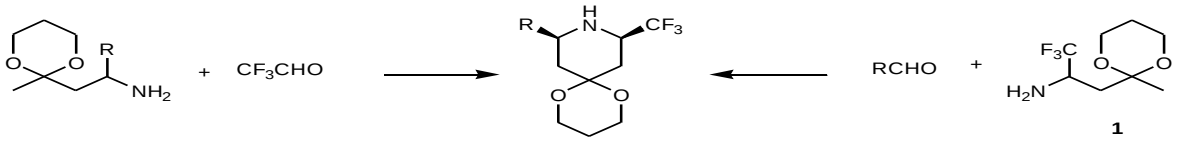
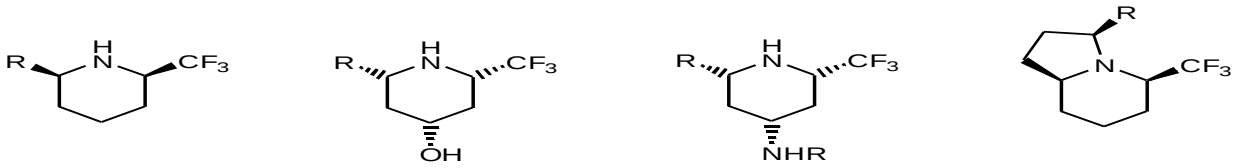
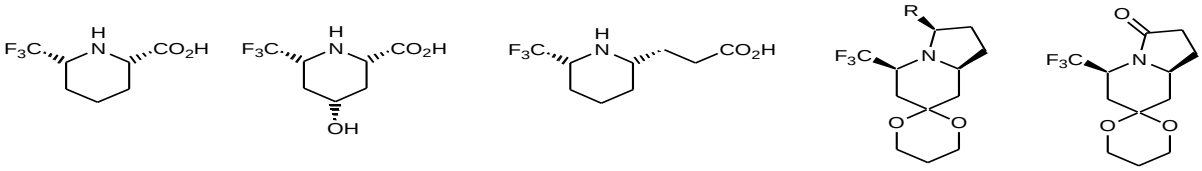
The intramolecular Mannich reaction of β-aminoketals offers a double opportunity for selective incorporation of a trifluoromethyl group at C-2 of a piperidine:



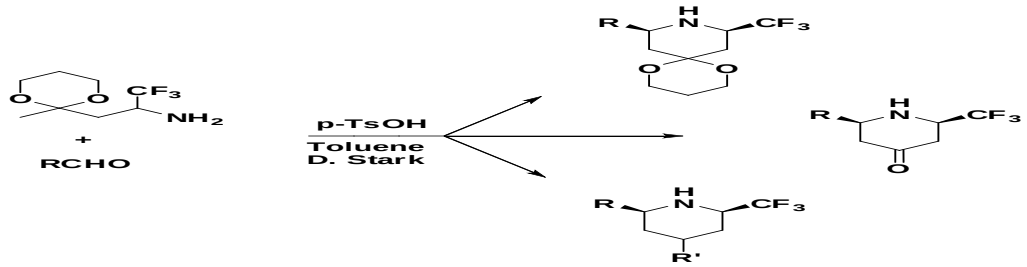
The validation of this strategy in enantioselective synthesis requires the amine 1 in a homochiral form. We propose a rapid access to (+)-1 and (-)-1, and together with its applications towards asymmetric preparation of various fluorinated N-heterocycles.



Besides this, we report the first enantioselective synthesis of Tfm-pipecolic acids, Tfm-piperidine-based analogue of GABA and polycyclic N-heterocycles of type Indolizidines and indolizidinones.



Recently, we have extended our work to synthesize novel derivatives of trifluoromethylated piperidines.



Detection And Analysis Of Various Textile Products For Heavy Metal Contents

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A total of nineteen textile accessories were tested for total metal concentration and results were compared with European Union/ United State regulated safety limits. Total Aluminum, Boron, Copper, Iron and Zinc concentrations were 187.54-330.064, 22.88-30.40, 50.97-13683.14, 27.402-121.98 and 38.015-3090.14 mg/kg respectively. In metallic textile sample category, Copper concentration in 4 out of 7 samples and Zinc concentration in 2 out of 7 samples exceeded safety limits. Copper and Zinc concentrations were found highest in metallic samples as compared to non-metallic and surface coating samples. The reason behind their highest concentration was the composition of these samples as these samples were made of brass which is an alloy of Copper and Zinc. Non-metallic samples contained Al, B, Cr, Cu, Fe, and Zn in considerable amounts but only chromium in only 2 samples exceeded the European Union safety limit. However, in 2 out of 6 surface coating samples, only Copper crossed its safety value. Al, Fe and Zn were also detected in sufficient amounts in these coatings. The reason behind detection of these metals in coating samples was that they were scratched from the surface of metallic accessories from where heavy metal get adsorbed. Cadmium, Cobalt, Mercury, Nickel and Lead were not detected in any of these nineteen samples. The data of this research work suggest the importance of quantification of metals in textile products that are more frequently encountered and easily available in local markets to evaluate the health risk these products can cause and besides Lead, Nickel and Mercury other metals also deserve attention.

Biosynthesis Of Copper Nanoparticles By Using Aloe Barbadensis Leaf Extracts And Study Of Application In Congo Red (Acid Red 28) Dye Removal.

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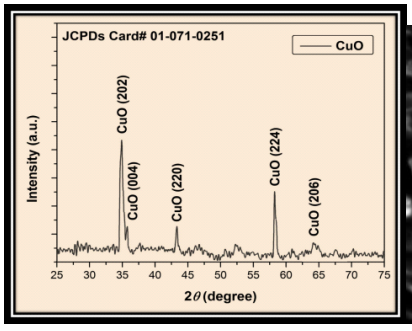
Development of green nanotechnology is generating interest of researchers toward eco-friendly biosynthesis of nanoparticles. In this study, biosynthesis of stable copper nanoparticles was done using aloe barbadensis leaf extract. First of all, we prepared leaf extract of aloe barbadensis in deionizedwater. This extract added to 1mmol of copper sulfate solution and observed the change in color of the solution from colorless to dark brown colored solution. The present study tracing of an object is a green synthesis of copper nanoparticles by theinteraction of leaf extract and copper salt and its dye removal efficiency. Copper oxide nanoparticles in this study examined the efficient removal of Congo red CR dye. The effect of variables like concentration, time, PH, adsorbent dosage also examined in this present study. This was noted that maximum PH 3, theconcentration of nanoparticles 1mg, maximum time 120mint was optimum condition for dye removal. Biosynthesis of nano particle put forward a cost-freeand environmentally suitable method of nano particle synthesis. The characterization of copper oxide nanoparticles like X-ray diffraction and SEM analysis showed thataverage particle size calculated was 40 nm. The shape of the coppernanoparticleswas spherical and cubic and their range of grain was 80-120nm.EDX of synthesized nano particles showed copper 38%.UV spectrophotometer analysis confirms peak of thecoppernanoparticles between 200-600nm.



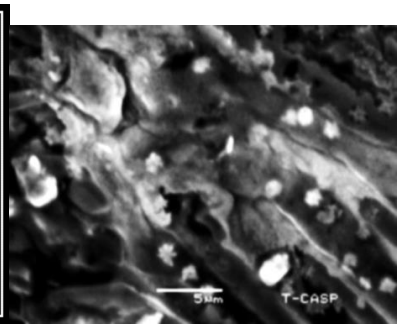


Figure 1sem images of copper nanopartical Figure 2 XRD of copper nanopartical

Variation in Nutritional and Antioxidant Attributes of *Moringa oleifera L.* Leaves at Different Maturity Stages

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The present work reveals variation in nutritional and antioxidants profile of *Moringa oleifera* leaves as function of four maturity stages. Percent yield and total phenolic contents (TPC) of 80% methanolic extract from *M. oleifera* leaves were found to be maximum (14.21 %, 95.26 mg/g) at 1st maturity stage and minimum (9.695 %, 38.22 mg/g) at the 4th maturity stage. Total flavonoids, ash, protein, vitamin C and *β*-carotene contents were found minimum at 1st stage and maximum at 4th maturity stage. Amino acids including valine, alanine, leucine and phenylalanine were identified with their least contents at 1st maturity stage (90.87, 53.07, 55.21, 48.65 mg/g) while maximum at 4th maturity stage (197.66, 114.3, 114.2, 104.5 mg/g, respectively). The level of different minerals such as Cu, Fe, Mn in *M.oleiefra* leaves at different maturity stages varied from 0.59 to 2.08, 21.96 to 58.68, and 5.56 to 13.84 mg/100 g, respectively. RP-HPLC analysis depicted the presence of quercetin as a major component (21.64 mg/kg) followed by benzoic acid, ferulic acid, sinapic acid, gallic acid, and *p*-coumaric acid with contribution at 13.03, 8.85, 3.39, 2.88, 1.59 mg/kg, respectively. Overall, a considerable variation in the content of different nutrients and phenolics was noted in *M.oleifera* leaves as maturity progressed. These results support the harvesting of *M.oleifera* leaves at an appropriate maturity stage to maximize the functional food and nutraceutical benefits of this valuable food commodity.

Chemical and Biological Attributes of Wild Thyme (*Thymus vulgaris L.*) Essential Oil

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This work presents the phytochemical composition and biological (antioxidant, antibacterial, hemolytic, and thrombolytic) potential of the essential oil (EO) isolated from aerial parts of wild thyme. The total phenolic and flavonoid contents in thyme EO (TEO) were 4.69 gallic acid equivalent (GAE) and 1.45 catechin equivalent (CE) mg/100 g, respectively. TEO exhibited considerable antibacterial activity against six bacterial strains; *S. typhi* (30 ± 1.41 mm) was found to be more sensitive to the tested TEO. Using gas chromatography-mass spectrometry (GC-MS) analysis, 13 components were identified; the major compound was carvacrol (76.00%), followed by o-acetyl thymol (5.63%), *α*-pinene (5.05%), and spathulenol (4.97%). Some other compounds like *ρ*-cymene (3.27%), ledenene (2.53%), *α*-myrcene (0.87%), *γ*-terpinene (0.86%), *α*-linalool (0.34%), *ρ*-menthenone-8-ol (0.24%), caryophyllene (0.07%), isoaromadendrene epoxide (0.06%) and isoborneol (0.02%) were also detected. The hemolytic and thrombolytic activities of TEO have shown that it has no cytotoxic effect. These results support the utilization of Wild TEO in nutra-pharmaceutical industry due to its potential antioxidant and antimicrobial characteristics.

Synthesis of amantadine derived thiourea derivatives as potent inhibitors of alkaline phosphatase with anti-inflammatory action

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This work targets the synthesis of aryl thiourea derivatives (4a–l) of pyrazole based nonsteroidal anti-inflammatory drug named 4-aminophenazone, as potential inhibitors of intestinal alkaline phosphatase enzyme. The derivatives were screened against calf intestinal alkaline phosphatase to unravel their anti-inflammatory potential. Compound 4c (3-methyl substituted derivative) of the series turned out as the lead candidate with IC50 value 0.420 ± 0.012 μM, many folds better than reference standard used (KH2PO4 IC50 = 2.8 ± 0.06 μM and l-Phenylalanine IC50= 100 ± 3.1 μM). Kinetic studies of the active member suggested non-competitive binding mode. The results were further supported by molecular dynamic simulations for deep insight about the protein behavior against active inhibitors 4c and 4g during docking analysis synthesized derivatives. Further study about the biochemical properties in addition to RO5 analysis of synthesized derivatives suggested the therapeutic potential of newly synthesized series of aminophenazone based thioureas (4a–l

Molecularly Imprinted Polymers for the Emerging Dye Acid Black-1 and its Quantification via Liquid Chromatography

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Molecularly imprinting polymer was successfully synthesized for the dye acid back-1 using Meth acrylic acid, ethylene glycol and azo-bisisobutyronytrile in the ratios of 2:11:49 (Template: monomer: cross linker). The novelty of the project was the packing of the newly synthesized MIP in the stainless steel column and their evaluation in the separation analysis of different dyes. In accordance with lock and key model the dye being imprinted in the polymer showed long retention time. The other dyes were also resoled by the MIP packed column with somewhat poor chromatographic performance. The thermo kinetic and thermo dynamic studies of the newly synthesized molecularly imprinted polymers were also carried out for the maximum output of the MIP. FTIR and SEM snapshots of the MIPs were exhibited as the characterizations. The synthesized polymeric substances possess excellent thermal, chemical, and mechanical stability and can be reused for several hundred times.

Adsorption characteristics of magnetic nanoparticles composite activated mango peels hydrochar for Decontamination of Cr (VI) ions from Aqueous Solution

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Activated hydrochar (ACH) prepared from low-cost mango peels a biomass modified with iron oxide magnetic nano composite (ACH/Fe_2O_3) material and tested for removal of Cr (VI) ions from aqueous solutions. The surface characteristics of the activated hydrochar before and after nano composite modification were measured and characterized by different techniques FTIR, XRD, SEM, EDS and BET for nitrogen adsorption porosimetry. The results showed that impregnation of activated hydrochar with iron oxide increased surface area and composite material introduced more acidic functional groups and improved the adsorption ability compared to the original activated hydrochar. The effects of adsorbent dose, contact time and initial Cr (VI) ions concentration on the adsorption of Cr (VI) ions by ACH/Fe_2O_3 were investigated. Equilibrium isotherm and kinetic data follows Langmuir isotherm and pseudo second order kinetic model. The uptake rate of chromium (VI) ions in a fixed-bed column experiment controlled by external mass transfer and intra-particle diffusion throughout the entire adsorption period. Based on obtained results ACH/Fe_2O_3 was promising for the elimination of Cr (VI) ions with obtained equilibrium adsorption capacity of 40.28 mg/g at the optimized bed height, flow rate and Cr (VI) ions concentration. The experimental breakthrough curves results by adsorption process were compared and were successfully fitted with kinetic models Adams - Bohart, Thomas and Yoon - Nelson in their linearized forms. Based on these results ACH/Fe_2O_3 is a promising sorbent to remove Cr (VI) ions from aqueous solution.

Spectrophotometric Determination of Nickel via Diathiocarbamate Complex

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In this study glyphosate complex was synthesized with nickel in aqueous media using ammonia as a buffer and 2% Carbon disulphide for a thiocarbamate formation. A yellow coloured Ni (II) glyphosate complex from glyphosate with Ni (II) salt was formed.

Different parameters were optimized for the synthesis of this complex. The optimum wavelength was found to be 390 nm. The maximum amount of complex was found at pH 12, as which it was stable also. The amount and volume of CS_2 was optimized at 2% and 2ml. Figures of merits which consist of Mean (0.64974), Standard deviation (0.225), Relative standard deviation (34.66), Limit of detection (0.675), Limit of quantification (2.25), calibration curve range (6-30), correlation coefficient (R^2) (0.9276) was calculated.

Silver nanoparticles of *Haloxylon recurvum* Plant extract and its application for degradation of Methylene blue dye

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The biosynthesis of Silver nitrate nanoparticles (AgNPs) is convenient, economical, eco-friendly, less energy-intensive. These prepared nanomaterials were used to eliminate the toxic and hazardous materials from aqueous solutions. Naturally occurring phyto constituents such as flavonoids and Phenolics in the *Haloxylon recurvum* can act as stabilizing agents during AgNPs formation process. This study presents the biogenic synthesis of AgNPs using *Haloxylon recurvum* plant extract. The developed *Haloxylon recurvum* were designated as HRS-AgNPs and initially characterized using various instrumental techniques including UV–Vis spectroscopy, Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) the optimally yielded HRS-AgNPs were then employed to test their methylene blue dye degradation potential. The degradation of dye suggests that HRS-AgNPs may also be exploited against other related and emerging contaminants in cost-effective manner.

Green Synthesis of MOFs for Resorcinol Adsorption

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Alcohol and alcohol-based compounds especially resorcinol is documented as emerging contaminants in water and are considered as major menaces to public healthiness all over the world. Synthesis of operative adsorbents to alleviate water contamination having high level efficacy is a major challenge for all researchers. Herein, two zeolitic imidazolate frameworks (ZIF-8 and ZIF-67) were synthesized by the reaction of 2-methyl imidazole with zinc and cobalt metals displaying excellent adsorption capacities (ZIF-8 = 478.39 & ZIF-67 = 538.13 mg/g) for highly toxic pollutant resorcinol. From thermodynamics study it was concluded that adsorption for resorcinol elimination is endothermic, followed by spontaneous process and physical adsorption process takes place as indicated by ΔH_{ads} (30.473 KJ/mol). Langmuir isothermal model and pseudo 2nd order kinetics is best fitted for adsorptive removal of resorcinol and separation factor values for 30 – 100 ppm resorcinol concentration was in the range of 0.0239 – 0.1312 which displayed that adsorption process is favorable. Furthermore, these MOFs have the same organic linker and same topology but different adsorption capacities. This difference is due to the presence of zinc and cobalt metals having different electronic configuration which results in different porosity (ZIF-8 = 1278 and ZIF-67 = 1876 m_2/g) and adsorption capacities.

Structure-Based Design and Synthesis of Trolox–1,3,4-Oxadiazole Hybrids with Potential Multi-Target Bioactivities

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We have focused our research on the synthesis of oxadiazole-based Trolox derivatives following multi-step reaction and assessment of their anticholinesterase inhibitory activities. Trolox was esterified with ethanol in the presence of a catalytic amount of sulfuric acid and further subsequent substitution with hydrazine hydrate yielded the acyl hydrazide. The acyl hydrazide upon condensation with various substituted aldehydes resulted in the corresponding Schiff's bases. The cyclization of Schiff's bases was carried out in iodine to obtain the target oxadiazoles of Trolox. The structures of the synthesized compounds were confirmed via UV, ^{1}HNMR, and Mass spectroscopic techniques. The studies of bioactivities both *in silico* and *in vitro* for the synthesized compounds reflect that they can act as leads for the design and synthesis of drugs.

Application of Carbon Sorbent derived from *Citrus X sinensis* (Orange) Peels for the Removal of Insecticides and Herbicides from Aqueous Resources

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The present study focuses on the adsorption of insecticides and herbicides from solution by carbonaceous adsorbent prepared from orange peels (AC-OP). The conversion of orange peels into AC-OP causes an increase in the removal capacity of the pesticides from 79% to 88% for chlorpyrifos and from 73% to 92% for pendimethalin for dried peels to AC-OP. This economic and environment friendly adsorbent is prepared from abundantly available orange peels for the adsorption of pesticides from water. This in turn is very useful in waste water treatment. The adsorbents were characterized with the help of Fourier transform infrared spectroscopy. Furthermore, the adsorption efficiency of dried fruit peels was compared with carbon sorbent prepared from orange peels. The effect of time, pesticides concentration, temperature and adsorbent dose were studied in batch adsorption studies. The experimental data shows an increase in uptake of pesticides with increase in the concentration of pesticides solution. The Qe (mg/g) value for AC-OP is increased from 3.61 to 4.15 mg/g for chlorpyrifos and from 4.1 to 4.68 for pendimethalin.

ORR (oxygen reduction reaction) for green energy technologies

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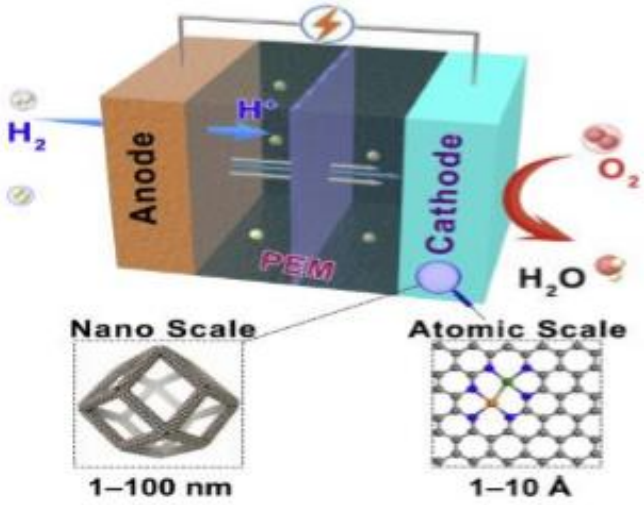
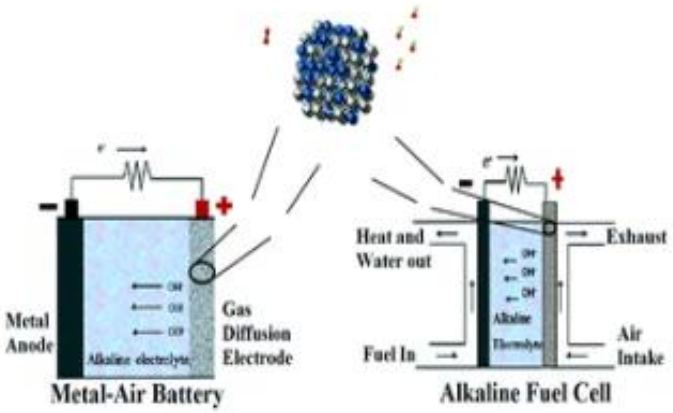
The growing population, greater energy demands and environmental pollution due to the excessive use of non-renewable resources put an emphasizes on the development of robust and efficient ORR (Oxygen reduction reaction) electrocatalyst to cope with the demands of the growing world and to make world better and safer place for living, for the present and future generation. The importance of Oxygen reduction reaction electrocatalyst can be estimated from the recent progress and research in both academic and industrial areas. Among the different fuel cells, proton exchange membrane fuel cells and metal-air batteries have attracted great attention owing to high efficiency in terms of cost, stability, low pollution and being safer, they are promising candidates for green energy systems. Rechargeable metal-air batteries operate under functionally more complex electrocatalysts than fuel cells. The key processes in metal-air systems are battery discharge process (ORR) and battery charging process (OER). To increase the sluggish kinetics in both PEMFCs and metal-air batteries, development of cathodic oxygen reduction reaction electrocatalyst is indispensable. Pt, Au, Ru Ag, Pd are highly efficient catalyst for oxygen reduction reaction. For the conversion of chemical energy into electrical energy, the four-electron process is catalyzed by metal surface, but the major bottleneck of precious metal is their high cost and scarce nature. An electrocatalyst with low cost, high activity, durability and stability for cathodic ORR is therefore, highly desirable for widespread applications of green energy technologies. The recent trend involves the development of catalysts based on non-precious metals in order to counteract the cost-effective issue for the commercialization of fuel cells and green energy technologies.



$$O_2 + 2H_2O + 4e^- \longrightarrow 4OH^-$$



Phosphatized copper oxide nanoparticles for electrochemical nitrite detection

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Phosphatized copper oxide nanoparticles have been synthesized by hydrothermal method for nitrite detection and their formation is confirmed by using electrochemical methods. To investigate the electrochemical sensing performances, cyclic voltammetry and different other electrochemical techniques; linear sweep voltammetry, electrochemical impedancespectroscopy and controlled potential electrolysis are employed on modified GCE. Several important electrochemical sensor parameters havebeenevaluatedfornitriteoxidationsuchaspH, different concentrations, varying time for phosphatization of modified electrode materials etc. The measuredresultsshowthattheaspreparedmodifiedelectrodematerialexhibitsdetectionlimitof 96.3 µM (S/N=3) and high analyticalsensitivityof0.413MAcm-2.Meanwhilethephosphatized copper oxide nanomaterial displays durability, long-term stability and anti-interference ability; when it is subjected for controlled potential electrolysis.

Synthesis, Characterization, Biological Evaluation and In Silico Studies of Trolox-Based Acylhydrazones

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In our research work we have focused on the synthesis of Trolox-based acylhydrazones following multi-step reaction and assessment of their antioxidant and anticholinesterase inhibitory activities. Trolox was esterified with ethanol in the presence of a catalytic amount of sulfuric acid and further subsequent substitution with hydrazine hydrate yielded the acyl hydrazide. The acyl hydrazide upon condensation with various substituted aldehydes resulted in the corresponding Acylhydrazones. The structure of the synthesized compounds was characterized by spectroscopic techniques via UV, ^{1}HNMR, and Mass spectroscopic techniques. Evaluation of biological activities both in silico and in vitro of the synthesized compounds reflect that they can play effective role in the synthesis of bioactive drugs.

Plasma miR-146a signature as a diagnostic and prognostic marker for pediatric acute lymphoblastic leukemia

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MicroRNAs (miRs) are small noncoding RNAs that have shown their role in the development and progression of acute lymphoblastic leukemia (ALL). The present study aims to analyze the plasma miR-146a expression as a potential diagnostic and prognostic signature in pediatric patients of ALL. A total of 86 study subjects were included in the study including pediatric patients, controls and follow up cases. MicroRNA was extracted from the plasma of all the subjects and complementary DNA (cDNA) was synthesized using reverse transcription. The relative quantification was performed using real time PCR and normalized fold expression was calculated by $2^{-\Delta\Delta Ct}$ method. Normalized fold expression of miR-146a was analyzed in pediatric patients before and after treatment. Pre-treatment expression in pediatric patients was significantly higher when compared with age and gender matched healthy controls ($P<0.0001$). Receiver operating curve (ROC) analyses showed AUC of 1 for pediatric ALL (95% CI: 0.960 to 1.00) exhibiting 100% sensitivity and 100% specificity ($P<0.0001$) highlighting its diagnostic potential. After treatment, the miR-146a levels showed significant reduction in expression of miR-146a levels in pediatric patients compared with controls ($P<0.001$) that indicates its prognostic significance. Clinicopathological correlation showed that miR-146a expression in plasma was independent of these factors demonstrating its clinical significance. Moreover, target prediction analysis performed using bioinformatics approach showed specific genes regulated by miR-146a that may be utilized as potential therapeutic targets for all.

High Paid Skills In the Field of Chemistry; Learn & Earn

Dr Rizwana Mustafa
Founder Scientific Pakistan

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A chemistry degree can give you access to a high-paying job in healthcare, manufacturing, tech, and biotech. Even if you don't wind up in a chemistry role, this degree makes you a uniquely-equipped employee and gives you a competitive edge when applying for jobs. But, unfortunately, after getting a degree in Chemistry, students have to face a lot of problems in the job market. The major reason behind this is not to be familiar and equipped with the emerging skills, tools and practical knowledge of the subject. This talk is focused on how you can identify, learn for free and apply these skills to get high paid jobs either in the industry or freelance marketplace. These skills are not only making you financially strong but helping you to find good positions in higher studies.

Anti-HCV potential of flavonoids isolated from *Rhynchosia pseudo-cajan*: In-vitro and in silico approach

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Hepatitis C virus (HCV) has become a leading cause of hepatocellular carcinoma and liver cirrhosis making it a major global health concern. To date, there is no vaccine available in the market to challenge this disease and current focus is on developing anti-HCV drugs with better efficiency. Flavonoids represent an important family of compounds with diverse pharmacological properties. Here, we have isolated eleven known flavonoids (**1-11**) from *Rhynchosia pseudo-cajan* and evaluated for anti-NS5B polymerase and anti-HCV potential. All isolated compounds (**1-11**) were screened for *in-vitro* anti-NS5B polymerase and anti-HCV activity. As a results all compounds (**1-11**) were found to be displayed significant anti-HCV and anti-NS5B polymerase activities in the *in-vitro* assay. Compounds **7** (quercetin) and **8** (rutin) were found to be most potent anti-HCV agents retarding its replication by 81.8 and 89.4%, respectively and their effective concentration were safe showing no cytotoxicity to the host cells. Molecular docking studies were also performed, to know the active pharmacophore in these isolated compounds at atomic level. It may be concluded that the flavonoids derivatives compounds **7** (quercetin) and **8** (rutin) have good potential and can be introduced as anti-HCV drugs. These data are the first description of **8** (rutin) possessing *in-vitro* anti-HCV activity.

Reverse Osmosis - The Future of Fresh Water Production by Desalination

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The availability of good quality drinking is one of the burning issues of the modern industrialized world. The increasing scarcity of fresh water in most of the developing countries has shifted the emphasis on the utilization of brackish and marine water reservoirs for the production of drinking water through the desalination of brackish and marine water. The two major desalination technologies are thermal desalination and membrane desalination. Today, the majority of the World's desalination industry has been shifted to membrane desalination due to its cost-effectiveness and environmentally friendly nature. Among the different membrane desalination techniques like microfiltration, ultrafiltration, nanofiltration, and reverse osmosis; reverse osmosis is the technologically and qualitatively most advanced desalination method. This review provides a background of the different water desalination techniques and the evolution of the reverse osmosis (RO) technique over the last few decades as the leading method for the desalination of marine and brackish water for the production of potable water. A state-of-the-art reverse osmosis water treatment plant containing all its essential elements is presented diagrammatically to provide a pictorial understanding of the process.

Synthesis of MnO2 Doped Cu_2O/Cu@C MOF as an Efficient Catalyst for CO_2 Reduction Reaction

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In the research of clean energy, the key challenge is the carbon dioxide (CO_2) and carbon monoxide (CO) conversion into value-added products. For this purpose, the electrocatalyst for CO_2 reduction reaction (CO_2RR) promotion is required. In this research work, a copper-based metal-organic framework (Cu-BTC MOF) was pyrolyzed into an oxide-derived nanoporous carbon (Cu_2O/Cu@C) structure that was then doped with MnO_2 for CO_2 reduction. The synthesized electrocatalysts were characterized by Fourier transform infrared spectroscopy (FTIR). The peaks that appeared at 721 cm^{-1}, 728$^{-1,}$ and 820 cm^{-1} confirmed the presence of the Cu-O functional group in Cu-BTC, Cu_2O/Cu@C, and MnO_2 doped Cu_2O/Cu@C catalyst respectively. While the appearance of a small intense peak at 984 cm^{-1} confirmed the presence of Mn-O group in MnO_2 doped Cu_2O/Cu@C. The crystallinity and average crystallite size was confirmed by powder X-ray diffraction (XRD). The average crystallite size of Cu-BTC was 98.89 nm while the crystallite size of Cu_2O/Cu@C was 48.26 nm. Thermogravimetric analysis (TGA) revealed that Cu-BTC was stable up to 350 ^oC, Energy Dispersive X-ray spectroscopy (EDX), and scanning electron microscopy (SEM) revealed the elemental composition and surface morphology. All the techniques revealed significant evidence of successful synthesis of MnO_2 doped Cu_2O/Cu@C catalyst.

