# CHAPTER 9

# CHEMISTRY

## Doctoral Theses

064. AGGARWAL (Komal)
**Synthesis of Novel Heterocyclic Compounds, their Biological, Photophysical and Theoretical Studies and also Application as Sensors.**
Supervisor : Prof. J. M. Khurana
Th 22067

*Contents*

1. Synthesis of novel 12-ary1-8,9,10,12-tetrahydrobenzo[*a*] xanthene-11-thiones and evaluation of their biocidal effects 2. DBU: A proficient catalyst for one-pot synthesis of biologically important spiropyrans in aqueous medium 3. Synthesis of benzo [*a*] xanthenes, effect of hydroxy1 group on their photophysical properties, solvatochromic studies and estimation of dipole moment 4. X-ray diffrantion, spectroscopic characterization and quantum chemical calculations by DFT and HF of novel 2-hydroxy-12-(4-hdroxypheny1)-9,9-dimethy1-9,10-dihydro-8*H*-benzo[*a*]xanthen-11(12*H*)-one 5. A green catalyst free synthesis of diazaspiro heterocycles and their photophysical studies solvatochromic analysis and TDDFT calculations PART VA: An efficinet catalyst free synthesis of nitrogen containing spiro heterocycles *via* [5+1] double Michael addition reaction PART VB: Photophysical studies, solvatochromic analysis and TDDFT calculations of diazaspiro compounds 6. Synthesis of novel indeno-furan based derivatives and their application as colorimetric and fluorescent pH sensors and sensors for detection of $Cu^{2+}$, $Pb^{2+}$ and $LA^{3+}$ PART VIA: Synthesis of some novel indeno-furan based derivatives and their application as colorimetric and fluorescent pH sensors PART VIB: Phenazine containing indeno-furan based multianalyte colorimetric and fluorescent sensor for the detection of $Cu^{2+}$, $Pb^{2+}$ and $LA^{3+}$ 7. Summary and conclusions. List of publications.

065. AMREETA PREETAM
**p-Dodecylbenzenesulfonic Acid Catalyzed Synthesis of Arenes and Heteroarenes.**
Supervisor : Prof. Mahendra Nath
Th 22415

*Abstract*

Development of green synthetic strategies for long term sustainability of environment has received considerable attention in recent years. The build-up pressure against the use of hazardous organic solvents or reagents for carrying out various organic reactions has alarmed researchers due to health, safety and environmental concerns and thereby initiated the search of eco-friendly approaches for the synthesis of various biologically useful molecules. In this context, surfactant combined catalysts have demonstrated their ability in constituting various environmentally benign protocols in the past. Among these, p-dodecylbenzenesulfonic acid (DBSA) has emerged as an efficient Brønsted-acid surfactant combined catalyst for carrying out diverse water-sensitive organic reactions in water as well as under solvent-free conditions. The main

objective of this thesis is to develop efficient and environmentally benign methodologies for the construction of diverse aromatic and heteroaromatic compounds by using DBSA as a Brønsted acid surfactant combined catalyst. The work presented in this thesis is divided into five chapters. The first chapter gives an overview on DBSA-catalyzed organic transformations with main focus on C-C, C-N and C-O bond forming reactions. Second chapter presents an eco-friendly methodology for the synthesis of materially important 1,3,5-triarylbenzenes by using 20 mol% of DBSA under solvent-free conditions. Chapter-3 describes an ambient temperature synthesis of various medicinally important pyrrolo- and indolo[1,2-a]quinoxaline derivatives via DBSA-catalyzed Pictet-Spengler reaction of 1-(2-aminophenyl)pyrrole or 1-(2-aminophenyl)indoles with a wide range of aromatic aldehydes, acetophenones or isatins. Chapter-4 discusses about the microwave-assisted eco-friendly one-pot multi-component synthetic strategy for a variety of xanthene analogues under solvent-free conditions. Chapter-5 presents efficient synthetic protocols for novel 2,3-disubstituted-4-thiazolidinones and spiro[indole-thiazolidinones] by reacting various aldehydes or isatins with primary amines and thioglycolic acid in the presence of 10 mol% of DBSA in water at ambient temperature.

*Contents*

1. p-dodecylbenzenesulfonic acid catalyzed organic transformations: An overview. 2. An efficient synthesis of 1,3,5-triarylbenzenes by using p-dodecylbenzenesulfonic acid as a bronsted acid catalyst. 3. Environmentally benign syntheses of pyrrolo-and infolo[1,2-a}quinoxalines via p-dodecylbenzenesulfonic acid catalyzed pictet-spengler approach. 4. p-dodecylbenzenesulfonic acid accelerated green synthesis of diverse xanthenes under solvent-free microwave conditions. 5. On water synthesis of 4-thiazolidinones and spiro[indole-thiazolidinones] using p-dodecylbenzenesulfonic acid as a bronsted acid surfactant combined catalyst. Summary.

066. ANURADHA
**Ceramic Based Nanocarriers: Synthesis, Characterization and Some Biomedical Applications.**
Supervisor : Dr. Indrajit Roy
Th 22059

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1. Introduction 2. Literature review 3. Experimental and characterization techniques 4. Fluorophore-doped calcium phosphate nanoparticles for non toxic biomedical applications 5. Europium doped nanophosphors and applications in vitro optical biomaging 6. Synthesis and characterization of iron phosphate NPs and applications in magnetically guided drug delivery 7. Synthesis and characterization of indium oxide NPs and applications in light activated therapy 8. Conclusion. Publication.

067. AZAD (Neeta)
**Novel Pyruvate Dehydrogenase Kinase (PDHK) Inhibitors Based on in Silico Studies.**
Supervisor : Prof. Rita Kakkar
Th 22421

*Abstract*

Chapter-1 (Introduction) The Pyruvate Dehydrogenase Complex (PDC) is one of the largest multi-enzyme complexes found in living cells, its activity is regulated by the Pyruvate Dehydrogenase Kinase (PDHK) isozymes, which catalyse the phosphorylation of PDC, causing its inactivation. Too much activity of PDHK reduces metabolism, causing conditions such as obesity, heart ischemia and insulin resistant diabetes. PDHK isozymes need to be inhibited in order to reactivate PDC. Chapter-2 (Computational Techniques) describes the various computational techniques applied in this thesis. Chapter-3 (Discovery of some potent PDHK inhibitors using pharmacophore modeling), a pharmacophore model has been generated and 3D-QSAR (Quantitative Structure Activity Relationship) studies performed on a set of fluorinated compounds having known activities for the PDHK inhibition. A class of 50 fluorine-containing compounds with known $IC_{50}$ values (ranging from 0.1 μmol $L^{-1}$to 100.0 μmol $L^{-1}$) were selected for developing a common pharmacophore hypotheses and 3D-QSAR model. In Chapter-4 (Computational testing of doxifluridine and its metabolites as PDHK1 inhibitors by the molecular docking method), the metabolites of doxifluridine were discussed. A theoretical comparison of 5'-dFUR and 5-FU was done to support the better therapeutic index of 5'-dFUR. Chapter-5 (Molecular Docking: A computational tool for structure based drug design applied to fluorinated PDHK2 inhibitors), the molecular docking method was performed on a library of fluorinated molecules. ADME properties and various descriptors were also calculated and analysed. In Chapter-6 (Long term inhibition of PDHK isozymes with AZ12 and its analogues), we tried inhibiting all the four isozymes of PDHK so as to maintain the long term effect of inhibitors and hence the long term activity of the PDC complex. In Chapter-7 (Concluding remarks), the implications of the present work and the necessary criteria that a molecule must satisfy in order to be called a good drug have been discussed.

