CHAPTER 10

CHEMISTRY

Doctoral Theses

01. AMIT KUMAR
Methodology for the Synthesis of Various *N,O*-Containing Heterocycles and [2] pseudorotaxanes from Sugar Based 24-crown-8.
Supervisor : Prof. Ashok K. Prasad
Th 23844

Abstract
(Not Verified)

The thesis entitled : "Methodology for the Synthesis of Various N,O-Containing Heterocycles and [2] pseudorotaxanes from Sugar Based 24-crown-8" is divided into four chapters. The work presented in Chapter I entitled "Synthesis of a Small Library of Unsymmetrical Coumarinyl-1,4-dihydropyridines" describes the design and synthesis of unsymmetrical coumarinyl-1,4-dihydropyridines from 4-formylcoumarin, ammonium acetate and b-keto ester in good yields. The work presented in Chapter II entitled "Greener Multicomponent Synthesis of a Small Library of 4-Aryl-1,4-dihydro-oxochromeno[3,2-b]oxoindeno[6,5-e]pyridine" describes the design and synthesis of a small library of 4-aryl-1,4-dihydro-oxochromeno[3,2-b]oxoindeno[6,5-e]pyridine from 4-aminocoumarin, aromatic aldehydes and indane-1,3-dione under microwave irradiation in excellent yields. The work presented in Chapter III entitled "Metal Catalyst Free Route to E-1-(Tri-O-benzyl-D-glucalyl)-2-phenylethene and its Diels-Alder Adduct" describes the synthesis of E-1-(tri-O-benzyl-D-glucalyl)-2-phenylethene and its Diels-Alder Adducts. The work presented in Chapter IV entitled "Design and Synthesis of Sugar-Aza-24-crown-8 Derivatives and their [2]pseudorotaxanes" describes the design and synthesize three new sugar-aza-24-crown-8 as an alternative to the dibenzo-24-crown-8. These ones are without phenolic oxygens and have sugar based rigid structure with regular oxy-ethylene units. A new synthon approach having seven-atom (O-C-C-O-C-C-O) would provide the new cavity for secondary ammonium ions. Thence we describe the formation of [2]pseudorotaxane from a sugar-aza-24-crown-8 and a secondary ammonium ion as the guest.

Contents

1. Synthesis of a small library of unsymmetrical coumarinyl-1,4-dihydropyridines 2. Greener multicomponent synthesis of a small library of 4-aryl-1,4-dihydro-oxochromeno[3,2-*b*]oxoindeno[6,5-*e*]pyridine 3. Metal catalyst free route to E-1-(Tri-O-benzyl-D-glucalyl)-2-phenylethene and its diels-alder adducts 4. Design and synthesis of sugar aza-24-crown-8 and its [2]pseudorotaxanes with *N*-(9-Anthracenylmethyl)benzyl ammonium hexafluorophosphate .Summary .List of publications .Workshop and Conferences attended.

02. DEVLA

Antimycobacterial and Antileishmanial Activity of Analogues of Chromone-Dihydropyridines, Coumarins and Some Natural Products.

Supervisor : Prof. M. Thirumal

Th 23875

Abstract
(Not Verified)

The quest to discover drugs for healing has always been influenced by prevailing socio-economical and cultural factors. Drug discovery and use of medicines has fascinated mankind and led to the path of scientific endeavour. Mycobacterium tuberculosis and Leishmania donovani remains a major source of global morbidity and mortality, which is exacerbated by their ability to readily evolve resistance. It is well acknowledged that drug resistance has become a major bottleneck in combating these deadly diseases. To overcome this problem; initiatives have to be made in the area of drug discovery and development to identify novel chemical entities (NCEs) with high efficacy, maximum safety, minimum side-effects and cost effectiveness, also keeping in mind that to curb drug resistance; these NCEs should be multi-targeted. Keeping in view the current scenario of these diseases, in the current study an attempt has been made to discuss all the important aspects related to these infectious diseases for which India is endemic and aims at discovering potential antimycobacterial and leishmanicidal NCEs which can be explored and exploited for drug development in future. Libraries of novel chromone-dihydropyridine and coumarin derivatives along with some natural products' crude soluble extracts (CSEs) from medicinally important plant E. alba and fungi F. oxysporum were evaluated for their antimycobacterial and antileishmanial potential. The results showed chromone-dihydropyridine and coumarin derivatives as antimycobacterial as well as leishmanicidal agents and were found to be non-hemolytic as well as non-cytotoxic towards human THP1 cell line as compared to the current first line drugs (Isoniazid and Amphotericin B) for these diseases. Also, the CSEs of E.alba and fungi F. oxysporum also showed leishmanicidal and antimycobacterial potential. These promising results by NCEs can be used as a lead for the future drug discovery and development.

Contents

1. Introduction and review of literature 2. Assessment of *In vitro* antimycobaterial potential and cytotoxicity study of chromone-dihydropyridine derivatives 3. *In vitro* anti-tubercular study of a novel series of coumarin – sugar triazole derivatives 4. Leishmanicidal activity of 7-amino-4-methylcoumarin and its analogues on *L. donovani* promastigotes and amastigotes 5. Preliminary screening of selected chromone-dihydropyridine and coumarin – sugar triazole analogues for their leishmanicidal activity against *L. donovani* promastigotes 6. Preliminary screening of natural crude extracts of plant *eclipta alba* and fungi *fusarium oxysporum* for their leishmanicidal activity against *L. donovani* promastigotes and antimycobacterial potential against M. tuberculosis .Summary and future perspective .Appendix .List of publications, workshops and conferences.

03. DIXIT (Ashish)

Development of Catalysts for Asymmetric Henry Reaction and Alcoholysis of Epoxides.

Supervisor : Dr. Surendra Singh

Th 23861

Abstract
(Verified)

Thesis entitled "Development of Catalysts for Asymmetric Henry Reaction and Alcoholysis of Epoxides" reveals synthesis and modification of chiral Salalen ligand synthesized from (S)-proline. Synthesized Salalen ligands were used for Cu and Mn complexes and these complexes were evaluated in asymmetric Henry reaction. Organocatalysts synthesized from DABCO and Bronsted acids were applied for the alcoholysis of epoxide at ambient temperature. This thesis contains the general introduction to the chirality and methods used for the asymmetric synthesis. It also comprises of different catalytic methods used for the asymmetric Henry reaction. It also gives brief introduction to alcoholysis reaction of epoxides. We also describe the development and synthesis of chiral Salalen ligands from (S)-proline and their in situ generated Cu complexes using Cu(OAc)2.H2O in isopropanol at 35°C. These in situ generated Cu(II) complexes were evaluated for asymmetric Henry reaction between benzaldehyde and substituted benzaldehydes and nitromethane to produce corresponding Henry product in 22-99% yield and 66-92% enantiomeric excess. Chiral Mn (III) Salalen complexes were synthesised and applied in asymmetric Henry reaction and β-nitro alcohols were obtained in 7-84% yields and 17-71% enantiomeric excesses. The Henry product was obtained in opposite configuration (R) compare to enantiomer obtained from Cu Salalen complex of the same ligand. We have in situ generated Cu complexes from the chiral Salalen ligand and these Cu(II) complexes act as catalysts for asymmetric Henry reaction using 4-methoxyphenol as an additive in toluene at 25°C to afforded corresponding Henry product in moderate yield and enantiomeric excess. We also developed Salts of 1-(Chloromethyl)-DABCO as organocatalysts and evaluated for the alcoholysis of epoxides at ambient temperature to yield β-alkoxy alcohol in excellent yield. The catalyst was also capable for alcoholysis of less reactive epoxides like glycidyl ethers and epichlorohydrin.

Contents

1. Introduction 2. Synthesis of chiral salalen ligands and their *in-situ* generated cu-complexes for asymmetric henry reaction 3. Synthesis and characterization of C1-symmetric chiral Mn(III)-salalen complex and their application in asymmetric henry reaction 4. Synthesis and characterisation of new chiral salalen ligands and application of their in sity generated Cu(II) in asymmetric henry reaction 5. Slats of 1-(chloromethyl)-DABCO : a highly efficient organicatalyst for the alcoholysis of epoxides. Summary and List of Publications.

04. DROLIYA (Preeti)
Physicochemical Studies of Molecular Interations in Multi-Component Solvent Systems.
Supervisor : Dr. Anil Kumar Nain
Th 23872

Contents

1. Introduction 2. Experimental methods 3. Temperature and concentration dependence of volumetric, acoustic, viscometric and optical properties of tetrahydrofuran + alkyl acrylate binary mixtures at different temperatures 4. Volumetric, ultrasonic, viscometric and optical behaviour of binary mixtures of acetonitrile with some alkyl methacrylates : An experimental and theoretical study 5. Physicochemical study of binary mixture of benzonitrile with some alkyl

methacrylates using volumetric, ultrasonic, viscometric and refractive index methods 6. Probing intermolecular interactions of benzylmethacylate in acetonitrile/ benzonitrile binary systems using physicochemical methods 7. Theoretical calculation of ultrasonic speeds in mixtures using scaled particle theory from experimental ultrasonic speed and density of pure components 8. Correlating models of viscosity .summary .List of publications.

05. DUMOGA (Shweta)
Design and Synthesis of Peg Based Macromolecular Carriers of Anti-Cancer Drugs for Targeted Diagnostic and Therapeutic Applications.
Supervisors : Dr. Surendra Singh and Dr. Dipti Kakkar Thukral
Th 23850

Abstract
(Verified)

The objective of this research work is to develop potential and desirable nanocarriers based on lipid and polymer systems to encapsulate the anticancer drugs for the treatment of various types of carcinomas. For this, the lipidic and polymeric systems have been designed to reduce the side effects of anti-cancer drugs like methotrexate and iron chelators. In lipid carrier systems, we formulate the stearic acid based solid lipid nanoparticles to encapsulate the novel chemotherapeutic (methotrexate) and incorporate the PEG-stearate to enhance the stealth property of the drug loaded carrier system. The effect of pegylation on these formulations is the main goal of this work for in-vitro and in-vivo studies. Thereafter, PEGylated solid lipid nanoparticles were prepared and modified with incorporation of PEG-biotin to enhance the selectivity of these drug loaded carrier system towards cancer. In these systems, the 2-Benzoyl pyridine thiosemicarbazide (BPT) and its analogue 2-Benzoyl pyridine-4-ethyl-3-thiosemicarbazide (BP4eT), which are iron chelators, were encapsulated and used as anti-cancer drugs. These systems have been used for in-vitro and in-vivo studies. The other system is based on block copolymers. Poly glutamic acid-poly ethylene glycol-poly glutamic acid (GEG) tri-block copolymer and Poly glutamic acid-poly ethylene glycol-folate (EGFA) have been synthesized. Thereafter, nano formultaion of these systems were prepared and physico-chemically characterized. (MTX) was used as novel anticancer drug and encapsulated in these systems. Thereafter, drug release study of MTX from these nanoparticles was done at different pH and measured the kinetics of these drug loaded nanoparticles by fitting the release data in different kinetic models. Biological evaluation of the prepared M-GEG and M-EGFA nanoparticles has been evaluated for cervical cancer by using the folic acid (biomarker) with di-block. For biological studies, HeLa cells were used as model cell line. These nanocarriers can be a good drug vehicle for clinical trials.

Contents

1. Introduction and literature search 2. Formulation of pegylated MTX encapsulated solid lipid nanoparticles, their physico-chemical characterization and biological evaluation 3. Design of biotin functionalized pegylated 2-benzoylpyridine thiosemicarbazone (BPT) and 2-benzoylpyridine-4-ethyl-3-thiosemicarbazone (Bp4eT) encapsulated SLNs for targeted delivery of chemotherapeutics 4. Synthesis of poly (Glutamic acid)-*b*-Poly(Ethylene glycol)-*b*-Poly (Glutamic acid) (GEG) and poly (Glutamic acid)-*b*-Poly(Ethylene glycol)-Folate (EGFA) and preparation of their nanoparticles 5. In-vitro and in-vivo evaluation of block copolymer based M-EGFA and M-GEG nanoparticles for treatment of cervical cancer 6. Summary and conclusions .List of publication/conferences.

06. DUTTA (Sriparna)

Fabrication of Sustainable Magnetically Retrievable Core-Shell Nanocatalysts and their Applications in Industrially Significant C-H Activation, Tandem Oxidative Cyclization, Reductive Amination and Enamination Reactions.

