Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2018, 7 (4):726-773

(International Peer Reviewed Journal)

Abstracts

of

International Conference on

STATE OF KNOWLEDGE OF CHEMISTRY IN INDUSTRY AND ENVIRONMENT

22-24 June, 2018 (SKICE)

Organized by

Journal of Applicable Chemistry
(www.joac.info)

SVRM College
Nagaram*Guntur Dist., Andhra Pradesh, India*

(Sponsored by University Grant Commission (UGC), India)

Key Note Address

Creating New Opportunities in Chemical Industry Through Data Driven Approaches

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Chemical technology has been traditionally of great importance in contributing to the life style of population in general and certainly play a pivotal role on the economy of nation, in general. The type of materials we employ largely define the civilization and developing smart and intelligent functional materials is interesting in its own right. Computational and theoretical approaches greatly aid in decoding the relationship between the structure and function of molecules and provide much strength to the experimental efforts. While chemists were primarily concentrating on covalent bond formation and breaking, the knowledge on non-covalent interactions is essential to understand the macromolecular structures and assemblies. In designing, intelligent polymeric materials, some aspects such as bonding, binding, aggregation and adhesion require a better understanding of non-covalent interactions. In this talk I would like to discuss some of the grand challenges and opportunities and address how these challenges can be met by judicious interplay between data driven approaches, modelling with experiment. A few case studies will be taken and explained about the importance of adopting an integrative approach to tackle grand challenges in science in general and chemistry in particular.

Invited Lectures

NanoChemistry

IL 1. Why are nanomaterials different? Design of nanoporous materialsand their applications

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Nanoporous materials are the class of nanomaterials which have length scale ranging from 1-100nm. Microporous (2nm), Mesoporous (2-50nm) and Macroporous (> 50 nm) materials are promising materials have unique properties such as low density, considerable thermal conductivity, gas permeability, significant surface/volume ratio, optical properties, mechanical strength and stabilityhence, such materials are having diverse applications in organic synthesis, heterogeneous catalysis, bio-filtration, adsorption, degradation of dyes and toxic metals, electronics/spintronics, electrochemical sensors, miniature primary cells, aerospace technology, supercapacitors, tissue engineering, cosmetics, computers, self-cleaning cars, paint, food, thermal underwear, defence, targeted drug delivery system, tele-communication, fuel cell technology, and robot surgery. Surface plasmon resonance, dispersion and quantum confinement effect (<10nm) will control their fluorescence properties. Porous materials of coinage metals such as gold, silver and copper are promising catalytic materials can be used for the conversion of several toxic organic reagents such as

o-nitrophenol to p-aminophenol, and o-nitroaniline to 1,2 benzene diamine. Some can be used as sensors and supercapacitors also. In this lecture, porous materials of some precious metals and their applications will be discussed.

IL 2. Nanocomposites and Mixed oxides as Reusable Catalysts for Organic Synthesis and Water treatment

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New generation materials, bimetallic oxides and their nanocomposites have wide-ranging applications as adsorbents, catalysts, membranes etc. These materials possess excellent thermal stability and other advantages are their crystalline structure, shape selectivity, and scope to modify to their structure and surface properties. The combination of heterogeneous catalysts with potential for recyclability and multi-component reactions (MCRs) deliver excellent yields of varied value added organic moieties, with superb selectivity and atom economy in green solvents at moderate conditions in short reaction times.

Although, the generation of ozone is energy intensive, its high oxidation potential and marginal side effects, make ozone, a choice oxidant in water treatment. To enhance its efficacy, various advanced oxidation processes (AOPs), in combination with H_2O_2, Fenton agent, UV/Visible light and/or varied catalysts and additives have been explored. The aim of such approaches is to either to enhance ozone solubility or to increase the production of highly reactive hydroxyl radicals in the system. With chemical industry's increasing needs and stringent environmental protection legislations, green approach based heterogeneous catalysts are perfect choices in drinking and wastewater treatment.
Based on our experiences, the details of ozone initiated advanced oxidation processes for toxic organics' degradation and microbial deactivation; and one-pot reactions for value added conversions will be described.
Keywords: Ozone, disinfection; advanced oxidation processes; Catalysed oxidation; Value added conversions.

IL 3. Modified Semiconductor oxide Nanomaterials for Industrial Applications

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Semiconductor oxide, titania was first reported for the production of hydrogen by water splitting in 1972. From 1990, Semiconductor oxides have been widely utilized in Advanced Oxidation Process for environmental remediation. Nanomaterials, particularly modified semiconductor oxide nanomaterials, have been developed in recent years for multiple applications in the fields of wastewater treatment, air purification, organic synthesis, fuel cells, hydrogen production from water and sterilization. Photoconductivity and electrocatalytic activity of these modified semiconductor oxide materials make them useful for solar cell and methanol fuel cell applications. Thin film coating of these materials is useful for the treatment of industrial effluents. We had developed a number of coupled and co-doped semiconductor oxides and characterized. This lecture will cover the multiple applications of some of these solar active Semiconductor oxide materials

Speciation-Quantum Chemistry-Experiment

IL4. C-N coordination bonds - New Concept in Chemistry

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Chemical bonding plays a major role in determining the drug-receptor, inhibitor-Enzyme, Drug-DNA interactions. Divalent N(I) compounds ($::N(\leftarrow L)_2^{\oplus}$) are systems with bicoordinated nitrogen in N(I) formal oxidation state. It was found that several therapeutically important compounds including like biguanide derivatives (metformin.HCl and proguanil.HCl), (thiazol-2-yl) guanidine derivatives (famotidine, ebrotidine, zaltidine, tuvatidine, tiotidine), guanylthio-urea derivatives and pyridyl-2-thiazolamine derivatives, etc. belong to this class with low-valent state of nitrogen. This class of compounds has been found to be characterized by two lone pairs on the central nitrogen, very similar to the central carbon in carbones ($::C(\leftarrow L)_2$). The new bonding environment for nitrogen (named Nitreones) is clearly different from the nitrenium ions $NR_2^{\oplus}$. Our previous in silico studies on guanylthiourea class of compounds have shown similarity in the molecular electrostatic potential surfaces of the guanylthiourea derivatives in protonated form and pyrimidine nucleus of pyrimethamine. In protonated form guanylthiourea derivatives show divalent N(I) character which is essential to predict the activity of the active moiety. This class is further being developed as a potential nucleus for antimalarial drug therapy. In vitro studies were carried out and two compounds from this class have shown activity in micro-molar range (100μM and 400nM).

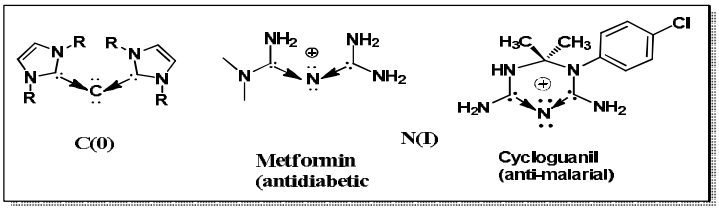

Fig. Structural representation of C(0) and N(I) species

IL 5. Micro solvation (MicSolv) in nature: Chemical speciation (CS) in micro_solvation of ion-pairs (Mips)

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Background: The evolution of biomolecules, metabolism for survival and food/water cycle in bio-life mostly involve water from simple amino acids to functioning of protein machinery. Solvation of proteins, DNA, nucleic acids in presence of salts, organic moieties, vesicles in different compartments of cells/organs of living species is very complicated in terms of concentration ranges, specificity, selectivity and reactivity of a species or reactions. But, this phenomenon plays a subtle role in formation/continuation/threatening and termination of processes throughout the life span of a species.

Micro Speciation in nature: In natural systems viz. bio-fluids, biological cells, oceans, mist/aerosols in atmosphere and ground water salts are present in varying amounts along with other chemical compounds.

Historical results: The work flow of predicting macroscopic properties from microscopic study and vice versa is coveted research pursuit of last century. The scale and resolution of micro- and macro-

picture continuously changed with advances in measurements through instrumentation. The computations opened a new complimentary dimension. Now with growing accumulation of results (KIDs) and cut throat competition of accuracy and reproducibility opened best of both worlds in looking at structures of species and their properties

Experimental Probes: The experimental probes viz. DRS, Raman/2D-IR, VSFG spectra and ultrasonic absorption and CQC (MD) confirm that strongly ionized divalent magnesium salts (chloride and sulphates) form solvated complexes, ion pairs and triple ions in water/interfaces and as intermediates in exchange reactions. But their relative distributions of concentrations depend upon solute concentration.

Divalent cations: Buchner et al. recorded dielectric spectra of $MgSO_4$ in the concentration range (0.08 to 2.2 M) at 25°C over the frequency range min< D/G HS <20 using a Hewlett-Packard model 85070M dielectric probe system based on a HP 8720D vector network analyzer (VNA).

State-of-Knowledge: An in depth study of conformer formation in micro solvated species and the subtle differences with those from gaseous phase are of primary step to probe into environmental evolution/formation/distribution/of both pollutants as well as essential molecules.

Computational Probes: The static DFT studies of $CuCl_2(H_2O)_{1\ to\ 10}$ micro-solvates in gas phase and aqueous solutions show CIPs and SIIPs of different conformer structure. It is inferred that seven water molecules are minimum required for solvation of $CuCl_2$. When the number of molecules of water in hydration shell exceeds seven, it results in dissolution of Cl. The H-bond between FHS and SHS of $CuCl_2$ has a role in micro-solvation process.

Environment

IL6. Treatment of Industrial Waste water with Ozonation

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In recent years, the issues of wastewater treatment have become one of the most important environmental problems. Taking into consideration the increased demand of water use for different purposes (drinking, household, agricultural, industrial, hydro energy and so forth) related to the current world population growth rate and the fact that, according to the different assessments, the world will be threatened by the lack of water resources in a few decades, the improvement of wastewater treatment system is very important and actual. For the creation of efficient wastewater treatment system, the development of such methods of wastewater cleaning, the application of which will be cost-effective and more efficient, is very important.

Nowadays ozone, as a strong oxidant, has a wide application in oxidation processes. It is used for the removal of organic pollutants from wastewaters. The application of ozonation in the treatment process of highly polluted wastewaters is more efficient. Ozone can be used in the treatment processes of such wastewaters that are treated for the use of drinking and other purposes. Taking into consideration the strong oxidizing property of ozone and the fact that ozone is converted to molecular oxygen after oxidation, the application of ozone in oxidation processes is more efficient.
Ozonation is one of ecologically clean perspective methods for the treatment of industrial wastewaters, as in this case chemical reagents, such as potassium permanganate, chlorine and so forth which cause the secondary pollution of water, aren't applied. Ozonation can be applied in the different stages of water treatment process.

Ozonation is used widely for the decontamination of different wastewater compounds, such as phenol and its derivatives (chloro-, nirtro-, amino-,alkyl-phenols), polyphenols, the complex compounds of

phenolic nature (hydrolysis lignin, lignosulfonic acids, water-soluble gums, hydrolyzed and condensed tannins, the materials of humine nature and …..), alkylbenzene sulfonates, alkylphenol polyethylene glycol ethers,cyanides, dyes and so on.

IL 7. Novel Adsorbents for Waste Water Treatment

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Large amount of waste water is generated by industrial, agricultural and domestic activities.Major content of waste waters is heavy metals and textile dyes which end up in natural bodies affecting livings organisms. Hence, it is important to develop an effective method for removal of these pollutants from waste water. Various methods used for removal of metal ions and dyes include chemical precipitation, solvent extraction, ion exchange, oxidation/ reduction, membrane separation, adsorption etc. Among these methods, adsorption process is preferred due to its high efficiency, cost effectiveness, and availability of various adsorbents. In our laboratory we have developed various cost effective novel adsorbents from sugar cane bagasse, hen feathers, and leaves of couroupita guianensis, cestrum nocturnum, saraca indica, barleria cristata plants for removal of heavy metal ions (Cu, Ni, Cr) and textile dyes (methylene blue, indigo carmine, eosin Y, crystal violet, reactive red). For this purpose, batch adsorption process was used. Various parameters: pH, contact time, adsorbent dosage, particle size, adsorbent concentration was optimized in order to achieve effective removal. In most of the cases removal was > 90 %. The adsorbents were characterized before and after adsorption using FTIR, FESEM, EDX, XRD techniques. The developed method was successfully applied to industrial effluents. The adsorbed metal ions/ dyes were recovered using various eluents such as HCl, HNO_3, KCl, NaOH and adsorbents were regenerated for further use. The study also covered kinetics and thermodynamics of adsorption process along with adsorption isotherms. The results obtained for some of the representative systems will be discussed in the talk.

Green Chemistry

IL 8. Microwave assisted synthesis of Nitrogen heterocyclic analogous as a green chemistry approach: Their biological evaluation

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Microwave assisted organic synthesis (MAOS) approach is a nonconventional technique of organic synthesis, which is more advantageous over conventional synthetic approach. In these conscious days of deteriorating environment, it is welcome addition to the list of green chemical synthetic methods. This method is also energy saving in this era of energy crisis as nobody want conventional tedious methods for driving a chemical reaction. Microwave-assisted heating under controlled conditions has been shown to be an invaluable technology for medicinal chemistry and drug discovery applications since it often dramatically reduces reaction times, typically from days or hours to minutes or even seconds. Many reaction parameters can be evaluated in a few hours to optimize the desired chemistry. Hence, compound libraries can be rapidly synthesized, so that the lead identification and lead optimization in the pharmaceutical research become an easier and efficient. The problem associated with waste disposal of solvents has been overcome by solvent less synthesis under microwave irradiation. Moreover, the biological activity of the compounds depends on structure of molecule and it has been observed that heterocyclic compounds are more biological active as compared to others.

Pyridine and its derivatives are the important chemical compounds with tremendous applications in medicinal field. The pyridine is found to have a large number of biological activities those including antiviral, anticancer, antimicrobial, antidiabetic, antitubercular, antidote, antileishmanial, antioxidant, antichagasic, antithrombin, anticoagulant etc along with most of the traditional biological activities. Pyridine is also a very active neutraceutical found in the form of vitamin B3 i.e., Pyridoxine, which attracts attention of synthetic Chemists for the synthesis of newer biological active candidate. Another important aim of this study is to develop and to apply more efficiently, environmentally benign strategies for future sustainable growth of reaction pathways, as the environmental protection has become a global concern. Under the framework of green chemistry, an efficient procedure for the synthesis of pyridine analogous contributing various heterocyclic moieties such as, triazine, benzothiazepin, pyrazole, etc., via microwave irradiation to offer newer analogous of pyridine with improved potency that compared with standard drugs, is described in this study. The comparative study of non-conventional microwave induced synthetic approach with conventional heating approach has also been done. Spectral characterization of final synthesized compounds was carried out using FTIR, ^{1}H &^{13}C-NMR and mass analysis. All the synthesized compounds were screened for their different biological potential. The implementation of Microwave assisted organic synthesis that has lower environmental impact forms a part of Green Chemistry.