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068. BADHANI (Bharti)
**Investigation of Varied Facets of Gallic Acid : An in Silico Approach.**
Supervisor : Prof. Rita Kakkar
Th 22416

*Abstract*

This thesis deals with in silico studies on gallic acid and its modifications in order to optimize the respective biologically beneficial characteristics. The thesis consists of seven chapters. In Chapter 1 (Gallic acid: A versatile antioxidant with promising therapeutic and industrial applications), we have reviewed the bioavailability and the biosynthetic pathway of gallic acid. In addition, a survey of various in vitro, in vivo and in silico studies providing the structure and function of this molecule, along with a comprehensive overview of factors responsible for its high antioxidant activity has been undertaken. Chapter 2 (Computational techniques) describes the various

computational techniques applied in this thesis. Density Functional methods and various docking techniques and tools to develop pharmacophore and 3D-QSAR models are reviewed in detail. Chapter 3 (An investigation of the structural and electronic properties of gallic acid and its anions in gas and aqueous phase) deals with an in-depth analysis of the structural and electronic features of gallic acid and its anions. In Chapter 4 (Influence of intrinsic and extrinsic factors on the antiradical activity of gallic acid), we have studied the various possible pathways for free radical scavenging by gallic acid. In Chapter 5 (In silico studies on potential MCF-7 inhibitors: A combination of pharmacophore and 3D-QSAR modeling, virtual screening, molecular docking and pharmacokinetic analysis), pharmacophore modeling and 3D-QSAR studies were performed. The pharmacophore model was further utilized to identify novel anticancer molecules. Chapter 6 (Structural, electronic and reactivity parameters of some triorganotin(IV) carboxylates: A DFT analysis) deals with triorganotin(IV) hydroxycarboxylates previously shown to possess anticancer ability. A thorough investigation of $R_3SnL$ complexes in the gas and aqueous phases was undertaken. In Chapter 7 (Concluding remarks), we have discussed the implications of the present work in understanding the structural, electronic, antiradical and anticancer properties of galloyl derivatives.

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069. BAG (Narmada)
**Development of Functionalize of Semiconductor Quantum Dots for Non-Invasive Imaging.**
Supervisors : Dr. Firasat Hussain and Dr. Rashi Mathur
Th 22054

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070. BANSAL (Prerna)
**DFT Studies of Trans-Resveratrol as an Antioxidant and Anti-Ageing Drug for Activating Sirtuins.**
Supervisor : Prof. Rita Kakkar
Th 22050

*Abstract*

This thesis deals with the computational studies on the structural and electronic properties of the polyphenol trans-resveratrol.
This is mainly a plant polyphenol which is produced in response to stress, injury, ultraviolet irradiation and fungal infection as a part of their defense mechanism. It has multiple health benefits including antioxidant, anti-inflammatory, anticarcinogenic, antiestrogenic, inhibition of platelet aggregation, anti hyperglycemic and neuroprotection. Among various health benefits, the antioxidant role is the most important where it has been found to have huge potential to combat oxidative and nitrosative stress by scavenging reactive radicals which damage biomolecules and results in ageing. It has also been found to delay ageing by activating the proteins called Sirtuins by varying NAD levels similar to calorie restriction. These Sirtuin proteins slow down the activity of other proteins responsible for metabolism and hence delays ageing. Thus in our studies,we have performed the computational studies on the electronic structure and properties of trans-resveratrol responsible for its extraordinary antioxidant action.
We have investigated various antioxidant descriptors and associated radical scavenging pathways that largely depends upon the philicity of radicals.
We have also performed computational studies on the various molecules which are similar to trans-resveratrol in their action and suggested a pharmacophore model to identify the features that enhances the binding of trans-resveratrol like molecules to sirtuin proteins.
In addition to that, we have also selected some naturally occuring polyphenols and flavanoids to assess the putative binding sites of them in the sirtuin protein using computational studies. We have thus concluded that trans-resveratrol has got huge potential in the future.

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071. BARUAH (Anupaul)
**Generalized Approach to Investigate Various Folding Phenomena and Intrinsic Disorder in Proteins by Sequence Design and Mutation.**
Supervisor : Dr. Parbati Biswas
Th 22058

*Abstract*

A self-consistent mean-field based model is developed to design sequences for a three-dimensional lattice protein and Cα chain backbones of real protein conformations. The unfolded ensemble of conformations are generated by a coarse-grained Monte Carlo simulation with a 6-12 Lennard Jones potential and restrictions in the Cα- Cα pseudo bond lengths. A generalized foldability criterion identifies the ensemble of sequences compatible to the target conformation by maximizing the sequence entropy. The design procedure utilizes both positive and negative design elements by including the unfolded ensemble of conformations. This protein design approach is applied to rationalize various protein folding related phenomena, like protein misfolding, protein

fold switch and intrinsic disorder in proteins. The role of structural flexibility and mutations in protein misfolding is investigated. A method is proposed to predict misfolding probability of mutated sequences. An effort to understand the physics behind protein intrinsic disorder is made, in the energy landscape perspective. A sequence information based method is suggested to predict order/disorder and measure the conformational entropy of a given sequence. The general sequence and energy landscape characteristics are also identified for proteins that switch fold. The overall consistency of the results suggests that the method developed is generalized and may, in principle, be applicable to any target topology to explain a broad array of folding phenomena.

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072. BASKARAN T.
**Silicate Moiety Intercalated Layered Double Hydroxide (LDH): As Potential Support and Catalytic Materials.**
Supervisors : Dr. A. Sakthivel and Dr. J. Christopher
Th 22424

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073. CHADHA (Nidhi)
**Computational Modeling Approaches and Analysis of Ligands Involved in the Biochemical Pathways.**
Supervisors : Dr. Marilyn Daisy Milton and
Dr. Anjani Kumar Tiwari
Th 22062

*Abstract*

Computational modeling approaches plays an important role in the interdisciplinary field of chemistry and biochemistry. In systems medicine, the understanding of these associated biochemical pathways is a fundamental challenge along with drugs and their mode of action where a small drug molecule interacts with target protein associated into the biochemical pathways. Also the key issue which are need to be addressed are the elucidation of drug targets for the search of new drugs or novel

targets for existing drugs. This can be further accomplished by incorporating the biological information about the drug targets which is of essence for studying the biochemical pathways computationally. With the aim of implementation of computational chemistry to replace the traditional laboratory research, in this thesis, we introduced the computational workflow for the detailed knowledge, analysis and validation of biochemical pathways and existing or new drug assessment. The introduction, Chapter 1 provides an overview of the thesis, statement of the problem, which explains the purpose, motivation and results of the research. Chapter 2 describes the theoretical and technical background of computational methods implemented in the thesis. Chapter 3 consists of two sections followed by brief introduction about the quest for computational studies for ligands and metal complexes and their corresponding physicochemical behaviour of them in in vivo environment. Chapter 4 includes two sections involving the theoretical investigation into structural and functional analysis of AChE and PAH enzymes involved in biochemical pathways for neurological cascades. Chapter 5 describes the computational modeling of important targets for neuroimaging; serotonin receptor subtypes, $5HT_{1A}$ and $5HT_7$. Chapter 6 involves the computational workflow for the development of acetamido-benzoxazolone based ligands for imaging of TSPO for neuroinflammation in the brain. Chapter 7 summarizes the thesis and suggests directions for future research.

