

CHAPTER 10

CHEMISTRY

Doctoral Theses

101. AERRY (Swati)
Synthesis and Characterization of Polymers and Polymeric Nanoparticles for Applications in Drug Delivery.
Supervisor : Dr. Subho Mozumdar
Th 18061

Abstract

Nanomaterials have been synthesized of thermosensitive moiety with variable sizes in order to broaden the area of applicability of these materials in drug delivery. Syntheses of NIPAM based copolymers have been optimized and by modulating various parameters nano as well as microgel materials have been synthesized. Applications of these have proven by recording and explaining their release behaviour, employing a model protein drug and finally the cytocompatibility of these copolymers has been studied. The pH sensitive polymers have been devised and synthesized with the aim of producing an enteric coating material. The polymers have been tested for successful polymerization and a detailed analysis has been done to explain their experimentally noted behaviour towards different pH.

Contents

1. Introduction. 2. Literature review. 3. Materials, methods and instrumentation. 4. Temperature dependent synthesis of NIPAM-VP nanogel and microgel particles. 5. Morphological analyses of NIPAM-VP microgel particles formed at different concentrations of the chemical crosslinker. 6. In vitro release kinetics study of microgel particles encapsulating bovine serum albumin. 7. Synthesis and characterization of a pH-sensitive polymer. 8. Cytotoxicity study of synthesized thermo and pH responsive polymers. Conclusion.

102. AGGARWAL (Nisha)
Synthesis of Novel Nalidixic Acid Based Derivatives and their Evaluation for Various Biological Activities.
Supervisors : Prof. J.M. Khurana and Dr. Rajesh Kumar
Th 18059

Abstract

This work has synthesized a variety of novel heterocycles and their applications in medicinal and agrochemical field. The synthesis of nalidixic acid based hydrazone derivatives and their evaluation for antifungal activity against *Rhizoctonia bataticola*, *Sclerotium rolfsii*, *Rhizoctonia solani*, *Fusarium oxysporum* and *Alternaria porri*, insecticidal activity against *Spodoptera litura*, *Callosobruchus maculatus* and *Tribolium castaneum* at 0.1% dose and nitrification inhibitory activity has been studied.

Contents

1. Nalidixic acid - An important tool for developing biomolecules.
2. Synthesis of nalidixic acid based hydrazones and their evaluation for various biological activities.
3. Synthesis of nalidixic acid based acyl hydrazines and their evaluation for various biological activities.
4. Synthesis of nalidixic acid based 1,3,4-thia/oxadiazole derivatives and their evaluation for antibacterial activity.
5. Synthesis of nalidixic acid based 1,2,4-triazole derivatives and their biological evaluation for antimicrobial activity.
6. Summary and Conclusions.

103. AHUJA (Gauri)
Synthesis, Spectral, Catalytic and Structural Study of Some Transition Metal Ion Complexes with N, O Donor Tetradentate Bis Benzimidazolyl Diamide Ligands.
Supervisor : Prof. Pavan Mathur
Th 18077

Abstract

Briefly introduces metalloenzymes containing Copper, Iron and Nickel. Complexes synthesized have been characterised by elemental analysis UV-visible spectroscopy, IR Spectroscopy, cyclic voltammetry, EPR, magnetic susceptibility Mossbauer study and HNMR analysis. The results obtained have been given with each chapter.

1. Introduction. 2. Theory of technique utilized in the identification of ligands and their complexes. 3. Synthesis and characterization of copper (II) complexes with tetradentate diamide ligands : Spectral, structural and oxidation of aminophenols & amines. 4. Synthesis, spectral, electrochemical and mossbauer of Iron (III) complexes with tetradentate diamide ligands and their utilization in the oxidation of alcohols & olefins. 5. Synthesis, spectral, ¹HNMR and fluorescence of nickel (II) complexes with tetradentate diamide ligands.

104. AJEET KUMAR

Preparation and Characterization of Inorganic and Polymeric Nanoparticles for Applications in Catalysis and Delivery of Bio-Active Molecules

Supervisor : Dr. Subho Mozumdar
Th 18060

Abstract

It has synthesized various inorganic nanoparticles using a soft chemical route. The optimized procedure of reverse microemulsion using cyclohexane/TX-100/nhexanol/water system has been used and nanoparticles of nickel, nickel oxide, copper and copper oxides have been successfully synthesized. Also synthesized nanoparticles for catalyzing various organic reactions and check the recyclability of the catalysts. The effects of concentration of the nanoparticles and the solvents on the reaction rates of the organic reactions have also been studied. Copper nanoparticles have been successfully used for the synthesis of thiazolidine (TZD) derivatives, naphthoquinone derivatives and for click reaction using highly viscous heteropolysaccharide (Guar-gum) as a stabilizer. Gold nanoparticles have been successfully functionalized with L-Proline using cysteine as linker and used for asymmetric aldol reaction in recyclable PEG.

Contents

1. Background and motivation. 2. Literature review. 3. Materials, methods and instrumentation. 4. Soft chemical route for the synthesis of metal and metal oxide nanoparticles. 5. Applications of copper nanoparticles. 6. Applications of nickel nanoparticles. 7. Application of gold nanoparticles. 8. Applications of polymeric nanoparticles for the delivery of bio-active molecules. Summary and Conclusions.

105. ARORA (Bharti)
Structural Studies on Single nucleotide Polymorphisms (SNPs) Associated DNA Sequences in Human MGMT Gene.
 Supervisor : Prof. Shrikant Kukreti
 Th 18051

Abstract

This work has studies the structural aspect of SNP associated DNA sequences within functional MGMT gene associated with various diseases, (including cancer). Biophysical and biochemical methods (Gelelectrophoresis, UV-thermal denaturation and circular dichroism (CD) spectroscopic techniques and bioinformatic approaches are used to investigate the structure.

