

CHAPTER 10

CHEMISTRY

Doctoral Theses

089. AGASTI (Nityananda)
Preparation and Characterization of Silver Nanoparticles.
Supervisors : Prof. N. K. Kaushik and Prof. A. N. Maitra
Th 16281

Abstract

This has produced silver nanoparticles with various stabilizing agents like myristic acid, stearic acid, octyl amine, hexadecyl amine and glycine and formulate each synthetic route at ambient reaction conditions and to avoid harsh reaction conditions. Characterize silver nanoparticle synthesized by several investigative tools like UV-Vis, FTIR, XRD, ¹H NMR, Fluorescence, TEM, TGA and DTA, the effect of various reaction parameters like pH of the medium, concentration of both precursor and reducing agent on synthetic routes, the interaction pattern of silver nanoparticles with biomolecules like amino acids and nucleic acid base pairs, the chemical sensing behavior of silver nanoparticles towards heavy metals like mercury. It has synthesized also Ag-Cu alloy nanoparticles with myristic acid as stabilizing agent and to study their optical properties.

Contents

1. Introduction. 2. Experimental techniques. 3. Synthesis and characterization of glycine stabilized silver nanoparticles. 4. Synthesis and characterization of silver nanoparticles stabilized by myristic acid. 5. Synthesis and characterization of silver nanoparticles stabilized by stearic acid. 6. Synthesis and characterization of silver nanoparticles stabilized by octyl amine. 7. Synthesis and characterization of ultrafine silver dusts. Appendices.

090. ATHEYAYA (Himanshu)
Design, Synthesis and Characterization of Modified Tetraoxans and Tetraoxane-Aminoquinolines as Antimalarial Agents.
Supervisor : Dr. Diwan S. Rawat
Th 16287

Abstract

Describes the geographical and economical incidence, life cycle and various treatment methods and control (traditional and modern day treatment) of malaria. Identifies various drug targets such as (cell cycle, metabolic pathways, mitochondrial targets, cytosolic targets, food vacuole targets and membrane targets. Antimalarials drugs, their classification and more of action is also discussed. Deals with the synthesis and characterization of symmetrical tetraoxanes. Describes the tetraoxane-aminoquinoline conjugates. Reveals that chloroquine exhibit potent activity against : HIV-1/AIDS and has shown great promise against chikungunya fever.

Contents

1. Malaria : An overview. 2. Synthesis, characterization, solid state thermal stability and antimalarial activity of symmetrically substituted tetraoxanes. 3. Synthesis, characterization and antimalarial activity of nitrogen containing tetraoxanes. 5. Synthesis and characterization of chloroquinoline-imine derivatives and chloroquinoline-triazole conjugates. Summary.

091. BRAJESH KUMAR

Design and Synthesis of Bioactive Peptides.

Supervisor : Dr. Satish Kumar Awasthi

Th 16282

Abstract

It Studies the design of several synthetic tryptophans rich cationic hexapeptides and synthesized on solid support using Fmoc Chemistry. A general schematic representation of sequence of hexapeptide is Ac-RRWWKX-NH₂ in which X are different amino acids (like arginine, lysine, tryptophan, histidine, asparagine, aspartic acid, tyrosine, glutamine, serine, threonine, alanine, glycine, leucine, and phenylalanine). All these peptides were synthesized by Fmoc Chemistry on Rink Amide MBHA resin. The crude peptides were purified by Sephadex G10 and analyzed by mass spectrometry.

Contents

1. Design, synthesis and characterization of antimicrobial peptides. 2. Design, synthesis and characterization of nucleobase tripeptide conjugates. 3. Design, synthesis and characterization of desotamide analogs.

092. CHAVHAN (Pandurang Maruti)
Synthesis and Characterization of Metal Oxide Thin Films by SOL-GEL Process.
 Supervisors : Prof. N. K. Kaushik and Dr. R. K. Sharma
Th 16265

Abstract

Attempts to synthesize new transparent conducting thin films by a low temperature sol-gel process. The primary objectives of the present work are the synthesis of multicomponent metal oxide thin films and mixed multicomponent oxide thin films by low temperature sol-gel route. The aim of this thesis is the development of sol-gel processing techniques to produce a transparent conducting multicomponent oxide (TCMO) thin films materials suitable for device fabrication.

Contents

1. Introduction. 2. Thin films deposition and characterization techniques. 3. Synthesis and characterization of $12\text{CaO}\cdot 7\text{Al}_2\text{O}_3$ [C12A7] thin films by Sol-Gel process. 4. Synthesis and characterization of $12\text{SrO}\cdot 7\text{Al}_2\text{O}_3$ [S12A7] thin film by Sol-Gel process. 5. Synthesis and characterization of $12\text{BaO}\cdot 7\text{Al}_2\text{O}_3$ [B12A7] thin films by Sol-Gel process. 6. Synthesis and characterization of $6\text{CaO}\cdot 6\text{SrO}\cdot 7\text{Al}_2\text{O}_3$ and $6\text{SrO}\cdot 7\text{Al}_2\text{O}_3$ thin films by Sol-Gel process. 7. Summary and conclusion.