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074. CHAUHAN (Manmohan Singh)

**Syntheses of Recyclable Organocatalysts and their Application in Asymmetric Reduction, Diels-Alder Reaction and Ring Opening of Epoxides.**

Supervisor : Dr. Surender Singh

Th 22071

*Abstract*

Research studies were done on the Syntheses of Recyclable Organocatalysts and Their Application in Asymmetric Reduction, Diels-Alder Reaction and Ring Opening of Epoxides. The preparation of enantiomerically pure compounds is an important area of contemporary synthetic organic chemistry. Asymmetric catalysis is one of the key tools for synthesis of enantiopure compounds. We have developed ionic liquid tagged chiral catalysts for asymmetric reduction of ketone and Diels-Alder reaction between cyclopentadiene and ∝,β-unsaturated aldehydes. The ionic liquid of prolinol modified with ionic liquid having ether linkage is stable catalyst for the asymmetric reduction of ketone with $BH_3.SMe_2$. Ionic liquid (5 mol%) with ester linkage of McMillan catalyst having hexafluorophosphate counter anion acts as catalyst in presence co-catalyst trifluoroacetic acid(5 mol%) for the Diels-Alder reaction between cyclopentadiene and crotonaldehyde, gave 94% conversion of product with exo/endo(1/1.1) and 90% ee of endo product. The effect of the counter anion of ionic liquid was also studied. These catalysts are recovered and reused upto 4-5 times. Different acid salts of amines were

synthesized and used as organocatalysts for the ring opening of epoxides with amines for the synthesis of amino alcohols.

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1. Introduction 2. Synthesis of recoverable and reusable Macmillan catalyst and its application in asymmetric diels-alder reaction Section A: Macmillan's catalyst modified with ethanol amine derived and its application in asymmetric diels-alder reaction Section B: Macmillan's catalyst tailored with ionic and its application in asymmetric diels alder reaction 3. Asymmetric reduction of ketones catalyzed by α,α– Dipheny1-(*L*)–prolinol modified with imidazolium ionic liquid and $BH_3.SMe_2$ as a recoverable catalyst 4. Synthesis of benzenaminium salt as organocatalyst and its catalytic activity in synthesis of β–amino alcohols by ring opening of epoxide with amines Section A: Synthesis of *N*-fluorobenzenaminium tetrafluroborate as organocatalyst and its catalytic activity in synthesis of epoxides with amines Section B: Synthesis of recoverable and reusable benzenaminium salt (Anilinium salt) for opening of epoxides with amines. Summary. List of publications.

075. CHHATWAL (Megha)
**Fabrication of Molecular Films Based on Metal-Polypyridyl Complexes.**
Supervisor : Prof. Satish K. Awasthi
Th 22454

*Contents*

1. Introduction : A brief overview on molecular films comprising polypyridyl complexes 2. Electropolymerization : Modification of electrodes (glassy carbon/ ITO-coated glass) via electroactive polymer films 3. Electropolymerized films as information reservoirs : Electrical modulation of films to store multi-state volatile memory 4. Covalent immobilization : Grafting of covalently-assembled monolayers on $SiO_x$ surface. List of publication

076. DEBNATH (Anamika)
**Synthesis, Characterization and Biological Evaluation of Metal Complexes of Some Selected Quinolones in Presence of Nitrogen Containing Heterocyclic Compounds.**
Supervisor : Dr. Dhanraj T. Masram
Th 22043

*Abstract*

Qunolones are broad spectrum synthetic antibiotics containing 4-oxo-3- carboxylic-1,4-dihydriquinolone skeleton. In this research I have synthesized some metal complexes of Nalidixic acid, Norfloxacin and Enoxacin with some biologically important metal ions. Then synthesized metal complexes were screened against some bacterial infections and fungal infections. It has been found that synthesized metal complexes give better anti microbial result comparatively than their parents quinolones.

*Contents*

1. Quinolones and metalloquinolones 2. Synthesis of mixed ligand complexes 3. Characterization of synthesised mixed ligand metal complexes 4. X-ray

crystallography analysis of metal complexes 5. Antimicrobial evaluation of the synthesised metal complexes. Future prospects. List of Publication.

077. DEORI (Kalyanjyoti)

**Morphology Controlled Synthesis and Characterization of Metal Oxide and Noble Metal Based Hybrid Nanocrystals as Efficient Enviromentally Friendly Catalyst for Multiple Applications.**

Supervisor : Dr. Sasanka Deka

Th 22061

*Abstract*

We have synthesized $CeO_2$ nanoparticles exposed in (100) and (111) surfaces and explored them as heterogeneous catalyst for the first time in the oxidation of para-xylene (pX) to terephthalic acid (TA) in a very environmentally benign reaction condition where water was used as the solvent. The above mentioned catalysis results can be further improved by improving the quality of ceria nanocrystals in terms of morphology to achieve the maximum number of active surfaces, i.e. only (100) facets in cubic topology. This newly established $CeO_2$ nanocubes showed breakthrough in catalytic performance, enabling quantitative pX conversion and absolute selectivity in terephthalic acid (>99%) in water at a temperature in the range 30−85 °C and one bar of oxygen pressure without the use of a bromide ion promoter and acetic acid. Similarly effect of different morphologies of $CeO_2$ nanocrystals viz., nanorods, nanocubes and nanopolyhedra developed by one new surfactant assisted colloidal process have been investigated in aromatic alcohol and toluene oxidation also. Later on, the as-synthesized $CeO_2$ nanocubes were used as model seed material for growing some noble metals like Au on to the surface of ceria to develop a new kind of material called hybrid nanocrystals (HNCs) where different shapes and properties are connected together in a single particle. The electrocatalytic activity of $CeO_2$ with cubic topology and Au-$CeO_2$ HNCs were then investigated for water splitting and methanol oxidation reaction. Continuing the idea of morphology controlled synthesis, a simple solvothermal strategy has been developed to synthesize highly stable CoO and $Co_3O_4$ NPs with controlled size and morphologies viz., nanocubes, hexagonal platelets, nanosphere etc., and studied their electrochemical activity, without adding any large area support or a conductive filler where, the hexagonal platelet $Co_3O_4$ particles exhibited comparatively better characteristics with high specific capacitance that suited for potential applications in supercapacitors.

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078. GARG (Parul)

**Synthesis of Novel Imidazolium Salts and their Applications in Metal-Catalyzed C-C Bond Forming Reactions and Development of Novel Synthetic Methodologies for Metal-Free C-N Bond Formation.**

Supervisor : Dr. Marilyn Daisy Milton

Th 22047

*Abstract*

The thesis entitled "Synthesis of Novel Imidazolium Salts and their Applications in Metal-catalyzed C-C Bond Forming Reactions and Development of Novel Synthetic Methodologies for Metal-free C-N Bond Formation" presents some novel synthetic methods, which includes synthesis and characterization of novel unsymmetrical N, N'-disubstituted imidazolium salts for application as preligands in transition-metal-catalyzed C-C bond forming reactions such as Heck-Mizoroki and Suzuki-Miyaura cross-coupling reactions and development of novel synthetic C-N bond forming methodologies for the synthesis of N-(hydroxyalkyl)cinnamamides and 2-aryl/heteroaryloxazolines under metal-free conditions. The thesis is divided into seven chapters. Chapter 1 gives an overview of recent advances made in C-C and C-N bond forming reactions. Chapter 2 describes the synthesis and characterization of novel unsymmetrically N, N'-disubstituted imidazolium salts with electronically inequivalent and flexible side arms incorporating a variety of functional groups such as hydroxyl, ammonium, phenyl, naphthyl etc. Chapter 3 explores the in situ catalytic performance of the synthesized novel unsymmetrical N, N'-disubstituted imidazolium salts as preligands in palladium catalyzed Heck-Mizoroki reaction of aryl bromides with methyl and ethyl acrylate under aerial atmosphere. Chapter 4 explores the in situ catalytic performance of the synthesized novel unsymmetrical N, N'-disubstituted imidazolium salts as preligands in palladium catalyzed Suzuki-Miyaura reaction of aryl halides with phenyl boronic acid under aerial atmosphere. Chapter 5 describes a direct and efficient synthetic methodology for the synthesis of a variety of N-(hydroxyalkyl)cinnamamides from cinnamates and aminoalcohols utilizing inexpensive, non-toxic and readily available $Na_2CO_3$ as the base. Chapter 6 describes the synthesis of a variety of 2-aryl/heteroaryloxazolines from nitriles and aminoalcohols under metal- and catalyst-free conditions and antioxidant properties of 2-aryl/heteroaryloxazolines using the DPPH (diphenyl picryl hydrazyl) assay method. Chapter 7 summarizes the research work reported in this thesis along with the important conclusions inferred from this work.