IL 9. Green synthesis of diverse heterocyclic library consisting macrocycles and bis-heterocycles

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Heterocycles are among the most frequently encountered scaffolds in pharmaceutically relevant substances and are essential for the human well being. The remarkable ability of heterocyclic nuclei to serve both as biomimetics and reactive pharmacophores has largely contributed to their unique value as traditional key elements of numerous drugs. Certain possible modifications on the heterocyclic ring may lead to new products with better biological profiles. Macrocyclic rings are commonly found structural units within the frame work of a variety of natural products, which is the main reason for the growing importance of such class of compounds. Moreover for an equal number of atoms, cyclic analogues inherently possess a lower number of rotatable bonds than their acyclic analogues. As a result cyclic counterparts are more conformationally restricted than their acyclic analogues, which potentially can impart higher target binding, selectivity and improved oral bioavailability. The relevance of compounds composed from two or more heterocyclic rings for drug discovery, irrespective of the target, bis-heterocyclic compounds are identified as the most potent ones. Among the top 50 prescription drugs there are twelve bis-heterocycles. As a part of our research program towards the green synthesis of bioactive molecules and above observations prompted us to take up the green synthesis of diverse heterocyclic library consisting macrocycles and bis-heterocycles.

IL 10. Hydrogen Energy: The future fuel

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Increasing energy demand results in severe stress on the current energy infrastructure, and damage the health of global environment. Traditional fossil energy sources are ultimately limited. The growing gap between increasing demand and shrinking supply will have to be met increasingly from alternative primary energy sources. In order to initiate sustainable development and to overcome these energy issues, long term potential actions need to be taken soon.

Hydrogen is one of the most plentiful element in the universe; however, only around 14 % of the atoms in the earth crust are hydrogen, and most of which resides in chemical combination with oxygen as water. Therefore, hydrogen, must be produces to fulfill the energy need in an eco-friendly way. Although a wide range of technologies have been utilized to produce hydrogen economically in an eco-friendly manner, the greatest challenge for hydrogen production is providing hydrogen that is cost competitive. In this regard, this talk will highlight the recent progress in hydrogen production and different methods, which have been utilized for hydrogen production. In particular, the photo electrochemical and photo catalysis will be elaborated in details.

Keywords: Fossil fuel; energy demand; hydrogen; photo electrochemical; photo catalysis.

IL 11. Role of Fuel Cellin Future Energy Generation

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The future energy crisis is an important problem for the present scientists to pursue solutions. Usage of natural energy sources to overcome this energy crisis is the best option and the next problem has to focus is the storage of energy. Fuel cell (FC) is a good alternative energy source that can efficiently generate electricity by consuming fuels and oxygen. FC has fuel flexibility. Hydrogen is the cleanest fuel with highest energy density in terms of mass. Both hydrogen and oxygen can be synthesized by water splitting using photo-catalytic processes and fuels like methanol can be produced from bio-degradable garbage. Hence, more environmental friendly fuels are there. This means that solutions for the usable energy crisis can be sought from our own surroundings instead of depending on crude oil. However, there are some drawbacks in FC systems especially the slow kinetics of oxygen reduction at cathode and the expensiveness of catalyst used for it. During my presentation, attention is given to how this overcome, what extend present researches help to commercialize the fuel cell technology, our latest findings of Catalyst for fuel cell cathode and what are the research area ahead to develop.

Chemistry – State-of-knowledge

IL 12. Crystal structure, DNA binding, cleavage, antioxidant and antibacterial Studies of Cu(II) metal complexes with heterocyclic Schiff bases

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The present work focuses on the preparation of Schiff bases by condensation of furan-2-yl-methanamine / 3,5-dimethylisoxazol-4-amine with substituted salicylaldehydes and their Cu(II) complexes. The Schiff bases and their complexes have been structurally characterized by elemental analysis, magnetic susceptibility measurements, spectral techniques and TG-DTA. The ligands and their metal complexes have been crystallized by slow evaporation / diffusion methods for X-ray diffraction studies. Based on the analytical and spectral data a square planar geometry is assigned for all complexes. The ligands and their complexes have been screened for antimicrobial activity against bacteria (Bacillus thuringiensis, Streptococcus pneumonia, Escherichia coli and Pseudomonas putida) by paper disc method. It is found that the Cu(II) complexes showed more activity than corresponding Schiff bases. Binding studies of these complexes with Calf thymus DNA (CT-DNA) have been investigated by UV spectra and viscocity measurements. It is found that these complexes are binding through intercalation to CT-DNA. Further DNA cleavage

experiments have also been investigated by agarose gel electrophoresis on pBR322 and it is observed that these Cu(II) complexes are capable of cleaving supercoiled plasmid DNA in the presence of H_2O_2 and UV light. Antioxidant studies of the Cu(II) complexes revealed that they exhibit significant antioxidant activity against DPPH radical.

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IL13. Progress and Sustainability: A Chemist's Perspective

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The rapid growth of science and technology over the last three centuries has resulted in a progress has essentially been driven by commerce and profit. Uncontrolled exploitation of resources and disregard of environmental health has reached unsustainable levels. This talk will discuss the role chemistry has played so far and the role it needs to play in restoring the chemical balance and achieving sustainable progress.

IL 14. Philosophy of Science and Chemistry

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Science is highly specialized knowledge of the physical universe. Its method is empirical, it is observational and experimental. It does not believe in anything unless it is testified by reason and experience. Its object is to enhance knowledge for human welfare. Science is not concerned with extra phenomenal world which is beyond experience. On the other hand, Philosophy is knowledge purse. It studies truth of the entire universe. This knowledge is higher than, and, comprehensive. Its method is reflective or deep thinking and object is deliverance of man from misery, ignorance and parochial thinking. During the past twenty-five years there has been a large upsurge of interest in the field of philosophy of science and chemistry. Now philosophers of science realize that they have paid great attention to physics and more recently biology, they have completely neglected the central science of chemistry, although it is earlier said that chemistry of philosophy is a barren land.

This paper brings the focus on the neglect of philosophy of chemistry, which was very unfortunate and that there is much to be learned from paying greater philosophical attention to set of issues defined by the philosophy of chemistry.

IL 15. Micellar Liquid Chromatography (MLC)

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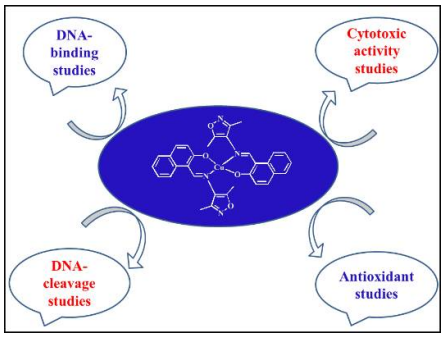
Micellar liquid chromatography (MLC) is a reversed-phase liquid chromatographic (RPLC) mode with a mobile phase containing an aqueous solution of surfactant above than its critical micellar concentration (CMC). The thought of using pure micellar solutions as mobile phases in RPLC is extremely smart due to the lesser charge and toxicity, and the low environmental contact. In practice, however, the accumulation of a small amount of organic solvent to the micellar solution is preferred to reach retention in practical time windows, and improve peak symmetricity and resolution. Micellar mobile phases have been used with many bonded stationary phases (mostly C8, C18 and cyanopropyl). The majority of common surfactants are the anionic sodium dodecyl sulphate (SDS), cationic cetyltrimethylammonium bromide (CTAB), and non-ionic Brij35. MLC is a charming example of the compensation of secondary equilibria in RPLC. The primary



equilibrium is solute partitioning between mass solvents (i.e. water or hydro-organic mixture) and the stationary phase. A secondary equilibrium is established with the micelles in the mobile phase. Both equilibria are affected by a range of factors, such as the type and concentration of surfactant and additives temperature, ionic strength and pH.

Studies in MLC have been focused essentially on surfactant adsorption, retention behavior, measurement of partition coefficients, development of peak efficiency and selectivity. This knowledge has allowed a theoretical explanation of MLC, and improves the understanding and use of the technique. The distinctive capabilities of micellar mobile phases are recognized by the ability of micelles to selectively compartmentalize and classify solutes at the molecular level. The mobile phase in MLC includes a surfactant above the CMC. This results in 3 types of interactions namely: stationary phase, bulk solvent and micellar pseudophase.

The MLC methods developed and validated as per ICH guidelines. This enables the researchers as well as pharmaceutical industry personnel to apply these green analytical methods for the quantitative analysis of the drugs in combination dosage forms. The entire work carried out by considering the factors like legibility of analytical methods, cost and quality.

IL 16.Macromolecules: Their Applications in Every Day Life

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A macromolecule is a very big molecule, commonly created by the polymerization of smaller subunits (which are called monomers). They are typically composed of thousands of atoms. The macromolecules themselves are called polymers because they are made up of many of monomeric units. In my presentation, I will be presenting on design, synthesis and applications of various metal containing conjugated polymers (MCCPs) and metallosupra molecular polymers (MSPs). In MCCPs the metal complexes are formed on covalently connected conjugated polymers containing ligand groups, hence the polymer backbone is stable and irreversible.

The strong interaction between organic and inorganic components also creates unique photophysical, electrochemical and photochemical properties. These hybrid conjugated polymer materials have found potential applications in sensors, solar energy conversion, electroluminescence,nonlinear optics, and photo refraction.Polymers formed by coordination of metals to bi- or multifunctional ligands are called MSPs. Coordination polymers often blend together the properties of both their organic and inorganic counterparts, e.g. the flexibility of organic polymers combined with the increased thermal stability associated with inorganic species. MSPs find diverse of applications in catalysis, sensing and media storage. In this presentation, I will be talking on 2,6-bis(pyrazolyl)pyridine based MCCPs, terpyridine based MSPs and their applications optics and optoelectronics.

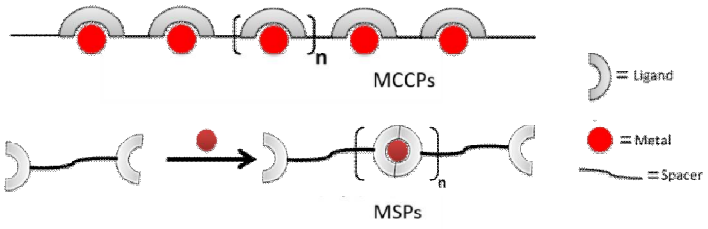

Figure: Schematic representation of MCCPs and MSPs.

IL 17. Contribution Study to the chemical composition of the volatile oil in the leaves of Thymus vulgaris L. and determination of the Anti-bacteriall activity and anti-Leishmanial vitality

MHD Isam Hasan Agha*, Ramah Baaj
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Thymus spp. is widely distributed plant in Syria, where it is used for its antiseptic and decongestant properties.We conducted this study to extract the essential oil from this plant and to determine the main components of this oil in addition to determine its antibacterial and anti leishmania activity compared withthe antibiotic ceftriaxone.The plant material *Thymus vulgaris* L. was obtained from the local market in Damascus, where the plant samples were dried (the moisture was 4%) and the volatile oil is extracted using Clevenger apparatus (water destillation), where100 g of thyme leaves powder steam distiledwith 500 ml water). The extracted volatile oil components were analyzed with GC/ FID. The results of the GC/FID showed that the most important ingredients in the volatile oil werecarvacrole and thymole (73.1%, 7.2% respectively).Antibacterial activity of the volatile oil has been determined on isolates of pathogenic identified bacteria and against the vitality of leishmania strains prepared from public health laboratories andHospital of Dermatologyof Damascus University, where it was determninedthe anti bacterial activity compared withceftriaxone and also determined the anti leishmaniavitality.

In this study it was found that the volatile oil of *Thymus vulgaris* has high anti-bacterial properties, and it has been found to have effectiveness against anti leishmania vitality.
Keywords:*Thymus vulgaris L*., Volatile oil, anti- bacteria, anti- leishmania,

Oral Presentations

OP 1.High removal of chromium (VI) ions from aqueous solution using modified activated carbon-based palm kernel shells

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The occurrence of heavy metals in wastewater presents a serious discharge problem due to their high toxicity and ecological aspects. The present study investigates the removal of chromium (VI) ions from aqueous solution using modified activated carbon-based palm kernel shells. The experiments were carried out under batch mode at room temperature by varying the key parameters of adsorption viz. pH, adsorbent dose, contact time and initial concentration on the percentage removal of chromium (VI) ions. The analysis of experimental results showed that, the adsorption equilibrium was reached within 45 min with 95% of percentage removal of chromium (VI) ions which seems to be pH and initial concentration dependent. The adsorption isotherms models namely, Langmuir, Freundlich, Tempkin were confronted to the experimental data. Freundlich well fits these data with R^2 closed to unity and the value of $1/n > 1$ implying a homogeneous surface of the modified activated carbon. The pseudo first order, pseudo second order, Elovich and Intraparticle diffusion models were tested to identify the mechanism involved on the adsorption of chromium (VI) ions. The results of kinetic study showed that the pseudo second order was adequately fitted. This study revealed that, the modified activated carbon based palm kernel shells can be used as low cost adsorbent for the removal of chromium (VI) in aqueous medium.
Keywords: Activated carbons, Biomass waste, Heavy metal, Pollution, Kinetic, Equilibrium.

OP 2.Treatment of industrial water in the Iraqi oil refinery

Dr. Ali Ali abdulkhabeer ali alyasiri*, Mariam Alwan Abdalrida Mushtaq Attia, Mohammed qassim
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In the present work, oil wastes were treated in the water used in the process of separating crude oil into the basic derivatives in the separation and treatment units in the refinery.Various laboratory tests have been done for contaminated industrial water before and after treatment. The results obtained showed a clear difference in water quality assessment using sawdust compared to the mechanical insulation method used in the refinery.
Key words: Treatment, Industrial wastewater, oil refinery, sawdust method, mechanical method.

OP 3. DNA interaction, anticancer, antioxidant and biological activity studies on Cu(II), Co(II) and Ni(II) complexes of benzothiazole derivatives

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Metal complexes of the type [Cu/Co/Ni(L^1H)$_2$] **1**, **2** and **3**, [Cu/Co/Ni(L^2H)$_2$], **4**, **5** and **6** (L^1H =2-benzo[d]thiazol-6-ylimino)methyl)-4-methoxyphenol and L^2H=2-benzo[d]thiazol-6-ylimino)methyl)-4-methylphenol) are synthesized and characterized by elemental analysis, NMR, Infrared, UV–

visible, ESI mass, magnetic moments, ESR, TGA, and powder XRD. Based on the experimental data a square planar geometry has been proposedfor all the complexes. The interaction of metal complexes with calf thymus DNA (CT-DNA) was investigated using UV-Vis absorption and fluorescence spectroscopy. The binding constant (K_b) estimated from the absorption spectral study and the quenching constant (K_{SV}) calculated from related fluorescence quenching data indicate a non-covalent interaction between the metal complex and DNA base pair. The competitive studies revealed that the complexes **1-6** could interact with CT-DNA through intercalation mode. Moreover, the metal complexes exhibited good cleavage ability against the pBR322 DNA even at low concentrations in the presence of activators, H_2O_2 as well as UV light and it is found that the Cu(II) complexes cleaved DNA more effectively compared to Co(II), Ni(II) complexes. In addition, the in vitro free radical scavenging, antimicrobial activity and cytotoxic potential of all the complexes were examined.

Keywords: RP-HPLC, Isocratic, Paracetamol, Ketoprofen.

OP 4. Extraction of Chromium from Ferrochrome Slag

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Leaching of chromium from ferro chrome slag (Kothavalasa) using hydrochloric and nitric acid media was attempted. Rate of leaching in both acids was found to be firstorder kinetics. Extraction of chromium (VI) by Tri methyl amine (TMA) dissolved in chloroform from nitric acid media has been carried out. Effect of concentrations of metal and TMA on the extraction has been studied. Attempts were also made to strip chromium from the organic phase with 0.2M NaOH. The extracted species are identified as$TMA\ H^+\ CrO_3\ X^-$.

Key words: Leaching - Chrome slag- Solvent extraction - Tri methyl amine (TMA).

