Functionalized Hydroxyethylamine Based Peptide Nanostructures as Potential Inhibitors of Falcipain-3, an Essential Proteases of *Plasmodium Falciparum*

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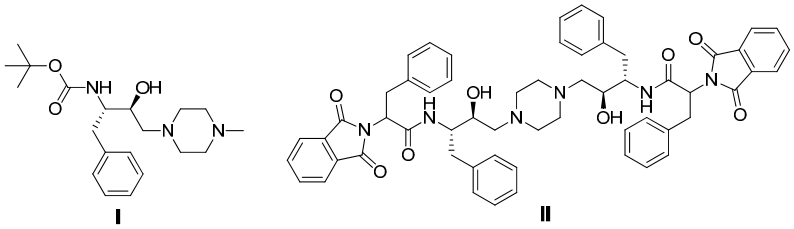
Self-assembled peptide based nanostructures gained enough popularity due to their easy biocompatibility and numerous potential applications. An extensive research has been carried out towards the development of novel functionalized peptide-based self-assemblies with strong potential of applications such as cell encapsulation, stem cell differentiation, immune response and drug delivery. Besides, peptide-based self-assemblies are of much interest due to their low cost, specific molecular recognition, easy tailoring of their chemical and biological functionalities and also their biomimetic nature. Several peptide nanohydogels have been reported to possess strong biological applications and also used as encapsulating metrices for target drug delivery. An excellent model of self-assembly of hydroxyethylamine based peptide nanostructures was synthesized and characterized by DLS and TEM. Spherical nano structures of **I** and **II** were observed with particle size ~50 and ~80 nm, respectively. Further, **I** and **II** were screened against anti-malarial target, falcipain-3 (FP3), a crucial cysteine protease involved as a major hemoglobinase of Plasmodium falciparum. Interestingly, compound **II** completely inhibited the activity of FP3. The effective concentration (1.5 M) of **II** found to be more potent than **I**. This biochemical result was substantiated by molecular-docking studies indicating **II** to be best inhibitor of FP3. This is the first report showing that bis hydroxethylamine based peptide nanostructures could be very effective inhibitor of malarial cysteine proteases.



I **II**

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POSTER

Synthesis of Biologically Important N/O- containing Heterocycles using Task Specific Acidic Ionic Liquid $[NMP]H_2PO_4$

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Multicomponent reactions (MCRs) have attracted the attention and interest of synthetic organic chemists for building highly functionalized organic molecules from readily available starting materials in single step. MCRs exhibit inherent flexibility and selectivity for creating molecular complexity and diversity coupled with minimization of time, labour, cost and waste production. In recent years, one of the concepts of green chemistry focuses on providing alternating reaction conditions and media. In this context, ionic liquids have gained recognition as possible environmentally benign alternatives to more volatile organic solvents. Therefore, MCRs performed in ionic liquids are of immense interest.

Task specific acidic ionic liquid *N*-methyl-2-pyrrolidonium dihydrogen phosphate ($[NMP]H_2PO_4$) is considered as environmentally benign medium and can be prepared in one step without use of any organic solvent unlike other ionic liquids. We have examined the efficiency of $[NMP]H_2PO_4$ as a catalyst and reaction medium for different MCRs. We report herein, one-pot synthesis of the biologically important benzo[*a*]phenazines *via* condensation of aldehydes, 2-hydroxy- 1,4-naphthaquinone, *o*-phenylene diamine and cyclic 1,3-dicarbonyl compounds; benzo[*a*]xanthenes *via* condensation of aldehydes, 2-naphthol/ 2,6-dihydroxy-/2,7-dihydroxy naphthalene and cyclic 1,3-dicarbonyl compounds; benzo[*b*]xanthenes *via* condensation of aldehydes, 2-hydroxy- 1,4-naphthaquinone and *N*,*N*-dimethyl barbituric acid; pyrimidoquinolines *via* three component condensation of aldehydes, 6-amino-1,3-dimethyl uracil and cyclic 1,3-dicarbonyl compounds.

POSTER

Photophysical Properties of Novel Benzo[*A*]Xanthenes And Benzo[*A*]Pyranophenazines - Solvatochromic and DFT Studies

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Development of new fluorescent organic compounds with high functionality has been the subject of intense study because of rapidly expanding applications of organic fluorescent materials for electroluminescence (EL), dye lasers, sensors, probes, and phototherapeutic agents. Benzo[*a*]xanthenes and benzo[*a*]pyranophenazines are of interest because they have been used in photodynamic therapy and can be used as dyes, pH-sensitive fluorescent materials. Absorption and emission spectra of benzo[*a*]xanthenes and benzo[*a*]pyranophenazines were studied at 298 K in solvents of different polarity for the first time. It was observed that an increase in the solvent polarity led to an increase in the Stokes shift. The solvent effect on the spectral properties of benzo[*a*]xanthenes and benzo[*a*]pyranophenazines has been investigated by using the Lippert–Mataga and Reichardt–Dimroth methods in order to obtain an insight about specific solvent-fluorophore interaction. Bakhshiev's and Kawski-Chamma-Viallet's correlations were used to determine the excited state dipole moment, ground state dipole moment and their ratio. The nature and extent of solute solvent interactions were described by multi-linear correlation using the three-parameter Kamlet-Taft and the new four-parameter Catalán polarity scales. Multiple regression analysis indicates that both non-specific solute–solvent interactions and specific solute–solvent interactions play an important role in the position of the Stokes shift. The polarizable continuum model using IEF-PCM was considered to calculate excitation energies in methanol. The HOMO and LUMO energies have been performed by TD-DFT (B3LYP/6-311G (d, p)) approach.

POSTER

Targeting tumor Associated hCA isoforms IX and XII by 4-functionalized Pyrazoles Bearing Benzenesulfonamide Moiety

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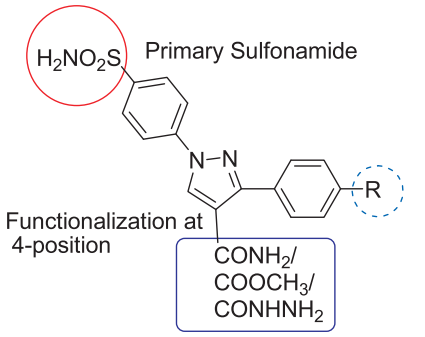
Carbonic anhydrases (CAs, EC 4.2.1.1) belong to the group of zinc metalloenzymes and play an important physiologic role by catalyzing the reversible rapid hydration-dehydration reaction of carbon dioxide to bicarbonate anion and protons. Primary sulfonamides were identified as the first and one of the most important class of α-family of CA inhibitors (CAIs) that has given many clinically used drugs. Perusal of literature reveals that pyrazole scaffold has been an important pharmacophore and privileged structure present in various CA inhibitors. Motivated by these findings, coupled with our ongoing research in the field of pyrazoles and other heterocyclic compounds of potential medicinal interest, [1,2,3] we turned our attention towards the synthesis and evaluation of benzenesulfonamide bearing 4-functionalized pyrazoles as novel CAIs. We have designed and synthesized a small library of novel 4-functionalized 1,3-diarylpyrazole compounds bearing a primary sulfonamide group on the phenyl ring at N-1 position of pyrazole scaffold with different functionalities at C-4 such as carboxamide, ester, and hydrazinocarbonyl, and evaluated them against four human carbonic anhydrases hCA I, II, IX and XII. Most of the tested compounds exhibited excellent CA inhibitory activity profile showing low nanomolar < 5nM potency against the tumor associated CA IX and XII.