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079. GAUTAM (Seema)
**Synthesis, Characterization and Biological Evaluation of Transition Metal Complexes with Some N,O and N,S Donor Polydenate Ligands.**
Supervisor : Dr. Sulekh Chandra
Th 22418

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characterization of nickel(II) ($3d^8$) complexes with polydentate ligands ($L^1$-$L^6$). 6. Synthesis and characterization of sopper(II) ($3d^9$) complexes with polydentate ligands ($L^1$-$L^6$). 7. Biological evaluation : Antimicrobial activity of polydentate ligands ($L^1$-$L^6$) and their metal complexes.

080. GROVER (Sonia)
**Synthesis, Characterization and Application of Nanocomposites of Metal Oxide, Conducting Polymers and Carbon Material for Supercapacitor Device.**
Supervisor : Dr. Raj Kishore Sharma
Th 22044

*Contents*

1. Introduction 2. Experimental techniques 3. MWCNT supported conducting polymer and $MnO_2$ nanocomposites for supercapacitor electodes: Role of $MnO_2$ dispersion in performance evolution 4. Fabrication and electrochemical investigation of various nanostructures of conducting polyaniline 5. PANI nanotube wrapped GONR nanocomposites for supercapacitor electodes 6. Interaction of PNT with metal oxides (I) PANI nanotube suppoted $RuO_2$ nanocomposites for supercapacitor electrodes (II) PANI nanotube supported $MnO_2$ nanocomposite for supercapacitor electodes 7. Conclusion and future prospects. List of Publications.

081. JAIN (Shilpa)
**Montmorillonite Based Excipients as Delivery Vhicle for Extended Release of Drugs.**
Supervisor : Prof. Monika Datta
Th 22063

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**SECTION (I) :** 1. Introduction to drug delivery systems 2. Recent review of literature 3. Selection of drugs 4. Analytical techniques used in present work
**SECTION (II) :** 1. Methodologies 2. Montmorillonite as a drug delivery vehicle 3. Organo montmorillonite as a drug delivery vehicle 4. Motmorillonite polymer composites as a drug delivery vehicle 5. Montmorillonite polymer beads as a drug delivery vehicle 6. Summary 7. Future prospects. Credentials.

082. JUNEJA (Ridhima)
**Micro-Emulsion Mediated Synthesis of Polymeric Naoparticles and their in Vitrostudies.**
Supervisor : Dr. Indrajit Roy
Th 22074

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1. Introduction 2. Literature review 3. Experimental and characterization techniques 4. Micro-emulsion mediated modulation of nanoparticle dimensions for optimal in vitro biomedical use 5. Surface modified PMMA nanoparticle with tunable drug release and cellular uptake 6. Synthesis and in vitro studies for biodegradable PCL nanoparticles with magnetic doping 7. Iron oxide nanoparticles doped niosomes for magnetically assisted drug delivery 8. Conclusion.

083. KADIYALA (K. Ganesh)

**Development of Ligands for Transporter and Receptor Targeted Molecular Imaging.**

Supervisors : Dr. M. Thirumal and Dr. Anupama Datta

Th 22417


*Abstract*

In brief, the aim of the thesis focuses on the design and synthesis of molecular imaging agents for transporter and receptor targeted imaging using molecular imaging techniques. The thesis was divided in to four objectives. In the first objective an acyclic bifunctional chelating agent ($H_2$pentapa-en-$NH_2$) was synthesized in >95% yield and conjugated with methionine for LAT1 imaging. After conjugation with L-methionine ($H_2$penetapa-en-$met_2$) properties were studied with $^{99m}$Tc. SPECT and Biodistribution studies reveal uptake was largely in kidney and $H_2$penetapa-en-$met_2$ was targeted towards tumor with T/M of 6.52. In the second objective the LAT1 targeted probe (DOA-Act-Met) was prepared using DOTA chelating agent having good binding affinity towards $^{68}$Ga and $^{157}$Gd after conjugation with methionine. The efficacy of the ligand was proved by its successful radiolabeling with $^{68}$Ga and $^{157}$Gd that ensured minimal cytotoxicity and significant cellular uptake in U-87MG cancer cells. Receptor binding studies suggests the participation of LAT1 in tumor uptake. In the third objective a piperazine derivative (N-(2-(4-(2-Methoxyphenyl)piperazin-1-yl)ethyl)-N-$^{11}$C-methylpyridin-2-amine), was synthesized labeled with $^{11}CH_3$. In the PET studies of rat brain, the highest uptake of radiolabeled-ligand was in the cerebellum, followed by moderate uptake in thalamus and striatum where the mGluR1 are high. The lowest uptake was detected in the pons where the mGluR1 are less. PET with the synthesized probe may useful for determining the density and the occupancy of mGluR1 in the brain. In the fourth objective estradiol derivatives ($E_2NO_2$ and $E_2CF_3$) were synthesized in high purity. The synthesized probe ($E_2CF_3$) inhibited the growth of the MDA-MB-231 and it was comparable to that of tamoxifen. The cell growth inhibition induced in MDA-MB-231 cells by $E_2CF_3$ was due to cell cycle arrest and apoptosis. Finally, the action of $E_2CF_3$ on ER-negative breast cancer cells may open new avenues for therapy and diagnosis in MRI and PET imaging.


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084. KALOTRA (Anil Kumar)

**Synthesis Characterization and Applications of Functionalized Silica Gel as Efficient Sorbent for the Slective Extraction and Determination of Cr(III), Cu(II), Ni(II) and Mo(VI) Ions.**

Supervisor : Prof. R.K Sharma

Th 22045

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preconcentration and recovery of Cr(III) ions 4. Silica functionalized with 4-hydroxy-2-phenyl phthalazine-1(2H)-one: Novel Organic-inorganic hybrid sorbent for selective extraction and determination of Cu(II) ions 5. Selective extraction and determination of ni(II) ions using 2-[3-(-formylphenoxy)-2-hyroxypropoxyl benzaldehyde (FPHB) functionalized silica gel 6. Synthesis, characterization and application of novel organic-inorganic hybrid 2'-hydroxy chalcone functionsalized silica gel for the selective extraction and determination of Mo(VI) ions. Summary. Publication.

085. KHERA (Mansi)
**Corrosion Mitigation of Aluminium in Acidic Medium by Using Some Phosphonium Compounds.**
Supervisor : Prof. Gurmeet Singh
Th 22056

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1. Introduction 2. Literature review 3. Experimental procedures 4. Weight loss measurments 5. Galvanostatic polarization studies 6. Electrochemical impedance spectroscopy 7. Temperature kinetic studies 8. Surface morphological studies-I, scanning electron microscopy 9. Surface morphological studies-II, energy dispersive spectroscopy 10. Quantum chemical calculations 11. Conclusions.