OP 5. Synthesis, *in silico* docking studies and evaluation of antidiabetic, antioxidant activities of novel quinoxaline, hydrazide-hydrazone, 1,2,3-triazole hybrid derivatives

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Backdrop:Quinoxaline moiety and its derivatives belong to class of nitrogen containing heterocyclic compounds with broad range of biological activities and pharmacological applications. These are rare in nature, synthetic quinoxalines are included in various antibiotics such as levomycin, echinomycin and actinomycin, well-known to inhibit the growth of Gram-positive bacteria and are also active against transplant tumors. Quinoxaline exhibits antitubercular, antimicrobial, antiviral, antiprotozoan, antiparasitic, antidiabetic, anticancer, anti-inflammatory, antimycobial and cytotoxic, anticandida, antioxidant, anticonvulsant activities. Moreover, Hydrazide–hydrazones comprise a class of organic compounds, which attracts the attention of medicinal chemists due to the fact that they contain azomethine group (–NH–N=CH–) connected with carbonyl group, which is responsible for their different pharmaceutical applications. They have anticancer, anti-inflammatory, antiviral, anticonvulsant and antiprotozoal activities. In addition, 1,2,3-triazoles have occupied an important role not only in organic chemistry but also in the medicinal chemistry due to their easy synthesis by click chemistry and attractive features as well as numerous biological activities. Some unique features like hydrogen bond formation, stacking and dipole-dipole interactions of triazole compounds have increased their importance in the field of medicinal chemistry as they bind with the biological target with high affinity due to their improved solubility.

We report in this communication, synthesis of quinoxaline-hydrazide-hydrazone-1,2,3-triazole molecular hybrids through the molecular hybridization approach. The synthesized compounds were analyzed by spectroscopy (1H, 13C, FT-IR & LC-MS) and screened for antidiabetic and antioxidant activities. Some of the compounds showed good antidiabetic activity as compared with standard antidiabetic drug acarbose.

OP 6.Removal of Coliform bacteria and Escherichia coli from waste water through bio-adsorbent column of activated carbon

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New bio-adsorbent carbon materials were synthesized from the leaves and veins of Mucuna pruriens plant, which are locally available in abundance. The synthesized carbon was activated using HNO_3 and found to be having high surface area of 918 m^2g^{-1}. Scanning electron microscopy analysis of the carbons reflects open pore sizes, shapes and dimensions having complex disorganized surface structures. A sand-supported carbon has been developed using this synthesized activated carbon for its possible use in the removal of coliform bacteria and Escherichia coli (E. Coli) from raw water samples. The removal percentage of E. coli was found to be 100% as confirmed from the McCardy most probable number table. Similarly, the removal percentage of coliform bacteria was found to be 99 %. This activated carbon synthesized from locally available plant possesses the characteristics of good low cost adsorbents which can be easily used for the removal of bacteria from water by adsorption method.

OP 7. Synthesis, Characterization And Evaluation Of In Vivo Anticancer Activity Of Some Novel 2, 5-Disubstituted 1, 3, 4-Oxadiazole Derivatives Against Hcc Rat Model

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Backdrop:Hepatocellular carcinoma (HCC) is the most common type of primary liver cancer in adultsand is the most common cause of death in people with cirrhosis. It occurs in the setting of chronic liver inflammationand is most closely linked to chronic viral hepatitis infection (hepatitis B or C) or exposure to toxins such as alcohol or aflatoxin. Certain diseases, such as hemochromatosis and alpha 1-antitrypsin deficiency, markedly increase the risk of developing HCC. Metabolic syndrome and NASH are also increasingly recognized as risk factors for HCC. As with any cancer, the treatment and prognosis of HCC vary depending on the specifics of tumour histology, size, how far the cancer has spread, and overall health.

The present communication deals with the synthesis, characterization, and evaluation of in vivo anticancer activity of some novel oxadiazole derivatives against HCC rat model. Hepatocellular carcinogenesis was induced chemically in rats by injection of a single intra peritoneal dose of diethyl nitrosamine (DEN) at a dose of 50 mg/kg b. wt. followed by weekly subcutaneous injections of CCl_4 at a dose of 3 ml/kg .b. wt. for 6 weeks. The activity was evaluated by administration of synthesized compounds at 100 mg /kg body weight in albino Wistar rats by oral route against DEN and CCl_4 induced hepatocellular carcinoma and all the compounds were displayed potential capability to restore normal hepatocellular status by inhibition of portal tract necrosis, centrilobular degeneration, fibrosis and anaplasia which was indicated by reduction in α-fetoprotein (AFP) by the synthesized compounds

(AB1-AB8), a potential tumour marker raised in liver cancer. In addition, it was also found that all the synthesized compounds restored the levels of SGOT, SGPT and ALP at the same dose.
Key Words: Hepatocellular carcinoma; cirrhosis; necrosis, α-fetoprotein; tumour marker etc.

OP 8. Synthesis and biological screening of some novel pyrimidine based thiazoles

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A series of novel 4-[4-(4-substituted-phenyl)-6-(2-hydroxy-phenyl)-pyrimidin-2-yl]-1-thia-4-aza-spiro[4.5]decan-3-ones **(9a-f)**were synthesized in good yields from the final intermediate 2-[6-(4-substituted-phenyl)-2-clohexylideneamino-pyrimidin-4-yl)-phenols**(7a-f)** and by using salicylaldehyde **(1)** as starting compound. The chemical structures of the newly synthesized compounds were elucidated by their IR, NMR and MS spectral data. Further, all the title compounds were screened for their antimicrobial activity against various microorganisms.
Keywords: pyrimidine based thiazoles, antimicrobial activity.

OP 9. Electrochemical determination of Atorvastatin at SDS modified carbon paste electrode

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Sodium dodecyl sulfate immobilized modified carbon paste electrode (SDS modified CPE) was employed for the determination of Atorvastatin. The modified CPE displayed very good electrochemical catalytic activity compared with bare CPE. Several parameters such as scan rate, concentration and pH were investigated by the cyclic voltammetric technique. At SDS modified CPE peak currents of atorvastatin was increased significantly indicating high sensitivity. The low detection limit (LOD) and low detection quantity (LOQ) of atorvastatin has been found to be 0.707×10^{-5} M and 2.359×10^{-5} M with a correlation coefficient of 0.99876. The application of the modified electrode in the determination of atorvastatin has good selectivity and high sensitivity.
Keywords: Atorvastatin, Sodium dodecyl sulfate, Carbon paste electrode, Cyclic Voltammetry.

OP 10. Synthesis of Some Heterocyclic Azo Dyes from Pyridone Derivatives and their Biological study

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Heterocyclic coupling compounds such as 6-hydroxy 4-methyl-2-oxo-1,2-dihydro pyridine-3-carbonitrile, 6-hydroxy 4-dimethyl-2-oxo-1,2-di hydropyridine-3-carbonitrile, 1-ethyl-6-hydroxy-4-methyl-2-oxo-1,2-dihydropyridine-3-carbonitrile were synthesized by ethyl acetoacetate, ethyl cyanoacetate and ethanol in one step reaction. A series of heterocyclic azo dyes were synthesized by diazotization of 4-nitro aniline by concentrated hydrochloric acid, followed by coupling with synthesized heterocyclic coupling compounds. Synthesized heterocyclic azo dyes were characterized by UV-Vis, IR, ^{1}H-NMR, element analysis and Mass spectral techniques. The synthesized heterocyclic azo dyes were screened for biological activity. The results of these study revealed that the newly synthesized compounds are potent biological agents.
Keywords: 4-Nitro aniline; azo dyes; biological activity.

OP 11. An Investigative Study on Quality of Groundwater in selected Tribal habitations by WQI and Multivariate Factor Analysis

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This study is to assess the groundwater quality collected from some selected parts of Tribal habitations in Eastern Ghats of Addateegala Mandal of East Godavari District, Andhra Pradesh, India. Twelve ground water samples were collected during pre and post monsoon seasons and were characterized for physicochemical parameters viz., pH, EC, TA, TDS, TH, Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, F^{-}, Cl^{-}, SO_4^{2-}, NO_3^{-}, and PO_4^{3-}. Water Quality Index (WQI) methodology has been applied to physicochemical parametric values to classify the ground waters into categories based on their quality index.
The multivariate factor analysis is performed for pre and post monsoon chemical data set. The microbial analysis has also been carried out to assess the bacterial contamination of waters. WQI for 67% of groundwater samples is good, 33% poor during pre-monsoon while 33% excellent, 58% good and 9% poor during post-monsoon period based on WQI and factor analysis the quality of water has been explained.
The parametric values indicated slight alkaline nature of waters and hardness. Higher values of hardness indicated the encrustative nature of waters and make the waters unsuitable for domestic purposes. The presence of *E.coli, Enterobacter, Klebsiella,Proteus* and *Pseudomonas* confirmed the bacterial contamination of waters. Based on the analytical data, it is concluded that the waters are to be further treated suitably for minimizing the dissolved solid content in waters by ultrafiltration (or) nanofiltration methods and by disinfection methods for the removal of the microbial contamination of waters before consumption for drinking to protect the health of the public residing in the tribal habitations.
Keywords*:* Groundwater, quality, parameter, characterization, bacteria.

OP 12.Recent Advances and Challenges in Anticancer Therapeutics With Nano techniques

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Review: Nanotechnology is a field that has given new hope in the early detection and treatment of cancer which is considered a challenge to the scientific community. Specific targeting of cancer cells is a major challenge faced by conventional therapeutic approaches in cancer treatment.Cancer nanotechnology is a branch of nanotechnology concerned with the application of both nano-materials and nanotechnology approaches to the diagnosis and treatment of cancer. Nanoparticles are developed to overcome several limitations of traditional drug delivery systems and are taking over as distinct therapeutics for cancer treatment. Potential cancer nanotechnology involves design of multifunctional nanoparticles, regulated delivery and release of drugs, and detecting cancer cells with great specificity and sensitivity and overcoming the serious side effect of conventional chemotherapeutics to the immune system.
Key words: Nanomedicines, anticancer therapeutics, nano devices.

OP 13. Anti-diabetic and anti-oxidant activities of crude extracts of *Kigelia Africana* (Lam.), *sterculia foetida* L.

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To explore antidiabetic and the anti-oxidant activities of crude plant extracts of *kigelia Africana (stem), Sterculia foetida (stem),* primarily plant samples *kigelia Africana* (stem), *Sterculia foetida* (stem) were extracted with four solvents viz. n-hexane, ethyl acetate, methanol and waterbased on the ascending order of the polarity. Further crude extracts of plant samples were analysed for phytochemicals such as alkaloids, flavonoids, phenols etc. The quantitative estimation of phenols, flavonoids, alkaloids was performed with the help of double beam U.V spectrophotometer. The evaluation of anti oxidant activity was determined by DPPH method. To assess the antidiabetic activities of crude extracts, *in vitro*α-amylase inhibition method was performed. It is concluded that aqueous extract of *kigelia Africana* (stem), methanol extract of *Sterculia foetida* (stem) are potential source of anti-oxidant and the anti-diabetic properties.
Keywords:*Kigelia Africana; Sterculia foetida*; *in vitro*α- amylase inhibition; anti-diabetic activity, anti-oxidant activity.

OP 14. Quality Evaluation of Ground Water near Granite Mining Area

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The main aim of the present research study is to evaluate the quality of ground water near mining activity area in East Godavari District of Andhra Pradesh. Ground water samples were collected during pre and post monsoon seasons from the nearby granite mining activity areas and characterized for physicochemical parameters viz., pH, EC, TDS, TH, TA, Ca^{+2}, Mg^{+2}, Na, K, Cl^{-}, So_4^{-2}, Po_4^{-3}, No_3, and also for bacterial species for evaluating the quality. The results revealed the unsuitability of waters for drinking or domestic application. The microbial analytical data of these waters also confirmed the presence of bacteria viz., *E.Coli, Klebsiella, Enterobacter*, *Proteus* and *Pseudomonas*, indicating the microbial contamination of waters. The waters are to be treated properly before considering them for utility.
Keywords*:* Ground water, mining, quality, drinking, health.

OP 15. A Facile Green Reduction of Graphene-Silver Nanocomposite using Betel Leaf Extract for the Photocatalytic Degradation of Water Pollutants

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In this report, the insitu synthesis of a nanocomposite of silver decorated on reduced graphene oxide sheets (BRG-Ag) using betel leaf extract as stabilizing and reducing agent is presented. The formation of nanocomposite is confirmed by UV-Vis, FT-IR and Raman spectroscopic techniques. The XRD results revealed the BCC structure of Ag nanoparticles with a particle size of 28 nm. The sheet structure of BRG and uniformly distributed Ag NPs on these sheets is confirmed by HRSEM

analysis. The obtained BRG-Ag nanocomposite exhibited good photocatalytic efficiency (95% in 2 h) against a model pollutant, methylene blue in sun light.
Keywords: Graphene, Silver, Betel leaf extract, Green synthesis, nanocomposite.

OP 16. Preparation of Guar gum Nano Particles for drug delivery applications

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Guar gum Nano particles play a dynamic role in the targeted drug delivery. Nano particles are widely used in drug delivery systems. Due to their smaller size, measured drug release potential, directing ability, enhancement of beneficial efficacy. The guar gum Nano particles are widely used in various industrial applications like food, paper, textile, petroleum, and pharmaceuticals. NPs are low-cost, non-toxic, biodegradable, amenable, biocompatible. The properties of Nano Particles make a perfect solid for mounting drug delivery interpretations.

This paper describes the design and preparation of guar gum Nano particles based on Nano precipitation method. This method is used to measure the synthesis and characterization of Guar gum Nano particles. With enhanced physicochemical and biological properties, Guar gum Nano particles becomes a potential method of replacing traditional medicines and the next generation tools for drug delivery applications. The synthesis and characterization of Guar gum Nano particles are reported.

OP 17. Production of Bio-Gas from Co-Digestion of Kitchen Waste and Cattle Manure: A Case Study of GMRIT Food Waste

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Backdrop:According to United Nations Development Programme (UNDP), 40% of the food produced in India is getting wasted and a 2.1million tonne of wheat is being wasted. According to the agriculture minister Rs. 50,000 crores worth of food produced is wasted.

The present attempt is to utilize the food wasted in the hostel of GMRIT and to produce bio-gas using this food waste. While kitchen waste(KW) & cattle manure(CM) is employed for co-digestion 8.4kg, 2.1kg respectively (KW/CM ratio 4) along with 41.5 litres of water with Hydraulic Retention Time (HRT) of 18 day (maintained) at 37degree Celsius for mesophilic bacteria in order to achieve 50% of methane production results are achieved and are being further studied.
Keyords:Kitchen waste, Cattle manure, Hydraulic Retention time, Biogas, Mesophilic bacteria and Co-Digestion.

