Commissioner of Collegiate Education, T.S. Hyderabad

National Science Day Celebrations - 2022

RUSA, TSCHE, NCSTC, DST (GOI) & TSCOST Sponsored

A two day National Seminar on

"Emerging Trends in Chemical and Materials Science Research"

(ETCMSR-2022)

25th & 26th FEBRUARY 2022

ISBN 978-93-91576-61-5

Organized by

DEPARTMENT OF CHEMISTRY

SR & BGNR Govt. Arts & Science College (Autonomous) Khammam - 507 002.
Telangana, India
(Reaccredited at B++ by NAAC)

RUSA & TSCHE Sponsored

Two day National Seminar on

“EMERGING TRENDS IN CHEMICAL AND MATERIALS SCIENCE RESEARCH”

(ETCMSR-2022)

On the occasion of “National Science Day Celebrations-2022”

25Th & 26 Th FEBRUARY 2022

Supported and Catalysed by

Telangana State Council Of Science & Technology

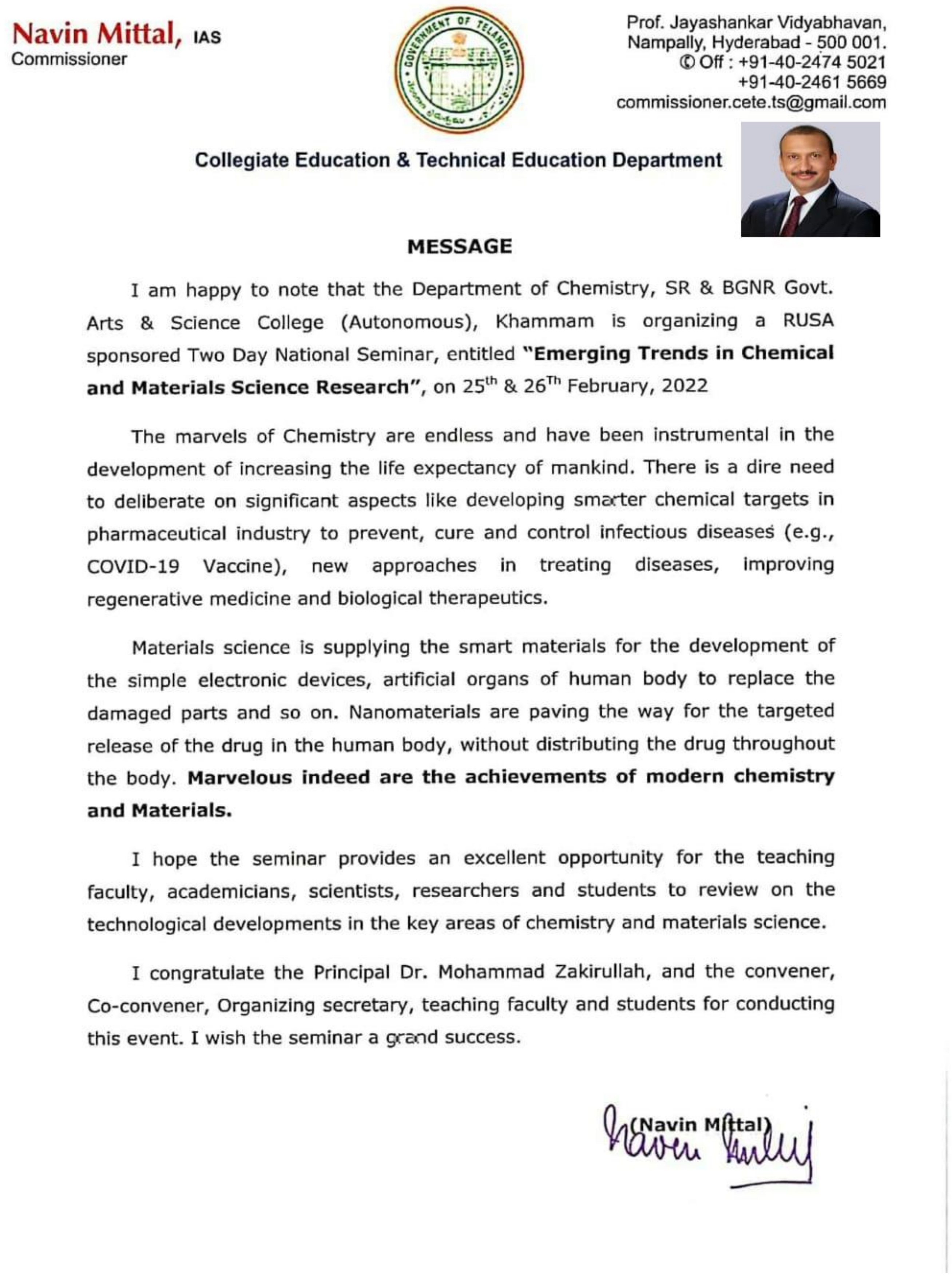
(TSCOST)

Organized by

DEPARTMENT OF CHEMISTRY

SR&BGNR. Govt. Arts & Science College (Autonomous),
Khammam
(Re-accredited at ‘B^{++}’ by NAAC)

Dr. P. Ramesh	**Dr. V. Shanti Kumar**	**Dr. M. Subramanyam**	**Dr. Mohd. Zakirullah**
Convener	**Co-convener**	**Organising Secretary**	**Chairman & Principal**



Navin Mittal, IAS
Commissioner

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Collegiate Education & Technical Education Department

MESSAGE

I am happy to note that the Department of Chemistry, SR & BGNR Govt. Arts & Science College (Autonomous), Khammam is organizing a RUSA sponsored Two Day National Seminar, entitled **"Emerging Trends in Chemical and Materials Science Research"**, on 25th & 26Th February, 2022

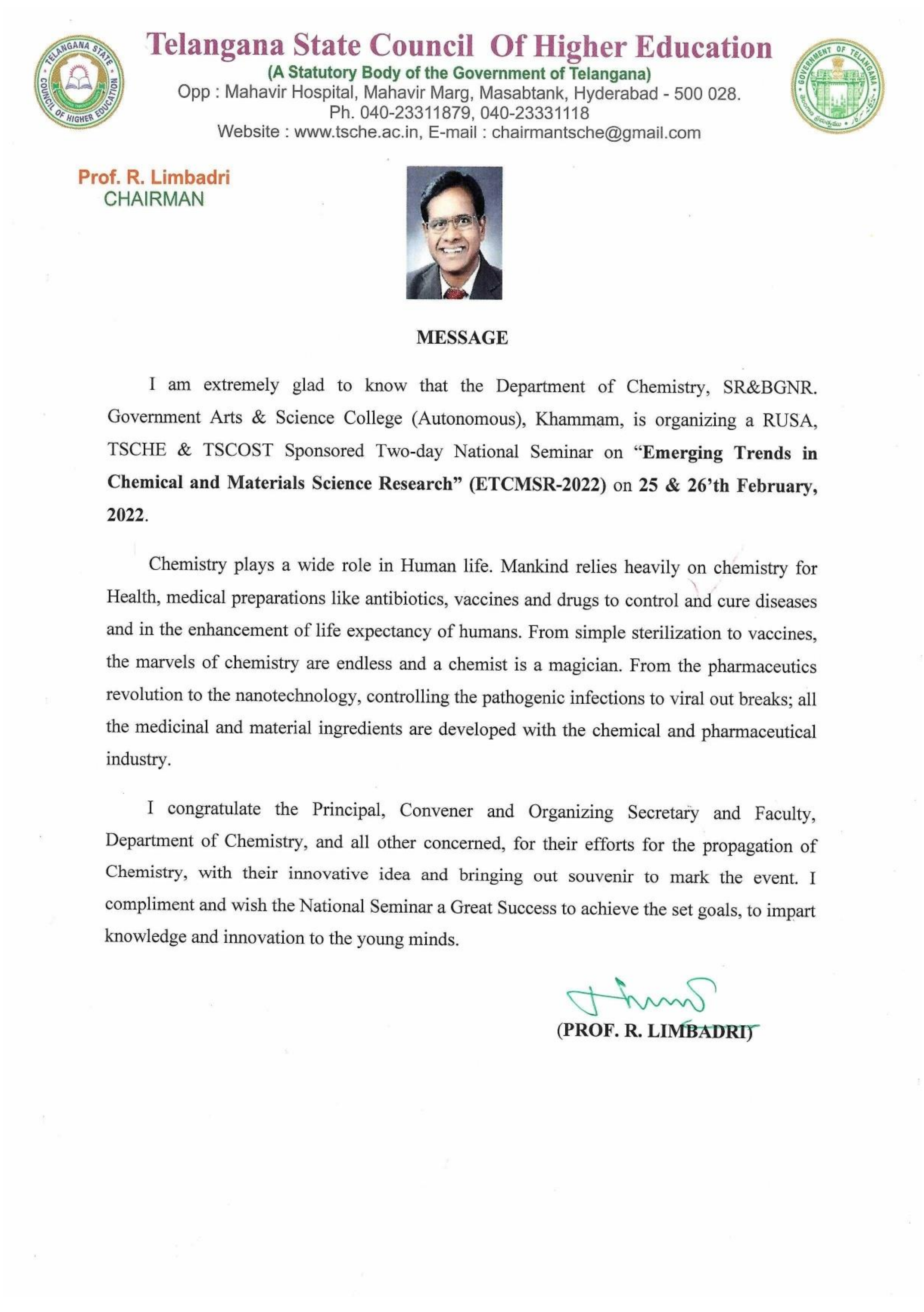
The marvels of Chemistry are endless and have been instrumental in the development of increasing the life expectancy of mankind. There is a dire need to deliberate on significant aspects like developing smarter chemical targets in pharmaceutical industry to prevent, cure and control infectious diseases (e.g., COVID-19 Vaccine), new approaches in treating diseases, improving regenerative medicine and biological therapeutics.

Materials science is supplying the smart materials for the development of the simple electronic devices, artificial organs of human body to replace the damaged parts and so on. Nanomaterials are paving the way for the targeted release of the drug in the human body, without distributing the drug throughout the body. **Marvelous indeed are the achievements of modern chemistry and Materials.**

I hope the seminar provides an excellent opportunity for the teaching faculty, academicians, scientists, researchers and students to review on the technological developments in the key areas of chemistry and materials science.

I congratulate the Principal Dr. Mohammad Zakirullah, and the convener, Co-convener, Organizing secretary, teaching faculty and students for conducting this event. I wish the seminar a grand success.