Supervisor : Prof. R. K. Sharma

Th 23851

Abstract
(Verified)

The entire work has been divided into six chapters. Chapter 1 elucidates the background, motivation and the current status of the research work. It provides a succinct overview on the substantial progress made in the fabrication of nanostructured catalysts with special emphasis on the protection and functionalization of the magnetite nanoparticles (Fe3O4). Chapter 2 throws light on the different physico-chemical techniques employed for the complete characterization of the magnetic nanocatalysts at nanoscale and the synthesized products. Through Chapter 3, we disclose the fabrication of an efficient organic-inorganic hybrid nanocatalyst possessing core-shell morphology for the synthesis of pharmaceutically significant polysubstituted oxazoles obtained via the tandem oxidative cyclization approach. Through Chapter 4, we report the synthesis of a highly efficient and magnetically retrievable catalytic system (Cu-2QC@Am-SiO2@Fe3O4) through the covalent immobilization of quinoline-2-carboxaldehyde (2QC) on amine functionalized silica coated ferrite nanosupport followed by metallation with copper acetate. A robust and efficient core shell structured magnetically retrievable nickel nanocatalytic system fabricated via the covalent immobilization of 2-acetyl furan on the surface of amine functionalized silica coated magnetic nanosupport followed by its metallation with nickel acetate has been reported in Chapter 5. Finally, Chapter 6 deals with a core shell hetero-nanostructure comprising of an in-situ generated naphthoquinone cobalt complex covalently tethered onto the surface of a silica coated magnetite nanosupport that was developed for catalyzing the enamination of β-carbonyl compounds. Advanced computational studies via DFT calculations were performed for gaining an insight into the mechanistic process. Further, all the synthesized nanocatalysts were characterized by using different physic-chemical techniques such as powder X-ray diffraction (PXRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive X-ray spectroscopy (EDS), energy dispersive X-ray fluorescence spectroscopy (EDXRF), atomic absorption spectroscopy (AAS), inductively coupled plasma spectroscopy (ICP-MS), vibrating sample magnetometry (VSM) etc.

Contents

1. Introduction 2. Aspects of instrumentation and experimental techniques Fabrication of core-shell-structured organic-inorganic hybrid nanocatalyst for the expedient synthesis of polysubstituted Oxazoles *via* tadem oxidative cyclization pathway 4.Quinoline-2-carboimine copper complex immobilized on amine functionalized silica coated magnetite nanoparticles : a novel and magnetically retrievable catalyst for the synthesis of carbamates *via* C-H activation of formamides 5. Nickel (II) complex covalently anchored on core-shell structured SiO_2@Fe_3O_4 nanoparticles : a robust and magnetically retrievable catalyst for direct one-pot reductive amination of ketones 6. Exploiting a core-shell structured organic-inorganic hybrid material as catalyst for chemoselective synthesis of β-enamino

carbonyl compounds : an experimental and DFT mechanistic investigation. Summary. List of publications

07. GAHLYAN (Parveen)
Synthesis, Biological and Metal Sensing Studies of Some *N*-Heterocyclic Compounds.
Supervisor : Dr. Rakesh Kumar
Th 23871

Abstract
(Not Verified)

This thesis is divided into four chapters, i.e. Chapter I, Chapter II, Chapter III and Chapter IV. In Chapter I , a library of 22 novel 1H-1,2,3-triazol-4-yl-methyl tethered 3-pyrrolyl isatin derivatives have been synthesized by the reaction of 1-(2-propynyl) isatins with various azides using click chemistry approach, followed by condensation of the resultant 1,2,3-triazole tethered isatins with 4-hydroxy proline in presence of InCl3 as catalyst. Cytotoxicity studies of newly synthesized compounds revealed that six of the compounds were three-fold more potent than the commercially available reference drug tamoxifen against MDA-MB-231 and relatively safe towards HEK-293 cells. In chapter II, a library of fluorescent 1,4-dihydropyridine linked bis-triazoles has been synthesized through Hantzsch synthesis by the condensation of o/m-chloro substituted benzaldehyde, ethyl 3-oxo-4-propargyloxy butanoate and ammonium acetate in presence of Ba(NO3)3 as catalyst followed by the click reaction of resultant bis-alkynyl-1,4-dihydropyridines with various azides. Anti-breast cancer evaluation of all the synthesized derivatives revealed that two compounds showed better anticancer activity than the standard drug tamoxifen against breast carcinoma (MDA-MB-231) cell line. In Chapter III, a water-soluble ferric (Fe3+) ion sensor has been synthesized using one-pot multicomponent Hantzsch synthesis, followed by Cu(I) catalyzed “Click reaction”. The synthesized probe showed selective binding towards Fe3+ ion among various metal ions tested in aqueous medium. The probe has also been tested for its application in biological systems. In Chapter IV, a new isatin-triazole tethered rhodamine based fluorescent probe has been synthesised using click chemistry approach. The synthesised probe exhibits a selective binding towards Cu2+ and Fe3+ ions through turn-on fluorescence response The probe was also applied in human primary glioblastoma brain carcinoma cells (U-87) for monitoring of Cu2+ ions which demonstrates its application in biological systems.

Contents

1. Design and synthesis of 1*H*-1,2,3-triazol-4-methyl tethered3-pyrrolylisatins as potent anti-breast cancer agents 2. Design and synthesis of *bis*-triazolylated-1,4-dihydropyridines as potent anti-breast cancer agents 3. Design and synthesis of *bis*-triazolylated-1,4-dihydropyridine based hydrophilic probe for selective detection of Fe^{3+}ion 4. Isatin-triazole tethered rhodamine based dual sensor for selective recognition of Cu^{2+} and Fe^{3+}ions and its application in live cell imaging .Summary.

08. GARG (Vineeta)
KOH/DMSO Assisted Chemo-, Regio- and Stereoselective Hydroamination of *N*-Heterocycles/ Nucleobases using Activated and Unactivated Alkynes.
Supervisor : Prof. Akhilesh Kumar Verma
Th 23852

Abstract
(Not Verified)

we have envisaged a versatile and efficient regio−, chemo− and stereoselective synthetic approach to produce a broad range of functionalized (E) and (Z) styrylpyrazole and benzpyrazole derivatives which can be used as precursors for the synthesis of biologically active molecules. we report a one-pot hydroamination reaction of carbazoles, aza-carbazoles and γ-carbolines with electron-rich and electron-deficient alkynes to yield a variety of (Z) and (E) styrylcarbazoles derivatives. The protocol was driven via alkyne i.e. electron-donating alkyne provides (Z)-selective product and electron-withdrawing alkyne provides (E)-selective products. we demonstrated the new strategy for the synthesis of styryl purines and pyrimidines, chemo-, regio- and stereoselectively in metal free environment, affording the product in good yields (55-70%). A new and direct approach for the synthesis styrylated N-vinylated heterocycles via alkene-alkyne replacement/substitution is demonstrated under KOH/DMSO catalytic system. The protocol was well employ on substituted aliphatic and aromatic terminal alkynes and offers the substituted products in moderate yields.

Contents

1. Chemo-, regio- and stereoselective *N*-alkenylation of pyrazoles/ benzpyrazoles using activated and unactivated alkynes 2. Substrate controlled region- and stereo-selective synthesis of (*Z*) and (*E*) *N*-StyrylCarbazoles, Aza-carbazoles and γ-Carbolines *via* hydroamination of alkynes 3. Alkali-matal-hydroxide catalyzed chemo-, regio-, and steroselective hydroamination of DNA and RNA nucleobases : synthesis of 9-(Arenethenyl)purines as dual Src/Abl kinase inhibitors 4. Unprecedent reactivity of hydroxyl/alkoxy alkenylated *N*-Heterocycles in KOH/DMSO system .Summary of the work .Copies of the publications

09. GAUR (Rashmi)
Designing, Characterization, and Application of Magnetically Retrievable Transition Metal Nnano Catalysts for CO_2 Fixation and other Organic Transformations
Supervisor : Prof. R. K. Sharma
Th 23869

Abstract
(Verified)

The advancement in the field of green chemistry and nanotechnology has introduced magnetically retrievable nanomaterials which provide immense surface area, excellent activity, economic viability, selectivity, recyclability and long-life time to the catalyst. The most significant and unique characteristic is that they are magnetically separable, which offers a good alternative to filtration and centrifugation methods. These outstanding features impart remarkable transformations in organic synthesis that drive researchers towards designing new sustainable nanocatalysts. In this thesis, magnetically retrievable transition metal nanocatalysts has been synthesized and characterized using various physico-chemical techniques such as FT-IR, XRD, XPS, SEM, FE-SEM, TEM, EDS, VSM, AAS, ICP-OES and ED-XRF. Furthermore, their applications have been investigated for different organic transformations which include C-O, C-N, C-S coupling reactions, fixation of CO2, oxidation of thiols, and reductive homocoupling of aryl halides. The work compiled in present thesis has

been divided into six chapters. Chapter one describes the introduction of magnetically retrievable nanocatalysts and their applications in catalysis. It describes various synthetic protocols of magnetic nanoparticles, followed by functionalization. It also incorporates relevant literature that serves as background for the work described in the ensuing chapters. This second chapter deals with the detailed description of theory and principles of the instrumental techniques required to carry out entire research work such as XRD, TEM, SEM, FE-SEM, FT-IR, ICP, EDS, XPS, VSM, Mössbauer Spectroscopy and GC-MS. Third chapter describes the synthesis of a magnetically retrievable, maghemite-copper nanocatalyst for different types of C-O, C-N, and C-S cross coupling reactions. Chapter four deals with a magnetically retrievable copper-based nanocatalyst and applied for the fixation of CO2. Fifth chapter presents the synthesis of magnetically retrievable, easily generated, chemically stable, and environmental friendly silver based nanocatalyst for the oxidation of thiols. Sixth chapter describes the synthesis of palladium-based magnetic nanocatalyst for reductive homocoupling of aryl halides.

Contents

1. Introduction 2. Instrumentation and theory of techniques used for the characterization of magnetic nanocatalysts 3. Magneticcopper-based nanocatalyst : applications for ligand-free cross-coupling (C-O, C-S and C-N) reactions 4. An eddicient copper-based magnetic nanoxatalyst for the fixation of carbon dioxide 5. Aerobic ocidation of thiols to disulfides by silver-based magnetic nanocatalyst 6. Magnetically retrievable palladium nanocatalyst for reductive homocoupling of aryl halides .Summary and list of publications.

10. GUPTA (Shruti)
Synthesis of Nitrogen Containing Heterocyclic Conjugates using Multicomponent Reaction Approach.
Supervisor : Prof. J. M. Khurana
Th 23848

Abstract
(Not Verified)

This thesis entitled “Synthesis of Nitrogen Containing Heterocyclic Conjugates using Multicomponent reaction approach” presents some novel synthetic methods. The subject matter of the thesis has been divided into five chapters. Each chapter I to V has been subdivided into sections (1) Introduction, (2) Results and Discussion, (3) Experimental and (4) References. The chapter wise brief account is given below. Chapter I consists of two parts. Part A describes an efficient synthesis of novel alkyl 7-aryl-5-hydroxy-5-methyl-1,3-dioxo-2-phenylhexahydropyrazolo[1,2-a][1,2,4] triazole- 6-carboxylates in ethanol-water using DBU as catalyst. Synthesis of dehydrated derivatives by dehydration of corresponding hydroxy pyrazolotriazoles has been reported using H2SO4 (10 mol%) in ethanol under reflux in Part B. A facile and efficient catalyst free one-pot synthesis of 3,4-dihydro-2H-naphtho[2,3-e][1,3]oxazine-5,10-diones by one-pot reaction of 2-hydroxy-1,4-naphthoquinone, aromatic amines and formaldehyde in glycerol at 50°C forms the subject matter of Chapter II. Chapter III describes efficient method for the syntheses of novel 1-aryl-5-hydroxy-2-imino-2,10a-dihydro-1H-chromeno[2,3-b]pyridine-3-carbonitriles in excellent yields by simply stirring the components magnetically at room temperature or by simply grinding the components i.e. 3-formylchromone, aromatic amines and malononitrile in equimolar amounts at room temperature under catalyst and solvent free conditions. A catalyst free one-pot three component reaction of

triphenylphosphine, dialkyl acetylene dicarboxylates and 5-arylidene-1,3-dimethylpyrimidine-2,4,6-triones for the efficient synthesis of spirophosphoranes by stirring the components in tetrahydrofuran (THF) at room temperature has been described in Chapter IV. Chapter V has been divided into two parts. Part A describes an efficient synthesis of novel substituted spiro[acenaphthylene-1,3'-pyrrolizin]-2-ones by one-pot three component reaction of acenaphthenequinone, α-amino acids (L-proline or L-thioproline) and 5-aryl-3-methyl-4-nitroisoxazoles in refluxing methanol while Part B reports a one-pot four component reaction of ninhydrin, o-phenylenediamines, α-amino acids (L-proline or L-thioproline) and 5-aryl-3-methyl-4-nitroisoxazoles for the synthesis of substituted spiro[indeno[1,2-b]quinoxaline-11,3'-pyrrolizines in refluxing methanol under catalyst free conditions. Chapter VI is a summary and conclusions of the work reported in this thesis.