OP 18. Synthesis, characterization, DNA binding and nuclease activity of Iron(III) complexes of isonicotinoyl hydrazones

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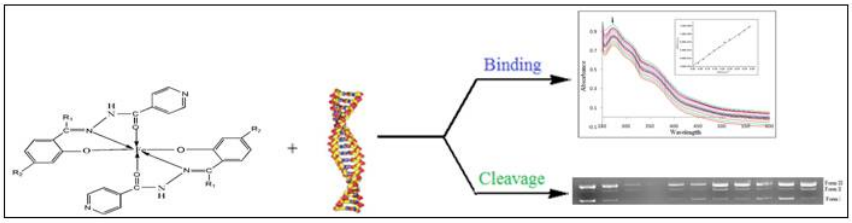
A series of iron (II) complexes of isonicotinoyl hydrazones have been synthesized and characterized based on elemental analysis, molar conductivity, magnetic susceptibility measurements, infrared and

electronic spectroscopy. Electrochemical behaviour of these complexes is investigated by cyclic voltammetry. The DNA binding constants K_b of the complexes are determined systematically with spectrophotometric titrations by using Calf Thymus DNA (CT-DNA). Cleavage activities of these complexes have been investigated on double stranded pBR 322 plasmid DNA by gel electrophoresis in the absence and in presence of oxidant. The complexes behave as efficient chemical nucleases with hydrogen peroxide activation in the presence of reductant (DTT).



Key words: Bioinorganic Chemistry, iron (III) complexes, isonicotinoyl hydrazones, DNA binding, DNA cleavage.

Op 19 Waste Management-Through the Lens of Chemistry and Policy Framework

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This paper incorporates the core area of managing waste in different countries around the Globe, including some good innovative ideas for doing it, and the latest available statistics. For the ease of data management and analysis, the paper takes a close look at solid waste management.The paper looks into Waste Management within two frames of reference; *firstly*, with the Chemistry Lens; and *secondly*, through a Policy Framework. The chemistry will help to understand the environmental hazards it can create if mishandled or not handled at all. Policy Framework will analyse innovative ideas of Waste Management. The literature review revealed that in developed economies there are some projects, cases, and regions where waste innovative waste management techniques have worked really well. It has also been found that waste management has two sides; one is to get rid of environmental pollutants while other is to achieve Go-Green status.

OP 20. Microwave Assisted Synthesis and Biological Screening of Dihydropyrimidine Derivatives Using DABCO an Efficient Catalyst

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The simple and green synthetic method proposed for the synthesis of biologically active multifunctional dihydropyrimidin-2-(1H)-one/ thione derivatives of series (5-phenyl-5,8-dihydropyrimido[4,5-d]pyrimidine-2,4,7(1H,3H, 6H) -trione) by the use of highly efficient DABCO as catalyst using microwave. The multicomponent condensation was carried out with the yield of new derivatives in high yield within desired time period. The catalyst can be reused and recovered easily at mild reaction condition and MWI technique always guarantees desired results with eco-friendly

output. Further, the structural features of newly synthesized compounds were confirmed by IR, ^{1}HNMR, ^{13}CNMR, Mass spectroscopic techniques. The biological screenings were done against gram +ve bacteria and gram –ve bacteria and anti-fungal activities using cup-plate diffusion method

Keywords: Dihydropyriminies, Biginelli reaction, DABCO Catalyst, Microwave Assisted method, Anti-microbial activities.

OP 21.Simultaneous determination of Paracetamol and Ketoprofen by RP-HPLC Technique

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An accurate and precise RP-HPLC Technique for the simultaneous determination of Paracetamol and Ketoprofen in pharmaceutical dosage form has been described. The method involves an isocratic elution of drug in a stationary phase of YMC, C4(150 x 4.6 mm, 3 µm) column. The mobile phase composition of methanol and 0.1% (v/v) orthophosphoric acid in the composition ratio of 70:30 v/v with a flow rate of 0.9 mL/min at 254nm of detection has been used. The injection volume is 10 µL. The developed method has been validated for specificity, linearity, range, precision, accuracy, limit of detection, limit of quantification, ruggedness and robustness.

The retention times for Paracetamol and Ketoprofen are found to be 1.50 and 6.27 min respectively. Quantitative linearity has been observed over the concentration range of 50 to 500 µg mL^{-1} for Paracetamol and 20.05 to 200.54 µg/mL for Ketoprofen respectively. The regression equations of concentration of Paracetamol and Ketoprofen are obtained as y = 1319x+8671, y = 5280x + 29575 respectively where y is the peak area and x is the concentration of drug (µg/mL). The % recovery of Paracetamol and Ketoprofen are found to be in the range of 97% to104 %. All the validation parameters are within the acceptance range.

OP 22. Structural and spectroscopic studies ofHydro tris (3, 5 dimethyl pyrozyl borate) by density functional method

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The DFT study of Hydro tris-(3,5 dimethyl pyrozyl borate) represented as $[HB(C_3N_2HMe_2)_3]^-$, that belongs to the class of scorpionate ligands involves structural investigation, spectroscopic studies (IR, UV) using (B3LYP) hybrid functions with 6-31G+(d, p) and 3-21G basis sets. Frontier orbital analysis was carried to find the interactions between HOMO-LUMO. Title molecule was analyzed by Natural bond orbital analysis and first order hyperpolarizability calculations using basis set 6-31G+ (d, p) method. NBO analysis has been carried out to study the stability of the molecule arising from hyper conjugative interactions and charge delocalization. These results shows the existence of intramolecular charge transfer (ICT) within the molecule. UV-Vis spectrum and its electronic properties such as, oscillator strength and wavelength were calculated by Time dependent Density Functional methods. Molecular electrostatic potential (MEP) and thermodynamic properties such as standard heat capacities ($C_{p,m}$), standard entropies (S_m) and standard enthalpy changes (H_m) of the title molecule have been calculated.

Keywords: B3YLP, hyperpolarizability, TD-DFT, ICT, NBO analysis.

OP 23.ThermodynamicExcess Properties and FTIR Spectroscopic Studies of Binary Mixtures Containing Propiophenone and 2-Alkoxy Ethanols at Temperatures 303.15K, 308.15K, 313.5K and 318.15K

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Densities ρ, viscosities η and ultrasonic speeds of sound of binary mixtures of Propiophenone (PPH) with 2-Alkoxy Ethanols [2-Methoxy Ethanol, 2-Ethoxy Ethanol, 2-Butoxy Ethanol] have been measured over the entire composition range from 303.15K to 318.15K and at atmospheric pressure 0.1MPa. The experimental data has been used to calculate various acoustical parameters like excess molar volume V^E, excess ultrasonic velocity U^E, acoustic impedance Z, excess acoustic impedance (Z^E), isentropic compressibility K_S, excess isentropic compressibility K_S^E, intermolecular free length L_f, excess intermolecular free-length (L_f^E) were calculated and the computed results were fitted with the Redlich Kister equation to estimate the binary coefficients and standard deviation between experimental and calculated data. At different concentrations, FTIR analysis has been done for the above binary mixtures to confirm the hydrogen bonding presence.
Keywords: Ultrasonic speed, impedance, excess molecular volume, Intermolecular free-length, isentropic compressibility.

OP 24. A Study on Physico Chemical parameters to assess Ground water quality in Post Monsoon season at Coastal regions of East Godavari District in Andhra Pradesh, India.

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One of the essential natural resources for sustaining life and environment is water and maximum demand of drinking water is met by the ground water. Over the last few decades the ground water quality has been declined. A systematic and continuous water quality monitoring is required to assess the principle pollutants in contaminated water and provide necessary remedial methods for better sustainability of the population at coastal habitations. This study was carried out by subjecting 164 ground water samples collected from 82 villages (12 Mandals of coastal zone are Tuni, Shankavaram, Tondangi, Gollaprolu, Pitapuram, U.Kothapalli, Kakinada Rural & urban, Samarlakota, Karapa, Kajuluru and Tallarevu) in Post Monsoon season (Nov-2017) and analysed for ten Physico-chemical parameters viz pH, Total Alkalinity (TA), Total Hardness (TH), Total Dissolved Solids (TDS), Electrical Conductivity (EC), Chloride (Cl^-), Calcium (Ca^{+2}), Magnesium(Mg^{+2}), Nitrate (NO_3^-) and Fluoride (F^-). Obtained results of the analysisevaluatedthat almost all parameters were exceeding the permissible limits of drinking water prescribed by standards of BIS, ICMR and WHO. Statistical data of each parameter viz pH is ranging from 6.8-8.1, Total Alkalinity in mg/l is (211-1430), Total Hardnessin mg/lis (217 - 1782), Total Dissolved Solids in mgL^{-1} is (366 – 5517), Electrical Conductivity in µmhos cm^{-1} is (546 – 8234), Chloride in mgL^{-1} is (34 – 2655), Calcium in mg/lis (36-437), Magnesium in mg/l is (24-236), Nitrate in mg/l is (2.0 – 126) and Fluoride in $mgL^{-1}$is (0.14-0.93). Except pH and Fluoride all the parameters were exceeding the standard permissible limits of drinking water. This study revealed that the ground water of the selected coastal habitations of the study area is unsuitable for the drinking purpose. Due to lack of awareness and drinking water resources, population which is being resides in and around the study area may be utilised this water

without proper water purification. Instant need is required to take necessary action for the applicable water treatment to prevent the population from adverse health effects in this region.
Key Words: Physico-chemical parameters, Ground water quality, Permissible limits, Coastal regions, Water purification.

OP 25. Role of Fuel Cell in Future Energy Generation

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The future energy crisis is an important problem for the present scientists to pursue solutions. Usage of natural energy sources to overcome this energy crisis is the best option and the next problem is to focus is the storage of energy. Fuel cell (FC) is a good alternative energy source that can efficiently generate electricity by consuming fuels and oxygen. FC has fuel flexibility. Hydrogen is the cleanest fuel with highest energy density in terms of mass. Both hydrogen and oxygen can be synthesized by water splitting using photo-catalytic processes and fuels like methanol can be produced from bio-degradable garbage. Hence, more environmental friendly fuels are there. This means that solutions for the usable energy crisis can be sought from our own surroundings instead of depending on crude oil. However, there are some drawbacks in FC systems especially the slow kinetics of oxygen reduction at cathode and the expensiveness of catalyst used for it. Attention is given how to overcomethis, what extent present researches help to commercialize the fuel cell technology and what are the research areas ahead to develop this FC technology.

OP 26. Synthesis of Styrylpyrazoles and isoxazoles Towards Potential Antitubercular Agents

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A series of styrylpyrazoles and isoxazoleswere synthesized by modifying the structure of Hispolon by bioisosteric replacement of 1,3-diketo functional group with the corresponding pyrazole and isoxazole moieties and characterized by spectral data. These compounds were subjected to *in vitro* anti-tubercular activity screening against Mycobacterium tuberculosis (H37Rv) strain. The synthesized compounds showed varied anti-tubercular activity ranging from 100 to 1.6 µg/mL. Among the tested compounds isoxazoles showed better anti TB activity with IS-02 showing maximum potency with MIC of 1.6 μgmL^{-1}. In the pyrazole series the compounds PY-01 and PY-02 showed highest potency with MIC of 3.2 μgmL^{-1}. The most promising compounds showed negligible antibacterial and highlighting their highly selective antimyco bacterial effects. The drug-inhibitor studies using the compound IS02showed slight synergism with corresponding hispolon, rifampicin, streptomycin but did not show any appreciable synergism with INH.
Key words: Isoxazole, pyrazole, antitubercular, antibacterial, mtbFabH, ketoacyl synthase inhibition.

OP 27. Synthesis and Characterization of Oxadiazole Scaffolds for Assessing Medicinal Potentials

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We report 1-phenyl-3-(3,4,5-trimethoxyphenyl)-1H-pyrazole derivatives as a series of novel 1, 3, 4-oxadiazoles through iodine-catalysed oxidative cyclization of the hydrazone derivatives in the

presence of K_2Co_3 and DMSO as solvent in good to excellent yields. The structures of all the newly synthesized compounds were characterized by IR, ^{1}H NMR, ^{13}C NMR and HRMS. Further the synthesized compounds were evaluated for their antimicrobial and anti-oxidant activities.
Keywords: Oxadiazoles, Derivative, Anti-microbial, Anti-oxidant activity.

OP 28. Molecular Interactions in Binary Mixtures Containing Halo-Substituted Carbonyl Compound + Alkoxy Alkanols+ Amines + Xylenes at Various Temperatures

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Densities, viscosities and ultrasonic velocities of binary mixtures containing halo-substituted carbonyl compounds with alkoxy-alkanols, amines, and xylenes were measuredat various temperatures and ambient pressure. From experimental data, parameters were calculated and fitted into the Redlich-Kister equation. The parameters of excess functions are found sensitivefor the intermolecular interactions between the binary mixtures. Theoretical values of viscosity of the binary mixtures were calculated using empirical relations and theoretical equations. The relative merits of these relations and theories were discussed.
Keywords: Ultrasonic velocity, viscosity, redlich-kisterequation, carbonyl compounds.

OP 29. Quality Evaluation of drinking Water Sources

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In the present investigation, efforts are made on Characterizing waters collected from drinking water sources for physicochemical parameters to assess their quality. Water samples were collected as per the standard procedures of sampling from different locations in Tuni and Kotananduru of East Godavari District. pH indicated slight acidic nature and slight basic nature. TDS crossed permissible limit of drinking water standards in majority water samples and indicated the presence of soluble solids in waters. Higher EC indicated the Saline nature of waters. Elevated levels of Total Hardness indicated the hardness of waters. Total Alkalinity crossed the permissible limits which can alter the taste of waters. In some samples fluoride levels are higher than 1 ppm. In somesamples Chloride levels crossed the permissible limit. Higher Nitrate values indicated the discharge of Agricultural run-off into the water sources. Lower values of Sulphate indicated the non discharge of Industrial effluents into water sources. The research results revealed that the waters are chemically contaminated and hence should be treated properly before consideration for drinking or domestic utilization.
Keywords: Water, Parameter, drinking, quality.

OP 30. Quality Evaluation of Ground waters in Agricultural activity areas for assessment of their Potentials for Application

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Water is a natural resource which is vital for the survival of all ecosystems on the earth. Agricultural activities with their intensive utilization of agro chemicals pose a significant potential for negative impact on the quality of ground water. Expansion and intensification of cultivation are among the predominant global changes of this century. Use of chemical fertilizers and pesticides has contributed to the tremendous increase in food production over the past 50 years.
The current paperdeals with the impact of agricultural activities on ground water quality near agricultural activity areas in East Godavari District, Andhra Pradesh, India. Ground water samples were collected and characterized for a range of physicochemical parameters viz., pH, EC, TDS, TH, Ca^{2+},Mg^{2+},TA,Na^{+},K^{+},Cl^{-},SO_4^{2-}, PO_4^{3-}, F^{-}, NO_3^{-}. Irrigation parameters were determined to evaluate the quality of ground waters for assessing their potentials for application. The results revealed that waters are slightly alkaline. Higher values of EC in case of certain water samples indicate their saline nature. Higher TDS indicated the presence of soluble solids in waters. Higher TH indicated the encrustation of waters on water supply systems and makes the waters unsuitable for domestic purposes.
Keywords: Ground water, Agriculture, Characterization, Parameter, Application

OP 31. Biomaterials in Tissue Engineering Applications\

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Tissue engineering is one of the prominent approaches in which natural or synthetic biomaterials could interact with the cells to promote the tissue regeneration activities and restoration. Fabrication of polymeric scaffolds plays a major role as a backbone in the field of tissue engineering; which would mimic the function of extracellular matrix due to its various physical, chemical and biological properties. Several natural and synthetic polymers have been widely used for the bone regeneration such as natural biopolymers viz. collagen, gelatin, alginate, chitosan and synthetic viz. polylactide, polyglycolide, polycaprolactone, poly (lactide-co-glycolide) and ceramic materials like hydroxyapatite, bioglass etc. However, these materials found to have limitations like pore size and its distribution, morphology, hydrophilic properties, mechanical strength, cell attachment and proliferation and differentiation. To overcome these defects, composite materials like a combination of natural and synthetic polymers or bioceramics and synthetic polymers have been designed and successfully used in hard and soft tissue engineering.