086. M. SARATH BABU
**Electrochemical Studies on Rough Glassy Carbon Electrodes in Room Temperature Ionic Liquids : Experimental Validation of Theories.**
Supervisor : Prof. Rama Kant
Th 22423

*Abstract*

We developed a theory for the influence of uncompensated solution resistance on quasi-reversible charge transfer at an arbitrary rough electrode. The significant deviation from the quasi-reversible behavior is explained as arising from the kinetics of the system, the resistivity of the solution and morphological irregularity of the interface. The morphological irregularity of electrode is characterized through a structure factor or power spectrum (PS) of roughness. The PS is obtained from SEM image using our recently developed CV-SEM method. The PS obtained from SEM image shows a finite fractal nature of roughness which is observed in the intermediate and high wavenumber. This analysis provide fractal dimension ($D_H$), lower cutoff length scale ($\ell$), upper cutoff length scale (L) and topothesy length ($\ell_s$). Our theory predicts the anomalous response on these finite fractal electrodes in the chronoamperometric measurements. Theory also accounts for the influence of uncompensated solution resistance. For experimental corroboration in RTIL on glassy carbon rough electrode, electrochemical active area, roughness factor (R*) and diffusion coefficient are obtained from chronoamperometric (potential step) measurements. Also, we have validated our recent theoretical model for anomalous behavior of electric double layer impedance on a heterogeneous electrode. This model validates the presence of single and double state compact layer depending upon the biased potential on the glassy carbon rough electrode in room temperature ionic liquid (GC|RTIL). Finally, we experimentally validated various theoretical equations obtained through the roughness power spectrum based analysis at heterogeneous glassy carbon electrodes in room temperature ionic liquid (GC|RTIL).

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087. MEENA KUMARI

**Synthesis of Biologically Potent Heterocyclic Compounds and PEG-glycerol Based Amphiphilic Co-polymers for Drug Delivery Applications.**

Supervisor : Prof. Sunil K. Sharma

Th 22051

*Abstract*

The work presented in thesis entitled “Synthesis of Biologically Potent Heterocyclic Compounds and PEG-glycerol Based Amphiphilic Co-polymers for Drug Delivery Applications” is divided into four chapters. The research work carried in chapter I entitled “Chemo-enzymatic Synthesis of Azido-glycerol and PEG based Amphiphilic Polymers and Study of their Transport Potential” is focused on developing some amphiphilic dendron grafted polymers as efficient ‘Nanotransporters’ and comparing their transport potential and other physico-chemical properties with their respective non-dendronized analogs. The work presented in chapter II described the “Synthesis of Azobenzene Grafted Polymeric Amphiphiles and Study of their Self-assembly, Photoresponsive Behavior and Transport Potential”. The azobenzene moieties were incorporated in the chemo-enzymatically synthesized block co-polymer following “Click Chemistry” approach, to sense the responsiveness of resulting azobenzene grafted amphiphilic polymers towards light. The resulting polymeric amphiphiles were further evaluated for their photoisomerization behavior, encapsulation potential for Nile red and Curcumin and photoresponsive release profile. The work presented in chapter III described the “Chemo-enzymatic Synthesis of Amphiphilic Tricomponent Co-polymers and Study of their Physico-chemical Properties and Transport Potential”. Herein, we have designed block co-polymers using poly(ethylene glycol bis(carboxymethyl) dipropyl ester, azido-glycerol and aliphatic diols (butane-1,4-diol/octane-1,8-diol). The synthesized block copolymer, poly(2-azidopropan-1,3-dioxy)-poly(octane-1,8-dioxy)-poly(oxyethylene-600)oyl) was then functionalized with various hydrophobic chains ($C_{12}$/$C_{18}$) and propargylated folic acid. The functionalized polymers formed stable supramolecular assemblies in the aqueous solution and has shown good encapsulation potential for Nile red. The work presented in chapter IV described the “Synthesis of Novel-N-alkyl 5-(5-methyl-2-hydroxybenzoyl)2-pyridone derivatives and Evaluation of their Anti-proliferative Activity”. Herein, we have synthesized a series of 24 N-alkyl 5-(5-methyl-2-hydroxybenzoyl) substituted 2-pyridone derivatives by the triethylamine catalyzed reaction of various primary amines with (E)-ethyl 3-(6-methyl-4-oxo-4H-chromen-3-yl)acrylate. Out of synthesized 24 derivatives, the six representative compounds were evaluated for their anti-proliferative activity against three human cancer cell lines namely HeLa, HT-29 and SK-OV-3.

*Contents*

1. Chemo-enzymatic synthesis of azido-glycerol and peg based amphiphilic polymers and study of their transport potential 2. Synthesis of azobenzene grafted polymeric amphiphiles and study of their self-assembly, photoresponsive behaviour and transport potential 3. Chemo-enzymatic synthesis of amphiphilic tricomponent co-polymers and study of their physico-chemical properties and transport potential 4. Synthesis of novel n-alkyl 5-(5-methyl-2-hydroxybenzoyl 2-pyridone) derivatives and evaluation of their antiproliferative activity. Summary.

088. NAGPAL (Ritika)
**Synthesis and Characterization of Covalently Linked Pophyrinoids with Graphene and Polyaromatic Hydrocarbons.**
Supervisor : Prof. S.M.S. Chauhan
Th 22068

*Contents*

1. Graphene and graphene models: Synthesis, soectral analysis and applications 2. Materials from covalently linked hexabenzocronene with porphyrins 3. Synthesis and characterization of novel calixphyrins and their applications in anion binding 4. Synthesis of bisporphyrins covalently linked to polyaromatics and their interaction with diamines 5. Synthesis of various triaryl corroles and their application in biomimetic oxygenation and oxidation of polyaromatic compounds. Synopsis. Publication.

089. PRAMOD KUMAR
**Synthesis of (S)-Proline Derived Chiral Salalen and Salan Transition Metal Complexes and Their Catalysis in Asymmetric Strecker and Henry Reactions.**
Supervisor : Dr. Surendra Singh
Th 22456

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1. Introduction. 2. Prolinamide based chiral Mn(III) salalen and salan complexes and catalytic activity in asymmetric strecker reaction. 3. Asymmetric henry reaction catalyzed by chiral Cu(II) salalen and salan complexes derived from (S)-proline. 4. (S)-pyrrolidine containing chiral Mn(III) salalen and salan complexes as catalysts for the asymmetric henry reaction. 5. (L)-proline derived N-alky1 and N-benzyl substituted chiral salan Cu(II) comlexes in asymmetric henry reaction.

090. PURI (Aditi)
**Synthesis, Characterization and Applications of Functionalized Silica for Slective and Cyclic Recovery of Zn(II). Cu(II) and Pb(II).**
Supervisor : Prof. R. K. Sharma
Th 22425

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1. Introduction 2. Instruemntation and theory of the techniques used. 3. Chemically modified silica gel with 1-[4-[(2-Hydroxy Benzylidene) Amino]Phenyl}Ethanone : Synthesis characterizatin and application as an efficient and reusable solid phase extractant for selective removal of Zn(II) 4. Diacetylmonoxime functionalized silica Gel : An efficient and recyclable organic-inorganic hybrid material for selective removal of

Cu(II) 5. Silica-based magnetically driven nano solid phase with new functionality of efficient removal of Cd(II) 6. Acetoacetanilide-functionalized $Fe_3O_4$ nanoparticles for selective and cyclic removal of Pb(II).

091. RAM KISHAN
**Synthesis, Structural Aspects, Solution Behaviour and Reactivity Studies of Half Sandwich Ruthenium(II) and Rhodium(III) Complexes Ligated by Monoanionic Sym N,N',N"-Triarylguanidines and Half Sandwich Ruthenium(II) Complexes Ligated by Neutral Sym N,N'-Diarylthiourea.**
Supervisor : Dr. Natesan Thirupathi
Th 22422

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1. Introduction. 2. Results and discussion. 3. Appendixes.

092. RANGARAJAN (T. M.)
**Study of Palladium-Catalysed Carbon Oxygen Bond Forming Reactions.**
Supervisors : Dr. R. P. Singh and Dr. Raj Pal Singh
Th 22069

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1. Introduction 2. Pd/brettphos ligand catalysed c-o cross-coupling reactions Part A: Brettphos ligand supported palladium-catalysed c-o bond formation through an electronic pathway of reductive elimination: Fluoroalkoxylation of activated aryl halides Part B: Mild and efficient palladium/ brettphos-catalysed methoxylation and deuteriomethoxylation of activated aryl bromides 3. A genral, mild and efficient palladium-catalysed 2,2,2-trifluoroethoxylation of activated aryl bromides and bromo-chalcones 4. A genral and efficient palladium-catalysed rapid c-o bond forming reaction of fluoroalcohols with bromo-chalcones.