Contents

1. DBU mediated one-pot synthesis of bovel 5-hydroxypyrazolo[1,2-α][1,2,4]triazoles and their dehydration to novel pyrazolo[1,2- α][1,2,4]triazoles 2. One-pot catalyst free synthesis of 3,4-dihydro-2*H*-naphtho [2,3-*e*][1,3]oxazine-5.10diones using glycerol as a green media 3. Synthesis of novel5-hydroxy-chromeno[2,3-*b*]pyridines under catalyst and solvent free conditions 4. Catalyst free synthesis of functionalized triphenyl phosphanylidene -7,9-diazaspiro[4,5]dec-1ene-2-carboxylates 5. Catalyst-free one-pot regioselective synthesis of spiropyrrolizines and spiropyrrolothiazoles using 1,3-dipolar cycloaddition reaction 6. Summary and conclusions .List of publications.

11. GUPTA (Sonal)
Nano Chitosans for Sorption of Heavy Metals and Dyes from the Industrial Waste.
Supervisors : Dr. P. S. Jassal and Dr. Rajendra Singh
Th 23864

Abstract
(Not Verified)

This thesis describes the removal of anionic, cationic dyes and heavy metal ions by chitosan nanoparticles (CHNPs) and low molecular weight chitosan nanoparticles (LMWCNPs) from the aqueous solution. CHNPs gained more attention as waste water treatment because of their better stability, non-toxicity and biocompatibility. Main purpose of using nanoparticles is its wide surface area. Chitosan is a hydrophilic polymer with positive charge which is obtained by deacetylation of chitin. CHNPs were prepared by ionic gelation technique. Adsorption efficiency of CHNPs is very high because of surface area increase along with increase the adsorption efficiency of dyes and metal ions on surface area. CHNPs were characterized by X-Ray powder diffraction (XRD), scanning electron microscopy (SEM), Energy Dispersive X-ray analysis (EDAX), and Fourier transforms infra-red (FTIR) and Thermo gravimetric analysis (TGA). CHNPs were also used to removal dyes and metal ions from the real sample which is collected from Tirrupur town which is situated in Tamilnadu. Presence of dye was analyzed by using UV-Visible spectrometer, Double beam and metal ions were detected by the help of the 797 VA Computrace. Effect of pH and Effect of temperature on the adsorption are also discussed. The experimental data were determined by using the Langmuir isotherm model, Freundlich isotherm model. The Kinetic data were also determined by pseudo first order and second order kinetic. The result fitted well the pseudo second order kinetics. Comparison of CHNPs and LMWCNPs for the adsorption of dyes was also discussed in this thesis. Conclusion of above mentioned work, we conclude that the CHNPs are effective to adsorption of dyes and metal ions.

Contents

1. Introduction 2. Review of previous work 3. Scope and objective of present work 4. Materials and method 5. Adsorption of cationic dyes on chitosan and its nano composites : equilibrium isotherm studies 6. Adsorption of anionic dyes onto chitosan adsorbent : batch studies 7. Selective adsorption of heavy metal ions from aqueous solution using chitosan nanoparticles 8. Heavy metal ions and dye concentration in textile industries wastewater of Tirrupur city in India .Summary, References and List of publications.

12. JASMIN KAUR
Theoretical Models for Curved Metal Nanoelectrochemical Systems.
Supervisor : Prof. Rama Kant
Th 23858

Abstract
(Not Verified)

We have developed theories for curvature dependent electronic and electrochemical work function (WF), for planar and curved geometries that find their relevance in various surface and electrochemical phenomena at metal surface. WF is framed as the work against electrostatic self-capacitive energy of a circular disc of radius of electronic screening length. Contribution of surface curvature is characterized by mean and Gaussian curvature. WF for metal electrode with adsorbed solvent dipoles is modelled for the partial to full surface coverage of solvent. We show that change in local WF is due to redistribution of surface charge caused by local surface curvature and adsorbing dipoles. Theoretical result is corroborated with experimental variation in measured WF due to partial and multilayer adsorption of water on Fe thin films, and a negative shift in oxidation potential for Ag nanoparticles in solution. Due to their direct relationship we developed a generic theoretical approach to address the WF and potential of zero charge moderations due to linkage of rod shaped organic dipoles at the metal surface. A theory for electrode structure and curvature dependent electrostatic potentials at plane of closest approach in an electrochemical interface is also developed. Inner interfacial region of EDL is considered with account of finite electronic spill over at metal electrode followed by solvent dipoles oriented by intrinsic field of metal. Electric potential across inner interfacial region is obtained in term of metal electron density profile at interface. Site dependent potential at outer Helmholtz plane is obtained in terms of IHP potential through modified Gouy-Chapman-Stern model of EDL. Generalized theory for influence of metal electronic characteristics and solvent dependent heterogeneous rate constant and electrochemical exchange current density for nanostructured metal electrodes is developed. We generalized Marcus approach for the metal electrodes by accounting electronic contribution from metal surface in formation of activated complex.

Contents

1. Introduction : electronic and electrochemical aspects of nanostructured metal electrodes 2. Theory of local work function of curved metal nanostructures 3. Theory of local work function and potential of zero charge for metal nanostructured electrodes in presence of dipolar solvent 4. Theory of local work function and PZC for systems with molecular self-assembly over nanostructured metal electrodes 5. Model for potential at inner outer Helmholtz layer and zeta potential of nanostructured metal electrodes 6. Theory of exchange current density and charge

transfer kinetics on metal nanostructured electrodes 7. Summary and future perspective.

13. LALWANI (Shubra)
Iron based Oxides/Sulphides for Supercapacitive Charge Storage and Electrocatalytic Energy Conversion.
Supervisors : Dr. Raj Kishore Sharma
Th 23862

Abstract
(Not Verified)

In summary, Chapter 1 gives a brief of the introduction to supercapacitors and electrocatalysts, chapter 2 mentions all the techniques employed for the structural and electrochemical characterization of iron based oxides/sulphides and their respective composites. In chapter 3 we describe charge storage ability of magnetite nanoparticles immobilized on graphene nanoribbons with different mass loading of magnetite nanoparticles and fabricating it as a solid state supercapacitor. Chapter 4 gives a brief of different morphologies of Cobalt ferrite on varying the concentration of surfactant, out of which nanorods with mesopores and edges outstand amongst the other morphologies. In Chapter 5, iron cobaltite nanostructures with varying reaction time were studied to obtain the electrochemically best nanostrip morphology with an excellent cycle life and charge storage. Further, after an elaborated study of mixed Fe-Co spinel oxides Chapter 6 describes the performance of sulphides in comparison to oxides. Fe-Co sulphides are synthesized in equimolar ratio with much better conductivity and thus are utilized for dual application. Further to observe the synergistic effect quantum dots (Chapter 7) of iron cobalt oxide were decorated on graphene nanoribbons. Chapter 8 concludes all the research work in brief.

Contents

1. Introduction 2. Characterization techniques and evaluation parameters 3. In-situ immobilized magnetite nanoplatelets over holey graphene nanoribbons for high performance solid state supercapacitor 4. Edge enriched cobalt ferrite nanorods for symmetric / asymmetric charge storage 5. Iron cobaltite nanostrips as in asymmetric supercapacitors 6. Bifunctional iron cobalt sulphide for supercapacitive charge storage and electrocatalysis 7. Quantum dots of iron cobaltite on graphene nanoribbons for high voltage symmetric supercapacitors 8. Conclusions.

14. MEENA (Kalawati)
Novel Methodologies for the Synthesis of Nitrogen/Oxygen Containing Heterocyclic Conjugates and Antimicrobial Studies.
Supervisors : Prof. J. M. Khurana and Dr. Amita Malik
Th 24313

Abstract
(Not Verified)

The subject matter of the thesis has been divided into six chapters. The chapter wise brief account is given below. Chapter I describes an efficient catalyst free synthesis of novel indeno[1,2-b] chromenone derivatives by hetero-Diels-Alder reaction of electron deficient 2-(arylmethylene)-1H-indene-1,3(2H)-diones as heterodienes and electron rich enaminones as heterodienophiles in [bmim]BF4 at 80oC or in acetic acid at 80oC. A new, diversity oriented protocol for the synthesis of alkyl 5-hydroxy-

pyrazolo[1,2-a][1,2,4]triazoles by one-pot three component condensation of aromatic aldehydes, 4-phenylurazole and ethyl/methyl acetoacetate in presence of catalytic amount of L-proline in, [bmim]BF4 at 80°C has been reported. Synthesis of alkyl pyrazolo[1,2-a][1,2,4]triazoles by dehydration of alkyl 5-hydroxy-pyrazolo[1,2-a][1,2,4]triazoles using [bmim]HSO4 at 80oC also has been reported in Chapter II. Chapter III reports a facile and convenient approach for the synthesis of spiro[indolo-3,10'-indeno[1,2-b]quinolin]-2,4,11'-triones by one pot-pot three component condensation of enaminones, isatin and indane-1,3-dione in presence of catalytic amount of CAN in EtOH :H2O at 80oC. Antimicrobial studies of the synthesized compounds have also been reported. Chapter IV describes synthesis of a series of novel 2-(3-alkyl/arylaminopropoxy)-12-aryl-9,10,dihydro-8H-benzo[a]xanthen-11(12H)-one derivatives from 2-hydroxy-12-aryl-9,10-dihydro-8H-benzo[a]xanthen-11(12H)-ones by two step sequence involving its reaction with 1-bromo-3-chloropropane in presence of K2CO3 in dry acetone followed by amination with aryl/alkyl amines in dry DMF in presence of KI at 100oC. The synthesized compounds were screened for antibacterial studies. Chapter V describes catalyst free synthesis of novel spiro isoxazolo[5,4-b]pyridine/quinolines by three component condensation of isatins, 5-amino-3-methylisoxazole and 1,3-dicarbonyls in ethylene glycol at 80ºC. Chapter VI describes catalyst free regioselective synthesis of benzo[d]-imidazo[2,1-b]thiazole derivatives by one-pot three component condensation of phenylglyoxal, cyclic enolizable carbonyl compounds and 2-aminobenzothiazoles by heating the components in glycerol at 80oC or simply by grinding the components in glycerol at ambient temperature . Chapter VII is a summary and conclusions of the work reported in this thesis.

Contents

1. An efficient synthesis of novel indeno[1,2-*b*]chromenones *via* hetero-Diels-Alder reaction of 2-(arylmethylene)-1*H*-indene-1,3(2*H*)-diones with enaminones 2. One-pot synthesis of 5-hydroxy-pyrazolo[1,2-α][1,2,4]triazoles and their dehydration using ionic liquids as reaction media 3. One pot three component synthesis of spiro[indolo-3,10'-indeno[1,2-*b*]quinolin]-2,4,11'-triones and their antimicrobial studies 4. Synthesis of novel 2-(3-aryl/alkylaminopropoxy-12-arylxanthenes and their antibacterial studies 5. An efficient catalyst free approach for the synthesis of novel isoxazolo[5,4-*b*]pyridines/quinolones *via* one-pot three component reaction in ethylene glycol 6. Catalyst free one-pot regioselective synthesis of benzo[*d*] imidazo[2,1-*b*]thiazoles by heating or grinding in glycerol 7. Summary and conclusions. List of publications.