K_i <5nM against hCA IX
K_i<10nM against hCA XII

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POSTER

Benzenesulfonamide Bearing 1,2,4-triazoles as Selective Potent Inhibitiors of Tumor Associated hCA Isoforms IX and XII

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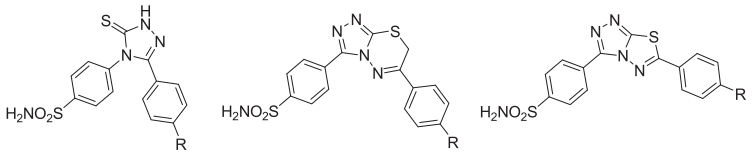
Carbonic anhydrase is the omnipresent class of metalloenzymes which catalyzes the reversible hydration and dehydration of carbon dioxide. Out of the 16 different CA isoforms discovered so far in the α-class, dimeric transmembrane glycoproteins hCA IX and XII having extracellular active sites are marker for a broad spectrum of hypoxic tumor types and promote tumor cell survival by acidification of extracellular hypoxic environment. Thus specifically targeting the tumor associated isoforms hCA IX and XII over the main off target isoforms hCA I and II, which have a physiological relevance, is considered to be a promising strategy in the cancer therapy. Sulfonamides are the most widely investigated class of CA inhibitors possessing significant inhibitory power against many isoforms. Possessing a wide spectrum of biological activities, indeed the class of heterocyclic compounds containing 1,2,4-triazole scaffold has been attracting the attention of researchers for a long time. 1,2,4-Triazole moiety has been found to be present in the skeleton of various natural products and a large number of compounds containing this moiety exhibits antimicrobial, antitubercular, analgesic, anti-inflammatory, anti-convulsant, antiviral and antidepressant activities. In our present study, we have developed new benzenesulfonamide CA inhibitors bearing 1,2,4-triazoles as the core scaffolds exhibiting excellent inhibitory potential against hCA isoforms IX and XII. [1,2]



K*i* <10 against hCA IX
K*i* < 5 against hCA XII

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POSTER

Elucidation of the mode of action of formulations of Four Plant Products- Clove, Pepper, Nutmeg and Cardamom against Pathogenic Yeast, *Candida albicans*

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Since the last three decades, emergence of superficial and invasive mycoses caused by opportunistic pathogens have resulted in increase of morbidity and mortality in immunocompromised and hospitalized patients. Dimorphic, opportunistic and otherwise commensal *Candida* spp. are reported to stand fourth among all microorganisms in causing nosocomial blood stream infections globally. Among all other *Candida* spp., *Candida albicans* is reported to be the most virulent form. Limitations in availability of broad spectrum antifungals with minimum side effects and emergence of drug resistant strains contribute as major factors which hinders the control and treatment of fungal infections.

There is a constant demand for new antifungal agents and therapeutic strategies to combat candidiasis by reversal of MDR. The objective of this study is to elucidate the anti-*Candida* effects and mode of action of formulations of four natural plant extracts- clove, pepper, nutmeg and cardamom either singly or in combination with other known drugs. The natural products were extracted using isopropanol followed by subsequent distillation and emulsification by ethylacetate and the active components of these formulations were characterized by GCMS. The formulations of the plant extracts showed antifungal effects on laboratory and clinical isolates of *Candida albicans* as confirmed by both broth microdilution and spot assays. The growth inhibition was found to be in the order clove> pepper> nutmeg> cardamom. Formulations of clove and pepper revealed 80% growth inhibition at respective concentrations of 3.125µl/ml and 25µl/ml (v/v) whereas formulations of nutmeg and cardamom were able to kill 70 - 75% cells at around 100µl/ml. The formulations of the natural plant products showed synergism with different classes of known drugs viz. azoles, polyenes and allylamines. Fluorescence polarization studies revealed 4-14% increase in rigidity of the membrane of *Candida* cells treated with the formulated plant extracts and altered sterol content in the treated cells. Treated cells showed alterations in the cell morphology, cell wall thickening, membrane aberrations and cytoplasm displacement as confirmed by Electron microscopy.

The antimicrobial effects observed may be due to the phenol, polyphenols, terpenoids, flavanoids, alkaloids and quinones present in the plant extracts. Further investigations are underway. This study has the potential to contribute to the development of new therapeutic strategies for clinical applications in the treatment of Candidiasis.

Acknowledgements:DBT grants (BT/PR5110/MED/29/497/2012 and BT/BI/12/045/2008), DST PURSE grant support is gratefully acknowledged.

POSTER

Hexa-peri-hexabenzocoronene–porphyrin as a Model for Graphene-porphyrin Conjugate

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The new synthetic carbon allotrope graphene is a two dimensional sheet of sp^2 hybridized carbon with remarkable thermal, mechanical and electronic properties. Since graphene is a zero band-gap semiconductor, proper functionalization and/or modification of its structure is mandatory to open a band-gap, which represents an important prerequisite for many possible applications in the field of molecular electronics. In this regard, chemical modification of graphene with various organic functionalities to introduce band-gap can be done with the development of interesting photo/redox activity profiles. Achieving high efficiency in a synthetic system for producing electricity using sunlight requires efficient light absorption from around 400 nm to the 1000 nm region. The highest efficiencies require tandem photoconversion systems with two or more photoactive components that cover this spectral region. To study this approach, graphene model system namely hexa-peri-hexabenzocoronene (HBC) and tetraaryl-porphyrins are covalently attached where the porphyrin building block was supposed to serve as a light harvester.

The covalent interaction of hexabenzocoronene with porphyrins have been examined through various spectroscopic techniques with their possible applications in solar cells, supramolecular chemistry and material chemistry.

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POSTER

Structure guided Design, Synthesis and Biological screening of Pyrimidine based novel Antimalarials.

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Malaria, one of the most important parasitic protozoan diseases of human beings, because of its prevalence, virulence and drug resistance which affects public health in developing regions of the world. According to WHO report it has been found that half of the world population is at risk of malaria [1]. Recently, it has re-emerged as a devastating parasitic disease in tropical and sub-tropical regions. 400-500 million cases are diagnosed annually and 2-3 million children below the age of five are infected which leads to death [1]. Previously the treatment of malaria was relied upon chloroquine but the demise of chloroquine due to the emergence of resistant P. falciparum strains new antimalarial drugs are desperately needed that must meet the requirements of rapid efficacy, minimal toxicity and low cost [2].

In our work, we have designed and synthesised novel pyrimidine based antimalarials keeping in mind that these novel molecules should be highly specific to target proteins. These molecules inhibit dihydroorotate dehydrogenase (DHODH) enzyme which is essential for the survival of malarial parasites. DHODH is an important enzyme that catalyses the fourth and rate-limiting step in de novo pyrimidine biosynthesis [3].

Key Words: Antimalarials, Pyrimidine, DHODH

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POSTER

Montmorillonite-Polymer Nanocomposites: Synthesis, Characterization and In Vitro Drug Release Studies

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The drawback associated with the conventional anti-hypertension tablets includes fluctuation in drug plasma level leading to requirement of multiple dosing. Therefore, there is a strong need for the development of oral extended release formulation.

The present work is aimed at developing Montmorillonite – Poly lactic – co - glycolic acid (Mt–PLGA) nanocomposites as a sustained release drug delivery vehicle for an anti-hypertension drug.

Drug loaded Mt–PLGA nanocomposites were synthesised by double emulsion solvent evaporation method. The drug encapsulation efficiency and drug loading capacity of synthesized products were estimated with the help of HPLC technique. The physical status of Mt and drug within synthesized nanocomposites, their particle size and surface morphology were evaluated with the appropriate analytical techniques. Results have been compared with the analogous drug incorporated PLGA nanoparticles.

The methodology developed has resulted in high loading and encapsulation efficiency. By tuning the multiple parameters two types of Mt-drug-PLGA nanocomposites (intercalated and exfoliated) were obtained. The drug-PLGA nanoparticles and Mt-drug-PLGA nanocomposites were found to be 50-100 nm in size (as confirmed by TEM data) which is in the range of intestinal uptake.

In vitro release profile of the drug from the nanocomposites (Intercalated and exfoliated) was recorded in simulated gastrointestinal fluids. The results indicate that presence of Mt within nanocomposites provide a better sustained release character to the encapsulated drug as compared to commercial formulation of the drug and the synthesised drug-PLGA nanoparticles.

Thus, on the basis of our work it could be concluded that Mt based PLGA nanocomposites has promising potential for developing into an extended release formulation for oral administration of selected anti-hypertension drug.

Keywords: Montmorillonite, Poly lactic-co-glycolic acid, anti-hypertension drug, encapsulation efficiency, sustained release drug delivery

POSTER

A Novel Three-Stranded G-quadruplex formation In Promoter Region of Human Myosin *(MYH7)* Gene

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Gene promoters are enriched in Guanine rich sequences that potentially fold into G-quadruplex structures. Such quadruplex structures were implicated in the regulation of gene expression by interacting with various transcription factors. G-rich regions are abundant in transcriptional regulatory regions of genes active in the lung, heart and brain. The G- enrichments in these tissues may indicate that these tissues have evolved certain mechanisms to utilize G-quadruplex structure to regulate gene transcription. On exploring the genome for search of G-tracts it was interesting to find that promoter of MYH7 gene is rich in Guanines and coincidently, is the best studied cardiac gene promoters so far. Mutations in this gene are associated with familial cardiomyopathy, dialted cardiomyopathy and laing early-onset distal myopathy. Enrichment of MYH7 gene in G-rich sequences could possibly play a critical role in its regulation. With this view in mind we adopted biophysical and biochemical approach to study 23-mer G-rich sequences from promoter location of Human Myosin b gene *(MYH7)*. Herein, using polyacrylamide gel electrophoresis (PAGE), UV-Thermal denaturation (UV-Tm) and Circular dichroism (CD) we demonstrate the formation of an unprecedented three stranded-G-quadruplex structure by the said sequences. A model is proposed for the novel three stranded parallel G-quadruplex structure which could possibly act as a regulatory element in the promoter region of Human Myosin b gene