Synthesis of Cu-Based Metal Organic Frameworks for CO_2 Reduction

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In the recent decades, because of extensive utilization in catalysis as well as structural properties and controllable surface functionalities, metal organic frameworks (MOFs) have gotten a remarkable attention for material scientists. In this study we have reported a strategy on developing MOF as a facile and highly efficient electrocatalysts for significant electrochemical carbon dioxide reduction (CO_2RR) as it is a beneficial process for conversion of CO_2 into useful energies, hydrocarbons and chemicals. A potential and dynamic electrocatalyst was synthesized and coded as PS1 and PS2 by pyrolyzing the prepared S1 and S2 MOFs, which were prepared by hydrothermal method using copper salt and 2,5-dihydroxy terephthalic acid as linkers. After pyrolysis, as organic linker was removed and nano-porous carbon matrix was obtained. All synthesized samples were characterized by using techniques such as x-ray powder diffraction (XRD), scanning electron microscopy (SEM), energy dispersive x-ray spectroscopy (EDS), thermo gravimetric analysis (TGA) and Fourier transforms infrared spectroscopy (FTIR). All of the results obtained by techniques showed that the prepared catalysts were successfully synthesized. On the bases of the characterization results it was expected that promising PS1 and PS2 electrocatalysts materials have attainable unsaturated metal sites and incredible textural properties which exhibit the outstanding performance towards electrochemical application of CO_2 reduction reactions.

Oxygen Reduction Reaction by using non-precious metals, like Cobalt Nickle Nanowires

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The electrocatalytic performance of alloy nano-catalysts may be efficiently enhanced by modifying their physical characteristics (ensemble, geometric, and ligand effects) to obtain model surface structure and compositions for proton exchange membrane fuel cell (PEMFC) use. Using a surfactant-free, thermal single-phase solvent technique, highly catalytic Iron Nickle nanowires (Co_n Ni_{100-n} NWs) with a modest lattice strain and helix type shape are created. Co_nNi_{100-n} NWs are exposed through the (111) facets, and their shrinking or expanding lattice parameters may be controlled by alloy compositions, according to X-ray diffraction studies. Electrochemical data suggest that their high catalytic activity is linked to lattice shrinkage, facets, and bimetallic compositions, with greater activity when the Fe/Ni ratio is 50:50, which is backed up by a comparative study. The Co_nNi_{100-n} NWs have dramatically increased electrocatalytic activity and stability for the oxygen reduction process when compared to nanoparticle type platinum metal catalysts with comparable metal compositions (Co_nNi_{100-n} NPS).

Layered Double Hydroxide Nanosheets and Their Derived Nanocomposites toward Efficient Oxygen Evolution Reaction

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In a variety of applications, layered double hydroxide (LDH)-based materials have gotten a lot of interest because of their distinct layered structure with high specific surface area and distinct electron dispersion, resulting in superior electrocatalytic performance. Furthermore, the presence of several metal cations imparts a degree of tunability to the host layers; the distinct intercalation properties result in flexible ion exchange and exfoliation. Thus, by altering the morphology, composition, intercalation ion, and exfoliation, their electrocatalytic performance may be tuned. However, their limited conductivity restricts their electrocatalytic effectiveness, prompting researchers to integrate them with conductive materials in order to boost their electrocatalytic activity. Another issue impeding their electrocatalytic activity is the LDHs' enormous lateral dimensions and bulk thickness. Introducing defects and tuning the electronic structure of LDH-based materials are thought to be useful ways for increasing the number of active sites and improving intrinsic activity. Because of the distinct benefits of LDH-based materials, their derivatives have also been employed as improved electrocatalysts for water splitting. Recent development on LDHs and their derivatives as improved electrocatalysts for water splitting is included in this article, current methodologies for their design are given, and key problems and prospects of LDHs are explored.

Silver metal-based nanocomposites for electrocatalytic reduction of CO2 into CO

Multi-Target Bioactivities

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Silver metal base electrodes are known to be the most common type of electrocatalyst for CO2RR. Here we mention Ag@CuO, an efficient electrocatalyst for the selective production of CO from CO2RR. The use of CuO as catalyst support for Ag catalysts to improve the reduction of CO2 to CO. Oxide-derived copper has produced/attracted high-interest rates due to its superior performance in terms of CO2 reduction reaction (CO2RR), Faradaic efficiency, lower overpotential, increasing conductivity and provide silver NPs uniform distribution on the surface. The deposition of silver NPs on copper oxide has shown improved catalytic performance over silver nanoparticles for the CO2RR to CO. Ag@CuO, is a more selective and efficient electrocatalyst that exhibited an enhanced current density and significantly improved Faradaic efficiency, additionally lower overpotential with high stability. Through electrochemical experiments and structural characterization, we also investigated the role of the CuO support in enhancing the catalytic sites, specifically to its ability to maintain the Ag nanoparticles at their most catalytically active size and its ability to stabilize the $CO_2^{\bullet-}$ intermediate and enhance the electrocatalytic performance.

Synthesis of Chiral Nanomaterials in the Presence of Purine Nucleotides

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A key component of DNA, nucleobases, nucleosides, and nucleotides has emerged as a viable building block for the creation of functional nanomaterials. The use of biomolecules as templates in the synthesis of nanomaterials provides a good technique for controlling and regulating their morphologies and other properties. In this study, we demonstrate the formation of different chiral morphologies of Cu/Pd nanoparticles by employing purine nucleotide as a morphological inducer. Furthermore, we study the effect of purine nucleotides on the preparation of chiral Cu/Pd, nanoparticles with spherical and hexagonal morphologies. In the presence of Purine nucleotides (ATP, GTP), Cu/Pd nanoparticles were successfully constructed. Transmission electron microscopy (TEM), scanning electron microscopy (SEM), X-ray diffraction (XRD), and chiral dichroism (CD) spectra were used to characterize the produced chiral metallic nanoparticles. The Cu/Pd chiral nanoparticles were used for a variety of applications due to their controlled shape. The research provides a potential approach for production of nanomaterials with controllable morphologies and various applications in optoelectronic devices, sensing or imaging, chemosensory, energy materials and bio-probes.

Fabrication of cobalt doped zinc ferrite nanoparticles with sulfur doped graphitic carbon nitride photocatalytic material

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In this project, zinc ferrite (ZF), and a series of Co doped zinc ferrite (Co@ZF) nanoparticles by varying percentage of cobalt (0.5, 1, 3, 5, 7, and 9 wt %) were prepared by using hydrothermal method and subjected to photocatalytic degradation of methylene blue taken as standard drug. The photocatalytic study revealed that degradation of methylene blue was enhanced as the concentration of cobalt increased up to 5 wt %. The degradation efficiency reached its pinnacle about 78 % for 5 % cobalt doped zinc ferrite and minimum about 57 % for pure zinc ferrite after 180 minutes. Then the composite of 5 % Co doped zinc ferrite were made with varying percentage of sulfur doped g-C3N4 (10, 30, 50 and 70 wt %). These nanoparticles and nanocomposites were characterized by XRD and FTIR to confirm their morphology. The photocatalytic efficiency of nanocomposites was enhanced due to synergistic effect of 5 % Co doped zinc ferrites and sulfur doped graphitic carbon nitride. The significant increase in degradation of methylene blue was observed by nanocomposite of 50 % sulfur doped graphitic carbon nitride with 5 % cobalt doped zinc ferrites and 91 % degradation was achieved after 180 minutes.

Synthesis of Bromide Bridged Mercury(II)-*N*-Heterocyclic Carbene Complexes to Prepare Ytterbium-NHC Complexes *via* Redox-Transmetallation Reaction

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The study to explore the practicability of a synthetic route for the metallation: redoxtransmetallation method (RTM) for the synthesis of ytterbium-carbene complexes. It was involved with the preparation of benzimidazolium salts (**4-6**) by symmetrical and nonsymmetrical substitution on benzimidazole. The salts were subjected to *In-situ* process for metallation to get [Hg(II)-NHC] complexes of type [(HgBr-NHC)(μ2Br)2] (**7-9**). Crystals of complexes **7** and **8** appeared successfully which were characterized by X-ray Crystallography. Both **7** and **8** showed tetrahedrally dinuclear nature with two bromide bridging units which were connecting both the metal centers. After that, the aforementioned RTM was employed under inert atmosphere wherein metal centres of three newer mercury(II)-*N*-Heterocyclic carbene [Hg(II)-NHC] complexes were reduced to metallic mercury under the action of metallic ytterbium.

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

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

Isothermal investigation of adsorptive Removal of Murexide Dye by *Pyrus communis* biowaste

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The purpose of this work is to investigate the detoxification of an anionic dye, Murexide on activated carbon, derived from *Pyrus communis* biowaste. The obtained adsorbent used, was characterized by Bohem titration, pH of point of zero charge (pH_{PZC}) and SEM. The different experimental parameters of the adsorption process such as: temperature, contact time, initial dye concentration and adsorbent dose were investigated. For the optimization of the process parameters, the effects of pH, adsorbent dosage, initial dye concentration and temperature were investigated. The regeneration process of the exhausted adsorbent was studied to assess the economic and operational feasibility. According to the obtained findings; it is proposed that the activated carbon prepared from *Pyrus communis* biowaste retains a high potential for Murexide elimination and is suitable for large-scale usage.

Extraction Optimization of Phenolic Compounds and Flavonoids of Propolis

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Recently use of propolis as natural medicine is increased enormously, healing effects of propolis is assumed to be because of its highly biologically active natural substances. These substances include the derivatives of cinnamic acid, phenolic acids, substituted benzoic acids, amino acids and flavonoids, to date more than 300 compounds have been identified in propolis. The quality, the color. The aroma and hence the composition of propolis varies with varying seasons, botanical and geographical conditions. Little information is available in the literature regarding composition of Pakistani propolis. It is therefore it is important to investigate the chemical composition of Pakistani Propolis. Proper extraction strategy is very important for accurate measurement of active compounds and there are many factors such as temperature, solvent composition etc. which effects the extraction efficiency.

This study is conducted to optimize factors effecting the extraction of total phenolic compounds and total flavonoids of propolis using multivariate optimization. Solvent composition, extraction temperature and time were selected as independent variable, whereas extraction efficiency was recorded as response variable. All three parameters were changed at 3 levels and a design of fifteen (15) experimental runs were conducted. Total polyphenol contents extracted of propolis were determined using Folin–Ciocalteu (FC) colorimetric method, whereas, total flavonoid contents were determined using AlCl3 colorimetric method. Temperature was found to be most significant term in case of total phenolic compounds, whereas extraction of flavonoids had direct significant relationship with time. Amount of total phenolic compounds extracted at optimum conditions i.e. at 55℃, 60 min and with 62% ethanol was 22.6 µg/g. Total flavonoid extracted were 33.1µg/g, using 90% ethanol, at 65℃.

A Review on Chemical Profile and Anti-Bacterial Activity of Achillea millefolium L

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Bacterial diseases are a great challenge in the health system and the treatment of these diseases continues to be a big problem in the modern day. Natural product medicines have been used since the ancient times to treat microbial diseases and proved to be efficient drugs to cure ailments. Achillea millefolium L. has proven to be an efficient anti-bacterial drug due to the presence of many secondary metabolites including flavonoids, sesquiterpenoids and phenolic acids. The phenolic acids and flavonoids are mainly responsible for the antibacterial activity of A. millefolium. Different studies showed that A. millefolium extracts, obtained from different areas, affect the anti-bacterial properties due to different composition of the secondary metabolites present. Achillea millefolium L. showed great anti-bacterial potential against many common bacteria like S. aureus, E. coli, K. pneumoniae, P. aeruginosa, S. epidermidis, B. cereus etc. Majority of the studies showed that the essential oils possess the highest anti-bacterial activity against S. aureus and low activity against E. coli. A lot of research work is done on A. millefolium along with its chemical composition and pharmacological activities but no data is available regarding its anti-bacterial activity in detail. Therefore, the main focus of this review is to present a comprehensive view of the anti-bacterial properties of Achillea millefolium against different types of gram positive and gram negative bacteria which will be a good contribution in literature and promising for future research in pharmacological fields.

Fabrication of Mo^{6+} a Photocorrosion resistant and hexagonal ZnO modified Photocatalyst for the decontamination of chloroacetic acids in sunlight

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In an effort to develop photocorrosion resistant sunlight active photocatalyst for water decontamination, the surface of hexagonal ZnO was altered by impregnating Mo^{6+} at its surface by a facile route. The synthesized powders were optically characterized by DR, PL and Raman spectroscopy. As evaluated by cyclic voltammetry, compared to pure ZnO, the synthesized catalysts exhibited substantially high stability under illumination. The XRD and XPS analysis evaluated the structure and chemical states. The HRTEM analysis revealed a homogeneous distribution of the Mo^{6+} at the surface without the formation of individual particles and altering the hexagonal geometry. The synthesized catalysts efficiently removed 50 ppm of mono and dichloro acetic acid. Using an innovative approach, the progress of the photocatalytic degradation process was monitored by ion chromatography by measuring the successive increase and decrease in the concentration of chloride and chloro-acetate ions. The mineralization efficiency of the as synthesized catalysts, in comparison to pure ZnO, was estimated by measuring TOC after the exposure. The kinetics of degradation as well as mineralization process was evaluated by applying Langmuir-Hinshelwood kinetic model or the estimation of rate constants.

Hybrid Quinoline-Thiosemicarbazone Therapeutics as a New Treatment Opportunity for Alzheimer's Disease – Synthesis, In Vitro Cholinesterase Inhibitory Potential and Computational Modeling Analysis

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Alzheimer's disease (AD) is a progressive neurodegenerative disorder and the leading cause of dementia worldwide. The limited pharmacological approaches based on cholinesterase inhibitors only provide symptomatic relief to AD patients. In this context, we herein report a series of quinoline-thiosemicarbazone hybrid therapeutics as selective and potent inhibitors of cholinesterases. A facile multistep synthetic approach was utilized to generate target structures bearing multiple sites for chemical modifications and establishing drug-receptor interactions. The structures of all the synthesized compounds were fully established using readily available spectroscopic techniques (FTIR, 1H- and 13C-NMR). In vitro inhibitory results revealed compound 5b as a promising and lead inhibitor with an IC50 value of 0.12 ± 0.02 μM, a 5-fold higher potency than standard drug (galantamine; IC50 = 0.62 ± 0.01 μM). The synergistic effect of electron-rich (methoxy) group and ethylmorpholine moiety in quinolone thiosemicarbazone conjugates contributes significantly in improving the inhibition level. Molecular docking analysis revealed various vital interactions of potent compounds with amino acid residues and reinforced the in vitro results. Kinetics experiments revealed the competitive mode of inhibition while ADME properties favored the translation of identified inhibitors into safe and promising drug candidates for pre-clinical testing. Collectively, inhibitory activity data and results from key physicochemical properties merit further research to ensure the design and development of safe and high-quality drug candidates for Alzheimer's disease.

ASSOCIATION OF INFLAMMATORY MARKERS AMONG PATIENTS WITH DIABETES MELLITUS AND PERIPHERAL ARTERIAL DISEASE

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Diabetes mellitus (DM) is major risk factor for peripheral arterial disease (PAD), coronary arteries disease and cerebral vessel disease. Hemostatic laboratory parameters of PAD patients are unknown. We investigated the biochemical profiling, inflammatory and vascular endothelial dysfunction markers and frequency of polymorphism in promotor region of diabetes associated genes between DM and PAD patients. This study was conducted on 500 patients consist of 2 groups. Group 1 consist of 250PAD and DM patients, group 2 consist of 250 DM patients and 100 healthy control from male and female sex. Blood serum, plasma and red blood cells were used for the estimation of biochemical profiling, inflammatory and vascular endothelial dysfunction markers and genomic study by using the Beckmann chemistry analyzer, ELISA and PCR equipment. Lipid profile (Triglycerides, Total cholesterol, HDL, LDL), cardiac enzymes (CKMB, CPK, AST), renal profile (Urea, Creatinine), Coagulation profile (PT, apTT), LFT (ALT) and CRP were significantly higher ($P<0.0001$) in DM with PAD cases compared to DM patients and healthy controls ($P< 0.05$). Our findings showed that the risk of heart failure, renal failure, diabetic foot ulceration, limb amputation is higher in DM with PAD patients as compared to DM patients and healthy control.

In-vitro evaluation of antiproliferative potential of various fractions of Silybum marianum using HeLa and HepG2 cell lines

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Silybum marianum (Milk thistle) has been proven to possess anticancer, lactogenic, neuroprotective, immunomodulatory, hepatoprotective and anti-inflammatory properties. The current study was designed to evaluate the antiproliferative potential of aqueous and various organic fractions (ethanolic, petroleum ether, ethyl acetate, chloroform, n-butanol) of S. marianum against cancerous (HeLa, HepG2) and noncancerous (BHK) cell lines. The MTT assay was performed to access the cytotoxicity of all these fractions and IC50 values were calculated. The cytotoxicity of these fractions was also confirmed through crystal violet and trypan blue assays. All the tested fractions of S. marianum possessed significant antiproliferative potential. Interestingly, ethyl acetate fraction of S. marianum exhibited the highest antiproliferative activity amongst all the other tested fractions with an IC50 of 13.07 µg/mL, 18.92 µg/mL and 76.15 µg/mL against HeLa, HepG2 and BHK cell lines respectively. Therefore, it is concluded that S. marianum possess strong anticancer activity against both cervical and liver cancer and low cytotoxicity against normal cell line so it could be used as a source of potent anticancer compounds having high efficacy and minimal side effects.

Effect of clomiphene citrate on ovulation induction and hormones of infertility with inflammatory effects on gingiva

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To determine the effect of clomiphene citrate on ovulation induction and its effects and evaluation on gingival inflammation. This was a clinical trial on 50 patients using clomiphene citrate [CC] for ovulation induction and 50 patients with control. These women were examined for dental hygiene, plaque and gingival index bleeding on probing, gingival clavicular fluid any inflammation, dental caries. The results were compared with a control group of 50 women who did not use ovulation medicines. Clomiphene citrate is used for ovulation induction. It alters the hormonal level in serum and also leads to gingival inflammation. Despite similar plaque levels (P 0.05), women using CC for more than three cycles had higher levels of gingival inflammation (P &lt 0.01, P &lt 0.001, and P &lt 0.001, respectively), bleeding (P &lt 0.001), and GCF volume (P &lt 0.001) when compared to the control group and to the users of CC for three cycles. It is concluded that hormonal disturbance in infertility and drugs used in this study may cause gingival inflammation.

Role of A^3-coupling in heterocyclic synthesis

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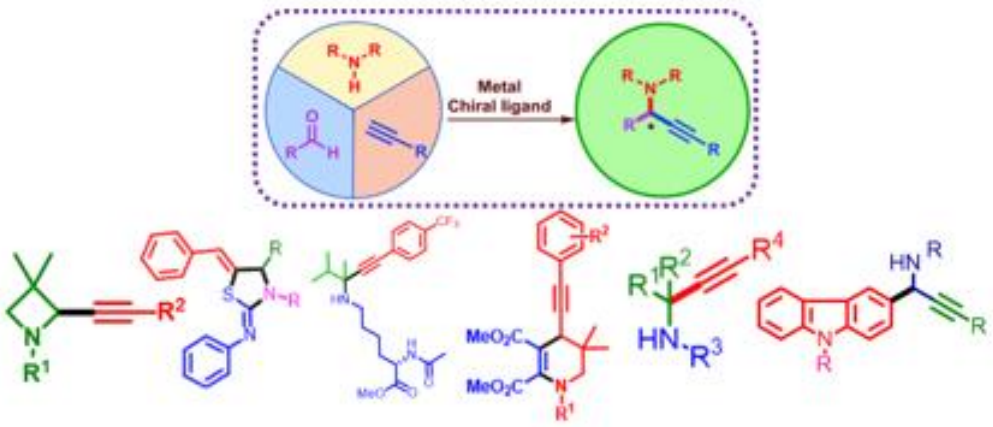
With increasing demand of new entities in medicinal and pharmaceutical industry, the need of new synthetic strategies especially using cheap and earth abundant starting materials is highly wished. A^3-coupling is one of such reactions that has attracted the intention of many chemists due to its versatile ability to build variety of heterocycles in just one or two steps. This talk will focus on our work on A^3-coupling where synthesis of *tri*- and *tetra*-substitutes propargylamines, azetidines, thiazolidines and dihydropyridines etc. have been accomplished using A^3-, KA^2- and IA^2-couplings.



Mechanism of apoptosis in Leishmania tropica promastigotes induced by Pentavalent Antimonial

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In pursuit of safe drug candidates for the treatment of the parasitic diseases like leishmaniasis, a series of heteroleptic pentavalent antimonials have been selected. As their predominantly substituted benzoates and carboxylates form with some complexes fit in acetato ligands. Therefore, using acetate ligands, pentavalent antimonials were screened for their antileishmanial activity and the significant antileishmanial potential was found. Furthermore, the interpretation of the molecular phenomena that are linked to apoptosis prompted in Leishmania tropica by pentavalent antimonials is predicted to distinguish novel targets for therapeutic purpose against leishmanial diseases.

Photocatalytic Degradation and Electrochemical Detection of Malachite Green Dye

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Access to clean water and safe aquatic environment are two of the primary sustainable development goals (SDGs). Despite all the ambitious targets, about 80% of industrial wastewater remains untreated and makes its way directly to freshwater bodies which seriously hampers the progress in fully achieving the SDGs. One of the most common classes of industrial pollutants is dyes. Many research teams are engaged in developing chemical and biological methods to convert these harmful pollutants into environmentally benign products. However, gaps are still there to develop a method which could avoid secondary pollution and which could be economical and efficient. With this consideration, we offer a photocatalytic degradation method and an electrochemical platform for following the kinetics and extent of the degradation of Malachite Green dye using lanthanum doped ZnO as photocatalyst. Lanthanum doping enhances the photocatalytic properties of ZnO. To obtain the best photocatalytic activity, the amount of dopant was optimized by comparing the degradation efficiencies of different percentages of dopant in the catalyst using UV-Vis spectroscopy. The extent of degradation came out to be 92 percent in the presence of 2% doped La-ZnO. The dye degradation was also probed in solutions of different pH from acidic to basic through neutral conditions to obtain evidence of the maximum degradation. In acidic media of pH 3 and 5, 48 and 72% degradation was achieved in 270 and 250 minutes respectively. In a solution of pH 7, 92% of the dye was found to degrade in 220 minutes while in pH 9 and 11 the degradation reached 92 and 99% in 180 and 40 minutes respectively. Evidently, 2% La-ZnO and pH 11 proved as the best conditions for photocatalytic degradation of the Malachite Green dye. Using these optimized conditions, electrochemical method was applied to monitor the leftover amount of dye in samples subjected to photocatalytic degradation. The electrochemical response of Malachite Green was recorded at a glassy carbon electrode using square wave voltammetry. For electrolyte optimization, various electrolytes such as PBS, HCl, BRB, NaOH, NaCl, and KCl were tested. The dye showed maximum current response in 0.1M PBS. Further enhancement in the signal of Malachite Green was achieved by pH optimization from 3 to 11. Deposition potential and accumulation time were also examined and then under optimized conditions, degradation of the dye was investigated by recording the current response during the photocatalytic degradation process. Results obtained from both spectroscopic and electrochemical techniques showed that the degradation process follows 1st order kinetics with a photocatalytic degradation efficiency of 99% in 40 minutes. The results were supported by naked eye evidence of color change of the dye solution from blue to colorless in the stated time. The obtained results hold great promise in the context of water purification for safeguarding human and aquatic lives from the effects of toxic dye effluents.

Synthesis of thienyl libraries via Palladium catalyzed cross-coupling reactions: A focus on computational and biological studies

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Functionalization of heterocycles is useful for synthesis of various organic molecules. Suzuki-Miyaura reaction has emerged as a convenient method to build C-C bonds in synthesizing organic molecules. A library of thienyl derivatives has been synthesized in presence of Tetrakis (triphenyl phosphine) palladium (0) in moderate to good yields. Reaction conditions were optimized and various functional groups were well tolerated. Density functional theory (DFT) investigations on synthesized derivatives were performed in order to explore the structural properties. The pharmaceutical potential of synthesized libraries was investigated through various bioassays (antioxidant, antibacterial, antiurease, haemolytic and antithrombolytic activities). From results, it is concluded that synthesized molecules could be a potential source of therapeutic agents.

Experimental Analysis of Excited State Dynamics in Anderson POM@Porphyrin Hybrids in Relevance to Third-Order Nonlinear Optical Properties

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This work accounts for the active contribution of life time decay in the field of nonlinear optics, especially for an energetic donor acceptor couple(porphyrin and polyoxometalate(POM)). Currently, two POM free porphyrins(Di-Tris-N@Por and Di-Tris@Por) and their two hybrids with POM(Di-Tris-NPor@Di-AndPOM-1 and Di-TrisPor@Di-AndPOM-2) have been studied keenly in nanosecond(ns) time span and resulted life times(τ1 and τ2) have been compared with nonlinear optical parameters. The results demonstrated that Di-Tris-NPor@Di-AndPOM-1 exhibited better third-order nonlinear optical susceptibility χ3, second hyperpolarizability χ and nonlinear absorption β and Di-TrisPor@Di-AndPOM-2 than Di-TrisPor@Di-AndPOM-2. This superiority of nonlinear optical parameters was supported by life time decay studies and electrochemical studies. It is revealed that more relaxation time in excited states lower will be the NLO response. The lifetime decay(τ1) value of Di-Tris-NPor@Di-AndPOM-1 is 3.86ns which is higher than DiTrisPor@Di-AndPOM-2 possessing lifetime decay(τ1) value of 2.45ns. Moreover, lower energy of charge separated state(-0.88 ev) of Di-Tris-NPor@Di-AndPOM-1 indicates the facile electron transfer in Di-Tris-NPor@Di-AndPOM-1 than Di-TrisPor@Di-AndPOM-2 which experienced more energy of charge separated state. Rapid intersystem crossing is also responsible for the electron transfer from porphyrin moiety to POM moiety.

S-Aralkylated 5-(4-methoxyphenyl)-4-phenyl-4*H*-1,2,4-triazole-3-thiols: As suitable Alzheimer's disease drug candidates

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Our efforts lay emphasis on synthesis of *S* aralkylated 5-(4-OMeC_6H_5)-4-phenyl-4*H* 1,2,4-triazol-3-thiols like pharmacologically active candidates to counter neurodegenerative disorder; Alzheimer's disease. A synthetic strategy was instigated by esterifying 4-methoxybenzoic acid through Fisher esterification's methodology. Hydrazinolysis of corresponding ester was performed under reflux with methanolic hydrated hydrazine to afford 4-methoxybenzohydrazide (**I**) which refluxing with phenyl isothiocyanate (**II**) in MeOH to yield a reactive intermediate (**III**). The later underwent base-catalyzed intermolecular cyclization to furnish 5-(4-OMeC_6H_5)-4*H*-1,2,4-triazol-3-thiol (**IV**). Ultimately, **IV** was aralkylated at thiol position with aralkyl halides **V(a-l)** in polar aprotic solvent and catalytic amounts of LiH to provide *S*-aralkylated 5-(4- OMeC_6H_5)-4-phenyl-4*H*-1,2,4-triazol-3-thiols **VI(a-l)**. Modern spectral analysis data explicitly established all the substitutions on nucleophilic *S*-atom of parent 1,2,4-triazol-3-thiol ring. Effective anti-cholinesterase potential depicted in 3-(phenylpropylthio)-5-(4-OMeC_6H_5)-4-phenyl-4*H*-1,2,4-triazole**;** **VIc** (IC_{50}; 3.26±0.35 µM) against acetyl cholinesterase; AChE and 3-(phenethylthio)-5-(4-OMeC_6H_5)-4-phenyl-4*H*-1,2,4-triazole; **VIb** (IC_{50}; 8.52±0.54 µM) against butyrylcholinesterase; BChE enzyme as compared to standard Eserine for both enzymes ($IC_{50;}$ 0.04±0.01 µM). Molecular modelling analyses had been conducted to recognize the interconnection of these compounds with enzymes that suggested key interactions (Docking is made to untie the active binding sites). Anti-proliferative activity results showed **VIg** and **VIj** with -Cl groups on benzylic ring as promising candidates with HCT-116 cell viability of 14.83 % and 3.09 % respectively.

POSTER PRESENTATION

Antioxidant, antibacterial and antifungal potential study of Salvia macrosiphon Boiss. Stem extracts

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The aim of present research work was to evaluate the Salvia macrosiphon Boiss. of Lamiaceae (mint family), using biochemical and biological assays. Plant's phytochemicals extraction was performed in methanol, butanol and water by mechanical shaking process. TPC and TFC were determined by Folin-Ciocalteu and aluminum chloride colorimetric procedures, respectively. The highest TPC (99.61±3.45 mg GAE/g) and TFC (234.72±7.12mg CE/g) were obtained in butanol and methanol, respectively. Regarding the antioxidant potential methanol extract showed the highest DPPH° scavenging potential (78.0±2.0%) and reducing activity (0.923±0.020 absorbance). The antibacterial activity of butanol extract against P. aeruginosa were found highest (ZOI = 23±2.00 mm). Antifungal study of methanol extract showed the ZOI (11 ±0.67mm) against F. brachygibbosum. The results revealed that the methanol stem extract of S. macrosiphon bear significant medicinal value and could be used for formulating phytomedicines and food preservers.