093. DEEPA
Development of Novel Radiopharmaceuticals : Synthesis, Characterization and their Biological Evaluation for Targeted Imaging and Therapy.
 Supervisors : Dr. Harish Chandra and Dr. Anil Kumar Mishra
Th 16544

Abstract

Focuses on the development of novel radiopharmaceuticals for the diagnosis/therapy of tumor. This includes synthesis of promising poly dentate BFCs, their conjugation with various bio-molecules, biological evaluation of BFCs-conjugated biololecules, optimization of radiolabeling methods and to perform SPECT studies on tumor-bearing mic/normal rabbit using a dedicated, high-resolution/high-sensitivity SPECT camera. In addition in vitro and in vivo studies were performed to investigate the distribution patterns and confirm specificity of the

radiopharmaceuticals in targeted tissues and normal tissues and organs of mice.

Contents

1. Introduction and objectives. 2. Synthesis, characterization and biological evaluation of indole and benzimidazole derivatives. 3. Design, synthesis and characterization of DTPA-bis (Amide) derivatives. 4. Synthesis of bifunctional chelating agents and their conjugation with biomolecules. Summary.

094. DHAWAN (Ashish)
Synthesis of Novel Bioactive Chromans, β -Amino Alcohols and Polymeric Antioxidants.
 Supervisor : Prof. V. S. Parmar
Th 16286

Abstract

In this the synthesis of twenty-two novel chroman derivatives has been achieved and the effect of chroman derivatives has been examined on the modulation of cytokine-induced expression of ICAM-1 in human endothelial cells. The chroman derivatives, synthesized are found to be potent inhibitors of TNF- α induced expression of ICAM-1 on human endothelial cells. The structure-activity studies indicated that the nature of functionality (Ester or amide) and the nature and positions of substituent(s) in the aromatic ring have significant effect on the inhibition of TNF- α induced expression of ICAM-1 on endothelial cells.

Contents

1. Synthesis and anti-inflammatory activity of novel chromans. 2. Synthesis and anti-microbial activity of novel β -aminoalcohols. 3. Design, synthesis and evaluation of novel polymeric antioxidants. Summary.

095. GARG (Bhaskar)
Synthesis and Anion Binding of Calix[4]pyrroles and Related Macrocycles.
 Supervisor : Prof. S. M. S. Chauhan
Th 16276

Abstract

This work has studied the synthesis of calix[4]pyrroles and

N-confused calix[4]pyrroles and their applications in anion binding, Functional chromophoric calix[4]pyrroles by reaction of calix[4]pyrrole with electrophiles and their applications in anion binding and anion sensing, Calix[4]pyrroles with reduced symmetry and non covalent interactions, Metallo-calix[4]pyrroles and their applications in biomimetic oxidation of hydroxymethylfurfural and related compounds, Heteroatom-bridged calix[4]pyrroles and related spectral characterization and reactions of macrocycles, Chromogenic urea and thiourea and anion interactions in different reaction conditions.

Contents

1. Synthesis of calix[4]pyrroles and N-confused calix[4]pyrroles and their applications in anion binding. 2. Synthesis of functional chromophoric calix[4]pyrroles by reaction of calix[4]pyrrole with electrophiles and their applications in anion binding and anion sensing. 3. Synthesis of calix[4]pyrroles with reduced symmetry and non covalent interactions. 4. Synthesis of metallo-calix[4]pyrroles and their applications in biomimetic oxidation of hydroxymethylfurfural and related compounds. 5. (A) Synthesis of heteroatom-bridged calix[4]pyrroles and related spectral characterization and reactions of macrocycles. (B) Synthesis of chromogenic urea and thiourea and anion interactions in different reaction conditions.

096. KAUSHIK (Shikha)
Formation and Stabilization of DNA Triple Helices.
 Supervisor : Dr. Shrikant Kukreti
Th 16261

Abstract

The structure of a pyrimidine motif triplex formed inter- and intramolecularly at the 12-bp duplex target present in the BOLE1 gene of human herpes virus-4 (HH4) genome using a designed pyrimidine their strand under varied solution conditions, the structure of a pyrimidine motif triplex (inter-and intramolecular) containing a naturally occurring highly conserved 11-bp long oligopurine oligopyrimidine DNA sequence found in human c-jun protooncogene, the purine motif triplex formation (inter-as well as intramolecular), containing human c-jun protooncogene target, the solution status of triplex binding ligands (coralyne, sanguinarine and berberine and the effect of triplex binding ligands on duplex and triplex stability in solution has been studied.