POSTER

Sodium Chloride Promoted Greener Approach for the Synthesis of Highly Functionalized Pyridines

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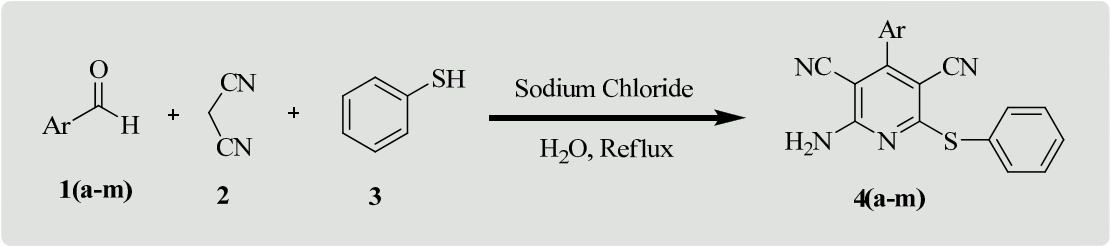
In the present work, sodium chloride promoted synthesis of highly functionalized pyridines in aqueous medium is described. This synthetic protocol offers some significant advantages such as easy availability of catalyst, operational simplicity, simple work up procedure and higher product yields.

Keywords: Pyridines, Sodium Chloride, Aqueous Medium, Green chemistry.



POSTER

Three-Component Metal-Free Arylation of Isocyanides

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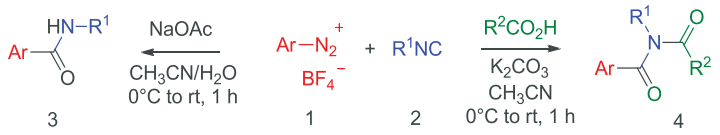
Metal-free arylation of isocyanides may be performed under addition of isocyanides to benzenediazonium salts in the presence of sodium or potassium carboxylates. The reaction involves nitrilium intermediates which may be trapped by water or carboxylic acids to form amides and imides after Mumm rearrangement.



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Though the efficiency of isocyanides[1] as strong ligands for transition metals has been recognized very early, the disclosure of metal catalyzed arylation of isocyanides[2] has only been explored quite recently[3]. In most of these studies, the formation of a metal-aryl complex starting from aryl iodide or bromide is followed by isocyanide insertion and trapping of the metal-imidoyl complex with various nucleophiles. These three-component couplings are mostly described with palladium and suffer from the high coordinating nature of isocyanides which often limits their efficiency to the use of bulky isocyanides. To circumvent these difficulties, the choice of a metal with moderate affinity for isocyanides or the development of metal-free arylation would be highly desirable. It is in this context that we herein present new three-component couplings involving isocyanides and aryl diazonium salts.

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POSTER

Synthesis of Ruthenium Complex of 1-[5-(4-aminophenyl)10,15,20-tri-(4-methylphenyl)porphyrinatozinc]-4-(2-pyridyl)-1,2,3-triazoles as Sensitizers for Photodynamic Therapy (PDT)

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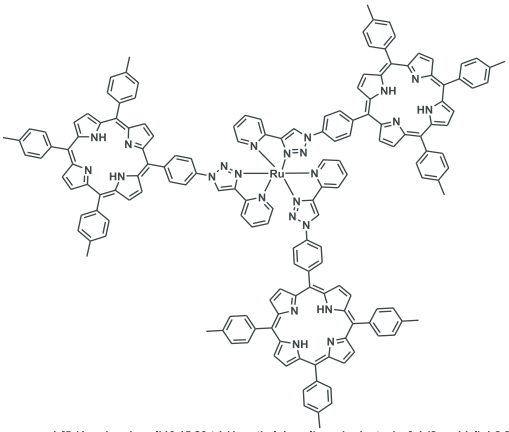
Photodynamic therapy (PDT) is an emerging treatment for different types of cancers. It involves the inactivation of living cells by the combined action of light, a photoactive molecule called sensitizer and molecular oxygen. A variety of sensitizers are being used in PDT. These include porphyrins, chlorins, bacteriochlorins, phthalocyanines, porphycenes, squaraines, cyanines, rose bengal, methylene blue, aminolevulinic acid, and their derivatives. Among these, porphyrins have attracted much attention as sensitizers due to their higher cellular affinity and very low dark toxicity. Photoinduced electron transfer or energy transfer processes in metalloporphyrin and ruthenium polypyridine complexes are of special interests in mimicking photosynthetic molecules, which makes them useful in photodynamic therapy, solar cells and molecular devices. The covalent linkage of zinc porphyrin with ruthenium(II)tris(bipyridine) complexes have been synthesized and intramolecular electron transfer or energy transfer between the $Ru(bpy)_3$ and porphyrin free base and their zinc complexes have already been reported. In present work, we have synthesized porphyrin containing 1,2,3-triazolyl-pyridine ruthenium complexes as PDT sensitizer. Click reaction is a Cu(I) catalysed azide-alkyne cycloaddition, which is an important, simple and efficient method for the synthesis of 1,4-aryl functional 1,2,3-triazoles. The required porphyrin was synthesized by the reaction of 5(4-azidophenyl)-10,15,20-triarylporphyrinatozinc with 2-ethynylpyridine to give 1-[5-(4-aminophenyl)10,15,20-tri-(4-methylphenyl)porphyrinatozinc]-4-(2-pyridyl)-1,2,3-triazole (A) using click reaction. It was further complexed with ruthenium(II)chloride to get the desired $Ru(A)_3$ complex and characterised by UV-visible, NMR and other spectroscopic techniques.



1-[5-(4-aminophenyl)10,15,20-tri-(4-methylphenyl)porphyrinatozinc]-4-(2-pyridyl)-1,2,3-triazole (A)

POSTER

Unexpected Effects of the Alteration of Structure and Stability of Myoglobin and Hemoglobin in Ammonium-Based Ionic Liquids

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The nature of solvent-biomolecule interactions is generally weak and non-specific, addition of ionic liquids (ILs), which emerged as novel and new class of solvents, strengthening the stability of some proteins whereas the same ILs weaken the stability of some other proteins. Although ILs are commonly used for the stabilization of biomolecules, the bimolecular interactions of their stabilization/destabilization is still an active subject of considerable interest and this approach has been limited. To reveal the impact of ILs on the stability of protein, a series of protic ILs possessing tetra-alkyl ammonium cation $[R_4N]^+$ with hydroxide $[OH]^-$ anion were synthesized. In this study, we report structural stability of heme proteins such as myoglobin (Mb) and hemoglobin (Hb) in a series of ammonium-based ILs such as tetramethyl ammonium hydroxide $[(CH_3)_4N]^+[OH]^-$ (TMAH), tetraethyl ammonium hydroxide $[(C_2H_5)_4N]^+[OH]^-$ (TEAH), tetrapropyl ammonium hydroxide $[(C_3H_7)_4N]^+[OH]^-$ (TPAH) and tetrabutyl ammonium hydroxide $[(C_4H_9)_4N]^+[OH]^-$ (TBAH) by fluorescence and circular dichroism (CD) spectroscopic studies. Our experimental results elucidate that less viscous IL carrying smaller alkyl chain such as TMAH is strong destabilizer of the heme proteins as compared to the IL carrying bulkier alkyl chain which is more viscous IL such as TBAH. Therefore, our results demonstrate that the addition of these ILs to the heme proteins decrease their thermal stability allowing the protein to be in unfolded state at lower temperature than their structure in their native state. Further, we describe the molecular structural interaction of the heme proteins with ILs (molecule like a ligand) by PatchDocking method.

POSTER

Synthesis and characterization of Porphyrins coordinated to ruthenium(II) polypyridyl complexes

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The versatility of porphyrins and metalloporphyrins as photo sensitizers is due to their structural and photophysical properties[1]. When coupled to their tumor targeting ability macrocycles like porphyrins are preferred for PDT as a treatment for cancer[2]. Ruthenium based cancer drugs have been of great interest over the past two decades in part due to their similarities to iron in biological systems, their numerous stable redox states under physiological conditions and the extensive library of synthetic complexes incorporating ruthenium.[3]

Coordination of two $[Ru(bipy)2Cl]^+$ moieties (where bipy = 2,2'-bipyridine) to the pyridyl nitrogens in the 5,10-positions of *meso*-5,10-bis-(4-pyridyl) 15, 20-bis-(4-methoxyphenyl) porphyrin gives the new diruthenium porphyrin complex. Electronic transitions associated with the ruthenium porphyrin complex include an intense Soret band and four less intense Q-bands in the visible region of the spectrum. An intense π–π^* transition in the UV region associated with the bipyridyl groups and a metal to ligand charge transfer (MLCT) band appearing as a shoulder to the Soret band are also observed.

