

1ST NATIONAL CONFERENCE ON INNOVATIONS IN CHEMICAL SCIENCES & TECHNOLOGY
(NCICST 2015)

**1ST NATIONAL CONFERENCE ON
INNOVATIONS IN CHEMICAL SCIENCES &
TECHNOLOGY (NCICST)**

21st August 2015

Book of Proceedings

Editors

**Dr Priy Brat Dwivedi
Dr Malar Retna**

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Message of Correspondent Secretary



It is a matter of happiness that the Department of Chemistry is organizing the National Conference on “Innovations in Chemical Sciences and Technology (NCICST – 2015) on 21st August 2015.

Conference of this stature provides the necessary inputs for academics for research activities and all the stake holders, may that be resource persons, delegates, students and other participants all take a lot of positive vibes and food for thought from such events. Educational institutions get a thirst to move ahead and plan future activities from such occasions.

I extend my heartfelt felicitations to the Department of Chemistry and all those associated with NCICST 2015 activities and wish the conference all success.

Adv.M.Joseph Raj

Correspondent -Secretary

Message of CEO GIAP Journals

It's a great moment that GIAP Journals and Department of Chemistry of Scott Christian College (Autonomous) Nagarcoil, Kanyakumari are jointly organizing 1st National Conference on Innovations in Chemical Sciences & Technology (NCICST) 2015. We expect NCICST to serve as a platform where academicians, educators, researchers and students meet, discuss and share current trends in research and education.

We are hopeful that outcomes of NCICST to be fruitful for society in terms of new informations, new research in resolving challenges of human society by chemistry education and research.

I heartily congratulate Organizing Committee of NCICST for creating this wonderful opportunity for knowledge sharing and collaborations. I also thank management, administration, teaching and non-teaching staff and students of Scott Christian College (Autonomous) Nagarcoil, Kanyakumari for arranging this conference in their campus. We expect more academic collaborations in near future.

Rajni Dwivedi

Co-Founder, CEO,

GIAP Journals

Message of Principal



It gives me immense pleasure to learn that the Department of Chemistry is organizing a National conference on “Innovations in Chemical Sciences and Technology (NCICST – 2015) on 21st August 2015. The Department of Chemistry has taken a right step in organizing such a conference and in a way it is a bold step too! I congratulate them on this constructive venture. I am sure that the conference “NCICST-2015” will serve as a platform for our teachers, students and scholars and other experts in the field to interact with each other and share their knowledge and expertise on the advances in the field of chemistry. It is the foremost duty of every education institution to update and adapt itself rapidly to the needs of today’s world to make education for research successful, meaningful and more relevant to society needs.

Holding conferences, listening to experts in relevant field for having fruitful interaction with those experts and scholarly would be a rich learning experience for our teachers and students. They would be stimulated to take up research projects which I am sure would address the need of the society. I congratulate the conveners of this conference.

Dr.M.Edwin Gnanadhas

Principal

Message of President CSI, India



I am very pleased to learn that the 1st National Conference on Innovation in Chemical Sciences and Technology (NCICST) 2015 is being jointly organized by GIAP Journals, Mumbai, Department of Chemistry & Research Center of Scott Christian College (Autonomous), Nagercoil in collaboration with the Association of Chemistry Teachers, Mumbai on 21st August, 2015 at Scott Christian College, Nagercoil. The core objectives of this conference such as encouraging teachers and students in research activities, sharing of knowledge between the industry and academia and create better academic environment among chemistry departments and good chemistry teachers are quite encouraging. The wide range of topics selected for the conference is all very relevant to today's needs and I am sure that the participants of the conference especially the students will benefit much from this.

Chromatographic Society of India (CSI), which is celebrating its 15th successful year has been quite dedicated in the past in propagating the education of chromatographic techniques and related spectroscopic techniques. CSI has organized several seminars and symposia in the past and has supported similar events wherever possible. I am very pleased that the NCICST-2015 is being organized in Nagercoil, which is away from the major cities and wish that more such conferences are arranged in the remote towns in India that will create a better atmosphere for the young minds for better exposure and participation.

I am happy to be a part of this conference and wish the organizers all the success they deserve in their efforts and wish all the participants to take reap the maximum benefits out of this conference.

Dr.G. Ramakrishnan

President, Chromatographic Society of India

Message of Secretary ACT, Mumbai



Association of Chemistry Teachers (ACT) was launched in 2000 to serve as an apex national body of Chemistry educators to promote excellence in Chemistry Education.

The main objectives of ACT are:

- 1) To advance Chemistry education by means of curriculum development and innovations in teaching and evaluation methods,
- 2) To organise subjected related activities like workshops and conferences, competitions for students and Chemistry popularisation programmes in different parts of the country,
- 3) To explore and nurture talent in Chemistry with special reference to the Indian National and International Chemistry Olympiads,
- 4) To forge a synergistic relationship between academia, industry and research institutions for mutual benefit,
- 5) To actively collaborate with International Science Teacher Associations for exchange of ideas and organisation of joint programmes.

NCCT 2015 will be held along with National Symposium on "Innovative Methods in Chemistry Education" IMCE 2015 on October 8-10, 2015 at Lucknow University, Lucknow under the convenorship of Prof Sudha Jain, former President ACT.

ACT Awards

- 1) ACT Life Time Achievement award to honour a superannuated teacher in recognition of his distinguished services to Chemistry and research
- 2) Shri Anupam Sinha-ACT Best Chemistry Teacher Award to honour an undergraduate teacher
- 3) ACT Best Woman Chemistry Teacher Award.

I am very happy to know that GIAP Journals is organising National Conference on "Innovations in Chemical Science and Technology" NCICST 2015 on August 21, 2015 at Scott Christian College, Nagercoil, Kanyakumari. The participants will be immensely benefitted by their interactions with the eminent faculty of the conference. ACT is proud to be associated with NCICST 2015. Prof P B Dwivedi, Secretary NCICST 2015 and Dr Malar Retna, Convenor NCICST 2015 and all their colleagues have worked very hard to ensure the grand success of the conference and deserve hearty congratulations.

I wish the conference great success

Prof Dr D V Prabhu

General Secretary Association of Chemistry Teachers
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Message of Convener

We the Department of Chemistry, Scott Christian College (Autonomous) putforth the National Conference on Innovations in Chemical Sciences and Technology NCICST- 2015 covering the concepts in order to update the various version of chemistry. It is the sincere hope of organizers of NCICST 2015, that the deliberations and proceedings of the conference will be fruitfully utilized by researchers in forth coming days.

I take this opportunity to express my gratitude to all the organizers and faculty members of the Department of chemistry for their sincere efforts. And I will feel grateful if this conference could contribute its mile to the world and society to bring up prosperity and enlightenment.

Dr.A.Malar Retna

Convener NCICST

INVITED LECTURES

**REMOVAL OF CONTAMINANTS FROM DRINKING WATER WITH IRON(III),
IRON(VI) AND IRON(0)**

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Presence of certain heavy metal ions like arsenic, chromium etc. above a certain amount in drinking water makes it toxic and unfit for consumption. Along with heavy metal ions drinking water is frequently contaminated with microorganisms such as *E. coli*, which is one of the species in the faecal coliform group, and has been used as an indicator for the faecal contamination in a given water sample. The Gram-negative cell wall of *E. coli* is complex and can survive for variable periods in natural waters. Worldwide concern over the presence of these contaminants in water bodies have prompted much research and policy development focusing on the removal of these pollutants from drinking water.

Iron in its various oxidation states has long been used for its various end applications. Hexacyanoferrate(III), in which iron exists in its (III) oxidation state has been used as an oxidant presumably due its cheap availability, less complexity involved in the estimation and its capability to act in acidic and alkaline medium both. Recently iron ferrate, in which iron exists in its lesser known (VI) and (V) oxidation states has been used both as oxidant and coagulant for industrial effluents and wastewater treatment also apart from being used as very powerful oxidizing agent for various organic and inorganic substrates. Treatment of infected water with ferrate kills harmful organisms (e.g., bacteria and viruses) and controls/ removes the odor precursors. A new generation of environmental remediation technologies includes nanoscale iron nano particles that provides cost-effective way to many of the most challenging environmental cleanup problems. Due to large surface area and high surface reactivity, iron nano particles become very effective for the transformation and detoxification of a wide variety of common environmental contaminants, such as heavy metals, inorganic compounds, chlorinated organic solvents, organochlorine pesticides, and PCBs Present work deals with the use of hexacyanoferrate(III), ferrate ions and zero valent iron nanoparticles in the removal of contaminants from polluted drinking water.