(Navin Mittal)



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Prof. R. Limbadri
CHAIRMAN

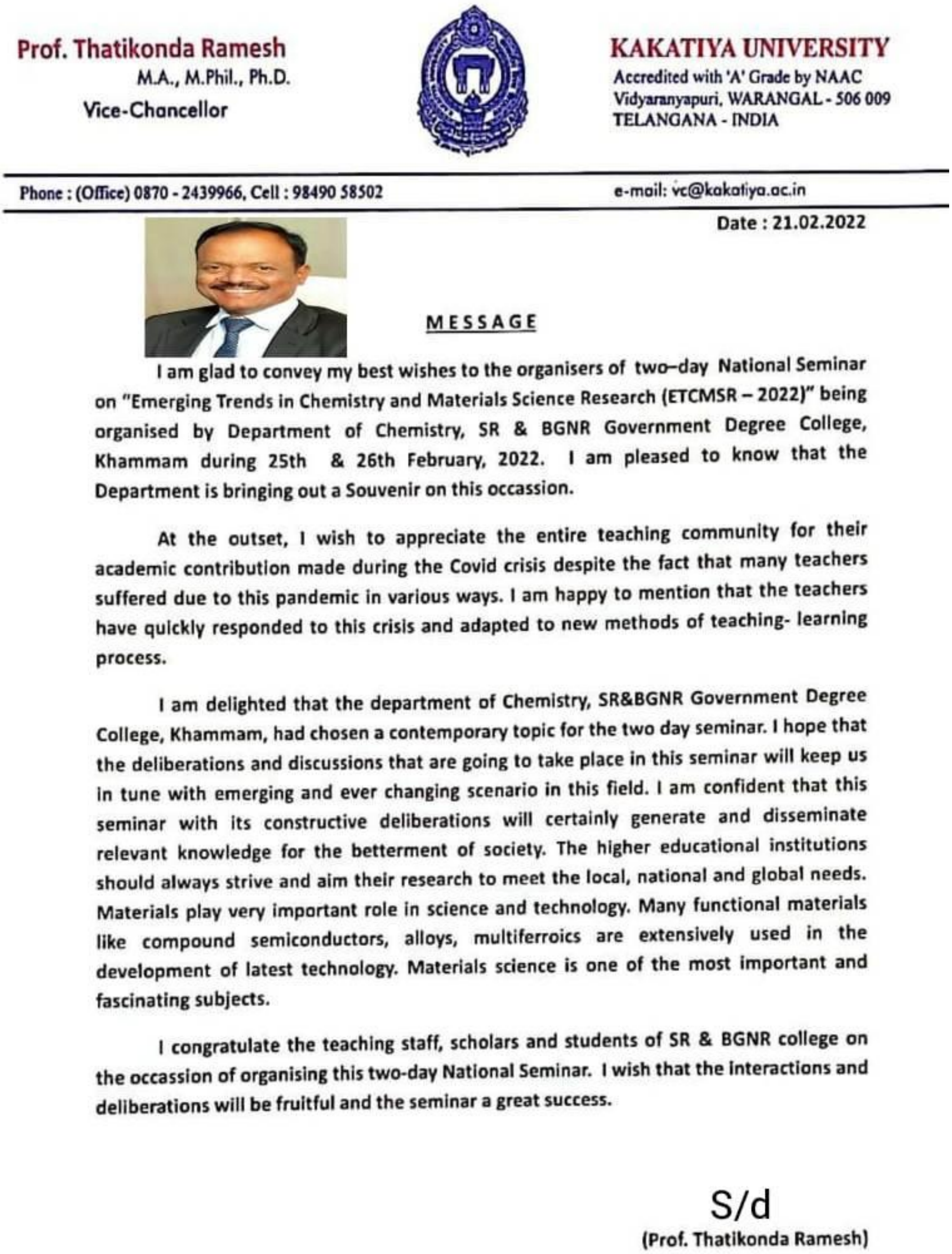
MESSAGE

I am extremely glad to know that the Department of Chemistry, SR&BGNR. Government Arts & Science College (Autonomous), Khammam, is organizing a RUSA, TSCHE & TSCOST Sponsored Two-day National Seminar on "**Emerging Trends in Chemical and Materials Science Research" (ETCMSR-2022)** on **25 & 26'th February, 2022**.

Chemistry plays a wide role in Human life. Mankind relies heavily on chemistry for Health, medical preparations like antibiotics, vaccines and drugs to control and cure diseases and in the enhancement of life expectancy of humans. From simple sterilization to vaccines, the marvels of chemistry are endless and a chemist is a magician. From the pharmaceutics revolution to the nanotechnology, controlling the pathogenic infections to viral out breaks; all the medicinal and material ingredients are developed with the chemical and pharmaceutical industry.

I congratulate the Principal, Convener and Organizing Secretary and Faculty, Department of Chemistry, and all other concerned, for their efforts for the propagation of Chemistry, with their innovative idea and bringing out souvenir to mark the event. I compliment and wish the National Seminar a Great Success to achieve the set goals, to impart knowledge and innovation to the young minds.

(PROF. R. LIMBADRI)



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Vice-Chancellor

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Date : 21.02.2022

MESSAGE

I am glad to convey my best wishes to the organisers of two–day National Seminar on "Emerging Trends in Chemistry and Materials Science Research (ETCMSR – 2022)" being organised by Department of Chemistry, SR & BGNR Government Degree College, Khammam during 25th & 26th February, 2022. I am pleased to know that the Department is bringing out a Souvenir on this occassion.

At the outset, I wish to appreciate the entire teaching community for their academic contribution made during the Covid crisis despite the fact that many teachers suffered due to this pandemic in various ways. I am happy to mention that the teachers have quickly responded to this crisis and adapted to new methods of teaching- learning process.

I am delighted that the department of Chemistry, SR&BGNR Government Degree College, Khammam, had chosen a contemporary topic for the two day seminar. I hope that the deliberations and discussions that are going to take place in this seminar will keep us in tune with emerging and ever changing scenario in this field. I am confident that this seminar with its constructive deliberations will certainly generate and disseminate relevant knowledge for the betterment of society. The higher educational institutions should always strive and aim their research to meet the local, national and global needs. Materials play very important role in science and technology. Many functional materials like compound semiconductors, alloys, multiferroics are extensively used in the development of latest technology. Materials science is one of the most important and fascinating subjects.

I congratulate the teaching staff, scholars and students of SR & BGNR college on the occassion of organising this two-day National Seminar. I wish that the interactions and deliberations will be fruitful and the seminar a great success.

S/d
(Prof. Thatikonda Ramesh)

Prof. G. BRAHMESHWARI
M.Sc., Ph.D.
HEAD

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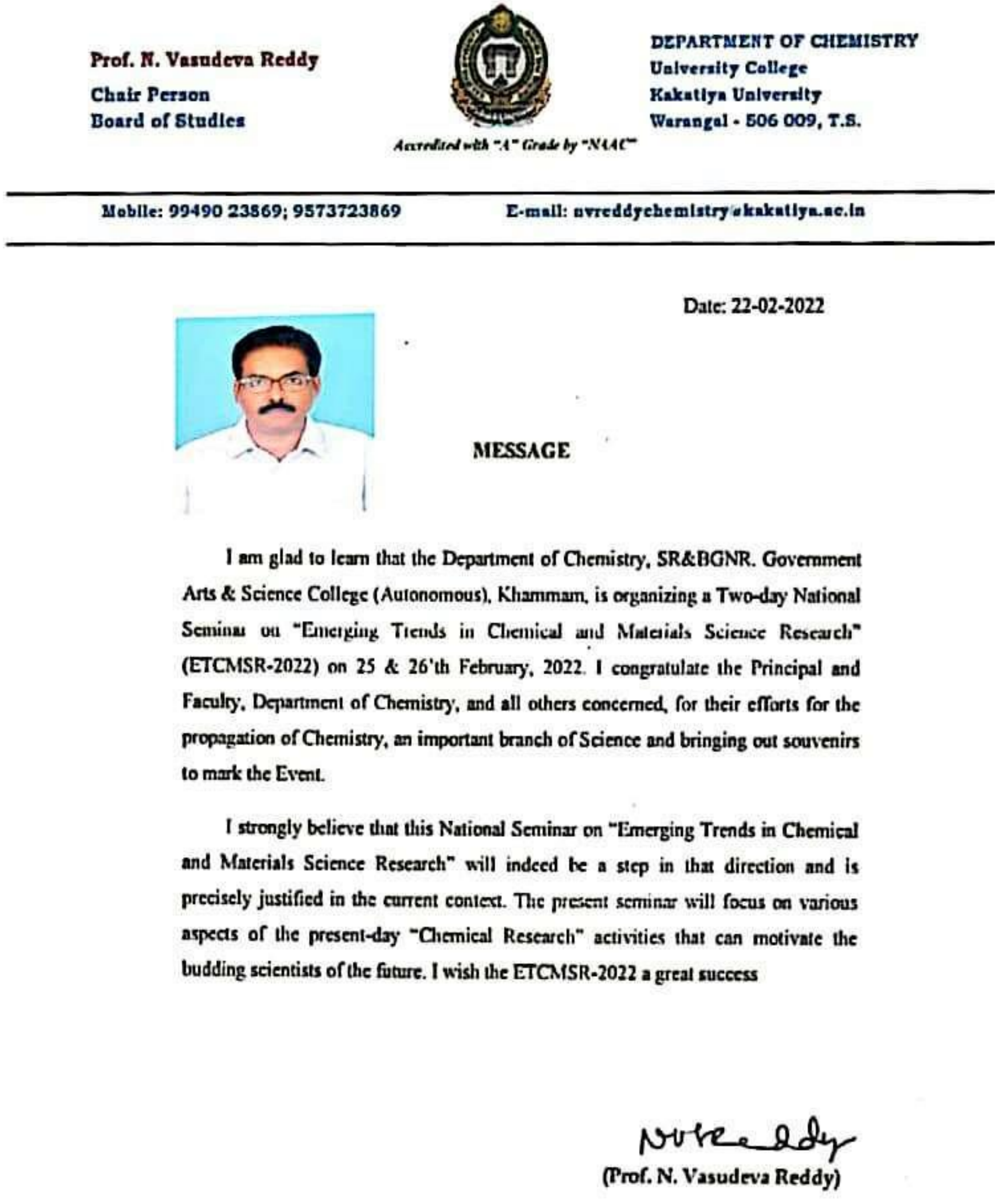
MESSAGE

I am happy to know that the Department of Chemistry, SR&BGNR Govt. Arts & Science College (Autonomous) is going to organize a Two day National Seminar on “Emerging Trends in Chemical and Materials Science Research”(ETCMSR-2022) on 25th & 26th February , 2022.