Contents

1. Introduction. 2. Materials and Experimental Techniques. 3. Bioinformatic approaches to study human MGMT gene 4. Biophysical and biochemical analysis of intron 1 Region polymorphism. 5. Biophysical and biochemical analysis of enhancer region polymorphism. 6. Conclusions. Bibliography.

106. AVNEET KAUR
Theoretical Designing of Electrically Conducting Polymers Using Genetic Algorithm.
 Supervisor : Prof. A K Bakshi
 Th 18064

Abstract

The present work have used the strategy of copolymerization to design novel conducting polymers. Copolymeric systems, are obtained by alternating the epitaxial growth of the two semiconductors copolymerization of different monomers chemical or electrochemical oxidation can effectively modify the structures and properties of conducting polymers.

Contents

1. Electrically conducting polymers: An Introduction. 2. Strategies for designing low band gap polymers. 3. Methodology. 4 Investigation of electronic and conduction properties of model binary copolymers. 5. Study of effect of changing band discontinuities and band widths on optimum solution obtained using GA. 6. Designing of type-I and type-II ternary polymeric superlattices

using genetic and ant algorithms: A comparative study. 7. Investigation of electronic and conduction properties of ternary copolymer (PTP-PITN-PINTP). 8. Summary and Conclusions.

107. BHARDWAJ (Saurav)
Synthetic Transformation and Nano Technology.
 Supervisor : Prof. M Kidwai
 Th 18065

Abstract

This work has carried out various organic synthesis using metal nanoparticles, Cu, CuO, TiO₂, Au, Fe₃O₄. The synthesis of 3-aryl-2,4-pentanedione and 2-aryl diethylmalonate using CuO-nanoparticles as a heterogeneous catalyst have been reported. It also has reported a novel and efficient protocol for oxidation of secondary alcohols into ketone using nanocrystalline titanium (IV) as catalyst in green solvent PEG and the synthesis of α -amino phosphonates using Cu-nanoparticles as selective and efficient catalyst for the synthesis of α -amino phosphonates.

Contents

Introduction. 1. A novel method for the synthesis of β -enamionones using Cu-nanoparticles as catalyst. 2. C-arylation reaction catalyzed by CuO-Nanoparticles under ligand free condition. 3A. An economical oxidation protocol for the conversion of secondary alcohols into ketones using heterogeneous nanocrystalline Titanium(IV) oxide as a sole catalyst. 3B. Transformation of amines to oximes using heterogeneous nano Crystalline Titanium (IV) oxide as a green catalyst. 4A. A new method for the synthesis of α -amino phosphonates via A²-P coupling using Cu-nanoparticles as heterogeneous catalyst. 4B. Synthesis of triazoles using mobilized heterogeneous Au-nanoparticles as catalyst. 5A. Mobilized gold nanoparticles as sole catalyst for the oxidation of secondary alcohols into ketones. 5B. Fe₃O₄ nanoparticles : a robust and magnetically recoverable catalyst for synthesis of β -amino carbonyl compounds via Mannich reaction.

108. BHASKARA NAND
Some Green Approaches for the Development of Novels Synthetic Methodologies and the Synthesis of Biologically Important Heterocycles.
 Supervisor : Prof. J M Khurana
 Th 18058

Abstract

This work presents some novel synthetic methods, which include (i) aqueous sodium hypochlorite mediated chemoselective oxidation of chalcogenides to monoxides and dioxides by microwave exposure, (ii) application of [bmin]BF₄ ionic liquid as green and rapid protocol for the synthesis of polyfunctionalized pyrano[2,3-c]pyrazoles, (iii) 1,8-diazabicyclo[5,4,0]undec-7-ene (DBU) catalysed efficient and green protocol for the synthesis dihydropyrano[c]chromenes, dihydropyrano[b]pyrans, 4H-benzo[h]chromenes, 4H-chromenes and tetrahydrocyclopenta[b]pyrans in aqueous medium, (iv) an efficient and convenient approach for the synthesis of novel 2-hydroxy-12-aryl-8,9,10,12-tetrahydrobenzo[a]xanthene-11-ones using pTSA in ethanol and (v) synthesis, spectral and crystal studies of antimalarial xanthene-chloroquinoline conjugates.

Contents

1. Aqueous sodium hypochlorite mediated chemoselective oxidation of chalcogenides to monoxides and dioxides by microwave exposure. 2. Rapid synthesis of polyfunctionalized Pyrano [2,3-c]pyrazoles via multi-component condensation in room temperature ionic liquids. 3. DBU : A highly efficient catalyst for one pot synthesis of substituted dihydropyrano[c]chromenes, 4H-benzo[h]chromenes and 4H-chromenes in aqueous medium. 4. An efficient and convenient approach for the synthesis of novel 2-Hydroxy-12-aryl-8,9,10,12-tetrahydrobenzo[a]xanthene-11-ones using pTSA in ethanol. 5. Synthesis, spectral and crystal studies of antimalarial xanthene-chloroquinoline conjugates. 6. Summary and conclusions.

109. BHATIA (Sumati)
Novel Synthesis of Sugar-PEG Based Polymers for Drug Delivery Application, Taxol Side Chain and Bioactive Dihydropyridine Analogs, and Biocatalytic Resolution Studies on Dihydropyrimidinones.
 Supervisor : Prof. Ashok K Prasad
 Th 18223

Abstract

It has exploited different reaction conditions using different molar ratios sodium meta-periodate and potassium permanganate as catalyst in different water miscible solvent systems like acetonitrile, tetrahydrofuran, acetone and dioxane as reaction

medium. To develop an inexpensive methodology for the oxidative cleavage of taxol side chain precursor using potassium permanganate and sodium meta-periodate as oxidizing agents in acetone-water as reaction medium. Further it has also done enzymatic resolution of biologically active racemic acylated DHPMz using Novozyme-435 (*Candida antarctica* lipase immobilized on polyacrylate, Lewatit).