093. RITU PAYAL
**Photophysical Investigations of Some Biologically Active Thymol Based Schiff Bases Using Absorption and Fluorescence Spectral Studies in Homegeneous and Heterogeneous Media.**
Supervisors : Dr. M. Thirumal and Prof. R. C, Rastogi
Th 22060

*Contents*

1. Introduction 2. Materials and methods 3. Excited state dipole moments: A solvatochromic study 4. Effect of $H_0$/pH/H_ on absorption and fluorescence spectra: A prototropic study 5. Solubilization in CTAB, SDS and Tx-100 micelles: A CMC and binding constant study. Concluding remarks.

094. SAHU (Satya Narayan)
**Synthesis of Functionalized Thiophenes and N-Arylated Piperidones from 2H-Pyran-2-Ones.**
Supervisor : Dr. Ramendra Pratap
Th 22455

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1. A green approach for the synthesis of thieno[3,2-c]pyrans from 2-pyranones and their photophysical properties. 2. A multicomponent approach for the synthesis of tetrasubstituted thiophenes. 3. Hydrazine mediated synthesis of thieno[3,2-c]pyridones from 2-pyranones. 4. Synthesis of N-arylated piperiodones and its ketals from 2-pyranones. List of publications.

095. SAINI (Mukesh Kumar)
**Syntheses and Characterization of Novel Self-Assemled Polyoxometalates and the Catalytic Application in Oxidation Reactions.**
Supervisors : Dr. Firasat Hussain
Th 22049

*Abstract*

The thesis entitled "Syntheses and characterization of novel self-assembled polyoxometalates and its catalytic application in oxidation reactions" describes the synthetic approach to isolate new self-assembled polyoxometalates and their systematic analytical characterization and its application as catalysts in some organic oxidation processes. Polyoxometalates (POMs) chemistry is an emerging area of research interest in which the syntheses of new POM compounds enhance the versatility of these nanoclusters in various fields such as catalysis, medicine, bioscience, and material science. Catalysts based on POMs are excellent candidates for the organic oxidation processes due to their inherent stability, redox behavior of their constitute elements and finally their better capacity to utilize green oxidants. The thesis consists of historical background, variety of POMs compounds, and synthesis of starting POM materials. Further, the thesis includes the syntheses and development of a series of Peacock and Weakley type dimeric lanthanoid containing $[Ln^{III}(PW_{11}O_{39})_2]^{11-}$ [$Ln^{III}$ = $Y^{III}$, $Pr^{III}$, $Nd^{III}$, $Eu^{III}$, $Gd^{III}$, $Tb^{III}$, $Dy^{III}$, $Ho^{III}$, $Er^{III}$, $Tm^{III}$, $Yb^{III}$] and a tetrameric $[(PY_2W_{10}O_{38})_4(W_3O_8)(OH)_4(H_2O)_2]^{22-}$ complexes, as an oxidation catalyst for the variety of alcohols in water using $H_2O_2$ as a green oxidant. Details about chemical kinetics and re-usability of catalyst for alcohol oxidation processes were also studied along with effect of temperature and addition of oxidant. In addition the synthesis of novel dimeric open Wells-Dawson Ni(II) – containing 19 – tungstodiarsenate $[\{Ni(H_2O)_4\}_2\{Na(H_2O)\}\text{-}As_2W_{19}O_{67}(H_2O)]^{9-}$ anion and its characterization by various analytical techniques such as FT-IR spectroscopy, single crystal X-ray diffraction, ICP-AES, thermogravimetric analysis, and magnetic studies using vibrating sample magnetometry. Finally, its application in styrene oxidation catalysis was investigated. The isolated polyanion is a guanidinium cation directing POM complex having an open Wells – Dawson type molecular structure. The effect of temperature and quantity of $H_2O_2$ were also taken under consideration for the styrene oxidation in presence of minimum amount of catalyst loading.

*Contents*

1. Polyoxometalates an introduction and experimental part 2. The use of rationally synthesized, a series of dimeric $[Ln^{III}\ (PW_{11}O_{39})_2]^{11-}$[$Ln^{III}$=$Pr^{III}$-$Yb^{III}$] complexes as an oxidation catalyst for the alcohols in water using $H_2O_2$ as a green oxidant 3. Synthesis, characterization and catalytic activity of guanidinium cation directing Ni(II) - containing an open Wells - Dawson 19-tungstodiarsenate $[\{Ni(H_2O)_4\}_2\{Na(H_2O)\}As_2W_{19}O_{67}(H_2O)]^{9-}$ polyanion 4. Yttrium containing dimeric and tetrameric keggin type phosphotungstates: Syntheses, crystal structure, and catalytic activity for alcohol oxidation in water using $H_2O_2$ as an oxidant. List of publications.

096. SETHI (Swarndeep Kaur)

**Design and Synthesis of Novel Peptidic and Non-Peptidic SPECT Radiopharmaceuticals and MR Contrast Agents for Imaging of Central Nervous System.**

Supervisors : Dr. Marilyn Daisy Milton and Dr. Raunak

Th 22055


*Abstract*

Molecular imaging is a technique which monitors and records the spatiotemporal distribution of molecular and cellular processes for biochemical, biological, diagnostic and therapeutic applications. The purpose of molecular imaging is to improve understanding of biology and medicine through non-invasive in vivo investigation of cellular molecular events involved in normal and pathologic processes. Molecular imaging can be divided into four categories of techniques, viz., Nuclear imaging which encompasses techniques like PET, SPECT. Other three are optical imaging, magnetic resonance imaging (MRI) and ultrasound. Nuclear medicine imaging (specifically SPECT) and MRI are the two major techniques taken up in the thesis. The work described in the thesis is an aim to design, synthesize and biologically evaluate novel acyclic and cyclic ligands frameworks with target specific peptidic and non peptidic biovectors for the targeted SPECT and MR imaging. This has been fulfilled through a.) Design and synthesis of a bisconjugated bifunctional chelating agent DTPA with triazaspirodecanone for SPECT imaging of $D_2$ receptors. This innovative and novel conjugate gives SPECT imaging probe with ease of synthesis, excellent radiolabelling yield, stability and purity. b.) Design and synthesis of DO3A-bis(triazole-triazaspirodecanone) as MRI contrast agent by using “click” chemistry. The longitudinal relaxivity of the biocompatible DO3A-bis(triazole-triazaspirodecanone) ligand shows that the synthesized conjugate is a suitable MRI contrast agent and c.) The solid phase synthetic protocol using Fmoc chemistry applied for the synthesis of novel KDP peptide for SPECT and MR imaging respectively. Relaxometric studies have been carried out for the MR imaging agent giving the longitudinal relaxivity values higher than the known DO3A-peptide analogues. Each technique, is unique in itself but has its own advantages and disadvantages.