Chemistry research will help human life to face major challenges which are raised in the society, such as creating and securing supplies of energy and food improving and maintaining accessible health and developing and ensuring sustainable management of water and air quality.

“I wish the Seminar a grand success”

(Prof.G.Brahmeshwari)



Prof. N. Vasudeva Reddy
Chair Person
Board of Studies

Accredited with "A" Grade by "NAAC"

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Date: 22-02-2022

MESSAGE

I am glad to learn that the Department of Chemistry, SR&BGNR. Government Arts & Science College (Autonomous), Khammam, is organizing a Two-day National Seminar on "Emerging Trends in Chemical and Materials Science Research" (ETCMSR-2022) on 25 & 26'th February, 2022. I congratulate the Principal and Faculty, Department of Chemistry, and all others concerned, for their efforts for the propagation of Chemistry, an important branch of Science and bringing out souvenirs to mark the Event.

I strongly believe that this National Seminar on "Emerging Trends in Chemical and Materials Science Research" will indeed be a step in that direction and is precisely justified in the current context. The present seminar will focus on various aspects of the present-day "Chemical Research" activities that can motivate the budding scientists of the future. I wish the ETCMSR-2022 a great success

NVReddy
(Prof. N. Vasudeva Reddy)

S.R &B.G.N.R. Govt. ARTS & SCIENCE COLLEGE
(Autonomous)
KHAMMAM - 507 002, Telangana
NAAC B++& ISO Certified 9001:2015

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Dt: 22-02-2022.

MESSAGE

I am happy to note that the Department of Chemistry, SR&BGNR. Government Arts & Science College (Autonomous), Khammam, is organizing a RUSA, TSCHE & TSCOST Sponsored Two-day National Seminar on “**Emerging Trends in Chemical and Materials Science Research” (ETCMSR-2022)** on 25 & 26 th February, 2022. Chemical science is instrumental in the development of modern medicine, from diagnosis to life saving drugs, antibiotics and vaccines, thus increasing the life expectancy of the mankind.

I extend warm greetings to the convener, co-convener, organizing secretary and the faculty of the department of chemistry for their untiring efforts in organizing a Two-day National Seminar on important area of today’s science which focuses and seek to answer the challenges like AIDS, Hepatitis-B to COVID-19 viral out breaks, constantly pose a great threat to humanity, in spite of the fact that science has marvelously controlled non-communicable diseases, with minimizing the side effects on one hand and environmental pollution on the other hand.

I hope the seminar provides an excellent platform of opportunity for the teaching faculty, academicians, scientists, researchers and students to review and discuss on the technological developments in the key areas of Chemistry and Material Sciences, for the continuous education on human health and environment.

I am thankful to the RUSA & TSCHE for providing financial assistance to conduct the Two-day National Seminar. I am grateful to the Telangana State Council of Science & Technology (TSCOST) for extending financial support to organize the programme on the occasion of ‘**National Science Day Celebrations-2022**”.

Finally, I congratulate the Convener, Co-convener, Organizing Secretary and Faculty, Department of Chemistry for conducting this event. I wish the Seminar a grand success.

(Dr Mohammad Zakirullah)
Principal

RUSA, TSCHE & TSCOST sponsored

Two day National Seminar on

“Emerging Trends in Chemical and Materials Science Research” (ETCMSR-2022)

25Th & 26 Th February, 2022

Organized by
DEPARTMENT OF CHEMISTRY
SR&BGNR. Govt. Arts & Science College (Autonomous), Khammam
(Re-accredited at ‘B^{++}’ by NAAC)

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Co-convener : Dr. Vadiga Shanti Kumar
Organizing secretary : Dr. Madala Subramnyam

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About the Institution

Sri Rama and Bhaktha Gentela Narayana Rao Govt. Arts & Science College, **Khammam** was established in the year 1956 under private management initially. The then Honorable Chief Minister Sri Boorgula Rama Krishna Rao and the then District Collector of Khammam Sri G.V. Butt, took the initiative for its establishment along with a committee formed with the elite of the town. The primary objective was to provide higher education to the students of the marginalized rural sections and Tribal community of Khammam District. The College was named after the Chief Donor, **Sri Rama and Bhaktha Gentela Narayana Rao**. The College was taken over by the state government on 1-09-1959 and it acquired permanent affiliation to the Osmania University in 1972. Eventually the affiliation is transferred to the Kakatiya University, Warangal.

About the Department

Department of Chemistry is one of the oldest departments in this college. It was started along with establishment of SR&BGNR. Govt. Arts & Science college (A) in 1956 .The department offering two years M.Sc., Chemistry (Post Graduation) and three years B.Sc., Physical Sciences and Life Sciences (Under Graduation) courses to the student community. It consists of four big well equipped laboratories, one Research Laboratory and eight eminent faculty members. The Under Graduate and Post Graduate curriculum contains Drug chemistry, Spectroscopy, Green chemistry, polymer chemistry, Separation techniques(i.e., Solvent extraction, chromatography), Heterocyclic chemistry, Natural products chemistry, stereochemistry, surface chemistry, Organometallic compounds, Analytical chemistry, Bioinorganic chemistry, photochemistry, Nanomaterials, in such a way to compete in academic and industrial areas at national and international scenario. We are conducting extension lectures to the students on different topics by inviting eminent professors from various universities, scientists from various research institutions (OU, KU, NIT, IICT, NIPER, etc) and industrial personnel from various industries.

Conducting various activities like field trips, study projects, (**like State Level Jignasa Projects Student Study Projects**), visiting industries, research institutes like IICT, NIT, NIPER etc, to impart knowledge and exposure on industrial knowledge among the students. We are encouraging the students to participate in workshops, seminars, conferences, symposiums, conducted by various institutions and organizations. The department faculty is engaged in various innovative projects funded by UGC. Conducting this seminar will helps the student community and the society to interact with the leading academics, scientists, researchers, industry personnel to exchange and share their knowledge and research results about all aspects of health and Environmental protection through lectures and presentations. During this seminar, it is expected that challenges encountered and the solutions to be adopted in sustainable development and Human health and environmental protection would be discussed.

Theme of the Seminar

Chemistry has provided the backbone in understanding the structure, organization and functions of living matter. The ability of plants to derive energy from sunlight and animals and humans to derive energy begins with chemistry and the principles of thermodynamics and basic of food itself are made of chemical and biological structures-Amino acids, sugars, lipids, Nucleotides, Vitamins, minerals and hormones.

Chemists and the chemical sciences have been integral to the development of modern medicine from diagnostics to drugs and the creation of the Pharmaceutical industry. The result has been a steady improvement in our health as life expectancy over the past century. Numerous challenges to human health still remain. Deadly infectious diseases including Malaria, Cholera and Tuberculosis may have been largely conquered in high income regions of the world but remain a major threat in poorer regions such as Africa. Even in richer nations infectious diseases remain a constant threat, the swine flu pandemic in 2009, Novel COVID-19 outbreak in 2020 and the dramatic increase of antibiotic resistance has made clear.

Modern health systems are struggling to cope with the demand for novel and more effective vaccines, antibiotics, as pathogens develop resistance to existing treatments. There is an urgent need for new drugs to fight multi-resistant infectious agents as our present vaccines, antibiotics become ineffective due to global misuse in medicine and the food industry.

Corona virus disease (COVID-19) is an infectious disease caused by the SARS-CoV-2 virus. Most people infected with the virus will experience mild to moderate respiratory illness and recover without requiring special treatment. However, some will become seriously ill and require medical attention. Older people and those with underlying medical conditions like cardiovascular disease, diabetes, chronic respiratory disease, or cancer are more likely to develop serious illness. Anyone can get sick with COVID-19 and become seriously ill or die at any age.

The best way to prevent and slow down transmission is to be well informed about the disease and how the virus spreads. Protect yourself and others from infection by staying at least 1 metre apart from others, wearing a properly fitted mask, and washing your hands or using an alcohol-based rub frequently. Get vaccinated when it's your turn and follow local guidance. In the treatment of COVID-19 various drugs like Azithromycin, Doxycycline, Favifirvir, Remedesivir, Bavesuzumab, Tocilizumabplays vital role. Invention of Covaxin, Covishield, Sputhnik, Pfizer covid-19 vaccines are controlling the spread of corona virus in the entire world.

Non-infectious diseases such as cardiovascular disease, cancer, diabetes and Alzheimer’s disease are becoming more prevalent. Millions of people are dying worldwide every year, which are major causes for death. Non-infectious diseases are caused by combined genetic and environmental factors, and cannot be cured, only controlled by current drugs. It has been predicted that, by 2030, non-infectious diseases will account for 69% of all deaths worldwide. This represents a significant challenge for modern science. In this connection it is the time to invent more efficient drugs to prevent, cure and control the non-infectious diseases. Developing innovative modes of drug delivery and new approaches to treat diseases, including personalized medicines, regenerative medicine and improved biological therapeutics are the need of the hour.

There is a growing need for public awareness about the environmental issues and for effective implementation of environmental regulations. Further, the pace of development of environmental science programs is not adequate. This has resulted in a gap in knowledge and environmental regulations between developed and developing countries. There is thus, a need for continuous education about human health and environment which needs a forum for exchange of ideas and knowledge. It is important that the student community need to participate in such forums.

Finally, it’s not only a question of what we can synthesize, but also how we do it. Since human growth and economic pressures are now forcing the chemical community to search for more efficient way to perform chemical transformations. Developing new route for Eco-friendly reactions i.e., **GREEN CHEMISTRY or GREEN SYNTHESIS** and their use in the chemicals, drugs, medicines etc, synthesis is keenly noticeable in all industrial countries since it reduces the reaction steps, selective towards target compounds with cheaper price. Hence “**Better Chemistry-Better Human health-Better Environment”.**

Therefore, the proposed National seminar on **“Emerging Trends in Chemical andMaterials Science Research”-(ETCMSR-2022)** aims to bring together leading academics, scientists, researchers and students along with industry personnel to exchange and share their knowledge and research results about all aspects of health and Environmental protection through lectures and presentations. During this seminar, it is expected that challenges encountered and the solutions to be adopted in sustainable development and Human health and environmental protection would be discussed.

Expected outcome

Conducting this seminar will helps the student community and the society of this rural area to interact with the leading academics, scientists, researchers, industry personnel to exchange and share their knowledge and research results about all aspects of health and Environmental protection through lectures and presentations. During this seminar, it is expected that challenges encountered and the solutions to be adopted in sustainable development and Human health and environmental protection would be discussed.