Contents

1. Introduction. 2. Experimental. 3. Structural status of pyrimidine motif (Parallel) triplexes. 4. Structural status of purine motif (Antiparallel) triplexes. 5. Stabilization of parallel/antiparallel DNA triple helices. 6. Conclusions. Bibliography.

097. KUNDRA (Hema)
Synthesis and Characterization of Value Added Products from Fly Ash.
Supervisor : Prof. Monika Datta
Th 16293

Abstract

Studied the developing a cost effective, synthetic methodology based on hydrothermal method of synthesis for the conversion of a fly ash into a technologically important and a value added single product for better and useful utilization of fly ash. The chemical and physical nature of any reaction product is highly dependent on the reaction parameters. In order to develop a novel method for the conversion of fly ash into a value added product/s, product performance has been monitored as a function of reaction parameters.

Contents

1. Introduction. 2. Literature survey : Methodologies for the conversion of fly ash into zeolite/s. 3. Experimental. 4. Result and discussion. 5. Conclusion. 6. Future prospects and summary.

098. OJHA (Himanshu)
Design and Biological Evaluation of Some 2, 4, 6 Triazine Antimalarials : A Combined Computational and Experimental Study.
Supervisor : Prof. Rita Kakkar
Th 16278

Abstract

This has studied the s-triazine derivatives chemistry at the molecular level by Quantitative structure-activity relationship (QSAR). The chemical structure is quantitatively correlated with a well defined activity such as biological activity or chemical reactivity. The QSAR is the paradox of structure activity relationship by employing the finite amount of data.

Contents

1. Introduction. 2. Qsar and drug design. 3. QSAR studies of 2, 4, 6-trisubstituted-1,3,5-triazine derivatives. 3. QSAR studies of 2, 4, 6-trisubstituted-1,3,5-triazine derivatives. 4. Synthesis and characterization of the designed triazine derivatives. 5. Density functional calculations on the synthesized triazine derivatives. 6. Evaluation of biological activity of the synthesized triazine compounds. 7. Conclusions & Perspectives. Bibliography and appendix.

099. MALHOTRA (Shashwat)
Synthesis of Novel, Bioactive Spiro-(Indoline-isoxazolidines) and Isatin Derivatives, and Biocatalytic Transesterification Reactions on Polyhydroxy Compounds.
 Supervisor : Prof. V. S. Parmar
Th 16288

Abstract

It studies the regioselective synthesis of novel esters of glycerol, G1 generation analogues of glycerol and related compounds by biocatalytic transesterification using B-Boc-glycine 4-nitrophenyl ester as the acylating reagent by carrying out the lipozyme-catalyzed transesterification of glycerol in dioxane using B-Boc-glycine 4-nitrophenyl ester as the acylating agent at two different temperatures to afford mono- and di-esterified products.

Contents

1. Synthesis and anti-inflammatory activity of novel, bioactive spiro (indoline-Isoxazolidines). 2. Synthesis and anti-inflammatory activity of novel isatin derivatives. 3. Biocatalytic transesterification reactions on polyhydroxy compounds. Summary.

100. MAMGAIN (Ritu)
Synthesis and Characterization of Biologically Relevant Nitrogen and Oxygen Heterocycles.
 Supervisor : Dr. Diwan S. Rawat
Th 16264

Abstract

It deals with the development of some novel antimicrobial agents by synthesizing new nitrogen, sulphur and coumarin conjugate derivatives and evaluated their in vitro antibacterial, antifungal activities.

1. Synthesis and antimicrobial activity evaluation of substituted coumarins and coumarin-triazole conjugates. 2. Synthesis and antimicrobial activity evaluation of nitrogen heterocycles related to theophylline and triazoles. 3. Synthesis and antimalarial activity of tetraoxane and 4-amino-quinoline derivatives. 4. (A) DBU-catalyzed three-component one pot synthesis of highly functionalized pyridines in aqueous ethanol. (B) Convenient synthesis of 1,8-dioxo-dodecahydroxanthones. Summary.
101. MOHAPATRA (Subash Chandra)
Synthesis and Characterization of Some Manganese (II) and Copper (II) Metal Ion Complexes of N,N'-bis(2-methyl benzimidazolyl)-2,2'-oxy Diethanamide, N,N'-bis(2-methyl benzimidazolyl) Pentane Diamide and its N-octyl Derivative.
 Supervisor : Prof. Pavan Mathur
Th 16270