15. MISHRA (Prashant Kumar)
Aero-Gel Based Metal Oxide Nanoparticles for the Rapid Uptake of Arsenic and Chromium from Water and their Superior Humidity Sensing Performance.
Supervisors : Dr. Rakesh Kumar and Dr. Pramod Kumar Rai
Th 23853

Abstract
(Not Verified)

Chapter 1, is detailed with general introduction about nanotechnology, its possible outcomes and applications in various field of sciences. Water crisis is one of the major concern for researchers in which arsenic and chromium play a major role. The techniques for removal of arsenic and chromium are embarked and explained. The importance of humidity sensors their working principle and mechanism has also

been explained in brief. Chapter 2, is separated into two parts, in part (a) the control synthesis of CeO2 NPs has been explained and the role of size, surface area and bulk density for the treatment of arsenic was demonstrated. In part (b), to increase the efficiency of CeO2 NPs the iron oxide was successfully doped up to 20%. The adsorption process was performed in presence of ultrasonic wave and as a resultant the efficacy of material was improved. In chapter 3, surfactant free one pot synthesis of TiO2, CeO2 and Ti@Ce oxide nanoparticles for ultrafast removal of Cr(VI) from aqueous medium have been explained. The impregnation of TiO2 on CeO2 NPs caused phase transformation of TiO2 from anatase phase to rutile phase. The removal mechanism of Cr(VI) was investigated using XPS analysis which illustrated the reduction of Cr(VI) to Cr(III) during adsorption process. In chapter 4, The excellent performance of synthesized materials as humidity sensors were demonstrated. CeO2 NPs exhibited low hysteresis, linearity, fast response/recover and sensitivity towards humidity. Moreover, the synergistic effect of iron in the matrix of ceria was also experienced during experimentation. TiO2 alone showed ultrafast response/recovery (2 s and 1.5 s), which is remarkable and attributed to 3-D morphology, defects, high surface area and ultrafine size of prepared material. Finally, the summary and future scope of the entire work are briefed.

Contents

1. General Introduction of nanotechnology and their applications for water purification and humidity sensing 2. Part (a) Surfactant free one pot synthesis of low density cerium oxide nanoparticles for the adsorptive removal of arsenic species from water Part (b) Aero-gel based cerium doped iron oxide solid solution for ultrafast removal of arsenic from water 3. Surfactant free one pot synthesis of TiO_2, CeO_2 and Ti@Ce oxide nanoparticles for ultra fast removal of Cr (VI) from aqueous medium 4. Highly responsive humidity sensor based on TiO2, CeO2 and solid solution of Fe@Ce oxide nanoparticles .Summary and future aspects .List of publications.

16. MISHRA (Pawan Kumar)
Development of Sustainable Methodologies : Efficient Synthesis of Small Bioactive Molecules.
Supervisor : Prof. Akhilesh K. Verma
Th 24312

Abstract
(Not Verified)

We have developed a simple, versatile and atom-economically benign tandem approach in aqueous media to provide a broad range of functionalized benzimidazolo-fused benzofuro[3,2-c]pyridines, benzofuro/ thieno[2,3-c] pyridines, and γ-carbolines in good to excellent yield. This methodology has gained significant attention due to the catalyst-free approach in H2O as a solvent which reduces the formation of by-products. We developed the two heterocyclic rings in one-pot under metal-free condition using easily accessible starting material via 6-endo-dig ring closure. Selective formation of the deuterated product confirmed the role of water in the designed approach. Alternatively, X-ray crystallographic data supported the formation of desired products. We have demonstrated a novel atom-economical and inexpensive approach for the synthesis of diversified of functionalized isoquinolines and azaanthracene derivatives from aryl-1,2-dicarbonyl and aryl/hetarylmethylamines in good to excellent yields. By this methodology, we could able to synthesized isoquinoline with cyano, ester, and halide containing substrates which will provide further derivatization of the product. By using our methodology,

we could able to replaced expensive alkynes as well as metal for the synthesis of these N-Heterocycles. The byproduct in the reaction is H2O which make the process environmentally benign. The designed represent Lewis acid catalyzed the efficient, straightforward and regiospecific synthesis of 1,3-diarylisobenzofuran derivatives via cascade hydroarylation/ cycloisomerization reactions between 2-formylarylketone and electron-rich nucleophile under metal-free condition. The isobenzofuran products further utilizing the synthesis of the cyclo-adduct product with DMAD by [4+2] reaction in good yield We have described a transition-metal-free strategy towards the synthesis of 2,3,5–trisubstituted 1H pyrroles from N–propargylamine under basic conditions. The N–propargylamine substrates were obtained via the three-component reaction between aldehydes, alkynes, and amines using 20 mol% copper catalysts. The reaction is also applicable to the synthesis of 2,4,5-trisubstituted pyridines with mild yields.

Contents

1. Metal-free regioselective tandem synthesis of diversely substituted benzimidazo-fused benzofuro/thienopyridines and γ carboline in aqueous medium 2. Base-promoted one-pot strategy for the synthesis of functionalized isoquinolines, benzo[*h*]isoquinolines and azaanthacenes 3. Lewis acid-catalyzed cascade hydroarylation/cycloisomerization reactions of 2-formylarylketones : an expedient approach toward isobenzofuran derivatives 4. Base-mediated direct transformation of N-propargyl amines into 2,3,5-trisubstituted 1*H*-pyrroles. .Summary of the work and Copies of the publications.

17. MISHRA (Vishwesh)
Platinum(II) Mediated C-H Activation of *sym N,N',N"*-Triarylguanidines and Palladium(II) Mediated N-H Activation of *N*-Aryl-*N',N"*-Dipyridylguanidines.
Supervisor : Prof. Natesan Thirupathi
Th 23857

Abstract
(Not Verified)

The reactions of *cis*-[Pt(OAc)$_2$(DMSO)$_2$] with two equiv of *sym N,N',N"*-triarylguanidines, [ArN=C(NHAr)$_2$] in toluene under reflux condition for 8 h afforded six-membered cycloplatinated guanidines, [Pt{κ^2(*C,N*)}(OAc){κ^1*N*(ArN=C(NHAr)$_2$)}] (*sym* = symmetrical; Ar = 2-MeC$_6$H$_4$ (**1**) and 2,4-Me$_2$C$_6$H$_3$ (**2**)) in 82% and 84% yields respectively. The salt metathesis reaction of **1** with one equiv of AgTFA in CH$_2$Cl$_2$ at RT afforded [Pt{κ^2(*C,N*)}(TFA){κ^1*N*(ArN=C(NHAr)$_2$)}] (**3**) in 94% yield. The reaction of *cis*-[Pt(TFA)$_2$(DMSO)$_2$] with one equiv of [ArN=C(NHAr)$_2$] in toluene under reflux condition for 8 h afforded six-membered cycloplatinated guanidines, [Pt{κ^2(*C,N*)}(TFA)(DMSO)] (Ar = 2-MeC$_6$H$_4$ (**4**), 4-MeC$_6$H$_4$ (**5**), 2,4-Me$_2$C$_6$H$_3$ (**6**) and 2-(MeO)C$_6$H$_4$ (**7**)) in ≥73% yields. The reaction of *trans*-[PtCl$_2$(PhCN)$_2$] with two equiv of [ArN=C(NHAr)$_2$] in toluene under reflux condition for 48 h afforded *trans*-[PtCl$_2${ArN=C(NHAr)$_2$}$_2$] (Ar = 2-MeC$_6$H$_4$ (**8**) and 2,4-Me$_2$C$_6$H$_3$ (**9**)) in 90% and 45% yields respectively. Complexes **8** and **9** were separately refluxed in MeOH for 8 h to afford six-membered cycloplatinated guanidines, [Pt{κ^2(*C,N*)}(μ-Cl)]$_2$ (**10** and **11**) in 93% and 96% yields respectively with concomitant formation of the respective guanidinium salts, [(ArNH)$_3$C]Cl as the byproduct.

Platinacycle **10** was treated with two equiv of AgTFA in CH_2Cl_2 at RT to afford six-membered cycloplatinated guanidine, [□$_2$(*C*,*N*)Pt(□-TFA)]$_2$ (**12**) in 94% yield. The new compounds were characterized by analytical techniques, multinuclear NMR (^{1}H, ^{13}C and ^{195}Pt) spectroscopy and further molecular structures of ten compounds were determined by single crystal X-ray diffraction.

Contents

1. Introduction 2. Results and discussion 3. Supporting information .Synopsis and Abstract.

18. NARANG (Payal)
Unravelling the Role of Additives on the Phase Transition Behavior of Thermoresponsive Polymers.
Supervisor : Dr. P. Venkatesu
Th 23859

Abstract
(Not Verified)

Chapter 1 delineates the introduction of polymers, its history and classification. The literature review of all the chosen TRPs for the present study is presented in this chapter to cover all the developments in the field of biopolymers. Chapter 2 includes the description of all the materials and methods used throughout the thesis work. The chapter describes the preparation of sample solution containing TRPs and additives. Chapter 3 dictates the role of several polyols with increasing C-chain length on the phase transition behaviour of PNIPAM. The polyols used are trehalose, sucrose, sorbitol, xylitol, erythritol and glycerol. Chapter 4 (a) and 4 (b). In the chapter 4 (a), the transition behaviour of polymer PVME is studied in presence of methylamine based osmolytes such as TMAO, betaine and sarcosine. Chapter 4 (b) unveils the influence of methylamine based osmolytes such as TMAO, betaine and sarcosine in altering the transition behavior of PVCL. Chapter 5 (a) and chapter 5 (b). Chapter 5 (a) highlights the role of urea, TMAO individually and their mixture in different ratios on the phase transition region of PNIPAM. Chapter 5(b) reveals the efficiency of particular concentration ratio of mixture of TMAO and SDS to bring the LCST of PNIPAM near to physiological temperature. Chapter 6 involves the impact of varying concentration of several additives such as TMAO, betaine, sarcosine, urea and GndHCl on the CMT behavior of PEG-PPG-PEG. The alteration in CMT behaviour of PEG-PPG-PEG is mainly depending on the structural arrangement and functionalities present in the particular additive. Chapter 6 involves the impact of varying concentration of several additives such as TMAO, betaine, sarcosine, urea and GndHCl on the CMT behavior of PEG-PPG-PEG. The alteration in CMT behaviour of PEG-PPG-PEG is mainly depending on the structural arrangement and functionalities present in the particular additive. Chapter 7 collects the conclusions of the work performed in investigating the phase behaviour of TRPs on presence of various additives. The thorough analysis of all the results concludes that the microscopic changes happening among the polymer on addition of additives are basically manifesting the its conformational change.

Contents

1. Introduction and review of literature 2. Materials and experimental techniques 3. Influence of a series of polyols on the phase transition behavior of poly(N-

isopropylacrylamide) (PNIPAM) 4(a). A molecular interplay for osmolytes induced phase behaviour of poly(vinyl methyl ether) (PVME) 4(b). A molecular interplay for osmolyte induces phase transition behavior of poly(N-vinylcaprolactum) (PVCL) 5(a). New endeavour to the cooperative behavior to trimethylamine N-oxite (TMAO) and urea towards the globular state of PNIPAM 5(b). An efficient study to reach physiological temperature with PNIPAM in presence of two differently nehaving additives 6. Scrutinizing the efficacy of various additives to modulate the micellization behavior of triblock copolymer 7. Conclusions.

19. NEELAM KUMARI

Design, Synthesis and Biological Evaluation of Benzoxazolone Based Probes for Neuroreceptor Quantification.

Supervisors : Dr. Sunita Bhagat and Dr. Anjani Kumar Tiwari

Th 23868

Abstract
(Not Verified)

The intend of the thesis is to present the idea of maneuvering benzoxazolone core for designing TSPO, 5HT1A/5HT7 and PDE10A targeted imaging probes/ radiopharmaceuticals for diagnostic purposes. As from the literature survey we have found that benzoxazolone is considered as a best bioisosteric scaffold so we can replace prevailing heterocyclic rings in existing pharmacophores to modify the skeleton in newer way. The systematic approach followed for achieving the concern objectives in every chapter is : in-silico screening of the proposed ligands for selecting the hits for wet lab synthesis followed by the chemical synthesis , hot labeling (11C and 99mTc labeling) and last but not least is the biological evaluation of the radiopharmaceutical by performing it's in vitro and in vivo experiments on various animal models. The designed ligands for three biological targets- TSPO, 5HT1A/5HT7 and PDE10A have been categorized in seven chapters. Chapter 1 covers the generalized introductions of the keywords utilized in the thesis. Chapter 2 involves the synthesis of 11C labelled PET radiotracers (MNBP) for demarcating the overly expressed TSPO region or inflammation region in ischemic rat model and chapter 3 is about designing the 99mTc labeled SPECT radiotracers, with two categories of chelating functionality - cyclic chelator (DOTA) and acyclic chelator (EDTA, PIC) for TSPO imaging in lung inflammated mice model. However Chapter 4 covers the designing and development of FITC conjugated benzoxazolone based TSPO ligand (FITC-MBP) for analyzing the TSPO over-expression during chemical or radiation induced inflammation and lung carcinoma. Chapter 5 and 6 is aimed for designing the specific probes for 5HT1A/5HT7 targeting through different modalities and in last chapter 7 11C labelled PET probe (DMQA) has been reported for locating PDE10A in rat brain.