Contents

1. Biocatalytic synthesis of novel Sugar-PEG based polymers for drug delivery applications. 2. Efficient and economical method development for the synthesis of side chain of taxol and its analogs. 3. Synthesis of rationally designed dihydropyridines and dihydropyrimidinones : Platelet anti-aggregation activity of dihydropyrimidinones. 4. Enzymatic stereoselective deacylation studies on dihydropyrimidinones.

110. DAVINDER PRASAD
Synthesis and Antibacterial Evaluation of 4-Thiazolidinones, Azoles and Azolo-Azine Conjugates.
 Supervisor : Dr. Mahendra Nath
 Th 18250

Abstract

Detailed synthesis strategy, characterization and in-vitro screening results of novel 4-thiazolidinones are presented. Synthetic procedure, characterization data and biological screening results have been discussed. Synthetic protocol, characterization and antibacterial screening results have been discussed.

Contents

1. Antibacterial Agents : An overview. 2. One-pot three-component synthesis and antibacterial evaluation of novel 2-Aryl-thiazolidin-4-one derivatives. 3. Synthesis of heteroarenes based [1,2,3]-Triazoles via click chemistry and their evaluation as antibacterial agents. 4. Synthesis, characterization and evaluation of 4-aminoquinoline-[1,2,3]-Triazole conjugates as antibacterial agents. 5. Synthesis and antibacterial evaluation of novel heteroarenes tethered dihydro[1,3]oxazines.

111. DHAND (Chetna)
Studies on Electrophoretically Deposited Nano-Structured Conducting Polyaniline Films for Application to Biosensors.
 Supervisors : Prof. Monika Datta and Dr. B D Malhotra
 Th 18071

Abstract

This work deals with the electrophoretic film fabrication of different PANI nano-structures including nano-patterned PANI, PANI nanospheres and PANI nanotubes onto ITO coated glass substrates. Electrophoretic technique has been applied for the first time to fabricate polyaniline-carbon nanotube composite with enhanced electrochemical characteristics. These electrophoretically deposited nano-structured PANI films have been utilized to immobilize desired enzymes [cholesterol oxidase (ChOx), lipase (LIP), glycerol dehydrogenase (GDH) via different immobilization methods [N-ethy-N²-(3-dimethylaminopropyl) carbodimide (EDC)-N-hydroxysuccinimide (NHS) chemistry or glutaraldehyde as cross-linker]. These prepared bioelectrodes have been explored for their biosensing characteristics pertained to cholesterol and triglyceride detection.

Contents

1. Introduction and literature survey. 2. Materials and characterization techniques. 3. Non-electrophoretically deposited Nano-structured conducting polyaniline film for cholesterol biosensor. 4. Electrophoretically deposited Nano-structured conducting polyaniline based matrices for cholesterol biosensor. 5. Electrophoretically deposited Nano-structured conducting polyaniline based matrices for triglyceride biosensor. 6. Summary and future prospects.

112. GAUR (Jitender)
Synthesis and Characterization of Complexes of Some Transition Elements with Nitrogen & Sulphur Containing Ligands.
 Supervisor : Dr. Raj Kishore Sharma
 Th 18221

Abstract

It describes the synthesis and characterization of complexes of Cu(II), Ni(II), Co(II), Zn(II), Ag(I), Rh(III), Pd(II) and Ru(III) with glyoxal dihydrazones (L_{1a}), dimine of glyoxal and ethylenediamine (L_{1b}) and their bis dithiocarbamates L_{2a} and L_{2b} respectively. It

also presents the biological activities of some of the synthesized complexes towards antifungal, antibacterial and anticancer activities against some widely spread fungi (*Rhizotonia solani*, *Rhizoctonia bataticola*), bacteria (*S. aureus*, *E. coli*, *B. subtilis*, *Pseudomonas*, Spp) and generally used cancer cell line (HeLa cell line). Copper complexes are also screened for catalytic activities such as oxidation of phenols and catechols by using molecular oxygen.

Contents

1. Introduction. 2. Experimental. 3. Characterization of ligands and their complexes. 4. Biological activities. 5. Catalytic activities. 6. Result and discussion. 6. Application of ligands : Synthesis of novel co-polymer of L1a and L2a for heterogeneous metal ions removal from water.

113. GHANTI (Epsita)
Studies on the Synthesis, Characterization and Properties of Ternary Phases in CuO/Cu₂O-Al₂O₃ System.
 Supervisor : Dr. R Nagarajan
 Th 18057

Abstract

The synthetic challenges in CuAl₂O₄ and CuAlO₂ preparation by altering the nature of the starting material thereby redefining the phase diagram has been undertaken. The basic principles of various analytical techniques such as FTIR, Raman, NMR, UV-Visible and DRS (Diffuse Reflectance Spectroscopy), TGA/DTA/DSC, Power X-ray diffraction, SEM (Scanning electron Microscopy), TEM, Elemental Analysis, BET Surface Area Measurement, Laser diffraction Scattering (LDS) have been extensively used for characterization of the compounds. The kinetics and the thermodynamics of conversion of CuAl₂O₄ + CuO to the nano sized CuAlO₂ phase from various precursor copper salts and aluminium salts by the solid state reactions are investigated.

Contents

1. Introduction. 2. Characterization techniques used for the present study. 3. Studies on the reactivity of different forms of bulk Al₂O₃ with CuO from various copper sources. 4. Synthesis and hydrolysis of heterobimetallic alkoxide, CuAl₂(OPr)₈ for CuAl₂O₄ spinel. 5. Synthesis and hydrolysis of heterobimetallic

β -diketonato alkoxide, $\text{CuAl}_2(\text{OPr})_4(\text{acac})_4$ for CuAl_2O_4 spinel. 6. Synthesis of metastable CuAlO_2 via ceramic method by evaluation of alternate precursors. Bibliography and appendix.