Cisplatin encapsulated ZnO Nanoparticles for target drug delivery in cancer patients

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Cisplatin $PtCl_2(NH_3)_2$, is a first metal-based anticancer drug. Its chemical name is cis-diamminedichloroplatinum. It is included in chemotherapy medication for various types of cancers such as breast cancer, lung cancer, brain tumor, germ cells tumors and is used intravenously. Cis-configuration in cisplatin is of great importance as it provides the complex to make the covalent bond. It results in the death of the cells (cancer cells). As Cisplatin is tremendously using for various cancers all over the world. It shows many side effects as well. Side effects include Diarrhea, neurotoxicity, nausea, vomiting, Ototoxicity, Hemolytic anemia. Besides all these side effects, nephrotoxicity is major concern. Kidney damage leads to serious complications in cancer patients. To reduce these side effects and to increase the medicine effect, target delivery system of drug delivery is promoted. This has been done by encapsulation of cisplatin with nanoparticles. Various types of nanoparticles such as Silver nanoparticles, titanium oxide nanoparticles etc could be used for this purpose. Nanoparticles are small sized particles having size between 1-100nm. They have important use in target delivery of drug. This results in minimum or zero side effects to patients. This study shows the use of ZnO nanoparticles for the encapsulation of cisplatin. Zn has an important role in cancer. ZnO nanoparticles interact with the cancer cells due to the fact that cancer cells can interact with the ZnO nanoparticles very efficiently. This study shows the methods for the synthesis of ZnO nanoparticles and the encapsulation of cisplatin with ZnO nanoparticles. The confirmation is done by spectroscopic techniques. This review study concludes that the cisplatin will release at target in minimum amounts. It will results in reduce dosage cycles and side effects.

Continuous Flow Adsorption of Crystal Violet Dye using Ficus religiosa Branches

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This research work presents the adsorption capability and efficiency of plant species i.e, Ficus religiosa branches, for crystal violet dye. This work is proposed to determine the effect of various parameters on the adsorption of crystal violet dye solutions onto Ficus religiosa from aqueous solutions in continuous adsorption process using packed columns with the help of peristaltic pump. The Ficus religiosa has been characterized by Fourier Transform Infrared Spectroscopy (FTIR), and Thermogravimetric Analysis (TGA). The parameters included the effect of change in concentration of dye solution and change in bed height. It was observed that with the increase in dye concentration, saturation time and breakthrough time was decreased. The time was maximum with the minimum concentration of dye solution. For packed columns, removal of dye depends upon the amount of biosorbent in the column. Diffusion of dye reduces at lesser bed height due to the occurrence of axial dispersions. As the bed height increased, the adsorption of dyes also increased. Optimum bed height was found to be 30cm. The results of present study indicated that the biomass from Ficus religiosa branches can be used for the removal of crystal violet through biosorption due to its low cost, effectiveness, and ease of operation.

Synthesis of Ternary Ferrite-Chitosan Microsphere for Photocatalysis of Selected Organic Dyes

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Water pollution has been increased significantly due to large scale urbanization and industrialization. The release of wastewater containing organic dyes from numerous industries is a big problem due to its carcinogenic and other health hazard effects. Photocatalysis using biopolymer coated ternary ferrites microspheres may offer efficient eliminating strategy for dyes from wastewater. Due to this reason, ternary ferrite chitosan microsphere was synthesized for removal of organic dyes from aqueous medium. In the current study, ternary ferrite Fe2Ni0.5Cu0.5 O4 (CNF-NPs) were synthesized by a facile approach as an efficient visible-light photocatalyst. For comparison the binary ferrite of the photocatalyst Fe2CuO4 (CF-NPs) and Fe2NiO4 (NF-NPs) were also prepared. The ternary ferrites were supported with chitosan microspheres Fe2Ni0.5Cu0.5O4-chitosan microspheres (CNF-CM) and binary ferrites as, Fe2CuO4-chitosan microspheres (CF-CM) and Fe2NiO4-chitosan microspheres (NF-CM).

FTIR analysis confirmed the synthesis of ternary ferrites nanoparticles and prepared photocatalyst. The XRD technique showed that the crystallite size of synthesized CNF-CM ternary ferrite nanoparticles was 18 nm based on Scherer's equation. The EDX images clearly confirmed the elemental composition of (CNF-NPs) ternary ferrites nanoparticles. The CNF-CM ternary ferrite chitosan microsphere has a smooth surface with a microspheres size of 860 µm based on SEM micrographs. The band gap of the photocatalyst was found in the visible region (2 eV) obtained from Tauc's plot.

The photocatalyst CNF-CM showed 93 and 90 % photocatalytic efficiency for Methylene Blue (MB) and Rhodamine B dyes, respectively at optimum conditions of pH 7.0, catalyst dosage 0.7 g, and initial dye concentration of 30 ppm in 160 min of sunlight irradiation.

Preparation of Propolis-Polymeric Composites for Apricot preservation

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Fruits are very perishable commodities with limited shelf life due to oxidative and microbial infections. Propolis has enormous captivating biological profile including potent antimicrobial, antioxidant, and anti-inflammatory activities. Inspired by these beneficial properties, propolis polymeric composites have been developed using propolis extract and agar to overcome the stated problem. These composites were characterized by chemical and spectroscopic methods, and then applied on perishable commodities such as apricot to observe their effect on shelf life. All composites were studied for found non-toxic and possess bacteriostatic potential.

Comparison of Antioxidant Activity of Plant Parts of *Annona squamosa*(L.)

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An increasing demand of natural additives, studies were performed to determine constituents that are responsible for antioxidant activity. In vitro scavenging activity of natural antioxidant of Annoneace family was performed due to some mutagenic effects that was observed in synthetic antioxidants. Extracts of different plant parts of Annona squamosa were prepared and in vitro scavenging activity performed which showed extract possess higher percentage of inhibition (97.99%) of DPPH radical scavenging activity than other extracts. The antioxidant potential was determined by free radicals using different concentration of extracts and sample, nitric oxide (70.96%), DPPH, hydrogen peroxide and super oxide (78.68%) of A. squamosa leaves, fruit pulp and bark. All extracts were found to express percent inhibition in dose dependent manner. Methanolic extract of fruit pulp, ethanolic extract of bark and methanolic extract of leaves exhibits higher antioxidant activity. The antioxidant potential was calculated in term of percentage inhibition and IC50 value. Result of Phytochemical analysis showed the presence of flavonoids, saponins, tannins, phenols and glycosides that are responsible for the inhibition of radicals by antioxidant activity. In vitro model clearly suggest that fruit pulp and leaves extract has higher antioxidant activity due to higher presence of flavonoids and phenolic constituents and extract of bark showed high percent inhibition and less IC50 that give more inhibition of free radicals. Synthetic antioxidants produce some toxic effect than natural antioxidant that helps to promote research toward green synthesis that exhibits more inhibition potential for free radical scavenging.

Des Mediated Synthesis Of Furylazoles - A Green Aspect Of Organic Synthesis

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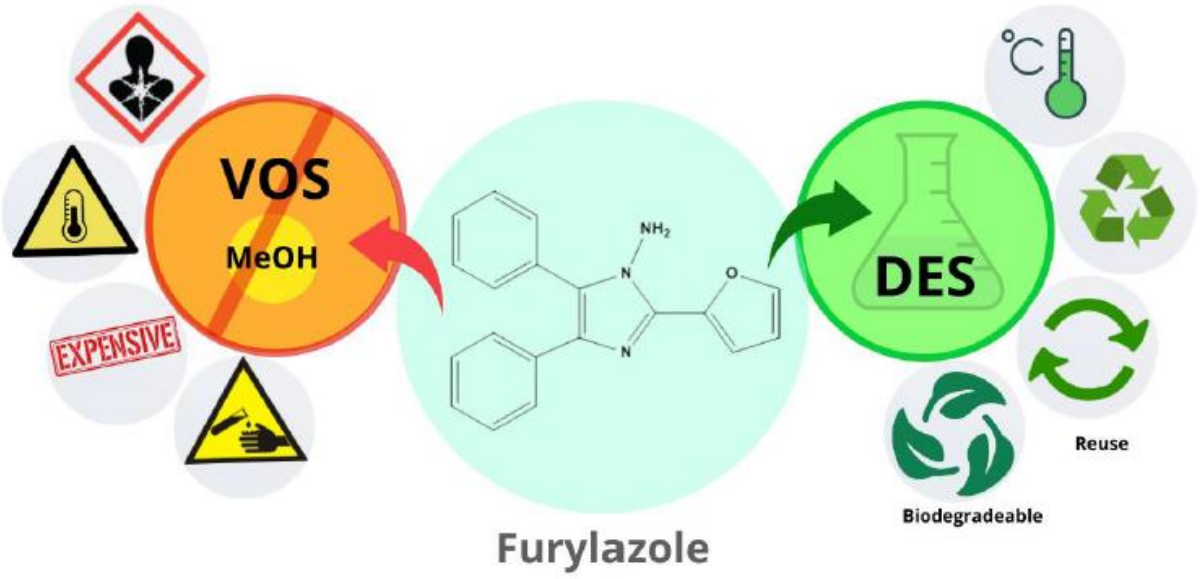
Organic synthesis requires volatile organic solvents as reaction mediums which impart atmospheric pollution due to high vapour pressure, low flash point, and toxicity. In this regard, DES has emerged as an eco-friendly alternative and sustainable media to accomplish the said goal. The exceptional pharmacological profile of azoles inspires to synthesize some furylazoles. For this purpose, MCR strategy was adopted and benzil, furfural, ammonium acetate, and 2,4-dinitrophenyl hydrazine were used to afford the target compounds employing deep eutectic solvents (DES). This green solvent has been prepared by mixing choline chloride and oxalic acid and play a dual role; as a catalyst and as a reaction medium. This approach additionally features high yield in lesser time as well as solvent reusability. All compounds were characterized by ^{1}H NMR and EI and HRMS.



Biosynthesis 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 chloroauric acid (HAuCl4) as precursor and NaOH used as accelerating agent to speed up the reaction. Synthesized gold nanoparticles were confirmed through the colour 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 limit of detection and limit of quantification for ferrous ion is 0.5 and 1.69 ppb respectively. The sensor was successfully applied to real water samples regarding the detection of Fe2+.

Solvent Free Synthesis Of Bisindolyl Methanes- A Green Approach Towards Sustainability

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Organic solvent exposure in synthesis is one of the most prevalent chemical health problems and need to be addressed to search for sustainable solution. In this research solvent free green methodology is used to synthesize biologically important compounds using solid supported SiO_2-$KHSO_4$ catalyst (5mol %) with maximal yield (89%) in an hour. The catalyst used is highly efficient, economical, non-toxic and readily available. This methodology has additional features including high yield, easy work-up and short reaction time. All characterizations were furnished by using DSC, TGA, FTIR, H_1-NMR and MS.

N-Substituted Indole

Bisindolyl methanes (BIMs)

Preliminary Assessment Of Selected Heavy Metal Residues In Different Types Of Cheese Consumed In Lahore, Pakistan

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Dairy products are considered as the most essential food in the human diet. While, human exposure to contaminated food products may cause health risks. Therefore, present study was a preliminary design to estimate the traces of selected heavy metals; Cu, Mn, Zn, Ni, Cd and Cr in some commonly marketed varieties of cheese, a dairy product. For this purpose, different cheese samples were collected from local supermarkets and fast food outlets from Lahore, Pakistan. Two digestion methods (D_1: aqua regia and D_2: nitric acid-hydrogen peroxide) were used to prepare samples prior to analyzing them through Atomic Absorption Spectrophotometer (AAS). Method-D_2 was screened out as a better digestion method herein, based on digestion time taken and metal detection results. The decreasing order of heavy metal mean concentrations in cheeses, digested via method-D_2, was as followed: Zn > Mn > Ni > Cu > Cd > Cr. Overall analytical results were comparable and in agreement with the documented literature data of recent years. Average concentrations of Zn (41.947 $mgkg^{-1}$), Mn (9.909 $mgkg^{-1}$), Ni (5.235 $mgkg^{-1}$) and Cu (5.051 $mgkg^{-1}$) were exceeding the permissible limits. Statistical study helped to identify some significant positive correlations among Zn-Cu, Mn-Cd and Mn-Ni. Such high levels of toxic metals could be attributed to the manufacturing quality. Hence, constant monitoring of such available food items and most importantly of their technological preparative steps are very crucial to assess the consumer's health concerns.

Nature Mimicked Antibacterial Zein Reinforced Thermosensitive Bone Regenerative Grafts

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Skeletal deformity is the second leading cause of disability worldwide. There has been a growing interest in the design of smart polymer systems that exhibit rapid changes in properties in response to chemical and/or physical stimuli. Temperature is the most often used stimulus in biomedical applications. Thermosensitive hydrogels have a low viscosity in the sol phase and high viscosity and elastic properties in the gel phase. They can be injected at the trauma site, so they offer a less invasive and more comprehensive filling of defected sites compared to prepared implant scaffolds. A series of novel *in situ* formed thermosensitive hydrogels were developed by using different ratios of Chitosan, Hydroxyapatite, Calcium glycerophosphate, and Zein. The installation of the temperature dependent phase transfer ability into chitosan, an unexplored economical and bioactive source of glycerophosphate, calcium glycerophosphate, was used. To improve mechanical and biological performance, Zein was used as a reinforcement material. Prepared composites existed in the sol phase at 10-12 °C and formed hydrogels at 37 °C in 4-7 minutes. FTIR revealed successful preparation of different compositions of hydrogels. Addition of Zein improved the mechanical properties. The highest mechanical strength at 40% strain 52.2 and young's s modulus of 850 MPa was obtained for a sample containing the highest Zein concentration. Prepared hydrogel showed good swelling property. Biodegradation analyses indicated that rapid degradation in first three days after that it slows down. Sample with higher amount of zein showed slow rate of degradation. SEM analysis revealed the presence of interconnected pores. *In vitro* cell culture assays and wound healing assays represented good biocompatibility, cell attachments and regenerative potential. Drug loaded hydrogels showed up to 92-98% drug delivery and good antibacterial activity. Prepared hydrogels offered good regenerative potential, thermosensitive gelling ability, injectability, biocompatibility and mechanical properties.

Green synthesis of aryl esters mesogens

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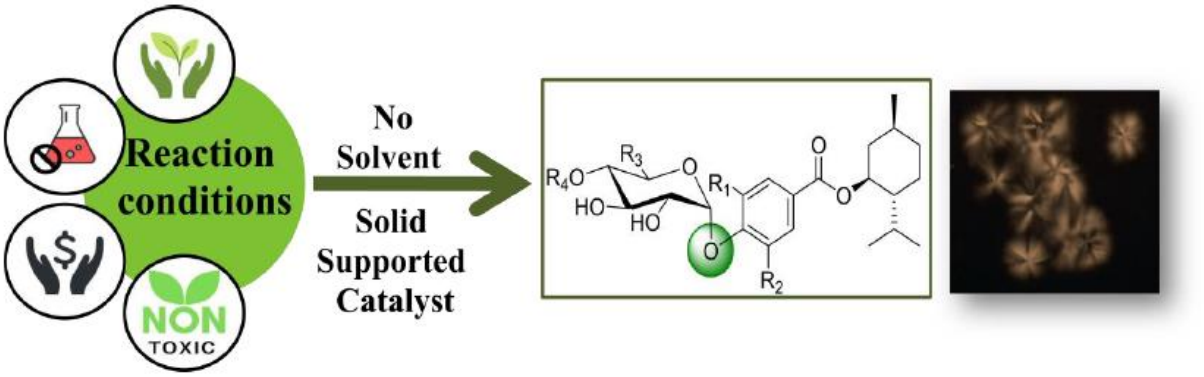
The environmental concerns addressed elimination of toxic solvents and reagents in the chemical reactions and doing them “neat” goes a long way towards achieving the goals of green atom economic chemistry. Therefore, this research have been designed to synthesize aryl esters that possess mesogenic properties by incorporating glycopyranosides by Fisher glycosylation using solid supported Si-H+ as a catalyst. All characterization was furnished by FTIR, 1HNMR, XRD, SEM, and thermal stability was studied by TGA and DSC while thermotropic liquid crystal behavior was observed under polarized optical microscope.



The comparative study of the Novel Indole Glucoalkaloid and Secoiridoid glucoside From *Tripterospermum chinense*

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In Asia 17 plants species of genus Tripterospermum are present. *Tripterospermum chinense* extensively distributed in South Asia. It is also used for the treatment of various diseases like cough, hemoptysis and pulmonary diseases by local habitat. The genus *Tripterospermum* comprise in higher amount in xanthones, flavonoids and iridoid glucosides which displays the numerous activities such as anti-hypertension and antivirus, inhibition of angiotensin-I-converting enzyme, Moloney murine leukaemia virus reverse-transcriptase cutaneous plasma extravasation and formyl methionyl-leucyl- phenylalanine-induced respiratory burst. In this review article comparison of the three papers is reported. In 2020 Tao Zhang reported that by using the Arial part of Tripterospermum with the process of extraction two new compounds are identified and their molecular formula are $C_{44}H_{57}O_{20}N_2$ and $C_{69}H_{100}O_{39}$. Tao Zhang also reported in 2012 that two other new compounds are extracted by using the arial part of this plant and the molecular formula of these compounds are $C_{66}H_{90}O_{37}$ and $C_{33}H46O19$. $C_{23}H_{29}NO_{11}$ and $C_{35}H_{52}O_{20}$ are the molecular formula of those compounds which are extracted and reported by Kai-Cheng Zhu in 2007. Further, their structural data can be determined by using IR study and the NMR. The most important point it helps to determine the chemotoxonomic data of various compounds. Further, the extracted compounds also exhibit the cytotoxic activity which is used against the man's stomach, colon, breast, cancer, and the cervical. The comparison of this study will inspire the scientist and shows the significance of the compounds which were isolated from the Tripterospermum.

Exploring The Therapeutic Potential Of *Olea Ferruginea*

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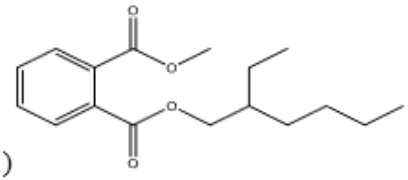
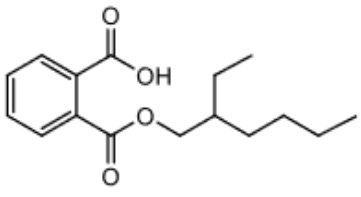
Curcuma Zedoaria is a perennial herb commonly known as white turmeric belonging to the Zingberaceae family and cultivated throughout tropical countries. Due to the presence of many Phytoconstituents Zedoaria plant is traditionally used in Ayurveda and other folk medicines for the treatments of different ailments like allergic, inflammation, microbial diseases, menstrual disorders, dyspepsia, flatulence, ulcer, and cancer. The methanolic extract of the fresh rhizomes of C. zedoaria were fractionated into numerous organic solvents and to evaluate their biological activities such as antimicrobial, cytotoxic, antioxidant, urease enzyme inhibiting, Leishmanicidal, anticancer and antitumor which showed significant activities. From the potential crude extract two phthalate esters, compound (1) and Compound (2) were purified and identified by the column and GC chromatography which showed significant activity against selected microbial pathogens like antioxidant, Cytotoxicity Assay, and DNA degradation analysis. The finding of our research confirmed the medicinal value of C. zedoaria and other complementary uses make it doubly attractive for incorporation in commercial-scale for the development of primary health care system.



(1)

Methyl -2-ethylhexylphthalate ester



(2)

1, 2-benzendicarboxylic acid, mono (2-ethylhexyl)

Composition and Biological Potential value of the Crude Extract of Curcuma Zedoria

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Medicinal plants have proven to be rich sources of biologically active molecules. The species belonging to genus Olea have been traditionally utilized both as a food agent and for medicinal purposes. Ethnobotanical studies on Olea ferruginea have proven its worth leading us to investigate its chemical and biological profile. During this research endeavor, a total of nine secondary metabolites were isolated and purified, including two new lignans. Among the seven known compounds, six have been reported for the first time from this plant species. Biological studies of the crude fractions and purified compounds revealed anti-microbial, anti-inflammatory, and leishmanicidal potential of the analytes. This plant has immense potential for the discovery of more structurally diverse and potent molecules. It's a surprise that it hasn't been explored much by the phytochemists. It does need attention and deeper investigations and we are already on track.

Comparison of Synthesis Methods of Gold nanoparticles

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Nanochemistry is an emerging branch of the materials and plays a significant role in many areas of science and society. Nanosized materials have brought about countless changes and new research. Nanoparticles have unique chemical and physical properties due to high surface area and volume ratio. Gold nano-particles can be synthesized by different methods. This study is actually on the comparison of three different methods of the synthesis of gold nano-particles. It is being noted that all three processes can synthesize gold nano-particles but under different reaction conditions and the color of gold particle is also different for every method. These particles have rod, cluster, sphere and shell type shapes with particle size > 30nm. The bio-synthesis of gold nano-particles are eco-friendly and safe for environment. These particles also have application in medical field for the treatment of cancer. Among the methods that are discussed, green synthesis is showing best results because the material that is used in this method is very cost effective. The spectrum of this method has also shown very sharp peak as compared to other methods.

Synthesis Of *B*-Lactams Functionalized And Functionally Diverse Tetrahydrothiadizine-2-Thiones In Search Of Potential Anti-Inflammatory Agents

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A series of new beta-lactam (cefaclor and cefadroxil) conjugates of thiadiazine-2-thiones (**1a-1g**, **2a**, **2b**) were synthesized in a phosphate buffer medium. The synthesized compounds were screened for their anti-microbial potential against *E.coli* and *P. aeruginosa.* All of the synthesized compounds were found active against both the strains, with Compounds **1e, 1f, 1g, 2a**, and **2b7-10,** and **11** showed significant activities against *Escherichia coli* (zone of inhibition (mm) =21, 24 22, 24 and 28) and *Pseudomonas aeruginosa* (16, 19 22, 24 and 30). The antinociceptive effect of the synthesized compounds was also evaluated by using the hot plate method. Compounds **1a, 1b, 1d, 1f, 1g,** and **2a** exhibited profound effects at 80 mg/kg dose, showing a significant increase in the latency time ($P<0.05$, $P<0.01$, $P<0.001$). Computational studies revealed that these compounds have a strong affinity with the binding site of the COX enzyme. Compound **11** was the most active (docking score -8.019), establishing four interactions with binding site residues.

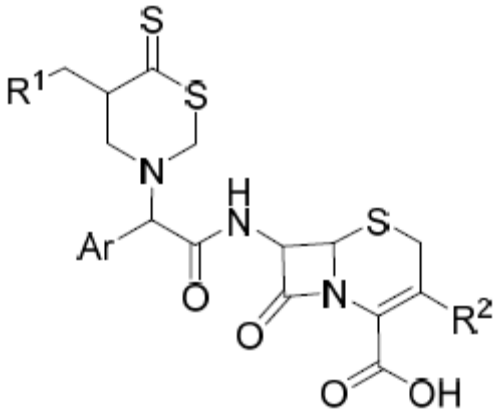

Fig: Structure of β-lactam conjugates of thiadiazine thiones**.**

Desymmetrization Construction Of Chiral Lactones By Synergistic Cu(II) Com - Plex And Organic Base

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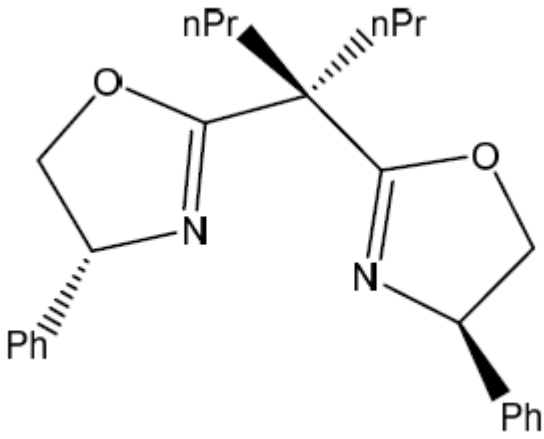
A highly enantioselective construction of quaternary carbon center has been realized by the desymmetrization strategy. Chiral enol lactones with up to 95% *ee* could be synthesized from prochiral dialkynoic acid under the catalysis of synergistic chiral Cu(II) complex and chiral $(DHQ)_2$-PHAL base.



Fig; Desymmetrization enabled by synergistic chiral Cu (II) complex and organic base

Solid phase extraction for the removal of lead and chromium from waste water using raw and chemically modified fuller's earth

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The present research work was executed in order to investigate the comparison of adsorption efficiency between raw Fuller's Earth (Gachini clay) and chemically treated Fuller's Earth (Gachini clay) as low cost and cheap adsorbent for the elimination of Chromium (Cr) and Lead (Pb) metals from their respective wastewater generated at laboratory scale. FTIR spectra revealed the presence of aliphatic hydrocarbons and unsaturated hydrocarbons responsible for the binding of metallic ions. FTIR spectra showed that chemically treated clay better removed metal ions from the aqueous medium. Process parameters like contact time, adsorbent dose, agitation speed, pH solution and temperature were determined by the adsorption of Cr and Pb metals during batch mode study experiment. The applicability of isothermal models and kinetics models i.e. Pseudo kinetic reaction of first and second order were also studied. The isotherm model of Langmuir best fits the experimental data, in case of chemically treated clay than Freundlich and Temkin as revealed by the R2 as well as the Qmax values for Langmuir (0.9617 and 24.996 mg/g for Cr and 0.9914 and 14.822mg/g for Pb) and Pseudo kinetic reaction of second order model best represented the adsorption kinetics for both Cr and Pb metals. Thermodynamics studies revealed that process proved to be spontaneous, exothermic and feasible in nature. The future research must focus on ways to enhance the efficiency of adsorbent by introducing new modifications, increasing active sites and to conduct these experiments on pilot and industrial scale.

Comparative Study of Anti-ulcer Activity of Different Extracts of *Ficus Religiosa* (Moraceae)

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An imbalance between protective mechanisms inside the gastro duodenal mucosa and damaging factors inside the lumen is termed as gastric ulcer [1]. Several plants have been reported and screened with the ever-rising interest in traditional medicine so that they can be used for the treatment of ulcer. An important natural medicinal plant of family Moraceae is Ficus religiosa which is distributed all over in India. Tannins, saponins, steroids, amino acids, flavonoids and carbohydrates are present in the stem bark and leaf of F. religiosa [2]. Prostaglandin analogues, antacids, anti-cholinergics, demulcents, cytoprotectants, H2 receptors and proton pump inhibitors are commercially available drugs used for the cure of gastric ulcer with various side effects. Herbal medicines are found to be better treatment of ulcer as compared to available synthetic drugs due to perceived effectiveness, fewer side effects, availability and lower costs [3]. In this study, the ethanolic and methanolic stem bark and leaf extracts of F. religiosa were tested for their anti-ulcer activity by using their different doses on different ulcer induced models of rats. The acute toxicity and phytochemical screening of F. religiosa extracts was also carried out. The results show that the different extracts of F. religiosa show significant anti-ulcer activity and even at high concentrations (2000mg/kg), the extracts are non-toxic. The ulcer index value is decreased by both ranitidine and F. religiosa extracts. The analysis of phytochemical screening identified the presence of proteins, carbohydrates, flavonoids, saponins, sterols and tannins. This comparative study will provide a convincing support to extend the existing therapeutic potential of plants for the use of natural medicines in the treatment of different diseases due to more compatibility of natural products with biological systems.

Preparation Of Sago Starch Hydrogels For Efficient Delivery Of Eugenol

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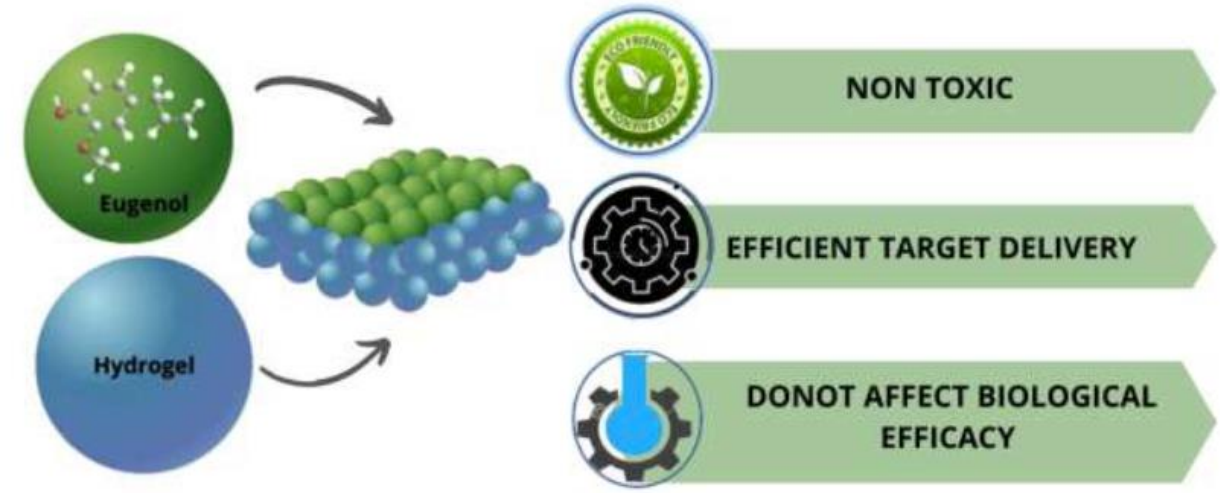
Eugenol is well known anti-microbial agent that is safe at limited dose of 2.5mg. kg^{-1} of body weight. In view of its safe transport to the target without the loss of its biological efficacy, it is required to load on a safe material which is biodegraded after its safe delivery. Therefore, the sago starch based hydrogels were prepared by solution casting method and loaded with eugenol. All prepared hydrogels were characterized by FTIR and SEM.



Comparative Study of Effects of Belamcanda Chinensis and Saffron (Crocus Sativus) from Family Iridacea, on Blood Glucose level and Blood Insulin Level in Rats

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For the treatment of hyperglycemia, the extract of Belamcanda chinensis (L.) leaves (BCLE) has been used as a traditional Chinese herbal medicine [1] and it has also been used for the cure of inflammation and for various other disorders [2] and Saffron, the dried stigmata of the flowers of the saffron (Crocus sativus L., Iridaceae) has several pharmacological effects and is considered as a powerful drug. Mohajeri et al. (2009) showed that saffron extract played a significant role in decreasing blood glucose and increasing insulin serum in diabetic rats [3]. In this comparative study, the effect of dried extract powder of B. Chinensis and Saffron (Crocus sativus) on blood glucose and blood insulin level was investigated by using KK-Ay mice, male Kunming mice and male Sprague-Dawley rats. This study revealed that both Belamcanda chinensis leaves (BCLE) and Saffron (Crocus sativus) belonging from family Iridacea had significant effect in decreasing the blood glucose level and also had significant effect on blood insulin level in these animals. These findings suggested that F2 an active component of Belamcanda chinensis displayed high hypoglycemic activity and thus it can be used as an efficient antidiabetic agent for the treatment of diabetes mellitus type II. This study encourages, that in future more researches should be carried out on these natural products and these should be considered in future therapeutic researches, as natural products seems to be less toxic and much affordable as well as quiet efficient therapeutic agents.