Abstract

Gives a brief review about the copper and manganese containing enzymes. Outlines the basic principle and brief instrumentation of the various techniques utilized to study the manganese (II) and copper (II) complex compounds. Also describes synthesis, spectral and structural characterization of the multidentate benzimidazole-diamides (GBOA, GBGA, O-GBGA) utilized for the complexation with Mn(II) and Cu(II) metal ions. Manganese(II) complexes have been synthesized by utilizing bis-benzimidazole diamide ligands (GBGA and GBOA) and characterized by their analytical Data, UV, IR, X-ray crystallography, EPR and Cyclic voltammetry. Copper(II) complexes have been synthesized by using the ligand N,N'-bis(N-octyl 2-methyl benzimidazolyl) pentanediamide)O-GBGA) and have been characterized by analytical Data, UV, IR, EPR and Cyclic voltammetry. Deals with the preparation of the copper(II) compounds in the reverse micellar media using CTAB and Triton-X-100 as surfactants with the ligand N,N'-bis(2-methyl benzimidazolyl)pentane diamide (GBGA). Effect of the nature of surfactant on the size of the hybrid solid is studied.

Contents

1. Introduction. 2. Theory of techniques utilized in the identification of ligands and their complexes. Synthesis and characterization

of bis benzimidazole diamide ligands. 3. Synthesis, spectral and structural studies of MN(II) complexes using bis benzimidazole diamide ligands. 4. Synthesis, spectral, electrochemical and functional studies of copper(II) complexes with N-octylated bis benzimidazole diamide ligand. 5. Copper (II) compounds synthesized in reverse micellar media, study on varying the compositions and surfactants. Summary.

102. MOHD. SAMIM
Chemical and Biological Studies with Metal Nanoparticles.
 Supervisor : Prof. N. K. Kaushik
Th 16268

Abstract

Studies the different macrophages reactivity with gold nanoparticles of different sizes. The macrophage injury and activation varies with size of Au nanoparticles with and without opsonisation. Different macrophage reactivity or injury may modulate the macrophage function which may in turn affect the ability for an antigen presentation or role in inflammation biology including tissue repair. It also reveals that different macrophage reactivity is observed with different types of nanoparticles (NP). Both the composition and the nanoparticles size appear to be important in determining the cellular toxicity of the NP. Gold nanoparticles were found to induce apoptosis. When Hoechst-PI staining was used to observe apoptotic/dead cells. With NP of same material, larger NP showed more cellular apoptosis thus showed more cytotoxicity than 10nm gold nanoparticles. Opsonising the NP by incubating the particles with 0.1% BSA prior to putting in the cell culture resulted in the reduction of their cytotoxicity. Hence opsonisation may result in increased biocompatibility of the NP.

Contents

1. Introduction. 2. Literature review . 3. Experimental. 4. Effects of size of copper nanoparticles on its catalytic behaviour in Ullmann reaction. 5. Effect silver nanoparticles : An efficient antifungal agent, its therapeutic effect on Malassezia furfur, a dandruff causing fungus. 6. Synthesis and characterization of gold nanorods and their application for photothermal damages of cell. 7. Evaluation of macrophage injury and activation by nanoparticles. 8 Conclusion.

103. PANDEY (Pratibha)
Preparation, Characterization and Application of Some Nanomaterials to Glucose Biosensor.
Supervisors : Prof. Monika Datta and Dr. B. D. Malhotra
Th 16280

Abstract

It deals with the preparation, characterization and application of nanoparticles such as gold (AuNPs), TiO_2 and Fe_3O_4 to glucose biosensing. Gold nanoparticles have been functionalized with inorganic molecules consisting of -COOH, -NH₂ -SH functional groups to facilitate attachment of biomolecules to gold nanoparticles surface. Glucose oxidase has been used as a model enzyme to study the importance of these nanoparticles for glucose biosensor with the synthesis of organic-inorganic nanocomposites films of both gold (AuNPs) and iron oxide (Fe_3O_4) nanoparticles for application to glucose biosensors.

Contents

1. Introduction. 2. Materials and experimental techniques. 3. Thiolated gold nanoparticles based glucose biosensor. 4. Gold nanoparticle-conducting polymer composite films based glucose biosensor. 5. Metal oxide nanoparticles based glucose biosensor. 6. Future prospects & summary.

104. PANDEY (Ravi Ranjan)
Organic-Inorganic Nanocrystalline Films for Catalysis and Sensors Applications.
Supervisors : Dr. Man Singh and Dr. K. K. Saini
Th 16267

Abstract

Understandes the mechanisms which influence the photocatalytic properties of TiO_2 , to design a photocatalyst with tailored properties for specific applications. Further the films of these catalysts are obtained on glass substrates, which exhibit desired catalytic efficiency and at the same time they are hard and inert to withstand the chemical or mechanical environment. Also develops, enhance surface chemistry, engineering for photocatalytic oxidation (PCO) using TiO_2 thin films by further modification with transition metals doping and its applications in current challenges in solid-liquid environmental remediation. Preparation of novel semiconduction-metals doped

films to understand the role of metal in promoting charge transfer from photoexcited semiconductor.