KEY NOTE

LECTURE

Influence of Nanotechnology on Traditional Medicine

Dr. K. Suresh Babu

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Abstract

Concurrent with human civilization, plants have been their true companions as source of food and medicine. These plants have contributed significantly in discovery, design and development of several modern medicines. Recent move of society towards nature for the treatment of various diseases where there is no satisfactory cure in modern medicine has diverted the attention of natural/medicinal chemists and biologists to unravel their chemical characteristics and biological activities together in order to define their therapeutic potential in the light of modern pathobiological understandings. This move has led collectively to rediscover, design and refine the therapeutic application of medicinal plants.

During last eight years, we have studied several medicinal plants guided by *in vitro* based bioassays to delineate the chemistry of medicinal plants responsible for biological activities. This effort has led to identify several potent multiple active medicinal plants, their active fractions and synergistic molecular compositions. We have identified particularly, several free radical scavengers, cytotoxic and α-glucosidase inhibitory principles present in substantial yield in Indian Medicinal Plants. Presence of multiple active phytochemicals in rich concentrations in some of the medicinal plants therefore offers exciting opportunity for development of novel therapeutics and also provides scientific justification for their use in traditional medicines. In addition, some of the compounds isolated from these plants also displayed potent insecticidal activities. Therefore, biologically activity based chemical characterization of these medicinal plants may provide scientific explanation for their use in traditional medicines and also redesign and develop preparations for novel therapeutic applications. The opportunities in the development of this therapeutics from natural products are divided into four topics. Each topic will be exemplified with suitable examples.

Nanotechnology is an interdisciplinary research field developed with an amalgamation of chemistry, engineering, biology, and medicine, and has various useful applications in NDDS, and development of novel treatments.

Nanoparticles are the end products of a wide variety of physical, chemical and biological processes some of which are novel and radically different, others of which are quite common place. Nanoparticles may be defined as submicron (<1µm) colloidal systems, generally, but not necessarily, made of polymers (biodegradable or not). Herbal drug in the nano carriers will increase its potential for treatment of different chronic diseases and health benefits. Treatment of chronic diseases like cancer using the targeted drug delivery nanoparticles is the latest achievement in the pharmaceutical drug delivery field. For instance, PLGA nanoparticles loaded with camptothecin (a cytotoxic alkaloid isolated from *Camptotheca acuminate*) and conjugated with antibodies against colorectal tumour cells. It was observed that the uptake of antibody-nanoparticles was increased in the cell compared to the nanoparticles without the antibody and increased cytotoxicity of camptothecin.

The combination of nanotechnology with traditional herbal medicine may provide a useful tool in designing future herbal medicine with improved bioavailability profile and less toxicity. Now a day's nanotechnology is rapidly expanding in the herbal industries include potentially field of medicines and cosmetics. Traditional Medicine will contribute to human health care in the 21st century. Still, there are many challenges to the safety and effective use of traditional medicine. But there is huge scope for nanotechnology based traditional medicines. It is long way to go..........

Keywords: Biological activities, traditional medicine, nanotechnology, targeted drug delivery.

INVITED

LECTURES

Diversity Oriented Synthetic Methodologies for the Molecules of Biological Interest

Prof. Mandava V. Basaveswara Rao
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Abstract

Methodologies to synthesize molecules of commercial value and their derivatives of biological importance is the attractive area of research, thereby creating library of known and unknown molecules having potential applications. Synthetic methods that allow rapid access to large number of diverse structural arrays is growing constantly, which served as a new driving force for the new innovations. In order to synthesize large number of molecules with high level of diversity and complexity, In addition to developing new synthetic techniques and reagents, organic chemists are exploring new methods to design and to evolve new molecules, strategies for new molecules leading to new source of diversity and improving the quality of compound libraries of natural product origin. This diverse new methodologies that will create structurally diverse compounds efficiently in high yields and with excellent purity and with wide range of functional groups as handles to expand them further. One of the richest sources of diversity in drug discovery is development of synthetic routes for the natural products and their derivatives.

Natural products isolated from marine and terrestrial origins, in addition to exhibiting biological activity, also serve as rapid scaffolds for further display of broad range of functionalities. For several years, we have been engaged in design and development of new efficient methodologies for a wide variety of heterocycles, displaying a range of skeletal and functional group diversity. The biological properties of heterocycles in general make them one of the prime interests of the pharmaceutical industry, storage device platforms for opto-electronic industry.

We have synthesized various heterocyclic skeletons initially and utilized them for making other heterocycles. All the synthetic methodologies reported by us are simple efficient and does not involve hitherto costlier chemicals, circuitous reaction pathways, drastic reaction conditions and corrosive molecules. We have exploited [4+2] cycloaddition reactions, [3+3]Cycloaddition reactions, indolo[2,3]quinodimethanes and dienolates, anion assisted aromatic annulations, heteroaromatic annulations and doubly handled reactions. Our aromatic and heteroaromatic annulation strategies are highly efficient, simple and results in variety of molecules with quantitative yields.

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Development of new Methodologies using Bismuth (III) and Iron (III) salts as green catalysts

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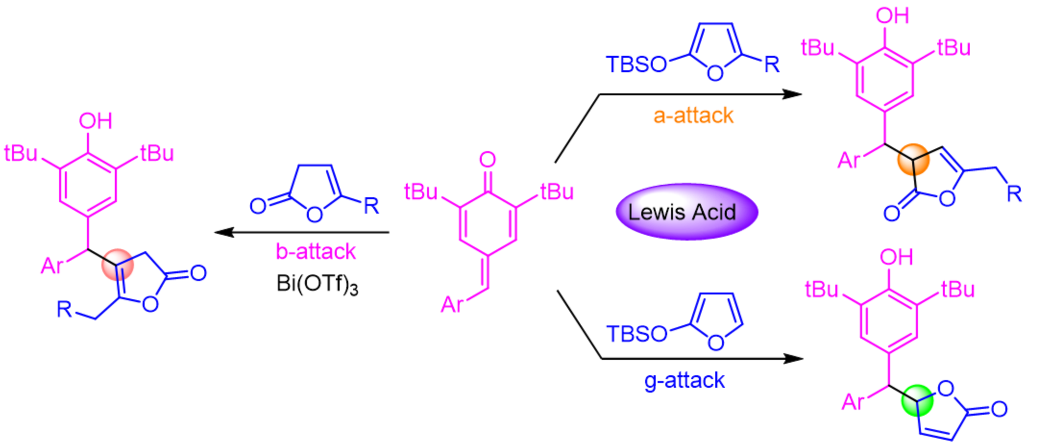
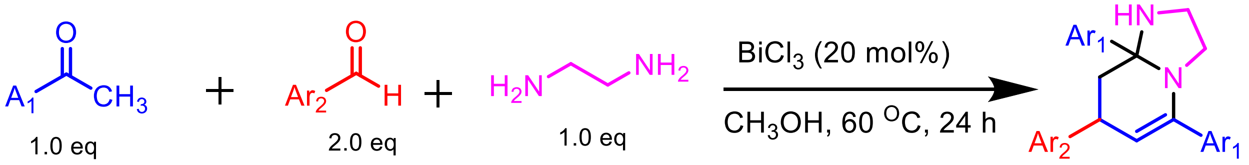
Our research is widely focused on Bismuth (III), Iron (III) salts catalyzed green reactions. A Lewis acid catalyzed regioselective C−C bond is constructed through β-addition of deconjugated butenolides with p-quinone methides in a 1,6-conjugate addition manner. Interestingly, Bismuth triflate lewis acid catalyzed vinylogous Mukaiyama−Michael reaction of silyloxyfurans with p-QMs proceeds selectively through α or γ position exclusively. The reaction is mild with broad substrate scope, thus allowing easy access to a wide range of bis-arylated α-/β-/γ-substituted butenolides.



The synthesis of nitrogen containing heterocycles is of particular interest in the pharmaceutical industry due to the range of biological activities exhibited by such compounds. Their synthesis using multicomponent reactions saves steps, and minimizes waste generation. The bismuth(III) chloride multicomponent synthesis of a series of hexahydroimidazo[1, 2-*a*]pyridines is a green protocol. Bismuth (III) compounds are especially attractive from a green chemistry perspective because they are remarkably nontoxic, non-corrosive and relatively inexpensive. The method avoids chromatography and an aqueous waste stream.



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Molecular Hybridization Approach: Accelerating the Design of New Anticancer Agents in Drug Discovery

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Cancer is a growing lead cause of mortality and accounts for the major morbidity worldwide. In the recent years, several approaches are being investigated to develop an effective cure, to curb the alarming increase in the number of cancer cases across the globe. The complex biological networks and heterogeneous nature of cancer displays a high degree of challenge at the tissue and cellular levels. Due to the proliferative nature of cancer cell and multi-drug resistance in cancer,[1] DNA becomes one of the most promising biological targets for developing anticancer agents. Hence, there is a need towards the exploration of nature inspired heterocycles and their derivatives to identify novel leads for cancer therapy. In cancer drug discovery, structural modifications and the fusion of pharmacophoric sub-units on these scaffolds aid the development of highly potent and selective hybrid molecules *via* molecular hybridization approach (**Figure 1**)[2]. It is a new concept in the drug design and development based on the combination of two different pharmacophoric moieties to produce a novel hybrid scaffold with improved affinity and efficacy, when compared to the parent drugs.

In continuation of our efforts in the design and synthesis of new chemical entities (NCEs) of anticancer agents, herein we combined the structural artifacts of several different bioactive heterocyclic scaffolds assembled as a new single hybrid. In this way, our research group have successfully generated a library of new compounds based on molecular hybridization approach by employing different heterocyclics such as isatin, 3-alkenyl oxindoles, β-carbolines, benzimidazoles, 1,2,3-triazoles/tetrazoles, podophyllotoxins, chalcones, pyrrolobenzodiazepines, thiazolidinediones, phenathrenes, etc., and tested their cytotoxicity on different human cancer cell lines by utilizing different *in vitro* assays. Some of the representative molecules have shown significant anticancer activity at nanomolar range in selected human cancer cell lines.