Catalytic Oxidative Desulfurization and De-ashing of Low Rank Coal Using Transition Metals Impregnation on Coal

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Catalytic oxidative desulfurization and de-ashing of the Dare Adam Khel coal was inspected by combination of catalytic and leaching oxidative process. During leaching process the coal was treated with base and acidic solutions consisting of HNO3 and KOH. The coal was subjected to oxidative desulfurization and de-ashing using H2O2 and HCOOH as oxidant. The most optimum conditions of temperature and time were found to be 70 °C temperature, 90 min stirring time using water as a solvent for coal, which has a very good effect on the desulfurization and de-ashing of Darra Adam Khel coal. The study was also extended from oxidative desulfurization and de-ashing to catalytic oxidation. During catalytic oxidation Sn was loaded on Activated carbon as catalyst. The oxidative desulfurization and de-ashing of the coal in the presence of Sn loaded on Activated carbon was reached to about 78 % desulfurization and 68 % de-ashing.

Heavy Metal Removal From Various Wastewater Samples Using Low Cost And Efficient Adsorbents

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The ability of wheat husk and bamboo to recover Cu, Cr, Mn, Ni and Zn from aqueous solutions was investigated on three parameters i.e. variations in pH, contact time and initial concentrations of metal. The bio-adsorbents were washed, dried and powdered up to the size of 112 µm followed by chemical activation with 0.3 M nitric acid (HNO3) solution for 24 hours, washing with distilled water until pH became neutral and then oven drying at 75˚C with constant mixing. The bio-adsorbents were applied to each metal ion solutions by preparing their 1M stock solutions made from copper (II) sulphate, potassium dichromate, manganese (II) sulphate, nickel chloride hexa-hydrate and zinc sulphate heptahydrate. The solutions were filtered and analyzed by atomic Absorption Spectrophotometer to check the efficiency of bio-adsorbents. Under optimized conditions of pH, contact time and concentration, the bio-adsorbents were allowed to react with metals in a digested industrial water samples i.e. paint. Wheat husk was found to be the most effective and low cost bio-adsorbent which has much high potential to be used for heavy metals removal from aqueous solution.

Comparative study of antimalarial activity of three different research article from Incacinaceae family

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Malaria is a worldwide disease caused by the plasmodium falciparum and plasmodium berghe. The research of natural product leads to the discovery of the many plants having ability against malaria disease; I. senegalensis is one of them. I.senegalensis is a leafy shoot plant having crawling roots, is used for the malaria treatment. It is found in sandy places mostly in Africa. Collected, identified, dried, crushed or grind the leaves or roots of I.senegalensis and treated with ethanol and methanol respectively. Mice are taken for the experiment. The LD50 is administrated to the mice and observed the effect. All mice were dead. The parasites are collected to infect the mice which divided into different groups, to calculate the paresitaemia. The group which is treated with the chloro-quine act as positive control and group treated with the normal saline is the negative control and thick film from tail blood of mice is prepared and percentage of suppression is observed in both cases. Doses of different concentration of plants extract is given to the mice and after 72 hours once again saline mixture from tail blood is prepared and % of suppression is observed. Anti-malarial activity of plant extract was also evaluated by ELISA. From the results we conclude that % of suppression of ethanolic root extract of I.senegalensis against malaria is greater than the methanolic leaf extract of I.senegalensis against malaria.

Synthesis And Functional Modification Of 3-Alkyl-5- Amino Tetrahydro-2*h*-1, 3, 5 Thiadiazine-2-Thiones In Search Of Bioactive Agents

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Herein, a series of biologically active, 3-alkyl-5-amino-1,3,5-thiadiazine-2-thione were synthesized by reacting selected primary amines with carbon disulfide, followed by cyclocondensation with formaldehyde and hydrazine in buffer medium. The synthesized, 3-alkyl-5-amino-1, 3, 5-thiadiazine-2-thione were further transformed into a series of 3-alkyl-5-arylidene-1, 3, 5-thiadiazine-2-thione All the synthesized compounds were characterized with the help of spectroscopic techniques including; FTIR, and H-NMR. The synthesized compounds were investigated for their antimicrobial, leishmanicidal and anti-inflammatory activities. Among the synthesized compounds 5-amino-3-propyl-1, 3, 5-thiadiazine-2-thione was found more active antibacterial agent than the standard levofloxacin.

Synthesis Of Biodegradable Galactomannan Hybrid For Anti-Iflammatory Drug Delivery

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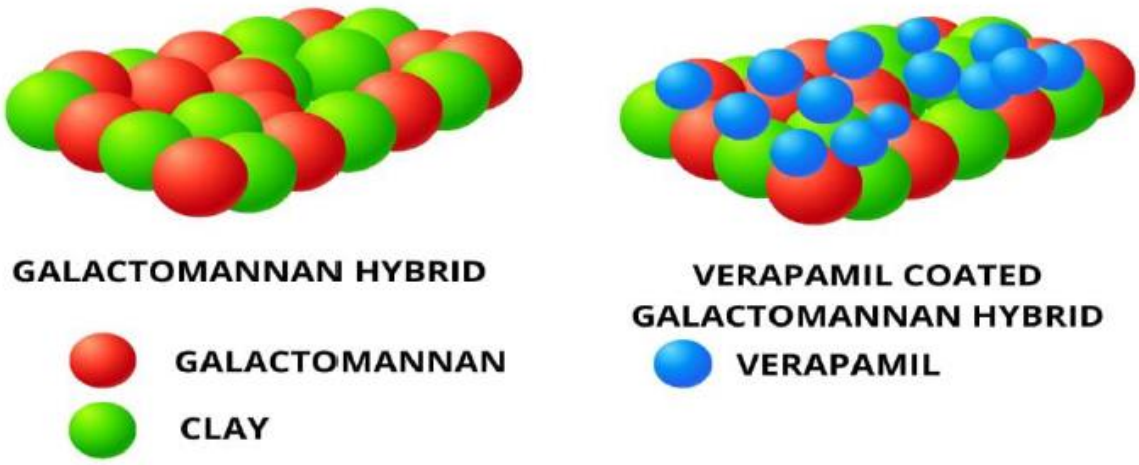
Biodegradable materials credited healthy environment and galctomannan are one of them with remarkable biomedical applications. Chemically modified heteroglycan galactomannan were prepared and intercalated with clay to form its hybrid and confirmed by their morphological studies. These composites have been employed for drug delivery application using verapamil, an anti-inflammatory drug, to investigate their efficiency by mathematical model.



Synthesis of ternary blend films for optoelectrical applications

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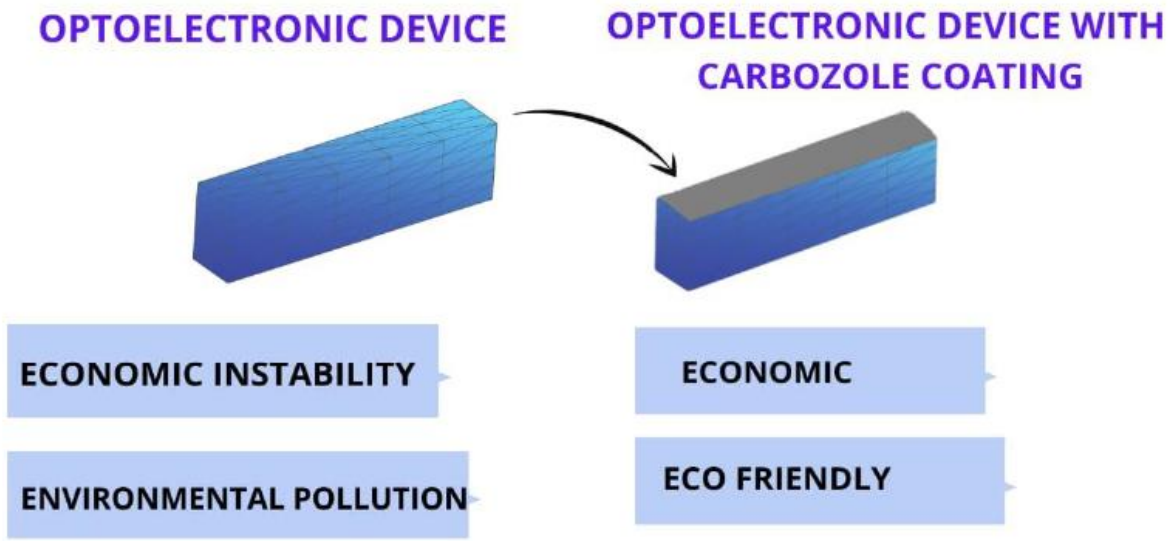
The incompetency of conventional optoelectronic devices for energy conservation is one of the major threats to environmental health and economic stability. In search of economical and ecofriendly devices ternary blends, loaded with carbazole were prepared. Their photoelectrical properties were investigated. Experimental conditions were optimized using response surface methodology. The adsorption of blend was calculated using Langmuir adsorption model. Also intermolecular interactions were confirmed using FTIR.



Plant Extract Induced Biogenic Preparation Of Silver Nanoparticles And Their Potential For Catalytic Degradation Of Toxic Dye

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In this study the synthesis of silver nanoparticles (Ag-nPs) was done by using the citrus fruit (citrus paradisi) peel extract as reducing agent and $AgNO_3$ as source of silver ions. The synthesized AgnPs suspension was turned light brown which indicates the successful preparation of the biogenic nanoparticles. The successful fabrication of nanoparticles was reported by observing the Surface Plasmon resonance (SPR) band in UV-Vis spectra. For the characterization of Ag-nPs different techniques such as FTIR, TGA and DLS were used. It was found that the Ag-NPs were excellent catalyst for the reduction of Congo red (CR), methylene blue (MB), Rhodamine B (RhB) and 4- nitrophenol (4-NP). In order to optimize the catalytic activity, the reduction of CR was carried out by changing the content of $NaBH_4$, CR and the catalyst. For determining the rate constant, the pseudo first order kinetic model was used. These results also showed that the Langmuir- Hinshelwood (LH) mechanism was followed by the catalytic reduction reaction. It was also reported that the green synthesized Ag-NPs catalyst can be very helpful for the treatment of various toxic dyes present in water sources.

Cycling performance degradation of Ni-rich layered NCM materials in full-cells: Effect of elevated temperature

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Lithium-ion batteries (LIBs) have dominated portable electronics and they are now opening potential applications in electric vehicles (EVs) and grid energy storage markets. For EVs, driving range anxiety is one of the main concerns for customers that requires development of high energy density LIBs. In this regard, Ni-rich layered cathode materials (LiNi1−x−yCoxMnyO2) with excellent electrochemical performance under harsh conditions are in urgent demand owing to their high capacity (over 200 mAh g−1) and relatively high working voltage (3.8 V). In this work, we evaluated the capacity fading of $LiNi_{0.85}Co_{0.10}Mn_{0.05}O_2$/Graphite full-cell at elevated temperature (45°C). A systematic failure analysis confirmed that it is the cathode material ($LiNi_{0.85}Co_{0.10}Mn_{0.05}O_2$) where elevated temperature causes structural degradation due to the formation of microcracks, decomposition of the electrolyte and higher resistance.

Synthesis of Starch-Clay nanocomposite films and their potential applications in food preservation

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Biodegradable starch-clay nanocomposite films were synthesized for their potential applications in food packaging. Bentonite clay was homogeneously dispersed into soluble starch solution in appropriate ratio at 90$_o$C using glycerine as plasticizer and acetic acid as a cross linking agent. Drying the solution resulted in the formation of films. The synthesized films were characterized by XRD, UV and FT-IR analyses. The films were also tested for their biodegradability and food preservation. The results proved that the prepared films are a promising substitute for petroleum-based food packaging materials.

Synthesis, characterization and photocatalysis of ternary metal complexes using salicyclic acid as a primary ligand

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In this study, $[Ce(sal)_3(Phen)_2]$ and $[Bi(sal)_3(Phen)_2]$ ternary metal complexes were synthesized. The products were characterized by Fourier-transform infrared spectroscopy (FTIR), UV-Visible (UV-Vis) spectroscopy and other spectroscopic techniques. The catalytic properties of prepared catalysts were evaluated against methylene blue as a model pollutant under ultraviolet irradiation, when H_2O_2 was present with the catalyst and under sunlight only in the presence of catalyst. The degradation efficiency of $[Bi(sal)_3(Phen)_2]$ catalyst was highest among all the catalysts. Results indicated that the produced catalysts may be employed as potential candidates for photocatalytic breakdown of synthetic dyes, and therefore are recommended for environmental cleanup.

Carbazole Interaction with Selected Phenols in a Micellar System of Cetyltrimethylammonium Bromide (CTAB)

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A group of selected phenols i.e. phenol, 2-Nitrophenol, 3-Nitrophenol, 4-Nitrophenole, 2,4,6-Trinitrophenol interaction was studied with a fluorescent probe carbazole in a micellar system of a cationic surfactant CTAB. CTAB concentration was optimized for maximum quenching of carbazole for each studied phenol. Interaction was studied in 0.02 and 0.1 mol/L CTAB. All the studied phenols resulted in the quenching of carbazole in both CTAB concentrations though lower CTAB concentration was found optimum for maximum quenching of the probe carbazole. Fluorescence quenching if carbazole by phenol is shown in figure.

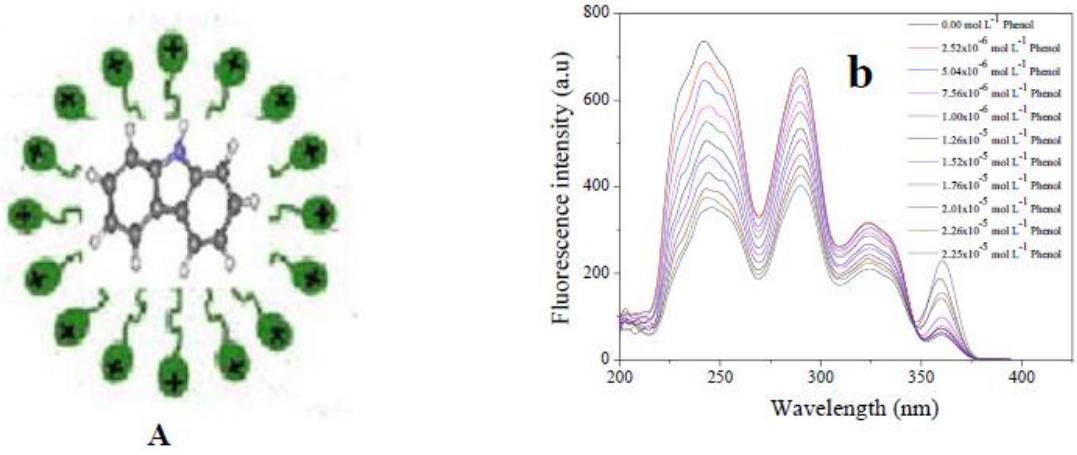

Figure (A) Partitioning of carbazole in micellar phase **(b)** Fluorescence quenching of carbazole by phenol

Fluorescence quenching of carbazole by phenols was treated with the Stern-Volmer equation that resulted in the constants of Stern-Volmer K_{sv}. K_{sv} shows the sensitivity of the method for the studied phenols (Table 1).

Table 1 Stern-Volmer constant (K_{sv}), detection (DL) and quantification limits (QL) for the studied phenols.

Quencher (Q)	K_{sv} mol L^{-1}	DL/mol L^{-1}	QL/ mol L^{-1}
2,4,6- Trinitrophenol	12.29×10^{4}	1.76×10^{-7}	5.898×10^{-7}
phenol	4.66×10^{4}	2.54×10^{-7}	8.47×10^{-7}
3-Nitrophenol	2.76×10^{4}	3.89×10^{-7}	1.39×10^{-6}
4-Nitrophenol	1.28×10^{4}	5.91×10^{-7}	1.97×10^{-6}
2-Nitrophenol	1.18×10^{4}	6.30×10^{-7}	2.11×10^{-6}

Nano-Structured Super Catalytical Clays For Production Of Biodiesel From Peach Waste Oil

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Biodiesel was determined as a good friendly and alternative source of petroleum diesel which is non-renewable. Mostly homogeneous catalysts were used to convert biodiesel from fatty acids of different feedstocks but for higher yield of biodiesel heterogeneous catalysts are more attention because of their good characters like reusability and not the production of wastewater. However, nowadays nanocatalysts have good quality and characters with different support composites. Present research experiments have investigated the production of biodiesel having good quality parameters which have similar characters like biodiesel international standards. Seeds of two types of fruits Prunus persica was collected from local markets, fruit and juice shops. There were the following steps: feedstock drying, raw material grindings, extraction of oil from dried seeds, filtration of oil, oil refined by charcoal, dehydration of oil with sodium sulfate, and vacuumed filtration. Nanocatalysts of zeolite with different clays composites were used to produce biodiesel. The calcinized composite of Bentonite clay with zeolite is the best catalyst to produce biodiesel because it has suitable pore distribution, higher surface area, and larger surface area. When the catalyst is combined into support, and structural qualities of catalysts are affected. Three parameters of transesterification were varied the biodiesel yield i.e., the concentration of catalyst, reaction time, and reaction temperature at same methanol ration and same stirring intensity. It was detected that peach oil gave a maximum yield of 99.1% respectively with 0.3% catalyst of Bentonite-Zeolite calcinized composite at 600C and at optimized reaction time was 4 hours for maximum biodiesel yield. Different physical quality parameters were observed i.e., pH, specific gravity, density, iodine value, saponification value, cetane number, cloud point and pour point, and acid value by various reactions. GS-MS analysis was used to characterize the composition of biodiesel samples. FTIR and SEM/EDX analysis were used to check the composition of nano-catalysts with support composites.

Surfactant Templated Synthesis Of Nanofibers By Dilute Polymerization Method For Energy Storage Devices

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Nanofibers of polyaniline (PANI), polypyrrole (PPy), and polycarbazole (PCz) were synthesized by dilute polymerization method using surfactants as soft micellar templates. Nanofibers were characterized by UV-vis spectroscopy, FTIR spectroscopy, XRD and their electrical conductivities were determined by four-point probe method. The association between polymer and surfactant monomers was observed to study the role of surfactant template in altering the properties of nanofibers. Nanofibers synthesized with surfactants showed improved properties, i.e., shape, size, and electrical conductivity, as compared to nanofibers synthesized without micellar templates. Nanofibers with improved conducting properties would be more convenient polymeric material for energy storage devices**.**

Synthesis, characterization and release study of drug-loaded collagen-chitosan hydrogel composites

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In the present work, collagen-chitosan hydrogel composites were prepared for controlled drug delivery. In the first step, hydrogels were prepared by using polyethylene glycol as crosslinking agent. Then 5-30% cinnamic acid was loaded in chitosan collagen composite hydrogels. Drug loaded hydrogel was characterized by Fourier transform infrared spectroscopy (FTIR). Drug release studies were carried out in vitro and the release profile indicated faster drug release in the beginning followed by a slower release. The swelling and degradation behaviour of prepared hydrogels was investigated through gravimetric analysis. These analyses suggested that drug loaded hydrogels have lower percentage swelling and degradation values as compared to simple hydrogel due to chemical bonding between drug and composite hydrogel. The prepared hydrogels have potential applications in pharmaceutical industry.

Synthesis Of Chitosan-Clay Composites For Water Purification

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In this work chitosan/bentonite (CS/Bt) hybrid composites were prepared for their potential applications in water purification. Polyethylene glycol (PEG) was used as a cross-linker in CCS/Bt hybrid composite formation. The composites were characterized with FTIR, SEM and XRD techniques. Chitosan, bentonite ratios were adjusted to prepare composites with good mechanical strength and high adsorption ability. Adsorbent applications of composites were checked with the adsorption of methylene blue dye and antimony. Adsorbent behavior of composites was evaluated by using various parameters i.e time factor, pH factor, concentration factor. These parameters were optimized during adsorption process to get maximum adsorption in a short period of time. When results were analyzed all composites showed good adsorption for both methylene blue and antimony.

Synthesis Of Structurally Diversified 3, 5 – Disubstituted – Tetrahydro – 2*h* – 1, 3, 5 – Thiadiazine – 2 – Thiones And Their Bioactivities

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Synthesis and biological evaluation of structurally diversified thiadiazine thiones including 2-(3-alkyl/aryl-2-thioxo-1, 3, 5-thiadiazinan-5-yl) propanoic acids and 4-methyl-2-(3-alkyl/aryl-2-thioxo-1, 3, 5-thiadiazinan-5-yl) pentanoic acids was carried out. Targeted compounds were synthesized by reacting primary alkyl/aryl amines with potassium hydroxide, carbon disulfide, formaldehyde and appropriate amino acids. Functionalization of selected synthesized compounds into ester analogue and consequently its conversion into hydrazide was carried out by using hydrazine hydrates. Spectral methods (IR, NMR and Mass spectra) were used for structure elucidation. The synthesized compounds were screened for their anti-nociceptive, antimicrobial, and antileishmenial activities.

Kinetics Of Pyrolysis Of Citrus Limetta Waste In Presence And Absence Of Zeolite

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Citrus Limetta is produced in large quantity in central and southern Punjab. After the consumption of the edible portion the waste is thrown away. In this study we have focused our attention on the use of juice squeezed citrus limetta waste for producing valuable components. The pyrolysis of juice squeezed citrus limetta waste was performed using thermogravimetry and pyrolysis gas chromatography mass spectrometry. TG/DTG profile showed a four step weight loss which was attributed to evaporation of water, degradation of hemicellulose, cellulose and lignin. Kinetic parameters in absence and presence of zeolite were determined from the thermogravimeteric data using Kissinger method. The oils obtained from catalyzed and uncatalyzed reaction was analyzed using GCMS. From the results it has been concluded that use of zeolite has not only reduced the activation energy but also improved the quality of oil produced. The oil obtained if upgraded would have potential applications in industries.

Comparison of Synthesis Methods of Zinc Stannate Nanoparticles

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Zinc Stannate (Zn_2SnO_4 or ZTO) is a mixture of ZnO & SnO_2 formed by non-toxic materials and is a metal oxide. It can be synthesized through various methods; hydrothermal synthesis, chemical synthesis, sol gel synthesis. Different characterization techniques were used in these methods. Hydrothermal synthesis of Zinc Stannate nanoparticles for antibacterial applications showed that Zn_2SnO_4 nanoparticles have great effect against Gram-positive and Gram-negative pathogenic bacteria. As it can be used as anti-bacterial agent to prevent infectious diseases and control the spread. Using spectroscopic techniques and XRD characterizations; Zn_2SnO_4 morphology was determined. SEM & TEM were used to study their particle size and shape. Using UV-Visible absorption spectrophotometer optical properties were analyzed. By FTIR spectroscopy, Zn_2SnO_4 nanoparticles presence was confirmed. It was observed that for the formation of Zn_2SnO_4, favorable growth occurs at high concentration precursor and decrease in reactant concentration results in the reduction of particle size i.e.; from 80 to 120 nm and band gap increases to 4.0eV. High reaction temperature is required i.e.; $\geq 200^0$C for small size. Through chemical synthesis, effect of temperature, time of reaction, reactant concentration on structural, morphological optical properties of particles was studied. 50 minutes time was best to synthesize Zn_2SnO_4.

Adsorption of Gentian Violet by Fish Scales as a Source of Biosorbent: Kinetic, Isotherm, and Thermodynamic Studies

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The aim of this research paper was to investigate the use of food industry waste as an adsorbent for the removal of gentian violet dye. Fish scale powder is an effective adsorbent for the removal of dyes. Phosphate, carboxyl, amine, and carbonyl groups are all found in fish scales and play an important role in the sorption process. For adsorption studies, the batch experiment method was used, and various parameters such as contact time, adsorbent amount (g), pH, dye concentration (mg/L), and temperature were investigated. The maximum percentage of removal was found at 1 g of adsorbent dose. The removal efficiency of dye declines as the initial concentration of dye is increased; the maximum percentage clearance was obtained at 20 ppm. The rate of dye concentration reduction increases over time, with the maximum percent clearance happening after 60 minutes. The kinetics were evaluated using pseudo-first order, pseudo-second order, and intraparticle diffusion models. The surface properties of fish scale powder were examined using a scanning electron microscope (SEM). The nature of the bonds and the numerous functional groups found on the surface of fish scales were disclosed using FTIR spectroscopy.

Preparation of surface modified tea waste as a low-cost adsorbent

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The present work deals with the enhancement of adsorption ability of tea waste for its potential applications in waste water treatment. Household chlorine bleach, base solution and acid solution were used for the modification of simple tea waste samples. The modified samples were characterized by Fourier Transform Infrared (FTIR) spectroscopy. The adsorption ability of the unmodified and modified samples was studied for the removal of methylene blue dye as a reference pollutant. Modified tea waste samples exhibited the highest adsorption capacity with respect to simple tea waste.

Photocatalytic degradation of Congo red dye by Fe/TiO_2 nanocomposites

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In this research work, Fe/TiO2 nanocomposites were synthesized via sol-gel method by using Titanium butoxide as a starting material. The structure, morphology and composition of the prepared samples were characterized by using Fourier transform infrared spectroscopy (FTIR). The prepared composites were used for the photodegradation of Congo red dye in direct sunlight. Different parameters like time, pH and catalyst concentration were varied to optimize the reaction conditions. The results showed that the photodegradation efficiency of Fe/TiO2 increases with increase in time, pH and catalyst concentration. Maximum 98.03% degradation was observed with Fe-doped Titania at pH 10. The results indicated the extra ordinary efficiency of the metal doped titania for the removal of harmful organic pollutant like congo red dye.

Coriandrum Sativum seedsasagreenlow-costbiosorbentforcrystal Violetdyeremovalfrom wastewater

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Thecurrentstudyfocusedonthecationictextiledye Crystalviolet'sadsorptionon Coriandrum sativum seeds powder collected from anindustrialdrain.The major goal of this study is to see how effective Coriandrum sativum seeds powder is at removing harmful crystal violet dye from batch adsorption Coriandrum sativum seeds parameters, isotherms, kinetic models and thermodynamics boundaries have been calculatedand elaborated. Adsorption parameters such as pH, adsorbent dosage, contactduration dye concentration and temperature on CV erection were recorded using a specific technique. Langmuir, Freundlich,D-R, and pseudo-first-order,pseudo-second-order,and intraparticle diffusion kinetic models were used and investigated.Under ideal conditions, such as a sieve diameter of 210 micrometers, pH7,adsorbent dose of 0.3g,contact and 50mint,dye concentration of 30ppm,and temperature of 10 Co,the maximum percent of dye was removed by75%. The experimental calculations were best fitted to Freundlich model along with second order kinetics display sets greater.Computed ΔG and ΔH valuesadjusted adsorption processs materialized to be spontaneous and exothermic.Concurrency ofestablished procedure with tap wateris 72% and regeneration capacity is71% that Coriandrum sativum is propitious adsorbed for decontamination of crystal violet.

Multistep Synthesis Of Bioactive Phenyl Based Pyrazolecoumarin

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Highly toxic nature of several bacteria is responsible for spreading diseases that have spurred the exploration of safe therapeutic agents such as natural products. Among these natural phytochemicals widely distributed pyrazole coumarin is a potential candidate for treatment of bacterial infections. This research work highlights the multistep synthesis of phenyl derivatives of pyrazole coumarins. The characterization of all compounds was done by spectroscopic methods. The antibacterial evaluation of all compounds was done against bacterial strain, staphylococcus aureus.

Antioxidant Potential Of Flavanoids Isolated From Indigenous Tea Decoction

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Tea is one of the most frequently consumed beverages that is consider for promising health since ancient times. It is rich in polyphenolic contents such as flavonoids which are natural antioxidants and regarded as key protective dietary component. This natural product was isolated from various types of teas that were locally available. This research has been carried out to evaluate the antioxidant potential of six different decoction of tea samples. The obtained results showed that all samples have good antioxidant potential including Ceylon tea that has the highest free radical scavenging activity at all concentrations while grey tea has the lowest activity among six samples of tea.

In Vitro Anti Inflammation And Hemolytic Study On Different Flower Extracts Of Mangifera Indica (Mango)

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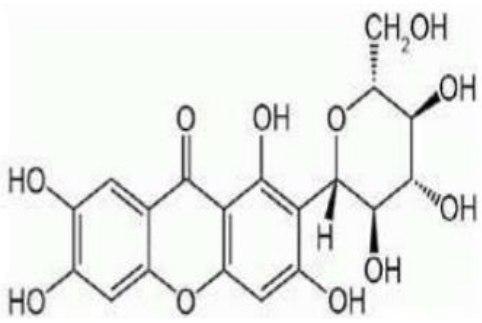
Inflammation is process, which leads to infections, vascular permeability, protein denaturation and membrane alternation in infected site. Inflammation can be treated with natural products that propose green and economic substitute with favorable health benefits. Pakistan is well known for its quality production of Mangifera Indica (Mango) that acquired antioxidant and anti-inflammatory properties. Present research was conducted to assess three different extracts (Ethanol, Methanol, Hexane, EDTA) of Mangifera Indica for their anti-inflammatory and anti-hemolytic activities. The obtained extracts were then evaluated by using albumin denaturation assay and membrane stabilization at different concentrations. It was observed that the extracts exhibit anti-inflammatory properties and best reactivity order was observed in water.

Mangifera indica linn. leave

Mangiferin powder



Mangiferin chemically structural formula

Halide Perovskite Materials for Catalytic Depolymerization of Lignin

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Lignin is an abundantly available bio-polymer found in paper and pulp industrial waste. Its catalytic depolymerization is the hot area of interest, for the material scientist around the globe, for its conversion to aromatic raw materials and fuels. In the current study, we synthesized metal halide perovskites with excellent light harvesting properties and used them for the very first time for the photocatalytic depolymerization of Lignin. The catalytic materials had been characterized by various instrumental techniques like PXRD, SEM, EDX, TEM and BET. The successful depolymerization of Lignin was monitored with UV-Visible spectroscopy and GCMS analysis. Lignin was successfully converted into smaller aromatic compounds of industrial significance like benzene, sinapyl alcohol and phenol. Results will be presented in the conference.