Contents

1. Introduction. 2. Materials and theory of methods used. 3. Enhanced hydrophilic and photo catalytic characteristics of nanocrystalline TiO_2 thin films doped with ruthenium (Ru^{3+}) ion. 4. Enhancement of hydrophilicity and photocatalytic activity of nanocrystalline TiO_2 thin films doped with tungsten (W^{6+}) ion. 5. Enhanced hydrophilic and photocatalytic characteristics of nanocrystalline TiO_2 thin films doped with palladium (Pd^{2+}) ion. 6. Glucose Biosensor based on the immobilization of glucose oxidase onto porous nanocrystalline titanium dioxide sol-gel matrix using amperometric detection. 7. Summary of the thesis.

105. PANT (Parul)
Synthesis, characterization and Applications of Functionalized Amberlite XAD-16 in Metal Ion Extraction and Catalysis.
 Supervisor : Prof. R. K. Sharma
Th 16262

Abstract

Describes the synthesis and applications of functionalized Amberlite XAD-16 in metal ion separation and catalysis by use of phenolic and polyphenolic compounds functionalized Amberlite XAD-16 chelating polymer in the field of metal ion extraction as well as in heterogeneous catalysis.

Contents

1. Introduction. 2. Theory of instrumental techniques used. 3. Solid phase extraction of metal ions from aqueous samples by gallic acid functionalized amberlite XAD-16. 4. Extraction behaviour of chrysin functionalized amberlite XAD-16 for Fe(III), Co(II), Ni(II), Cu(II). 5. Solid phase extraction and determination of metal ions in aqueous samples using quercetin functionalised amberlite XAD-16. 6. Application of gallic acid functionalized amberlite XAD-16-Zinc catalyst in esterification of acids and anhydrides.

106. RAVIVANSHI (Kuldeep Kumar)
Platinum (II/IV) and Gold (III) Complexes of Some Ligands Containing N and S Donor Atoms : Synthesis, Characterization, Thermal and Biological Studies.
 Supervisors : Prof. N. K. Kaushik and Dr. R. L. Gupta
Th 16269

Abstract

It studies the structural studies of the Platinum (II/IV) and Gold(III) complexes of Dithiocarbamates, Thiohydrazides and Thiohydrazone ligends. Characterization and thermal studies of these complexes were carried out with some physico-chemical methods. Biological studies on certain economically important microorganisms like fungi and bacteria. The transition metal complexes of Dithiocarbamates, thiohydrazide and thiohydrozone have been syntheized and characterized by elemental, spectroscopic and thermal analysis. The spectral (IR, ¹HNMR and UV-Vis) studies show that the coordination occurred through azomethine nitrogen and thioamide sulphur.

Contents

1. Introduction. 2. Methods and materials. 3. Synthesis of platinum (II/IV) and Gold (III) complexes. 4. Physio-chemical studies of the complexes. 5. Thermal studies. 6. Biological studies. 7. Results and discussions. Reference and summary.

107. SANJAY KUMAR
Some Novel Synthetic Organic Transformations.
 Supervisor : Prof. J. M. Khurana
Th 16275

Abstract

It deals with the novel synthetic methodologies developed in laboratory these include (i) Facile Reductive Dehalogenation of Organic Halides using Nickel Boride, (ii) Microwave Assisted Solent Free Oxidation of Organic Halides Using Aqueous Hydrogen Peroxide, Oxidation of Chalcogenides using Peroxo Complex of Molybdenum [MoO₅.H₂O.HMPA], Application of Tetrabutyl lammonium bromide (TBAB) as a Neutral and Efficient Catalyst for the Synthesis of Biscounarins and Dihydropyrano [c] chromene Derivatives in Water and under Solvent Free Conditions, Application of [bmim]Br and [bmim]BF₄ Ionic liquids as an Efficient and Recyclable Media for the Synthesis of

Octahydroquinazolinone and Biscoumarin derivative and an efficient, Catalyst free Synthesis of some Novel 2,3-Dihydroquinazolin-4(1H)-one in Aqueous medium.

Contents

1. Facile reductive dehalogenation of organic halides using nickel boride. 2. Microwave assisted solvent free oxidation of organic halides using aqueous hydrogen peroxide. 3. Oxidation of chalcogenides using peroxo complex of molybdenum ($\text{MOO}_5 \cdot \text{H}_2\text{O} \cdot \text{HMPA}$). 4. Tetrabutylammonium bromide (TBAB) : A neutral and efficient catalyst for the synthesis of biscoumarin and dihydropyrano[c]-chromene derivatives in water and solvent free conditions. 5. Ionic liquid : An efficient and recyclable media for synthesis of octahydroquinazolinones and biscoumarins. 6. An efficient catalyst free synthesis of some novel 2,3-dihydroquinazolin-4(1H)-ones in aqueous medium. 7. Summary and conclusions.