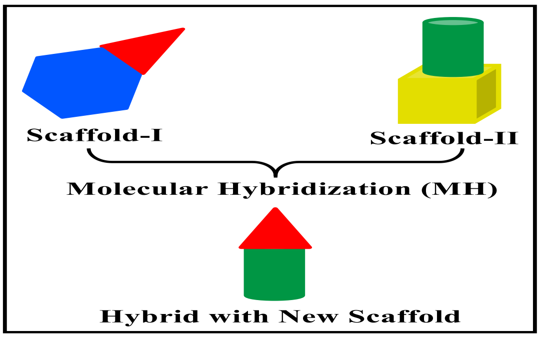

Figure 1. Molecular hybridization approach.

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Development of a Rapid and Cost-Effective and Feasible Method for the Evaluation of Vitamin D Deficiency Using Advanced Mass Spectrometry Based Methods

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Abstract

The change in lifestyle and work of the people has led to the emergence of new diseases and deficiencies over the world. One of the major deficiencies would be the vitamin D deficiency that may not sound too threatening, but has very great impact on the health and lives of people. The deficiency in turn causes many severe diseases and deficiencies such as rickets in children and osteomalacia, hypertension, myocardial infarction, Stroke, Diabetes, Atherosclerosis and cancer in adults. Moreover, the recent studies have greatly researched on the harmful impact of vitamin D deficiency is with the COVID -19 pandemic, where it has increased possibility of increasing the risk of lives in COVID patients. In Telangana especially in Hyderabad there are about 60-65 % of vitamin D deficit cases shooting up at orthopedics' clinic and moreover in rural areas the awareness over the requirement of Vitamin D is negligent along with ignoring mind set and cost issues for testing. More concerns over the children, senior citizens and women of Telangana is considered as the vitamin D deficiency can cause decreased calcium and phosphate absorption in turn causing bone related problems.

On viewing these problems, there comes the requirement of developing cost effective, sensitive and rapid testing methods for evaluating vitamin D concentrations for common people to afford without hesitation and can keep their health on-check. Hence the present study involves the gas chromatography coupled mass spectrometry with trimethylsilyl derivatization (TMS-GC-MS-MS) is the most suitable protocol for quantitative analyses of Vit-D3. Performance of method was evaluated and compared with LC-MS/MS and conventional immuno assay method. Method validation has been carried out with various blood samples. The limit of quantitation of TMS-GC-MS/MS method is 1.5 ng/ml with good linear correlation. Furthermore, the dietary intake and nutritional status of vegetarian and non-vegetarians were assessed by our validated method. As a result, this vitamin D nutrition survey demonstrates that most people have insufficient vitamin D. Our results can be used to develop dietary suggestions and monitor risk to improve health.

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Design and Synthesis of Spiroheterocyclics as Potent Anticancer and Antitubercular Agents

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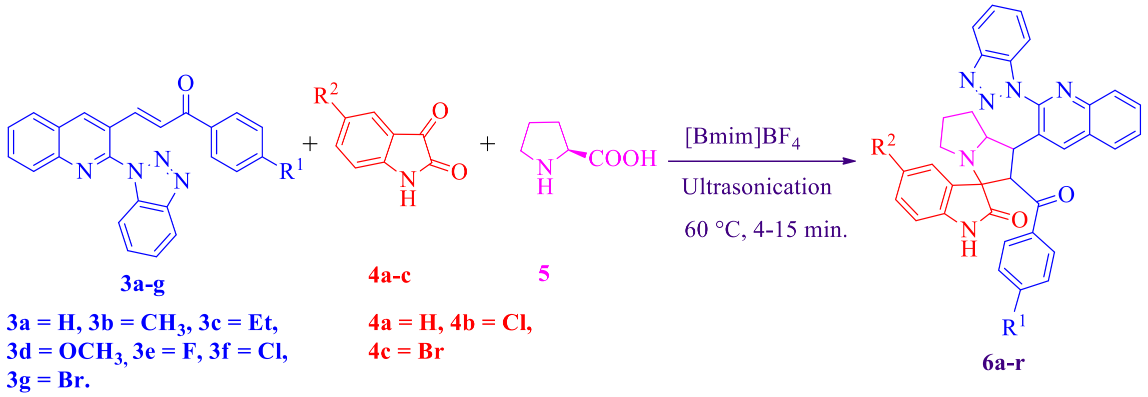
Abstract

The essential need for the potent anticancer and antitubercular agents with high selectivity and safety profile prompted us to synthesize a new series of spiroheterocyclics, spiropyrrolizidines. These compounds were synthesized by one-pot multicomponent [3+2] cycloaddition reaction under reflux/ultrasonication. Further, *invitro* anticancer and antitubercular activities were evaluated against human lung carcinoma (A549) and human cervical (HeLa S3) cancer cell lines and *Mycobacterium tuberculosis* H37Rv respectively.



3a-g

3a = H, 3b = CH_3, 3c = Et,
3d = OCH_3, 3e = F, 3f = Cl,
3g = Br.

4a-c

4a = H, 4b = Cl,
4c = Br

5

6a-r

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Design, Synthesis of Temperature and Co-ordination Dependent Superhydrophobic MOFs for Gas Separation and Oil Spills Cleanup Applications

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Porous coordination polymers (**PCPs**), which also known as metal-organic frameworks (**MOFs**) are emerged as potential materials of the decade, particularly forgas storage, separation, catalysts and sensors etc. However, PCPs existing in the literature were mostly instability with respect to moisture and bulk water. Besides these traditional **PCPs**, we have been designed and synthesized an organic rich low density, $BTMBH_3$=1,3,5-benzenetris(*m*-benzoic acid)) ligand. Using this novel ligand we achieved first time a series[1-3] of six new superhydrophobic porous coordination polymers (**SPCPs**), with molecular formulae, $\mathbf{Zn_4(\mu_3\text{-}OH)_2(BTMB)_2\supset Guest}$ **(1)**,$\mathbf{Zn_2M_2(\mu_3\text{-}OH)_2(BTMB)_2\supset Guest}$ [**M** = **Co** (**2**) and **Ni** **(3)**],$\mathbf{Pb(H\text{-}BTMB)\supset Guest}$ **(4)** and$\mathbf{M_4(OH)_2[(BTMB)_2(4,4'\text{-}Bipy)_3]\supset Guest}$ [**M** = **Zn** (**5**) and **Cd** **(6)**]. These interesting **SPCPs**, possesses an aromatic terminating low density surface that is highly corrugated over the nano-scale causes the superhydrophobic (self-cleaning) nature with contact angles >150°.[4-6] Moreover, this superhydrophobic nature is stable even at high temperature, whose stability depends on structure, metal coordination and guest species *etc*.

All these **SPCPs** exhibit very interesting gas separation and, oil and organic solvent spills cleanup applications. In this presentation, we discuss, synthesis, structures, characterizations, properties and applications these novel **SPCPs**. However, compound, **6**, converted from hydrophobic at RT to hydrophilic at 70°C.[6] This study can provide a roadmap for design and synthesis of novel superhydrophobic porous materials for the applications in the energy and securing the environment.

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Advancement of Nanomedicine in Cancer Therapy

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Nanomedicine has been considered a possibility since Richard Feynman originally described the concept of nanotechnology in his renowned Caltech address, "There's Plenty of Room at the Bottom," in 1959. Various types of environmentally sensitive polymeric nano carriers for cancer chemotherapy have been discovered in recent years. However, after systemic administration of the drug, the efficiency of drug release in the tumour microenvironment is reduced, owing to the early release of the drug prior to reaching the tumour cell.

An intracellular acid cleavable Schiff's base polymeric drug micelle for systemic and local administration of doxorubicin, an anti-cancer medication, has been developed. The polymer nanomedicine is composed of hydrophilic PEG chains of varying molecular weight that are covalently bonded to Doxorubicin via imine linkage. Such formulations prepared from nanoparticles of pH-sensitive PEG–drug conjugates mayalso be envisioned to be extended to formulate other hydrophobic drugs for local delivery with propellant-based inhalers to otherpulmonary disorders, thus broadening the impact of the proposed strategy.

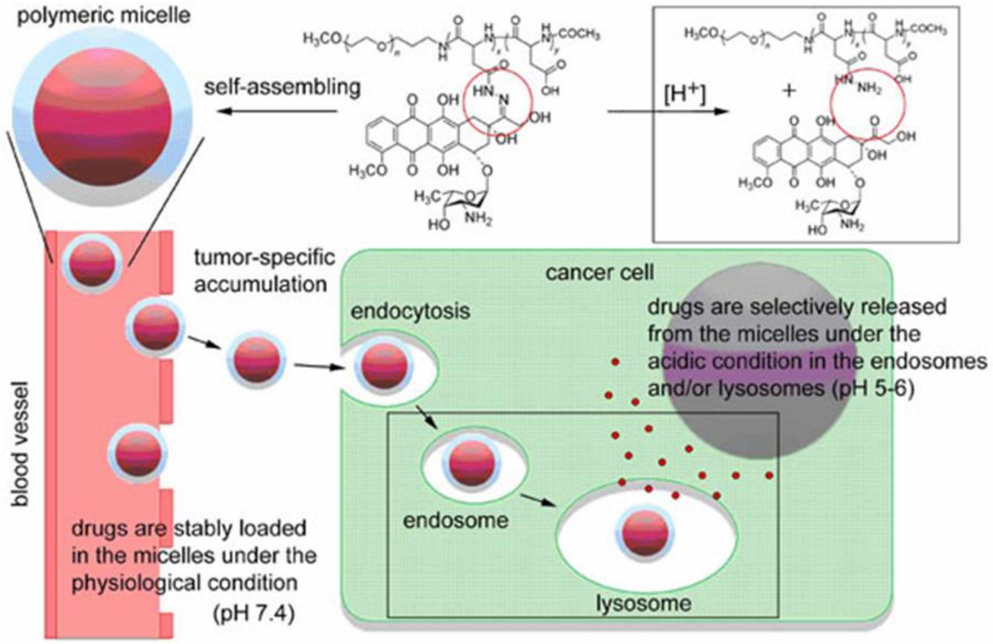

Fig. 1. Tumor-specific accumulation and intracellular pH-dependent drug release mechanism of micelle doxorubicin.

Key words: Nanomedicine, Cancer, Biomaterials, Polymers, PEG, Doxorubicin

Design and Synthesis of some Novel Heterocyclic Compounds and their Biological Evaluation

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Heterocyclic chemistry constitutes an essential branch of organic chemistry. Heterocycles are widely known to display a range of bioactive properties which are widely utilized in the pharmaceutical and agricultural sectors. Heterocyclic compounds, especially nitrogen heterocycles, are the most important class of compounds in the pharmaceutical and agrochemical industries, with comprising around 60% of all drug substances.