OP 32. Exploring nanomaterials with Scanning Electron Microscopy\

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Electron Microscopy is one of the most powerful tools for material characterization. It gives minute details of nanomaterials at high resolution. Microscopy methods and X-ray based characterization in nanomaterials are used to study and characterize a wide variety of nanomaterials used for various applications.Scanning electron microscopy is mostly non-destructive analysis technique for fast imaging and it is the great way to obtain information about topography and compositionof the specimen surface. These techniques are used for the determination of surface morphology and chemical characterization at the nanoscale, which are much useful in various industries such as microelectronics, semiconductor, plastics manufacturing and fabrication, metals processing, paints and coatings manufacturing, pharmaceutical, medical devices manufacturing and cleaning, electronics components, food processing and printed circuit board manufacturing etc. The focus of

this review is the fundamental understanding of scanning electron microscopy and x-ray based characterization techniques. It encompases instrumentation, sample preparation and different modes of analysis. The effective way of using this tool for characterizing micro and nanoscale features will be briefed

OP 33. Effect of Calcination Temperature on CO_2 Adsorption Studies of Rice Husk Ash prepared in different Atmospheres

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The existing carbon dioxide adsorption methods are environmental unfriendly. Thus, a search for new materials and technologies, which are ecologically safe, inexpensive and able to fulfill its role with little pre-processing is growing. One interesting approach is employing agro bio-waste as adsorbents for CO_2 adsorption. Rice husks from local areas are collected and washed with distilled water and subjected to calcination at different temperatures under different atmospheres. Among all the samples rice husk calcined at 600^0C in nitrogen and steam is showing promising results in terms of texture as well as adsorption of CO_2. All the samples are characterized for measuring surface area, pore diameter, X-Ray diffraction studies, FTIR. The adsorption break through with 10% CO_2 balanced helium at 70^0C for all the samples are studied. RHNW-6 has shown maximum break through adsorption capacity of 0.86 mmol g^{-1}. Recyclability has been carried out up to 10 cycles.

OP 34. Investigations on the removal of Lead (II) ions in Synthetic Wastewater - A model for Industrial Wastewater Treatment

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Presence of heavy metals in environmental systems may contribute to adverse effects on environmental and human health. This is a consequence of acute and chronic exposure contaminated air, water and food chain. They are non- biodegradable and are released into the aquatic environment from various industrial activities. Particularly cadmium, lead, chromium, nickel and copper are the most toxic metals of widespread in industrial wastewater.Hence, treatment of wastewater and possible removal of toxic pollutants are very essential before discharge. A number of adsorbents are in use in water treatment process. Most of the conventional treatment methods of metal removal are often limited by their operational cost and ineffectiveness at low concentrations. In this respect, a new search is in progress to identify cheap materials which may have higher potential for the removal of pollutanted water and wastewater systems. The use of activated biomass as adsorbents offers an attractive potential alternative to their conventional methods. In the current investigation, we introduced a new biocarbon material, which is produced from a medicinal plant for the metal removal. In a model trial, 2.5g 100mL^{-1} of biocarbon is used as adsorbent to the removal of Pb (II) ions with the initial concentration of 100 mg L^{-1}. At the equilibrium time of 180min, at a pH of 5.6. It is noticed that 98.85% l of Pb (II) ions removed. In real sample analysis, leather industry wastewater is tested and treated with the biocarbon material. The analytical results are very much promising. The removal process of metal ion on the biocarbon matrix is an ion-exchange mechanism and also mainly depends on the physical characteristics of the materials.

Keywords: Industrial wastewater, biocarbon, activated biomass, toxic pollutants.

Poster Presentations

Nanomaterials

PP01. Synthesis, characterization and applications of silver nanoporous materials using Tween – 80 as sacrificial template

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An elegant method is presented to synthesize Silver porous monoliths using Tween - 80 as sacrificial template. Dextran and Trimethylbenzene(TMB) were added as structural directing agents with Silica as reinforcing agents in situ to silver nitrate. The porous scaffolds of silver were characterized with Fourier transform infra red spectroscopy, Thermogravimetric analysis, Powder X-ray diffractometer, Scanning electron microscopy, and BET surface area analysis. Macroporous morphology with silver nanoparticles was reported with silver monoliths. As synthesized monolith showed good sensor activity against ethyl alcohol.

PP02. Synthesis, characterization and application of Calcium crosslinked Alginate/ Carboxymethylcellulose composite gel

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Novel polysaccharide sponges containing a network of capillaries and pore prepared by dissipative convective phenomenon followed by freeze drying of Ca^{2+} ion cross-linked sodium carboxymethylcellulose/sodium alginate hydrogels with and without dextran and reinforcing agents such as gold, TiO_2, Fe_3O_4, SiO_2 nanoparticles or Graphene oxide (GO) in situ have been reported. The ionotropic gels have capillaries of 10 to 50µm which comprised small pores, 1- 30 µm in size. The as synthesized gels were characterized by Fourier Transform Infra-red spectrometry (FTIR), Scanning electron microscopy (SEM), Bruner Emmett Teller (BET) Surface area study. Mechanical properties of composite sponges were also studied. The gels showed significant sensor activities against glucose.

PP03. Synthesis, characterization and applied applications of Silver monoliths using Triton X-705 as reducing agent with silica nanoparticles as reinforcing agents against iodate sensing and antimicrobial agents.

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Silver monolith with Triton X-705 as reducing agent encapsulating silica nanoparticles was synthesized by modified Sol-Gel method at room temperature which was used as a sensor against iodate by electrochemical method using 0.1M H_2SO_4 as supporting electrolyte. Glassy Carbon

Electrode was used as an indicator electrode. The fabricated sensor responses immediately to iodate over the concentration range of 0.1-5.0 µM with a detection limit of 10 µM and sensitivity of 0.68 µA µM-1 cm-2. Remarkably enhanced electrocatalytic performance of the Ag/Triton X-705/SiNPs was ascribed to the synergistic effect of hierarchical nanostructures with high surface to volume ratio, excellent conductivity and also the excessive electrocatalytic behavior of AgNPs. The fabricated Ag/Triton X-705/SiNPs was carefully characterized by X-ray powder diffraction (XRD) and scanning electron microscopy (SEM), (TEM), (FT-IR), TGA, BET techniques.

The antimicrobial activities of the as synthesized silver monolith were studied against some gram positive and gram negative bacteria such as *Escherichia coli* (MTCC 9537), *Salmonella enterica* (MTCC 734), *Staphylococcus aureus* (MTCC 1144), *Listeria monocytogenes* (MTCC 1143), *Klebsiellapneumoniae* (MTCC 109), *Clostridium* sporogenes (MTCC 1349), *Vibriovulnificus* (MTCC 1145) and *Bacillus subtilis* (MTCC 1272). Silver monoliths showed a significant antimicrobial activities against the chosen bacteria.

PP 04. Characterization of Green Nanoparticles from plant materials

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Nanotechnology is one of the fastest growing areas of science and technology which radically changed the way we diagnose, treat and prevent various diseases in human life. The various metals, like copper, silver, gold, and iron etc which are obtained from plants are known as Green Nanoparticle.

The use of eco-friendly synthesis of green Nanoparticles is known as 'Green Synthesis'. Green synthesis is preferred over conventional synthesis because it is cost-effective, single-step method that can be easily scaled up for large scale synthesis and does not require high pressure, temperature, energy and toxic chemicals.

Silver nanoparticles (AgNPs) are one of the most vital and fascinating nanomaterials among several metallic nanoparticles that are involved in biomedical applications. AgNPs play an important role in nanomedicine. AgNPs were isolated from plant materials and were characterized by different techniques like UV-vis spectroscopy, XRD, FTIR, XPS, SEM and TEM.

Keywords: Green Synthesis, Silver nanoparticles, Extraction, Spectral Methods.

PP05. Nanotechnology in catalysis

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Interest in nanoscience and in nanotechnology in recent years focused attention on the opportunity to develop catalysts that exhibit 100% selectivity for a desired product, thus minimising byproducts and waste. Currently, the research is more focused towards nanostructured catalysts with enhanced physiochemical properties. Nanoscale catalysts have high specific surface area and surface energy, which ultimately lead to the high catalytic activity. Nano-catalysts improve the selectivity of the reactions by allowing reaction at a lower temperature, reducing the occurrence of side reactions, higher recycling rates and recovery of energy consumption. Therefore, these are widely used in green

chemistry, environmental remediation, efficient conversion of biomass, renewable energy development and other areas of interest.

The benefits of moving to the nanoscale are best illustrated by gold. In its bulk form gold is relatively chemically inert, but in nanoparticle form it becomes active for a range of important catalytic reactions like oxidation of carbon monoxide to form carbon dioxide and the epoxidation of propene. The increasing role that nanotechnology is playing in modern catalysis has to do with the increasing surface-to-volume ratio with decreasing particle size which strongly increases the specific catalytic activity.

Key words: nanotechnology, green chemistry, selectivity, catalytic activity.

Pharmaceutical analysis

PP06. Synthesis, characterization, Cytotoxicity, DNA interaction and anitimicrobial studies on copper(II) complexes of p-tolylmethanmine Schiff bases

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Three copper(II) complexes with formulae **1**[Cu(L^1)$_2$], **2**[Cu(L^2)$_2$], and **3**[Cu(L^3)$_2$], where, $\mathbf{L^1}$ -(2-((E)-(4-methylbenzylimino)methyl)-4-nitrophenol, $C_{15}H_{14}N_2O_3$)),$\mathbf{L^2}$-(-2-((E)-(4-methylbenzylimino) methyl)-4-chlorophenol, $C_{15}H_{14}ClNO$)), and $\mathbf{L^3}$(2-((E)-(4-methylbenzylimino) methyl)-4,6-dichlorophenol, $C_{15}H_{13}Cl_2NO$))have been synthesized and characterized by elemental analysis, FT-IR, ^{1}H-NMR, ^{13}C-NMR, ESI mass, ESR, UV-Visible, magnetic susceptibility, SEM and TGA analysis. A survey on spectral and analytical data, assigned for all complexes has a square planar geometry through the coordination of azomethine (C=N) nitrogen and phinolic -OH donor atoms. The Schiff bases and their metal complexes were screened for their antimicrobial activity, the results revealed that metal complexes show more potent activity than free ligands and moderate to standard drugs. DNA binding titrations were also performed and indicated that all complexes bind to CT-DNA via an intercalation mode. Additionally, the metal complexes exhibited good cleavage ability against the pBR322 DNA even at low concentrations in the presence of activators, H_2O_2 as well as UV light. Further, *in vitro* cytotoxicity of the metal complexes against MCF-7 and KB3 cell lines was examined which shows higher activity and efficiently vanished the cancer cells even at low concentrations.

PP07. Comparison of Validated Spectrophotometric And HPLC Methods For Estimation of Cefpirome Sulphate In Pure And Pharmaceutical Dosage Form.

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We developed a quick and reliable green analytical method for the quantitative assessment of Cefpirome sulphate in pure and pharmaceutical formulations by using spectroscopic and chromatographic modes for quality control. The spectroscopic techniques devised for assay of Cefpirome sulphate comprise UV and IR. The novel HPLC method was progressed for determination of Cefpirome sulphate in pure and pharmaceutical formulation. UV method involves absorbance measurement at 270 nm serving phosphate buffer pH 6.8 as a solvent. In IR potassium bromide was employed to prepare discs, analysis was performed by marking the concentration of N-H group

existing at a wavenumber 3562 cm^{-1}, employing base-line technique. For both spectroscopic ways, absorbance was found to incline with concentration of 4-20 μgmL^{-1} (UV) and 10-50 w/w (IR) for Cefpirome sulphate. The correlation coefficient is 0.9998. Chromatographic distinction was accomplished on 250x4.6mm, 5µ particle size Phenomenex C18 column at 270 nm utilizing a mixture of methanol and water in the ratio of 60:40 as the mobile phase. Linearity for peak area was found in the concentration range of 2-10 μgmL^{-1} with correlation coefficient of 0.9999. All these methods have been successively applied for estimation of CPS and were validated according to ICH guidelines. F-test and t-test at 95% confidence level were used to check data obtained under different experimental setups; the calculated value was found to be less than the critical value.

PP08. Simultaneous estimation of Dapoxetine and Tadalafil in bulk and Pharmaceutical dosage forms by RP-HPLC method

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A simple, sensitive, linear, precise, and accurate method by gradient reversed-phase-high performance liquid chromatography for the simultaneous estimation of Dapoxetine and Tadalafil in bulk and in their combined tablet dosage form was developed and validated. The separation of the two drugs was based on the use of Zorbax SB C18 (100 × 4.6 mm, 3.5 µm) column in a gradient mode. Mobile phase consisted of potassium dihydrogen phosphate, tetrabutyl ammonium hydrogen sulfate, triethylamine adjusted to PH 3.0 with dilute ortho phosphoric acid (solvent A) and Acetonitrile and methanol was prepared in the ratio of 60:40, v/v (solvent B) was set with gradient programming for 20 min and was delivered at 1 ml/min flow rate and effluents are achieved with variable wavelength at 280 nm.Thestocksolutions were prepared by using A 60:40, v/v mixture of 0.05% triflouroacetic acid and acetonitrile was used as the diluent.The retention times of Dapoxetine and Tadalafil were found to be 6.913 and 9.483. The percentage assay of Dapoxetine and Tadalafil was found to be 99.92% and 99.32. Calibration curves were linear for Dapoxetine and Tadalafil at concentration ranges of 60-364 µg/ml and 40-122 μgmL^{-1} with the regression coefficient of 0.999 for all the two drugs and precise with (% relative standard deviation <2). The limit of detection for Dapoxetine and Tadalafil was found to be 0.05 µg mL^{-1} and 0.004 μgmL^{-1}, and limit of quantitation for Dapoxetine and Tadalafil was found to be 0.012 μgmL^{-1}, and 0.006 μgmL^{-1}, respectively.

PP09. Simultaneous Estimation of Canagliflozin and Metformin in Human Plasma by HPLC

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The combination of canagliflozin and metformin was recently approved for the treatment of type-2 diabetes. We developed a simple, sensitive, précised and accurate isocratic method for the simultaneous estimation of canagliflozin and metformin in human plasma using dapagliflozin as internal standard. Chromatography was performed on waters 2695 HPLC equipped with a quaternary pump. The separation was achieved by using Agilent C18 (150 × 4.6 mm, 5µm), buffer:acetonitrile (55:45%v/v) as mobile phase with 1mL min^{-1} flow rate. The detection of analyte was monitored at

250nm by using PDA detector. The extract method involves protein precipitation by using acetonitrile. Retention time of Canagliflozin, metformin and internal standard was found at 3.806, 2.246 & 5.476 min respectively. The peaks were found to be free of interference. The method is validated over a dynamic linear range of 0.02-2.00µg mL^{-1} and 0.20 to 20.00µg mL^{-1} for canagliflozin and metformin respectively, with a correlation coefficient of 0.999. The precision and accuracy of samples of six replicate measurements at lower limit of quantification (LLOQ) level were within the limit. The analytes were found to be stable in human plasma at-28°C for 37 days. The method was validated as per FDA guidelines. The stability, sensitivity, specificity and reproducibility of this method make it suitable for the determination of canagliflozin and metformin in human plasma.
Key words: Canagliflozin, Metformin, Isocaratic, Type-2 diabetes.