**STRUCTURE TAILORING AND CATALYTIC ACTIVITY ASSESSMENT OF
NANOMATERIALS FOR ENVIRONECONOMIC CONSTRUCTION OF
BIOLOGICALLY VITAL HETEROCYCLES**

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Giving consideration to escalating demand for novel pharmaceutically/ biologically imperative compounds, the most important goal for chemists is to develop more sustainable and greener synthetic protocols for drugs and fine chemical synthesis. The fusion of green chemistry and nanotechnology seems to be the preeminent way to develop the next generation of highly efficient processes. Therefore, we have investigated the synthesis of a variety of nanoparticles including CuO, ZnS, CdS, TiO₂; Al₂O₃ doped nanoparticles, etc. by wet chemical precipitation method with a narrow size distribution, which offers new means of tailoring materials structure to conquer the bottleneck in catalytic reactions. Moreover, this promising environ economic technique was extended for the synthesis of magnetically separable nanoparticles as well. The magnetic nature of these heterogeneous nanocatalysts allows its easy separation from the reaction mixture by the use of simple bar magnet, which is an additional attribute of this approach. Recently, we have extended our studies for the synthesis of metallic NPs decorated polycarbonate/ graphene oxide sheet. This hybrid material improved the catalyst recovery and prevents metallic NPs aggregation in reaction mixture that usually lacks in these components in isolation. The synthesized nanomaterials were fully characterized by various analytical techniques.

To further exploit the potential of the dynamic character of nanomaterials, we describe herein nanomaterials catalyzed one pot multi-component chemo/diastereo-selective synthesis of library of spiro and annulated heterocycles including pyrazolo[3,4-e][1,4]thiazepines, indoloquinolines and chromenonaphthyridines. Moreover, the synthesized compounds were screened for various biological activities and they have shown promising anti-mycobacterial and anti-oxidant activity.

**EVALUATION OF NANO STATIONERY PHASE (NSP) CAPILLARY COLUMNS
FOR GC-MS**

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Fused Silica Capillary columns was invented by Dr. Ray Dandeneau of Hewlett-Packard in 1979 and it was commercialized immediately thereafter. This changed the way chromatographers looked at GC as an analytical technique for various applications. Today majority of GC columns used for GC and GCMS are fused silica capillary columns. While 180u, 250u, 320u and 530 u ID columns are used mostly, the 100u ID columns have made a huge difference in the fast GC technology, where in, the analysis time can be considerably reduced as also the carrier gas consumption. In general there are 3 types of capillary columns available such as Wall Coated Open Tubular (WCOT); Support Coated Open Tubular (SCOT) and Porous Layer Open Tubular (PLOT) and under each category there are many variations of the inside of the column coating material . Based on the mixture to be separated one can select the right type of column for good chromatographic resolution.

It takes a long time for any innovation to take place in the column technology and it is interesting to note that one important column technology came into being in the recent past, thanks to the company, J&K Scientific from Canada. The columns are known as Nano Stationery Phase (-NSP-) columns. While the manufacturing process is a top trade secret it can be perceived that nano particles of the desired stationery liquid phase are coated and surface bonded on the inside walls of the fused silica capillary column. This presentation will compare the performance of these new NSP columns with the conventional stationery phase WCOT columns that are being used in our GC and GCMS. The various classes of compounds such as essential oils, Pesticides, petroleum products, drugs, etc are analyzed and the results compared. It is worthwhile to note that the new NSP technology does give good chromatographic separation with lesser length of column.

ORAL PRESENTATIONS

**ASSESSMENT OF INDOOR RADIATION DOSE RECEIVED BY THE RESIDENTS
OF NATURAL HIGH BACKGROUND RADIATION AREAS OF COASTAL
VILLAGES OF KANYAKUMARI DISTRICT, TAMIL NADU, INDIA.**

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Radiation exposure and effective dose received through two routes of exposure, viz. external and internal, via inhalation, by residents of coastal villages belonging to Natural High Background Radiation Areas (NHBRA) of Kanyakumari District and Tamil Nadu in India were studied. While the indoor gamma radiation levels were monitored using Thermo Luminescent Dosimeters (TLDs), the indoor radon and thoron gas concentrations were measured using twin chamber dosimeters employing Solid State Nuclear Track Detectors (SSNTDs, LR-115-II). The average total annual effective dose was estimated and found to be varied from 2.37 to 8.64 mSv.

Key words: Radon, Thoron, Effective dose

**A QUANTITATIVE EVALUATION OF CRACK PARAMETERS BY USING
PHOTOELASTIC ANALYSIS**

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Fracture process can be influenced by many parameters. Fracture toughness is an indication of the amount of stress required to propagate a pre-existing crack or flaw. Fracture toughness of a material commonly varies with grain direction. In the present work, the fracture behavior of cured epoxy resin under mode I loading is studied by analyzing results obtained in a single edge notch bending specimen.

In the present study, the fracture of an epoxy based thermoset specimen with single edge crack is analyzed using two dimensional photoelasticity. An attempt was made to study the effect of stress intensity factor with single edge crack. Fracture toughness and the ultimate strength of the single edge notch resin specimen was obtained using the four point flexural test with a universal testing machine.

The stress intensity factor is found near the crack tip. Stress intensity factors is determined using 2-D photoelasticity where plane polarized light is passed through a photoelastic material (epoxy resin) resulting in a colorful fringe pattern indicating the intensity of the stress. Cracks have a sharp tip and lead to stress concentration. Mode I fracture is the condition where the crack plane is normal to the direction of largest flexural four point bending.

Keywords: Composite Laminates, Photoelasticity, Fracture toughness

TROUBLE SHOOTING ISSUES OF BIODEGRADATION OF ORGANIC POLLUTANTS IN TROPICAL MARINE ENVIRONMENT

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Marine pollution occurs due to the entry of organized or unorganized, point or non – point land based releases of industrial, agricultural and residential waste. Biodegradable organic waste rich in microorganisms lead to potentially harmful effects and alter oxygen cycle, where as excessive inputs of nutrients like nitrogen and phosphorus stimulate algal growth leading to eutrophication. Thermodynamics play an important role in chemicals reactions occurring in ocean during degradation of organic waste. The rate of reactions is altered due to temperature and high salinities. This aspect is very crucial while predicting the self purification capacity of the water body. Adequate experimental work pertaining to the order of reaction and thermodynamic constants is essential to prove the basis of the predicted assimilative capacity of the system.

In Mumbai, huge quantity of domestic waste is generated. Due to land restrictions, complete treatment of tertiary level is not feasible. The Municipal administrators take the advantage of coastal location and discharge this waste into the ocean with just meagre preliminary treatment. The disposal practices are advanced and well planned but still expected purification or dilution is not achieved in the near shore region. This has resulted in spoiling the impact zone of coastal areas creating stress on the living biota and non compliance of the marine water quality standards.

Three major issues in coastal system, viz. Operation and control of waste discharges, degradation patterns of pollutants and self purification capacity needs systematic evaluation to maintain favorable conditions for aquatic life. Hence it is essential to study the reaction kinetics and thermodynamic behaviour of the biodegradation of carbonaceous waste occurring under highly saline conditions. Experiments are conducted to confirm the kinetics and thermodynamics of biodegradation of domestic waste water into marine water at variable salinities. The paper presents the findings of kinetic behaviour particularly the values for rate of reaction, Activation energy and related constants.

Key words: BOD, kinetics of biodegradation, thermodynamic aspects of BOD

A KINETIC INSIGHT INTO THE OXIDATION OF PERFUMERY PHENOLS USING POTASSIUM PERSULPHATE IN ACIDIC MEDIUM

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The isomeric phenols, Eugenol and Isoeugenol are widely used in the manufacture of perfumes. These phenols are found in the Indian spices, clove and nutmeg. Not much work has been reported on the kinetic aspects of the oxidation of perfumery phenols. We report herein the kinetic, mechanistic and thermodynamic studies of the oxidation of eugenol and isoeugenol by potassium persulphate ($K_2S_2O_8$) in acidic medium.

The oxidation rates of phenols were determined under first order kinetic conditions with respect to the inorganic oxidant and the progress of the oxidation was monitored by iodometric estimation of the unreacted oxidant at regular time intervals.

The effects of phenol and oxidant concentrations, ionic strength and temperature on the oxidation rates of phenols have been studied in detail. The oxidation rate increases with [phenol] but decreases with increasing oxidant concentration. K_2SO_4 was used to determine the effect of ionic strength on the oxidation rates of phenols in accordance with the Bronsted-Bjerrum equation.

From the effect of temperature (303-318K) on the reaction rate, the various thermodynamic activation parameters of the reaction were evaluated and interpreted. The energy of activation (E) was determined from the Arrhenius plot of log k versus 1/T. The formation of a rigid activated complex as an intermediate during the course of the reaction results in the reorientation of solvent molecules around the activated complex thereby curtailing the degrees of freedom of the reacting system. This explains the observed decrease of entropy of the reacting system.

The sequence of oxidation rates of phenols, isoeugenol > eugenol has been explained on the basis of isomeric and structural features of the phenols. Suitable reaction mechanisms have been suggested for the oxidation of the perfumery phenols under study.