The nitrogen containing heterocycles form a diverse class of organic molecules and were found to possess many types of biologically interesting activities including anti-bacterial, anti-viral, anti-fungal, anti-cancer, anti-tumor, anti-inflammatory, anti-hypertensive, anti-convulsant and anti-diabetic properties.

This study covers the synthesis characterization and anti-bacterial, anti-inflammatory anti-oxidant and cytotoxicity evaluation of some new heterocyclic molecules containing benzimidazole, piperazine, triazole nuclei.

Synthetic Strategy – The Disconnection Approach

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Chemists have two major goals, one is to unravel the secrets of nature-advancing horizons of knowledge and the other is to make human life as comfortable as possible. Industrial chemists synthesize pharmaceuticals, polymers (plastics) pesticides, dyestuffs, food colorings, perfumes, detergents and disinfectants. While research chemists synthesize natural products whose structure is uncertain, compounds for mechanistic investigations, possible intermediates in chemical and biological processes and even compounds which might themselves be useful for organic syntheses.

Before and during these syntheses chemist has to plan the work and how about to undertake. One has to draw possible routes to achieve success. The important analytical approach in organic synthesis is disconnection or synthon approach. We start with the molecule we want to make (the target molecule) and break it down by a series of disconnections into possible starting materials. At last we shall devise a route using different easily available starting materials.

Organic Materials based on Hetero Polycyclic Aromatic Hydrocarbons for Organic Thin-Film Transistors Applications

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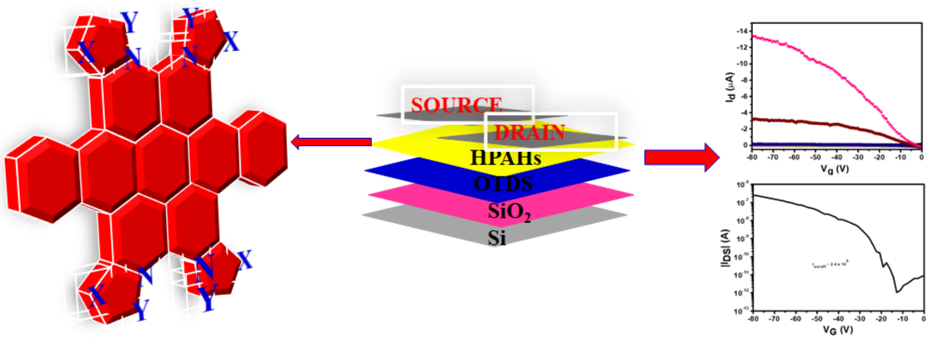
Abstract

The synthesis and characterization of a series of novel hetero polycyclic aromatic hydrocarbons (HPAHs) as a potential lead molecule in organic semiconductor devices with tetra-imidazolo or tetra-pyrazolo benzo-fused coronene as the main framework are reported. Incorporation of hetero atoms into polycyclic aromatic hydrocarbons (PAHs) by Corey-Fuchs reaction followed by photochemical cyclisation using iodine has been described for carrier mobility and hole transport properties. The synthesized coronenes, Tetraimidazocoronene (TIC), Tetraimidazobenzocoronene (TIBC), Tetraimidazodibenzocoronene (TIDBC), Tetrapyrazolocoronene (TPC), Tetrapyrazolobenzocoronene (TPBC), and Tetrapyrazolodibenzocoronene (TPDBC), have good physicochemical properties and are supported with DFT/TDDFT studies. On an ODTS-SiO_2 substrate at room temperature, the reported compounds were utilized to fabricate organic thin-film transistors (OTFTs) and shownhole mobilities in the range of 0.21-0.71 cm^2/Vs and with an on/off ratio of 10^4.



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Synthesis, antiproliferative and apoptosis induction potential activities of novel Bis(indolyl)hydrazide-hydrazone derivatives

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Abstract

In recent years, indole-indazolyl hydrazide-hydrazone derivatives with strong cell growth inhibition and apoptosis induction characteristics are being strongly screened for their cancer chemo-preventive potential. In the present study, N-methyl and N,N-dimethyl bis(indolyl)hydrazide-hydrazone analog derivatives were designed, synthesized and allowed to evaluate for their anti-proliferative and apoptosis induction potential against cervical (HeLa), breast (MCF-7 and MDA-MB-231) and lung (A549) cancer cell lines relative to normal HEK293 cells. The MTT assay in conjunction with mitochondrial potential assays and the trypan blue dye exclusion were employed to ascertain the effects of the derivatives on the cancer cells. Further, mechanistic studies were conducted on compound **5-bromo-1-methyl-N'-[(E)-(1-methyl-1H-indol-3-yl) methylidene]-1H-indole-3-carbohydrazide** to understand the biochemical mechanisms and functional interactions with various signaling pathways triggered in HeLa and MCF-7 cells. The above compound induced apoptosis via caspase independent pathway through the participation of mitogen-activated protein kinases (MAPK) such as extracellular signal related kinase (ERK) and p38 as well as p53 pathways. It originates the activation of pro-apoptotic proteins such as Bak and Mcl-1s and also strongly induced the generation of reactive oxygen species.

In downstream signaling pathway, activated p53 protein interacted with MAPK pathways, including SAPK/c-Jun N-terminal protein kinase (JNK), p38 and ERK kinases resulting in apoptotic cell death. The involvement of MAPK cascades such as p38, ERK and p38 on the above compound induced apoptotic cell death was evidenced by the fact that the inclusion of specific inhibitors of p38, ERK1/2 and JNK MAPK (SB2035809, PD98059 and SP600125) prevented the above compound towards induced apoptosis. The results clearly showed that MAP kinase cascades were crucial for apoptotic response in the above compound induced cellular killing and were dependent on p53 activity. Based on the results, compound was identified as a promising candidate for cancer therapeutics and these findings furnish a basis for further *in vivo* experiments on anti-proliferative activity.

Keywords: Bis(indole)hydrazide-hydrazone, anti-proliferative, apoptosis, MTT assay,mechanistic studies.

Study of NLO behavior of Proton Transfer Complexes via DFT Studies

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Exploring novel organic compounds those exhibit physical properties of interest by investigating the intermolecular interactions is one among the main objectives of solid state chemistry and crystal engineering due to their potential applications in non-linear optics (NLO). An extensive research has been carried in the present scenario in NLO field due to their requirement in the field of technology in day to day life. Hence the search for novel NLO compounds has grabbed the attention of material chemists.

Compared to inorganic materials, organic non-linear optical materials were explored more since they have several orders of higher magnitude and fast response time as they are made up of conjugated molecules where π-electrons move freely between donor and acceptor groups inducing charge transfer. Generally Proton transfer complexes possess high molecular polarizabilities, due to π-delocalized electronic systems, which show enhanced nonlinearities, hyper polarizabilities and appropriate physicochemical behaviour. The probability of hydrogen-bond formation between azoles and carboxylic acids provides a broad scope for the study of interactions. Carboxylic acids with amines forming molecular salts with non-covalent interactions in their crystal structure which can be explored for various applications via Density-functional theory (DFT) studies.

Artificial Intelligence-Based Smart Detection of Lung Disease from Chest X-Ray

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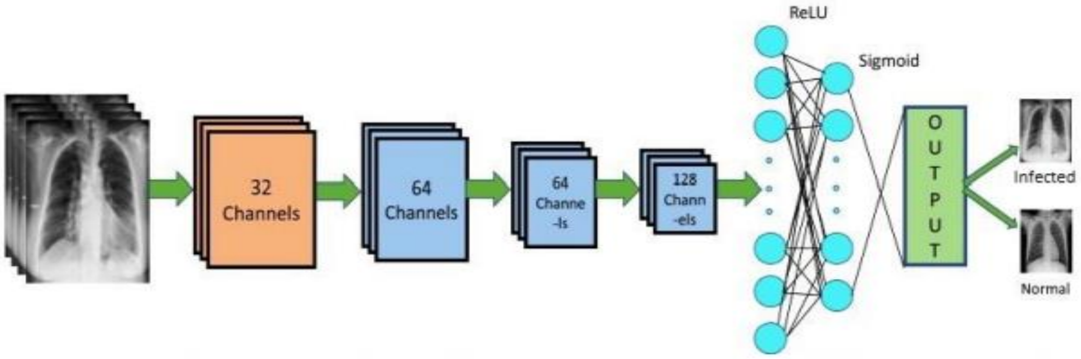
Abstract

In recent years, multi-fold improvement is viewed in the field of Artificial Intelligence hence playing a significant role in image classification especially the classification of medical images. In specific Convolutional Neural Networks (CNN) belonging to Artificial Intelligence performs well in the detection of several diseases such as heart disease, Dental diseases, Malaria, and Parkinson’s disease. CNN has a significant vision in the detection of lung disease utilizing the medical images of the patient such as X-rays. Lung disease is the basic symptom of the global pandemic disease COVID-19. This invention proposes a CNN model for the detection of lung disease where the model involves four layers namely input layers, convolutional layers, fully connected layers, and output layers.

The three-layered two-dimensional convolutional layers involve the ReLu activation function along with Max pooling making the detection process easier by training the model using the dataset. The proposed CNN model provides 97.4% of accuracy and 94.5% of precision. F1 score of the model is achieved as 97.60 and the curve area of Receiver Operating Characteristic (ROC) is obtained as 0.975.



Pharmaceutical co-crystals and their commercial opportunities"

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Pharmaceutical co-crystallization is an emerging approach to generate more number of new crystalline forms with changed physicochemical properties. These changes sometimes may lead to tremendous opportunities in the commercialization of co-crystals using the 505 b (2) filing route.