114. JAIN (Nidhi)
Novel Molecules Based on Trimethoxybenzenesulphonyl and Spiroindolyl Scaffold Possessing Lipophilic Character: Synthesis and Biological Activity & Study of Triterpenoids from Flowers and Fruits of Carissa Carandas.
 Supervisors : Prof. S C Jain
 Th 18067

Abstract

This work has synthesise molecule incorporating the structural features of both spiro indole and trimethoxy benzenesulphonyl group. The phytochemical investigation of some uninvestigated parts of medicinal plants, have been undertaken a detailed study of the chemical constituents of the flowers and the fruits of carissa carandas to isolate and characterize natural products.

Contents

1. Synthesis of novel 1,2,3-trimethoxy-5-(1-phenylsulphonylalkyl/alkenyl) benzene. 2. Synthesis of 1,2,3-trimethoxy-5-(1-phenylsulphonyl-7(Nheterocyclyl) heptyl) benzene. 3. Synthesis of 1'-(7-(phenylsulphonyl)-7-(3,4,5-trimethoxyphenyl)alkyl) spiro(1,3-dioxolane-2,3'-indoline)-2'ones. 4. Synthesis of 7-(phenylsulphonyl)-7-(3,4,5-trimethoxyphenyl) heptanal and its hydrazones, semicarbazones, thiosemicarbazones and oximes. 5. Synthesis of novel 1-(6-(N-heterocyclyl)hexyl)-3'-(2,3-dimethyl-5oxo-1-phenyl-3-pyrazolin-4-yl)spiro(2H-indol3,2'-thiazolidine)-2,4'diones. 6. Study of triterpenoids from flowers and fruits of carissa carandas. References and Summary.

115. KATHURIA (Abha)
Design and Synthesis of Oxygen and Nitrogen Containing Heterocyclic Compounds as Potent Anti-Platelet and Antimicrobial Agents.
 Supervisor : Prof. Sunil K Sharma
 Th 18073

Abstract

It has investigate the specificities of acetoxy derivatives of 7-aminocoumarins on CRTAase activity and also to delineate the structure activity relationship (SAR) with special reference

to the effect of N-acetyl amino group, the presence of alkyl group at C-3 position and the replacement of methyl group by trifluoromethyl group. It has observed that 7-N-acetylaminocoumarins are better substrate for CRTAase as compared to the acetoxy coumarin counterparts. The activity of 7-N-acetyl-amino-4-methylcoumarin is found to be even better than DAMC and MAMC which are so far considered to be best substrates for CRTAase. Also elucidated the action of CRTAase on a series of 8-acetoxy and 7-N-acetyl-amino quinolin-2-ones by studying their consequent effect on the enhancement of NO levels in platelets and inhibitory effect on ADP/Arachidonic acid (AA) induced platelet aggregation.

Contents

1. Design and synthesis of novel coumarins and quinolin-2-ones and evaluation of their Calreticulin Transacetylase activity. 2. Synthesis of benzopyrones and quinolin-2-ones as lead antimicrobial agents.

116. KUSHWAHA (Khushbu)
Studies on Azaphenothiazine Derived Pharmacophores & Synthesis of Triazolyl Derivatives of 2H-Chromen-2-One & Pyridine Using Click Chemistry.
 Supervisor : Prof. S C Jain
 Th 18052

Abstract

The synthesis is done with the formation of 3-azidopyridine obtained from 3-aminopyridine by first diazotizing the amine group and replacing it with azide. Synthesized azide is then reacted with propargyl bromide and secondary amines using CuI as catalyst in presence of water and triethylamines to yield the corresponding compound. It synthesized eight new compounds and characterized them on the basis of their complete detailed spectral data such as IR, ¹H NMR, ¹³CNMR and Mass. The newly synthesized compounds and intermediates are finally screened for their in vitro antibacterial and antifungal activity against various strains following cup-plate method against standard drugs Ciprofloxacin for bacteria and Miconazole for fungi.

Contents

1. Synthesis and X-ray structure of novel bis azaphenothiazines. 2. Synthesis of some aminoalkylated azaphenothiazines to discover a lead antimicrobial. 3. Synthesis of sulfoxide and

sulfonyl derivatives of azaphenothiazines. 4A. Synthesis of biologically active triazolyl 2H-chromen-2-ones using click chemistry. 4B. Synthesis of novel 7-O-(1,4-disubstituted-1H-1,2,3-triazolyl)4-methyl-2H-chromen-2-ones. 5. A green protocol for the one pot synthesis of triazolylpyridines.

117. LATA
Chemical Modification of 2, 4-Disubstituted Thiazoles in Search for a Bioactive Lead Molecule & Phytochemical Investigation of Momordica Dioica.
 Supervisor : Prof. S C Jain
 Th 18075

Abstract

This work has synthesized the molecule, 1H-indol-2,3-dione treated with 2-amino-4-(carboethoxymethyl)thiazole in the molar ratio in absolute ethanol to obtain hitherto unreported 3-hydroxyindole derivative which is fully characterized as 3-hydroxy-3-[2-amino-4-(carboethoxymethyl)thiazol-5-yl]-1H-indol-2-one. Twenty novel heterocycles are synthesized in good yields, and have been fully characterized on the basis of their detailed spectral interpretation and also by single crystal X-ray crystallographic studies in 3-hydroxy-1-methyl-3-[2-amino-4-(carboethoxymethyl)thiazol-5-yl]-1H-indol-2-one. The newly synthesized compounds are finally screened for their in vitro antibacterial and antifungal activity following cup-plate methods at 100 µg/ml against standard drugs Ciprofloxacin for bacteria and Micozole for fungi.

Contents

1. A novel method for the synthesis of Spiro[indole-pyran] by regioselective one-pot tandem reaction of 2-aminothiazole with indol-2, 3-dione. 2. Design and synthesis of novel triazolylthiazole of biological importance. 3. Synthesis of biologically active molecules by chemical modification of 2,4-disubstitutedthiazole. 4. A novel, one-pot, catalyst-free and economically efficient synthesis of 2, 4-disubstitutedthiazoles in water. 5. Phytochemical investigation of Momordica dioica.