Keywords: perfumery phenols, inorganic oxidant, kinetics, energy of activation, degrees of freedom, entropy of activation

SYNTHESIS AND CHARACTERIZATION OF COPPER NANO PARTICLES: APPLICATION, IN FIELD OF OXIDATION OF AROMATIC HYDROCARBONS CERIUM (IV) SULPHATE UNDER MICROWAVE IRRADIATION

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The catalytic oxidation with Cerium (IV) in aqueous solution offers an economic and environmentally safe alternative for oxidation reactions performed in synthetic laboratories and chemical industry. In this paper we have shown that the size of the copper nanoparticle is responsible for the yield of chemical change. The copper catalyst (non-nano) powder showed 21% conversion of naphthalene to α -naphthol in 3 min under our experimental conditions. Same quantity of copper nanoparticles (size, ~ 60 nm diameter) ready by turn PVP-EG capping showed 33% conversion of naphthalene to α -naphthol that inflated to concerning 43% when 8 nm diameter capped copper nanoparticles are used. Surprisingly, 5 nm size copper nanoparticles showed no change in the yield of about 41%. [Ce(IV)-Cu(II)sulphate] system in our experimental work shows 43%, 97%, and 96% yields for oxidation of naphthalene, phenanthrene, and anthracene respectively in the presence of copper nanoparticles.

Key words: Aromatic hydrocarbons, Cerium (IV), copper nanoparticles, PVP-EG capping, surface area.

ANTIMICROBIAL ACTIVITY OF MARINE FLOWERING AND NON- FLOWERING HALOPHYTIC PLANTS AGAINST SOME CHOSEN MICROBIAL PATHOGENS

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Marine plants are considered as a source of bioactive compounds as they are able to produce a great variety of secondary metabolites characterized by a broad spectrum of biological activities. Compounds with antioxidant, antiviral, antifungal and antimicrobial activities have been detected in mangroves, seaweeds and seagrasses. Marine plants are the source of amino acids, terpenoids, phlorotannins, steroids, phenolic compounds, halogenated ketones and alkanes and cyclic polysulphides. In this study, the antibacterial activity of flowering seagrass species viz., *Syringodium isoetifolium* and *Cymodocea serrulata* and non-flowering seaweeds viz., *A. anceps*, *G. corticata*, *S. wightii*, *P. pavonica*, *Ulvalactuca*, and *V. pachynema* was taken for this study. Interestingly it is found that, most of the ethanolic algal extracts control all the pathogens of antibiotic resistant organism, fish pathogens, poultry pathogens and human ophthalmic pathogens. The ethanolic algal extracts of antibacterial activity were evaluated by the well diffusion assay and the zone of inhibition ranged between 6mm to 13mm in the ethanolic extract. The maximum activity was recorded with ethanolic extracts of all the six marine plant species chosen for the present study.

ANALYSIS OF ANTICONVULSANT, ANALGESIC AND ANTI-INFLAMMATORY ACTIVITIES OF SOME NEW SYNTHETIC PYRAZOLINE DERIVATIVES

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3,5-diphenyl-4,5-dihydro-1-*H*-pyrazole compounds were synthesized by reacting acetophenone with the substituted aromatic aldehydes in presence of ethanol and sodium hydroxide followed by acidification with dilute hydrochloric acid followed by treatment with hydrazine hydrate in the presence of acetic acid and ethanol. The derivatives of these compounds were synthesized by making substitution at free N-(1*H*) position of 3,5-diphenyl-4,5-dihydro-1-*H*-pyrazole through Mannich condensation with formaldehyde and series of primary and secondary amines. The purification was done by column chromatographic technique by monitoring thin layer chromatography and the structures were confirmed by comparison of melting points, and infra-red spectral studies. *In vivo* anticonvulsant, analgesic, anti-inflammatory activities were done with albino mice for all the compounds by administering intra-peritoneal route. The compounds with dimethyl, diethyl and diphenyl substituted at free N-(1*H*) position showed good activity for all *in vivo* studies. The statistical analyses for multiple comparisons of biological studies were done by ANOVA test.

STUDIES OF SOLVENT EXTRACTION AND SUPPORTED LIQUID MEMBRANE WITH REACTIVE DYES FROM AQUEOUS SOLUTIONS USING ALIQUAT 336 AS CARRIER

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The liquid-liquid extraction (LLE) and supported liquid membrane (SLM) studies of reactive dyes namely Gold Yellow (GYHE-R) and Reactive Green HE 4BD (RGHE-4BD) from aqueous solution of acidic medium using aliquat 336 as the carrier has been investigated. Polytetrafluoroethylene (PTFE) membrane with 0.5 µm pore size has been used after impregnated with Aliquat 336 in dichloromethane. In liquid liquid extraction the following parameters had been optimized; pH of feed, diluent, carrier, strip and dye concentration and the same parameters have been applied to supported liquid membrane (SLM) study to transport dye from aqueous solution. The main advantages SLM study is; the extraction and stripping as single stage process and low consumption of carrier in the membrane phase compared to the solvent extraction process. The other parameters such as transport time, stirring speed and mechanism of dye transport has also studied. The percentage of transport of dye and flux rate increases with increasing time. The stability of membrane is satisfactory over 5 days.

Keywords: Feed phase; Aliquat 336; extraction; reactive dye; transport.

QUANTITATIVE PHYTOCHEMICAL DETERMINATIONS AND IN-VITRO CYTOTOXIC ACTIVITY OF MEDICINAL PLANTS

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The present study evaluates in-vitro cytotoxic activity of active extracts of medicinal plants. It evaluates anti-cancer activity of most active extracts of *I. pes-caprae* and *C. roseus*. This study focuses on the total phenol content and the total flavanoid content of the plant and searches into its medicinal potency based on the total phenol and total flavanoid content. The anti-cancer activity of the extract is found to be more significant than one another. The cytotoxic activity of *Ipomoea pes-caprae* and *C. roseus* showed better results. Methanol extracts of aerial and root of *Ipomoea pes-caprae* possess maximum anticancer activity is found to be 61.77% and 65.55%. Chloroform extract of *Catharanthus roseus* root was also active against MCF- 7 cells by exhibiting 64.34% of activity. These plants may be a source of new antibiotic compounds. These findings enriches our knowledge of the chemical constituents that are responsible for the medicinal uses of the plant and the anti-cancer potential of selected plants.

Keywords: *I. pes-caprae*, *C. roseus*, phytochemicals, cytotoxic, MTT assay.

**SYNTHESIS AND CHARACTERISATION OF COIR FIBRE REINFORCED EPOXY
COMPOSITES FROM PUNNAL OIL**

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Vegetable oil is readily available and inexpensive, can be used to synthesise various types of polymers. In our present study, epoxidised punnal oil has been synthesised from punnal oil via peroxy acetic acid generated 'insitu' by treating acetic acid with hydrogen peroxide as oxygen donor. The epoxidation is catalysed by using sulphuric acid. The epoxidation is confirmed by iodine value, oxirane oxygen analysis, fourier transform infrared spectroscopy (FT-IR), nuclear magnetic resonance (NMR) and thin layer chromatography (TLC) analysis. Natural fibers such as jute, sisal, banana, rice husk etc are locally available in abundance and have excellent physical and mechanical properties and can be used more effectively in the development of composite materials for various applications. Epoxy composite samples are prepared from the natural fiber with different ratios using triethylamine hardener and phthalic anhydride. The mechanical properties viz. tensile strength and the physical properties observed are discussed in detail.

Keywords: Punnal oil, Epoxidised punnal oil, Epoxy composites, Coir fibre, Chemical resistance

**OPTIMIZATION OF ADSORPTION PROCESS FOR REMOVAL OF
SULPHONATED DI AZO TEXTILE DYE**

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Treatment of textile waste water has emerged as a great matter of concern amongst scientific community because of essentiality and scarcity of this valuable natural resource. Various techniques have been employed for waste water treatment, amongst which use of natural materials have made a significant contribution in the area of sustainable environment. This paper focuses on the use of the seeds of Argemone Mexicana, a weed for removal of a textile dye from its synthetic solution. Optimisation of several parameters has been carried out for elimination of dye from water resource at neutral conditions. Variation in different parameters affecting decolorization of the dye from aqueous solution, have been studied at length. Maximum decolorization (About 60%) has been observed after four hours with 0.1 g of the elected natural adsorbent obtained after passing through sieve size of 300 µm.

Keywords: Adsorption, Argemone Mexicana, Decolorization, Sulphonated di azo dye, Textile effluent.