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POSTER

Versatile Chlorin and Bacteriochlorin-NIR Fluorophore Conjugates for Tumor Imaging and Photodynamic Therapy

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Near-infrared (NIR) fluorescence imaging techniques have advanced considerably over the past few years; presently, they are being investigated for more challenging biotechnological and biomedical applications[1]. One such application is the *in vivo* imaging of biological targets and disease[2]. *In vivo* NIR fluorescence imaging is usually conducted within the spectral range of 700-900 nm because tissues and body fluids do not absorb NIR light. As a result, this facilitates deep tissue imaging and tissue autofluorescence is minimized.

Exogenous probes belonging to a family of polymethine cyanine-based fluorophores are in widespread use as NIR imaging agents. However, these compounds are usually not tumor-avid and generally have short half-lives. A number of recent reports though indicate that designing bifunctional agents containing NIR probes and tumor-avid photosensitizers (PS) may serve function of tumor imaging and PDT agents as well[3,4].

In the present study we synthesized a series of chlorin and bacteriochlorin based photosensitizers linked with various fluorophores. The photophysical properties, *in vitro* photobleaching characteristics and the effectiveness of these multifunctional agents for tumor imaging, with or without PDT have been examined.

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POSTER

Fructo- and Isomalto-oligosaccharides against Diabetes: Validation by *in silico* and *in vitro* Experiments

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This study evaluates the relative beneficial effects of fructooligosaccharides (FOSs), isomaltooligosaccharides (IMOs) and their various combinations on two proteins namely PPAR- and DPP-IV, known to have diabetic therapeutic potential. *In silico* docking studies were performed by GLIDE program for various FOSs and IMOs for PPAR- activationand DPP-IV inhibition. A total of nine oligosaccharides from FOS and IMO were docked. Panose, nystose and kestose showed highest ranking binding mode with DPP-IV and PPAR- and were selected for *in vitro* study either alone or in various combination. On its own nystose showed most potent DPP-IV inhibitory activity with an IC_{50} of 146.8 µM while panose at 20.2 µM concentration showed 50% binding ability to PPAR- -LBD. Combinations of oligosaccharides tested namely Nys+Pan, Nys+Kes and Pan+Kes demonstrated significantly ($p<0.001$) different effect on PPAR- and DPP -IV bioassay. Combination index of Nys25+Pan25, Nys25+Kes25 and Pan25+Kes25 were found to be 0.123, 0.158 and 0.195, respectively. Thus this study showed that the application of Nystose and Pannose reduce the complications of diabetes more effectively.

Keywords: Diabetes mellitus, fructooligosaccharides, isomaltooligosaccharides, molecular docking, dipeptidyl peptidase-IV inhibitor, peroxisome proliferator-activated receptor- gamma agonists, synergistic effect.

POSTER

Iron Configuration in the Type 2 Diabetes Profile using Ion Chromatograph: Probable Role of a Peanut Protein

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Iron overload in blood serum has been related with early onset of type 2 diabetes mellitus [1]. A comparative study was made between iron status and insulin resistance together with prevalence of nephropathy in type 2 diabetic population of South Kolkata, India. It was found that an index obtained from ($BMI \times Fe^{3+}/Fe^{2+}$) directly varies with insulin resistance in female subjects. Over the counter use of iron medications may now be seriously questioned as free iron was found to be significantly increased in diabetic population. Peanut protein, conarachin I was found to have high iron binding efficiency and was studied for its chelation effect for free iron in the blood serum *in vitro* for formulating probable remediations.

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POSTER

Synthetic Design of New Chiral Co(II) Based Peptide Complexes As Efficient Hydrolytic Cleavage Agents

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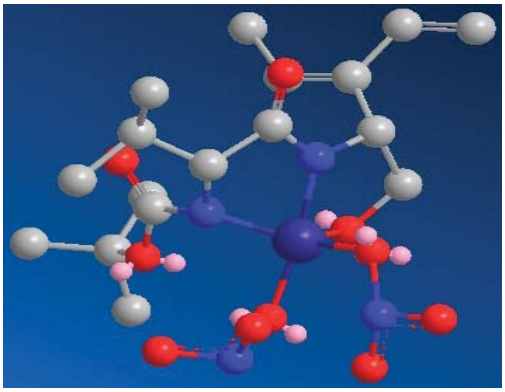
Amino–acid peptide conjugate complexes are of interest for application as targeted therapeutic delivery agents. Chiral Co(II) peptide conjugate complexes **1** & **2** (a,b) derived from condensation product of Boc–L–Valine & Boc–D–Valine & R/S-Phenyl glycinol in presence of coupling reagents DCC–DMAP were synthesised and thoroughly characterised. The stability of peptide conjugate was studied by Uv–vis and cyclic voltammetry which revealed complexes are quite stable. Preliminary DNA binding studies were carried out which revealed their strong propensity for ct–DNA. Further, cleavage efficiency of these complexes was evaluated by gel electrophoresis assay with pBR322 plasmid DNA. Co(II) complexes were found to be efficient hydrolytic cleavage agents and L–enantiomers of **1** & **2** were more promising than D–enantiomeric complexes.



Energy minimizes structure of Complex **1** (Ball and stick model)

POSTER

Synthesis of 2-alkyl-1, 3 thiazolyl-2-yl-quinazoline-4(3H)-one Derivatives: A New Class of Antibacterial & Antifungal Agents

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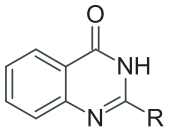
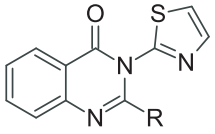
Since many years there has been an increasing interest in the chemistry of 4(3H)-quinazolinones, because of their broad biological activities. Many of the quinazolinones derivatives shows antibacterial, antifungal, antiviral, antitumor, anticonvulsant activities as well as the inhibitory effects for thymidylate synthase and poly- (ADP-ribose) polymerase [1-5].On the other hand, heterocyclic containing aminothiazole nucleolus also exhibit various pharmacological activities; reduction of blood pressure [6], anticonvulsant activity [7].Because of the established biological activities, our own interest to synthesize 2-alkyl-1, 3 thiazolyl -2-yl- quinazoline-4(3H) one and their derivatives, the present work aims, the synthesis of series of 2-alkyl-1, 3 thiazolyl -2-yl-quinazoline-4(3H)-one & its substituted derivatives.

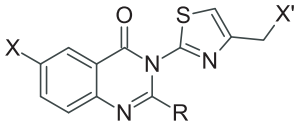
Anthranilic used as cheap raw material for preparation of 2-methylquinazolin-4(3*H*)-one, which was further coupled with 2-amino thiazole to prepare target molecule followed by substitution in aromatic and thiazole ring to prepare series of compounds [8]



R = -CH3, -CH2-CH3



R = -CH3, -CH2-CH3



X= -Cl,-Br,-I,-O-CH3, X' = Cl,-Br,-I,-O-CH3

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POSTER

Novel C_5-Curcuminoid and Aminoquinoline Based Molecular Hybrids: Synthesis and Investigation of Anticancer Activity

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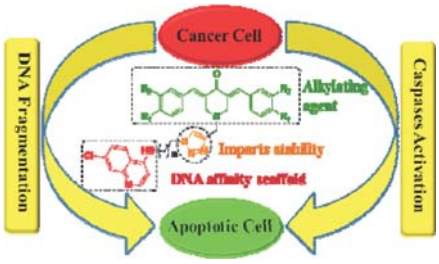
Cancer remains a principle cause of death worldwide with 7.6 million deaths in 2008 and expected to cross the figure of 13 million deaths by 2030 [1]. Cancer patients often receive a combination of therapies and palliative care such as surgery, radiation, chemotherapy etc. Anticancer drugs such as alkylating agents, antimetabolites, plant alkaloids, topoisomerase inhibitors and cytotoxic antibiotics have been used extensively in cancer chemotherapy [2-3]. Major problems associated with these existing drugs are their unfavorable side effects and their high cost in the market. Therefore, based on these findings, clearly there is a cogent need to develop novel, efficacious and affordable chemotherapeutic agents. Quinoline based molecules possess high ability to exhibit anti-proliferative and antitumor activity [4]. Similarly, the natural product 'curcumin' has shown a wide range of biological activities, including anti-cancer potential, anti-arthritis etc [5]. Previously we demonstrated that C_5-curcuminoid and 4-aminoquinoline based molecules exhibit potent anticancer and antimalarial activities [6-10]. Therefore, we anticipated that covalent hybridization of these two pharmacophores may lead to a molecule with improved anticancer activity. To test the hypothesis we covalently attached these pharmacophores *via* triazole linker. These hybrids were tested for anti-cancer activity on 60 human cancer cell lines, which represent diverse histologies. Our study has identified a set of hybrids that shows excellent growth inhibition at nano-molar concentration. The mechanistic investigation through series of assays shows apoptotic induction to cause anti-cancer activity.