Contents

1. Introduction and literature search 2. Development of acetamidobenzoxazolone based PET imaging probe for inflammation imaging in ischemic rat 2(a). Synthesis and biological evaluation of ^{11}C Labeled *N*-methyl-22(2-oxobenzo[d]oxazol-3(2H)-yl)-N-phenylacetamide based PET imaging probe for locating activated microglia in ischemic rat model 2(b). Design and synthesis of *N*-(2-methoxyoxyphenyl)-Nmethyl-2-(5-nitro-2-oxobenzo[d]oxazol-3(2*H*)-yl)acetamide as a PET imaging probe 3. Development of acetamidobenzoxazolone based SPECT imaging probe for TSPO mapping 4. Benzoxazolone based FITC conjugated florescent probe for assessing translocator protein (TSPO) expression in lung inflammation and tumor model 5. Synthesis and biological evaluation of arylpiperazinyl-alkyl benzoxzolone/

benzothiazolone based PET imaging probe for $5HT_{1A}$/$5HT_{7A}$ mapping 6. Synthesis of EDTA and FITC conjugated arylpiperazinylalkyl 2-benzoxazolones ligand as SPECT and optical imaging probe 7. Design, synthesis and biological evaluation of ^{11}C PET tracers for phosphodiesterase 10A (PDE10A) imaging .List of publication/conference papers/abstract.

20. PANWAR (Rahul)
Synthesis of Functionalized Carbocycles and Azaheterocycles from Ketene Dithioacetals.
Supervisor : Dr. Ramendra Pratap
Th 23863

Abstract
(Verified)

The thesis entitled "Synthesis of functionalized carbocycles and azaheterocycles from ketene dithioacetals" is submitted to the University of Delhi. In the thesis, we have reported the synthesis of various functionalized carbocycles and azaheterocycles from various ketene dithioacetals and 2H-pyran-2-ones via cyclization and ring transformation strategy. Ketene dithioacetals and 2H-pyran-2-ones are versatile precursors for the synthesis of various pharmacological important functionalized carbocylic and azaheterocyclic compounds. A wide variety of ketene dithioacetals was planned and used for the synthesis of various functionalized bioactive molecules taking advantage of good leaving group property of methylsulphanyl group. Presence of methylsulphanyl group in ketene dithioacetals make these molecules vulnerable for nucleophilic attack and most of the nucleophiles attacks at carbon containing methylsulfanyl group followed by loss of SMe group to afford the desired products. We have used various nucleophile sources to synthesized aromatic, heteroaromatic and nonaromatic hydrocarbons, oxygen and nitrogen-based heterocyclic compounds. Extensive research from many decades has given rise the new prediction in organic chemistry as well as they simply undergo base promoted substitution, elimination and addition reactions. In the thesis chapters, we have taken the advantage of applications of ketene dithioacetals and used them for the synthesis of diverse classes of functionalized carbocycles and azaheterocycles compounds. The whole work presented in the thesis has been divided into four chapters. Chapter 1 : In this chapter, we have explored the application of ketene dithioacetals and 2-(1-arylethylidene)malononitriles for the synthesis of functionalized benzenes. Chapter 2 : In this chapter, we have reported a regioselective approach for the synthesis of m-teraryls by using pyran-2-ones and2-(1-arylethylidene)malononitriles under basic conditions. Chapter 3 : In this chapter, we have reported a chemoselective approach for the synthesis of benzo[h]quinolines and benzylpyrans by using 2H-pyran-2-ones and 4-nitro-2-methyl benzonitrile. Chapter 4 : In this chapter, we have reported a water-mediated regioselective synthesis of 6,7-diaryl-5-oxo-2,3,5,6-tetrahydroimidazo[1,2-a]pyridine-6-carbonitriles.

Contents

1. Transition metal free strategic synthesis of multifunctional benzenes from ketene dithioacetals 2. Base mediated regioselective synthesis of *m*-teraryls from 2*H*-pyran-22ones and α,α-dicyanoolefins 3. Substituent directed chemoselective synthesis of highly sunctionalized benzo[*h*]quinolones and 4-benzylpyrans from 2*H*-pyran-2-ones 4. An unprecedented synthesis of partially reduced imidazo[1,2-α]pyridines from ketene dithioacetals .List of publications and Conferences attended.

21. PARUL

Synthesis, Characterization and Sinple in *vitro* Applications of Some Inorganic Based Nanoparticles.

Supervisor : Dr. Indrajit Roy

Th 24259

Abstract

(Not Verified)

The thesis entitled "Synthesis, characterization and simple in vitro applications of some inorganic based nanoparticles" reveals the synthesis of inorganic nanoparticles (ormosil, AuNPs, UCNPs etc) synthesized via micellar system or hydrothermal synthesis. The as-synthesized NPs were used for killing of cancer cells via photodynamic and photothermal therapy. Chapter 1 is the introduction chapter explaining the basic fundamentals of nanotechnology, significance of engineered nanoparticles, manipulation of its chemical or physical properties at nanoscale with potential applications in biomedicine. Chapter 2 comprises the literature review related to the research work included within this thesis. This chapter summarised the research work carried out till date regarding the various NPs in PDT for cancer killing. Chapter 3 provides the detailed experimental characterization techniques used throughout the research work embodied in this thesis. Chapter 4 contains the synthesis and characterization of Au@ORM NPs via micellar system. Owing to the enhancement in photodynamic therapy after Au aggregation over ormosil NPs using cancer cells in *vitro*. Chapter 5 contains the synthesis and characterization of MB-Si@AuNFs. The combination effect of PDT and PTT were investigated in cancer cells in vitro. Chapter 7 contains the synthesis and characterization of FL loaded NIO-IOVT NPs . We explored the magnetically induced PDT using these NPs for the enhance killing of cancer cells. Chapter 8 enlightens the conclusion of all these works embodied in this thesis, with their present and future significance.

Contents

1. Introduction 2. Literature Review 3. Experimental and characterization techniques 4. Gold nanoparticle enhanced photodynamic therapy from photosensitizer entrapped ormosil nanoparticles 5. Photosensitizer tagged gold nanoflowers as photodynamic and phototheramal agents 6. Silica-coated up-conversion fluorescent nanoparticle (silica@$NaYFa_4$:Yb,Ho) for photodynamic therapy 7. Iron oxide nanoparticles doped niosomes for magnetically assisted photodynamic therapy 8. Conclusions .Publications, conferences and workshops.

22. POKHRIYAL (Meenakshi)

Exploration of Materials to Identify New Structural Variants with Interesting Optical, Catalytic and Ionconducting Properties.

Supervisor : Prof. S. Uma

Th 23856

Abstract

(Not Verified)

Chapter 1 briefly summarizes the background literature of the solids dealt in the present thesis. A short introduction to the various structures and their compositional variants is included. Chapter 2, Section 2.1, deals with the synthesis

and characterization of Eu3+ doped phospho-silicate apatites. The CIE coordinates of the Eu3+ doped apatite samples resulted in red emission. Section 2.2 describes the results belonging to the incorporation of spectroscopically active ions into beyerite. Tunable colors in a wide range were possible by varying the relative doping ratios of Tb3+ and Eu3+ in the lattice. Section 2.3 deals with the single crystal as well as bulk synthesis of cadmium substituted layered perovskite. The SXRD measurements suggested the structure to be tetragonal, (S.G. *P4/mmm*). Chapter 3, section 3.1 and 3.2 deal with attempts to realize the extent of dissolution of rare earth oxides of the formula LnO1.5 ranging from relatively lighter to heavier in fluorite structured theories are described. Section 3.3 deals with the synthesis of mixed metal oxides and anion doped mixed metal oxide using single source precursor. Co2TiO4, CoTiO3 and C, N-doped SnO resulted from these reactions as revealed from various characterizations performed. Chapter 4 has been devoted fully for the work carried out on layered hydroxide compounds. Synthesis of acetate intercalated Co-La and Ca-Ln (Ln = Tb3+, Er3+ and Yb3+) constitute section 4.1 and 4.3. Synthesis of dodecyl sulfate intercalated Co-Y and its usage as an adsorbent constitute section 4.2. Section 4.4, deals with the microwave assisted synthesis of layered double hydroxide, LiAl2(OH)7.2H2O from LiAlO2 as well as LiAlH4. Exchange of the interlayer hydroxide ion with nitrate and chloride ions have also been successful. Chapter 5 The overall conclusions emerged from the present set of investigations summarized in this chapter. Additionally, its implications for futuristic applications to mankind are elaborated.

Contents

1. Background of the study 2. Investigation of materials belonging to apatite, beyerite and layered perovskite structural families 3. Application of epoxide gel synthesis, hydroxide co-precipitation and EDTA based molecular precursors for the generation of functional metal oxides 4. Novel ways of generating layered hydroxides 5. Conclusions and future directions. List of publications.

23. PRIYANKA KUMARI

Micronutrients Containing Clay Polymer Composite Film as Seed Coating Material for Better Plant Growth.

Supervisors : Prof. Ramesh Chandra and Prof. Monika Datta

Th 23865

Abstract
(Not Verified)

Nutrient reserves in the seed must be adequate to sustain growth until the root system can take over the nutrient supply function. During the early establishment phase of a plant, supply of nutrients comes partly from the seed reserves and partly from the soil. These nutrients are always not enough in the soil for healthy growth of plant. That is why fertilizers and nutrients are required for the soil. There are seventeen nutrients that are essential for the healthy growth of plants, They are divided into two main groups : mineral and non-mineral nutrients. Mineral nutrients are further classified as macronutrients and micronutrients. Micronutrients are essential for the early growth of plants and required in very small quantity. So, sprinkling of micronutrients into entire field will be wastage. Therefore, to overcome these problems there has been a need of biodegradable micronutrient/s encapsulated Clay- polymer composite film. This composite film creates a nutritious environment in the immediate vicinity of the germinating seed. This provides a

"boost" for the seedling in its critical early stages of development. This is environment friendly economical for farmers because it prevents excessive use. The synthesized micronutrients encapsulated Clay composite film was characterized by XRD, FTIR, TGA, SEM and TEM techniques. The quantitative estimation of the micronutrients was performed by flame atomic absorption spectrometry. The study of the release behavior of micronutrients in aqueous soil extract was. The release of micronutrients from Clay composite film was slow and extended. Therefore, Clay increases the holding time of nutrients in the composite film. Hence Clay has promising probability of providing extended release of micronutrients from polymer composite film. Finally it was observed that, the micronutrient coated seeds (rice and wheat) resulted in improved vegetative growth of especially where plant-available micronutrients in soil are limited.