**FORMULATION AND EVALUATION ENTERIC COATED MINI-TABLETS OF
DULOXETINE HYDROCHLORIDE IN CAPSULE**

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Duloxetine HCl is unstable in acidic pH and hence requires enteric coating. However, it is well-known that duloxetine is incompatible with many enteric coating polymers. The main objective of the present study was to develop and characterize an enteric coated mini tablet of duloxetine HCl in capsule with excellent stability and dissolution profile. In the optimization of excipient, it was found that polyplasdone XL at ratio 1:1 %w/w (duloxetine:polyplasdone XL) was the optimum superdisintegrant, PVP K29/32 at 2.5% w/w as the optimum binder and SLS at 2.5% as the optimum wetting agent based on the dissolution of the granules. From the process optimization, it showed that wet granulation method with binder added in the intra granular step was the optimum method based on the dissolution result which 90% of the drug content was released within 5 minutes in pH 6.8 phosphate buffer solution. The optimum formulation was compressed into mini tablet and subjected to optimization of enteric coating. Two types of polymer at various concentrations were used to compare their coating efficiency namely HPMC E5 and Acryl EZE. Acryl EZE at 8% was selected as the optimum coating polymer and concentration based on the dissolution profile. The dissolution was conducted for the first 120 minute in 0.1 N HCl medium and the subsequent 90 minutes in pH 6.8 phosphate buffer medium. There was no drug release in the first medium whereas 80% of the drug content was released in 60 minutes in the second medium. The dissolution profile was comparable with the dissolution profile of the marketed product. In conclusion, an enteric coated mini tablet formulation of duloxetine in capsule was successfully developed and characterized.

REAL TIME LEVEL CONTROL OF THE INDUSTRIAL SISO NONLINEAR SYSTEM

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Chemical processes present many challenging control problems due to their non-linear dynamic behavior and because of the inherent nonlinearity they are in need of enhanced control techniques. Proportional-integral-derivative (PID) control schemes continue to provide the simplest and yet effective solutions to most of the control engineering applications today. A number of processes in the chemical industries are controlled using PID controllers. The work described in this paper aims at controlling the level of a nonlinear process. The nonlinear process considered is a conical tank system whose parameters vary with respect to the process variable. Initially the system identification of the conical tank is done and identified to be a First Order plus Dead Time model (FOPDT). Set point Tracking and Load disturbance rejection tasks are considered. Simulations are carried out in MATLAB then Lab view software is used to monitor the operation in real time and the results are compared to verify their effectiveness. Performance indices such as Settling time, Percentage peak overshoot, Integral square error and Integral Absolute error are used for the assessment of controller performance. By comparing the results obtained it is shown that the use of Internal model control based PI provides a performance improvement.

POLYANILINE-GRAPHITE OXIDE NANO-COMPOSITE SENSOR FOR LPG DETECTION

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Recent advances in nanotechnology offer enormous opportunities to investigate new nano-structured materials for sensing applications. Sensors are of immense importance in environmental safety and personal protection for human beings. Among various sensors that are available commercially, sensors for monitoring organic and inorganic gases have drawn most consideration, due to their massive applications in day to day life. To detect, Liquid Petroleum Gas (LPG) is most important, due to its flammable nature, when it is used as a fuel in industrial and domestic purposes. An explosion is possible due to leakage, it has become quite common, and hence, it is indispensable to detect the leakage at initial stage. Recently, many semiconductor gas sensors have been developed for detecting LPG, but the operating temperature is high which consumes more power and also expensive. To overcome these drawbacks, presently a considerable attention has been focused on conducting polymers and intensively studied, to detect LPG at room temperature. By exposing the polymer to LPG, the resistivity of the polymer is altered. Among the polymers, polyaniline has occupied a unique position due to its easy method of synthesis, different oxidation states, low cost and can interact with chemical species at room temperature. The nano-structured polyaniline provides a larger surface area for the diffusion of gas molecules and the sensitivity is also increased by incorporating graphite oxide. This presentation reveals the synthesis of polyaniline-graphite oxide nano-composite by rapid mixing method (chemical polymerization) and it has also been characterized by UV-visible spectroscopy, FTIR spectroscopy, X-ray diffraction, Scanning Electron Microscope (SEM) and Transmission Electron Microscope (TEM) to study the suitability of the nano-composite material for LPG sensor. Finally, a prototype LPG sensor has been fabricated and evaluated.

Keywords: LPG, Polyaniline, Graphite oxide, Nanocomposite, Resistivity, Prototype.

SYNTHESIS AND CHARACTERIZATION OF NATURAL FIBRE REINFORCED POLYURETHANE COMPOSITES BASED ON CARDANOL

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In recent studies importance has been given to the use of natural products from renewable resources due to the decrease in the supply and price escalations of petroleum raw materials. Cardanol based resole type phenolic resin has been synthesized by condensing cardanol with furfural in a particular mole ratio using dicarboxylic acid catalyst such as phthalic acid. Polyurethane sheets were prepared by treating cardanol furfural resin with 4,4¹ – methylene bis(cyclohexylisocyanate) and the catalyst dibutyltindilaurate. Natural fibres are prospective

reinforcing materials and their use until now has been more traditional than technical. Among the various fibres sisal is of particular interest in that its composites have high impact strength besides having moderate tensile and flexural properties compared to other fibres. Fibre reinforced polyurethane composites have been prepared by treating sisal fibre (10%) into polyurethane. The physico chemical, spectral and thermal properties of polyurethane and fibre reinforced polyurethane composites have been studied.

Keywords: Cardanol, furfural, sisal fibre, polyurethane, 4,4¹ – methylene bis (cyclohexylisocyanate)

STUDIES ON METFORMIN HYDROCHLORIDE AND α -CYCLODEXTRIN INCLUSION COMPLEXES

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Metformin hydrochloride is an oral antihyperglycemic drug used in the management of type-2 diabetes. Inclusion complexes were prepared between Metformin hydrochloride and α - cyclodextrin in solid and solution state. Inclusion complexes were characterised using UV-VIS, Fluorescence and FTIR Spectroscopic Studies. Phase solubility studies were carried out which determined the 1:1 stoichiometry for the formation of inclusion complexes.

Keywords: Metformin hydrochloride, Antihyperglycemic drug, α -Cyclodextrin, Inclusion complex, Phase Solubility.

ANTIBACTERIAL ACTIVITY OF ZINC OXIDE NANOPARTICLE BY SONOCHEMICAL METHOD AND GREEN METHOD USING ZINGIBEROFFICINALE

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Nanoparticles have made a steady progress in all the branches of science. It is used in biological applications including nanomedicine. Zinc oxide is also known as Zincite generally seen in a crystalline form. Zinc oxide nanoparticles are multifunctional. It has effective antibacterial activity. This study focusses on the synthesis of zinc oxide nanoparticle by the sonochemical and green method, characterized by XRD, SEM and to determine the antibacterial efficacy of green and chemical techniques. Results prove that green synthesised Zinc oxide nanoparticle shows the enhanced biocidal activity. In addition the current study has demonstrated that the particle size variation and surface area to volume ratio of green synthesised Zinc oxide nanoparticles are responsible for significant high antibacterial activity. From the result obtained it suggested that the biogenic green fabrication is a better choice due to eco-friendliness.

Keywords: Sonochemical, zincite, antibacterial, green fabrication, efficacy.

ASSESSMENT OF INDOOR RADON, THORON AND THEIR PROGENY LEVELS IN RESIDENTIAL HOUSES OF HARDOI, UTTAR PRADESH, (INDIA)

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Radon, thoron and their progeny levels are significant natural sources of radiation exposure for general population in both living and working places. The concentration of radon varied from 15 Bq/m³ to 78 Bq/m³ with an average of 46 Bq/m³, while thoron concentration varied from 11 Bq/m³ to 26 Bq/m³ with an average of 18 Bq/m³. The concentration of radon progeny (EERC) varied from 10 Bq/m³ to 26 Bq/m³ with an average of 18 Bq/m³, while the concentration of thoron progeny (EETC) varied from 0.56 Bq/m³ to 1.91 Bq/m³ with an average of 1.11 Bq/m³. The value of equilibrium factor for radon varied from 0.19 to 0.76 with an average of 0.37 while for thoron it varied from 0.02 to 0.12 with an average of 0.06. Our experimental finding confirmed that the indoor radon, thoron and their progeny concentration were within internationally accepted norms.

Keywords: Pin hole dosimeter, DTPS, DRPS, Indoor radon & thoron concentration.

PREPARATION OF HOLLOW TiO₂ NANOSPHERES FOR BIOMEDICAL APPLICATIONS

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The present work reports the preparation of hollow TiO₂ nanospheres through sacrificial core templating method where, the sacrificial core of carbon spheres were indigenously synthesized and mixed into the starting ethanolic solution of titanium tetraisopropoxide (TTIP) under ambient condition. The solid obtained on the hydrolysis of TTIP were dried and calcined in air to acquire the hollow nanospheres of TiO₂ in anatase phase. The acquired samples were further doped with varying mole % of Mn(II) to invoke magnetism in the material. X-ray diffraction and thermal studies reflected the anatase to rutile phase transformation of TiO₂ at 550 °C when the dopant (i.e., Mn) concentration was increased from 0 to 6 mol % (with respect to Ti). The hollow and spherical morphology of the TiO₂ nanostructures were confirmed through scanning electron microscopic studies while their ferromagnetic behaviour (at 300 K) was affirmed through SQUID analysis. For intracellular applications, the biocompatibility of the nanospheres was tested through conventional MTT assay, performed on MDA-MB 231 cancer cell lines.