C_5-cucuminoid-4-aminoquinoline hybrids mode of action on cancer cell line

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POSTER

Functionalization of Ampicillin Via Green Route and Evaluation of Antibacterial Activity Including Against Resistant Bacteria

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The excessive use of antibiotics against the widespread pathogenic bacteria which are developing continuous resistance against them via smart selection and mutation process has forced the researchers to look for newer methods and techniques to design effective antimicrobial agents. In present study a new series of Ampicillin-based antimicrobial polymers (AMPs) were synthesized via greener routes as potential antimicrobial agents and their antimicrobial activity was studied against resistant bacterium. The above said AMPs were synthesized via lipase-catalysed esterification with polyethylene glycol (PEG) and ethylene glycol (EG) by simple PEGylation and acrylation methods, respectively. The resulting polymers were then transformed into nano-particles by emulsion method. The AMPs were characterized by different techniques i.e. FTIR , NMR, XRD, SEM, EDAX and TEM. The antimicrobial studies were carried out against two bacteria resistant and susceptible. The series of AMPs synthesized in present work has proved themselves more potent and efficient antimicrobial agents when compared against the parent compound Ampicillin.

Keywords: Ampicillin, Antimicrobial polymers, Resistant bacteria, Antibiotics.

POSTER

University of Delhi

PP-216

POSTER

Reagent-based DOS: Developing a Diastereoselective Methodology to Access Spiro Cyclic and Fused Heterocyclic Ring Systems

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ABSTRACT

We report herein a diversity oriented synthesis (DOS) approach to synthesize biologically relevant molecular scaffolds. Our methodology enables facile synthesis of fused *N*-heterocycles, spirooxoindolones, tetrahydroquinolines and fused N-heterocycles. The 2-step sequence starts with a chiral bicyclic lactam-directed enolate addition/substitution. This is followed by a ring closure onto the built-in scaffold electrophile, leading to stereoselective carbocycle and spirocycle formation. We used *in silico* tools to calibrate our compounds with respect to chemical diversity and select drug-like properties. We evaluated the biological significance of our scaffolds by screening in two cancer cell lines. In summary, our DOS methodology yields novel, diverse scaffolds resulting in compounds that can have significance in medicinal chemistry.

INTRODUCTION

Small molecules make excellent drugs because of their ability to modulate the functions of proteins in living systems.[1] There is a continuous ongoing effort in the chemical community to discover novel chemical scaffolds that will access new chemical space and reveal interesting biological activity. Diversity oriented synthesis (DOS) provides an ideal platform to access novel compounds and has demonstrated great utility in the generation of structurally complex and skeletally diverse small molecules.[2] Efficient synthetic strategies coupled with rational design leads to generation of small molecules with architectural diversity & complexity and acceptable physicochemical properties. Evans[3a], and later Schreiber[3b] have pioneered library generation using the DOS approach. Popular DOS strategies include the build/couple/pair (B/C/P) concept pioneered by Schreiber[4], the "click, click, cyclize" strategy by Hanson[6] and others by Park, Shair and Spring.[5]

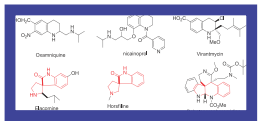
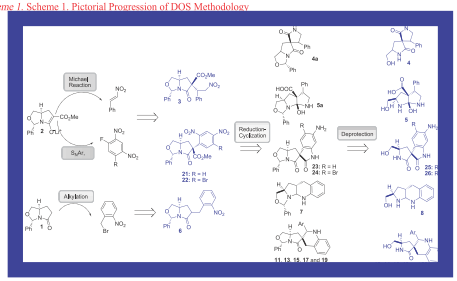


Figure 1. Biologically active spirooxoindoles, tetrahydroquinolines and pyroloquinolinolines

Biologically active spirocyclic indoles, tetrahydroquinolines and N-fused polycyclic ring systems provide a good platform to demonstrate the utility of our DOS methodology.[7] Spiroxoindolines *Elacomine* and *Horsfiline* (Figure1) are reported to have multiple biological activities (as antimalarial agents, inhibitors of p53:MDM2 receptors and as antimicrobial agents for both plant and human pathogens).[8] 1,2,3,4-tetrahydroquinoline (THQ) structures (like those present in *Oxamniquine*, *Nicainopril* and *Virantmycin*, Figure 1) are present in nature and exhibit antitumor & antibiotic properties, bradykinin antagonism and activity against a-adrenergic, histaminergic and muscarinic receptors.[9] Fused N-heterocycles show promising antiphlogistic activity in rats.[10] We aimed to keep our scaffolds as close to the *Rule of Three* as possible (M < 300; HBD ≤ 3 and HBA ≤ 3; clogP = 3; Number of rotatable bonds ≤ 3; Polar Surface Area = 60Å^2). These parameters are generally accepted to be most appropriate in creating fragment libraries.[11] Linear enantioselective synthesis of these scaffolds have been reported in the past.[12] However, to the best of our knowledge, this is the first reagent-based DOS methodology that allows access to these structurally diverse molecular scaffolds through common intermediates (**1** and **2**). We achieve skeletal diversity via a sequence that uses either an alkylation or a Michael addition or an S_NAr reaction on chiral bicyclic lactams (**1** and **2**). This is followed by cyclization of the intermediates (after nitro group reduction) to give polycyclic systems. The highlight of our methodology is a 3-step synthesis of 5 distinct natural product-inspired scaffolds. This methodology has an attractive *steps-per-scaffold-efficiency* while providing access to chemically complex end molecules.

Scheme 1. Scheme 1. Pictorial Progression of DOS Methodology



RESULTS AND DISCUSSION

Four unique bicyclic lactam based intermediates **3**, **6**, **21** and **22** were made using the protocol depicted in Scheme 1. Intermediate **3** was synthesized via by Michael addition of enolate of acyl bicyclic lactam **2** (generated with lithium diisopropyl amide (LDA) in tetrahydrofuran) to nitrostyrene at −78°C in ~50% yield and 9:1 diastereomeric ratio, separable by column chromatography. **2** in turn was synthesized by acylating **1** with methyl chloroformate and LDA at -78°C.[13] Utilizing two different hydrogenation conditions, the fused and the spiro- templates (**4**, **4a**, **5** and **5a**) were readily synthesized. Initial hydrogenation of **3** (H_2-Pd/C, 10% w/w) followed by *in situ* cyclization of the resulting amine provided the desired spirolactam **4a** and fused bispyrrolidine, **5a**. **4a** (70:30) was the major product under neutral hydrogenation condition (with EtOAc or IPA as solvent). On the other hand, during acidic hydrogenation (AcOH), the formation of **5a** was favored (60:40). TFA deprotection of the intermediates (**4a** and **5a**) generates **4** and **5** respectively.

In contrast, synthesis of interesting C(7) aminoaryl substituted ring fused system was initiated by alkylation of bicyclic lactam **1** with 2-nitrobenzylbromide in the presence of LDA at −78°C) to generate **6** in 80% yield as a 98:2 diastereomeric mixture (Scheme 3). The NOE studies of **6** confirmed the absolute configuration at C-7 as S (refer experimental). Reduction of the nitro group with 3 eq. of LAH, followed by *in situ* cyclization generated the desired fused system **7** in 56% yield. Chiral auxiliary removal was achieved upon treatment of **7** with TFA to generate alcohol **8** in 86% yield.