118. MATHEW (Bijoy P)
Synthesis and Antimicrobial Evaluation of Dihydro[1,3] Oxazine Derivatives.
 Supervisor : Dr. Mahendra Nath
 Th 18249

Abstract

Describes the syntheses, biological and material significance of various dihydro-1,3-oxazine derivatives. Some of the synthesized molecules have been evaluated for antimicrobial efficacy and preliminary screening results are presented. The antimicrobial profile of some of the compounds have also been evaluated. The synthesis, characterization and the preliminary invitro antibacterial activity results are discussed.

Contents

1. Syntheses, biological and material significance of dihydro[1,3]oxazine derivatives : An overview. 2. Environmentally benign synthesis and antimicrobial activities of naphtho[e][1,3]oxazines. 3. Synthesis and antimicrobial efficacy of coumarin based dihydro[1,3]oxazine derivatives. 4. Synthesis, characterization and antibacterial evaluation of thiocoumarin based dihydro[1,3]oxazines.

119. NITIN KUMAR
Synthesis and Biological Evaluation of Tetraoxane and Curcumin Analogues.
Supervisor : Prof. Diwan S Rawat
Th 18222

Abstract

The emergence of drug resistance by P.Falciparum against conventional antimalarial drugs has put enormous pressure on public health so there is an urgent need to introduce new chemical entities that can overcome the problem of drug resistance. A number of synthetic peroxides have been synthesized and screened for antimalarial activity, and among them tetraoxane class of compound have shown great promises. Some of these compounds have shown impressive in vitro antimalarial activity, antiproliferative and antituberculosis activity.

Contents

1. Tetraoxanes : Synthetic and medicinal chemistry perspective. 2. Synthesis, characterization and in vitro antimalarial activity evaluation of symmetrical and asymmetrical tetraoxanes. 3. synthesis, characterization and in vitro antimalarial activity of tetraoxane-amine/amide conjugates. 4. Tetraoxane-triazine/piperidone hybrids as potential antimalarial agents. 5.

Synthesis, characterization and in vitro anticancer activity of curcumin analogues and curcumin-triazoles conjugates.

120. PONNAN (Prija)
Computational Studies to Elucidate the Structure and Function of Acetoxy Drug : Protein Transacetylase Mediating Protein Acetylation Independent of Acetyl CoA.
Supervisors : Prof. R C Rastogi and Prof. H G Raj
Th 18053

Abstract

The present thesis studied the protein acetyltransferase function of human CR and glutamine synthetase of *M. tuberculosis* using computational biology and chemoinformatics methods. The computational approach to establish the relationship between a chemical structure and its biological activity and predicted the functional consequences of protein acetylation has been used. The docking studies gave evidence to the interaction of PA with TAase and subsequently assisted in elucidating the mechanism of action of TAase. The role of post translational modifications in nNOS and rGST by way of acetylation catalyzed by TAase utilizing PA, as analyzed by molecular simulation studies revealed that autoacetylation of CR triggers protein-protein interactions and modulates their substrate binding capacity. QSAR and ADMET analysis provided design strategies for the development of PA as candidate antimycobacterial drugs.

Contents

1. Introduction. 2. Application of QSAR and molecular modeling to delineate calreticulin mediated protein acetylation utilizing polyphenolic acetate as the acetyl group donor. 3. Computational studies to investigate the mechanism of CRTAase catalyzed acetylation of receptor proteins *Schistosoma japonicum* GST and rat neuronal NOS (nNOS). 4. 2D-QSAR, Docking Studies and in silico ADME prediction on polyphenolic acetates as substrates for protein acetyltransferase function of Glutamine synthetase of mycobacterium tuberculosis.

121. POONAM
Synthesis of Selected Azaporphyrinoids and Their Application in Catalysis, Supramolecular and Material Chemistry.
Supervisor : Prof. S M S Chauhan
Th 18062

Abstract

It has syntheses diferent functional porphyranooids and subporphyranooids and their applications in the field of catalysis, supramolecular and material chemistry. The structure of metal phthalocyanines obeys both the requirements. Self-assembled growth of carbon nanotubes by pyrolysis of metallophthalocyanines has been performed at different temperatures. The structure of CNTs formed is confiemed by UV-vis, TEM (transmission electron microscopy) and Raman spectroscopy.

Contents

1. Synthesis of functional metallophthalocyanines and their application as a ctalyst in the reduction of flavones adn isoflavones. 2. Synthesis of selected metallophthalocyanines, and their application in oxidative and reductive transformation of atrazine. 3. Synthesis of boron subphthalocyanines and their interaction with anions in different reaction condition. 4. Green synthesis of metalloporphyrazines and its application in supramolecular chemistry. 5. Synthesis of functional phthalocyanines and their reaction with graphene oxide and related carbon nanostructures.

122. RAJESH KUMAR
Theoretical Models for Diffusion, Reaction and Adsorption Admittance of Rough Electrodes.
 Supervisor : Prof. Rama Kant
 Th 18069

Abstract

It has developed a mathematical model of first order homogeneous chemical reaction coupled with electron transfer on random corrugated finite fractal electrode. Method of Green's function is used to obtain second-order perturbation expressions for concentration, admittance density and measured admittance for an arbitrary corrugated electrode. Analyzed the problem of impedance for a diffusion controlled charge transfer process across an irregular interface and developed a theoretical model for quasi-reversible charge transfer admittance on a random corrugated finite fractal electrode.