Keywords: TiO₂; hollow nanospheres; biocompatibility; carbon spheres; anatase; rutile.

FACILE SYNTHESIS OF SUPERHYDROPHOBIC MATERIAL FOR SELECTIVE REMOVAL OF SPILLED-OIL FROM WATER SURFACES

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The present work reports the preparation of superhydrophobic and oleophilic sorbent powder for the selective removal of spilled-oil from oil-polluted water surface. The sorbent powder was prepared by the surface modification of commercially available pure barium sulfate (BS) with palmitic acid via a simple one-step synthetic approach. The powder was observed to exhibit superhydrophobic character with a static water contact angle value of 152±2°. The powder also possesses sufficient buoyancy and exhibits high selectivity towards oil, vital for a sorbent for use in oil spill clean-ups. The oil sorption capacity of the sorbent material was also investigated.

Keywords: Superhydrophobic; sorbent; spilled-oil; contact angle; oil sorption capacity.

PREPARATION OF CHAIN EXTENDED POLYURETHANE AND ITS COMPOSITES BASED ON CASTOR OIL AND COIR FIBER

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The chain extended polyurethane was synthesized by reacting castor oil based polyol with 4,4'-methylenebis(cyclohexyl) isocyanate and chain extender such as malonic acid. The composites have been fabricated by incorporating the coir fiber into the neat polyurethane. The polyurethane and its composites were characterized with respect to their mechanical properties such as hardness, tensile strength, percentage elongation and Young's modulus. The morphology of neat polyurethane and its composites with coir fiber was studied using scanning electron microscope (SEM). These studies revealed the high performance character of the polyurethane composites with respect to the corresponding neat polyurethane.

Keywords: Castor oil, 4,4'-methylenebis(cyclohexyl) isocyanate, dibutyltin dilaurate, coir fiber, polyurethane composites.

EFFECT OF INCREASING NCO/OH MOLAR RATIO ON THE CHEMICAL AND MECHANICAL PROPERTIES OF ISOCYANATE TERMINATED POLYURETHANE PREPOLYMER DERIVED FROM BIO-MASS

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The study deals the effect of increasing NCO/OH molar ratio on the physico-mechanical properties of isocyanate terminated polyurethane prepolymer. The prepolymer was prepared using castor oil and toluene-2,4-diisocyanate. The NCO/OH molar ratio has been varied from 1.6 to 2.0. The formation of the prepolymer was confirmed by UV and FTIR spectroscopy. The results reveal that the curing time of the prepolymer decreased with increase in NCO/OH molar ratio. When NCO/OH molar ratio increased, the tensile strength of the polyurethane film increased, while percent elongation decreased due to increase in hard segment content.

Keywords: Polyurethane Prepolymer, Tensile strength, UV, FTIR

OXIDATION OF AROMATIC HYDROCARBONS BY CERIUM (IV) BY USING THE TRANSITION METAL IONS AS A CATALYST IN ACIDIC MEDIUM BY KINETIC METHOD

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Oxidation of toluene and ethyl benzene by cerium(IV) sulphate in aqueous sulphuric acid medium catalyzed by Iridium(III) chloride was studied. Change in the concentration of oxidant shows a specific effect that the rate increases in the beginning at low concentrations, it reaches to a maximum and further increase in oxidant concentration decreases the rate. Oxidation was highly selective as it oxidizes toluene to benzaldehyde and ethyl benzene acetophenone. It is proposed that the complex formed between cerium(IV) and the organic substrate in first equilibrium step gives another complex in the presence of iridium(III) which ultimately gives rise to products of oxidation. Order of the reaction follows first order kinetics at low concentrations tending to become zero order at higher concentrations of organic substrate in both the cases. Rate of the reaction follows direct proportionality with respect to catalyst concentrations, while the rate decreases sharply with increasing hydrogen ion and cerium(III) concentrations. Change in ionic strength of the medium and the effects of changing concentrations of acetic acid, Cl⁻ ions, and HSO₄⁻ ions on the rate were studied. The energy of activation, entropy of activation and free energy of activation values, which were found to be 8.80 and 7.04 (kJ mol⁻¹), -45.54 and -45.79 (J K⁻¹ mol⁻¹), 14.03 and 14.11 (kJ mol⁻¹) for toluene and ethyl benzene, respectively.

WATER QUALITY INDEX AND CORRELATION STUDY FOR THE ASSESSMENT OF GROUND WATER QUALITY OF ALLAHABAD CITY
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Water, the Nectar of Life', is fundamental resource which is essential for the survival of different sectors, such as agricultural sector, industrial sector and small business units. In the absence of proper planning, urbanization and industrial/agricultural activities have adversely affected many regions around the world. This has led to indiscriminate actions, including dumping of wastes into the water and washing and bathing in open surface water bodies. In the present study groundwater samples from five sampling locations were collected and the analyses were done for nine physicochemical parameters. Water quality index assessment was carried out by using physicochemical analysis results. Water quality index of the sampling locations of Allahabad city has been divided into five categories. Good water quality index has been put into location 1 while locations 2, 3 and 4 indicate bad quality index. Very bad water quality index has been denoted in location 5. Correlation, the descriptive relationship among the physicochemical parameters, were also studied and it was found that the highly positively correlated values were among the parameters TDS vs EC (r=1.00), TS vs TSS (r=0.91), Temp vs TSS (r=0.87), Phosphate vs TSS (r=0.823) and highly negatively correlation was shown among TA vs Chloride. The result shows that the water quality of Allahabad city is not good and there is an urgent need for

the preliminary treatment of water before it is used for the drinking purposes. There is also the need for the proper waste disposal and treatment system for the contaminants which seep in the groundwater and deteriorate groundwater quality. Awareness programmes should also be organized to educate the masses for the conservation and management of groundwater resources and the need to reduce of overuse and wastage of the groundwater resources should be emphasized. Sustainable water development in the city is needed to fulfill the demand of water for future.

KEYWORDS: Groundwater, Physico-chemical analysis, Industrialization, Water quality index, Correlation matrix.

WATER PURIFICATION: A BRIEF REVIEW ON TOOLS AND TECHNIQUES USED IN ANALYSIS, MONITORING AND ASSESSMENT OF WATER QUALITY

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Drinking water sources are regularly polluted by various human activities that cause severe health problems all over the world. In recent years, water quality research has drawn great attention of scientific communities. A lot number of tools and techniques are used for proper water quality analysis, monitoring and assessment. This paper includes brief information about some of them namely, physico-chemical water analysis (PCWA), adsorption, metal pollution index (MPI), water quality index (WQI), water quality modelling tools (WQMT) and multivariable statistical models that includes five multivariate data mining approaches i.e. cluster analysis (CA), principal component analysis (PCA), factor analysis (FA), multiple linear regression analysis (MLRA), discriminant analysis (DA). Present paper also explores the interaction between science and technologies and provides basic knowledge of emerging tools and techniques used in water purification.

KEYWORDS: Water purification, adsorption, metal pollution index, water quality index and water quality

BINDING OF RUTHENIUM(II)-POLYPYRIDYL COMPLEXES WITH POLYPHENOLS IN AQUEOUS MEDIUM

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The binding of three Ru(II)-polypyridyl complexes with polyphenols (gallic acid and quercetin) have been studied in aqueous medium at pH 11 by means of absorption spectral technique. The absorption and emission maximum of these complexes are in the range of 451-457 nm and 612-626 nm respectively. The binding constant (K_b) for these reactions are determined from the Benesi-Hildebrand equation using absorption intensity data. The observed binding constant values are sensitive to the nature of the ligand and the structure of the gallic acid and quercetin. Quercetin binds strongly with Ru(II) complexes than gallic acid owing to the presence of more phenolic -OH groups. Structural effect seems to play a vital role on the binding of the antioxidants with these complexes.

Keywords: Ruthenium(II)-polypyridyl complexes; polyphenols; Benesi-Hildebrand equation; binding constant; structural effect

SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL STUDIES OF COPPER COMPLEX OF PYRAZOLE DERIVATIVE

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Due to huge importance of pyrazole derivatives, considerable efforts have been made by several researchers, to prepare new compounds bearing a single substituent or more complicated systems, including the heterocyclic rings mainly at 1-, 3- and 4-positions. The literature survey revealed that excellent anti-inflammatory, analgesic (Farghaly et al., 2001; Balsamo et al., 2003; Youssef et al., 2007; Souza et al., 2001; Godoy et al., 2004; Souza et al., 2002; Prokopp et al., 2006), anti-microbial (Pimerova et al., 2001; Bekhit et al., 2008), anti-viral, anti-tumor (Park et al., 2005), anti-convulsant (Michon et al., 1995), anti-histaminic (Yildirim et al., 2005) and anti-depressant (Bailey et al., 1985) activities with some compounds containing the heterocyclic ring such as

pyrazole. Based on the above mentioned research outcomes, the objective of the study, a novel derivative (obtained from acetophenone and imidazole-2-carboxaldehyde by Aldol condensation and then followed by condensation reaction with thiosemicarbazide under basic condition) was synthesised. The corresponding copper(II) complex was also prepared. They were characterized by elemental, molar conductance, FTIR, ¹H NMR and UV-Vis spectroscopy. The electrochemical behavior of copper complex was studied and its salient features were discussed. It was concluded that the prepared copper complex may be mimic natural enzyme like SOD.