Chemical Modifications to Tailor the Performance of Hydroxyapatite

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The biological performance of a biomaterial is influenced by its surface characteristics. Biomaterials' surfaces can be modified to improve its performance. Chemical alterations can be accomplished through the chemical reaction of material functional groups with appropriate chemical reagents, grafting of a material with small molecules, and physical/chemical crosslinking. Bone grafts provide rapid healing in situations where natural healing is slow or impossible. Surgical tissue repair techniques have a significant risk of infection. Infections in wounds result in tissue necrosis, a delay in the healing process, and the failure of implants. Anti-infected tissue healing biomaterial is a great way to reduce the chance of infection. Functionalized mesoporous materials released antibacterial/bioactive compounds in a controlled manner and help to limit the risk of infection. Hydroxyapatite (HA) is a widely used synthetic bone repairing material because of its excellent biocompatibility, controlled bioactivity, and biodegradability. The surface of HA can be used to tune its properties. The *in situ* co-precipitation method was used to make a series of carboxylic acid functionalized hydroxyapatite (f-HA) particles, which were then tested for controlled drug delivery. The mesoporous f-HA with high surface area, surface charge, and low degree of crystallinity were prepared, which showed favorable and improved electrostatic interaction with the drug. This helped in improved loading and *in vitro* release of the drug. The surface area of the f-HA functionalized with 0.05 mole equivalent of tartaric acid was increased to 737 m2/g. Drug release from f-HA was effective against S. *aureus* and E. *coli*. The prepared f-HA samples are biocompatible according to *in vitro* cell studies with the MC3T3 cell line.

Antibacterial Functionally and structurally Graded Composite Membrane for Periodontal Regeneration

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Periodontitis is a bacterial gum disease, affects the delicate and firm structures that hold the teeth. It affects 90% of the world's population and causes more tooth loss than dental caries. Functionally graded materials have the potential to repair soft and hard tissue and provided a viable therapeutic option. In this work antibacterial, functionally, and structurally graded bilayer membranes were created by using a greener crosslinker 2,3-dialdehyde cellulose (DAC), Chitosan (CS), Oval albumin (OA) and copper substituted Hydroxyapatite (Cu-HA). Cu-HA samples of different substituted amount of Cu were prepared to optimize biological activity and antibacterial properties. CS and OA are biocompatible, biodegradable, and regenerative biopolymers, DAC is a safer crosslinker than other polyaldehyde-based crosslinkers, prepared by oxidation of cellulose. HA and Cu-HA were made using the co-precipitation technique. XRD demonstrated successful synthesis of phase pure Cu-HA, while EDS confirmed copper substitution. To assess the impact of crosslinkers on membrane strength and biological characteristics, four membrane samples were prepared by using CS, OA and CDS to facilitate the soft part of periodontitis, this is called as first layer. The second layer, including CS, OA, CDS and HA or Cu-HA samples, was prepared over the first layer. Presence of Cu-HA could help to regenerate hard part of periodontitis. Membranes were prepared using the freeze gelation process. Prepared membranes were tested by physical and biological characterization. Membrane swelling was good and decreased when crosslinker content was increased. Biodegradation was 45% up to 14 days. Thermal study indicates a loss of 50-54 percent weight up to 1000 °C. The contact angle measurement showed hydrophilic nature of prepared membranes. Cu-HA containing membrane showed antibacterial activity against E. coli and S. aureus. Prepared Membranes were non-toxic and promoted the growth of NIH3T3 cells as well as wound healing. The developed bilayer membrane has potential to treat periodontitis.

Assessment of Heavy Metals in Local Cosmetic Products by Atomic Absorption Spectrophotometer

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Many heavy metals are prohibited as ingredients in cosmetic products as they can cause serious skin diseases such as skin allergies and cancers. Some of the toxic elements and their compounds are water soluble and thus facilitate percutaneous absorption through moist skin. The contents of heavy metals (Pb, Cd, Cu, Ni, Cr, Zn, Sb) in 30 different samples of local cosmetic brands was determined by atomic absorption spectrophotometer.

In Vitro Biological Potential of Mustard Seed Extracts

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Phytochemical substances are ever attention grabbing due to their large therapeutic index. Rich composition of mustard seeds (calcium magnesium phosphorous and potassium) makes them a promising candidate in pharmaceutical chemistry. This research was designed to investigate antioxidant, anti-inflammatory and homolytical activity of extracts derived from mustard seeds by maceration method. All extracts exhibit promising results of anti-inflammatory activity.

Photodegradation of azo dyes by using metal incorporated ionic liquids

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The metals (Sb, Bi) containing ionic Liquids were synthesized by metathesis reaction followed by quaternization of anilines. They were characterized by FT-IR, NMR, atomic absorption spectroscopy and single-crystal XRD for their structural analysis. In this work, the photodegradation of organic pollutants that are emergent concerns in urban water, has been investigated with synthesized metals containing ionic liquids. The Sb and Bi containing ionic liquids have shown a very effective degradation of strong azo dyes and the activity increased several folds with just an increase in concentration from 8 to 10mg/L and resulted in complete degradation in a few minutes. The crucial photodegradation parameter like the amount of catalyst, pH of water and regeneration of catalyst were also examined. There was a very slight decrease in efficiency even after the 5th run. In comparison with Sb, Bi containing ionic liquids have shown higher photocatalytic activity. From these observations, it is supposed that Sb and Bi containing ionic liquids can be used as an effective catalyst for photodegradation of organic pollutants in water. In addition, more experiments are to be done for its electrochemical carbon dioxide reduction capability.

Multistep Synthesis Of Acetyl Substituted Thioxo –Pyrimidine Chromene -2-One

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An increase in inflammatory and non- inflammatory diseases has urged researchers to explore a potent hybrid. Broad range of biological characteristics of coumarins makes it a structural motif in several pharmaceuticals and an innocuous substitute for non-selective drugs. This study is ocused on multistep synthesis of acetyl substituted thioxo -pyrimidine chromeneha- 2- one. The synthesized compounds were characterized by spectroscopic methods.

Removal of methyl violet dye from wastewater by using eggshells

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The purpose of this research was to remove methyl violet dye from wastewater by using eggshells. Batch experiment was performed to check influence of different parameters on adsorption capacity such as pH, adsorbent dose, contact time, dye concentration and temperature. There was 88% removal of methyl violet dye from wastewater by using optimized conditions (pH 7, 0.6g adsorbent dose , 10 minutes contact time, 40ppm dye concentration and 0°C temperature). Pseudo-first-order, pseudo-second-order and intraparticle diffusion models were used to examine the adsorption process. Pseudo-second-order best fitted the adsorption process. SEM was used to investigate surface morphology. FTIR used for functional groups study. Adsorption isotherms such as Langmuir and Freundlich were used to study adsorption capacity. Langmuir was best followed by the adsorption process. Thermodynamic parameters (ΔH, ΔG and ΔS) were studied. From results it was found that process was spontaneous and exothermic. Removal of methyl violet by using eggshells was 88% from tap water.

Fabrication of bimetallic nanoparticles for environmental remediation

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In this research work, Aluminum-Nickel (Al-Ni) based Bimetallic nanoparticles (BMNPs) were fabricated by hydrothermal approach and characterized by scanning electron microscopy (SEM), Fourier transforms infrared spectroscopy (FTIR), and X-ray diffraction (XRD). The XRD and SEM analysis confirmed the alloy formation between Al and Ni. The synthesized photocatalyst was applied for photocatalytic degradation of azo class of dyes (Acid orange 7 and Direct violet 51) from aqueous medium. Different process parameters including pH, time, dose, and dye concentration were optimized. The result has shown that the highest degradation of acid orange was 88% at pH 2 by using 15 mg catalyst with 40 mL of 30 ppm dye within 120 min. The maximum degradation of direct violet was 84% at pH 2 by using 5 mg catalyst, 40 ppm dye solution within 60 min. To check the degradation rate of dyes, kinetic models was applied, and results demonstrated that Behnajady Modirshahla Ghanbery (BMG) model was best suitable to experimental data. The synthesized Al-Ni bimetallic NPs can serve as efficient and cost-effective catalyst.

Synthesis of iron oxide nanoparticles and thier application as nanofertilizer to increase the growth efficiency of zia maize plant

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The use of large-scale chemical fertilizer applications to improve crop production is not an acceptable choice in the longer term, because they reduce soil fertility, disrupt the balance of soil minerals and have major effect eco-system. The application of nanotechnology as a nanofertilizer in the agricultural sector is improving food productivity, addressing environmental issues and nourishing the world's growing population. Iron is an essential micro-nutrient and have ability to increase the fertility of soils for the growth of plants. It is needed for biochemical processes such as photosynthesis, respiration and many cellular activities. The effect on growth and metabolic functions of iron nanoparticles diverges differently across plants. The present research work was carried out in two steps: the first was to synthesize Iron-based-nanomaterials. These INPs wase characterized by suitable analytical technique, such as Fourier transform spectroscopy (FTIR), X-ray diffraction (XRD), and scanning electron microscope (SEM). In second step these synthetic INPs were applied as micronutrients on maize plant (Zea mays) at different concentration (50, 100, 150, 250 mg/kg) of soil and (50,100,150,250 mg/L) foliar application to check the effect of Iron-based-nanomaterials through different parameters (growth and biochemicals). The study revealed that the INPs have potential to replace conventional bulk-based fertilizer for better production and protection.

Comparison of Green Synthesis of ZnO nanoparticles

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Synthesis of nanoparticles is an increasing demand of present era due to their significant electrical, optical, catalytic, and magnetic properties. Nanoparticles are called wonders of modern science and they find their applications in paints, ceramics, gas sensing, cosmetics, drug delivery, catalysis, chemical storage, microcapsule reactors and in photoelectric materials. Nanoparticles are multifunctional materials. Among various Nanoparticles, ZnO are distinct type particles. There are several ways to prepare these particles but physical and chemical ways to prepare ZnO are toxic and hazardous. Therefore, synthesis of ZnO nanoparticles by using simple, novel, nontoxic, cost effective and environment friendly green methods was compared. By using facile green recipe highly pure, safe, and durable zinc Oxide nanoparticles canbe synthesized. Plants or plants extract can be used like; Solanum nigrum leaf extract, Euphorbia Jatropa latex and potato extract. These extracts act as stabilizing and capping agent. Synthesized particles were characterized by using different characterization techniques including XRD, FTIR, SEM-EDS and TEM. Furthermore, the functional groups, presence of Zn and O elements and purity of ZnO was confirmed by these techniques. The average particle size calculated was in the range of 15-30nm. As the particle size get smaller the band energy or band gap goes on increasing. Antibacterial activity and crystal structure of ZnO is prominent as particles get smaller.

Assessment of Quality of Olive Oil Commercially Available in Pakistan

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Olive oil is widely used as salad dressing, frying, cooking, and pharmaceuticals formulations. It is a highly health-beneficial and profitable food product due to its uniquesensory characteristics. The increase in product cost owing to growing demand creates olive oil to a certain extent to adulteration. Regretfully, it is common to blend high-quality olive oil with other vegetable oils and low-quality olive oil to increase profits. The main aim of the present study was to determine the concentration of various physicochemical parameters of olive oil available in the local market. Results of olive oil samples indicated that FFA was found in the range of 0.93 to 2.62%. β-carotene was observed in the range of 1.28 to 7.92 mg/kg. The amount of chlorophyll from lower to higher was observed at 2.42 mg/kg and 165.1 mg/kg. The CD and CT were observed at 0.08 to 1.26 and 0.35 to 2.10. Respectively, the oxidative stability was found in the range of 10.67 to 28.45 h. None of the analyzed olive oil could be recommended for cooking as they contain high FFA (>0.7%).

Bioremediation of Pymetrozine by *Plurotus eryngii* fungal biomass

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Owing to the significance of bioremediation technique, the present study is based upon the biological preparation of environmental friendly fungal biomass *P*leurotus eryngii (*P*. eryngii) and their exploitation for the removal of selected persistent pesticides. In current part of the study, removal of Pymetrozine (pyridine azomethines), a new class of insecticides was successfully accomplished with *P*. *eryngii* fungal biomass. The biomass was characterized by FTIR and SEM techniques to verify surface functionality and morphology. In the initial step of study various pesticides i.e Endosulfan, Bifenthriuon, azocyclotin, pymetrozine were screened for their biodegradation possibility by *p.eryngii*; amongst them Pymetrozine was degraded effectively and subjected to further optimization with UV-visible spectroscopic monitoring. The Response Surface Methodology (RSM) was employed for optimization of experimental variables owing to the fact that such statistical optimization decrease the number of experiments, improved the removal efficacy and reduced treatment time and overall research cost. A two level, three factors Central Composite Design (CCD) was used to evaluate the effects and interactions of the process variables for removal of Pymetrozine. Factors studied included pesticide concentration, reaction pH and time for utmost degradation of pymetrozine in water system. Results showed that *P.eryngii* was able to degrade 93.2% (0.02 mM pymetrozine) under aerobic conditions at pH 5 in 9 days. Hence, ***P.eryngii*** proved as cost-effective, eco-friendly, and an effective potential novel tool for removal of pymetrozine.

Development of Antiviral Fabrics, their characterization and application for prevention of Covid-19

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The COVID-19 pandemic is the worst and largest global public health outbreak of 21st century. According to WHO more than 5 million people have died and 250 million are affected with SARS-CoV-2, one of the major sources of infection spreading is the droplet released by the infected person through cough, exhale, or sneezing. These heavy droplets rapidly fall on different surfaces and cause infection to a healthy person, so the technology that can help to slow down the spread of vires is strongly needed. In this study, we designed antiviral coated fabric to combat the spreading of SARS-CoV-2. Copper ions and copper oxide nanoparticles were synthesized and subsequently deposited on to the surface of different types of fabrics in order to check their antiviral activity. The morphology and structure of uncoated and coated fabrics were examined by scanning electron microscopy, X-ray diffraction, FTIR, and elemental analysis. The results reveal that copper ions and copper oxide nanoparticles are crystalline and absorbed physically onto the different fabrics. The coating procedure is designed in such a way that any textile industry can apply it without any modification in its textile processes with text the dip and dry method. The process showed uniformity, simplicity, and very good adhesion on different fabrics. The results show that synthesized antiviral fabric can neutralize more than 99% of viruses according to ISO 18184 testing standard. This fabric can be widely used in the face mask, clothing, bedding, and aprons and the coating is remain efficient over more than 25 washes.

Hetero-catalytic Kinetics of CuO Nanostructures for Simultaneous Decolorization of Eosin Y and Rhodamine B in Aqueous Environment

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In an effort to save the environment from hazardous pollutants, we describe an exceptional synthetic route for the fabrication of heterocatalyst CuO nanostructures through a practical aqueous chemical growth route. The successful fabrication of heterocatalyst was confirmed via versatile analytical tool e.g. AFM, EDX, FTIR, SEM, XRD and zeta potential. All these characterization tools reveal exceptional phase purity, nanoflakes morphology, surface charge of (-36.5 ± 3 mV), average size of 18.7 nm and monoclinic structure respectively. The heterocatalytic kinetics of proposed nanocatalyst manifests outstanding degradation of Eosin Y and Rhodamine B dyes over ≥ 97% within 3 minutes of time period with a minute dose of CuO nanocatalyst from 120 to 140 µg simultaneously and individually under the sunlight. The minimum catalyst dose, cost-effective fabrication route, short time, supreme reduction percentage and exceptional recyclability ensure the propose nanocatalyst as an effective heterogeneous material for environmental remediation. Consequentially, the proposed CuO heterocatalyst is more realistic and promising aspirant for the successful degradation of hazardous and complex dyes from the aqueous medium at commercial level.

Synthesis of functionalized carbon material for the catalytic degradation of selected organic contaminants

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Environmental pollution is becoming a global issue with the rapid development of industrialization. Endocrine disrupting compounds (EDCs), a diverse class of emerging contaminants, have been recently detected in natural water. In the past few decades, the exploration of various photo-catalysts for splitting of water, degradation of organic contaminants and reduction of CO2 is one of the significant strategies for solving energy crisis, global environment pollution and climate change. Therefore, developing new efficient photocatalyst and broadening the scope of photo-catalyst response became a hot research topic in the field of environmental photo-catalysis. This research work is based on the synthesis of functionalized graphene based material that can work as heterogeneous photo-catalyst for the degradation of selected organic compound (BPA as the model compound). Bisphenol A (BPA), also known as 2,2-bis-(4-hydroxyphenyl) propane or 4,4′-isopropylidenediphenol, is used for the production of various polycarbonate and polysulphone plastics and epoxy resins. In this study, we have synthesized expanded NiSO4 intercalated GO flowers (NiSO4 Int. GO flowers) for the degradation of endocrine disrupting organic contaminants. Bisphenol A (BPA) was degraded photo-catalytically by synthesized NiSO4 Int. GO composite under UV light. The synthesized expanded NiSO4 Int. GO flowers presented high photo-catalytic activity for 100% degradation of BPA at pH 4 within 20 min. The morphology of synthesized material was characterized using SEM, XRD and BET and composition of synthesized NiSO4 Int. GO flowers was characterized by using FTIR. These findings are crucial for designing GO-based photocatalysts with high performance for degradation of persistent organic pollutants in wastewater and potable water.

Co-relation of particle size and catalytic efficiency of bio-carbon derived solid acid catalyst

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Hydrothermal carbonization is a promising upgrading process to convert low energy density lignocellulosic biomass materials to homogeneous energy-dense HTC biochar known as hydrochar. Carbon solid acids are atypical representatives and a new type of Bronsted acid catalytic material. So far they have been widely used in esterification, cellulose hydrolysis, alkylation etc. The cost-effective carbon-based catalyst possesses very high catalytic activity in the reduction of CO_2. This catalyst is non-corrosive, and renewable and has the potential to be used in the industrial production of biodiesel. Sulfonated porous carbons (PCs-SO3H) have been prepared from the carbonization of sucrose (monosaccharides) followed by one-step hydrothermal treatment. Carbon materials are sulfonated by treatment with H2SO4. Using the stronger sulfonating reagent, fuming sulfuric acid, resulting in much higher transesterification activity. The catalyst was characterized by FT-IR, XRD, SEM, and BET analysis. The catalyst was regenerated again by refluxing with concentrated sulfuric acid. For the catalytic activity test, the prepared catalyst with small particle size was studied for their ability to catalyze the esterification reaction of oleic acid with methanol. The results revealed that a green sulfonated hydrothermal catalyst with a small particle size has a high potential to esterify oleic acid into methyl esters about 93-96% conversions. The relation between the carbon particle size on esterification reaction, the sulfonation efficiency, reaction time, reaction temperature, methanol to oil molar ratio, and its performance as a catalyst was studied. Sulfonated porous carbons (PCs-SO3H) with small particle sized exhibited high efficiency for the esterification reaction and high performance for bio-diesel production. The catalyst can be recycled several-time with minimal loss of activity. The simple synthesis and low cost of the porous sulfonated carbons (PCs-SO3H) make the promising catalyst for esterification reaction and in many industrial applications to reduce the time to obtain the final product and increase the yield of the process if a preliminary sieving step is applied to the carbon.

A new electrochemical method for the detection of quercetin in onion, honey and green tea using Co_3O_4 modified GCE

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Quercetin (Qu) is the most abundant biologically active dietary flavonoid which belongs to the family of flavanols. It has numerous potential health care benefits and is widely used against different diseases but its excess consumption can also cause kidney cancer. Hence, we have synthesized ionic liquid-assisted Co_3O_4 nanostructures with a very simple and cost-effective method and utilized them to fabricate an electrochemical sensor for the highly sensitive determination of Qu. The material was prepared with different volumes of ionic liquid to examine its effect on the morphology and size of the material. The functionalities, composition and surface morphology of the material was studied with different sophisticated techniques like FTIR, XRD, EDX and FESEM, etc. which revealed that the prepared material is highly crystalline, with nano rod-like shape containing purely cobalt and oxygen elements in it. The electrochemical performance of the fabricated Co_3O_4/GCE sensor was just not found more selective but also highly sensitive for the determination of Qu in standards as well as in different dietary foods like honey, onion and green tea. Due to the high catalytic ability, large surface area and good conductivity of Co_3O_4 nanostructures the proposed sensor have shown maximum electrochemical response for Qu sensing in a wide range of detection from 0.01 µM to 3 µM with a very low limit of detection (0.0002 µM) and limit of quantification (0.0007 µM) respectively. The amount of Qu found in the food samples; Green tea, onion and honey were 3.473 mg/g, 15.58 µg/g and 5.367 µg/mL respectively.

Authentication of Halal fat ingredients in selected imported confectionery products marketed in Pakistan

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Halal authentication of fat ingredient is gaining attention owing to recent revelations related to pork and lard being mixed in confectionery and other food products and their sales of porcine fat listed in different super marts have surfaced. Therefore, present study aims is to investigate oil/fat quality for halal authentication. Different sample of selected imported confectionery products including chocolates n=30 (3×10) and biscuit (n=18 (6×3) were purchased from local super marts of Hyderabad, Islamabad, Karachi and connected areas. Oil /fat was extracted from chocolates and biscuit samples by soxhlet extraction method (AOAC, 2007). The extracted oil/ fat was analyzed by Gas chromatography fitted with flame ionization detector after methyl estrification. Result showed variable fat content in all imported chocolates and biscuits ranged between 11.5-32.5% with relatively higher content in chocolates (15.2 - 32.5 %) than biscuits (11.5 -21.5 %).Chocolate fatty acid composition showed plamitic, stearic and oleic as a dominating component with the exception of palm kernel based chocolates which were rich in lauric acid (42-52%) and Myristic acid (18-20%).Biscuits fatty acid composition showed palmitic and oleic as main ingredient comprising > 75% FA's in all type of biscuits categories. Overall milk based chocolates showed better profile with more stearic and oleic acid, which are considered better FA than palmitic acid. Among biscuits palm oil based biscuits with milk exhibited better profile with more MUFA. Pocrine fatty acids biomarkers i.e eicosadienoic acid (C20:2) and C-16:0/C-18:1 were found positive in few imported chocolate samples.

Green Synthesis of Copper Oxide Nanoparticles via Prosopis glandulosa for removal of Eriochrome Black T

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Metal oxide nanoparticles are currently the subject of extreme investigation and research inprogress from a diversity of perspectives. Nano-copper oxide is very interested because of its potential applications in many fields such as heterogeneous catalysts, anti-microbial, antioxidants, imaging agents, and drug delivery agents in the field of biomedicine. There are various routes for the synthesis of metal oxide nanoparticles which are potentially harmful to the ecosystem, but green method of synthesizing nanoparticles is significant due to its low cost, less toxicity and environment friendly role. EIn present study, *Prosopis glandulosa* leaves extract was employed to synthesize CuO nanoparticles using copper chloride precursor salt. Green synthesized CuO NPs were characterized using various spectroscopic techniques such as UV-Visible spectroscopy, FTIR, Scanning Electron Microscopy (SEM), Zeta Sizer, Zeta Potential and EDS. The UV–visible and FTIR study profile initially confirms the formation of CuO NPs. A distinct absorption peak at 270 nm confirms the formation and presence of CuO NPs. The SEM images revealed semispherical shaped CuO NPs. While Zeta sizer and Zeta potential measurements explained well arranged, size, and charge over the surface of CuO NPs, which was calculated to be 65 nm with desirable charge of – 1.42 mV. Furthermore, the CuO NPs were applied for catalytic reduction of Eriochrome black T (EBT). Different parameters were optimized including NaBH4, time of exposure under Microwave radiation, nanoparticle dosage. Catalytic reduction of EBT was achieved up to 95 % using 2 mg CuO NPs within 25 minutes.

Evaluation of Quality of Oil Present in Biscuits Prepared Through Industrial and Artisanal Process

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Biscuit is a popular food product produced by using wheat flour, carbohydrate and fat as its main ingredients. Among the bakery products, biscuits stand out most it is a food of daily consumption and greatly appreciated by consumers. The difference in artisan and industrialized biscuits indicates that 86% of consumption corresponds to artisan biscuits and only 14% processed biscuits such as sandwiches or chocolate, bakery, butter, cream and salts biscuits.

The present study deals with analyzing oil present in the industrially processed and artisanal biscuits commercially available in the local market. Eighteen different biscuits samples (twelve industrial and six artisanal) were collected from local market such as saltish, chocolate chip, coconut, peanut, and wheatable biscuits. The analytical tests were performed according to AOCS standard methods such as moisture, ash, oil/fat content, free fatty acid (FFA), peroxide value (PV) and color. The results indicated that moisture and ash content were found in the range of 0.53 - 1.58% and 0.41-2.1%, respectively. The fat content in different biscuit samples ranged between 7.03-21.75%.All biscuits have FFA and PV that fall within the allowable limits, i.e., 0.53 - 1.58% and 0.21-5.4 meqO2/Kg, respectively. Except for a few samples that crossed the allowable limits of PV, which shows that oil is slightly oxidized.

The results of present study shows that artisanal biscuits have the good quality as compare to industrial biscuits on the basis of free fatty acid and peroxide value.

Synthesis Of Functionalized Graphene Based Composite Materials And Their Applications

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Graphene is an exciting and widely studied material, which has a one-atom-thick 2D planar sheet of sp2-bonded carbon atoms in a honeycomb crystal lattice that exhibits extraordinary electronic, chemical, mechanical, thermal, and optical properties which made it a promising material in the 21st century. Due to its fascinating physical and electrochemical properties, it has been extensively utilized in the modification of electrodes in electrochemical sensors. Bisphenol A (BPA, (2,2′-bis(4-hydroxyphenyl) propane) is commonly known as an endocrine-disrupting compound that is widely used for the synthesis of some polymer materials such as Polycarbonate (PC) and Epoxy resins (Es). These polymer materials are used to produce food storage containers, beverage cans, feeding bottles, packaging materials, thermal papers, supply pipes, and many more. BPA has been exposed to humans and aquatic organisms due to the widespread use of packaging materials that leach into water and food which cause serious problems. The nanomolar concentrations of BPA can mimic estradiol hormone, causing changes in some cell functions and adversely affecting the functions of the brain, thyroid, ovary, and reproductive organs, leading to cardiovascular diseases, obesity, and carcinogenicity. Therefore, the regular monitoring of BPA in drinking water is quite essential. Recently, electrochemical sensors are considered as promising detection tools for simple, rapid, and accurate determination of BPA due to their simple fabrication, high sensitivity, and ease of sample preparation.

Herein, we have developed an electrochemical sensor based on graphene-based composite material (GBCM) for electrochemical determination of BPA. The prepared sensing material was characterized using FTIR, SEM, XRD, and EDS techniques. Conductivity was initially checked using Cyclic Voltammetry (CV) and Electrochemical impedance Spectroscopy (EIS) and different parameters were optimized. The LOD & LOQ of the proposed sensor for the detection BPA were calculated to be 0.041 and 0.13 μM, respectively.

Quality Evaluation of Commercially available Shampoos

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Shampoos are widely used cosmetic products for daily washing of the hair and scalp. Shampoos are mainly used to remove such as dirt, oil, unwanted particles which remove the dirt of human body. The evaluation of shampoos comprises quality control tests including visual assessment and measuring physiochemical controls such as pH, cleaning action test, foam stability (mL), viscosity (Nsm^2) and wetting time(s). The contents of pH, cleaning action, foam stability, viscosity in all the shampoos were ranged as (4.56-7.15, 11.35-31.1, 99.25-172.25, 0.81-2.44,) while the highest Surface Tension was observed in S7 and lower in S2. Wetting time in studied shampoos were ranged as (65.96- 254.28). Highest wetting time was obtained in S-9 which (254.28), lowest wetting time was obtained S3 (65.98). Great variations have been observed among the shampoos of different brands. Cheap and substandard shampoos contain cleaning action less than 18%. FTIR study was conducted in order to check the different functional groups present in shampoos.

Significance and impact of trace and toxic metals in different age groups consuming confectionery and nut products.

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Heavy metals (Pb, Ni, and Cr) were assessed in seven different categories of confectionaries and nut product which include ten brands of chewing gums, ten brand of batel nut, commonly found in retail stores and sells on major street in Jamshoro. The results indicated concentration of Pb, Ni, Cr, Cd and in the mean concentration of Pb, Ni, Cd and Cr in batel nut samples ranged from 0.53 – 5.18µg/Kg, 0.41 – 0.55 µg/Kg, 0.00 – 0.053 µg/Kg, 2.6 – 8.11µg/Kg respectively. While the mean concentration of Pb, Ni, Cr, Cd and in the mean concentration of Pb, Ni, Cd and Cr in chewing gum samples ranged from 0.01 – 8.73µg/Kg, 0.43 – 1.74 µg/g, 0.00 – 0.044 µg/Kg, 4.91 – 84.4 µg/Kg respectively. Higher concentration of all the studied metals were found in both batel nut and chewing gum samples. But as contrary to batel nut only a few samples of chewing gum were contaminated of heavy metals. All the confectionaries studied indicated presence of the studied metals (Ni, Pb Cd and Cr) at concentrations which exceeded the permissible limit of0.001µg/Kg prescribed by FAO/WHO (2011) .Therefore, consumption of those products may likely results to some adverse health effects.