Contents

Section-I : 1. Introduction to plant nutrients 2. Methods of providing micronutrients to plants. Section-II : 1. Comprehensive review of literature 2. Methodologies 3. Montmorillonite – polymer composite film for extended release of micronutrients 4. Bentonite – polymer composite film for extended release of micronutrients 5. Vermiculite – polymer composite film for extended release of micronutrients 6. Application of micronutrient containing clay polymer composite film in seed coating 7. Summary of the work reported 8. Future prospects of the work reported .Credentials

24. RAI (Gobind Ji)
Role of Excluded Volume on the Conformation and Rheology of Flexible Dendritic Polymers.
Supervisor : Prof. Parbati Biswas
Th 23874

Abstract
(Verified)

This thesis is devoted to study the conformation and rheology of flexible dendritic polymers by incorporating excluded volume interactions, which may be expressed in terms of the effective co-volume between the nearest non-bonded monomers, modelled through the delta function pseudopotential. The strength of such interactions is evaluated from the possible geometric orientations of the bonds. Chapter 1 provides the basic introduction of dendritic polymers. Dendrimers are perfectly branched, monodispersed acrylic polymers build around a core resembling a Cayley tree. Randomly hyper branched polymers represent imperfectly branched tree-like polymers with branch points scattered throughout the entire structure without well-defined generation of growth. In chapter 2, the mechanical and dielectric relaxation moduli of dendrimers with the excluded volume interactions are theoretically investigated within the framework of Rouse-Zimm theory. In chapter 3, the rheology and transport dynamics of the randomly hyper branched polymers with excluded volume interactions are investigated within the tenets of the Rouse-Zimm theory. In chapter 4, the rheology of dendrimers with excluded volume interactions is investigated and match with those reported in earlier theory, experiments and simulations. Excluded volume between the nearest non-bonded monomers of dendrimers is evaluated within the mean field approximation along the lines of Flory's theory. In chapter 5, we propose the present day picture of dendrimers as a

transition from a non-compact sphere to a dense space filling hyperbolic topology, which contradicts the existing perception of a dendrimer with a dense core and open periphery. The position of maximum in intrinsic viscosity represents the onset of this structural transition, which is accompanied by a change in the overall shape, characterized by a cross-over from the Euclidean to non-Euclidean dimensions.

Contents

1. Introduction 2. Intramolecular relaxation of flexible dendrimers with excluded volume 3. Effect of excluded volume on the rheology and transport dynamics of randomly hyperbranched polymers 4. Dynamics of dendrimers with excluded volume : a comparison with experiments and simulations 5. Topology driven structural transition of dendrimers with a dimensional sross-over .Bibliography.

25. RAKHEE
Isolation and Characterization of Bioactive Compounds from *Cordyceps Sinensis*.
Supervisors : Dr. Raj Kishore Sharma and Dr. Kshipra Misra
Th 23854

Abstract
(Verified)

Mushrooms are perhaps the most well-known, documented edible forest product and have a long and rich history. Prehistoric humans likely used mushrooms collected from the wild as food and possibly for medicinal purposes. Mushroom belonging to high altitude regions such as *Cordyceps sinensis* grows at Indian Himalayan region at different altitude ranges from 3,200 m to 5,000 m and has been traditionally used as herbal medicines. The Indian Himalayan Medicinal Mushrooms are growing in popularity due to its bioactive compounds and several pharmacological activities. However scientific research is not studied as systematically for isolation and characterization of bioactive compounds. Here in this study, we do the sequential isolation and further characterization using different techniques. *Cordyceps sinensis* is interesting, especially because of the pathogenic lifestyle on insects. This endangered species is a combination of fungus and dead insects that is why in present scenario it has been harvested widely. In brief, chapter 2 summarizes the material and methodologies of all isolation and characterization techniques, antioxidant and biochemical assays, proteomics study and bio-efficacy study. The chapter 3 depicts the qualitative and quantitative evaluation of *Cordyceps sinensis* crude sample in terms of phytochemical analysis, proximate analysis and Toxic metal analysis correspondingly. In brief, chapter 4 recapitulates about the proteomic study of several bioactive peptides specially of lower molecular weight, present in *Cordyceps sinensis*. *Cordyceps sinensis* has been evaluated in terms of separation and characterization of bioactive compounds of *C. sinensis* using semi-preparative HPLC, HPTLC, antioxidant assays, antibacterial activity, GC-MS analysis and bio efficacy study sequentially in chapter 5 and 6. Therefore, this study has been reviewed to isolate and characterise the bioactive compounds and their bio-efficacy evaluation of medicinal mushroom *Cordyceps sinensis*.

Contents

1. Introduction 2. Materials and methods 3. Phytochemical and proximate analysis of *C. Sinensis* 4. Proteomics analysis of *C. Sinensis* 5. Separation and characterization of bioactive compounds of *C. Sinensis* by semi-preparative HPLC 6. Fractionation, characterization & bioefficacy evaluation of phenolic rich fractions of

C. Sinensis 7. Conclusions and further perspectives .References and list of publications.

26. RAO (Devarapalli Chenna)
Synthesis of Functionalized Azaheterocycles, Bis (indolyl)methanes and Amides by Oxidative Annualation/Coupling Methods.
Supervisor : Dr. K. Gopalaiah
Th 23855

Abstract
(Not Verified)

The thesis elicit the following dissertations focussing on : (i) developing efficient synthetic method for accessing 2,4,6-trisubstituted pyridines; (ii) developing elegant synthetic route for construction of benzimidazoles; (iii) exploring novel approach for synthesis of quinoxalines by oxidative annulation of 2-azidoanilines with 2-arylethylamines; (iv) aiming for metal-free oxidative coupling between indoles and benzylamines to obtain bis(indolyl)methanes; (v) evolving the direct and efficient transformation for production of secondary amides through oxidative C-H bond activation of aldehydes. An efficient iron(II) bromide-catalyzed one-pot method was developed by oxidative annulation of benzylamines with arylmethyl ketones through C-N bond cleavage and trapping of ammonia, leading to 2,4,6-trisubstituted pyridine derivatives. Reaction mechanism proposed by isolating some key intermediates. Synthesis of 2-substituted benzimidazoles was accomplished by a simple and straightforward approach involving the oxidative annulation of 2-azidoanilines and 2-(aryl/heteroaryl)methanamines in the presence of copper(I) iodide catalyst. Various 2-azidoanilines were easily synthesized by ortho-selective C(sp2)-H functionalization of anilines using trimethylsilylazide as azide source and TBHP as oxidant. An ovel approach for synthesis of quinoxalines by copper(I) bromide catalyzed aerobic oxidative annulation of 2-arylethylamines with 2-azidoanilines at mild conditions, has been presented. A facile metal-free oxidative coupling of benzylamines with indoles for synthesis of a wide variety of functionalized bis(indolyl)methanes has been presented. Molecular iodine was used as catalyst under air atmosphere. Synthesis of secondary amides from benzylamines and aldehydes by oxidative C-H bond activation was performed at 90 oC using CuI as catalyst and TBHP as oxidant in DMSO under oxygen atmospheric conditions.

Contents

1. Iron(II) bromide-catalyzed oxidative annulation of benzylamines with arylmethylketones : construction of 2,4,6-trisubstituted pyridines by in situ ammonia trapping 2. Copper(I) iodide-catalyzed oxidative annulation of 2-azidoanilines with alkyl/2-arylmethanamines to construct 2-substituted benzimidazoles 3. Copper(I) bromide-catalyzed oxidative annulation of 2-azidoanilines and 2-arylethylamines : a simple route to construct quinoxalines via activation of C-H bonds 4. Iodine-catalyzed oxidative coupling between indoles and benzylamines : a greener method to bis(indolyl) methanes 5. Synthesis of secondary amides from benzylamines and aldehydes by copper-catalyzed oxidative C-H bond activation .Summary and Publications.

27. SAINI (Anupmana)
Synthesis of Quinoxalines, Quinazolines and Schiff Bases using Primary Amines.
Supervisor : Dr. K. Gopalaiah
Th 23847

Abstract
(Not Verified)

The thesis entitled "Synthesis of Quinoxalines, Quinazolines and Schiff Bases using Primary Amines" is to be submitted to the University of Delhi. The thesis deals with the studies related to the construction of N-heterocycles and Schiff bases via oxidative condensation/annulation reactions through activation of C-H bonds using inexpensive catalysts and oxidants. The present thesis has been divided into 5 chapters and brief details of the chapters are listed below : Chapter 1 provides a comprehensive overview of the construction of nitrogen heterocycles because of their tremendous importance in the field of medicine and industry. Several approaches that have recently appeared in the literature for the construction of wide classes of valuable N-heterocycles through oxidative condensation/annulation reactions in presence of suitable catalysts and oxidants are discussed in this chapter. Chapter 2 describes the one-pot, one-step synthesis of 2-substituted quinoxalines by copper(I) bromide-catalyzed oxidative coupling reaction of o-phenylenediamines and 2-aryl/hetarylethylamines under molecular oxygen as sole oxidant at room temperature. Chapter 3 describes the iron(II) bromide-catalyzed oxidative cascade reaction of readily available o-aminobenzyl alcohols with 2-aryl/heteroarylamines for the synthesis of 2-aryl/heteroarylquinazolines via trapping of in-situ generated ammonia in the presence of molecular oxygen at 110 oC. Chapter 4 describes a metal-free cascade reaction of o-aminobenzyl alcohols with benzylamines for the efficient synthesis of 2-substituted quinazolines using molecular iodine in DMSO at 110 oC. Chapter 5 describes the solvent-free synthesis of diverse imines by iron(II) bromide-catalyzed oxidative self and cross-condensation of primary amines. We intended to optimize a generalized method for the preparation of various functionalized imines. Therefore, our optimized conditions involves the use of FeBr2 as a catalyst (5 mol %) and molecular oxygen as oxidant at 110 oC under solvent free conditions.

Contents

1. Synthesis of *N*-heterocycles through oxidative condensation/coupling reactions 2. Synthesis of quinoxalines by copper-catalyzed oxidative coupling of *o*-phynylenediamines with 2-aryl/heatarylethylamines 3. Synthesis of quinazolines by iron-catalyzed oxidative cascade reaction of 2-aminobenzyl alcohols with benzylamines 4. Metal-free method to access quinazolines via oxidative condensation of 2-aminobenzyl alcohols with benzylamines 5. Iron-catalyzed synthesis of imines via self-or cross-oxidative condensation of primary amines .Summary and List of publications.

28. SANJAY KUMAR SAROJ
Studies on Various Aspects of Selected Mixed Metal Fluorides and Layered Inorganics Including Their Applications.
Supervisor : Prof. Rajamani Nagarajan
Th 24262

Abstract
(Not Verified)

Chapter 1 has dealt with the different structural families adopted by mixed metal fluorides. The important application aspects of fluorides, layered hydroxide salts and layered oxides have been included. Chapter 2 has been fully devoted to the mixed metal fluorides which have been further presented in six subsections. Section 2.1 describes rare earth and rubidium containing fluorides by the reaction of rare earth acetylacetonates with rubidium fluoride in non-aqueous solvent. Section 2.2 summarizes the results obtained from the room temperature synthesis of Rb2CoF6 (S. G. Fm-3m # 225) from RbCoF3 (S. G. Pm-3m # 221) employing a simple oxidation process. Section 2.3 is devoted to the hexagonal perovskite which is transformed into cubic RbNiF3 by applying chemical pressure of substituting Cd2+-ion for Ni2+-ion. Additionally, a transformation of RbNiF3 to double perovskite, Rb2NiF6 has also been demonstrated. Section 2.4 summarizes the reaction of tetragonal perovskite structured KCuF3 with H2O2 and its transformation to a cubic cryolite structure. Section 2.5 is devoted to the luminescence property to the perovskite structured RbZnF3 by doping of manganese (II), cerium(III), europium(III) and terbium(III) ions. Section 2.6 summarizes the work involving the upconversion phosphorescence for the rare-earth doped K3InF6, having cryolite structure. Chapter 3 dealt with layered hydroxide salts and layered oxide. Where in a synthesis of Zn and Cu containing layered hydroxide acetate was achieved by a titrimetric procedure. The swelling behavior of these systems with polyols has been examined. Layered oxides have been synthesized by the soft chemical route by employing NaOH and KOH fluxes. Chapter 4 the overall conclusions emerged from the present set of investigations is summarized. Additionally, its implications towards either practical application or to carry out advanced studies for futuristic applications to mankind are elaborated.