CHEMICAL ANALYSIS OF ENDOSULFAN

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Endosulfan is an easily available insecticide and mainly used for agricultural purposes. Hence most of the villagers use endosulfan for committing suicide. The recent cases reported in toxicological laboratories show that suicide with endosulfan is increasing these days. Endosulfan causes most degree of death because of its toxic effects. The toxicology division of forensic science laboratory plays vital role in analysis of poisons through Criminal Justice System. In every death case which is connected to the criminal justice system, the human viscera of deceased are sent to forensic sciences department for analysis. In a case report, the toxicology division received human viscera of a deceased from the forensic medicine department where a person was declared death after consuming endosulfan due to severe stomach pain. It was brought to toxicology division of forensic science laboratory where the type of poison was identified and estimated. Two methods such as thin layer chromatography and UV Visible spectrophotometric method were adopted to analyze the human viscera. The forensic analysis includes solvent extraction, identification and estimation.

Keywords: Endosulfan, thin layer chromatography, UV visible

DISTRIBUTION OF ORGANIC CARBON, PHOSPHORUS AND NITROGEN IN THE SEDIMENTS OF MANAKUDY ESTUARY

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Estuary is a transition zone between land and sea as well as freshwater and salt water. In the estuary, the water carrying agricultural, industrial and domestic wastes are deposited as sediment. Distribution of organic carbon, total phosphorus and total nitrogen in the sediments of Manakudy estuary has been studied. Based on their nature, five stations have been earmarked for sampling. The C/N ratio of these sediments are very high compared to the sediments from Mandovi estuary goa.

Keywords : Organic Carbon, Nitrogen, Phosphorus, Sediment, Estuary

MANAGING FORMER LANDFILL SITES: A CASE STUDY OF ECORESTORATION FROM KOCHI, KERALA

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This paper describes the dramatic success in the eco-restoration of a heavy-metal contaminated open garbage dump at the Amrita Institute of Medical Sciences (AIMS), a 1450-bed super-specialty hospital located in Kochi, Kerala, India. Today, the hospital caters to over 10 lakh patients annually. Inspired by our Chancellor's vision of zero-waste, the hospital undertook its journey with a view to also reducing massive greenhouse gas emissions that result from improper handling of waste. Today, the hospital manages its municipal solid waste on an industrial scale, composting some eight metric tonnes of organic waste daily. This case study outlines the path followed to achieve zero-waste. Alongside, the rehabilitation of a former dump site is described in detail at this very site are carried out all composting operations of AIMS. Within three years of the restoration activities, heavy metal concentrations in the contaminated soil reduced drastically. There was relatively low uptake of the

heavy metals by the plants; however, they might have been crucially responsible for providing a favorable environment for soil restoring microorganisms in their rhizosphere. Observable habitat-restoration continues at the site, including the return of birds and insects and other wildlife, making this an ideal site for further research and demonstration for community awareness and education.

Keywords: Zero waste, MSW, heavy metals, mycoremediation, phytoremediation.

SYNTHESIS AND CHARACTERIZATION OF ORGANICALLY MODIFIED Gd₂O₃ - NATURAL RUBBER COMPOSITES AS EFFECTIVE X-RAY SHIELDING MATERIALS

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Protective materials based on lead are the usual X-ray shielding materials but their extended use leads to severe health problems due to the toxic nature of lead. Moreover, lead based materials are not appropriate for absorbing the regular energy region of X-ray used in medical field and hence natural rubber composites containing modified Gadolinium oxide (Gd₂O₃) as filler is suggested as an alternative. Natural rubber composites were prepared with organically modified Gd₂O₃ at various filler loadings. The structural features of modified Gd₂O₃ were examined using FTIR, X-ray diffraction and SEM. The particle size of organically modified Gd₂O₃ was found to be in the nano range which contributes to the enhanced properties of the composites. The increase of filler loading improved the shielding effectiveness of the rubber composites. Examination of mechanical and X-ray shielding properties show the effectiveness of the material to be used as potential shielding materials.

Keywords: X-ray attenuation, rubber composites, natural rubber, gadolinium oxide, SEM.

A STUDY ON PHYTOPLANKTON DIVERSITY IN RIVER GANGA AT ALLAHABAD UTTAR PRADESH (INDIA)

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Presence of microscopic algae can cause taste and odour problems, water discoloration, or form large mats that can interfere with boating, swimming, and fishing. The present study was conducted to assess the phytoplankton assemblages which in turn can serve as a suitable method to assess the quality of river ecosystem. Diversity and density of phytoplankton in river Ganga in Allahabad at five sampling stations was conducted from March to April 2014. Plankton identified in the river mainly composed of the members of Bacillariophyceae, Chlorophyceae and Cyanophyceae families and their count was made by Sedgewick rafter cell method. The Palmer pollution index values were calculated to know the level of organic pollution and to support the data. On the basis of quantitative and qualitative estimates 15 significant algal species were identified which can tolerate high degree of pollution. The abundance of phytoplanktons in April was greater than in March. Abundance of phytoplanktons and algal bloom was maximum at Chhatnaghat whereas at Sangam low phytoplankton diversity was found. In general, moderate temperature, low current velocity and high transparency of water appear to be better the conditions for algal growth in the river Ganga. These findings highlighted the deterioration of water quality of the river due to industrial, commercial and anthropogenic activities. The status of phytoplankton diversity of river Ganga was quite low indicating that the river is highly polluted.

Keywords: Phytoplankton, Sedgewick rafter cell, Palmer pollution index, Phytoplankton diversity, Algal bloom

POWER GENERATION USING INDUSTRIAL FLUE GAS M.M.S. Khaleel Naina Mohammed¹ Arun Mithran² L.Gautam³ A Sivabalan⁴ Electronics and Communication Department, Chennai Institute of Technology khaleelmms@gmail.com, gautam51@gmail.com³

The demand for power is the major problem that the world is facing now a day's. So in our generation we engineers have planned to resolve this problem by introducing the new concept that is "POWER GENERATION USING INDUSTRIAL FLUE GAS".

Here in this method we are not going to use any sort of fuel the thing we are going to use is that only the dirt gas

that is being emitted by the industries and the gas which is left out into the atmosphere does not contains any toxic content in it . it is purely an eco friendly gas which has an lower temperature no toxicity and the main thing we are going to use here is that nano filter beds by means of which we capture the unstable electrons and that are combined together by electron acceptor and the flow of electrons is nothing but electricity.

A STUDY ON THE BIOACTIVE COMPOUNDS PRESENT IN LEAVES OF *DICHROSTACHYS CINEREA*

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Natural products from medicinal plants, either as pure compounds or as standardized extracts, provide unlimited opportunities for new drug because of the unmatched availability of chemical diversity. Due to an increasing demand for chemical diversity, seeking therapeutic drugs from natural products interest particularly in edible plants has grown throughout the world. Botanicals and herbal preparations for medicinal usage contain various types of bioactive compounds. The focus of this paper is on the analytical methodologies, which include the extraction, isolation and characterization of active components in leaves of *Dichrostachys cinerea*. The analysis of bioactive compounds present in the plant extracts involve the application of common phytochemical screening tests, physicochemical tests, chromatographic techniques such as HPLC and TLC were discussed.

Keywords: *Dichrostachys cinerea*, physicochemical, phytochemical, TLC, bioactive