We attempted to build in more diversity at this stage by reducing **6** to the amine **9**, converting it to the benzaldehyde imine **10** and finally subjecting it to a novel base mediated 1,6- ring closures intramolecular addition to the imine. This generated the corresponding spiro-tetrahydroquinoline **11**, containing a chiral quarternary C-center. We attempted cyclisation of the crude imine **10** using various bases (Triethyl amine [TEA], K_2CO_3, Cs_2CO_3 and KH) at various temperatures (70-80°C) under thermal condition gave the desired product in extremely low yield (2-5%). However using microwave heating at 160°C with t-BuOK as base provided the desired product spirotetrahydroquinoline **11** in 76% yield and 95% *de*. Deprotection (TFA) generated the alcohol **12** in 67% yield. Gratified with the optimized cyclisation conditions, we went ahead and converted several crude imines to spirotetrahydroquinolines (**11**-**20**) in decent yield (~65%) and good diastereoselectivity (>90%). The absolute configuration of these molecules was established by X-ray crystallography of one of the representative compounds **13** for which the single crystal was generated in acetonitrile

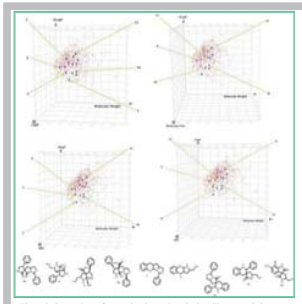


Figure 2. Comparison of our molecules against six drug like propertied relative to 1011 FDA approved drugs from GOSTAR database

Table 1. Cellular evaluation of the compounds against MCF-7 and HeLa cell lines

CONCLUSIONS

In summary, we have developed a 2-step sequence starting with a chiral bicyclic lactam-directed enolate addition/ substitution, leading to stereoselective carbocycle and spirocycle formation. A main objective of this paper - to explore new and diverse chemical space - has been achieved (Fig.2, ESP data and Fig.3, Drug-like properties). Additionally, we have demonstrated that the novel scaffolds and their derivatives show some biological activity in selected cancer cell lines. This DOS methodology serves to provide hits as starting points for medicinal chemistry campaigns.

ACKNOWLEDGMENT

The authors acknowledge GVK Biosciences Pvt. Ltd. for the funding and Dr. Raghuram S. Tangirala for his useful suggestions.

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Study of Interaction of Harmine with DNA Oligomers by Fluorescence Spectroscopy

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Harmine, a β–Carboline alkaloid, isolated from the seeds of Peganum *harmala* (Syrian Rue, family Zygophillaceae), recently has drawn attraction due to its antitumor activities. Harmine is widely distributed in nature, such as in various plants, marine creatures, insects, mammalians, human tissues and body fluids. Harmine (7-methoxy-1-methyl-9H-pyrido [3, 4-b] indole) is a tricyclic β-carboline alkaloid has antimicrobial, antiplasmodial, antifungal, antioxidative, antitumor, antimutagenic, cytotoxic and hallucinogenic properties. The mechanistic studies indicated that β -carboline derivatives inhibit DNA topoisomerases and interfere with DNA synthesis. They interact with DNA via intercalative modes and cause major DNA structural changes [1-5].

In present study, the interaction of harmine with 4 DNA oligomers viz. DNA-1: 5'-d(GATGGCCATC)$_2$, DNA-2: 5'-d(GATCCGGATC)$_2$, DNA-3: 5'-d(GGCAATTGCC)$_2$ and DNA-4: 5'-d(GGCTTAAGCC)$_2$ having AT/GC base specific central core was studied by fluorescence quenching method. The fluorescence quenching studies showed the binding of harmine with all four DNA oligomers having binding constant of 4.4×10^5 mole^{-1} with DNA-1, 5.5×10^4 mole^{-1} with DNA-2, 4.5×10^3 mole^{-1} with DNA-3 and 4.6×10^4 mole^{-1} with DNA-4. The results indicated that the binding of harmine with DNA oligomers with GC specific central core (DNA: 1) is greater as compared to other oligomers. This possibly indicated towards the binding preference of these alkaloids for GC specific sites.

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POSTER

An efficient one-step, chemo selective reduction of alkyl ketones over aryl ketones in β-diketones using LiHMDS and lithium aluminium hydride

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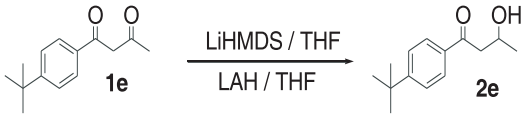
POSTER

Chiral β-hydroxy ketones are useful synthetic intermediates and have been used widely in the synthesis of natural products.[1] β-hydroxy ketones are very important synthetic intermediates in the synthesis of 1,3-diols, which are basic skeleton of polyene and poly macrolide antibiotics, for example, compactin, Rifamycin,[2] and Lonomycin A,[3] etc. There are many reported methods to synthesize β-hydroxy ketones, among them traditional aldol condensation, Mukaiyama aldol reactions[4] and boron mediated aldol condensations[5] of an aldehyde with ketone have been most widely studied. There are methods to synthesize β-hydroxy ketones starting from β-diketones such as ruthenium-BINAP catalyzed hydrogenation,[6] Pt/Al_2O_3 catalyzed hydrogenation, and reduction of both the ketones followed by selective oxidation, but these methods are poor chemo selective and step intensive.



We have developed an efficient, simple, fast one-step method for chemoselective reduction of alkyl ketones in the presence of aryl ketone in β-diketones using LiHMDS and LAH. This method will help researchers to prepare various β-hydroxy ketones, which are basic skeleton of many natural products and important synthetic intermediates in the synthesis of 1, 3-diols.

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Aminoquinoline-Pyrimidine Hybrids as Potent Nurr1 Agonists for the Treatment of Parkinson Disease

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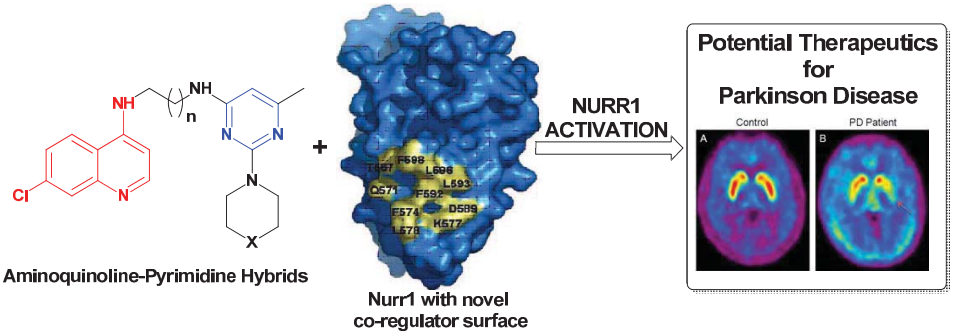
Parkinson disease (PD), primarily caused by the selective degeneration of midbrain dopamine generating neurons, is the most prevalent movement disorder and the second common neurodegenerative disorder after Alzheimer's disease affecting approximately seven million people globally. Currently, there is no cure for PD and only symptomatic treatments (e.g. L-DOPA) are available, which lose their efficacy over time, with associated severe side effects [1]. Thus, there is an ardent need to develop mechanism-based and/or disease modifying treatments for PD. Recent studies indicate that the orphan nuclear receptor Nurr1 is essential for the development and maintenance of midbrain dopaminergic neurons [2,3] and also for their protection from inflammation-induced death suggesting it as a promising target for the development of novel disease-modifying therapeutics for PD [4]. It does not possess a cavity for ligand binding but recently a novel hydrophobic interaction surface was identified that could serve as a molecular target for Nurr1 activating compounds. To address this possibility, a high-throughput assay system based on Nurr1's ability to directly activate tyrosine hydroxylase promoter function was established, which resulted in the identification of 4-amino-7-chloroquinoline scaffold as a potent Nurr1 activator. Moreover, linking this scaffold to various hetero-aromatics led to aminoquinoline-pyrimidine hybrids [5, 6] as promising Nurr1 agonists for the development of novel therapeutics for PD.



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POSTER

Synthesis, Characterization and Thermal Study Of 1,2,4-Triazole Derivatives

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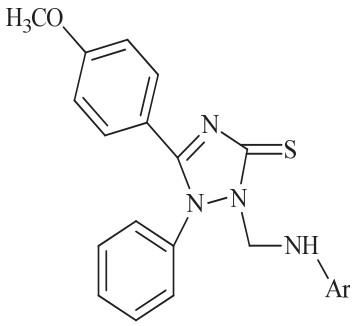
Three compounds of 1,2,4-triazole derivative were synthesized by condensation reaction. These synthesized compounds ($PM4_{a\text{-}c}$) have been characterized by various spectral techniques such as FT-IR, ^{1}H-NMR, ^{13}C-NMR and mass spectroscopy [1]. The thermal stabilities of these compounds ($PM4_{a\text{-}c}$) were investigated by simultaneous TGA and DSC methods. The decomposition steps and thermal behaviour of three compounds were investigated. The kinetic parameters such as order of reaction (n), energy of activation (E_a), pre-exponential factor (A), entropy of activation ($\Delta S^{\#}$), enthalpy of activation ($\Delta H^{\#}$) and Gibbs free energy of activation ($\Delta G^{\#}$) were evaluated by using Freeman-Carroll method [2-5]. The one step degradation for each compound and its correlation with thermal behaviour were also evaluated.