This talk will cover:

1. Introduction to pharmaceutical co-crystals
2. Design and synthesis of co-crystals
3. Patent life cycle and pharmaceutical co-crystal opportunities
4. FDA guidelines regarding the classification of pharmaceutical co-crystals
5. Case studies related to improved physicochemical and biopharmaceutical drug properties

ORAL, POSTER & PAPER PRESENTATIONS

OP/PP-1

Rapid identification of Limonoids in *Meliaceae* family plant species based on structure–fragmentation relationship study using Q-ToF-MS/MS analysis

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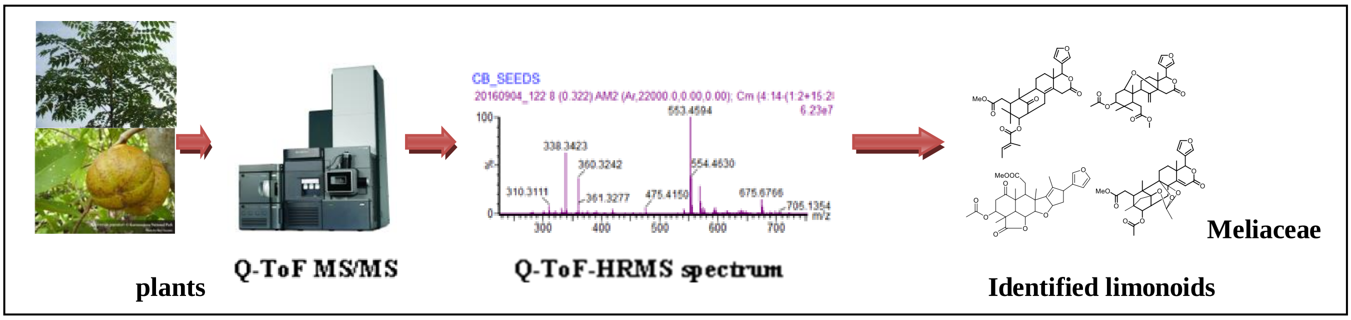
Abstract

Limonoids are highly oxygenated, modified terpenoids with a prototypical structure either containing or derived from a precursor with a 4,4,8-trimethyl-17-furanylsteroid skeleton and these limonoids found to be chemotoxonomic markers from the plants of the Meliaceae and Rutaceae families. Limonoids of Meliaceae plants vary due to seasonal and geograpical conditions and threfore, rapid identification of these constituents is desired.

The present study, based on positive ion mode electrospray quadrupole time-of-flight mass spectrometry (ESI-Q-TOF-MS/MS), which reveals the structure–fragmentation relationship of limonoids belonging to various sub-chemical classes such as mexicanolides, methyl angolensate, Trijugin, nimbolinin etc type class. Collision induced dissociation mass spectrometric analysis of these protonated molecules yielded key fragments due to the loss of neutral components like H_2O, CO_2, methanol, as well as McLafferty rearrangement and Retro-ene reaction. The fragmentation pattern of selected mass, coupled with high resolution analysis and database were utilized for the rapid identification of limonoids in Meliaceae species, namely *Cipadessa baccifea* and *Melia dubia*. Furthermore MS/MS spectra revealed different fragmentation pathways for different classes of limonoids which further aided dereplication.



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OP/PP-2

A Green Catalyst Iron tosylate hexahydrate $Fe(OTs)_3\cdot 6H_2O$ for the synthesis of α-aminonitriles through one pot three-component coupling reaction in water

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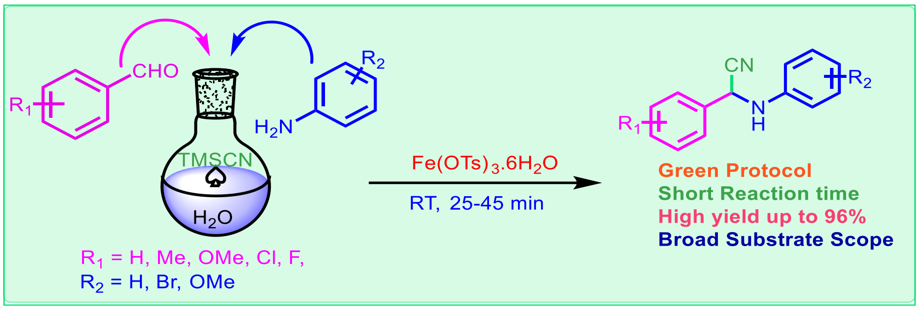
Abstract

An efficient and environmental friendly synthetic protocol has been presented to synthesize α-aminonitriles via one pot three component reaction of aldehydes, amines and TMSCN in the presence of Iron tosylate hexahydrate ($Fe(OTs)_3\cdot 6H_2O$) as a catalyst in aqueous media. Iron tosylate hexahydrate ($Fe(OTs)_3\cdot 6H_2O$), is a promising catalyst, introduced first time for the synthesis of α-aminonitriles in aqueous media as it is commercially available, inexpensive, non-toxic, operational simplicity and short reaction time with excellent yields.



Keywords: Strecker synthesis, Iron tosylate, TMSCN, water

References:

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OP/PP-3

Design and Synthesis of Indole-3-Glyoxamide Tethered β-Carboline Derivatives as Cytotoxic Agents: Apoptosis Induction and *in silico* Molecular Modeling Studies

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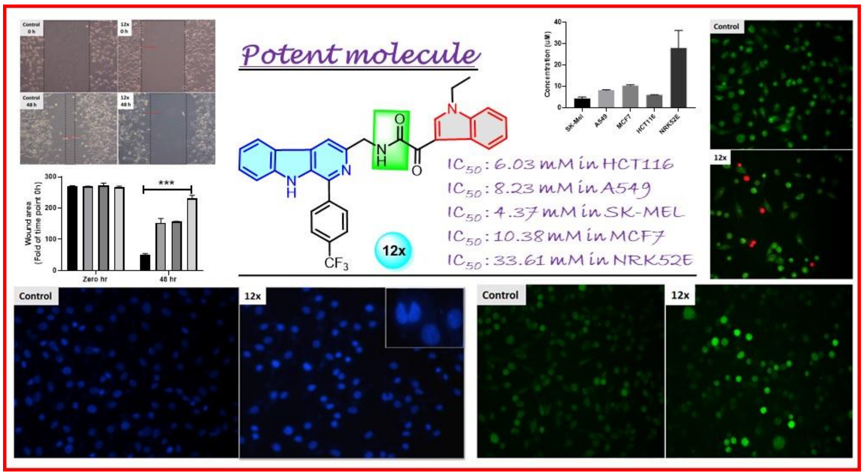
Abstract

National Cancer Act - strategically, the "war on cancer" was signed in 1971 to eradicate cancer by finding effective targeted drug therapies.[1] Following in time, continuous efforts are placed on developing promising anticancer agents as cancer remains public health concern worldwide.[2-4] In the same quest, a series of 25 compounds based on β-carboline tethered indole-3-glyoxylamide, conjoining salient pharmacophoric properties directing prominent cytotoxic agents were synthesized. The *in vitro* cytotoxic ability of the compounds was established, and many of the compounds exhibited remarkable cytotoxicity (IC_{50} <10 μM) on human cancer cell lines like HCT116, A549, SK-MEL and MCF7. Precisely, compound **12x** expressed the best cytotoxic potential against melanoma cancer cell line (SK-MEL) with an IC_{50} value of 4.37 μM. In addition, cytotoxicity evaluation against normal kidney cell line (NRK52E) entrenched the cytospecificity and selectivity index of **12x**. Wound healing assay inferred the inhibition of *in vitro* cell migration (metastasis) by compound **12x** in SK-MEL cells. The traditional apoptosis assays advised morphological and nuclear alterations such as apoptotic body formation, condensed/horseshoe-shaped/fragmented nuclei, and generation of ROS. Moreover, molecular modeling studies affirm the excellent DNA intercalation potential and stabilized interactions of **12x** with DNA base pairs. *In silico* prediction of physicochemical parameters revealed the promising drug-like properties of the synthesized derivatives.



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OP/PP-4

Potential Role of Iron Oxide Nanoparticles in Forensic, Food and Environmental Application

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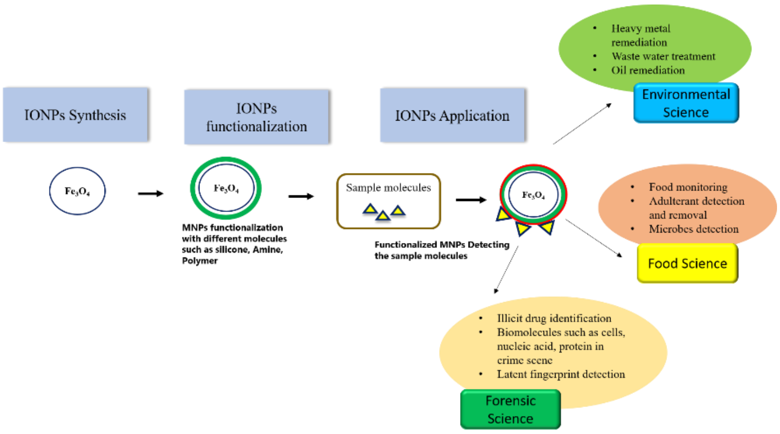
Abstract

The diversity in the application of iron nanoparticles (IONPs) is quite remarkable that draws attention among researchers. The basis for their diversity lies in their exceptional properties apart from the typical nano properties that eventually create space for upcoming and most required fields. Therefore, the present paper discusses about the significant role of IONPsin disciplines like forensic, food and environmental. IONPs aids in detecting the presence of the toxic compounds during food manufacturing, identifying the harmful adulterants in food items and deleterious pathogens. IONPs can also assist in solving crimes by identifying the sample types accurately such as n detection of illegal drugs and cells (sperm and epithelial cells) that are difficult to differentiate, also aid in making latent fingerprints visible. Among the new technologies IONPs also have great part in reviving the polluted environment by remediating heavy metals from soil, water, treating waste water, removing oils from sea waters and so on. Hence, in upcoming days it could be anticipated that IONPs can contribute to real-time applications in various disciplines.



Schematic overview of IONP applications in Food, Forensic and environmental science

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OP/PP-5

A photoinduced multicomponent regioselective synthesis of 1,4,5-trisubstituted-1,2,3-triazoles: transition metal-azide and oxidant-free protocol

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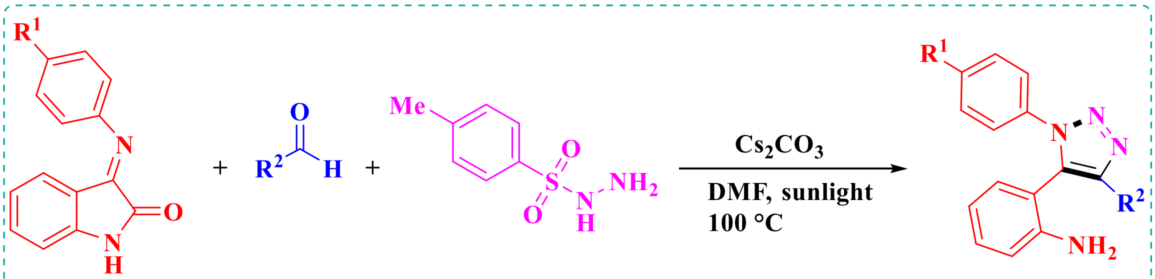
Abstract

A transition metal- and azide- free approach is explored to synthesize 1,4,5-trisubstituted-1,2,3-triazoles under sunlight. The reaction proceeds *via* C–N and N–N bond formations. These regioselective 1,2,3-triazoles are obtained from isatin Schiff bases, benzaldehydes and tosylhydrazine in the presence of base. This protocol offers the structurally diverse 1,2,3-triazole derivatives with 75-90% yields.