Contents

1. Introduction to Electrochemical response of disordered

electrodes: theoretical aspects. 2. Theory of gerischer admittance of rough electrode : Deterministic, stochastic and realistic fractal roughness. 3. Theory of gerischer admittance of corrugated electrode : Stochastic and finite fractals. 4. Theory of anomalous warburg admittance of realistic self-affine fractal electrode. 5. Theory of anomalous warburg admittance of corrugated self affine fractal electrode. 6. Theory of diffusion limited adsorption admittance of rough electrode : Deterministic, stochastic and realistic fractal roughness. 7. Theory for admittance of electrochemical reaction with adsorption on corrugated electrode : Stochastic and finite fractal models. 8. Theory of quasi-reversible charge transfer admittance on realistic self-affine fractal electrode. 9. Theory of partial-diffusion limited charges transfer admittance of random corrugated fractal electrode. 10. Summary and conclusions.

123. RAJNI
Electrochemical Investigation of the Corrosion Behavior of Mild Steel in 0.5 M H₂SO₄ in the Presence of Hetrocyclic N-substituted Pyridine Compounds.
 Supervisor : Dr. Gurmeet Singh
 Th 18056

Abstract

This work has determine the inhibition efficiencies of the selected inhibitor under chosen concentration and temperatures conditions and investigate the mechasism and mode of inhibition process by using galvanostatic polarization technique at different temperatures, temperature kinetics studies heats of adsorption of the corrosion process, impedance measurements at 308k, potentiostatic polarization study at 298k, surface characterization by scanning electron microscopy (SEM), atomic force microscopy (AFM), and quantum chemical calculations.

Contents

1. Introduction. 2. Literature Survey. 3. Experimental techniques. 4. Galvanostatic polarization studies. 5. Temperature kinetics studies. 6. Potentiostatic polarization studies. 7. Electrochemical impedance spectroscopy. 8 Scanning electron microscopy. 9. Atomic force microscopy. 10. Quantum chemical calculation. 11. Conclusions.

124. ROY (Kapil)
Structural Polymorphism at Locus Control Region (LCR) of β -Globin and Human Growth Hormone Gene Cluster.
 Supervisor : Prof. Shrikant Kukreti
 Th 18248

Abstract

An integrative approach has been adopted to address the issue of the structural and functional aspects of polymorphism. Various biochemical and biophysical techniques like UV-Visible absorption spectroscopy, UV-thermal denaturation, gel electrophoresis and circular dichroism spectroscopy has been carried out exhaustively to study the structural polymorphism in LCR to understand the possible mechanism of recognition of transcription factors, during gene transcription.

Contents

1. Introduction and review of literature. 2. Experimental. 3. Bioinformatics : Analyzing DNA sequences. 4. Biophysical and biochemical analysis of $(AT)_xN_{12}(AT)_y$ motif in the LCR of β -Globin gene. 5. Biophysical and biochemical analysis of deoxyoligonucleotides of the LCR of human growth hormone gene cluster. 6. Conclusions and bibliography.

125. RUCHI
Synthesis, Spectral and Antimicrobial Studies on Transition Metal Complexes of some Schiff's Base Ligands.
 Supervisor : Dr. Sulekh Chandra
 Th 18054

Abstract

In this work the synthesis and characterization of Manganese (II), Cobalt(II), Nickel(II) and Copper(II) complexes with four macrocyclic ligands and their use as antimicrobial compounds have been done. The synthesis and characterization of four ligands; L_1, L_2, L_3 and L_4 which are prepared by 2+2 condensation of precursor molecule have been done. The ligands have been characterized by elemental analysis, IR, mass and 1H NMR. The antimicrobial activity of macrocyclic ligands L_1, L_2, L_3 and L_4 and their complexes such as $MnCl_2, CoCl_2, NiCl_2$ and $CuCl_2$ for antifungal studies and their complexes such as $Mn(CH_3COO)_2, Co(CH_3COO)_2, Ni(CH_3COO)_2$ and $Cu(CH_3COO)_2$ for antibacterial studies. The antifungal and antibacterial activities are carried out using food poison and dual culture methods respectively.

Contents

1. Introduction. 2. Manganese(II),3d⁵. 3. Cobalt(II),3d⁷. 4. Nickel(II), 3d⁸. 5. Copper(II),3d⁹. 6. Antimicrobial activities of transition metal complexes. References and Summary.

126. SARAH JALAL

Design and Synthesis of Novel Pyridones and Benzopyran-2-ones as Potential Bio-active Compounds & Synthesis of Glycerol Based Mixed Esters and Dendrimer Building Blocks.

Supervisor : Prof. Sunil K Sharma

Th 18063

Abstract

It has studied the synthesis of novel 2-pyridone derivatives as potential antimicrobial agents, chemo-enzymatic of glycerol based mixed esters and dendrimer building blocks and benzopyran-2-ones as potential bio-active agents. 2-Pyridones are important heterocycles with great applicability in medicinal chemistry and this core structure is found in compounds with various biological/medicinal applications. 2-Pyridones have relatively simple structures and received attention as antimicrobial and antiviral. The antimicrobial activity of 2-pyridones has been evaluated against the fungal strains *Aspergillus fumigatus*, *Aspergillus flavus*, *Aspergillus niger* and *Candida albicans*. The anti-bacterial activity of 2-pyridones is also evaluated against the bacterial strains of *Streptococcus epidermidis*, *Streptococcus aureus* and *Pseudomonas aeruginosa*.

Contents

1. Synthesis of novel 2-pyridone derivatives as potential antimicrobial agents. 2. Chemo-enzymatic synthesis of glycerol based mixed esters and dendrimer building blocks. 3. Synthesis of benzopyran-2-ones as potential bio-active agents.

127. SHARMA (Raman Kumar)

Synthesis, Src Kinase, Anti-cancer and Platelet Aggregation Inhibition Activities of O-Aryl Glycosides, Chromonyldihydropyrimidinones and Aminocoumarin Analogs.

Supervisor : Prof. Ashok K Prasad

Th 18066

Abstract

The synthesis of O-aryl α,β -D-ribofuranosides and highly efficient

lipase-mediated separation of the α - and β -anomers using one of the acetoxy functions of peracetylated O-aryl α -D-ribofuranoside as handle has been done. The structure of synthesized compounds are unambiguously established by analysis of their spectral data (^1H -, ^{13}C NMR, IR, HRMS spectroscopy). Synthesized b-and a-O-arylribofuranosides are evaluated as Src kinase inhibitors.