PP10. An Investigative Study on Impurity Profiling of some Selected Drugs

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Impurity profiling for pharmaceutical compounds has a great significance while evaluation safety and efficacy of the drug product. The unwanted chemical substance in the drug is termed as impurity. The various sources of impurities in pharmaceutical products are reagents, heavy metals, ligands, catalysts, and the degraded end products obtained during / after manufacturing of bulk drugs by hydrolysis. photolytic cleavage, oxidative degradation, decarboxylation etc. Now, efforts are made on the impurity profiling studies on some selected anti depressive, anti allergetic, anti hypertensive and anti-inflammatory drugs. The strategies in impurity profiling include separation, identification, isolation or synthesis and characterization of impurities. In profiling of impurities, chromatographic and spectroscopic techniques such viz., TLC, GPLC, LC-MS, NMR, IR, LC-NMR, LC-NMR-MS and GC-MS etc., are being employed.
Keywords: Characterization, Chromatography, Impurities, Spectrometry

Air pollution monitoring

PP11. Prediction of $PM_{2.5}$ Concentration using Quadcopter - A Case Study from Rajam Town of Srikakulam District of Andhra Pradesh

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$PM_{2.5}$ is the fine particle matter with the size smaller than 2.5µm and is considered being one of the atmospheric pollutants whose effects are the greatest on the public health. The accurate measurement of $PM_{2.5}$ provides a crucial basis for health impact assessment and pollution management and control. Here, we propose propose a novel platform to manage drones monitoring of $PM_{2.5}$ in the outdoor environment. This project demonstrates the feasibility of Quadcopter equipped with dust sensors effectively and flexibility to measure three-dimensional $PM_{2.5}$ concentration within 8M altitude, particularly peak hours of a day and measured for three months. The present case study of Rajam of the average concentration of $PM_{2.5}$ was recorded as moderate as per CPCB norms. The experimental results show that in the $PM_{2.5}$ concentrations decrease when height increases. The increasing concentration rate of $PM_{2.5}$ concentrations is larger in the morning than in the afternoon. The results demonstrated that there are fluctuations in concentrations during different peak periods of the day.
Keywords: Dust monitoring, Quadcopter, 8M altitude, Peak hours of day, $PM_{2.5}$ µg m^{3-1}.

PP12 Development of new cloud point extraction procedure using mixed micelles of TX-114 and DOSS for the determination of Azocarmine G.

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A new cloud point extraction (CPE) procedure with spectrophotometry for the preconcentration and extraction of azocarmine G (ACG) has been developed using mixed micelles of Triton X–114 (TX–114) and Docusate sodium salt (DOSS) for the CPE of azocarmine G at pH 4.6. In this method the dye azocarmine G was extracted into the surfactant rich phase of mixed micelles of TX-114 and DOSS by heating the sample at 70°C for 20 minutes. Various parameters effecting the extraction of dye like pH, concentration of TX-114, concentration of DOSS, equilibrium temperature and equilibrium time were optimized. Under optimum conditions the linear range of azocarmine G was found to be 0.0–23.18 µg mL^{-1}. The corresponding limit of detection was found to be 4.125 ng mL^{-1}. The proposed method has been successfully applied to the extraction of azocarmine G in tap water and sea water. The recoveries were found to be in the range of 89.91-106.9 %.
Keywords:Cloud point extraction, mixed micelles, spectrophotometry, TX-114, DOSS

PP13. Molecular Interactions In Binary Mixtures Containing Halo-Substituted Carbonyl Compound + Alkoxy Alkanols+ Amines + Xylenes at Various Temperatures

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Densities, viscosities and ultrasonic velocities of binary mixtures containing halo-substituted carbonyl compounds with alkoxy-alkanols, amines, and xylenes were measuredat various temperatures and ambient pressure. From experimental data, parameters were calculated. The obtained values were fitted to the Redlich-Kister equation. The parameters of excess functions are found sensitivefor the intermolecular interactions between the binary mixtures. Theoretical values of viscosity of the binary mixtures were calculated using empirical relations and theoretical equations. The relative merits of these relations and theories were discussed.
Keywords: Ultrasonic velocity, viscosity, redlich-kisterequation, carbonyl compounds.

PP14. Studies on Water Quality Parameters of Kankipadu Mandal Krishna District

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In developing countries water pollution has become major concern now a day. We concentrated in assessment of water quality in and around the region of Kankipadu. In this study, the water quality has been assessed in terms of temperature, pH, Electrical conductivity, total suspended solids (TSS), total dissolved solids (TDS), total hardness (THA), temporary hardness (HAT), permanent hardness (PAH), chloride (CL), sulphate (SUL), Calcium (CA), magnesium (MG), phosphate (PO4), chromium

(CR), Biological oxygen demand (BOD), chemical oxygen demand (COD), Dissolved oxygen (DO), total alkalinity (ALK), and nitrate (NO). These parameters throw light in adopting apt steps to bring down the extent of water pollution.
Keywords: Water quality, parameters, COD, BOD, DO, Hardness of water etc.

PP 15. Bioconversion of crustacean waste to value added product

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Every year 6 million to 8 million tonnes of waste crab, shrimp and lobster shells are produced globally about 1.5 million tonnes in Southeast Asia alone. In spite of being highly rich in chitin content, this by-product is neither profitable nor environmentally friendly due to its extremely slow degradation in nature and it is underutilized and is thus wasted. Maritime industry has the problem of disposal of crustacean waste. This is an issue requiring serious attention with burgeoning global shellfish production which is dumping this by product continuously. Hence, bioremediation of this high voluminous waste will result in environmental cleaning and producing useful products from waste. Bioconversion of chitinous materials has been proposed as a waste treatment alternative for the disposal of crustacean wastes. Effective recycling and utilization of this grossly underutilized waste is of great economic and ecological importance. This review summarizes the use of this crustacean shell fish wastes and the various applications of chitin biopolymer and its derivatives which shows many biological activities (e.g., anti-cancer, antioxidant, and immune-enhancing) and can be used in the fields such as medical, cosmetic, food, and textile etc. Slow recycling of crustacean waste in nature results in accumulation of dumps leading to environmental pollution.
Keywords*:* Disposal of crustacean waste, maritime industry, chitin biopolymer and its derivatives.

PP 16. Synthesis, Biological activity & docking studies of 3, 5-diaryl isoxazoles having 1,4-dioxan ring

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Most of the 3, 5-diaryl isoxazole derivatives exhibit moderate to excellent biological activities in the field of medicinal chemistry. The synthesis, characterization and docking studies of a series of novel 3, 5-diaryl substituted isoxazole derivatives possessing biologically active pharmacophores like, 1, 4-dioxan ring and peptide bond are carried out. They are tested for anti fungal, anti viral, and anti cancer activity.
Keywords: Synthesis, Antifungal, Biological, Isoxazole, Derivative

PP17. Viscometric study of binary mixtures containing Propiophenone with alcohols 1-Propanol, 1-Butanol and 1-Pentanol at temperatures 313.15K and 318.15K

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The current study deals with densities 'ρ', and viscosities of binary mixtures of propiophenone (PPH) with 1-alcohols [1-Propanol, 1-Butanol, 1-Pentanol] measured over the entire composition range at

temperatures from 313.15K and 318.15K and at atmospheric pressure 0.1MPa. The experimental η data has been used to calculate deviations in viscosity (Δη) by correlating with theories like Grunberg Nissan (d), Hind(H_{12}), Katti –Chowdary (Wvis/RT), Tamura-Kurata(T_{12}) and Gibb's free energy(G^{*E}) activation relations. The deviations in viscosity with composition and temperature of the mixtures have been discussed in terms of molecular interaction in these mixtures. The parameters of these studied systems were found to be responsive towards molecular interactions. The computed results were fitted with the Redlich Kister equation to estimate the binary coefficients and standard deviation between experimental and calculated data.

Keywords: Density; Deviation in viscosity; molecular interactions; Viscosity theories.

PP18. Soil Contamination with Heavy Metals -Impacts on Human Health

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The health issues of longstanding, low-level exposure to soil impurities is of particular interest, and researchers,decision makers have both pointed optimum information in this sector. On the other side, the investigation of soil and human health is a hard task. The soil contaminantinvestigation in isolation does not favor the scientists a true picture of the complicated relationships between contaminants and health. This In-detailed Report from Science for Environment Policy draws on present research and number of case studies from different scientific disciplines that examine the interaction between polluted soils and human health. It demonstrates contaminant path from soil to the human and some of the different properties of soil are shortly examined. These are most vital factor in determining percentage of a contaminants are available in both to the human body, and for transport around the surrounding atmosphere. The most common contaminants of soil are heavy metals and mineral oil, and roughly three million areas are analyzed to have been potentially affected by activities that can pollute the soil. Diseases like cancers, nerve damage and low IQ level, kidney disease, and skeletal and bone diseases are serious concern. In many cases heavy metals and persistent organic chemical substances are of particular concern. Industrial activity can introduce heavy metals such as cadmium, arsenic and mercury in to soil through mining, smelting, agriculture and fossil fuels burning. Our degradation of materials containing heavy metals which includes paint, e- waste, and sewage also contributes to the pressure of heavy metal pollution. Organic hazard chemicals are also part of industrial effluents, and many are still extensively used. Composite mixtures of these industrial chemicals in the environment and in human bodies cause major challenges to scientists are trying to analyze the health problems of these widespread substances. There are many methodological contests relating to the study of soil, human biology, sampling techniques and their interactions between numbersof factors in soil and health. But the contaminants do not necessarily tell any disaster,

Keywords: soil contamination,heavy metals, human health, disease.

PP19. The construction of 2-halaaromatic/aryl/alkyl cyanamides libraries and further conversion into tetrazole compounds

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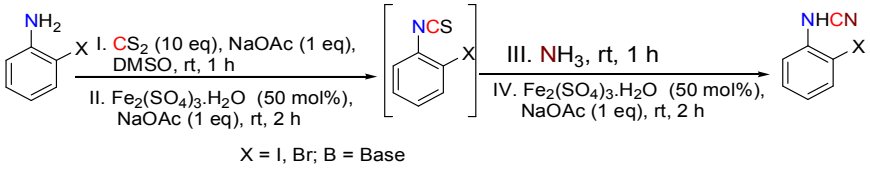
One pot multi step reaction towards the synthesis of 2-halo aromatic/aryl/alkyl cyanamides has been carried out in the presence of transition metal under mild reaction conditions. The cheap, air stable

and readily available iron source as a catalyst was developed for desulphurization. In addition, the scope ofsubstrate has been explored.



X = I, Br; B = Base

Keywords: Iron catalyst, Cyanamides, Room temperature, Multistep reaction, One pot reaction.

PP20. Role of Chemistry in Industry and Environment

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Everything is made of chemicals. Many of the changes we observe in and around are caused by chemical reactions. Chemistry is very important because it helps us to know the properties of matter. All the matters are made up of chemistry. Society tends to consider every manmade chemical as bad and everything natural as good. Just because something is natural does not automatically make it good for the health or the environment or unsafe if it is a manmade chemical.

Environmental issues such as climate change, water pollution and renewable energy have become increasingly important in day to day life. Many people perceive chemistry and the chemical industry as harmful to the environment. However, many new advances and scientific researches in the field of chemistry are helping us to develop more environment friendly materials and applications, while preserving the quality and the lifestyle we expect. Research in biological sciences and chemistry has revealed that industrial processes in chemistry could play a role in developing solutions to environmental problems such as climate change, waste management, recycling, energy efficiency etc. Without chemists we might never have truly understood these problems. Profound changes have been made and still are being made to provide alternative solutions. Over the years, the industry and wider public have become aware of the damaging effects of some past practices and the need to protect the environment. In the past, few were aware of the potentially negative effects our modern lifestyle might have on the environment, and rather saw only the positive potential for creating new, useful materials and products.

Industry has also developed a number of voluntary initiatives to raise the standards in dealing with health and environment issues and establish safe and sustainable systems in accordance with regulations. The industry publishes guidelines for the distribution and handling of chemical substances that require appropriate precautions. All these efforts guarantee that chemistry is carried out in a safer and more environmentally friendly way. Strengthening the science of chemistry through research and development is necessary to allow us maintaining a comfortable life in harmony with the environment and nature. It illustrates the greatest challenge of all disciplines of modern science, and most especially with those that pertain to the environment, integration of technology, nature and human beings.

PP21. Impact of Chemical Industry on Environment

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Many of our day to day activities involve chemistry broadly. Pollution, environmental disturbance and effects on human health are problems that manifest as society comes to rely more and more on chemical tools. Chemistry plays an vital role in the solving several of the environmental problems such as pollution because when you know more about chemistry you will know what are the effects of incorrect disposal of chemicals and when you know this you could minimize the pollution caused by chemicals. Careful handling of chemical products and a thorough testing of their effects is an essential step in reaping the benefits of chemistry. Applications of chemical science have contributed significantly to the advancement of human civilization. Hence industries that strictly follow the guidelines of sustainable chemistry principles in design of products and process that minimize the use and generation of hazardous compounds.

PP22. Synthesis and characterization of some Hydroxy Benzohydrazide derivatives to evaluate their microbial activities

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4-Hydroxy benzoic acid derivatives attracted the attention of synthetic chemists for their antifungal, antimutagenic, antisickling, estrogenic and antimicrobial activities. Aseries of 4-hydroxy benzohydrazide derivatives were synthesized by the condensation of hydroxyl benzohydrazide with fluoro benzaldehydes in the presence of C2H5OH and characterized by IR, ^{1}H NMR, ^{13}C NMR and MS spectral analysis. The derivatives were evaluated for their invitro antimicrobial activity against *E.Coli*, *Pseudomonas* (gram negative) and *S.aureus, B.subtilis* (gram positive) bacterial strains with control drug Streptomycin.

Keywords: Characterization, Derivative, Microbial activity, Bacteria

PP23. Identification and Characterization of Forced Degraded impurities of Fenoxazoline using Chromatographic and Spectroscopic Techniques

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A selective specific and sensitive HPLC method was developed for determination of Fenoxazoline degradation impurities. The chromatographic separation was achieved on Shimadzu LC-2010 with PDA system and Kromasil C18 column using gradient elution of mobile phase. We report herethe degradation products using different conditions. The degraded products were subjected to LC-MS to find out the impurities. Based on the mass of impurities, the structures were assigned. The proposed method was successfully employed for estimation of Fenoxazoline impurities in pharmaceutical preparations.

Keywords: Characterization,Fenoxazoline, Degradant, Impurities

PP24. Bio magnification of metals in plant species

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Ecosystem contamination and metal toxicity to plants is one of the major problems at global level. Metal contamination in agricultural environments can originate from atmospheric pollution, application of pesticides, chemical fertilizers and irrigation with poor quality waste water. Though, some of metals are bio elements (macro and micro nutrients) at normal concentration, they are hazardous in the plants when present in excess. Moreover, these metals have strong impact on human health through the food chain. Toxic metals or biometals as bio elements in higher concentrations constitute as xenobiotics. These metals can initiate acute or more dangerous and frequently occurring chronic diseases. However, anthropogenic activity and its effects on environment can also show that medicinal plants have also responded on the changing environmental conditions. Even literature indicated that there is currently only a limited understanding and quantification of some key parameters. Hence eco-friendly technologies such as phyto remediation have its potential for the removal of the harmful metals from the environment.
Key words: Metal, Bio magnification, Hazard, Plant, Environment.