108. SAVITA KUMARI
Effect of Ligand Architecture on the Structure and Properties of Nickel Complexes with Amide - Based Macrocyclic Ligands.
 Supervisor : Dr. Rajeev Gupta
 Th 16274

Abstract

It describes the design and synthesis of novel macrocyclic ligands and their coordination chemistry towards Ni(II) ion. The ligands H_2L^1 to H_2L^{13} have been designed to provide an identical donor-environment in conjunction with a 12 or 13 - membered macrocyclic ring around the metal center. The square planar Ni(II) center is housed quite tightly within the cavity of the 12 - membered ligands, while it is quite relaxed in the cavity of the 13 - membered macrocycles as evident by the Ni-N bond lengths and displacement of the Ni ion out the N_4 basal plane. In the case of copper (II) ion, the geometry is square - pyramidal where N_4 coordination is from the ligand whereas the 5th coordination comes from the O_{amide} of the neighboring unit. The effect of ligand planarity, non-innocent features and the electronic effects on the structural, spectroscopic, and redox properties of the nickel center are discussed. Electrochemical or chemical oxidation at the 1st redox potential results in the generation of an unstable "green species" that shows distinct features in the absorption spectrum and exhibits anisotropic EPR spectrum and thus confirms the existence of a rare square-planar Ni(III) species.

Contents

1. Introduction : A brief survey of the amide-based ligands and their coordination chemistry with nickel ion. 2. Synthesis and characterization of 12- and 13-membered amide-based macrocyclic ligands. 3. Studies on Ni(II) Complexes with 12 - membered amide - based macrocyclic ligands. 4. Studies on Ni(II) and Cu(II) complexes with 12 - membered amide - based macrocyclic ligands : Effect of electronic substituents. 5. Studies on nickel complexes with 13 - membered amide - based macrocyclic ligands.

109. SHAKYA (Gaurav)
Chemical & Chemoenzymatic Synthesis of Unnatural Pentofurano-Nucleosides of Importance.
 Supervisor : Dr. Ashok K. Prasad
Th 16266

Abstract

This study reveals that the lipase from *Pseudomonas aeruginosa* has been found to have remarkable selectivity towards the butanoylation of 3'-hydroxyl group in the presence of primary hydroxyl group of 2'-deoxynucleosides of thymine and adenine. Secondly, in case of ribonucleosides series, 3'-hydroxyl group of adenosine has been selectively butyrate even in the presence of secondary 2'-hydroxyl and primary 5'-hydroxyl group. Moreover, biocatalytic direct N-butanoylation in case of cytosine nucleosides have been achieved in excellent yields.

Contents

1. Lipase catalysed selective acylation studies on nucleosides.
 2. Chemoenzymatic synthesis of α -L-/ α -D-configured pentofuranosyl-nucleosides. Summary.

110. SHARMA (Deepti)
Synthesis of Novel Bioactive β -Amino Alcohols, Coumarinyl-dihydropyridines and Biotransformations on Nucleosides and their Precursors.
 Supervisor : Prof. Ashok K. Prasad
Th 16271

Abstract

Efforts are being made to identify new anticancer drug targets.

Kinases have become one of the most lucrative drug targets today. Tyrosine kinase Src is one of the important protein which is implicated in cancer. Src kinase is a family of protooncogenic tyrosine kinase. These protooncogenes become tumor inducing agents on activation. There are various anticancer drugs with an amino alcohol unit present in them. Daunorubicin and doxorubicin are the two such examples currently considered to be the most potent and clinically useful agents in cancer chemotherapy. A host of synthetic molecules used as drugs or pharmacological agents also contain the vicinal amino alcohol moiety. It also demonstrated the specificity of CAL-B (Novozyme 435) for regioselective deacylation of acyl groups at primary position over that at secondary position in peracylated azido nucleosides **45a-45c** and **50a-50c**. The arabino configured mono acylated azido nucleosides (46a-46c) were synthesized starting from L-arabinose in eight steps following the chemoenzymatic route. While the ribo configured mono acylated azido nucleosides (**51a-51c**) were synthesized from commercially available rithymidine in five steps following the chemoenzymatic route.

Contents

1. Synthesis and Src kinase inhibitory activity of 1-substituted-3-(N-alkyl-N-phenyl)aminopropan-2-ols. 2. Synthesis and antiplatelet activity study on some novel coumarinyl-dihydropyridnes. 3. Synthesis and lipase catalysed deacylation studies on 4-C-acyloxymethyl-3,5-di-O-acyl/4-C-acyloxymethyl-5-O-acyl-1,2-O-(1-methylethylidene)-O-D-erythro-ribofuranose : Precursors of bicyclonucleosides. 4. Synthesis and regioselective deacylation studies on azido nucleosides : Towards synthesis of 5'-O,2'-N-Linked oligonucleotides. Summary.