Keywords: Freeman–Carroll method, TGA and DSC analysis



Ar = Different aryl groups

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POSTER

Structural studies of symmetric DNA decamers containing (Pu-Pu-Py-Py) base specific central motifs

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Complementary Watson-Crick G-C and A-T pairs are the foundation of double helical nucleic acid structures, and current antisense oligonucleotide designed for drug therapy also rely on this complementarity for the specific interaction between antisense and target molecules.[1] 2D-NOESY is a convenient method for the structural elucidation of DNA decamer duplexes d-(GATGGCCATC)$_2$ (DNA-1) & d-(GGCAATTGCC)$_2$ (DNA-2) containing four 5'-(Pu-Pu-Py-Py)-3' motifs. The NMR assignment of the exchangeable and non-exchangeable protons of the DNA decamers was carried out in H_2O and D_2O respectively.

Sequential assignment of H6↔H1' NOE cross-peaks of purine residues showed relatively stronger intensity than pyrimidine residues in both DNA decamers. This suggests that the purine residue has C3'-exo type sugar puckering, whereas for pyrimidine remain in C2'-endo conformation. Pyrimidine base (T3) was found to have *Syn* type of geometry in DNA-1 while in DNA-2 bases attained a regular conformation and so such base perturbations were observed.

The line shape of the amino-proton resonances gives information on the rotation of the NH_2 group about the C-N bond. The observed NOEs indicated qualitatively that, in solution form, the DNA decamer helix has constitutively right handed and close to the B-form of DNA.

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POSTER

Synthesis and Non Covalent Interactions of Double Decker Porphyrin of Cerium

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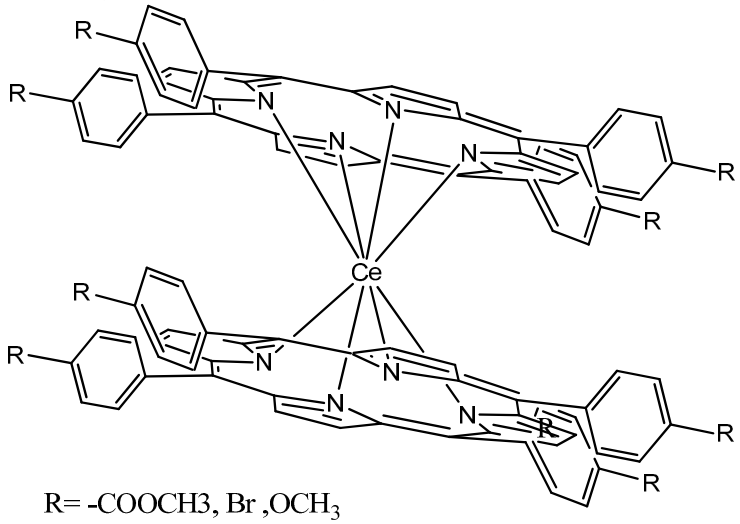
Cerium is one of the most important elements in lanthanide series that benefits plant growth. There has been increasing interest in the application of rare earth metals to medicinal plants in recent years. The double decker sandwitch structure of rare earth elements with chlorophyll has been proposed which acts as model system of special pair of bacteriochlorophyll. Various tetrasubstituted porphyrins have been employed for the synthesis of Ce(IV) double decker porphyrins. The allosteric binding of homoleptic and heteroleptic double decker porphyrins with silver(I) ions has been studied using UV–Visible spectroscopy. UV studies confirm the strong π-π interaction between two porphyrin rings. Further it also confirms that homoleptic double decker porphyrins containing symmetrical porphyrins exhibit pronounced allosteric effect as compared to homoleptic double decker porphyrins containing unsymmetrical porphyrins.



R= -COOCH3, Br ,OCH_3

POSTER

Synthesis of Pyrimidine Analogues of Triazole Linked Chalcone

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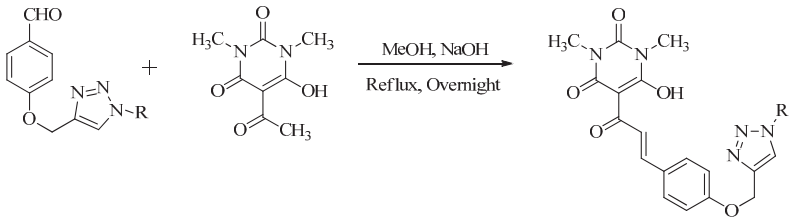
Chalcones are products of condensation of aromatic aldehydes with acetophenones in the presence of alkali. Chalcones and their derivatives constitute an important group of natural products and are an attractive molecular scaffold for the search of new biologically active molecules.[1] A number of chalcones having hydroxy, alkoxy groups at different positions have been reported to possess antimicrobial, anticancer, antitubercular and ,antiviral activities.[2]

In view of interesting pharmacological properties, we herein report the synthesis of triazole linked chalcone derivatives with an aim to develop new antibacterial agents with novel structure. The antimicrobial activity of these compounds have been evaluated *in vitro* by disc diffusion method against gram positive and gram negative bacterial strains and compared with standard drug gentamycin.[3]



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POSTER

Microwave assisted new route for synthesis of β-C-Glycoside

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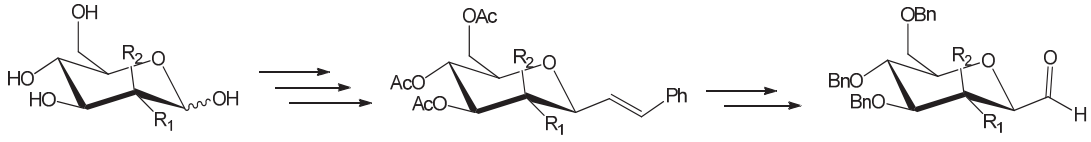
The C-glycosides are important class of Carbohydrate derivative as stable analogs of naturally occurring sugars[1]. They are resistant to chemical and enzymatic hydrolysis. These sugars mimetic possess an improved stability towards acid and bases also can play an interesting biological activity. Also C-glycosides are used as models in enzymatic and metabolic studies, because conformation of glucose, mannose and its C-linked analogs has little difference. C-glycosides are gaining the importance because of development in synthesis of C-linked disaccharides. They also found as precursor of various natural products. Amphidinol 3 (AM 3)[2], a bioactive secondary metabolite displays antifungal and hemolytic activity. Amphidinol 3 subunit can be synthesized from L-Mannose in a multigram scale easily. Ambruticine is an antibiotic which possess *in vivo* oral activity against fungal infection. Ambruticine subunit can be synthesized from D-Glucose. Many reports are previously published for the synthesis of C-glycosyl aldehyde[3]. In most of cases either yield is modest or starting materials are commercially expensive thus limiting their importance. A new DIPEA catalyzed tandom one pot mesylation and elimination reaction. Alkene was cleaved using $KMnO_4$ and $NaIO_4$ efficient route for the introduction of methylene group at anomeric position of pyranoside was developed via microwave assistance.



R_1 = OH D-Glucose
R_2 = OH D-Mannose

4a R_1=OAc
4b R_2=OAc

8a R_1=OBn
8b R_2=OBn

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POSTER

Standardization of homoeopathic drug *Rumex crispus*

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Rumex crispus Linn. (Yellow dock) is a perennial flowering plant in the family Polygonaceae and considered as a serious invasive weed in many areas. However, in traditional medicine the root of this plant has been used for the treatment of venereal diseases, rheumatism, hemorrhoids, bleeding and used synonymously with blood purifier, a tonic and laxative. Its roots are also largely recommended by herbalists for range of skin diseases, from spring eruption, to scurvy and as a tonic to the stomach and gastrointestinal system. The fruits have been given for the treatment of dysentery due to their astringent action (Grieve et *al*.) [1].The methanol extract of ripe fruit of *R.crispus* has been reported to demonstrate anti-oxidant activity both *in-vitro* and *in-vivo* models (Maksimović *et al*.) [2].The major chemical constituents of *R.crispus* are tannins and anthraquinones (Tayler *et al*.). [3]

In homoeopathy, *R.crispus* has been considered as one of the most potent drug and prescribed for treatment of bronchitis, chronic gastritis and intense itching of skin and anus (Boericke)[4]. It is, therefore, imperative to authenticate and document the standards to ensure its safety, efficacy and quality scientifically (Raina) [5]. In the present study, the physico-chemical standards viz., moisture content, alcohol content, wt. per ml., total solids, ash values, extractives values, T.L.C analysis and quantitative estimation of various phyto-chemicals have been determined for raw drug as well as finished product (mother tincture) of *R.crispus* and discussed. The data presented in this paper may be considered as physico-chemical standards for homoeopathic drug *R.crispus.*

Keywords: *Rumex crispus,* homoeopathic drug, standardization, T.L.C analysis

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POSTER

Polyaspartic based pH Sensitive Semi-Interpenetrating Absorbent Polymers

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Absorbent polymers have found various applications in the field of environment, drug delivery, personal hygiene products and for many other applications in the field of biomedical applications[1]. Research in the area of developing polyamino-acids based absorbent polymers have been reported[2,3]. Polyaspartic acid and acrylic acid based semi-interpenetrating polymers have been developed using different cross-linkers, N,N'-methylene bisacrylamide (NMBA), and Ethyleneglycol diethyleneglycol dimethacrylate (EGDMA). Free radical polymerization has been carried out using free radical initators viz. ammonium persulphate. The free radical polymerization has been carried out using thermal polymerization and microwave polymerization. The developed polymers have been characterized for their pH sensitivity. The absorbency and swelling characteristics have also been studied. The developed polymers have been characterized by IR, TGA, and NMR studies .EGDMA based polymers have given much better properties has compared to NMBA. Comparative study of the developed polymers has also shown positive results. The developed will have applications in the biomedical areas.