THERMAL DEGRADATION AND XRD STUDIES OF VEGETABLE OIL BASED NOVOLAC SCAFFOLDS FOR THE FORMULATION OF RESINS

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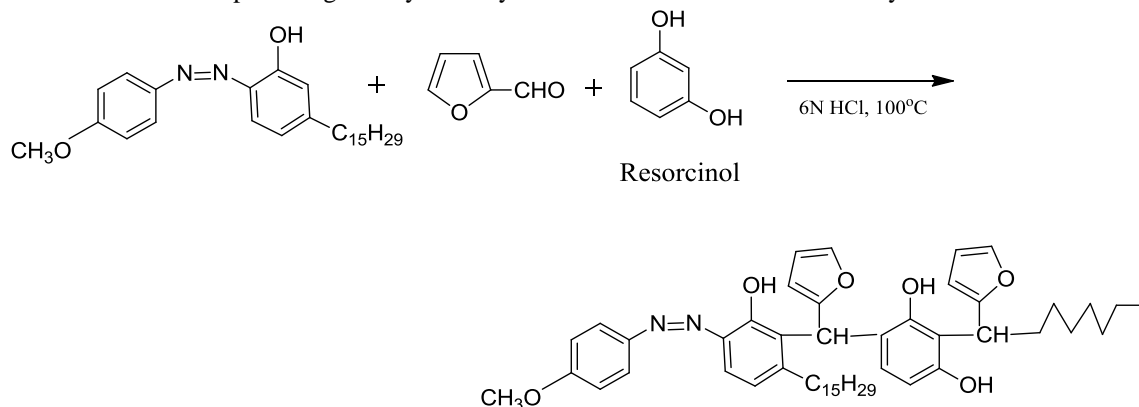
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Biomaterials, chemicals and energy from renewable resources have been the object of considerable interest in recent years. Vegetable oils are one of the cheapest and most abundant biological sources available in large quantities and their use as starting materials has numerous advantages such as low toxicity, inherent biodegradability and high purity. They are considered to be one of the most important classes of renewable resources for the production of bio-based thermosets. As a substitute to the use of conventional reinforcing synthetic resins, biobased resins were synthesized from cardanol, renewable and low cost industrial grade oil obtained by vacuum distillation of Cashew Nut Shell Liquid (CNSL), an abundant agricultural byproduct of cashew industry. On the other hand to further expand the field of application, cardanol-based novolac scaffolds, used in the formulation of thermosetting resins by blending with a conventional epoxy resin, especially designed to be compatible with conventional bisphenol-A epoxy resins. In the present study resins have been synthesized by condensing diazotized p-anisidine-cardanol dye with urea, resorcinol and furfural as condensing agent.. The resins have been characterised by FT-IR, ¹H-NMR and XRD studies. Thermal behavior of the resins has been studied by Thermogravimetric Analysis (TGA) and Differential thermal analysis (DTA). The DTA, SEM and XRD data indicated the percentage of crystallinity associated with the thermal stability of the resins.



Keywords: Diazotized p-anisidine, cardanol, furfural, thermal stability, crystallinity.

GROWTH AND CHARACTERIZATION OF A SEMIORGANIC NLO MATERIAL: L-HISTIDINEBARIUM CHLORIDE DIHYDRATE

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L-Histidine Barium Chloride dihydrate (LHBC), a semi organic nonlinear optical material was grown from aqueous solution by slow solvent evaporation method at room temperature. The LHBC crystals were characterized by X-ray powder diffraction analysis. The presence of functional groups was identified through Fourier Transform Infrared Spectroscopy. Thermogravimetric and Differential Thermal Analysis confirm that the crystal is stable up to 269°C. The mechanical properties of the grown crystals have been studied using Vickers microhardness test. The second harmonic generation behavior of LHBC crystal was tested by Kurtz-Perry powder technique.

Keywords: Crystal growth, X-ray diffraction, Optical material, Thermal studies, Nonlinear optics

DOCKING SCORE OF THE ISOLATED COMPOUND: 19-HYDROXY LOCHNERICINE - WITH DIFFERENT PROTEINS

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It evaluates the inhibitory effect of the isolated compound with different drug targets for the anti-cancer activities. The present investigation analyses the docking score of the isolated compound with different proteins. Two types of proteins (Drug targets) were chosen against cancer namely Human Epidermal Growth Factor and Crystal structure of human placental aromatase cytochrome P450. This result reveals that the compound 19-Hydroxy lochnericineshows hydrogen interactions with the docking energy of – 7.41 and -7.15 –8.83 kcal/mol. This reveals a significant interaction between the target proteins and the selected compound. Hence, the compound may offer therapeutic advantages in the treatment and prevention of diabetes and breast cancer.

Keywords: Isolated compound, *C.roseus*, Drug targets, cytochrome P450, ADMET, Docking scores.

PREPARATION OF MAGNESIUM HYDROXIDE NANOPARTICLES FROM BITTERN

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Magnesium hydroxide is an important inorganic material and has been widely used as neutralizing agent, flame retardant, smoke suppressant, desulphurizing agent and decolourizing agent. Magnesium hydroxide is very popular environmental friendly and thermally stable flame-retardant filler in composite materials. It has high decomposition temperature and good effects on depressing smoke. Magnesium hydroxide nanoparticles have favourable high flame retardant efficiency. It is also used to neutralize acidic waste streams and gases rich in sulphuric oxides, as anti-acid excipient in pharmaceuticals, in pulp and paper industry, as fertilizer additive and the important precursor for magnesium oxide.

In the present study nanoparticles of magnesium hydroxide were prepared from bittern. Bittern is the waste liquid formed during the production of salt. Since it is rich in magnesium, magnesium hydroxide nanoparticles can be prepared. Magnesium hydroxide nanoparticles with fiber like morphology were prepared by chemical precipitation process, with the bittern from the salt-pans of Tuticorin district used as Mg²⁺ raw material and ammonia water as precipitator. The nanoparticles were characterized by SEM, EDS and TG-DTA.

Keywords: Bittern, magnesium hydroxide, nanoparticles, chemical precipitation process, precipitator.

**PHYSICO CHEMICAL ANALYSIS OF GROUND WATER NEAR MUNICIPAL
SOLID WASTE DUMPING SITES IN ARUMUGANERI, THOOTHUKUDI
DISTRICT, TAMILNADU, INDIA**

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Ground water samples in and around from the dumpsite located in Arumuganeri were studied to assess the impact of Municipal solid waste on the ground water resources. Ground water samples were collected from the 5 different bore-wells in and around the dumpsites. The collected water samples were analyzed for parameters of Total Dissolved Solids (TDS), Total Alkalinity (TA), Total hardness, chloride and dissolved oxygen. The results were observed in each sample, compared with standards WHO, ICMR, ISI and thus an attempt was made to ascertain whether the quality of ground water is fit or not for drinking and other purposes.

Keywords: Ground water, MSW, Total hardness, Total Alkalinity, Water pollution.

**MOLECULAR STRUCTURE, VIBRATIONAL ASSIGNMENT, HOMO-LUMO AND
MULLIKEN ANALYSIS OF 2-[4-AMINO-2-(4-METHYLPHENYLAMINO)
THIAZOL-5-OYL] BENZOTHAZOLE (AMPATOB)**

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The compound 2-[4-amino-2-(4-methylphenylamino)thiazol-5-oyl]benzothiazole (AMPATOB) was prepared from 1-(4-methylphenyl)-3-(N-nitroamidino)thiourea and 2-(2-bromoacetyl)benzothiazole in the presence of triethylamine and characterised by FTIR, NMR and mass spectra. The geometry of the molecule was investigated and optimized with the help of B3LYP/ 6-31G density functional theory (DFT) method using Gaussian 09 software package. The calculated geometries such as bond lengths, bond angles, dihedral angles, atomic charges, harmonic vibrational wave numbers and intensities of vibrational bonds of the titled compound were investigated. The experimental ¹H NMR and IR spectrum was compared with theoretical value. The molecule consists of three ring systems, all are lying in one plane.

Keywords: Benzothiazole, DFT, B3LYP, Thiourea, Triethylamine

**STUDY OF EFFECT ON OXIDATIVE STABILITY AND RADICAL SCAVENGING
ACTIVITY OF SOYBEAN OILS BLENDED WITH COCONUT OIL**

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Coconut oil is consumed in daily diet especially in Southern India, owing to regional variations in food habits in country. The present study is focussed on blending regularly used oil with Soybean oil. SBO may protect against cancer of the breast and prostate. But consuming SBO directly as edible oil is not possible, due to its smell. Hence, blending SBO with other edible oils may exert beneficial influence. Here, blends (20%, v/v) of coconut oil (CO), with soybean oil (SBO) were formulated. Oxidative stability and radical scavenging activity of SBO and its blend with CO stored under oxidative conditions (60⁰C) for 24 days were studied by using ASTM. Due to blending, levels of polyunsaturated fatty acids (PUFA) decreased, while that of monounsaturated fatty acid (MUFA) content increased. Progression of oxidation was followed by measuring peroxide value (PV), p-anisidine value (PAV), % conjugated dienes (CD) and conjugated trienes (CT). Results: PV and OS showed inverse relationship at termination of storage. Levels of CD and CT in SBO, and blends, increased with increase in time. The impact of CO as additives on SBO, indicated markedly slow rate of oxidation.

Oxidative stability of oil blends was better than SBO, mostly because changes in profile of fatty acids and tocopherols, and also due to traces of minor bioactive lipids found in vegetable oils. The results suggest that

these oil blends could contribute as sources of important antioxidant related to the prevention of chronic diseases associated to oxidative stress, such as in cancer and coronary artery disease.

Keywords: Vegetable oil blends - soybean oil - oxidative stability - antiradical properties

PREPARATION OF SOYPROTEIN BASED NANOPARTICLE

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Soy protein based Nanoparticles were prepared via direct graft copolymerisation of soyprotein isolate(SPI) with ethyl methacrylate at a temperature of 120°C using benzoyl peroxide as a catalyst. The technique used here was emulsion polymerisation technique. The products obtained i.e., the graft copolymer and the homopolymer Poly(ethyl methacrylate)(PEMA) were separated from the product mixture by dissolving the mixture using chloroform in a separating funnel. The separated graft copolymer in the emulsion form was then spreaded over a glass plate to make a nano plastic sheet and the sheet was allowed to dry for 24 hrs at room temperature to remove chloroform from it. FTIR study confirmed the grafting of SPI and PEMA. XRD studies confirmed the presence of nanoparticles. TG-DTA, Hydrolytic stability, chemical resistivity and water absorption of the sample were studied. Grafting efficiency and grafting percentage of the sample were calculated.