Contents

1. Chemo-enzymatic synthesis, Sre Kinase inhibition and anti-cancer activity of O-Aryl glycosides. 2. Synthesis and antiplatelet activity of novel chromonyldihydropyrimidinones. 3A. Synthesis, Src Kinase inhibition and anti-cancer activity of novel 7-Aminocoumarin analogs. 3B. Synthesis, Src Kinase inhibition and anti-cancer activity of 3-Amino-2-hydroxypropyl analogs of 7-Aminocoumarins.
128. SHARMA (Satyasheel)
Peripheral Functionalization of meso-Tetraphenylporphyrins for the Synthesis of Novel Benzazolo-, Quinoxalino-and Dihydro-1,3-Oxazinoporphyrins.
 Supervisor : Dr. Mahendra Nath
 Th 18072

Abstract

Porphyrins are one of the most attractive class of natural products, often considered as the "pigments of life". They represent a ubiquitous class of naturally occurring heterocyclic compounds with many important biological representative including chlorophyll, prosthetic groups of various metalloenzymes/ proteins such as hemoglobin, myoglobin cytochromes, Vitamin B₁₂. Modifications at β -positions have been carried out with various functional groups including heteroaryl systems to generate several porphyrin molecules. The effort have also been successful to synthesize β,β' -fused imidazoloporphyrins and β -substituted azoloporphyrins bearing biologically important pyrazole and isoxazole ring systems. It has synthesized two new precursors, 5-(3,4-diaminophenyl)-10,15,20-triphenylporphyrin and 5-(3-amino-4-hydroxyphenyl)-10,15,20-triphenylporphyrin through regioselective introduction and functionalization of the substituents on a meso-phenyl group of the 5,10,15,20tetraphenylporphyrin. The synthesized compounds are characterized spectroscopically and their preliminary photophysical properties have been investigated.

1. An account on the synthesis and efficient peripheral functionalization of meso-tetraarylporphyrins. 2. Synthesis and spectroscopic characterization of novel nickler(II) 2-benzazolo-5,10,15,20-tetrahyenylporphyrins. 3. Synthesis and photophysical studies of novel meso-substituted benzazolyltriphenylporphyrins and β ,meso-benzoxazolyl-bridged porphyrin dyads. Synthesis and optical properties of meso-phenyl-fused quinoxalinoporphyrins. 5. Synthesis of meso-substituted dihydro-1,3-oxazino-porphyrins.

129. SINGH (Jyoti)
Theoretical Studies of CdSe Quantum Dots and their Interactions.
 Supervisor : Rita Kakkar
 Th 18068

Abstract

This deals with computational study on the structural and electronic properties of stoichiometric II-VI semiconduct quantum dots, particularly CdSe quantum dots, and their interactions. Also studied the interaction of the CdSe quantum dots with two surfactants, namely benzoic acid and benzoate and also the changes caused by installing a para substituent with no affinity for the nanocrystal quantum dots on the surfactant, keeping in the end functional group intact. The eight substituents used for both the mentioned cases comprise four electron donating groups (-OCH₃, -CH₃, -NH₂, -OH) and four electron withdrawing groups (-NO₂, -CN, -F, -Cl).

Contents

1. Quantum Dots - A brief introduction. 2. Computational techniques. 3. A DFT study of size dependent structural and electronic properties of stoichiometric II-VI quantum dots. 4. Transition metal doped CdSe quantum dots. 5. Interaction of CdSe quantum dots with para substituted benzoic acid and para substituted benzoate surfactants. 6. CdSe quantum dots as a sensor for detection of various gas molecules. 7. Conclusion & perspectives.

130. SINGH (Sukhev)
Synthesis of Coumarin-based Thiazines and Chalcones, and Fluoropicolates and their Dipeptides.
 Supervisor : Prof. Ashok K Prasad
 Th 18246

Abstract

It has reported greener and environmentally friendly microwave assisted synthesis of 7-methoxy-/7,8-dimethoxy-4-(1'-aryl-1'-oxoprop-2'-en-3'-yl)coumarins; a mimic of chalcone in which ring **B** is coumarin moiety instead of an aryl moiety. The synthesis of both diastereomers of 5-fluoropipercolates; the methodology employed relies on the sequence, electrophilic fluoromethoxylation (or fluorohydroxylation) by fluorinating agent selectfluor, and subsequent reductive demethoxylation (dehydroxylation) of pipercolate-based enecarbamates have also been discussed.

Contents

1(A). Synthesis and anti-inflammatory activity of novel Alkyl (\pm)-2-Amino-6-(coumarin-4'-yl)-4-alkyl-1,3-thiazin-5-carboxylates. 1(B). Synthesis of 7-Methoxy-/7,8-Dimethoxy-4-(1'-aryl-1'-oxoprop-2'-en-3'-yl)coumarins. 2 (A). Synthesis and characterization of fluoropipercolates. 2(B). Synthesis and conformational analysis of dipeptides involving fluoropipercolates and Boc-Glycine.

131. SINGH (Taruna)

Synthesis, Characterization and Reactivity Studies of Ruthenium(II) and Palladium (II) Complexes of N,N',N''-Triarylguanidines and N,N'-Diaryl Thiourea.

Supervisor : Dr. N Thirupathi

Th 18070

Abstract

This has undertaken the reactivity studies of N,N',N''-triaryl guanidines and N,N'-diaryl thiourea with palladium(II) and ruthenium(II) salts/presursors. New compounds synthesized in the present investigation have been characterized by various spectroscopic data. In addition, selected compounds have also been characterized by single crystal X-ray diffraction study.