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097. SHARMA (Atul Kumar)

**Synthesis of Benzoxazine, Pyridin-2(1H)-one and Benzopyrone Derivatives and Evaluation of their Biological Activity.**

Supervisor : Prof. Sunil K. Sharma

Th 22057

*Abstract*

I, Dr. Atul Kumar Sharma, have completed my Ph.D. to the Department of Chemistry, University of Delhi. As a research scholar, I have gained valuable experience in the field of chemistry, especially organic chemistry, as my PhD is entitled as "Synthesis of Benzoxazine, Pyridin-2(1H)-one and Benzopyrone Derivatives and Evaluation of their Biological Activity". The thesis contains three chapters focusing on synthesis of different types of heterocyclic compounds. The chapter I is Synthesis of benzoxazine derivatives and evaluation of their biological activity. In this section, considering 1,4-benzoxazin-3(4H)-one scaffold utilization as a privileged structure for the generation of several drugs and cyclic imides constitute an important class of compounds possessing great pharmacological potential,. A total of twenty benzylidinyl benzoxazine derivatives were synthesized in this category The chapter II is Synthesis of pyridin-2(1H)-one derivatives and evaluation of their biological activity. This section includes the discovery of 2-Pyridones derivatives that contain the great potency against DNA gyrase and topoisomerase IV of bacteria. It involves the synthesis of a series of eighteen N-alkylated 2-pyridone derivatives. The chapter III is Synthesis of benzopyrone derivatives and evaluation of their biological activity. In this chapter, it has been focused on Benzopyran-2-one (coumarin) compounds, which are an important class of biologically active molecules. A total twenty four coumarin derivatives were synthesized in this section. Besides that, I have also gained knowledge during my PhD course work in reaction mechanism, NMR spectroscopy, and synthesis of various compounds which qualified me to handle both class-room and laboratory works. I have always been encouraged and respected by supervisor (Prof. Sunil K. Sharma), advisors (Prof. A.K.Prasad and Dr. B.K. Singh) and colleagues during my research work. I am a firm believer in prompting discussion of established and new concepts learning from my lab-mates as well as colleagues. Thanking you.

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098. SHIV KUMAR
**Chemo-enzymatic Synthesis of Dendronized Polymeric Architectures for Biomedical Applications and Synthesis of Benzopyram-2-one Derivatives as Potential Antimicrobial Agents.**
Supervisor : Prof. Sunil K. Sharma
Th 22046

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099. SINGH (Poonam)
**Studies on the Low-Temperature Synthesis of Some Double Hydroxides, Their Derivatives, Oxyfluorides and Fluorides with Emphasis on Optical, Magnetic and Photocatalytic Properties.**
Supervisor : Prof. Rajamani Nagaranjan
Th 22426

*Abstract*

The thesis focuses on the low temperature synthesis of inorganic materials, their characterization, and the investigation of their potential applications as optical, magnetic as well as photocatalytic materials. As the thesis deals with three different classes of compounds namely layered hydroxides, oxyfluorides and mixed metal fluorides, a brief outline of the structural chemistry of these compounds along with relevant properties and applications are described.In Chapter 1, the important role played by materials research is highlighted. Among the various families of structures, perovskite, layered double hydroxides based on brucite and $K_2SiF_6$ structures have been described along with their wide variety of applications. Chapter 2 deals with the synthesis of novel layered hydroxide acetates containing zinc and lanthanides. The intercalation chemistry of layered hydroxide acetates containing organic, inorganic anions and polymeric moieties form the content of Chapter 3.Chapter 4 deals with the discovery of anion deficient oxyfluoride of $K_2CoO_{2-x}F_4$ (x = 1) from the oxidation reaction of perovskite structured $KCoF_3$. $K_2CoO_{2-x}F_4$ (x = 1) was found to possess $K_2PtCl_6$-type structure with the cobalt in IV oxidation state. Chapter 5 describes a simple and green mechanochemical synthesis of layered perovskite structure type fluorides, $A_2MF_4$ (A = K, Rb; M = Co, Cu, Mg, Ni). In Chapter 6, effects of A-site (Na, K, Rb) and B-site (Mn, Ni) mixing on the structure and properties of $AMF_3$ are presented.

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100. SIVA KUMAR REDDY KOTLA
**Transition-Metal-Catalyzed Novel Approaches for the Tandem Synthesis of Naphthyridines/Thienopyridines/Acridones/ γ– Carbolines and Isoquinolines from Alkynes.**
Supervisor : Dr. Akhilesh Kumar Verma
Th 22065

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101. SINDHU (Jayant)
**Multicomponent 1,3-Dipolar Cycloaddition Reaction Based Novel Synthesis of Biologically Important N/O/S Containing Heterocycles.**
Supervisor : Prof. J. M. Khurana
Th 22070

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1. 1,3-Dipolar cycloaddition reaction: An efficient tool for the synthesis of 1,2,3-triazoles and pyrolidines 2. Synthesis of 1,4,5-trisubstitued-1,2,3-triazoles using efficient, green and recyclable DBU-$H_2O$ catalytic system 3. Synthesis of biologically important 2,4-thiazolidinedione based molecular hybrids containing 1,2,3-triazole and spirooxindole moieties using multicomponent 1,3-dipolar cycloaddition reaction 4. L-proline: A versatile organocatalyst in the 1,3-dipolar cycloaddition based multicomponent synthesis of biologically important molecular hybrids containing 1,2,3-triazoles 5. Multicomponent synthesis of novel 2-aryl-5-(1-aryl-1H-1,2,3-triazol-4-yl)methylthio)-1,3,4-oxadiazoles using Cu(I) as catalyst and their antimicrobial evaluation 6. Summary and conclusions. List of publications.

102. SINGH (Anil Kumar)
**Synthesis of Novel Phthalimide Derivatives, their Antimalarial Activity and Non-Linear Optical Properties Evaluation.**
Supervisor : Dr. BK Singh
Th 22064

*Contents*

1. Synthesis of novel phthalimide derivatives and their antimalarial activity and solid state property evaluation, Section A: Synthesis of novel cyclic amine based phthalimide analogues and their antimalarial activity evaluation, Section B: Chiral Phthalimides: Evaluation of solid state, piezoelectricity and nonlinear optical properties 2. Synthesis of novel arylpiperazine base phthalimide derivatives and their antimalarial activity and solid state property evaluation, Section A: Synthesis of novel arylpiperazine based phthalimide analogues and their antimalarial activity evaluation, Section B: Crystal engineering directed second harmonic generation response of novel chiral phthalimides functionalized with arylpiperazines 3. Design and synthesis of novel hydroxyethylamine based phthalimides and their antimalarial activity evaluation. Summary.

103. SINGH (Arvind Kumar)
**Synthesis of Novel Micro-Mesoporous Aluminophosphate-Based Materials and their Catalytic Applications.**
Supervisor : Dr. A. Sakthivel
Th 22073

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1. Introduction 2. Experimental methods 3. Mesoporous SAPO-34 (M-S-34) molecular sieves: Synthesis, characterization and its catalytic application 4. Mesoporous SAPO-5 (M-S-5): Synthesis characterization and its catalytic application 5. Uniform mesoporous silicoaluminophosphate by vapor phase treatment (M-S-34-VPT): Its catalytic and kinetic studies in hydroisomerization of 1-octene 6. Synthesis and characterization of M-S-34 in the presence of ammonium hydroxide (M-S-34-N) and its catalytic behaviour for transalklation 7. Cobalt containing M-S-43: Synthesis, characterization and catalytic application in oxidation of benzhydrol. Future scope of the work. List of publications.

104. SINGH (Surjeet)
**Syntheses of Arenes and Heteroarenes from Ketene Dithioacetals.**
Supervisor : Dr. Ramendra Pratap
Th 22052

*Contents*

1. Synthesis of α-aminated aroyl/acetylnaphthalenes through [5C+1C] and [4C+2C] annu;ations 2. Synthesis of various N-heterocycles from 2-(1-cyano-2,2-bis(methylthio)vinyl)benzonitrile 3. Base promoted synthesis of functionalized benzo[h]quinolines and benzo[e] indenes 3.1: A one pot domino approach for the synthesis of arylated benzo[h]quinolines 3.2: Precursor dependent regioselective synthesis of partially reduced benzo[e]indenes through oxidative cyclization 4. A rapid regioselective synthesis of highly functionalized $\alpha,\beta-$ unsaturated ketones 5. Microwave assisted regioselective synthesis of sterically hindered teraryls from 2-pyranones. List of publications.