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POSTER

Synthesis, Characterization and Antimicrobial Activity of Some 1, 3, 4-Trihydro-4-aryl-6-(2-oxo-8-methylquinoline-3-yl) 2-oxopyrimidine

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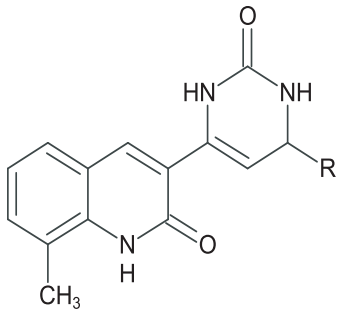
Quinolone derivatives possess high activity profile due to their wide range of useful biological properties including antibacterial and antimicrobial activity. On the other hand, oxopyrimidine derivatives were also showing remarkable pharmaceutical importance because of their diverse biological activities. In the last decade, biological interest in oxopyrimidine nucleus has been extended to several activities such as anti-inflammatory, antitumor, antiviral and antimycobacterial. Inspired from the biodynamic activities of oxopyrimidine and quinoloine derivatives, we have designed and synthesized a new series of hybrids molecules containing oxopyrimidine and quinolone scaffold for the biological evaluation.

All the synthesized compounds have been confirmed by spectroscopic method such as ^{1}H NMR, IR and Mass spectrometry as well as elemental analysis. The synthesized compounds were evaluated for their antimicrobial activity against *B. spinzi, S. aureus, S. aerogen* and *E. coli*. The details synthetic methodology and biological studies will be discussed in poster.



R= Aryl

POSTER

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Synthesis and Biological Evaluation of Some Dihydropyrimidine Derivatives bearing Substituted Quinoline Nucleous

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During last decade, there is a considerable evidence have been observed to find potential of thienopyrimidine derivatives and quinoline and its derivatives occupy a unique place in a field of medicinal chemistry due to their wide spectrum therapeutic activities. A series of dihydropyrimidine derivatives have been prepared by condensation of Aldehyde, Ketone and Thiourea in presence of alcoholic KOH as catalyst. All the synthesized compounds have been confirmed by spectroscopic techniques such as PMR, FT-IR, Mass spectra and Elemental analysis. All synthesized compounds have been also evaluated for Antibacterial and Antifungal activity.

POSTER

An Efficient Synthesis and Cytotoxic Evaluation of Novel Coumarins Against MCF-7 cell lines

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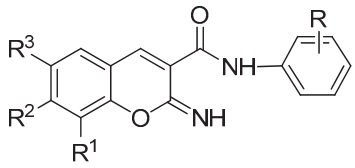
Cancer is a widespread lethal disease characterized by uncontrolled cell growth, invasion and sometimes metastasis. The therapeutic activity of most anticancer drugs is limited due to lack of selectivity for cancerous cells. Coumarins (known as 2*H*-1-benzopyrone-2-one) attracted intense interest from many decades due to their diverse biological activities such as anticancer, antiHIV, antibacterial, anticoagulant, antioxidant, anti-inflammatory, dyslipidemic, antitumor and antifungal [1-3]. Inspired from these results, we have decided to further explore 3-substituted coumarins by bioisosteric replacement at 2nd position with imine. Therefore, we have synthesized four series of novel 2-imino-2*H*-chromene-3(*N*-aryl)carboxamides **1** and evaluated their cytotoxic activity against MCF-7 breast cancer cell line. Compounds comprising 4-flouro and 3-methoxy phenyl ring exhibited significant cytotoxicity (IC_{50} = 15.5 µM), It is noteworthy that most of the synthesized compounds showed equipotent or better activity than standard Docetaxel. These novel 2-imino-2*H*-chromene-3(*N*-aryl)carboxamides have been identified as potential scaffolds for the further development of anticancer research.



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POSTER

Acid-Promoted Synthesis of Imidazolyl-pyrazole Derivatives via a Multicomponent Reaction under microwave irradiation

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A simple, efficient and expedient synthetic route has been developed for the construction of Imidazolyl-pyrazole derivatives via acid promoted multi-component reaction of substituted pyrazole aldehyde, ammonium acetate and diketone. The reaction proceeded smoothly with a range of functionalities to produce the imidazole scaffolds in good to excellent yields. Simple reaction conditions, easy work-up, avoid the use expensive reagents and low costs make this method valuable and attractive method to produce various tri-substituted imidazoles. The synthesized compounds were characterized by various analytical techniques such as 1H and 13C NMR, and Mass spectra. Various reaction conditions adopted and detail methadology for preparing the Imidazolyl-pyrazole derivatives will be discussed in the presentation.

POSTER

Highly Efficient and Eco-Friendly One-Pot Synthesis of Penta-Substituted Pyrrole Derivatives Under Catalyst-Free Conditions

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An eco-friendly and efficient one-pot synthesis of penta-substituted pyrrole derivatives via a four-component reaction of maldrum's acid, arylglyoxal monohydrate, dimethyl but-2-yne-dioate and amines under catalyst-free conditions in an environmentally friendly medium is described. The simple experimental procedure, catalyst-free reaction conditions, short period of conversion, and excellent yields are the advantages of the present method. Good chemical yields have been achieved without the need for chromatography and recrystallization or other purification methods. Detailed chemical synthesis and proposed mechanism will be discussed in in presentation.

POSTER

Synthesis and biological evaluation of (4-((5-(benzo[b]thiophen-2-yl) pyrazin-2-yloxy) methyl) piperidin-1-yl) (aryl)methanones.

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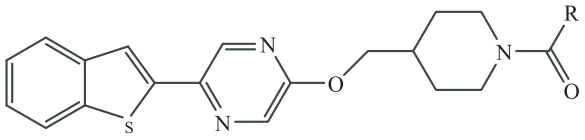
Pyrazine nucleus possesses remarkable pharmaceutical importance and biological activities, some of their derivatives occur as natural products. Pyrazine play an important role as intermediates for perfumes and food spices[1]. Extensive literature survey revealed very few published data on the synthesis of new pyrazine derivatives as potential anti tubercular [2], Cannabinoid (CB1) receptor antagonists [4] and HIV-1 Integrated inhibitors [5] agents. This observation prompted us to synthesize this nucleus so as to enhance the overall activities at resulting moieties can be evaluated. It was consider of interest to design and synthesize some 2-amino pyrazine derivatives shown as under.



Where R = various aryl acids

The constitution of all the synthesized compounds have been characterized by Elemental analyzer, FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy and further supported by mass spectroscopy. The purity of the compounds has been checked by thin layer chromatography.

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POSTER

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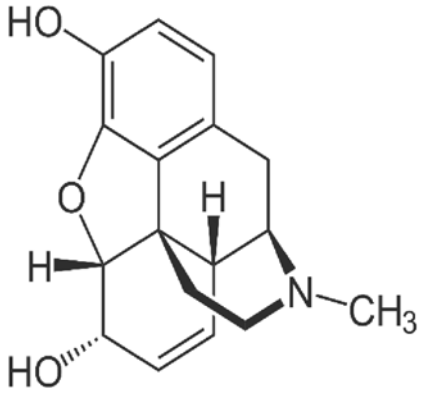

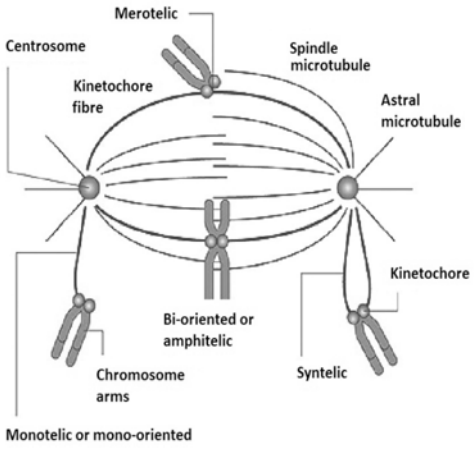

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