PP 25. Possible consequences of CNS depressant use and abuse

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CNS depressants are substances that can slow normal brain function. Because of this property some CNS depressants are useful in the treatment of anxiety and sleep disorders.Barbiturates such as Mephobarbital (mebaral) and Pentobarbital Sodium (membutal), which are used to treat the anxiety, tension and sleep disorders.Benzodiazepines such as Diazepam (valium), Chlorodiazepoxide HCl (Librium) and Alprazolam (xanax) are prescribed for anxiety, acute stress reactions and panic attacks.

Often the abuse of Barbiturates and Benzodiazepines occurs in conjunction with the abuse of another substance or drug such as alcohol or cocaine. In these cases of poly drug abuse, the treatment approach must address the multiple addictions.
Keywords*:* Anxiety and sleep disorders, barbiturates, mephobarbital, pentobarbital sodium, benzodiazepines, diazepam, alprazolam.

PP26. Fluroscence Studies Of Acid-Catalyzed Crosslinking With Pva

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The present study determines varying concentration of acid catalyzed cross linking poly vinyl alcohol (PVA) with Glutaraldehyde by Fluroscence Spectrometry. PVA with varying concentrations (1, 2, 3, 4, and 6%) of Glutaraldehyde (2.8, 3.2, 5.6, 32, 34%) of degree of crosslinking were observed maximum 34% of crosslinking density was observed due to the increase in the content of crosslinker glutaraldehyde. Rate of swelling ratio, diffusion coefficient is also determined. Changing the concentration of glutaraldehyde will affect the swelling of the film. The P^H did not affect the swelling and diffusion coefficient.
Keywords: hydrogel, poly vinyl alcohol, glutaraldehyde, swelling,diffusion.

PP27. Non Conventional Energy Resourses – Impact On Human Health

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The principle environmental and health impact of energy are due to the use of solid fuels like bio-mass, coal, charcoal, fuel wood for cooking and heating in simple devices that produce large amounts of pollutants. In communities fuel use is the main cause of atmospheric pollution through there is a variation among cities in the relative contribution of vehicles and point source.
In developing Countries the diesel fuelled vehicles are more prominently used, which shown impact on human health. Emission of nitrogen, sulphur and carbon dioxide lead to acid deposition far from their sources. These depositions cause damage to human environment.The energy use is the human activity most closely linked to potential climate change finally climate change is threat to have significant direct impact on human health and on ecosystem.
Key words: Solid Fuels, Atmosphere pollution, Point sources, Human health.

PP28. Characterization of Organic pollutants in water sources

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All life on earth is influenced and adapted by water. Natural water contamination is cumulative consequence of agricultural and industrial activities. These activities can introduce organic pollutants from the usage of fertilizers, pesticides and heavy metals etc., keeping in view the present scenario; it is proposed to characterize ground waters around industrial areas for physicochemical, metal ions and microbial species for evaluation of quality of waters for taking initiatives to protect the quality of waters.
Key words: water, Characterization, parameter, industry.

PP29. Isolation, Characterization and Phytochemical Analysis of Mangrove Plant Species

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The mangrove forests are widely spread along coastal line across the India. Keeping in view the importance of medicinal plants as natural products derived from the nature, it is proposed to carry out isolation of chemical compounds. It is followed by their separation , analysis of metal ions by ICP-MS technique from the plant species. It is also proposed to carry out analysis for antioxidants, nutrients and anti nutrients. The outcome of the present investigation can help the pharmaceutical industry to design new drugs.
Key words: Mangrove plants, Extract, Metal ion, Antioxidant, Nutrient, Anti nutrient.

PP30. Seasonal Variation of Physico-Chemical parameters of Groundwater in Proddatur Area of YSR Kadapa DT, AP-India

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People on globe are under tremendous threat due to undesired changes in the physical, chemical and biological disturbances in air, water and soil. Due to increased human population, industrialization, use of fertilizers and man-made activity, water is highly polluted with different harmful contaminants. Natural water contaminates due to weathering of rocks and leaching of soils, mining processing etc. It is necessary that the quality of drinking water should be checked at regular time intervals, because of contaminated drinking water, human population suffers from varied water borne diseases. The availability of good quality water is an indispensable feature for preventing diseases and improving quality of life. It is necessary to know details about different Physico-chemical parameters such as Hydrogen ion concentration, electrical Conductivity, total Dissolved Solids, Total Hardness, Calcium, Magnesium, Sodium, Potassium, bicarbonate, Chloride, Sulphate, Phosphate, Dissolved Oxygen, Biochemical Oxygen Demand, Chemical Oxygen Demand etc. for testing water quality. Proddatur area of YSR kadapa district was selected to determine the seasonal variation of groundwater quality in monsoon and summer seasons. In the present study, the results showed that most of the Physico-chemical parameters exceeded the permissible limits of WHO. The water Quality Index (WQI) showed that groundwater is not suitable for drinking purpose in all locations of the study area. So, it is necessary to adopt sound water purification methods in the study area.
Keywords: Industrialization, Contamination, Physico-chemical parameters, Permissible limit, Water Quality Index, Purification.

PP31. Solid waste management in open cast coal mines

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Unlike in other sector, there are no chemical processes involved in the winning of the coal. The mining is mainly two types- Opencast and underground modes. Opencast mining involves extraction of overlying material called as Over Burden (OB) and coal. Presently Stripping Ratio (Ratio of coal to OB) is also being planned in the opencast mines, which indicates that, more than 10 times of waste has to be removed than actual salable coal. Such a voluminous extent of over burden stacked in dump yards in open cast mines poses a great threat to the environment it not pragmatically handled. We report better understanding and broader perspectives of planning, operation and management of solid waste dumps in opencast mines. Further, this paper also discusses need for stabilization, slope stability, engineering and biological principles involved in reclamation of Over burden Dumps.
Keywords: Mining solid wastes, planning, operational, mine closure objectives, challenges, design criteria, biological engineering management of soil.

PP32. Biological Activities of Hydrazone Derivatives

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Hydrazones possessing an azometine -NHN=CH- proton constitute an important class of compounds for new drug development. The inspiration is from the development of novel compounds with anticonvulsant, antidepressant, analgesic, antiinflammatory, antiplatelet, antimalarial, antimicrobial, antimycobacterial, antitumoral, vasodilator, antiviral and antischistosomiasis activities. The critical knowledge bitsdeveloped are reviewed.
Keywords: Hydrazones, hydrazide-hydrazones, biological activity, isoniazid.

PP33. An Efficient Methodology Towards the Synthesis of (2*R*, 4*R*)-ethyl-4-methylpiperidine-2-carboxylate

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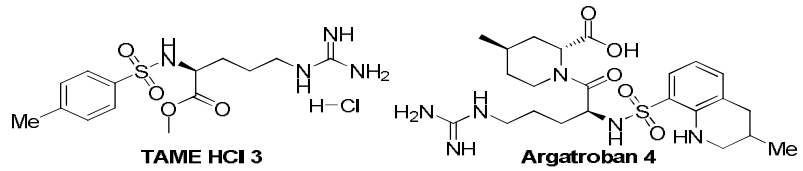
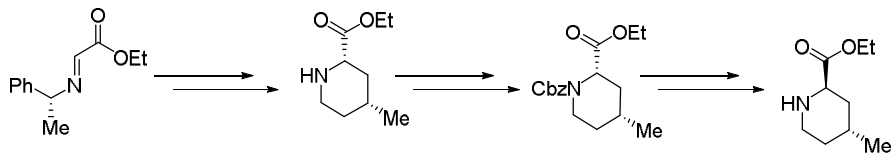
In the majority of natural products or medicinally important leads, so calledprivileged skeletal fragments can be identified. (2*R*,4*R*)-ethyl 4-methylpiperidine-2-carboxylate and (2*S*,4*S*)-ethyl 4-methylpiperidine-2-carboxylate are the important skeletal fragments in the medicinally important products and it is the key intermediate used in the synthesis of Argatroban. Argatroban is used as an anticoagulant in individuals with thrombosis and heparin induced thrombocytopenia. Historically, impressive synthetic work has been reported starting from two simple lead compounds TAME (*N*-Tosyl-l-Arginine Methyl Ester) and benzamidine. A highly enantioselective synthesis of (2*R*,4*R*)-ethyl 4-methylpiperidine-2-carboxylate was developed by using commercially available starting material. The product was isolated in high yield with excellent enantiomeric excess 99%.





Scheme

PP34. Fluorescence Studies of Chitosan Hydrogels By Using Glutaraldehyde Cross Linker

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Hydrogels are unique, consisting of a self-supporting, water-swollen three-dimensional (3D) viscoelastic network. It permits the diffusion and attachment of molecules. Despite of the vast importance of green chemistry synthesis and characterization, natural biopolymers eliminate the danger to health and environment. Polysaccharides are widely spread biopolymers with diversity of structure and properties. Chitosan is a natural cationic copolymer with hydrophilic nature. The present study determines the gelation of chitosan by varying the concentrations of glutaraldehyde. 30% of crosslinking density was observed due to the increase in the content of crosslinker glutaraldehyde. Changing the concentration of glutaraldehyde will affect the swelling. The pH did not affect the swelling and diffusion coefficient. The crosslinked hydrogel concentration was studied from fluorescence. Fluorescence microscopy is a rapid expanding technique, both in the medical and biological sciences. It is a fast, simple and inexpensive method to determine the concentration of an analyte in solution. With enhanced physicochemical and biological properties, of cross-linked chitosan hydrogels and its concentration studies were determined by fluorescence.
Keywords: Hydrogel, Chitosan, Glutaraldehyde, Swelling,

PP35. Binuclear Ni(II) and Co(II) complexes of bis aryl hydrazone and phenanthroline: Synthesis, spectroscopic, powder X-ray diffraction, fluorescence, FMO, ESP, docking and antimicrobial screening

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A Schiff base ligand $N^{1'}$, $N^{3'}$-bis (4-(methylthio) benzylidene)-5-nitrobenzene-1, 3-dihydrazide (**L**) has been prepared from condensation of 4- (methylthio) benzaldehyde with 5-nitrobenzene-1, 3-dihydrazide. The binucleated Ni(II) (complex **1** $C_{52}H_{45}Cl_2N_9Ni_2O_4S_2$, complex **2** $C_{48}H_{37}Cl_2Ni_2N_9O_4S_2$), Co(II) (complex **3** $C_{52}H_{47}Cl_4Co_2N_9O_4S_2$, complex **4** $C_{48}H_{37}Cl_4Co_2N_9O_4S_2$) and mixed ligand complexes have been synthesized from Schiff base and 1, 10-phenanthroline / 2, 9-dimethyl-1, 10- phenanthroline with good yield. The synthesized compounds has been characterized by elemental analysis, ^{1}H-NMR, ^{13}C-NMR, FT-IR, UV-Visible, magnetic moment, powder X-ray diffraction and molar conductivity measurements. From the analytical spectral data, octahedral and square planar geometry assigned to complexes. Further, the Schiff base and its metal complexes have been investigated for fluorescence activity, frontier molecular orbital determination and molecular docking studies. In addition, Schiff base and its metal complexes were screened for antimicrobial activity against bacteria; *Escherichia coli, Bacillus* subtilis and the fungi; *Sclerotium rolfsii*and *Macrophominaphaseolina*. From the results, it is found that the complexes showed potent antimicrobial activity compared to Schiff base.

PP36. Removal of Disperse dye from Aqueous Solution using Activated Carbon from Jackfruit Waste: Kinetics, Isotherms and Thermodynamics

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We report the preparation of activated carbon from Jackfruit waste. Batch mode experiments were conducted to know the adsorption capacity of prepared activated carbon for the removal of Disperse Blue 14 (DB14) from aqueous. The effect of dye concentration, contact time, temperature and adsorbent dose on the removal of dye was studied. The kinetic experimental models of pseudo-first-order, pseudo-second-order, Weber and Morris intra-particle diffusion model, Bangham's pore diffusion model and Elovich equations have been discussed to identify the rate and kinetics of sorption of dye. Results imply that adsorption of DB14 on the adsorbent nicely followed the pseudo-second order kinetics model and maximum adsorption capacity was found to be 93 mg g^{-1}. Equilibrium adsorption was investigated by the Langmuir, Freundlich, Temkin and D-R isotherms. The thermodynamics parameters of adsorption systems indicated spontaneous and endothermic process.
Key words: Activated carbon, Disperse Blue 14, Isotherms, Kinetics, thermodynamics

PP37. Non Conventional Energy Resourses – Impact on Human Health

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Traditional energy sources for food processing and heating have some impact on our environment and human health. This is due to the use of solid fuels like bio-mass, coal, charcoal, fuel wood for cooking and heating in a simple devices that produce large amount of pollutants. In some communities fuel use is the main cause of atmospheric pollution though there is a variation among cities in the relative contribution of vehicles.

In developing countries the diesel fuelled vehicles are more prominently used, which showed impact on human health. Emission of nitrogen, sulphur and carbon dioxide lead to acid deposition far from their sources. These depositions cause damage to human environment. The energy use in the human activity most closely linked to potential climate change to a level of threat human health.
Key words: Solid Fuels, Atmosphere pollution, Point sources, Human health.

PP38. Method for the determination of Flecainide acetate and its degradation impurities by UPLC-MS

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A sensitive UPLC-MS method was developed for the determination of Flecainide acetate in the presence of four related impurities (Impurities: A,B,D and E). The forced degradation study of

Flecainide acetate was carried out under acidic, alkali, neutral and oxidative conditions. Successful chromatographic separation of Flecainide acetate and its degradation products were achieved on a Waters Acquity BEH C18 column (100 mm x 2.1 mm x 1.7µ) using a mobile phase of solvent A (10 mM Ammonium formate) and solvent B (acetonitrile) in gradient elution. The gradient program employed to achieve the separation was (T_{min}/%Solvent B): 0/15, 1/15, 3/90, 5/90, 7/15, 9/15. The flow rate was maintained at 0.3 mL/min. The impurities were characterized and the fragmentation pathways for the impurities were proposed.

Keywords: Flecainide acetate; Forced degradation; UPLC; ICH, LC-MS method.

PP39.Kitchen Waste to Biogas – A Smart Energy

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Inadequate management of solid waste like uncontrolled dumping leads to several adverse effects like polluting the surface and ground water through lechate.It further results the breeding of flies, mosquitoes and other vector born diseases. Also, it leads to release of unpleasant odour and methne a major green house gas contributing to globalwarming. Here an attempt was made to manage the kitchen waste which is highly nutritive to microbes to synthesise methane by creating an ecofriendly and cost effective biogas plant especially in residential hostel's backyards.

Key words: Solid waste, Sold waste management, Biogas, Metahne.

PP40.Removal of Safranine using Chitosan as adsorbent –Effect of SDS micelles

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In the present study, Chitosan, a natural polyaminosaccharide employed as low cost adsorbent for the removal of safranine an azine dye. The results of studies both in the presence and absence of sodium dodecyl sulphate (SDS) micelles have been reported. The adsorption studies were carried out at different concentration ranges of dye from 5 – 100 mgL^{-1}, adsorbent dosage in the range of 0.25 - 2.0g and the surfactant concentrations in the range of 1×10^{-3} - 1×10^{-1} M at room temperature. The kinetic studies were carried out by varying the dosage of the adsorbent, concentration of the dye, concentration of the surfactant and at different time intervals. It was observed that the reaction was found to follow the Temkin adsorption isotherm and second order kinetics both in the presence and absence of surfactant (SDS).