Contents

1. Introduction. 2. Results and discussion. 3. Experimental. References. Appeneix.

132. SUDERSHAN KUMAR
Electrochemical Study of Polyurethane Based ABA Type amphiphilic Tri-Block Copolymers as Corrosion Inhibitors for Mil Steel in Acidic Medium.
 Supervisor : Prof. Gurmeet Singh
 Th 18247

Abstract

It has found some copolymer based cheap and environmentally safe substances that could be used for inhibiting the corrosion of mild steel. The use of such substances will achieve simultaneously, the economic and environmental goals. Some copolymer based compounds like PANIPAAm-PU, PNVP-PU, PTBA-PU, and PDMAEMA-PU are used as corrosion inhibitors for mild steel surface in sulphuric acid medium at different temperatures. These compounds are analyzed as corrosion inhibitors by carrying out with the help of following techniques : Galvanostatic polarization studies, Temperature kinetic studies, Electrochemical impedance spectroscopy, Potentiostatic polarization studies, Scanning electron microscopy studies, Atomic force microscopy and Quantum chemical analysis.

Contents

1. Introduction. 2. Literature survey. 3. Synthesis and characterization of the corrosion inhibitors. 4. Experimental procedure. 5. Galvanostatic polarization studies. 6. Temperature kinetics. 7. Potentiostatic polarization studies. 8. electrochemical impedance spectroscopy. 9. Scanning electron microscopy. 10. Atomic force microscopy. 11. Quantum chemical analysis. 12. Conclusions.

133. TYAGI (Neetu)
Studies on the Synthesis Structure and Photophysical Properties of KMF_3 ($M = Mg, Mn, Co, Ni, Cu$), $KZnF_3$, $KLaF_4$, and K_3VF_6 .
 Supervisor : Dr. R Nagarajan
 Th 18076

Abstract

This work describes the synthesis and characterization of a number of fluorocomplexes comprising of a series of KMF_3 compounds (with $M^{II} = Mg, Mn, Co, Ni, Cu$), $KZnF_3$, K_3VF_6 and $KLaF_4$ possessing cubic and disordered perovskite, cryolite, elpasolite and calcium fluorite type structures. The compounds

are structurally characterized by powder X-ray diffraction and transmission electron microscopy. The transmission electron micrograph of KCuF_3 showed the tetragonal lattice of the unit cell. The absorption spectra of the powder samples are collected using UV - Visible diffuse reflectance spectroscopy.

Contents

1. Introduction. 2. Characterization techniques. 3. Synthesis, properties and applications of KMF_3 ($M^{11} = \text{Mg, Mn, Co, Ni, Cu}$). 4. Synthesis of KZnF_3 nano-structures and optical properties characterization. 5. Synthesis of K_3VF_6 using vanadium (III) precursor and investigation of its optical and magnetic properties; preparation and properties of $\text{K}_3\text{V}_{0.7}\text{Zn}_{0.3}\text{F}_6$. 6. Synthesis of KLaF_4 : (Er & Mn) nanophosphors & their upconversion and downconversion properties.

134. TYAGI (Nidhi)
Synthesis and Spectral Studies of Iron(III), Manganese(II & III) and Copper(II) Complexes with Multidentate Benzimidazolyl Based Ligands and their Use as Catalysts for Some Organic Transformations.

Supervisor : Prof. Pavan Mathur
 Th 18074

Abstract

This work has synthesised and characterized Iron (III), Manganese(II), Manganese (III) and Copper (II) complexes with multidentate benzimidazolyl based ligands. Imine-N atom of benzimidazole is similar to the imidazole nitrogen of the histidine is known to be the coordinating atom in several iron, manganese and copper metalloenzymes. Benzimidazoles are therefore good mimics of Histidines; some of the ligands also have a amide coordination site besides benzimidazole groups. The metal ions stabilize, destabilize or modulate biological molecules by introducing conformation changes and by creating centers of activity in the bio-macromolecule.

Contents

1. Introduction. 2. Principles of techniques utilized in identification of ligands & their metal complexes and synthesis of ligands. 3. Synthesis, spectral and electrochemical studies of iron (III), manganese (II), manganese (III) and copper (II) complexes. 4. Studies of some iron (III) complexes as catalyst

for oxidation of 2-aminophenol & 1,2-phenylenediamine, catalytic transformation of 1,2-phenylenediamine to alkylated benzimidazoles and interaction with a polyhydroxy catechol like catechin. 5. Studies of some Mn(II) & Mn(III) complexes as catalyst for the oxidation of 3,5-ditert-butylcatechol and oxidation of alcohols to aldehydes/acids using Cu(II) complexes as catalyst.

135. UMESH KUMAR
Synthesis and Characterization of Nanostructured Semiconducting Materials and Composites.

Supervisors : Prof. Rita Kakkar and Dr S T Lakshmikummar
 Th 18055

Abstract

In the present work, the method pioneered by Murray, and modified by Peng, has been used to prepare Cadmium selenide (CdSe) nanoparticles of high quality. In addition, this method is further modified, using safer, cheaper and easily available oleic acid in place of toxic trioctyl phosphine oxide to make this synthesis greener. The synthesis of lead selenide and core-shell CdSe-ZnSe quantum dots has been carried out using TOP/TOPO and TOP/Oleic acid as capping agent. The optical, structural and morphological properties of the CdSe, Pbse and CdSe-ZnSe nanoparticles have been studied using various characterization techniques : X-Ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Transmission Electron Microscopy (TEM), Photoluminescence (PL), UV-VIS spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR) and Energy Dispersive X-ray analysis (EDX) measurements.

Contents

1. Introduction. 2. Experimental techniques. 3. Synthesis and optimization of cadmium selenide (CdSe QD's) and surface modification. 4. Photostability studies of CdSe/Polymernanocomposites: Application of CdSe QD's. 5. Synthesis and characterization of PbSe QD's and their photovoltaic applications. 6. Towards greener nanosynthesis of Core-shell CdSe-ZnSe quantum dots.