105. S. NAGA CHANDRUDU
**Synthesis of Imines and Nitrogen-Containing Heterocycles by Oxidative Coupling of Amines.**
Supervisor : Dr. K. Gopalaiah
Th 22048

*Contents*

1. Synthesis of imines by iron-catalyzed oxidative self-or cross-coupling of primay amines 2. Synthesis of 1,3-benzazoles by iron(II) bromide-catalyzed oxidative coupling of benzylamines wih ortho-substituted anilines 3. Synthesis of bis(indolyl) methanes by iron(II) triflate-catalyzed oxidative coupling of benzylamines and indoles 4. Metal-free oxidative coupling of benzylamines and indoles: novel method for synthesis of bis(indolyl) methanes. 5. Synthesis of quinoxalines by copper-catalyzed oxidative condensation of 2-arylethylamines and *o*-phenylenediamines. Summary. Publications.

106. THAKRAL (Priyanka)
**In-Silico Investigations on Molecular Engineering of Electrically Conducting Copolymers Using Particle Swarm Optimization Algorithm.**
Supervisors : Prof. A. K. Bakshi and Prof. Shrikant Kukreti
Th 22072

*Abstract*

The study focuses on blueprinting the molecular codes of novel copolymers with optimal electronic properties. An artificial intelligence strategy, viz., particle swarm optimization (PSO) algorithm has been employed for designing binary, ternary and quaternary copolymers corresponding to optimal electronic properties. The reliability and effectiveness of PSO methodology has been tested following which binary and ternary substituted copolymers based on thiophene, pyrrole and furan have been tailored. Also, this copolymerization scheme has been clubbed with donor - acceptor polymerization where binary, ternary and quaternary copolymers based on donor-acceptor-donor (D-A-D) framework have been designed with thiophene, pyrrole & furan as donors and carbonyl & dicyanomethylene as acceptor moieties.

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1. Electrically conducting polymers: An introduction 2. Molecular modeling strategies for tailoring intrinsically low band gap polymers 3. Methodology 4. Investigation of electronic properties of model binary and ternary copolymers 5. Molecular designing of novel copolymers based on derivatives of thiophene, pyrrole and furan 6. Atomistic crafting of donor-acceptor-donor (D-A-D) framework based heteroaromatic copolymers 7. in-silico tailoring of quaternary copolymers 8. Sumaary and Conclusions.

107. THAKUR (Anuj)
**Design, Facile Synthesis and Development of Novel Molecular Hybrids as Therapeutic Agents .**
Supervisor : Prof. Diwan S. Rawat
Th 22075

*Abstract*

Molecular hybridization approach in medicinal chemistry, which was introduced in the last decade, has gained much attention in recent times. It is expected that these hybrids, because of different molecular framework as compared to the parent molecules can combat drug resistance issues. Moreover these hybrids can act at multiple targets or can have dual mode of action which often delivers superior efficacy against multigenic diseases than the drugs with single mode of action. In addition, these hybrid molecules are free from any drug-drug interaction as observed in the case of combination therapy. Taking into account the molecular hybridization approach, we have designed different series of bioactive molecules such as 4-aminoquinoline-pyrimidine and 9-aminoacridine-pyrimidine hybrids which were evaluated for their antimalarial and anticancer activity. Also, diarylidenyl-piperidone (DAP) based $C_5$-curcumin hybrids were synthesised and exhibited excellent anticancer, antibacterial and antioxidant activities. Similar to the molecular hybridization strategy, the fragment based drug design approach deals with the identification of small chemical fragments which, in isolation, may bind only weakly to the biological target. But combining these fragments may generate a lead molecule, often a new chemical entity, with a higher potency. Integrating this approach with the MCRs (multicomponent reactions) has paved a way for the facile synthesis of diverse MCR-scaffolds incorporating the desired fragments and with eventual identification of highly potent molecules. However, existing protocols for MCRs suffers from various drawbacks such as long reaction times, low yields, tedious work-ups, expensive catalysts, recyclability issues, and some processes may not be feasible from an industrial point of view. Therefore, improving the existing protocols is always in demand. Towards this end, EDDF (ethylenediammoninum-diformate) was utilized as a novel organocatalyst for the facile synthesis of medicinally important 4H-pyrans including chromenes, xanthenes and various 3-substituted indoles through improved MCR approach.

*Contents*

1. Synthesis and evaluation of antimalarial and anticancer activity of 4-aminoquinoline-pyrimidine and 9-aminoacridine-pyrimidine hybrids 2. Aminoquinoline-pyrimidine based molecular hybrids: Role of flexible and rigid linker in the antimalarial activity 3. Synthesis, anticancer, antibacterial, antioxidant activity and ADME properties of $C_5$-curcuminoids 4. Improved MCR strategy for the synthesis of medicinally relevant scaffolds. Summary. List of publications and patents.

108. U. CHINNA RAJESH

**Design and Development of Nanocatalysts for Green and Sustainable Synthesis of Biologically Active Heterocycles.**

Supervisor : Prof. Diwan S. Rawat

Th 22420

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1.Hydromagnesite as a novel heterogeneous solid base catalyst for the synthesis of nitrogen & oxygen heterocycles. 2A. Hydromagnesite and carbon coated magnesium carbonate as recyclable nanocatalysts for A3 coupling and one-pot witting reactions. 2B. Copper stabilized on hydromagnesite (Cu(II)/HM) as recyclable nanocatalyst for one-pot synthesis of pyrrolo[1,2-a] quinolines. 3A. Functionalized ferrite as efficient magnetically retrievable nanocatalysts for multi-component synthesis of indolyl chromenes. 3B. Copper oxide supported hematite as magnetically recoverable nanocatalyst for multi-component synthesis of indolizines and pyrrolo[1,2-a]quinolines. 4A. RGO/ZnO nanocomposite as an efficient amphiphilic catalyst for the synthesis of 3-substituted indoles in water.4B. CuI/CSP nanocomposite as recyclable catalyst for one-pot synthesis of aminoindolizines and chalcones with anomalous selectivity.

109. VILVAMANI N

**Surface Modification and Functionalization of Nanoparticles using Metal Complexes.**

Supervisor : Dr. S. K. Awasthi

Th 22053

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1. Introduction: An overview on synthesis, surface modification and functionalization of nanoparticles I. Addendum 2. Transition metal ion-induced anisotropic architectures using 4,4'-dicarboxy-2,2'- bipyridyl silver naopetals 3. Bottom-up molecular-assembly of ru(II)-polypyridyl complex-based hybrid nanostructures decorated with ag nanoparticles 4. Functionalized ru(II)-polypyridyl complexes induced gold nanocomposites assembly IV. Addendum 5. Ru(II)-polypyridyl complexes grafted silica nanohybrids: Versatile hybrid materials for visible light photocatalytic activity.

110. YADAV (Pratik)

**Synthesis of Aromatic and Heteroaromatic Scaffolds Using Ketene Dithioacetals and 2-Pyranones.**

Supervisor : Dr. Ramendra Pratap

Th 22066

*Contents*

1. A rapid multicomponent "on water" synthesis of tetrasubstituted thiophenes from ketene dithioacetals 2. Tandem carbocyclization strategy for the synthesis of biaryls and bridge biaryls from functionalized 2-pyranones 3. Microwave assisted base dependent regiodivergent synthesis of phenanthrenes, chrysenes and fused oxygen heterocycles 4. Palladium catalyzed C-N bond formation for the synthesis of modified nucleobases.

111. YADAV (Preeti)

**Benzopyrenone and Quinolinone Derivatives & Dendritic Architectures : Study of Photophysical and Biological Applications.**

Supervisor : Prof. Sunil K. Sharma

Th 22419

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