Synthesis of mixed matrix proton exchange membrane and its application for fuel cell

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Proton-exchange mixed matrix membranes (PE-MMMs) have received considerable interest as promising materials. Proton-exchange membrane fuel cells (PEMFCs) are considered to be a promising technology for clean and efficient power generation in the twenty-first century. Fuel cells due to their particular properties are on the verge of creating a vast revolutionary change in the field of electricity. A novel proton exchange membrane consisting of 8-hydroxyquinoline-5-sulfonic acid intercalated Graphene oxide (HQSA Int. GO) as nanofiller has been successfully prepared by simple and scalable polymer blending methodology. Different compositions of PEMs were optimized by changing the loading amount of 8-HQSA-GO in the range of 5 to 25 mg. Prepared PE-MMMs were evaluated for their ion exchange capacity (IEC), water uptake %, water stability %, oxidative stability % and water content %. Different membranes exhibited IEC in the range of 0.9 to 1.3 mmol/g, water uptake in the range of 32 to 40 %, water stability in the range of 88 to 94 %, oxidative stability in the range 99 to 99.5 % and water content in the range of 14.7 to 20.4 %. The membrane with excellent performance in PEMFC was obtained when 15 mg of HQSA Int. GO was loaded. This membrane exhibited IEC of 1.3 mmol/g, oxidative stability of 99.4%, and water uptake of 34.5% and water content of 14.7 %. These results are in good comparison with PEM based on Nafion. Prepared HQSA Int. GO composite and its membranes were thoroughly characterized using FTIR, SEM, XRD and BET.

P-Doped $C_{24}N_{24}$ Fullerene as an Efficient Candidate for Scavenging of NO_2, a Contributor to COVID-19 Fatality

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Nitrogen dioxide is a toxic air pollutant released anthropogenically through combustion of fossil fuels in automotives or naturally through lightening. It is associated with medical conditions like cardiovascular diseases, hypertension, reduced lung function, chronic obstructive pulmonary diseases and is considerably linked with respiratory fatality. Recent studies illustrate that greater concentration of NO_2 also contribute to the fatality of COVID-19. Therefore, detection and sequestration of NO_2 from atmosphere is necessity of time. In this study, we have for the first time evaluated phosphorous doped porous carbon nitride fullerene ($C_{24}N_{24}$) for the removal of NO_2, using first principle analysis. The energetics, electronic properties, thermodynamic study, atom in molecule analysis and charge transfer analysis reveals that the P-doped $C_{24}N_{24}$ fullerene efficiently captured the NO_2 molecules from its N site through chemisorption. Moreover, the selectivity study indicates that P-doped $C_{24}N_{24}$ fullerene selectively captured NO_2 from gas mixtures containing NO, N_2O, SO_2, NH_3, H_2O, CO, CO_2 and O_2. Our results demonstrate that this study will help the scientists to develop novel, efficient and selective sensors for NO_2 in future endeavors.

Di allylcalix[4]arene incorporated polystyrene nanofibers for removal of endosulfan from aqueous environment

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The present work explores adsorption behavior of diallyl derivative of calix [4] arene based nanofibers for removal of α and β endosulfan isomers from aqueous media. The synthesized Poly Styrene (PS) and PS-calixarene diallyl derivative (PS-CLX) nanofibers were characterized by FTIR and SEM analysis. The efficiency of PS and PS-CLX nanofibers for removal of endosulfan was checked by performing batch adsorption experiments. Various parameters were optimized including pH (2-12), contact time (20-120 min), shaking speed (20-150 rpm) adsorbent dosage (1-10 mg) and pesticide concentrations (0.025 ppm – 0.3 ppm). The PS-CLX nanofibers showed maximum adsorption at pH 7 with contact time of 60 min, shaking speed of 120 rpm and adsorbent dosage of 7.5 mg. Freundlich and Langmuir adsorption isotherm models were applied to validate the sorption process. Kinetics study reveals that the adsorption follows pseudo second order rate equation. The modified method has also been applied to real water samples and the results showed that PS-CLX nanofibers were an effective adsorbent to remove endosulfan from waste waters.

Compare the nutritional status of essential minerals in milk of different cattle and humans: Estimated daily intake for children

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In present study, the comparisons of electrolytes, calcium (Ca), potassium (K), magnesium (Mg), sodium (Na) phosphorus (P), and essential trace elements, iron (Fe), zinc (Zn), copper (Cu) and selenium (Se) were carried out in milk samples of different cattle (cow, buffalo, goat, sheep, and camel) and human as total and soluble form (whey of milk). The sampling of milk was carried out from different farms, flocks and human from rural areas of Hyderabad city. The electrolytes and essential trace elements in milk, as total and soluble (whey) forms were determined by different techniques, after acid digestion method. The concentrations of Na, K Ca, P and Mg were significantly higher in camel milk, whereas, the contents of K were elevated in goat and sheep milk. As compared to the different cattle, human milk had the lowest concentrations of all selected essential trace elements except Se. The percentages of all elements in whey milk were found in the range of 20 to ≥ 95% of their total contents in whole milk samples of different cattle and human. The estimated daily intake of all elements was calculated for infants <0.6 month to 10 years old children via consuming milk of cattle and humans. It is notable that milk of each species has a specific individual pattern of electrolytes and essential trace elements, which might be an indicator of relative nutritional importance for human of all age groups.

Comparative Study for the Synthesis of Graphene Oxide

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This comparative study comprises of various methods for the synthesis of graphene oxide. Graphene oxide is a low density material having a thickness of about 1 nm. Graphene is made up of carbon atoms that are bonded together in a regular pattern of hexagons. It is usually synthesized by hummer's method. In this work three methods are reported for the synthesis of graphene oxide. Hydrothermal synthesis, modified hummers method and Improved Hummers method results in the formation of graphene oxide. Hydrothermal synthesis method is a chemical free synthesis approach because it only involve the sugar and deionized water. It is considered green approach to obtain our desired product because no toxic chemicals are used in this method. In recent years more attention is given for the synthesis of graphene oxide because of it wide range of applications .Improved Hummers method also gives the good prospects to obtain desired product. This method provide good result and also eco-friendly as it does not involve the use of NaNO3. Modified hummers method results in the synthesis of graphene oxide and involve the use of NaNO3. The modified Hummers method is considerably less important because of toxic gases NO2/ N2O4. The Characterization techniques used to study the morphological and physiochemical features are UV-Vis spectroscopy, FT-IR and XRD. The presence of oxygen having functional group within GO was confirmed by FT-IR and XRD spectra.

Quantitative analysis of macronutrients and oil quality of snacks commonly consumed in Rural Sindh, Pakistan

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Snacking is considered as the routine habit in Pakistan between meals. Snacks comprises of ready-to-eat mixes, chips, nimkos and other light processed foods. Quality of snacks is vital for maintaining a healthy diet, managing hunger between meals, and keeping correct blood sugar levels. On the shelf, multiple complex reactions take place during the usage life that bring drastic changes in sensory, physical, chemical, and nutritional properties of the oil in food. For assessing these problems, we designed our research to evaluate macronutrients and oil quality parameters by using standard AOAC methods for determining physicochemical parameters such as free fatty acid (FFA), peroxide value (PV) by titration; conjugated diene (CD), conjugated triene (CT), and para-anisidine(P-AV), by using UV-visible spectroscopy; trans-fatty acid by FT-IR spectroscopy and, total oxidation (TOTOX) in different oils of snacks consumed by rural population (Matiari) of Sindh, Pakistan. Samples of snacks obtained and categorized broadly as biscuits, cakes, chips and nimko. Oil was extracted using Soxhlet extraction method. Highest oil content was found in nimko (33.2%), followed by biscuits (20.72%), cakes (16.56%), and lowest in chips (15.89%). The values obtained for various quality parameters of oil was found above the permissible limit which indicate that the oil in snacks is oxidized. Furthermore, trans-fatty acids were found in 55% of samples which indicate that use of poor-quality hydrogenated oil in production of snacks Also, higher values of P-AV indicate secondary oxidation and may be due to longer storage than actual shelf life.

Green Synthesis of Silver Based Bimetallic Nanoparticles Using Bombax Ceiba Flower Extract and Their Morphological, Optical, and Catalytic Application

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Nobel metal nanoparticles have provided much application in bio-medical industries besides photocatalysis. Consequently, bimetallic nanoparticles synthesized by reduction of two metals combined by inter-metallic interactions in over nucleation process. Ongoing exploited the Noble bimetallic nanoparticles such as Ag/Au, Pd/Pt, Ag/Pd and Ag/Ni have been applied in various areas like catalysis and medical ailments. Especially Ag/Ni bimetallic nanoparticles offering wide potential applications in biomedical industries. There are various routes for synthesis of nanoparticles, which are more expensive, toxic, and potentially harmful to the eco-systems but green strategy diverse for the synthesis of metal nanoparticles entities have significant role due to its environment friend viability and implies a simple, low-cost, with owing to their biomedical and catalytic applications. In present study, Silver based bimetallic nanoparticles were synthesized by green method using flower extract of *Bombax ceiba* plant. For extract preparation, flowers of *Bombax ceiba* were collected from NCEAC Hostel University of Sindh, Jamshoro. The synthesized bimetallic nanoparticles were subjected under different characterization tools. The UV–visible and FTIR study profile initially confirms the formation of Ag/Ni Bimetallic Nanoparticles. A distinct absorption peak at 461 nm confirms the formation and presence of Ag/Ni BMNPs. The SEM images revealed untwined combined form rhombohedron shaped Ag/Ni BMNPs. While Zeta sizer and Zeta potential measurements explained well arranged, mono-dispersity, size, and charge over the surface of Ag/Ni BMNPs, which was calculated to be 50.06 nm with a desirable charge of -8.4 mV. Furthermore, the Ag/Ni BMNPs were applied for catalytic degradation of 4-nitrophenol (4-NP). Different parameters were optimized including NaBH4, time of exposure under Microwave radiation, bimetallic nanoparticles dosage. Catalytic reduction of 4-NP was achieved up to 99% using 120 µg Ag/Ni BMNPs within 60 seconds.

Synthesis of metal-free Biomass-derived Electrocatalyst and its electrochemical applications

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Water oxidation reaction is a bottleneck in water splitting for energy generation. Currently, metal based catalysts are used for water splitting. The precious metal oxide such as RuO2 and IrO2 show excellent catalytic activity for oxygen evolution Reaction (OER). However, the large scale application of energy generation through water oxidation is still not possible due to high cost and scarcity of the noble metal based catalyst. Hence, to make water splitting cost effective there is a need to develop alternate new material that could replace state-of-the art expensive metals. In this pursuit, an abundant and cost effective catalyst based on biomass is synthesized by facile pyrolysis method. The as prepared biomass derived catalyst named as Nitrogen Doped Carbon Matrix (NCM). Potentiometer having three electrode systems is used to study the electrochemical properties of the catalyst. The activity of material is calculated by using linear sweep voltammetry and chronoamperometry. The catalyst showed overpotential of only 330 mV. Furthermore, controlled potential analysis and tafel slope demonstrate the high stability and fast kinetics of the metal free catalyst towards Oxygen evolution Reaction respectively.

Adsorption of methylene blue through electrospun nanofiber polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP) incorporated Silica nanoparticle (SiNPs)

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Textile industry plays a significant economic growth but create serious environmental problem, it is very essential to remove colored dye from waste water. Therefore, the simple and delicate technique based on spectrophotometry was developed for the adsorption of methylene blue through electrospun nanofibers. So we developed polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP) incorporated silica nanoparticles (SiNPs) based electrospun nanofibers. Synthesized (PVDF-HFP) incorporated (SiNPs) based electrospun nanofibers were characterized by AFM, FT-IR spectroscopy and UV-visible spectrophotometer. AFM images show that the synthesized electrospun nanofibers of PVDF-HFP incorporated (SiNPs) are smooth and beadles. The synthesized electrospun nanofibers of PVDF-HFP incorporated (SiNPs) were used for adsorption of methylene blue. For the adsorption of methylene blue (MB), the known amount of methylene blue standards ranging from 50-1000 ppm were used. The adsorption isotherms of MB dye on electrospun nanofiber of PVDF-HFP incorporated (SiNPs) fitted with the Langmuir model, and the adsorption kinetics followed the pseudo-second-order model. The maximum actual adsorption capacity of electrospun nanofiber of PVDF-HFP incorporated (SiNPs) found 588.32 mg/g, which was larger than other adsorbent materials and any other electrospun nanofiber. Furthermore, the electrospun nanofibers of PVDF-HFP incorporated (SiNPs) exhibited adsorption equilibrium within 90 min, and good selectivity was achieved.

Template Assisted Imprinted Materials For The Selective Adsorption Of Tribeneuron

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Tribeneuron methyl is a sulfonylurea herbicide which is applied to broadleaf weeds and crops. As it is applied in the form of foliar spray so it remains in the environment for a longer period of time and also gets into water and pollutes the water causing great damage to human and aquatic life. In this research work, we have prepared two types of molecularly imprinted materials (MIMs) and conducted a comparative study to investigate their extraction efficiency for Tribeneuron methyl from aqueous solutions. The MIP (molecularly imprinted polymer) was prepared using vinyl acetate, acrylic acid and acrylonitrile as monomers and EGDMA as a cross linking agent. While, MIS (molecularly imprinted ormosil) was synthesized using APTES as monomer, TEOS as reticulating agent and tribeneuron methyl as template molecule. Both the MIMs were characterized through FTIR. Various experimental parameters were optimized as well as cross reactivity's evaluation were performed. The relative study of both MIP and MIS for the removal of the herbicide showed that MIP is more selective with higher adsorption capacity towards tribeneuron methyl as compared to MIS. A percentage recovery of 96% was obtained at pH 7 using MIP as a selective sorbent material. Furthermore, the MIP could be reused for 5 successive cycles without the loss of efficiency. In future, the MIP will be applied for the selective adsorption of the herbicide from real water samples of agricultural runoff.

Synthesis Of Biodegradable Plastic By Using Cellulose Extracted From Waste Clothes

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Pakistan being a developing country is striving on different grounds to keep pace with the advancing world. Among the trending challenges being faced by our nation, the prime one is the plastic pollution. Currently, government has restricted the use of plastic bags and focusing to replace with biodegradable ones. The next goal needs to be the replacing of disposable plates made of thermocol with the nontoxic and biodegradable materials. Keeping in view the current scenario of environmental pollution, we fabricated biodegradable plastic using cellulose from waste clothes. The process of synthesis involved the extraction of cellulose followed by its oxidation. In the next step, different plasticizers were tested to modulate the durability and porosity of the bioplastic. The finally obtained bioplastic was then tested for its solubility and biodegradability. The bioplastic was insoluble in aqueous medium and took 5 days in the soil to degrade. The synthesized bioplastic was casted into plates. Further research is being conducted to cast into different shapes and introduce in the market as a replacement of non-biodegradable disposable utensils.

Structural elucidation and dielectric studies of Aluminium doped Copper-Nickel ferrites

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Al doped Copper-Nickel based spinel ferrites $Cu_{0.7}Ni_{0.3}Fe_{2-x}Al_xO_4$ are prepared by using sol-gel synthesis route. The characterization techniques like X-ray diffraction, Fourier transform infra-red spectroscopy, impedance analyzer, EDAX and Scanning electron microscopy are employed. Phase analysis confirmed a cubic spinel structure having a single phase. Scanning electron microscopy images showed the uniform formation of nanoparticles. Elemental stoichiometry is confirmed from EDAX spectra. The size of crystals lies within the range of 28.38–30.04 nm. The lattice constant decreases from 8.614 to 8.604 Å with the increase of quantity of Aluminium. The M-O oscillations at octahedral and tetrahedral sites are confirmed by Fourier transform infra-red spectroscopy. Dielectric studies are performed by using impedance analyzer within frequency range 1 MHz–3 GHz. Dielectric constant is prominently affected with Aluminum substitution. It attained 16.1 value at 2.3 GHz for $Cu_{0.7}Ni_{0.3}Fe_{1.7}Al_{0.3}O_4$. Furthermore, $Cu_{0.7}Ni_{0.3}Fe_{1.7}Al_{0.3}O4$ showed maximum dielectric loss of 0.4 at 2.5 GHz and the quality factor is enhanced up to 1500 with doping of Aluminum at quantity of $x = 0.3$. The best dielectric behavior of the material indicated that they are strong candidates for high-frequency devices as well as super-capacitors.

Sodium alginate derived silane crosslinked hydrogels to study angiogenic potential and wound healing efficacy in chick and mouse models

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Silane crosslinked biopolymer based novel pH-responsive hydrogels were fabricated by blending the anionic sodium (alginate) with poly(ethylene glycol). Tetraethoxysilane (TEOS) was used, as a crosslinker due to its nonhazardous nature. Different concentrations of PEG 600 was used to study its impact on physical and chemical properties of the prepared hydrogels along with the controlled release of drug. This study comprised of three basic phases: fabrication of hydrogels coupled with characterization, to assess the angiogenic potential along with toxico-pathological effects of hydrogels in chick embryos and to check wound healing efficacy in mouse model. The prepared samples were characterized and analyzed by FTIR, SEM, TGA, DSC, swelling response in water, buffers and electrolyte solutions. Chorioallantoic membranes (CAM) assay was performed to study *in-vivo* angiogenesis and toxicological analysis through implanting prepared hydrogels on chorioallantoic membranes of developing chicks at 7^{th} day of incubation. Gross pictures were taken and embryo were recovered at day 9^{th} and 14^{th} of incubation for further analyses (morphological and histological). Amniotic fluid sampling was done to perform the enzymatic assays. Finally, Full thickness wounds were excised on mice dorsolateral skin to assess the wound healing effect of hydrogels by measuring wound contraction. Lidocaine (LDC) was successfully loaded on suitable hydrogel to study its release mechanism. The in vitro drug released profile was examined in simulated gastric fluid (SGF), simulated intestinal fluid (SIF). LDS was released in a controlled way up to 87% in 80 min. This study reported that the addition of PEG 600 to alginate biomaterials using TEOS cross-linkers remarkably improved angiogenesis and accelerated wound healing in chick and mouse models, respectively. These results endorsed that the hydrogels could be practiced as a smart intelligent material for controlled drug delivery at physiological pH, as well as for other biomedical applications i.e. wound healing, and tissue engineering.

Versatile applications of bi metallic metal organic framework

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Metallic organic frameworks are formed by the combination of metals and organic linkers. They may be mono metallic, bi metallic or tri metallic. They are also known as coordination polymers. They have gained much importance not only in chemistry but also in different fields due to their properties like porosity, thermal stability, exceptional morphology, durability and lower density. Bi metallic metal organic framework can be used in a variety of applications like anti microbial activity, dyes adsorption, waste water treatment, photo catalysis, gas adsorption, bio sensors, drug delivery etc. Present study deals with the versatile applications of a bi metallic metal organic framework. A bi metallic copper zinc MOF synthesized by solvothermal method was applied in anti microbial activity and dyes adsorption. Bi metallic MOF was synthesized by using benzene dicarboxylic acid (BDC) as liner and copper and zinc as metals. This MOF was used in anti bacterial activity. Minimal inhibition concentration (MIC) was performed by using MOF against gram positive and gram negative bacteria. Test tubes were taken with bacteria and minimal quantity of MOF added in different ppm solutions. Change of clouded to clear solution indicated bi metallic MOF (0.018 gram) has shown anti bacterial activity. Zone of inhibition method was also applied to confirm anti bacterial activity. Bacteria were added in Petri dishes and holes were made to add different ppm solution with MOF (0.015 gram) in bacteria. Appearance of grayish zones confirmed that MOF is efficient against anti bacterial activity and can be used in bio medical applications. Bi metallic MOF was also used for dyes adsorption. Two dyes i.e. Reactive golden and Reactive black were absorbed by using MOF (0.003 gram). UV results confirmed that by increasing time duration dyes are absorbed to a greater extent. Hence bi metallic MOF are efficient to perform different applications in different fields.

Amazing biotransformational derivatives of dydrogesterone

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Biotransformation is one of the well-known methods to obtain biologically active compounds in which pure enzymes, partially pure enzymes, whole cell cultures of plants, animals or 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. Biotransformation of dydrogesterone (**1**) by using human volunteers and animals, fermentation with cell suspension cultures and fermentation with fungal cultures afforded amazing derivatives **2**-**16**.

We obtained two derivatives by incubation of dydrogesterone (**1**) with *Gibberella fujikuroi* using standard two-stage fermentation protocol with interesting biological activities. Structures of these metabolites were deduced through modern spectroscopic techniques.

Green Synthesis, Characterization and Cholinesterase Inhibitory Potential of Gold Nanoparticles

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Delphinium uncinatum and Erythrophyleum guineense plants extracts were used for the green synthesis of gold nanoparticles. The SEM study showed the synthesis of gold nanoparticles of E. guineense (GE) and D. uncinatum (GN) below 100 and 300 nm, respectively. The gold nanoparticles of E. guineense (GE) has irregular sound shape while D. uncinatum (GN) has cylindrical shape showed by the micrographs. Similarly, the XRD spectra showed peaks at about 38.1°, 44.43°, 64.6° and 77.64° can be indexed to (111), (200), (220) and (311) orientation, respectively, which confirmed the synthesis of gold nanoparticles. It means that the synthesized gold nanoparticles of E. guineense (GE) and D. uncinatum (GN) are crystalline in nature. It was confirmed by UV/visible spectra that both plant extracts reduce the gold slat and as a result high quantity of gold nanoparticles were formed and confirmed by EDX spectroscopy. In this study, the gold nanoparticles of E. guineense (GE) and D. uncinatum (GN) were screened out for their in-vitro cholinesterase inhibitory activity in concentration ranging from 62.5 to 1000 µg/mL, which showed excellent inhibitory activity.

Antimicrobial activity of coal derived fulvic acid

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Fulvic acid is a subclass of different compounds recognized as hemic substances, which are by-products of organic deterioration from microorganisms. Fulvic acid is low molecular weight fraction of coal has high solubility in water. Different locally present coal samples were studied to extract fulvic acid. Fulvic acid is found abundantly in peat, weathered coal, lignite, and other humified substances. Fulvic acid contains mixture of closely related compound aromatic polymers with the presence of aromatic rings, quinone carbonyl, ketone carbonyl, carboxyl, phenolic hydroxyl, and alkoxyl groups. Extraction and purification of crude fulvic acid were optimized for different physico-chemical variables. Moreover, to evaluate the bio efficacy of extracted samples of fulvic acid in-vitro antimicrobial activity of fulvic acid was studied against different pathogens e.g., *Macrococcus, Escherichia coli, Bacillus subtilis, Aspergillus flavus & Aspergillus Niger*. The fulvic acid has an antimicrobial spectrum wider than any recommended antibiotic; it acts synergistically with the ciphlofloxin. Fulvic acid salts, esters, or derivatives in pharmaceutical arrangements are operative for treating inflammation, eczema, acne, bacterial or fungal infections.

Synthesis, characterization and application of starch phosphate-*g*-polyacrylic acids as adsorbents for removing ammonia and phenol

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Starch phosphate was prepared by treating starch with monosodium phosphate (NaH_2PO_4) and disodium phosphate (Na_2HPO_4) at 170℃. This starch phosphate was further treated with different amount of acrylic acid in the presence of potassium persulfate (KPS) to prepare three different types of starch phosphate-*g*-polyacrylic acids (SP-*g*-PAA1, SP-*g*-PAA2 and SP-*g*-PAA3). These SP-*g*-PAAs were then characterized by proton nuclear magnetic resonance (^{1}H NMR) and Fourier transform infrared (FT-IR) spectroscopy. Integration results of the ^{1}H NMR spectra of the SP-*g*-PAAs showed that SP-*g*-PAA3 had the highest amount of PAA, followed SP-*g*-PAA2 and SP-*g*-PAA1, respectively. Crystallinity of starch, starch phosphate and the SP-*g*-PAAs was checked from their x-ray diffraction XRD analysis. The XRD analysis showed that starch phosphate and SP-*g*-PAAs had amorphous nature which revealed that starch has lost its crystallinity after modification. The thermal properties of the modified samples were checked by thermogravimetric analysis (TGA) and differential thermal analysis (DTG) which also confirmed the successful grafting of PAA on starch phosphate. Finally the SP-*g*-PAA1, SP-*g*-PAA2 and SP-*g*-PAA3 were utilized for ammonia and phenol adsorption. SP-*g*-PAA3 which had the highest PAA content, showed the highest adsorption efficiency towards ammonia and phenol (ammonia; 7.47 mmol/g and phenol; 1.02 mmol/g) which was followed by SP-*g*-PAA2 (ammonia; 5.73 mmol/g and phenol; 0.9 mmol/g) and SP-*g*-PAA1 (ammonia; 2.33 mmol/g and phenol; 0.61 mmol/g). These adsorbents could effectively be used as additives in cigarette filter to reduce the concentration of these harmful ammonia and phenol in the cigarette smoke.

Non enzymatic Electrochemical Sensor based on Tin Oxide Nanostructures for Simultaneous determination of two Vitamins

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In this study, we report a simple and easy procedure for the fabrication of electrochemical sensor for simultaneous determination of two essential vitamins; Vitamin C and Vitamin B_6 using Tin oxide (SnO_2) nanoparticles. We opted a facile synthesis route for the fabrication of SnO_2 nanoparticles. The synthesized material was characterized through FTIR, XRD, EDS, TEM and SEM analysis to evaluate different functionalities, crystalline structure, material purity and morphological texture of SnO_2 NPs. For the evaluation of charge transfer kinetics, the prepared material was exploited for electrochemical characterization via cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) which exhibited excellent conductive behavior of SnO_2 NPs. For the first time, the capability of SnO_2 NPs was investigated in simultaneous determination of VC and VB_6 through the modification of glassy carbon electrode (GCE) using Nafion® as sandwich between material and the base electrode. The SnO_2/ Nafion®/GCE showed exceptional response in the simultaneous determination of VC and VB_6 under optimized parameters such as scan rate 70 mV/s, potential range from -0.6 to 1.4 V and PBS pH 7.0 as supporting electrolyte. Under the linear dynamic range from 10 to 140 µM for AA and 5 to 120 µM for VB_6, the SnO_2/ Nafion®/GCE displayed low limit of detection calculated as 0.067 and 0.048 µM for AA and VB_6. The prepared nano electrochemical sensor retained reliable stability, good reproducibility and anti-interference behavior in real sample analysis. The analytical applicability of SnO_2/ Nafion®/GCE was investigated in different pharmaceutical formulations with acceptable percent recoveries.

Effect of temperature, and concentration on potentiometric titrations of chitosan and its based biosorbents

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The present work focuses on the characterization, potentiometric titration studies of a novel and efficient chitosan based biosorbents. The surface structure of the chitosan and its based bio sorbents were identified and characterized by X-ray diffractometry (XRD), FTIR spectroscopy, point of zero charge (PZC), scanning electron microscopy (SEM) coupled with energy dispersive X-ray analyses (EDX). A comprehensive study of the potentiometric titrations of chitosan and its based biosorbents in the presence of Na^{+}, Cd^{2+}, Zn^{2+}, Ni^{2+}, Pb^{2+}, Cu^{2+}, were conducted under different experimental conditions of temperature, concentration and pH. The affinity of metal cations evaluated from the potentiometric titration data was found to be divalent transition metals higher than alkali metal. The deprotonation of chitosan and other based biosorbents was observed to be dependent upon the concentration, temperature of metal cations present in the system.

The changes in enthalpy (ΔH) and entropy (ΔS) connected with the surface deprotonation of the chitosan/electrolyte interface were measured. Thermodynamic parameters showed that the positive value of enthalpy was the driving force for the deprotonation of the chitosan and other biosorbents surface.

Effect Of Clarified Rice Syrup On Quality Of Glutenfree And Sugar-Free Bread

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Clarified rice syrup is a good sugar replacer for sugar free bread. Gluten-free products may reduce the risk of diabetes and can also be helpful in minimizing celiac disease. The products made from clarified rice syrup and gluten free flour have less moisture content that helps to increase the shelf life of products due to minimal microbial attach and improve its nutrition and quality. Four different formulations were prepared, characterized, and compared with a control using standard methods. Selected physico-chemical properties, texture profile analysis, sensory evaluation, and stability studies were done. Specific loaf volume of bread, protein and carbohydrate contents were significantly decreased, whereas ash and fat contents were significantly ($P<0.05$) increased with the addition of clarified rice syrup in comparison to the control. Texture profile analysis revealed that hardness, gumminess, and chewiness were increased while cohesiveness was decreased when clarified rice syrup was added. The results of sensory analysis showed that the taste attribute of the bread was significantly increased ($P<0.05$) with the addition of clarified rice syrup. The results obtained were promising with the addition of clarified rice syrups as a substitute of sucrose in gluten free bread with improved physico-chemical properties and acceptable.

Effect of temperature, pH and concentration on adsorption studies of chitosan mixed cellulose biosorbent

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The use of biopolymers such as chitin, chitosan & cellulose are particularly important because of their unique biological properties including non-toxicity, biodegradability & biocompatibility. the aim of this study was the development of chitosan-based bio-sorbent in combination with cellulose to form composite adsorbent beads for adsorption purpose at various pH (6, 6.5, 7, 7.5) & temperature ranges(303, 313 and 323 K). The physicochemical properties were characterized by FTIR (Fourier-transform infrared) spectroscopy), SEM (scanning electron microscopy), XRD (X-ray diffraction), DSC(Differential Scanning Calorimetric), The method used for synthesis of the beads by using the solvent of NaOH.. The adsorption studies were conducted under optimum concentration for maximum yield of beads. The different adsorption models were applied on experimental data and Langmuir model was better fit due to higher regression coefficient values. The adsorption extent showed that the developed blend beads could be applied as adsorbent for the metal removal from industrial contaminated water.

Assessment of selected heavy metals contamination and its sources in urban soil and ground water of district Hyderabad, using GIS and multivarient analysis

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To investigate influence of soil-water, rock-water interaction on the quality of ground water, soil, rock and ground water samples were collected from district Hyderabad. A total 415 soil and 118 ground water sample were collected from of district Hyderabad.from areas with buildings, roads, and other structures. Spatial maps of elements were prepared using GIS software which highlighted the hotspots of metal contamination from various environmental sources, the highest concentration of Zn (125.1 mg kg^{-1}) and Pb (76.4 mg kg^{-1}) was found in city center which suggested traffic emission mostly from the vehicle smoke and other contamination sources. Moreover, the second highest concentration of Pb was observed in the surface soil associated with the Phulleli canal, passes through the Hyderabad city, which is under threat of waste material disposal because of anthropogenic and industrial activities. In case of Ni, three hotspots were observed including the industrial area of Hyderabad, the city Centre and the Phulleli canal with the average concentration of 57.0 mg kg^{-1}. Ground water samples from district Hyderabad, Pakistan were collected to study the concentration of 10 elements including potential hazardous elements to evaluate their natural and anthropogenic origin and their possible effects on living organisms including human health. Risk assessment was quantified by the hazard quotient (HQ) and cancer risk for both adult and child. The non-carcinogenic risks as depicted by HQs of all the metal(loid)s were below the recommended HQ threshold of 1 for both child and adult. The potential risks and combined effect of all metal(loid)s through ingestion of groundwater was assessed using hazards index (HI). The carcinogenic risk assessments in this study were based only on concentrations of As, Cd and Cr in groundwater.