Keywords: Nanoparticles, Copolymerisation, homopolymer, emulsion.

ELUCIDATION OF REACTIVITY DESCRIPTORS AND NBO ANALYSIS FOR AN ANTI-MALARIAL DRUG 5-(4-CHLOROPHENYL)-6-ETHYL-2,4-PYRIMIDINEDIAMINE USING DENSITY

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The present work elucidates the reactivity descriptors for 5-(4-chlorophenyl)-6-ethyl-2,4-pyrimidinediamine at DFT based B3LYP/6-31G(d) level theory in order to analyze its reactivity and site selectivity. Reactivity descriptors such as ionization energy, chemical potential, molecular softness, hardness, electrophilicity index and Fukui function have been determined to identify the nature of reactivity of 5-(4-chlorophenyl)-6-ethyl-2,4-pyrimidinediamine. The atomic descriptor $f(k)$ has been introduced to determine the local reactive sites of the molecular system during electrophilic, nucleophilic and radical attacks. For calculating the Fukui functions $f(k)$, the individual atomic charges calculated by the MPA scheme (Mulliken population analysis) have been used. In order to analyze the chemical reactivity, various global and local quantities have been utilized. The electron density based local reactivity descriptors; local hardness also known as intermolecular reactivity descriptor, local softness and the Fukui function also known as more reliable intramolecular site selectivity descriptors were recommended to explain the chemical selectivity or reactivity of particular site of a chemical system. The new descriptor, electrophilic index, to quantify the classification of the global electrophilic nature of a molecule and Fukui function (FF), one of the universally used local density functional descriptors to exemplify chemical reactivity and site selectivity have been studied. The NBO analysis clearly illustrates the existence of strong N-H...N intermolecular hydrogen bonding in 5-(4-chlorophenyl)-6-ethyl-2,4-pyrimidinediamine. The difference in stabilization energy associated with the hyperconjugative interactions are considerable which is due to the accumulation of electron density in the N-H bonds drawn not only from $n(N)$ of the hydrogen-acceptor but from the entire molecule leading to its elongation and concomitant red shift of the N-H stretching wavenumber.

Keywords: Fukui Function; Reactivity Descriptors, NBO analysis; Drug activity; Density Functional Theory; Pyrimidine ring;

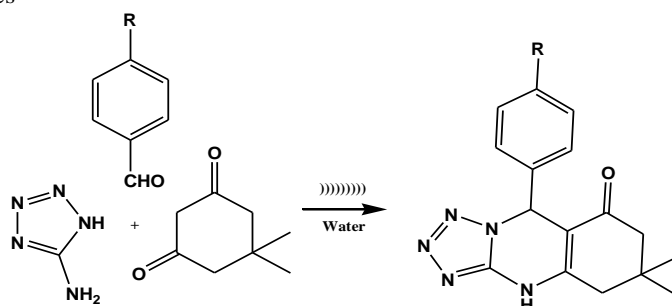
SYNTHESIS, SPECTRAL CHARACTERIZATION, ANTIMICROBIAL SCREENING AND MOLECULAR DOCKING STUDIES OF SOME NOVEL TETRAZOLOQUINAZOLINONE

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Quinazolinone derivatives have attracted attention as an important class of heterocyclic compounds in the field of drugs and pharmaceuticals. Tetrazole ring containing compounds represent an important class of heterocyclic nitrogen compounds and their derivatives are characterized with a broad spectrum of biological activity. The new series of tetrazoloquinazolinone derivatives were synthesised with excellent yields by the reaction of 5-amino-tetrazole – monohydrate and dimedone with corresponding aryl aldehydes in water under ultrasonic irradiation. The structures of all newly synthesised compounds are confirmed by FT-IR, ¹H, ¹³C NMR, HSQC and Mass spectral studies



R= H, CH₃, OCH₃, Cl, F, Br, NO₂, (CH₃)₂CH, (CH₃)₂N

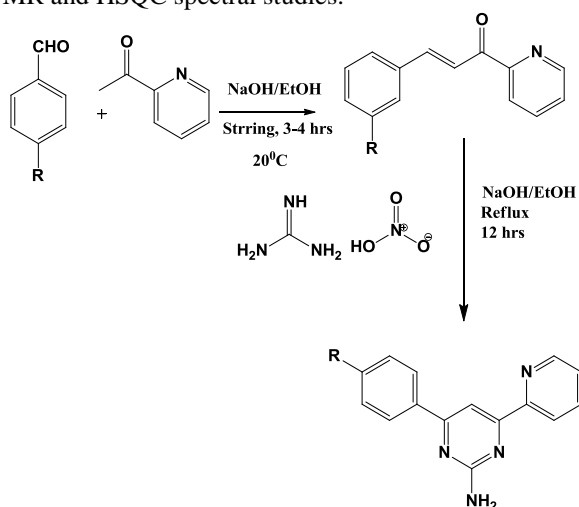
SYNTHESIS AND SPECTRAL STUDIES OF BIOLABILE 2-AMINO -6-((PYRIDINE-2-YL)-4-ARYLPYRIMIDINES DERIVATIVES

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Pyrimidines are considered to be a consequential precursor because they are integral part of the genetic material sagacious, DNA and RNA as nucleotides and nucleosides. Many pyrimidine derivatives have been found to be important pharmacophore for various drugs. A series of 2-amino-6-(pyridin-2-yl)-4-arylpyrimidines are synthesized by the condensation of (E)-3-phenyl-1-(pyridine-2-yl) prop-2-en-1-ones with guanidine nitrate in the presence of ethanolic sodium hydroxide solution. The structure of the synthesized compound are confirmed by FT-IR, GC-MS, ¹H, ¹³C NMR and HSQC spectral studies.



R: H, Cl, Br, F, CH₃, CH₃O, NO₂, CH(CH₃)₂

CATALYSIS BY AMBERLYST A 21: A GREENER APPROACH TO 4,5,6,7-TETRAHYDRO-1H-INDAZOL-3(2H)-ONES VIA EFFICIENT CONSTRUCTION OF CYCLOHEXANONE DERIVATIVES

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The 4,5,6,7-tetrahydro-1H-indazol-3(2H)-one derivatives have been synthesized in good yields via a two-step method in a single pot. The initial step involved the construction of cyclohexanone ring from aromatic aldehydes and β -ketoester in i-PrOH using an inexpensive and reusable catalyst (i.e., Amberlyst A-21) under mild reaction conditions. The utility of this catalyst has been demonstrated in synthesizing a range of cyclohexanone derivatives. The catalyst can be recovered and recycled, which makes this procedure simple, convenient, economically viable, and environmental friendly.

Keywords: Amberlyst A-21; catalysis; cyclohexanone; indazole

**ANTILITHIATIC ACTIVITY AND PHARMACOGNOSTIC STUDIES OF SCOPARIA
DULCIS**

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Abstract

Scoparia dulcis Linn has been widely reported to have pharmacological uses arising from its wide spread uses. The different extracts were prepared by successive extraction with petroleum ether, chloroform, ethanol and water using soxhlet distillation method. Phytochemical analysis of plant extract revealed the presence of alkaloids, carbohydrates, glycoside, tannins, starch etc. Thin layer chromatography and Gas chromatography-mass spectrometric analysis revealed the presence of different components in the plant extract. Among the 50 components obtained, 10 important organic compounds were analyzed. All these compounds are found to be having some medicinal application. UV visible spectroscopic analysis of extract of Scoparia dulcis reported four chromatogram figures which showed prominent peaks having maximum absorption of 666 nm corresponded to wavelength of methylene blue and brilliant blue.

FTIR spectroscopic analysis reveals the presence of important functional groups like-OH,-NO₂,-SO₃,-SH, -COOH, NH₂, R-X etc. Antibacterial activity of petroleum ether, chloroform, and ethanol and water extracts of stems and leaves of Scoparia dulcis reveals that chloroform and ethanol extracts shows maximum resistance against Staphylococcus while ethanol and aqueous extracts showed maximum resistance against Klebsiella pneumonia. The exciting fact came out of the study is that water extract of Scoparia dulcis showed great potential to dissolve the Calcium oxalate crystals ie, the plant extract shows invitro antilithiatic activity for kidney stones. Thus Scoparia dulcis act as a source of different valuable organic compounds that are having medicinal applications and have a beneficial effect on kidney stone problem.

Key words: Scoparia dulcis, Antibacterial activity, Antilithiatic activity, Calcium oxalate dissolution method, Gas chromatography-mass spectrometry.