Key words: Adsorption studies, Temkin adsorption isotherm, Safranine dye, Chitosan

PP41.Impacts of Aqua cultural Activities on Ground Water Quality

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Some areas of East Godavari district of Andhra Pradesh are with hectic Aqua cultural activities which cause concern on the nearby water sources. Hence it is necessary to evaluate quality of waters near

aqua cultural activities to suggest the public residing in the nearby habitations for utility of water sources for drinking or domestic purposes The present research work is around the characterization of ground water samples collected near aqua cultural activities for physicochemical parameters to assess the quality of waters. pH values indicated slight alkaline nature.Higherconductivity indicated the saline nature of waters.TDS crossed the permissible limit indicating the presence of dissolved salts in waters which can change the taste of waters. Higher TH and Ca^{2+} ion concentrations indicated the hardness of waters which make them unsuitable for domestic purposes. Mg^{2+} Ion concentrations crossed the limits in majority of samples. Higher chloride ion concentrations indicated the concern.The research results revealed that the waters are not suitable for drinking or domestic purposes. They are to be treated properly before consumption either for drinking or for domestic purposes.

Keywords: Water, parameter, Characterization, Aquaculture, drinking

PP42.Water Quality near Agricultural Activity locations in West Godavari District

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Water is ubiquitous. but contamination cause health hazards in human and animal life. Keeping in view the hectic agricultural activity in west godavari district of Andhra Pradesh, India, wecarried out analysis of ground waters near agricultural activity areas. Ground water samples were collected and analyzed for physicochemical parameters to monitor their quality. pH indicated the slight alkaline nature of waters. Higher EC indicated the saline nature of waters. Higher TDS confirmed the presence of soluble solids. Total Alkalinity levels are within the permissible limit. Higher Total Hardness and calcium ion concentrations indicated the hardness of water which makes them unsuitable for domestic purposes. Chloride ion concentration crossed the permissible limit. The waters are to be treated properly by using the available treatment methods before use either for drinking or domestic purposes.

Key words: Ground water, Agriculture, Parameter, drinking

PP43.Isolation and characterization of forced degradative products of an Anti-psychotic drug by spectroscopic techniques

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HPLC method was developed for the determination of degradation products of an anti- psychotic drug Levosulpiride. The chromatographic separation was achieved on Shimadzu LC-2010 with PDA system and Hypersil BDS C18 (250x4.6 mm) column using isocratic elution of mobile phase. The present research study is focused on the degradation of the drug using different forced degradation conditions (as per ICH guidelines). One major degradation product was observed in the base and oxidative degradations while no degradation products were observed in acid, thermal and photolytic degradations respectively. The major degraded products were isolated using semi-preparative HPLC. The degraded products were subjected to LC-MS to find out the products mass. The structures of the degradative products were characterized using IR and NMR techniques.

Keywords: Levosulpiride, reverse phase HPLC

PP44. Quality Evaluation of Subsurface Waters near a Non -Point Source

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Subsurface waters are source of drinking water to many rural based communities. Nonpoint source like agricultural runoffs contaminate these waters due to seepage. As a part of the present proposed research study, representative samples of subsurface waters are collected and analysed for physicochemical parameters viz., pH, EC, TDS, TH, Ca^{2+}, Mg^{2+},TA,Na+, K+, Cl^-, SO_4^{2-}, PO_4^{3-},F^-, NO_3^-. Metal ions which include Al, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd, Pb, As, U were also analysed by ICP-MS technique. Further the water samples are analysed for MPN count and *bacterial species* to evaluate the quality of subsurface waters for consideration for end user applications. Higher levels of pH, TDS, TH, TA, and Chloride indicated the unsuitability of waters for drinking and domestic utility. The metal ion concentrations are within the permissible limits of drinking waters. Though majority of water samples are not with MPN count they are observed with pathogenic bacteria like *Klebsiella, Proteus, Enterobacter, Pseudomonas* and *E.Coli* indicating the microbial contamination of these waters. Hence these waters are to be treated properly by suitable treatment methods before considering them for drinking or domestic purposes.
Keywords: Subsurface water, nonpoint, bacteria, heavy metal, drinking

PP45. Hydro geochemistry Evaluation of Ground Water using Multivariate Factor Analysis

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The present research is aimed to evaluate the quality of ground water in Srikakulam region of Andhra Pradesh by characterizing ground water for physicochemical parameters viz., pH, EC, TDS, Na, K, Ca^{+2}, Mg^{+2}, Cl^-, HCO_3^-, NO_3^-, SO_4^{-2}, PO_4^{-3} collected near Kalingapatnam creek stream joining the sea in Srikakulam district during pre monsoon and post monsoon seasons. The multivariate factor analysis is performed for pre and post monsoon chemical data set. It provided an insight into the source of parameters which are mainly responsible for the water quality variations which occur in the area including the sea water intrusion. The present research study elucidated the effectiveness of factor analysis in evaluating the hydro geochemistry of ground water quality in this coastal region which is dominated by natural and anthropogenic activities.
Key Words: Ground Water, Quality, Factor analysis, Coastal region. Monsoon

PP 46. Impact of Sewage Drainage Water System on Ground Water Quality in Different Areas in and around Chirala Mandal, Prakasam Dist., A.P., India

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Water is one of the most important natural resources and need to be conserved and managed properly. Due to increased population and urbanization, ground water pollution increases in many

different ways. The objective of the study is to access the effect of leachate generated from sewage water on ground water quality by comparing results with WHO water standards. Water samples are collected from different areas in and around Chirala Mandal, Prakasam district, A.P during post monsoon season. Assesment of ground water quality for suitability for drinking and domestic purposes has been carried out. It has been assessed by examing various physico chemical parameters such as PH, EC (Electrical Conductivity), Total hardness, Alkalinity, TDS (Total Dissolved Solids), HCO_3, CO_3, Ca, Mg, Fe, F, Cl. Results are compared with WHO water standardsfor drinking purpose. Overall view of samples reveal that water samples which are collected nearer to sewage drainage water system exceed the permissible limits in Hardness, Alkalinity, Electrical conductivity, TDS(Total Dissolved Salts), HCO_3.

Keywords*:* Leachate, WHO and Physico chemical parameters

PP 47. Quality Evaluation of Ground Water near a Point Source in an Urban Area

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In the present scenario of urbanization especially in Metro, Urban and semi urban areas, the accumulation of domestic wastes are enormously increasing and management of the municipal solid wastes have become very difficult. The domestic wastes are being deposited even in and around residential localities by municipal or metro authorities in some urban areas. The municipal dump yards act as a point source of pollution. Percolation or leaching of the solid substances from these wastes enter the ground water around the dump yard can change the chemical characteristics of ground water in the nearby areas. The presence of microbial content can also contaminate the ground water and can cause health hazards.

In the present research programme, efforts are made on characterization of ground waters near a Municipal dump site in Kakinada city of Andhra Pradesh for Physicochemical parameters, viz., pH, EC, TDS, TH, Ca^{+2}, Mg^{+2}, TA, CO_3^{-2}, HCO_3^-, OH^-, Na^+, K^+, F^-, Cl^-,SO_4^{-2}, NO_3^-, PO_4^{-3}. The ground waters are also characterized for *bacterial spps* to assess the bacterial contamination of the waters in the study area. The research results revealed that the waters are chemically contaminated and indicated their unsuitability for drinking and domestic utility. The presence *of bacteria viz., E.Coli, Klebsiella, pseudomonas, proteus and Enterobacter* confirmed the *bacterial* contamination of waters.

Key Words: Ground Water, Point Source, Parameter, Irrigation, *Bacteria*

PP 48. Simultaneous Determination of 2-Chloro Methyl Propionate, 1, 4-Di-Bromo Butane and Para Anisic Aldehyde in Mebeverine HCl API and its Pharmaceutical dosage forms by GC-MS with SIMmode

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In this study we have developed Gas Chromatography–Mass Spectrometric (GC-MS) Selected-Ion-Monitoring (SIM) method for determination and quantification of 2-Chloro methyl propionate (2-CMP), 1,4-Dibromo butane(1,4-DBB) and Para Anisic Aldehyde (PAA) as angenotoxic impurities in Mebeverine HCl API(MEB) at ppm level and validated as per International Council of Harmonization (ICH) guidelines.

In this method mass selective detection was developed and validated for the trace level analysis of three impurities. All these three impurities are simultaneously determined by a GC–MS method using VF-624 Capillary column (60m×0.32mm×1.80µm) with Helium as carrier gas and a flow rate of 2.0 $mLmin^{-1}$. Chromatographic separation of 2-CMP,1,4-DBB and PAA were achieved in 7.91 min,13.69 min,18.45 min and m/z values was 63,55,135 on SIM mode.The proposed method is specific, accurate, precise, linear, rugged and robust for the determination of the three genotoxic impurities in API of Mebeverine HCl and hence is of wide applicability in pharmaceutical industries.
Keywords: Mebeverine HCl, GC-MS, Method development, Method Validation

PP 49. Feasibility study report on estimation of Dabigatran Form II content in Form I by FT-IR spectroscopy and DSC

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The aim of the present work is to provide analytical methods for estimation of Dabigatran Form II content in Form I using different techniques like FT-IR spectroscopy, DSC (Differential Scanning Calorimetry), X-ray diffraction study and Raman Spectroscopy. The results show that estimation of Dabigatran Form II content in Form I can be performed by all the above methods as they show prominent difference between Dabigatran Form II and Form I. Dabigatran form I is having advantageous properties for pharmaceutical use. Dabigatran etexilate is a new type of thrombin inhibitors, is the prodrug of dabigatran, and it belongs to non-peptide thrombin inhibitors.
Keywords: Dabigatran, FT-IR Spectroscopy, DSC, X-ray Powder Diffraction, Raman Spectroscopy

PP 50. Structural identification of degradants of moexipril by LC-MS/MS

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A gradient LC-MS method was used for the identification and characterization of degradants of moexipril using liquid chromatography electrospray ionization tandem mass spectrometry (LC/ESI-MS/MS).

Moexipril was subjected to hydrolysis (acid, base and neutral), oxidation, photolytic and thermal degradation conditions as mentioned in ICH guidelines Q1A (R2). The drug degraded under hydrolysis, oxidation and photolytic conditions, but it was stable under thermal conditions. In total, five degradants were formed and separated on an Agilent XDB C-18 column (4.6 × 150 mm, 5µm) in a gradient elution method. Four degradants (D1, D2, D4 and D5) under acidic conditions, three degradants (D2, D3 and D4) under basic conditions and three degradants (D1, D4 and D5) under neutral and oxidative stress conditions were formed. In addition, two degradants (D4 and D5) were formed under photolytic stress conditions.

To elucidate the structures of degradants, fragmentation of moexipril and its degradants was studied by using LC-MS/MS and accurate mass measurements (HRMS) data. The fragment ions in the production tandem mass spectra of all the degradants were compared with those of moexipril and assigned the probable structures for the degradants.
Keywords: Moexipril, liquid chromatography, Mass Spectrometry, HRMS data, Degradants.

PP 51. Synthesis, Spectroscopic Characterization, DNA binding propensity, Nuclease efficacy and Antimicrobial activity of Cu(II), Ni(II) and Co(II) Complexes derived from Schiff bases

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Two Schiff base ligands and their binary metal complexes $M(L_1)_2$ and $M(L_2)_2$ where M=Cu(II), Ni(II), Co(II) and L_1H=2-((E)-(4-(trifluoromethoxy)phenylimino)methyl)-4-methylphenol, L_2H =2-((E)-(4-(trifluoromethoxy)phenylimino)methyl)-5-methoxyphenol were synthesized and characterized by elemental analysis, NMR, IR, UV–visible, mass, magnetic susceptibility, ESR, TGA and powder XRD. Based on the experimental data square planar geometry around the metal ion is assigned to all the complexes. The interaction of synthesized metal complexes with calf thymus DNA was investigated by using UV-visible absorption spectra, fluorescence and viscosity measurements. The experimental evidence showed that all the metal complexes strongly bound to CT-DNA through an intercalation mode. DNA cleavage experiments of metal(II) complexes with supercoiled pBR322 DNA have also been explored by gel electrophoresis in the presence of H_2O_2 as well as UV light, and it is observed that the Cu(II) complexes cleaved DNA more effectively compared to Co(II), Ni(II) complexes. Finally in vitro by paper disc method the compounds were screened for antibacterial activity against few pathogens such as E. coli, P. aeruginosa, S. saphyphiticusand S. aureus and fungal species C. albicans and A. niger. It is observed that the complexes have potent biocidal activity than their free ligands.

Keywords: Schiff base, Transition metal (II) complex, DNA interaction, Biological activity.

PP 52. A Review on Boron Pollution and its Removal Techniques

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Boron is one of the minor elements in natural water and one of the seven essential micronutrient elements required for the normal growth of most plants. Boron is a commonly known drinking water contaminant that affects the reproductability of living organisms. In nature boron appears mostly as boric acid (H_3BO_3) and borax, ($Na_2B_4O_7.10H_2O$). In aquatic systems, it exists primarily as undissociated boric acid and borate ions.

The main sources of boron in surface water are urban wastewater containing detergents and cleaning products, industrial effluents and chemical products used in agriculture. When water with high boron concentration is used for irrigation, boron compounds form complexes with heavy metals like Pb, Cu, Co, Ni, Cd etc. and increase the potential toxicity. In recent years, boron toxicity has gained an increasing interest because of the greater demand for desalinated water, in which boron concentration may be very high for healthy irrigation. There is no easy method available for the removal of boron from water and wastewater. Structural studies have indicated that in borates, the boron atom usually combines with either three or four oxygen atoms forming [BO_3] or [BO_4] groups. The commonly used Reverse Osmosis (RO) desalination systems are not efficient enough in boron removal since boric acid might be transported through RO membranes in a manner similar to water. Conventional ion exchange is also inapplicable due to poor ionization of boron acid and requires periodical regeneration of resins when the ion exchange capacity becomes saturated. Biological treatment is inefficient because of the complex boron chemistry. Each database was searched for the entire dates available. An extensive survey of the literature has been conducted related to

technologies that have been developed for boron removal from wastewater. Only the publications concerned with the removal of boron from aqueous solutions have been reviewed and summarized.

PP 53. Pesticide Residues in Selected Vegetables collected from Local Markets in Vijayawada City

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Vegetable samples of green chilly, cabbage, tomato and brinjal were collected from market in five regions of Vijayawada municipality in April 2017. Selected vegetables were tested for the presence of pesticide residues like pyrathroids, organo chlorine compounds and organo phosphorous compounds using a gas chromatograph equipped with electron capture and thermo sensitive detectors. The samples tested, viz. chilly, cabbage, tomato and brinjal were found to have pesticide residues well above the permissible limits. Among the organo chlorine compounds, α-endosulfan was detected.
Keywords: Pesticide residue, Vegetable samples, Gas chromatograph.

PP 54. Isolation and Identification of Bio-active Photochemical Compounds from *Ventilago Denticulata* stem using GC-MS

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The present study explores the primary phytochemistry using gas chromatography-mass spectroscopy (GC-MS). The in vitro anti microbial study (against gram positive bacteria and gram negative bacteria) was performed on n-hexane (50%)+Benzene (25%)+25% ethanol stem extract of Ventilago denticulata. Preliminary phytochemical screening revealed that plant contains 17 bio-active compounds with different concentrations. Qualitative analysis shows the presence of various components of therapeutic importance including tannins, saponins, phenolic compounds, glycosides, flavonoids.
The present study provides information about the availability of some bio active phyto constituents, which can be useful to provide dietary elements and it may also help in developing new drug formulations.
Keywords: Gas chromatography, Mass spectroscopy, Photochemical, Identification.