Synthesis, characterization and optical properties of novel PPy/MnO_2 composite

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The oxidant ferric chloride was used to synthesize polypyrrole from pyrrole monomer. The FTIR and UV-visible spectroscopy were used to characterize the synthesized polypyrrole. FTIR spectra of polypyrrole exhibits all of its distinctive peaks, including 3304 cm^{-1} (C-C stretching vibration), 623 cm^{-1} (C=C stretching vibration), 1437 cm^{-1} (C-N stretching vibration), 1272 cm^{-1} (C-H stretching vibration) and 1150 cm^{-1} (C-C stretching vibration). Polypyrrole has an absorption peak at 439 nm according to UV-visible analysis. The nanosheets of MnO_2 were prepared by the chemical reaction of HCl, $KMnO_4$ and Sodium dodecyle sulphate. The synthesized nanosheets of MnO_2 were characterized by FTIR and UV-visible spectroscopy. The FTIR analysis of MnO_2 nanosheets shows Mn-O vibration peaks at 972 cm^{-1}, 1553 cm^{-1} and 2985 cm^{-1}. UV-visible study of MnO_2 nanosheets shows absorption at 371 nm. The nanocomposite of PPy/MnO_2 was prepared by the reaction of pyrrole, ferric chloride and MnO_2 nanosheets. The FTIR and UV-visible spectra displayed all of the nanocomposite's distinctive peaks, including 510 cm^{-1} (Mn-O vibration), 1184 cm^{-1} (C-C stretching vibration), 1294 cm^{-1} (C-H stretching vibration), 1476 cm^{-1} (C-N vibration) and 1549 cm^{-1} (C=C stretching vibration), and 393 and 444 nm, respectively.

Synthesis and Optical Investigation of Sodium Dodecylsulfate andPerchloric Acid Doped Polyindole Salt via Benzoyl Peroxide as Oxidant

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In this work, double doped PlN-SDS-$HClO_4$ salt was successfully prepared by chemical polymerization process at room temperature. The indole monomer was polymerized using benzoyl peroxide (BPO) as oxidant whereas perchloric acid ($HClO_4$) and sodium dodecyl sulfate (SDS) were used as dopants. The structural composition as well as incorporation of SDS and $HClO_4$ into PlN chain was confirmed through FTIR analysis. The polymerization of indole into PIN-SDS-$HClO_4$ salt and its optical properties were investigated through UV-Vis spectroscopic technique. The modified electronic band structure was confirmed via Tauc plots and band gap energy values. The least optical band gap of PIN-SDS-$HClO_4$ salt was found to be 2.44 eV. Additionally, the influence of different concentration of BPO on the percent yield, structural composition, and optical properties of PlN-SDS-$HClO_4$ salt was evaluated. The maximum percent yield obtained for PlN-SDS-$HClO_4$ salt is 33.66%.

Mineral Elements Composition And Dpph Free Radical Scavening Activities Of Acetonic Extract Of FENUGREEK

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The proximate analysis, phytochemical screening, metallic screening, and antioxidant properties of aqueous and acetonic extracts of Fenugreek were investigated in this work. Moisture, ash, total acidity, and pH of Fenugreek were found in proximate analysis to the nutritional profile of Fenugreek aqueous extract (moisture, ash, pH, and total acidity). All of the outcomes were expressed in the percentage. Moisture and ash content were determined to be 43.3% ± 0.19% and 39.42% ± 0.7%, respectively. Total acidity (0.12% ± 0.01%) and pH (6.39% ± 0.9%) were also investigated. Saponins, carbohydrates, phenolic compounds, flavonoids, protein & amino acid, phytosterols, gum & mucilage, and tannins were detected in selected neutraceutical plants using phytochemical screening. The presence of alkaloids, saponins, tannina, gum & mucilage, carbohydrate, phytosterols, protein and amino acida, and flavonoids was confirmed in the aqueous extract of Fenugreek seeds. However, the findings for glycoside detection were negative. The atomic absorption spectrophotometer (AAS) and flame photometer were used to conduct a quantitative mineral analysis of F. Greek seeds for the detection and quantification of five metals, including (Ni, Cu, Zn, Fe, and Mn). The findings indicated that the metals tested were present in varying quantities. Fe has the greatest concentration (0.856 ± 0.0082 ppm), followed by Ni (0.551 ± 0.026 ppm). Mn had the lowest concentration at 0.036 ± 0.0047 ppm, followed by Zn at 0.067 ± 0.0159 ppm, while Cu was not detected. Antioxidant activity of Fenugreek acetonic extracts was determined at various concentrations (250, 125, 50, 25, 10, and 5 µg/mL in ethanol). Antioxidant activity was found in the acetonic extract of Fenugreek, with values of 62.42 ± 0.81 µg/mL. Rutin was used as a reference for the plant extract, and it showed activity of 15.12 ± 0.32 µg/mL.

Synthesis of flurbiprofen derivatives and their biological activities

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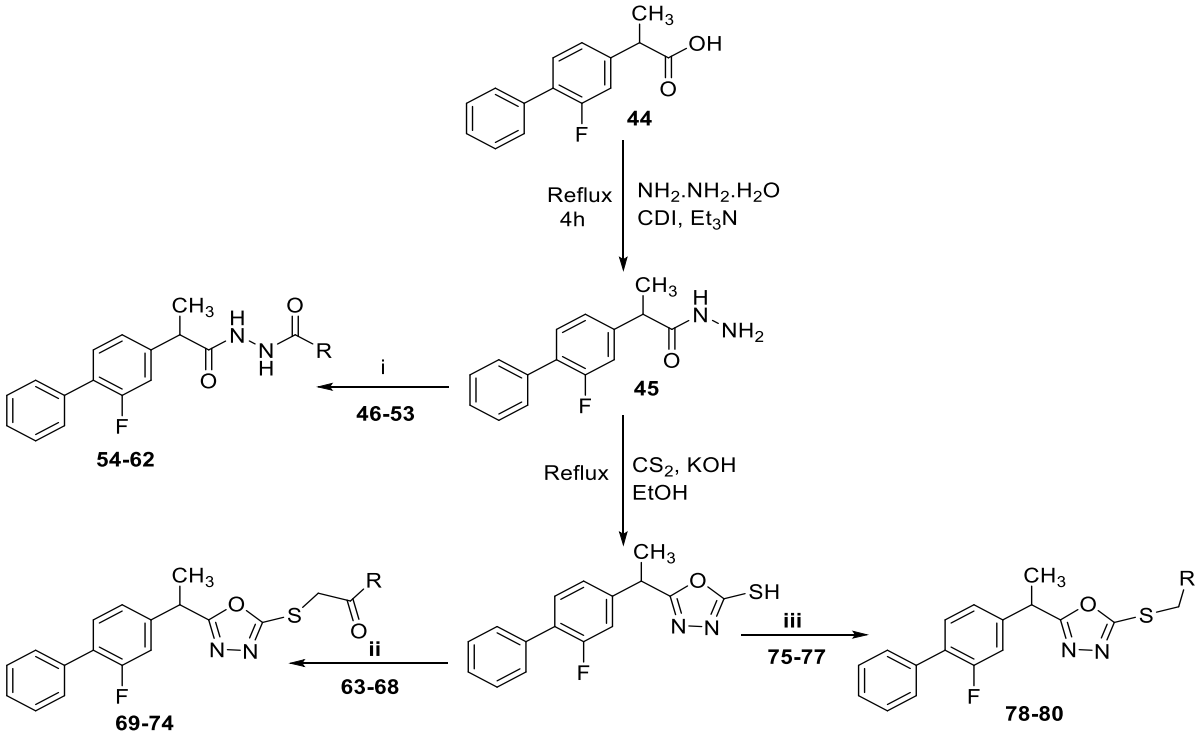
Flurbiprofen derivatives **1-18** were synthesized by two step reaction. First step was hydrazide synthesis followed by oxadiazole formation. Synthetic compounds were characterized by spectroscopic techniques such as ^{1}H-NMR and EI-MS. Compounds were screened for their α-amylase activity. Most of the compounds showed excellent α-amylase activity.



i) Substituted Benzoyl Chloride, Pyridine Refluxed 8-10 hrs. ii) Phenacyl Bromide, EtOH, K_2CO_3, Refluxed 15-20 hrs. iii) Benzyl Chloride/Bromide, K_2CO_3, EtOH, Refluxed 4-5 hrs.

Scheme: Synthesis of 1, 3, 4 -oxadiazole derivatives **1-18**

Evaluate the impact of oil well drilling activities on vanadium contents in soil, ground water, vegetables, fruits and feed crops: Impact on human

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The global use of petroleum hydrocarbons for energy and raw materials in various applications has increased with extensive release of a wide variety of contaminants into the environment, affecting soil, groundwater and translocation to vegetation. The population near by the petroleum industries can be effected due to contaminate environment of heavy metals including vanadium.

The dispersal of vanadium (V) in water, soil, vegetables, fruits and animal feed sampled from the nearby area of oil well drilling fields (saman-1 and saman-2) of the district Tando Allayar, Sindh Pakistan has been carried out. For comparative determination, same environmental (water and soil), vegetable, fruits and animal feed samples were collected from agricultural land (nonindustrial area), termed as control samples. The total and bioavailable forms of V was determined in soil. The V in vegetable, grass, fruit and biological samples (scalp hair and blood) was determined by electrothermal atomic absorption /ICP OES, after acid digestion. The ooccupational exposure to vanadium was evaluated in refinery worker population resided in nearby villages as exposed, whereas for comparative purposes office workers of metropolitan city without any industrial exposure were selected.

Novel fluoride selective voltammetric sensing method by amino phenylboronic acidzirconium oxide nanoparticles modified gold electrode

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A novel fluoride selective voltammetric method has been developed by using the 3-aminophenylboronic acid (APBA)-zirconium oxide (ZrO2) nanoparticles modified gold (APBA-ZrO2- NPs/Au) electrode for sensitive detection of F- at trace levels in water and toothpaste. A coprecipitation approach was applied to synthesize ZrO2 nanoparticles (ZrO2-NPs) using Salvadoraoleoides leaves extract and characterized by UV-Visible spectroscopy, Fourier transform infrared (FT-IR) spectroscopy, Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), and X-Ray Diffraction (XRD) for morphological and structural analysis. The APBA-ZrO2-NPs/Au electrode was fabricated by coated of ZrO2-NPs on the surface of Au electrode by drop costing method followed by electrochemical polymerization of APBA. The reduction response of peak current of potassium ferricyanide was achieved by the interaction of the phenylboronic acid with F-to produce the boronate anions. Thus, the method was optimized in detailed for successive electrochemical detection of F-. Two linear relations were observed in reduction peak current and logarithm of F- concentration in the range of 1.0×10–9 – 3.0×10–4 M and 3.0×10–4 – 1.0×10–2M, respectively. The limits of detection (LOD) and limit of quantification (LOQ) were calculated as 3.0×10–10 and 1.0×10–9 M, respectively. Interference of other competing anions, including chloride, bromide, iodide, acetate, sulphate, carbonate, and nitrate, was also investigated. Furthermore, the developed APBA-ZrO2-NPs/Au was employed to the fast detection, wide range of response, and high selectivity of F- in water and toothpaste samples.

Impact of heavy metals on rice varieties by different fertilizers

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The current study is designed to assess the physicochemical characteristic like (pH, electrical conductivity (EC), bulk density (BD), salinity, organic matter (OM), and total nitrogen (TN) and heavy metals (Cd, Cr, Ni, and Pb) in rice farmland amendments with synthetic fertilizer (SF) and organic synthetic fertilizer (OSF) followed by the phytoextraction capacity of minerals by different rice varieties of upper Sindh. Similarly, the changes in the phytoextraction capacity of minerals by selected rice varieties are also evaluated at different growth stages will also be evaluated. Different varieties of rice such as Super 515, Diamond, Anmol, Guard 50, Guard LP 18 and Komal crops growing on synthetic fertilizer (SF) and organic synthetic fertilizer (OSF) paddy soil, and irrigation water were collected from different rice farmlands in Upper Sindh region of Pakistan (Kashmore, Tangwani, Kandhkot and Buxapur). The bulk density was found higher in paddy soil amended with synthetic fertilizer (SF) as compared to the soil amended with organic synthetic fertilizer (OSF). The decrease in BD in soil amended with OSF may be attributed to the OM, which may be increased due to the application of livestock manures. pH, EC, OM and TN were found to be lower in paddy soil amended with SF and compared to paddy soil amended with OSF. Input of heavy metals (Cd, Cr, Ni and Pb) were found lower in paddy soils amended with synthetic fertilizer (SF) as compared to the organic synthetic fertilizer. Whereas the input of heavy metals by irrigation water in case of SF and OSF rice fields were same because of the application of same river water. The concentrations of Cd, Cr, Ni, and Pb were found lower than the recommended values set by food and agriculture organization (FAO) in the irrigation water. Thus, input of heavy metals from irrigation water is very low. The heavy metal concentration in different parts of rice crops were higher in rice varieties grown on the soil amended with OSF at different stages as compared to those rice varieties grown on the soil amended with SF except stage three, which did not show a significant difference ($p < 0.05$).

Kinetics Of The Thermal Decomposition Of Catalyzed And Un-Catalyzed Polylactic Acid

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With world modernization, the usage of fossil fuel has been increased day by day, due to which their reservoir decreases rapidly. So, it is the prime focus of researchers to get energy from renewable resources. One of the main target is to degrade waste material i.e. biomass and plastic waste and to convert it into fruitful products. In present study Polylactic acid was thermally decomposed in the temperature range of 300 ºC to 360 ºC using thermogravimetry and pyrolysis gas chromatography-mass spectrometry. The oil was extracted, which was characterized using GC-MS and FTIR. To know the kinetic parameters i.e. collision frequency and activation energy, TG analysis was carried out of polylactic acid with and without molecular sieve as catalyst and kinetics parameters were determined using Kissinger method. The properties of oil obtained were compared with commercial fuel and was found comparable. Therefore, the study would have potential application in industries if implemented on commercial scale.

Synthesis of functionalized carbon material for the catalytic degradation of selected organic contaminants

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Environmental pollution is becoming a global issue with the rapid development of industrialization. Endocrine disrupting compounds (EDCs), a diverse class of emerging contaminants, have been recently detected in natural water. In the past few decades, the exploration of various photo-catalysts for splitting of water, degradation of organic contaminants and reduction of CO2 is one of the significant strategies for solving energy crisis, global environment pollution and climate change. Therefore, developing new efficient photo-catalyst and broadening the scope of photo-catalyst response became a hot research topic in the field of environmental photo-catalysis. This research work is based on the synthesis of functionalized graphene based material that can work as heterogeneous photo-catalyst for the degradation of selected organic compound (BPA as the model compound). Bisphenol A (BPA), also known as 2,2-bis-(4-hydroxyphenyl) propane or 4,4′-isopropylidenediphenol, is used for the production of various polycarbonate and polysulphone plastics and epoxy resins. In this study, we have synthesized expanded NiSO4 intercalated GO flowers (NiSO4 Int. GO flowers) for the degradation of endocrine disrupting organic contaminants. Bisphenol A (BPA) was degraded photo-catalytically by synthesized NiSO4 Int. GO composite under UV light. The synthesized expanded NiSO4 Int. GO flowers presented high photo-catalytic activity for 100% degradation of BPA at pH 4 within 20 min. The morphology of synthesized material was characterized using SEM, XRD and BET and composition of synthesized NiSO4 Int. GO flowers was characterized by using FTIR. These findings are crucial for designing GO-based photocatalysts with high performance for degradation of persistent organic pollutants in wastewater and potable water.

Nutritional Profiling of Vegetables Grown in Larkana Division

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Vegetables are the fresh edible parts of herbaceous plants that offer vital nutritional elements that may be used to help the body generate and repair itself. Vegetables are important for keeping the body's alkaline reserve healthy, mainly for their high carbohydrate, phytochemicals, and mineral contents. In this study, five selected vegetables were collected from the Larkana division, such as Spinach, Brinjal, sponge gourd, Lotus root and Okra studied to assess their proximate analysis and mineral composition. Proximate analysis of all the selected vegetables revealed that the moisture contents, ash, fat, and fiber in vegetables ranged 90.5 – 65.7, 7.7 – 1.66, 3.39 – 0.550, and 16.7 – 2.05 %, respectively. The contents of Ca, K, Mg, and Na in vegetables were ranged from 0.42 – 0.16, 1.68 – 0.07, 5.66 – 1.50, 1.99 – 0.81 mg/g, respectively. Whereas the Fe, Zn, Cu, Mn, and Cr levels were observed in between 20.8 – 3.9, 7.42 – 2.07, 12.0 – 2.00, 28.9 – 1.81, 5.11 – 1.61µg/g, respectively.

Leaching of phthalates from plastic packaging into juices

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In present study an attempt is made to study the leaching of PAEs from plastic packing into juices. After market survey different brands of juices such as Nestle, Polly, Maza, Cappy, Joiner, Smile, Mogu Mogu and so on were collected and labeled without brand identity in order to full fill ethical issues. Total 45 samples (15×3) were collected and analyzed. The juices were classified as citrus, stone, mix fruit, berry and fleshy fruit juices. Leached PAEs were extracted with dichloromethane and further cleaning up procedure was also performed for juices with silica gel packed column. In addition plastic bottles were also analyzed by FTIR for characterization. Results indicate that all juices were acidic with pH ranges from 2.25 to 3.73. Gas Chromatographic analysis showed that extent of leaching was different among brands; mix fruit juices showed more PAEs leaching (71.93µg/L) followed by strawberry juices (31.35 µg/L), citrus fruit juices (20.64 µg/L) and fleshy fruits juices (18.61µg/L). Overall studies indicate that juice packed in plastic bottles are more prone to phthalate leaching owing to acidic pH and high temperature exposure in our Country, therefore phthalate should be replaced with other plasticizers.

Pyrolysis Behaviour Of Karanja (*Pongamia Pinnata* L.) Seed Press Cake: Evaluation Of Abandoned Anthill As Catalyst

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Fossil fuel supplies are rapidly depleting as a result of increasing industrialization and population. Furthermore, excessive usage of fossil fuels has led to the release of a variety of harmful gases as well as global warming. As a result, it is necessary to seek for inexhaustible, renewable, and environmentally friendly energy sources. In this study, bio oil was produced from the pyrolysis of karanja seed press cake without and with a catalyst. The anthill used as a catalyst in this study was collected from the local area and characterised by SAA, EDX, SEM, XRF and XRD. The pyrolysis experiment was carried out without and with an anthill catalyst in an indigenously made furnace in an inert atmosphere at a temperature range of 310 to 400^{o}C. The pyrolysis oil was collected at an optimised temperature from the experiment and analysed through GC-MS and FTIR. The compounds identified for the obtained bio-oil from non-catalytic pyrolysis were in the range of C_5 to C_{19} while the compound identified for bio-oil obtained from catalytic pyrolysis were in the range of C_2 – C_{63}. Furthermore, TG analysis of the karanja seed press cake without and with anthill was carried out at different heating rates of 3, 12, 20, and 30^{o}C/min.TG and DTG of karanja seed press cake showed four step weight loss in the temperature range of 30-800 ^{o}C. Kinetics parameters were determined by applying different kinetic equations i.e. Kissinger-Akahira Sunose, Friedman, and Kissinger equations. The average activation energy for non-catalytic reaction was calculated from KAS and FM models as108.101 and 120.553 kJmol^{-1} while the frequency factor calculated were 6.75 x10^{16}and 9.01 x10^{10} min^{-1} respectively. The average activation energy was reduced to 95.2547 and 104.51 kJmol^{-1} respectively by loading a catalyst to a sample while the frequency factor were calculated as 1.51 x10^{10}and 3.48 x 10^{12} min^{-1} respectively. Kissinger equation gave activation energy values for hemicelluloses, cellulose and lignin as 99.768, 182.908, and 199.536kJmol^{-1} without catalyst and with catalyst it was lowered to 74.826, 83.14, and 108.08kJmol^{-}. So, from the results, it was concluded that the catalyst played a key role in lowering the activation energy for the pyrolysis reaction. Comparing catalytic pyrolyzed products with non-catalytic products of karanja seed press cake revealed that catalyst has great impact by not only lowering the pyrolysis temperature as well activation energy but also increased the number of compounds with enhanced quality of bio-oil.

Synthesis of functionalized graphene based composites and their application in water purification

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Although about 71% of the Earth's surface is covered by water, only 3% is fresh water which is also contaminated by organic and inorganic pollutants due to human activities. Especially, the surface water bodies are contaminated with various treated or untreated effluents from different resources. This problembecomes more acute with less developed countries owing to the lack of resources and civic management. Recently, Graphene oxide due to its many promising properties has been introduced as a unique material and has received considerable attention in the scientific community. In the field of adsorption, Graphene oxide based materials show effective adsorption and removal capacity for the organic pollutants from aqueous media. So, in this study we have made an attempt to synthesize Grapheneoxide Based Composite (GOBC) to remove EDCs from aquatic environment. In orderto investigate the sorption potential of synthesized material;fixed-bed column experiments were performed for the removal of most injurious EDC Bisphenol A (BPA).The fabricated materials were characterized by FTIR, SEM, EDX, BET and XRD.Bed-column experiments were conducted to study the effects of important parameters such as column bed depth in the range of 0.1 to 0.4 cm, flow rate in the range of 0.5 to 1 mL/min and concentration of BPA in the range of 200 to 300 ppm. Different models like Adam-Bohart model, Thomas model and Yoon-Nelson model were applied to the experimental sorption data. The sorption data fitted well withThomas and Yoon–Nelson models. The prepared GOBC showed good sorption capacities for BPA with excellent kinetics.

Pharmacophore modelling of Urease Inhibitors by In-Vitro, Kinetics and Molecular docking Approach

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The ureases are important class of enzyme which occur in jack beans, soybeans, and seeds of other plants. These are also found in some animal tissues and microorganisms which lived in the intestine of living organism. It is very harmful to mammals due to over production of ammonia. The sources of urease are different bacteria in mammals, which are found in the intestine of mammals like humans. Urease plays major role in the intensification of *H. pylori* poison. It catalyses the reaction in which, conversion of urea into carbon dioxide and ammonia occur. It has also ability to neutralize gastric acid and stop the infection of *H. pylori* which occurs at lower pH in the stomach of humans. The synthetic approaches towards the production of urease inhibitors give new way to control disorders associated with urease. Natural and synthetic clinical entities are major contributor to overcome the hyperactivity of the enzyme. The main purpose of this research is to determine the new inhibitors of urease and to check their mechanism of action. For this purpose, high-throughput mechanism is carried out which is based upon spectro-photometric assay procedure. The new inhibitors both natural and synthetic can be used for the treatment of number of diseases caused by the rapid action of urease enzyme.

Porous Silica Monolith Activated Carbon Composite for the Adsorption of Cadmium and Mercury

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Porous silica monolith particles were synthesized by the renovated sol-gel process using the sophisticatedly controlled heating steps and nitrogen environment. The silica particles were coupled with activated carbon using 2-aminopropyl triethoxysilane as the cross binding agent. The resultant composite was thoroughly investigated using the Scanning electron microscopy, Field transmission infra-red, and X-ray diffraction which confirmed the formation of silica monolith@activated carbon composite. The newly synthesized composite was evaluated for the adsorption of cadmium and mercury which come up with excellent results Ca. 98.5% adsorption of cadmium. A method was also developed for the detection of mercury using the N-phenylbutan thioamide as the ligand.

Adsorptive Removal of Imidachlopiride and Carbofuran Pesticides Using the Silica Monolith Anchored Graphene Oxide

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Partially porous silica monolith materials were synthesized by the acid catalyzed sol-gel process while the graphene oxide sheets were synthesized by the hummer's method. The silica particles were anchored upon the surface of graphene oxide sheets by the one step procedure using the esterification protocol. The resultant materials showed excellent resulted when used as adsorbents for the removal of imidachlopiride and carbofuran. X-ray diffraction, Field transmission infra-red, and zeta potential were carried out as the characterizations for the newly synthesized materials. The thermo kinetic and thermo dynamic studies were carried out. The adsorption of both the pesticides followed the Freundlich isotherm. All the key parameters of adsorption were optimized for the best output of the adsorbent materials.

Low Cost Adsorbent for The Removal of Dye from Waste Water

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Dyestuff production units and dyeing units have always had a pressing need for techniques that allow economical pre-treatment for color in the effluent. The effectiveness of adsorption for dye removal from waste waters has made it an ideal alternative to other expensive treatment options. In the present study, the kinetic of the adsorption of two dyes; methylene blue and Congo red onto activated almond shell has been explored. The result the equilibrium time for the adsorption of methylene blue Congo red was attained in 1 hour. The data obtained from kinetic interpretation using Elovich, Bingham and intrapartickle diffusion models show that the adsorption of dyes on almond shell fitted to linear equation from which it is concluded that the adsorption process is a diffusion controlled process and can be effectively used as potential adsorbent for removal of Congo red and methylene blue with higher adsorption effectively.

Synthesis of Selected Acetylcholinesterase Inhibitors Based on Benzimidazole-2-Thiol Nucleus

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The focus of our research was to explore *in silico* anti-acetylcholinesterase potential. Initially a library of 360 benzimidazole-2-thiol(2-MBI) based acylhydrazone ligands was built and subjected to virtual screening. The library was reduced to only 5 ligands after analyzing the physicochemical properties and binding affinities to the active site of the enzyme. We were able to synthesize only two of the ligands in our lab in a step wise manner. Benzimidazole-2-thiol was first alkylated with 2-bromobutane. The resulting thioether of benzimidazole upon esterification with ethylchloroacetate and subsequently treatment of the esterified product with hydrazine hydrate yielded the respective acetohydrazide which was then coupled with 4-hydroxybenzaldehyde to the desired products.

Fabrication of high efficiency visible light Z-scheme heterostructure g-C_3N_4 Fe_0/TiP and degradation of rhodamine 6G

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We produced and investigated an outstanding and less expensive photocatalytic composite material of g-C3N4Fe_0/TiP. By employing a simple process involving the chemical reduction of zero valence iron. X-Ray diffraction (XRD), UV-vis Spectrum, Energy Dispersive Spectrum (EDS), Scanning Electron Microscopy (SEM), Raman Spectroscopy, and Transmission Electron Microscopy were used to evaluate this ternary photocatalyst g-C3N4Fe_0/TiP. It has been shown to have strong visible light activity in a wide variety of pH settings, and it can photo catalytically breakdown Rhodamine 6G (Rh 6G) in 60 minutes under visible light. The enhanced harvest of more visible light and the better separation of photo-excited electrons and holes via Z-scheme and heterojunctions mechanisms, as well as the time required for the complete removal of (Rh 6G) to the photocatalysis system, which aided in the formation of reactive species and pollutant degradation, from 60 to 90 minutes. The characterization results reveal that the synthesized photocatalyst and evaluated photocatalysis degradation system have a potential application possibility.

Utilization of photovoltaic energy for the spark assisted pyrolysis and copyrolysis of Dara Adam Khail coal and waste polyethylene into oil and gas

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A novel idea of the use of photovoltaic energy as high energy spark for the pyrolysis of coal and plastics is presented. This study is also focused to investigate the pyrolytic liquification of coal from Dara Adam Khail of the KPK through pyrolysis and copyrolysis with waste polyethylene. The spark is initiated through discharge of a lead battery using graphite rod and the battery was recharged using solar panels. This study is also focused on the fabrication of suitable reactor for the spark or discharge pyrolysis. Each of these reactors were batch reactors, made of stainless steel and working in distillation mode. The reaction conditions for the pyrolysis were investigated by varying length and girth of graphite rod, heating time and reactor load. Each of the reaction was carried out in the temperature range of 900-1000 oC. This high temperature was attained using direct current and short circuiting. Both the pyrolysis and copyrolysis reactions were found to produce gaseous, liquid and solid products. The vapours of the pyrolysis reaction were condensed using cold traps. The amount of gases was found greater than oil due to the high temperature however in copyrolysis oil was greater. The gaseous products of pyrolysis were analyzed for its chemical nature using chemical traps containing aqueous solution ammoniacal cuprous chloride for the analysis of alkynes and Baeyer's solution for the analysis of olefins. The oil product of pyrolysis was analyzed using GC-MS and FTIR. The oil product was found to contain Hydrocarbons. The gaseous product is composed of alkenes, alkynes, alkanes and hydrogen in addition to small quantities of carbon dioxide and carbon monoxide.

Comparison of Synthesis Methods of Titania (TiO2) Nanorods Voltametric Determination of BPA in Exposed Bottle Water

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Titania nanorods can be synthesized by diverse methods. Nanochemistry has wide applications in electronic, optical and sensing devices. This study is on the comparison of different methods of the synthesis of Titania- nanorods. Methods are being compared based on techniques as transmission electron microscopy (TEM), scanning electron microscope-energy dispersive x-ray analysis (SEM-EDX), x-ray diffraction (XRD), and Fourier transform infra-red (FTIR) and modified sensors. The electrolytic activity of the modified sensor was studied by cyclic voltammetry as well as electrochemical impedance spectroscopy (EIS).

A highly sensitive electrochemical sensor based TiO_2- nanorods modified carbon paste electrode (CPE/TiO_2 NRs) for the determination of bisphenol A (BPA) in bottled water was successfully studied. The composition of TiO_2NRs,pH of BPA solution, as well as scan rate have been investigated. The linear range of detection for BPA using the CPE/TiO_2 NRs was found to be between 6 x 10^{-4} M and 10^{-2} M with a limit of detection of 0.08µM.