Contents

1. Background of study 2. Mixed metal fluorides : synthesis, structure, reactivity, properties and applications 3. Engineering inorganic-inorganic hybrids using layered hydroxides and oxides 4. Conclusions and future directions .List of publications

29. SHARMA (Shalini)
Synthesis, Characterization and Application of Hybrid Nanoparticles in Drug Delivery.
Supervisor : Dr. Indrajit Roy
Th 23867

Abstract
(Not Verified)

The thesis entitled “Synthesis, characterization and application of hybrid nanoparticles in drug delivery” reveals the synthesis of hybrid nanoparticles (metal-organic frameworks) synthesized from metal ions and the organic ligands. The as-synthesized MOFs were used for anticancer drug delivery, photodynamic therapy, photothermal and photo-antibacterial applications. Chapter 1 is the introduction chapter explaining the basic fundamentals of nanotechnology, significance of engineered nanoparticles, manipulation of its chemical or physical properties at nanoscale with potential applications in biomedicine. Chapter 2 comprises the

literature review related to the research work included within this thesis. This chapter summarised the research work carried out till date regarding the nanoscale metal-organic framework, in addition to nanoscale coordination polymers for various biomedical applications. Chapter 3 provides the detailed experimental characterization techniques used throughout the research work embodied in this thesis. Chapter 4 contains the synthesis and characterization of iron (III)-carboxylate metal organic framework MIL-88 B using DMF as a coordinating solvent via micellar system. Owing to the superparamagnetic nature of this NMOF, we investigate their magnetically aided drug delivery and photodynamic therapy using cancer cells in *vitro*. Chapter 5 contains the synthesis and characterization of anti-cancerous MOF (MIL-53) composed of copper ions with the anticancer drug gallic acid as the linker itself. The combination effect of GA induced toxicity and light induced toxicity were investigated in cancer cells in vitro and in vivo. Chapter 6 contains the synthesis and characterization of anticancer NCPs of alendronic acid (AL) with the non-toxic and biocompatible zinc ion in the aqueous environment at moderate temperature. Chapter 7 contains the synthesis and characterization of biocompatible, cubic shaped, citric acid coated silver containing Prussian blue analogue. We explored their anticancer, antibacterial and photothermal properties. Chapter 8 enlightens the conclusion of all these works embodied in this thesis, with their present and future significance.

Contents

1. Introduction 2. Literature review 3. Experimental and characterization techniques 4. Magnetic nanoscale metal-organic frameworks for magnetically aided drug delivery and photodynamic therapy 5. Copper-gallic acid metal-organic framework for drug delivery and photodynamic therapy 6. Zinc-alendranic acid nanoscale coordination polymers in drug delivery 7. Silver-prussian blue nanoparticles for combined-thermal applications 8. Conclusion .List of publications .Conference and workshop.

30. SHARMA (Shilpa)
Synthesis, Characterization and Evaluation of Polyaspartic Acid Based Superabsorbent Polymers for Wound Healing.
Supervisor : Dr. Amita Malik
Th 23849

Abstract
(Not Verified)

Wound management and wound care has gained importance in recent years. Advances have been made to achieve wound management with better absorption systems using superabsorbent polymers (SAPs). Wound healing is a multi-stage dynamic biological process related to tissue growth and regeneration. SAPs are class of upcoming polymeric material that embraces different biomedical and pharmaceutical applications. Superabsorbent Polymers are three dimensional hydrophilic crosslinked polymeric networks with proficiency to absorb and retain large amount of fluids. SAPs change their volume when in contact with fluids and are termed as Stimuli responsive polymers. Polyaminoacids have been studied in past few years for SAP synthesis. Polyaspartic acid is water soluble and biodegradable polyaminoacid, respond to the change in external environment and are being used as drug delivery system.

Contents

1. Introduction 2. Materials and methods 3. Synthesis, characterization and evaluation of polyaspartic acid and acrylic acid based superabsorbent polymers 4. Synthesis, characterization and evaluation of polyaspartic acid and 2-acrylamido-2-methylpropane sulfonic acid based superabsorbent polymers 5. Synthesis, characterization and evaluation of polyaspartic acid, sodium alginate and 2-acrylamido-2-methylpropane sulfonic acid based superabsorbent polymers 6. Conclusions and future prospects .References .List of publications

31. SHIV SHYAM
Design and Synthesis of N, O & S Containing Heterocyclic Molecular Hybrids as Blodynamic Agents.
Supervisor : Prof. Diwan S. Rawat
Th 24261

Abstract
(Not Verified)

In chapter 1, the effect of structural modifications on the linker of the previously synthesized 4-aminoquinoline-pyrimidine hybrids has been studied in order to examine their antiplasmodial activity and pharmacokinetic behavior. The terminal free -NH of diamine linker was substituted with appropriate aryl/heteroaryl functionality (furfuryl and pyridin). The resulted compounds showed moderate to excellent in vitro antiplasmodial activity against both the strains (W2 and D6) of P. falciparum. In addition, to understand the mechanism of action; heme binding and molecular docking studies of best active compounds were performed. ADME properties were predicted to assess the pharmacokinetic behavior of the synthesized compounds. In chapter 2, molecular hybrids comprising imidazo[1,2-a]pyridine-triazole and imidazo[1,2-a]pyridine-amidoether pharmacophores have been synthesized since these pharmacophores are well known for their wide range of biological activities including anti-TB activity. Synthesized compounds were evaluated for their in vitro anti-mycobacterial activity against M.tb H37Rv strain which showed moderate activity. In chapter 3, imidazopyridine-oxadiazole pharmacophores have been synthesized since these pharmacophores are well known for their wide range of biological activities including anti-TB activity. All the synthesized compounds were screened against M.tb H37Rv strain with good anti-tubercular activity. In chapter 4, benzothiazole hydrazono-amidoether derivatives were designed as possible anti-tubercular agents. This design was based on the literature that proposes functionalization of substituted benzothiazole hydrazono-amidoether may improve their anti-TB activity.

Contents

1. Synthesis and antimalarial activity evaluation of *N*-Substituted 4-aminoquinoline-pyrimidine hybrids 2. Synthesis and anti-tubercular activity of imidazo [1,2-α]pyridine-triazole and imidazo[1,2-α]pyridine-amidoether hybrids 3. Synthesis of imodazopyridine-oxadiazole molecular hybrids as anti-tubercular agents 4. Synthesis of substituted benzothiazole hydrazono-amidoether hybrids as anti-tubercular agents .Summary .List of publications .Conferences, seminar and workshops.

32. SHIVANI

Design, Synthesis and Biological Evaluation of Synthetic Probes for Tumor and Alzheimer's Diagnosis.

Supervisors : Dr. Rakesh Kumar Sharma and Dr. Sweta Singh

Th 23846

Abstract

(Not Verified)

The thesis entitled "Design, Synthesis and Biological Evaluation of Synthetic Probes for Tumor and Alzheimer's Diagnosis" is submitted to University of Delhi. The thesis is divided into four chapters i.e. Chapter 1, Chapter 2, Chapter 3 and Chapter 4. The introductory chapter (Chapter 1) of the thesis discusses the importance of molecular imaging probes. Radiopharmaceuticals could be introduced with the help of prosthetic groups, acyclic and macrocyclic chelators. Acyclic chelators serve high complexation rates and flexible cation coordination. Development of SPECT and PET in recent times has helped in understanding and management of the disease like cancer and neurological disorders. Chapter 2 focuses on the design, synthesis and preliminary biological evaluation of DTPA conjugated D-Glucose as tumor targeted SPECT imaging agent. Imaging of glucose-related molecular events using PET, SPECT radioligands has been developed successfully in recent times. Bivalent approach is introduced to incorporate two biovectors in one molecule resulting in better target binding and accomplishment of desired effect at much lower concentration than the monovalent counterpart. Chapter 3 includes design, synthesis and preliminary biological evaluation of thymidine-DTPA based SPECT probe for imaging of cell proliferation. DNA targeting in the proliferating cells is direct approach for tumor diagnosis. Thymidine (specific for DNA over RNA) derivatives get incorporated in the newly synthesised DNA strands of proliferating cells thus allowing thymidine to be used in monitoring the overexpression of TK1 in the proliferating cells. Here two moieties of N-3 modified thymidine has been conjugated with acyclic chelator, DTPA. Chapter 4 revolves around the design, synthesis and preliminary biological evaluation of a novel imidazo-oxazolopyridine derivative for PET imaging of β-Amyloid aggregates (hallmarks of Alzheimer's disease). Imaging of β-Amyloid is important for the diagnosis, staging of AD and monitoring the progress of the therapy. Here, two already established β-amyloid tracers are conjugated and evaluated.

Contents

1. Introduction and objectives 2. Synthesis and biological evaluation of a Tc-99m labelled diethylenetriaminepentaacetate-bis-deoxyglucose complex {[^{99m}Tc]-DTPA—bis(DG)} as a potential SPECT based imaging probe got tumor imaging 3. Synthesis and preliminary evaluation of a novel ^{99m}Tc labelled DTPA-bis-Thymidine derivative as a tumor imaging agent 4. Synthesis and preliminary evaluation of a nover ^{18}F labelled imodazo-oxazolopyridine derivate as a β-amyloid imaging agent .Summary and List of publications.

33. SHYAM LAL

Synthesis and Evaluation of Novel Fluorescent Heterocyclic Chemosensors.

Supervisor : Dr. Sunita Hooda

Th 23873

Abstract
(Not Verified)

Herein we have presented the synthesis and structural characterization of three newly synthesized chemosensors (L1, L2 and L3), styrene - acrylonitrile co-polymer based membrane sensor (SA) and heteroleptic metal complexes (Mn+) of curcumin and 2, 2'-bipyridine. Synthesized chemosensors (L1, L2 and L3) and styrene - acrylonitrile co-polymer based membrane sensor were employed to their metal ion sensing study and selective detection study of Cu2+, Fe3+, Hg2+ and Pb2+ metal ions in aqueous medium with UV-Visible, fluorescence and electrode potential techniques. Chemosensor (L1) upon the addition of 10 equivalents of Cu2+ and Fe3+ ions, shows notable color change, light yellow and yellow color of L1 in the solution as well as on paper strips with good binding constant 6.46 x 103 M-1 for L1 + Cu2 and 6.46 x 103 M-1 for L1 + Cu2 respectively. Chemosensor L2 display good binding constant for L2 + Cu2+ (2.4 x 105 M-1) and L2 + Hg2+ (7.46 x 105 M-1) which indicate good interaction of chemosensor with Cu2+ and Hg2+ ions in 10% HEPES solution. Chemosensor (L3) indicate high binding constant (*K*b, 1.45 x 105 M-1), and Stern-Volmer constants (*K*SV 1.2 x 105 M-1) with Cu2+ ion. Chemosensor (L3) upon the addition of 10 equivalents of Cu2+ ion, show notable color change, visible color changes in few seconds just by dipping the paper strips in the solution of metal ions from colorless to green. Fabricated polymer membrane sensor, over a concentration range of 1x10-5 -1x10-1 mol L-1 revealed a best Nernstian response for Pb (II) ions with a slope of 39.60 mV/decade. All the heteroleptic metal complexes showed 1 :1 stoichiometry and an insight from the data, the copper complex exhibit remarkable activities against used microbial strains.

Contents

1. Introduction 2. Instrumental techniques 3. A highly selective chemosensor for Cu^{2+} and Fe^{3+} ions in aqueous medium : spectroscopic, computational and cell imaging studies. 4. Curcumin based fluorescent chemosensor for slelctive detection of Cu^{2+} and Hg^{2+} ions in awueous medium 5. Iburprofen based fluorescent chemosensor for selective detection of Cu^{2+} ion in aqueous medium 6. Styrene-acrylonitrile copolymer based membrane sensor for selective detection of Pb^{2+} ions in aqueous medium 7. Synthesis, characterization and antimicrobial evolution of heteroleptic metal complexes of curcumin and 2, 2'-bipyridine .Summary.

34. SINGH (Amit Kumar)
Synthesis of Hydroxyethylamine and Quinoline Based Maleimide Derivatives for the Inhibition of Malarial Parasite.
Supervisor : Dr. B. K. Singh
Th 23860

Abstract
(Not Verified)

Due to increasing resistance of malarial parasites against all the existing drugs of malaria *i.e.* quinine, chloroquine, proguanil, sulfadoxine-pyrimethamine, mefloquine, atovaquon. In fact the recent medicine given to patient *i.e.* artemisinin-base combination therapy (ACT) has also shown resistance, increased from 2% to 30 %. There is no back-up drug for ACTs and infect no drug has been introduced since 1996. Malaria is the major cause for death of children under 5 years old, taking a life of a child in every two minutes. So in chapter I, we have designed, synthesized, characterized, antimalarial activity and inhibition constant have been done. After carrying out antimalarial activity, it has been observed that hydroxyethylamine

based derivatives having bulkier amino acid *i.e.* leucine, isoleucine and phenylalanine were showing better antimalarial activity as well as inhibition of plasmepsin II and IV enzymes of malarial parasite. Chapter II, describes the synthesis of hybrid molecules having two pharmacophore units *i.e.* quinoline and *N*-phenylmaleimide clubbed together *via* Wittig reaction. As quinoline, which is found in most of the antimalarial drugs, so we have clubbed it with other bioactive moiety *N*-phenylmaleimide. The idea of making hybrid molecules have been introduced, for the better result in respect to biological activities. Such molecules are known as hybrid molecules. These molecules have drawn the attention of synthetic as well as biochemists for certain advantages *i.e.* enhanced potency by self-synergy within one molecule that may not be achieved by the traditional combination of separately doses, reduce risk of developing drug resistance, improved pharmacokinetic properties, reduce the toxic side effects and may provide the advantage of reduced cost. Chapter III, here we have taken three bioactive moieties *i.e.* quinoline, *N*-phenylmaleimide and 1,2,3- triazole and clubbed them together in a single molecule *via* Vilsmeier-Haack reaction, Wittig and Click reactions, for the search of better result.