111. SHARMA (Smriti)
Functionalization of Carbon and Boron Nitride Nanotubes with Carbenes : A Density Functional Study.
 Supervisor : Prof. Rita Kakkar
Th 16283

Abstract

It has studied the electronic structures of these nanotubes and the effect of functionalization by carbenes. State of the art density functional studies were use to obtain the optimized geometries of armchair and zigzag nanotubes, which were then functionalized with various carbenes. The effect of increasing

diameters of the nanotubes was studied and it was found that the effect of curvature is pronounced for small diameters, which have almost sp^3 hybridization at the carbon atoms, which gradually becomes sp^2 on increasing diameter. It also found that functionalization leads to opening up of the band structure of the nanotubes. While the pristine tubes are metallic, functionalization leads to an almost uniform band structure.

Contents

1. Introduction. 2. Computational theory and methodology. 3. Functionalization of carbon nanotubes with carbenes. 4. Interactions of carbenes with boron nitride nanotubes. 5. Diameter effects on addition chemistry of methylene on nanotubes. 6. Periodic single-walled carbon nanotubes with sidewall functionalization. 7. Conclusions & perspectives. Bibliography.

112. SHUKLA (Gauri)
Conjugation to Biological Vectors as Scintigraphic and Intracellular Therapeutic Agents for Cancer.
 Supervisors : Dr. Anil Kumar Mishra and Dr. Harish Chandra
Th 16292

Abstract

It attempts to verify the proposition and highlights the work carried out as metallopharmaceuticals and its biological evaluation for scintigraphy and therapy. The potential targeting biologically active vectors taken for the studies are the folate, antibody and amino acid (methionine) followed by the studies for construction of a drug delivery with PEG as polymer. It also represents a comprehensive account of the synthesis of a new conjugate for therapy and imaging in good yield and its biological evaluation as a drug candidates in cell cultures and animal models.

Contents

1. Introduction. 2. Scientific background. 3. Folate receptor-mediated targeting of therapeutics and imaging. 4. Targeted therapy with radiolabeled antibody conjugates. 5. Radiolabeled amino acids analogues for application in oncology. 6. Conjugates of anticancer agents with PEG (Poly Ethylene Glycol). Summary. Bibliography.

113. SINGH (Dev Raj)
Synthesis and Industrial Applications of Novel Macrocyclic Ligands.
Supervisor : Dr. Sulekh Chandra
Th 16277

Abstract

This work studied the six macrocyclic ligands synthesized thereafter and then used as metal ion selective PVC based membrane electrodes as electroactive materials. These macrocyclic compounds are highly sensitive and selective towards some specific transition and heavy metal ions. The electrodes developed have been analysed by testing some practical samples and using them as electron indicator electrode Macrocyclic compounds.

Contents

1. Introduction. 2. Materials and instruments used and synthesis and characterization of macrocyclic ligands. 3. (I) Development of Poly(Vinyl chloride) based Ni^{2+} -selective electrode using macrocyclic ligand L_1 as an ionophore. (II) Development of Poly(Vinyl chloride) based Zn^{2+} -selective Electrode using triaza macrocyclic ligand L_2 as an ionophore. 4. (I) Development of Poly(Vinyl chloride) based Cu^{2+} -selective Electrode using macrocyclic ligand L_3 as an ionophore. (II) Development of Poly(Vinyl chloride) based La^{3+} -selective electrode using macrocyclic ligand L_4 as an ionophore. 5. (I) Development of Poly(Vinyl chloride) based Pr^{3+} selective electrode using macrocyclic ligand L_5 as an ionophore. (II) Development of Poly(Vinyl chloride) based Nd^{3+} selective electrodes using macrocyclic ligand L_6 as an ionophore. Summary.

114. SINGH (Jyoti)
Studies on Coordination Complexes with Synthetically Designed Tetradentate Amide-Based Ligands.
Supervisor : Dr. Rajeev Gupta
Th 16279

Abstract

It is a detailed study on various coordination modes of the amide-based ligands. Various amide-based ligands are synthesized to explore their coordination chemistry towards different transition metal ions. The ligands with rigid backbone afforded

mononuclear complexes, however, dinuclear, trinuclear and chains were isolated with ligands having flexible backbone. The di- and tri-nuclear copper(II) complexes show interesting magnetic properties. Coordination complexes supported with amide-based ligands also show interesting electrochemistry and tend to stabilize the higher oxidation state of the metal ion.