A good linear relationship was found among the electrochemiluminescence (ECL) intensity as well as the increased BPA concentration within 0.01-5.0mg/L, with a correlation coefficient of 0. 9972.The detection limit was 0.66 x 10^{-3} mg/L. Good recoveries between 96.0% as well as 105.0% with a relative slandered deviation of less than 4.8% were obtained in real water samples. ECL sensor can be successfully working to BPA detection in environmental aqueous samples. The modified sensor was fruitfully applied for the determination of BPA in a real sample bottled drinking water with fine stability, good repeatability as well as good agreement results contrast to other methods.

Utilization of wild plants juices for the preparation of bio rechargeable batteries

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In this work the juices extracted from leaves of the four wild plants Rumex dentatus, Alovera, Calotropis and Castor plant were used for the preparation of rechargeable bio battery. This work is based on the idea that plant juices contain antioxidant compounds which may pass through electrochemical redox reaction. The bio-rechargeable battery was prepared by coupling each of the juice with the juice extracted from the bitter orange through salt bridge. Each of the juice acts as the half-cell of battery. The current generated was harvested through the graphite electrodes. The juice was used as redox material in two versions i.e. the fresh juice and the juice obtained by boiling of the leaves. The voltage of each battery was measured before and after charging. It was also observed that the voltage of these batteries increased after charging. Optimum conditions for the maximum voltage and power of the battery were investigated by varying the concentration of the electro-active species, the power of the charger, the porosity of the salt bridge boiling time and pH of the medium. In addition to the voltage, the power, and stability of each battery were also investigated. The current and voltage of each of the bio-battery were determined both in open and closed circuit conditions. The Power and stability of each battery was investigated using the loads i.e. LEDs. The compounds responsible for electrochemical process were analyzed using FTIR and cyclic voltammetry. Five cell battery of each plant was found to be used as stable source of power for small electric devices**.**

Kinetic study of thermal degradation of polypropylene using florisil as catalyst

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Plastic has an essential role in today's world. Due to their low cost, longevity, adaptability, light in weight and high hardness, Plastic items are quite applicable and common in our everyday lives. Owing to their widespread use and non-biodegradability, plastics cause problems on the environment. Plastic waste is either landfilled or incinerated after it has been disposed of. However, these actions in turn also pollute the air, water, and land. Therefore, the focus of our research is on environmentally beneficial processes. In this regard, Pyrolysis is the appropriate solution since it has two benefits. One reduces waste plastic, while the other produces usable goods that may be used as an energy source. In the current work, polypropylene was pyrolyzed in a Pyrex glass reaction vessel by placing it in an indigenously constructed furnace in the presence of a florisil catalyst at temperatures ranging from 350 to 430 °C in an inert nitrogen atmosphere. The parameters were optimized for maximum yield of oil and the most suitable circumstances for maximal oil yield were found to be a constant flow of nitrogen, 410°C of temperature, 3% of catalyst, and a 40-minute of reaction duration. In addition, the obtained oil was analyzed through Gas Chromatography/Mass Spectrometry (GCMS). Moreover, the kinetic measurements for the polypropylene thermo-catalytic decomposition in the presence of florisil as catalyst were investigated using the Ozawa Flynn Wall (OFW) and Kissinger-Akahira-Sunnose (KAS) methods in a thermo balance system at heating rates of 3, 12, 20, and 30 °C/min in a nitrogen atmosphere. Using florisil catalyst activation energy (Ea) and pre-exponential factor (A) were determined to be in the range of 102.7395-173.0766kJ/mol and $7.09x10^{8}$-$9.32954x10^{11}$ min^{-1} respectively. The catalyst can be seen to have enhanced the quality as well as the quantity of the oil produced while reducing the activation energy. As a result, florisil was discovered to be a good catalyst for transforming polypropylene into useful compounds. As a result, the laboratory work on model polypropylene might be applied to waste polypropylene on a commercial scale.

P-Doped $C_{24}N24$ Fullerene as an Efficient Candidate for Scavenging of NO_2, a Contributor to COVID-19 Fatality

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Nitrogen dioxide is a toxic air pollutant released anthropogenically through combustion of fossil fuels in automotives or naturally through lightening. It is associated with medical conditions like cardiovascular diseases, hypertension, reduced lung function, chronic obstructive pulmonary diseases and is considerably linked with respiratory fatality. Recent studies illustrate that greater concentration of NO_2 also contribute to the fatality of COVID-19. Therefore, detection and sequestration of NO_2 from atmosphere is necessity of time. In this study, we have for the first time evaluated phosphorous doped porous carbon nitride fullerene ($C_{24}N_{24}$) for the removal of NO_2, using first principle analysis. The energetics, electronic properties, thermodynamic study, atom in molecule analysis and charge transfer analysis reveals that the P-doped $C_{24}N_{24}$ fullerene efficiently captured the NO_2 molecules from its N site through chemisorption. Moreover, the selectivity study indicates that P-doped $C_{24}N_{24}$ fullerene selectively captured NO_2 from gas mixtures containing NO, N_2O, SO_2, NH_3, H_2O, CO, CO_2 and O_2. Our results demonstrate that this study will help the scientists to develop novel, efficient and selective sensors for NO_2 in future endeavors.

Green fabrication of graphene oxide-based membranes for ultrafast water purification and heavy metals separation

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Important achievements have been done on the progress of next -generation for filtration and purification membranes by using graphene oxide-based materials. These membranes proved several novel mass-transport properties that are impossible in state of art. Traditional membranes produce them ideal in fields including water desalination, separation, conversion and energy storage etc. Nevertheless, the major areas of these membranes are elimination of contaminants from water. The huge amount of sea water with high quantity of salts needs to be cleaned. Laminated Because of their molecular filtration capabilities, graphene oxide membranes offer more potential in membrane processing; yet, owing to the unstable interlayer spacing and electrostatic interaction, these membranes exhibit poor selective retention of cations.. Herein, graphene oxide (GO) is crosslinked by two green approaches, Onion extract (OE) and Quercetin (Q) membranes, (GO/OE) and (GO/Q) respectively to acquire the selective retention of salts by the controlling tuning of surface charge and configuration. The GO/OE membranes showed an excellent rejection efficiency 97% of Pb^{2+}, 91% of Cr^{6+} and 87% of As^{3+} with high water permeance ~460±20 $Lm^{-2}h^{-1}bar^{-1}$ as compared to GO membranes. We have also compared these results with Quercetin (Q) membranes (GO/Q) which is active ingredient of onion. The (GO/Q) membrane showed good rejection efficiency 78% of Pb^{2+}, 73% of Cr^{6+} and 68% of As^{3+} with high water permeance ~1150±10 $Lm^{-2}h^{-1}bar^{-1}$. These membranes showed better water separation performance having a low operating pressure and a high salt rejection efficiency and stability more than 60 days. The outstanding efficiency was observed along with the thick structure and positive charge of GO/OE.

Silver sulfide and zirconia composite based visible light photocatalyst for the degradation of organic pollutants

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Three new composites based on Ag2S/ZrO2 were synthesized by using hydrothermal and sonochemical methods. In these synthesized composites Ag2S to ZrO2 ratios were 1:1, 2:1 and 3:1 respectively. It was found that composite of the ratio 2:1 have displayed strong photocatalytic properties for the degradation of methyl orange (MO) and Rhodamine B (RhB). Composites were characterized by FTIR (Fourier-transform infrared) spectroscopy, PXRD (Powder X-ray diffraction) analysis, SEM (Scanning electron microscopy), EDX (Energy-dispersive X-ray) and BET (Brunauer, Emmett, and Teller). These synthesized composites were tested for photocatalytic efficiency under solar-light irradiation. The effect of photocatalyst dose, time interval, dye concentration and pH were evaluated on the degradation efficiency of methyl orange (MO) and Rhodamine B (RhB). It was observed that the degradation efficiency of these organic pollutants decreased by increasing the concentration of dye and solution's pH while it increased with increasing the irradiation time and catalyst dose. Almost 99% degradation efficiency was achieved by adding 0.025 g of catalyst at 20 minutes.

Synthesis of multiresposive composite hydrogel for removal of selective antibiotics from drinking water

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Current research has claimed to remove a diverse range of antibiotics present in ground water which comes from medical, municipal, and agricultural means. An environmental-friendly, reusable and recyclable chitosan built composite hydrogel have been synthesized via free radical copolymerization for selective removal of antibiotics from drinking water. The composite hydrogel have been characterized by using solid state Nuclear Magnetic resonance (^{13}C-NMR, Fourier Transform Infra-red spectrophotometer (FT-IR), Zeta-Nanosizer and Laser Light Scattering (LLS), respectively to study the structure, stability, swelling, physicochemical responses and Adsorption kinetics at air water interface. The highly porous structure and the pendant group of chitosan coordinated chemically with the selective antibiotic at various pH ranges (4- 7.2). An 85 % of antibiotic solution has been cleared using the composite hydrogel which has been investigated spectroscopically. Further, the composite hydrogel with five time reusability has been explored while retaining its chemical identity. The synthesized composite hydrogel may have the potential to interact with the antibiotic present in drinking water in the same way as determined in vitro and can be potentially applied at industrial level with controlled physicochemical responses.

Processing of Agricultural Waste via Biocompatible Ionic Liquid to Produce Food-Grade Glucose

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Agricultural waste material can be use productively to fulfill the future demands of food, fine chemicals, fuel and energy. We used two agricultural residues abundantly available in Pakistan to produce food-grade glucose using a biocompatible ionic liquid. This biocompatible ionic liquid is based on food-grade cholinium hydroxide and lysine and has potential to remove undesirable components from agricultural cellulose such as, lignin and hemicellulose. The obtained pure cellulose pulp was subsequently hydrolyzed into glucose by using food-grade enzymes. The optimum delignification efficiency of the IL is 87% at 120 °C after 8 h pretreatment. The optimum yield of food-grade sugar was 77% from cellulose pulp after processing at 100 °C for 8 h. The analysis of the pulp and lignin was made using compositional analysis, FT-IR, TGA, and SEM techniques, whereas glucose was quantified using HPLC. The food-grade glucose may be used in the food industry or pharmaceuticals, but this study aims at synthesizing mycoprotein in the future.

Utilization of Agricultural Waste for Efficient Mass Production of Carboxymethyl Cellulose

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Carboxymethylcellulose (CMC) has found various applications in many industries such as paper, textile, pharmaceutical, food, paint and others. In Pakistan, it is imported 4629 tons every year that costs 1666 million PKR and we have no local production unit. This project is aimed to launch a pilot plant for mass production of this important cellulose derivative. For the purpose, local agricultural waste material is successfully converted into cellulose using different methods such as alkaline, acidic, peroxide, ionosolv and many other methods. Cellulose, in turn, is etherified using monochloroacetic acid or sodium monochloroacetate. Produced CMC is optimized for reaction conditions, characterized for its structure and physical properties and is tested for various applications. Product is successfully scaled up to 1 Kg using our industrial collaboration and now we are about to launch our own pilot reactor.

Volumetric studies on understanding the salvation behavior and sweetness response of erythritol in aqueous KCl solution at different temperatures

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Sugar alcohols have vast application in pharmaceutical and sugar industry due to their role in in controlling blood glucose level and metabolic rate. Volumetric study provide information about solvation behavior and sweetness response. Solvation behavior and sweetness response of sugar alcohol namely erythritol was investigated in the presence of KCl in the term of expansibility and compressibility. The density of erythritol in water and in the presence of 1% KCl was studied at temperature (20–45) oC using density sound velocity meter.The density data was further used to calculate the volumetric parameters such as partial molar volume, partial specific volume, partial transfer molar volume, expansibility and Hepler's constant. Partial specific volume of erythritol in water (0.70-0.71 cm3g-1) and in aqueous 1% KCl (7.2 –7.5 cm3g-1) have been measured that used in industry to specify the sweeteners. Positive trend of apparent molar volume showed that strength of solute-solvent interaction in binary and ternary system. The decrease in thermal expansion coefficient with temperature show structure making behavior of erythritol. All parameters provide a complete picture of solvation behavior as well as mode of interactions in binary as well as ternary system .These information can played a role in food industry and pharmaceutical industry.

Michael Reaction as a tool for Construction of C-C bond

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The Michael additions of Cyclohexanone to b-nitrostyrene and 4-Methoxy-β-Nirostyrene were studied. The reactions employ small organic molecules Pyrrolidine as a catalyst under mild reaction conditions and do not require pre activation of the carbonyl donors. The conditions were optimized and under these optimized conditions Michael Products were obtained.

CoCu-MOF derived nanomaterials for efficient oxygen evolution reaction

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Metal organic frameworks are considered as an ideal precursor for various nanomaterials. Herein, we report the synthesis of CoCu-MOF through hydrothermal method. The formation of MOF was confirmed through powder XRD analysis. This bimetallic MOF was then further treated in different atmospheres i.e., Air and argon at different temperatures i.e., 700,800 and 900℃. Each of the resulting compound was evaluated for OER activity in alkaline medium. Under air atmosphere, spinel CuCo2O4 is formed, which is confirmed through crystallographic (powder XRD) analysis. Spinel CuCo2O4-900 shows best activity for OER at a current density of 20mAcm-2 with 300 mV overpotential, with a tafel slope of 60 mVdec-1, which is much higher than that obtained by calcining Co-MOF and Cu-MOF individually under air. Under argon atmosphere, CoCu-NPs@N-doped porous carbon is formed, which is also confirmed through powder x-ray analysis. CoCu-NPs@N-doped PC-900 shows best activity, with an overpotential of 310mV@20mAcm-2, with a tafel slope 70 mVdec-1, which is also higher than materials obtained by calcining individual MOFs under argon. Both CuCo2O4-900 and CoCu-NPs@N-doped PC-900 how excellent stability for 15 hours for continuous OER evaluation. The energy dispersive X-ray mappings and X-ray photoelectron spectroscopy (XPS) studies were carried out to investigate the presence of elements/oxidation state in the synthesized material.

AgCu Alloy supported on porous carbon for selective electrochemical reduction of CO2

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The electrocatalytic CO_2 reduction is an alternative to fossil fuels since it can simultaneously satisfy the energy demand and mitigate the detrimental effect of CO2. The current project has been designed initially to synthesize an efficient silver and copper base bimetallic novel catalyst AgCu Alloy supported on porous carbon for selective reduction of Carbon dioxide to Carbon monoxide. In this work, we synthesized AgCu Alloy supported on porous carbon through pyrolysis of silver deposited on copper benzene-1,3,5-tricarboxylate (BTC), under H2 environment at high temperature treatment. The AgCu Alloy supported on porous carbon perform better than conventional Ag or Cu based catalysts. The AgCu Alloy supported on porous carbon catalyst derived from Ag@CuBTC is an efficient and selective catalyst for electrocatalytic reduction of CO2 to CO, which exhibited an enhanced current density and significantly improved faradaic efficiency, additionally lower overpotential with high stability. The metal-organic frameworks (MOFs) will be synthesized in special designed high-pressure vessels known as autoclaves by mixing copper metals and organic ligand(benzene-1,3,5-tricarboxylate) in a suitable solvent like ethanol stirred and put in an electric oven at 150 °C for 72 hours, followed by cooling and collection of crystals by filtration and dried in a vacuum oven. The electrochemical experiments will be done using cyclic voltammetry techniques. Gas chromatography was used to identify the gaseous products of CO2RR. High-performance liquid chromatography for liquid products. The synthesized material has been characterized by various analytical techniques, i.e., Transmission Electron microscopy and Scanning electron microscopy, Energy dispersive X-ray spectroscopy, Powder X-ray diffraction, X-ray photoelectron spectroscopy etc.

Biogenic synthesis, characterization and application of FeO and Ag nanoparticles in degradation of toxic dyes

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Metal organic frameworks are considered as an ideal precursor for various nanomaterials. Herein, we report the synthesis of CoCu-MOF through hydrothermal method. The formation of MOF was confirmed through powder XRD analysis. This bimetallic MOF was then further treated in different atmospheres i.e., Air and argon at different temperatures i.e., 700,800 and 900℃. Each of the resulting compound was evaluated for OER activity in alkaline medium. Under air atmosphere, spinel CuCo2O4 is formed, which is confirmed through crystallographic (powder XRD) analysis. Spinel CuCo2O4-900 shows best activity for OER at a current density of 20mAcm-2 with 300 mV overpotential, with a tafel slope of 60 mVdec-1, which is much higher than that obtained by calcining Co-MOF and Cu-MOF individually under air. Under argon atmosphere, CoCu-NPs@N-doped porous carbon is formed, which is also confirmed through powder x-ray analysis. CoCu-NPs@N-doped PC-900 shows best activity, with an overpotential of 310mV@20mAcm-2, with a tafel slope 70 mVdec-1, which is also higher than materials obtained by calcining individual MOFs under argon. Both CuCo2O4-900 and CoCu-NPs@N-doped PC-900 how excellent stability for 15 hours for continuous OER evaluation. The energy dispersive X-ray mappings and X-ray photoelectron spectroscopy (XPS) studies were carried out to investigate the presence of elements/oxidation state in the synthesized material.

COMPUTATIONAL ANALYSIS OF NIGELLA SATIVA DERIVED PHYTOCHEMICALS AGAINST BEAK AND FEATHER DISEASE VIRUS

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This in-silico study was aimed at computer aided drug discovery of phytochemicals against beak and feather disease virus BFDV, belonging to family Circoviridae. In this research, 21 out of 52 phytochemicals were selected from Nigella sativa belonging to a family Ranunculaceae, as they passed the criteria of drug likeliness through ADMET analysis. The binding affinity of already discovered inhibitor (ATPase inhibitor) is -5.5 kcal/mol. Through the docking analysis it has been found that 5 out of 21 selected phytochemicals have binding affinities ≥ -7.3 kcal/mol. It means that these 5 phytochemicals can be used to inhibit the main capsid protein of BFDV. 5 out of these 21 phytochemicals were found to have the best inhibitory activities. The 5 best phytochemicals with their binding affinities are Rutin -8.8 kcal/mol with seven hydrogen bonds. Beta amyrin showed the binding affinity of -8.3 kcal/mol with one hydrogen bond. The binding affinity shown by Hederagenin was observed as -7.8 kcal/mol and one hydrogen bond. In addition, Taraxerol and Stigmasterol showed -7.6 kcal/mol and -7.3 kcal/mol binding affinities respectively with one hydrogen bond each. The highest binding affinity against BFDV capsid was shown by Rutin -8.8 kcal/mol and the lowest binding energy was shown by ascorbic acid as -5.4 kcal/mol. In addition, ZINCPharmer was used to search for the similar compounds as of Rutin. Neohesperidin was evaluated as the similar phytochemical showing binding affinity of -8.0kcal/mol, which is less than Rutin. Hence, the docking result indicates that Rutin forms the strongest complex and ascorbic acid forms the weakest complex with BFDV capsid protein. Through analysis, it is concluded that phytochemicals such as Rutin, Beta-amyrin, Hederagenin, Taraxerol and Stigmasterol are candidate inhibitors for targeted proteins and can help in drug formulations, after in vitro and in vivo analysis. This study provides a path for drug development against BFDV for obstructing the massive global outbreak.

Green Synthesis, morphological and optical studies of Zinc Oxide (ZnO) Nanoparticles and their Application

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Metal oxide nanoparticles (NPs) have been extensively synthesized and utilized in different areas because of their distinctive optical, physio-chemical, thermal, and biologic attributes. In fact, as compared to the organic NPs, metal oxide NPs indicate unique stability, lower toxicity, and higher heat resistance and selectivity. Among the metal NPs, zinc oxide nanoparticles (ZnO NPs) are highlighted due to their numerous applications in the plastic, cement, lubricants, paints, adhesives, pigments, packaging, cosmetics, and textile industries. On the other hand to synthesize (ZnO NPs) is easier, and simple. In the present study, ZnO NPs were synthesized by a simple and cost-effective method using Solanumm melongena peel extract and zinc nitrate tetrahyderate as precursors. The synthesized ZnO NPs were characterized by UV-visible spectroscopy, Fourier transforms infrared (FTIR) spectroscopy, Zeta Sizer, Zeta Potential, energy dispersive X-ray (EDX) analysis. The UV–visible and FTIR study profile initially confirms the formation of ZnO NPs. A distinct absorption peak at 276 nm confirms the formation and presence of ZnO NPs. The SEM images revealed semispherical shaped ZnO NPs. While Zeta sizer and Zeta potential measurements explained well arranged, size, and charge over the surface of ZnO NPs, which was calculated to be 50 nm with desirable charge of – 7.1 mV. Furthermore, the ZnO NPs were applied for catalytic reduction of bromocresol green. Different parameters were optimized including NaBH4, time of exposure under Microwave radiation, nanoparticle dosage. Catalytic reduction of bromocresol green was achieved up to 95 % using 5 mg ZnO NPs within 35 minutes.

Metal organic framework as an adsorbent for Boron uptake

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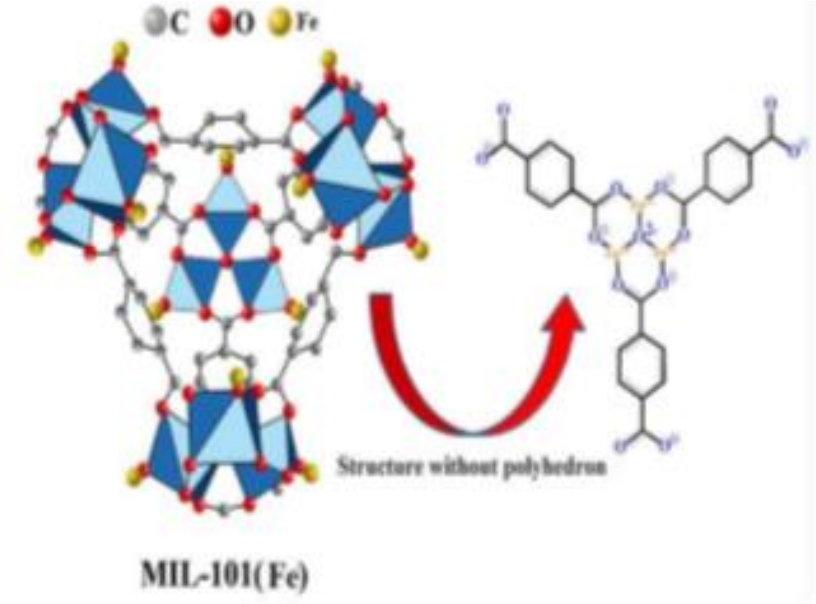
The advanced porous materials, known as coordination polymers, are MOFs, have a broad spectrum of applications, assembled from two basic components: Metal atoms (ions) also called secondary building unit and organic linkers that are multifunctional polyatomic organic bridging ligands, are bonded together by form porous materials. Metal-organic frameworks are the emerging class of the material having large surface area and high porosity, these characteristic advantages had made them a desired candidate for application in many fields. The applications of metal-organic framework in various fields including drug delivery, gas storage, cancer treatement, chemical catalysis, biosensors, medical imaging and adsorption. MOFs with long term water stability are the desired material for adsorption applications in the aqueous conditions for purification purose. The reported adsorbent were costly and undstable at drastic conditions. Therefore, an efficient adsorbent with maximum boron uptake desirable to minimize the cost and improvement in efficiency of boron separation process. The wellknown parameter for selection of boron adsorbent is its adsorption capacity. For the first time, an iron-based waterstable metal-organic framework (MOF) MIL-101(Fe) that has molecular formula [Fe3O(OOC-C6H4-COO)3(H2O)3]n Cl·(H2O)x was investigated for the removal of boron from water. The structure was confirmed by X-ray diffraction (XRD), scanning electron microscopy (SEM), and the thermogravimetric analysis (TGA). In a batch adsorption procedure, the boron adsorption kinetics, isotherms, thermodynamics, mechanism, were investigated. At 25 degrees Celsius, MIL101(Fe) exhibited a high adsorption performance of 958 mg/g at pH = 10. For purpose of kinetic analysis, the psuedo-first-order model and the pseudo-second-order model were used. The process is controlled by entropy change rather than enthalpy change in the system, implying extensive adsorption (chemisorption). Noteworthy, the traditional boron removal adsorbents have a lower boron adsorption capability as compared to MIL-101(Fe).


C O Fe
Structure without polyhedron
MIL-101(Fe)

Synthesis, Structure Elucidation & Biological evaluation of Arylated Pyridines & Quinolines by TM Catalyzed Suzuki Miyaura Cross Coupling & Buchwald-Hartwig Amination

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Transition metal catalysis is important because of its intriguing chemistry and wide range of applications, allowing for the creation of carbon-carbon (C-C) and carbon-heteroatom (C-X) bonds. The superiority of palladium (Pd0) and nickel (Ni) -catalyzed methods are attributed to the fact that they are usually one pot reactions. By using noval approach of Suzuki Miyaura cross coupling (Nobel award 2010) & Buchwald-Hartwig amination new biologically active Het-Aryl compounds are synthesized. These arylated pyridines & quinolines have shown excellent antibacterial, anti fungal and antimicrobial actvities. They've also found uses in the feild of Organic Electronics (OE) as OLEDs, SMOCs & Photovoltaic dyes (DSSCs). Structure of these compounds are confirmed by 1H-NMR, 13C-NMR, EI-MS, FTIR and single crystal X-Ray crystallography.

Evaluation of indole-picolinamide hybrid molecules as carbonic anhydrase inhibitors: Biological and computational studies

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Carbonic anhydrases (CAs), a class of enzymes of different forms act as a biocatalyst and regulates CO2/HCO3- and some reactions of hydrolysis. Deficiency of CAs leads to different disorders (cerebral calcification, osteoporosis, renal tubular acidosis, etc.) as it maintains the fluid balance in many parts of the body like eyes, stomach, kidney etc. There were many enzyme activators reported which activates central nervous system (CNS) of humans causing problems in the memory and learning activities. Moreover, reported inhibitors of carbonic anhydrase inhibits the activity of glaucoma, epilepsy, altitude sickness etc. The study was designed in order to prepare a series of indole-picolinamide hybrid compounds as potent and selective inhibitors of bovine carbonic anhydrase II as its abnormal level can cause tumorigenesis (formation of cancer cells, conversion of normal cells to cancer cells) and ureagenesis (metabolism of nitrogenous waste i.e., urea of protein) as well. A multistep scheme was designed to produce desirable structures having markable sites to modify the compounds chemically and induced interactions between drug and receptor. FTIR, 1H-and 13C-NMR, spectroscopic techniques were used for the establishment of all the synthesized structures. Out of all only compound 1a was observed as a potent inhibitor of the bovine CA II during the in vitro studies with the IC50 value of 0.04398 ± 0.00946 µM, more potent than the standard (acetazolamide IC50; 0.96 ± 0.18 µM). The level of inhibition of compounds varies with the addition of the different substitutions like trifluoromethane, methylmorpholine etc. The results of the in vitro studies were more confirmed with the molecular docking which showed important interactive pose along residues of amino acids. The compound's suitable mode of inhibition was obtained by kinetic studies. In short, the pharmacokinetic (ADME) properties along with the data of performed activities ensured that the designed drug can be used as inhibitor of bovine carbonic anhydrase II.

Ionic Liquids for Extraction of Hydrogels from Mucilaginous Seeds and Its Application

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Ionic liquids are molten organic salts having melting points less than 100 °C. These are highly designer and tailormade solvents with vast adjustable properties. They have excellent dissolution powers for organic, inorganic, biopolymeric compounds are an excellent media for extraction of useful compounds from natural sources. Mucilage of different seeds possesses significant chemical and physical properties such as high water absorbing capacity, stabilizing and emulsifying properties. Traditional chemical and physical methods for extraction of mucilage (hydrogel) from different seeds suffered from various drawbacks. In this work, we used ionic liquids first time for the purpose. Process is optimized for different parameters and application of extracted mucilage was checked for stabilization of gold nanoparticles.

Green and Chemical Synthesis of Fe_2O_3 and their applications in antibacterial and photocatalytic activity

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Novel approach for the synthesis of Fe2O3 was established by chemical and green method. In the chemical synthesis of iron oxide nanoparticles, ferric III chloride was used as precursors and NaOH as stabilizing agent. The eco-friendly approach for the synthesis of Fe2O3 nanoparticles has been employed by using onion extract which acts as reducing agent. The confirmation of synthesized iron oxide nanoparticles were done by using Fourier transform infrared spectroscopy (FTIR) Ultraviolet Visible spectroscopy and X-ray diffraction (XRD). The optical properties of nanoparticles were determined by using UV-Visible spectroscopy and band gap was established via Tauc and Wood relation. The crystallite sizes of nanoparticles were calculated using Debye Scherrer and Williamson-Hall equations using X-ray spectrum for both chemical and green method. The photocatalytic activity of nanoparticle was observed against methylene blue in the presence of sunlight. The decrease in band gap results in increase in the percentage degradation with relation to crystallite size of nanoparticles.

Production Of Biodiesel From Waste Vegetable Oil Using Waste Egg Shell Based Heterogeneous Catalyst

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With the increase in energy demand all over the world, it is necessary to find alternative to fossil fuels as source of energy. Biofuels have gained importance in recent years as they are reusable and eco-friendly. In this study, a green synthesis method has been carried out using waste vegetable oil (WVO) as a feedstock for biodiesel production. A renewable heterogeneous alkali catalyst was prepared by extraction of calcium oxide (CaO) from waste egg shells and calcinating it at 900ºC for 4h. CaO was then doped with a metal i.e., cobalt (Co/CaO) by co-precipitation method using cobalt nitrate hexahydrate [Co $(NO_3)_2.6H_2O$]. It was then used for the conversion of WVO into biodiesel via transesterification under optimized conditions. Concentration of the catalyst (Co/CaO) was varied in different transesterification reactions to study its effect on the yield of biodiesel. CaO and Co/CaO were characterized by using Fourier Transform Infrared Spectroscopy (FTIR), Energy Dispersive X-Ray Spectroscopy (EDX) and Scanning Electron Microscopy (SEM) techniques for determination of chemical composition and surface morphology of the catalysts. Fatty acid alkyl esters present in the prepared sample of biodiesel were determined by Gas Chromatography-Mass Spectrometry (GC-MS). Different fuel properties were studied including cloud point, flash point, density and viscosity. This study emphasized on biodiesel production by green process from WVO using waste organic material as a catalyst source.

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)