Contents

1. Design and synthesis of dydroxyethylamine based inhibitors of plasmepsin II, IV enzymes of malarial parasite 2. Design and synthesis of new class of quinolone based maleimide derivatives for antimalarial activity 3. Design and synthesis of new class of triazolyl-quinolone based maleimide derivatives for antimalarial activity .Summary and List of published paper.

35. SINGH (Ashwani Kumar)
Design and Synthesis of Newer Chiral Organocatalysts for Enantioselective Synthesis of Heterocyclic Compounds and Experimental and Theoretical Study of Intramolecular O••O Interaction in β-Keto Carboxylic Esters.
Supervisor : Prof. Satish Kumar Awasthi
Th 23870

Abstract
(Not Verified)

This thesis addressed to develop asymmetric organocatalysts for few important organic transformation reactions i.e. carbon-heteroatom bond formation. Simple organic molecule used as a promising chiral organocatalyst in asymmetric transformation and act as alternative in addition to metal containing catalysts. Among these organocatalyst, the catalyst having 1, 2, 4-triazole, guanidine, imidazolidinone, urea, thiourea, amidine and amide groups act as an efficient chiral catalyst in asymmetric conversion reactions. This thesis includes five chapters which brief descriptions are given below. Chapter I is introductory which discussed brief introduction of earlier reported asymmetric synthesis methods for asymmetric small organic molecule synthesis. Chapter II includes synthesis of *s*-triazene based phase transfer asymmetric organocatalysts, their characterization and its application in enantoselective synthesis of flavanone from 2-hydroxychalcone in higher yield and better enantioselectivity. Chapter III consists of screening of the *s*-triazine catalysts having guanidine functional group for the enantioselective synthesis of 2-aryl 2, 3-dihydro-4-quinolones from 2-aminochalcones. Chapter IV discusses L-proline and *s*-triazene based bi-functional chiral organocatalysts and its role in synthesis of most important biologically active heterocyclic compounds, 3-hydroxy-2-oxindole from 2-oxindole. Chapter V consists of experimental (TGA, DSC, single crystal x-ray diffraction and IR) and theoretical study (QTAIM and NBO) of intramolecular oxygen

- oxygen interaction in structurally rigid quinolone carboxylate and bis ethoxycarbonyl vinyl aniline.

Contents

1. A brief history, approaches and overview of asymmetric catalysis 2. Synthesis of asymmetric *s*-triazine based organocatalyst and its application in enantioselective synthesis of flavanones 3. An efficient enantioselective synthesis of 2-aryl 2, 3-dihydro-4-quinolones via protecting group free aza Michael addition reaction 4. An effective and efficient asymmetric synthesis of 3-hydroxy-2-oxindoles by reduction of 3-benzylidene indolin-2-one, a Knoevenagel condensation product of 2-oxindole 5. Experimental and theoretical study of intramolecular oxygen-oxygen interaction in structurally rigid quinolonecarboxylate and bisethoxycarbonylvinyl aniline. Publication.

36. TEKURI (Chandra Sekhar)
Synthesis and Photophysical Properties of β-Modified *meso*-Tetraaryl-porphyrins Docorated with Fused Nitrogen and Oxygen Heteroaromatics.
Supervisor : Prof. Mahendra Nath
Th 24260

Abstract
(Not Verified)

The primary goal of this dissertation is to synthesize the novel π-conjugated porphyrinoids through peripheral functionalization of *meso*-tetraarylporphyrins involving *β*-positions and study their electronic properties. These newly prepared *β*-substituted and *β*,*β*'-fused *meso*-tetraarylporphyrins are expected to be useful for a wide variety of applications in medicinal and material chemistry. The work presented in this thesis is divided into four chapters. The first chapter presents a brief account on the synthesis and electronic properties of *β*-substituted pyrrolo- and indolo[1,2-*a*]quinoxalinoporphyrins. These newly designed porphyrins were synthesized in good yields *via* a Pictet-Spengler reaction of copper(II) *β*-formyl-5,10,15,20-tetraarylporphyrins with 1-(2-aminophenyl) pyrrole or 2-(3-methyl-indol-1-yl)-phenylamine in the presence of *p*-dodecylbenzene sulfonic acid (DBSA) as an acidic catalyst in 1,4-dioxane at 25-40°C followed by oxidation using aqueous potassium permanganate. Chapter 2 discusses about the trichloroacetic acid promoted one-pot three-component synthesis and photophysical properties of novel nickel(II) *β*,*β*'-chromeno[3,4-*c*]pyridin-5-one-fused 5,10,15,20-tetraphenylporphyrins. These porphyrins were synthesized by the reaction of nickel(II) 2-amino-5,10,15,20-tetraphenylporphyrin with 4-hydroxycoumarin and aromatic aldehydes in 1,2-dichlorobenzene containing trichloroacetic acid under reflux condition. Chapter 3 deals with the synthesis of benzoquinoxalino[2,3-*β*]-5,10,15,20-tetraarylporphyrins *via* the condensation of various copper(II) 2,3-diamino-*meso*-tetraarylporphyrins with 4-N-substituted naphthaquinones in presence of 10 mol% trichloroacetic acid in chloroform under reflux condition. The photophysical studies revealed a significant red-shift in the absorption and emission spectra of these molecules. Chapter 4 describes the synthesis, spectroscopic characterization and optical properties of novel benzo[*a*]quinoxalino porphyrins and benzo[*a*]chromeno[2,3-*c*]quinoxalinoporphyrins. The preliminary photophysical results are found to be significantly encouraging and henceforth may prove useful for the designing of diverse π-extended porphyrinic systems as light harvesting materials and photosensitizers in photodynamic therapy applications.

Contents

1. Synthesis and electronic properties of β-subsitituted pyrrolo-and indolo[1,2-α]quinoxalinoporphyrins 2. Trichloroacetic acid promoted one-pot three-component synthesis and photophysical properties of novel nickel(II)β,β'-chromemo[3,4-c]pyridine-5-one-fused 5,10,15,20-tetra-phenylporphyrins 3. Synthesis, characterization and photophysical properties of benzoquinoxalino[2,3-β]-5,10,15,20-tetraarylporphyrins 4. Novel benzo[α]quinoxalinoporphyrins and benzo[α]-chromeno[2,3-*c*]quinoxalinoporphyrins : synthesis, spectroscopic characterization and electronic properties. .Summary .Publications.

37. TOMAR (Richa)
Synthesis, Characterization and Dielectric Properties of Complex Perovskite Oxides.
Supervisor : Prof. M. Thirumal
Th 23866

Abstract
(Not Verified)

Herein we have presented the synthesis and structural characterization of three newly synthesized chemosensors (L1, L2 and L3), styrene - acrylonitrile co-polymer based membrane sensor (SA) and heteroleptic metal complexes (Mn+) of curcumin and 2, 2'-bipyridine. Synthesized chemosensors (L1, L2 and L3) and styrene - acrylonitrile co-polymer based membrane sensor were employed to their metal ion sensing study and selective detection study of Cu2+, Fe3+, Hg2+ and Pb2+ metal ions in aqueous medium with UV-Visible, fluorescence and electrode potential techniques. Chemosensor (L1) upon the addition of 10 equivalents of Cu2+ and Fe3+ ions, shows notable color change, light yellow and yellow color of L1 in the solution as well as on paper strips with good binding constant 6.46 x 103 M-1 for L1 + Cu2 and 6.46 x 103 M-1 for L1 + Cu2 respectively. Chemosensor L2 display good binding constant for L2 + Cu2+ (2.4 x 105 M-1) and L2 + Hg2+ (7.46 x 105 M-1) which indicate good interaction of chemosensor with Cu2+ and Hg2+ ions in 10% HEPES solution. Chemosensor (L3) indicate high binding constant (*K*b, 1.45 x 105 M-1), and Stern-Volmer constants (*K*SV 1.2 x 105 M-1) with Cu2+ ion. Chemosensor (L3) upon the addition of 10 equivalents of Cu2+ ion, show notable color change, visible color changes in few seconds just by dipping the paper strips in the solution of metal ions from colorless to green. Fabricated polymer membrane sensor, over a concentration range of 1x10-5 -1x10-1 mol L-1 revealed a best Nernstian response for Pb (II) ions with a slope of 39.60 mV/decade. All the heteroleptic metal complexes showed 1 :1 stoichiometry and an insight from the data, the copper complex exhibit remarkable activities against used microbial strains.

Contents

1. Introduction 2. Ba-Ni-Ta System 3. $Ba_3ZnTa_{2-x}Nb_xO_9$and $Ba_3Zn_{(1-x)}Ni_xTa_{(2-x)}Nb_xO_9$ 4. (1-x) $Ba_8ZnTa_6O_{24}$ – (x) $Sr_8ZnTa_6O_{24}$ and (1-x) $Ba_3ZnTa_2O_9$ – (x) $Ba_8ZnTa_6O_{24}$Systems 5. Synthesis of new hexagonal and cubic perovskites 6. Order-Disorder Transitions for $Ba_3ZnTa_2O_9$ using NaCl-KCl Flux. Publications and Conferences.

38. WADI (Ishan)
Biological Evaluation of Dual Stage Antiplasmodial Potential of Novel 4-Amino-7-chloroquinoline Appended [1,2,3]-Triazoles.
Supervisors : Prof. Mahendra Nath and Dr. Neena Valecha
Th 23845

Abstract
(Verified)

Malaria is a tropical disease which remains a global health problem despite the availability of effective tools. Drug resistance and absence of safe and effective transmission-blocking drugs are the two major roadblocks which have severely halted the progress of malaria elimination campaigns. One way to combat these problems is to develop safe and effective antimalarials. In the present work, 4-amino-7-chloroquinoline appended [1,2,3]-triazoles are screened for their ability to simultaneously target asexual stages and gametocytes of *P. falciparum*. The study begins with development of a continuous *in vitro* culture of asexual stages and gametocytes of *P. falciparum*. Further, a very simple and cost effective gametocytocidal-drug screening assay was optimized, and methylene blue was investigated as a gametocytocidal agent. Then, ADMET properties of newly synthesized group of quinoline-triazole hybrids were predicted using *in silico* tools and their cytotoxicity evaluated on VERO cells. Further, their dual stage antiplasmodial potential was investigated. After optimizing the asexual stage culture and gametocyte production in *P. falciparum*, two field isolates RKL-9 and JDP-8 were identified as high gametocyte producers and were deemed suitable to screen gametocytocidal drugs. Methylene blue was found to target gametocytes by either completely eliminating gametocytes or rendering them morphologically deformed with IC50 (late stages) as 106.4 nM. Addition of [1,2,3]-triazoles to 7-chloroquinoline nucleus resulted in formation of compounds that demonstrated potency in nanomolar range against chloroquine sensitive strain (3D7) of *P. falciparum* with three compounds showing IC50 of <100 nM against chloroquine resistant field isolate (RKL-9). Further, the lead compounds were also observed to be causing morphological deformations in gametocytes with IC50 < 15 μM. All compounds displayed attractive ADMET profile whilst majority demonstrated little or no cytotoxicity. Our results prove that these newly synthesized compounds may be used as prototypes for the development of effective multi-stage antimalarial drugs against *P. falciparum*.

Contents

1. Introduction and review of literature 2. Establishment of a continuous *in vitro* culture for asexual stages of *P. falciparum* 3. *In vitro* production and cultivation of gametozytes Indian field isolates of *P. falciparum*. 4. Development of gametocytocidal drug assays and investigation of methylene blue as a gametocytocidal agent against Indian field isolates 5. Dual stage antiplasmodial activity of novel 4-amino-7-chloroquinoline appended [1,2,3]-Triazoles. 6. Conclusions. Bibliography. Summary. Appendices and Publications.