Contents

1. Introduction : An overview of the coordination chemistry of the amidebased ligands and their biological relevance. 2. Studies on nickel(II) complexes with tetradentate amide-amine based ligands. 3. Studies on copper(II) complexes with tetradentate amide-amine based ligands. 4. Studies on nickel(II) and copper(II) complexes with tetradentate amide-pyrrole based ligand containing flexible backbone. 5. Studies on copper(II), nickel (II), manganese(III) and iron (III) complexes with tetradentate amide-pyrrole based ligand containing rigid backbone. Summay.

115. SUMIT KUMAR
Design and Synthesis of 3-(3-Chromonyl) Acrylic Acid Derivatives and Synthesis and Applications of PEG Based Amphiphilic Polymers.
 Supervisor : Dr. Sunil K. Sharma
Th 16285

Abstract

It studied the effect of variation of hydroxyl group position on benzene ring, replacement of ester linkage by amidic linkage, and replacement of hydroxyl group by its acetate derivative in addition to the earlier work done on this class of compounds by synthesizing a series of chromone carboxylic acid esters (534) based on 3-(4-oxo-4H-1-benzopyran-3-yl) propenoic acid (20) in which the hydrogen bond between the carboxylic acid group and the carbonyl group is sterically impossible and these compounds were evaluated for their ICAM-1 inhibitory activity on human endothelial cells as well as their effect on NADPH-catalyzed rat microsomal lipid peroxidation.

Contents

1. Synthesis of 3-(3-Chromonyl)acrylic acid derivatives. 2. Synthesis and applications of PEG based amphiphilic polymers.

116. VATS (Ishwar Dutt)
Designing, Synthesis and Biological Activity of Endogenously Occurring Opiate Peptides.
 Supervisors : Dr. Mahendra Nath and Dr. Santosh Pasha
Th 16284

Abstract

Gives a detailed overview of opioids, opioid receptors and the mechanism of induction of opioid analgesia. Also describes the side effects associated with opioids and their explanation as hypothesized by different models/mechanisms ; the detailed designing concept of different chimeric peptides ; the synthesis of some standard peptides like Dynorphin A (1-13), endomorphine-1 etc. on Wang resin ; the pharmacological studies of synthesized chimeric peptides along with some standard peptides. Concludes from the present pharmacological studies that designed chimeric peptides predominantly act as opioid agonist and anti-opioid (-RF_{amide}) site also contributes towards total observed analgesia via indirect activation. Also conclude that either incorporation of D-amino acid or increase in lipophilicity of peptide or both causes a considerable increase in analgesia and also alters opioid receptor specificity. Importantly, the non-specific behavior of synthesized chimeric peptide agonists in turn enhance its potency to induce tolerance free analgesia. Finally got a potent analgesic chimeric peptide (CP-3) which does not show any sign of tolerance during 6 days of chronic treatment.

Contents

1. An overview of Opioid and Anti-Opioid System. 2. Designing of Novel Chimeric Opioid Peptides. 3. (A) Synthesis, Purification and Characterization of Chimeric Peptides. (B) CD Studies of Chimeric Peptides. 4. Pharmacological Studies of Synthesized Chimeric Peptides. 5. Mechanism Based Molecular Study of Novel Chimeric Peptides. Summary.

117. VIKRAM SINGH
Synthesis Characterization and Studies of Selected Sulpha Drugs and Their Metal Complexes.
 Supervisor : Prof. N. K. Kaushik
Th 16556

Abstract

In this work the selected Schiff bases derived from sulphonamide

and aldehydes and ketones are prepared by the modification of known literature methods. The obtained sulpha drugs are screened for potential antifertility agent. Selected metal complexes are also prepared. The number of synthesized metal complexes of sulfa drugs has been increasing; the interaction of metal ions with drugs administered for therapeutic reasons of considerable importance.

Contents

1. Metal complexes of sulpha drugs ; an overview. 2. Experimental. 3. Results and discussion. 4. Biological studies. 5. Summary. Bibliography.

118. YADAV (Yogesh)
Synthesis and Anti-Viral Activities of Pyrazolyl Nucleosides and Potential β -Naphthol Based Selective Estrogen Receptor Modulators.
 Supervisor : Prof. V. S. Parmar
Th 16263

Abstract

The broad spectrum biological activities of pyrazoles and base modified nucleosides containing them are undertaken to synthesize novel pyrazolyl nucleosides. In the present work the synthesis of ten novel pyrazole nucleosides have been achieved by obtaining the corresponding pyrazole-based nucleosides to couple the hydroxyl-protected chlorosugar with the desired pyrazole derivative through one of the N-atoms.

Contents

1. Synthesis and Anti-viral activities of novel pyrazole nucleosides. 2. synthesis of β -Naphthol based potential selective estrogen receptor modulators. Summary.

M.Phil Dissertations

119. CHANDRA MOHAN
Synthesis of New Series of ACID Catalysts : Heteropoly ACID Intercalated Clay.
 Supervisor : Prof. Monika Datta