- **One pot three component**
- **Broad substrate scope**
- **Transition metal free**
- **High regioselectivity**
- **Azide free**

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OP/PP-6

Synthesis, Characterisation of new Sacubitril Derivatives exhibits Various Biological activities

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Abstract

We have attempted to identify Sacubitril derivatives[1] as lead compounds for different biologically active compounds. A total of Twenty-two compounds belongs to these libraries of the Sacubitril derivatives were synthesized. All the newly synthesized compounds structures were determined by NMR, Mass, FTIR and CHN analysis. Few compounds structures were confirmed by single crystal X-ray diffraction.

The newly synthesized compounds were screened for Anti-cancer activity with A549 cells in vitro by MTT Assay, all these compounds were evaluated against the bacterial strains they are E.coli (MTCC 9721), P. aeruginosa (MTCC 9800), S. aureus (MTCC 11949), B. subtilis (MTCC 9800)&antifungal activity by *Candida Albicans* (ATCC 10231). Among these Series few compounds exhibited potent anti-TB activity (6.25 µg/mL) compared to the standard drug ethambutol (1.56 µg/mL). Further, the anti-TB activity of the compounds was evaluated against *M. tuberculosis* in the nutrient starvation model. To determine the toxicity nature, the potent anti-TB active compounds were evaluated against RAW 264.7 cells.

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OP/PP-7

N-Boc Protection of Amines using Picric Acid as a Catalyst under Solvent Free Condition

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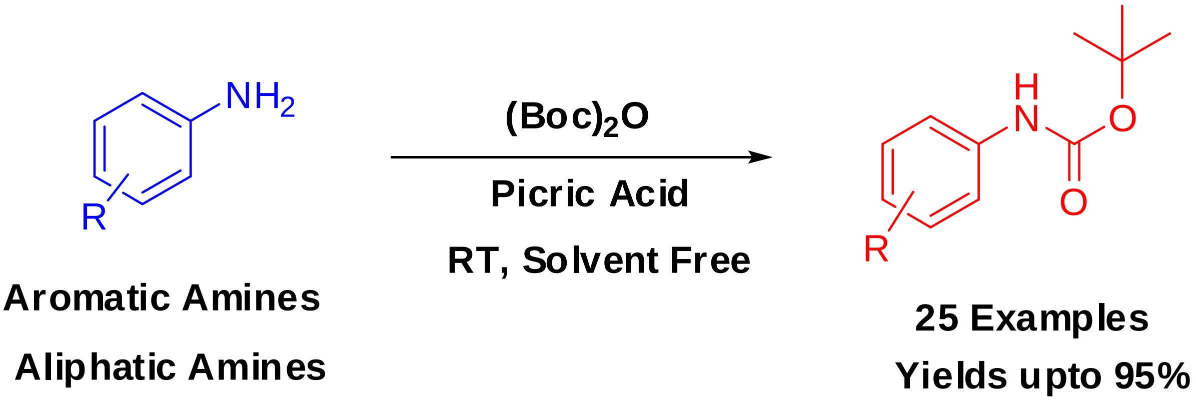
Abstract

A simple, efficient, and eco-friendly protocol for the N-Boc protection of the amine moiety in a variety of compounds with di-*tert*-butyl dicarbonate under Picric acid catalyst and solvent free conditions at room temperature is described. The corresponding monocarbamate is obtained in excellent yields on short reaction times (up to 50 minutes). This method represents a reasonable alternative to the previous reported protection procedures. Aromatic amines and aliphatic amines (up to 25 examples) also protected in good yields (up to 95%) under this reaction conditions.



OP/PP-8

Synthesis of novel pyrimido[4,5-*c*]isoquinoline containing 1,2,4-oxadiazoles as potent anticancer agents

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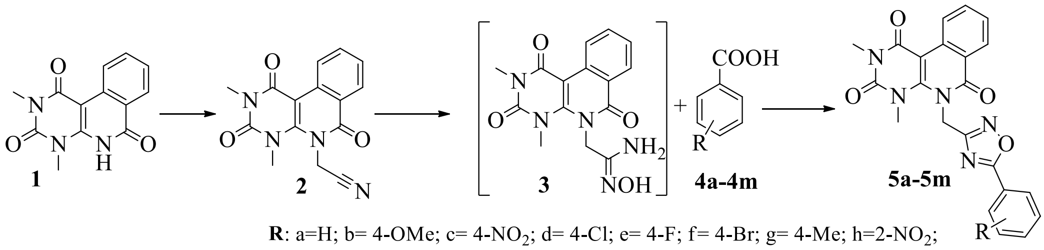
Abstract

A number of new 1,2,4-oxadiazoles coupled pyrimido[4,5-*c*]isoquinoline has been synthesized in good to excellent yields by the one pot method. All these hybrids were evaluated for their in vitro anticancer activity against three human cancer cell lines namely A375 (melanoma), MCF7(breast) and A549 (lung) using MTT assay and out comes revealed that three compounds like **5e**, **5j** and **5m** displayed superior inhibitory activities against all the cell lines than the standard. Molecular docking studies have also been conducted to complement the experimental results.



R: a=H; b= 4-OMe; c= 4-NO$_2$; d= 4-Cl; e= 4-F; f= 4-Br; g= 4-Me; h=2-NO$_2$; i= 2,3-diMe; j=3,5-diCl; k=3-Me; l=3-NO$_2$; m= 2-F,4-CF$_3$

Keywords: One-pot; Pyrimido[4,5-*c*]isoquinoline; 1,2,4-oxadiazole; Anticancer activity; Molecular docking.

OP/PP-9

LC-MS guided isolation of novel constituents from *Usnea longissima*

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Abstract

Lichens are nutritionally specialized fungi living in symbiotic association between fungi and algae. Several lichen species have been used in traditional medicine for centuries and are gaining considerable interest as an alternative medicine for the treatment of various ailments in different parts of the world. Several *Usnia* species are available in the North-east region of India and most of them became part of folklore medicine in the tribal areas. LC-MS guided isolation is an effective method, both in finding new natural products and characterizing trace components in a complex mixture of natural products.

As part of continuing studies in the identification on novel bio-active constituents from medicinal flora, we conducted phytochemical analysis of ***Usnea longissima*** using HPLC–MS system, which indicated the presence of several peaks with their corresponding molecular weights. Further guided by the MS/MS spectra, we have isolated three compounds (1-3), of which one compound is a new secondary metabolite. The individual compounds were identified using exact molecular masses from their MS/MS spectra. Moreover, all the isolates were screened for their anti-cancer activity against a panel of cancer cell lines.

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OP/PP-10

Design, synthesis, biological evaluation and molecular docking studies of some Novel Pyrano Chrysin Derivatives

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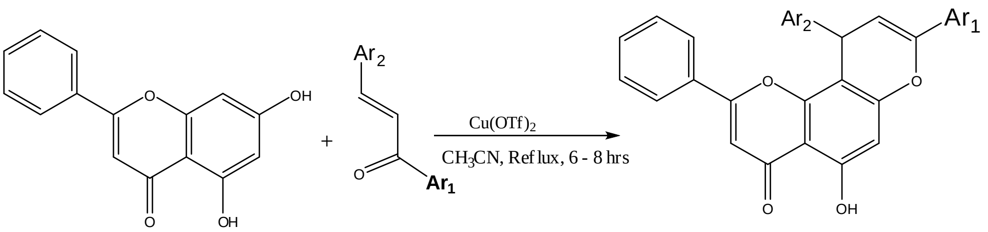
Abstract

Chrysin is a widely distributed flavone, mainly isolated form an Indian medicinal plant ‘*Oroxylum indicum*’. Chrysin (5,7-dihydroxyflavone) has been reported to exhibit many biological activities which includes antibacterial, antiinflammatory, antiallergic, antioxidant and anticancer activities[1-2].

As part of our investigations on the structural modifications of chrysin, Pyrano[2,3*H*]chrysin derivatives, 2-Hydroxy-3-Chrysino Dithiocarbamate Derivatives and Novel C (7) Modified Analogues of Chrysin have been synthesized and studied for their antimicrobial earlier[3-5]. In continuation of our work on synthetic modifications of chrysin, herein we report the synthesis of a series of novel pyrano chrysin analogues in which chrysin ring system is fused with pyran ring, with a view to enhance their biological activity. The antimicrobial assay and molecular docking studies are in progress.



Chrysin (I) Chalcone **(IIa-l)** Pyrano Chrysin **(IIIa-l)**

Scheme

Keywords: Chrysin, Pyrano Chrysin Derivatives, biological activities, molecular docking studies.

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OP/PP-11

Correlation Studies in the Oxidation of 5-Oxo Acid by N-Bromophthalimide: A Kinetic and Semi-empirical Approach

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ABSTRACT

The kinetic and mechanistic aspects of oxidation of 5-oxo acids by N-Bromophthalimide (NBP) in acid medium have been studied. The reaction exhibits first order each in [NBP] and [acid] & [oxo acid]. The reaction is failed to induce polymerization of acrylic monomers and no induction is observed over a wide concentration range of reagents. Variation in ionic strength has no effect on the reaction rate, while reaction rates are enhanced on lowering dielectric constant of the medium. Electron-releasing substituents in the phenyl ring of the substrate greatly accelerate the rate, whereas the rate retardation by electron-withdrawing substituents is observed, which is further supported by the electronic properties obtained by performing semi-empirical calculations on the substrates (5-oxoacids) with different substituents in the phenyl moiety.

The linear free energy relationship is verified by linearity in Hammett plots. The reaction constant (ρ) is negative and decreases with increase in temperature. From the intersection lines in the Arrhenius and Hammett plots, the isokinetic relationship is evaluated. Based on the experimental evidences, a plausible mechanism is proposed and rate law explaining all the kinetic results has been derived and verified.

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OP/PP-12

Synthesis of Multisubstituted Indanedione Based Spiropyrans via Oxa-Michael/Michael Cascade Reaction

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Abstract

Cascade reactions have emerged as efficient methods for the synthesis of complex structural compounds from simple precursors over the last ten years. This methodology involves two or more bond forming synthetic transformations (i.e., C-C, C-O, C-N, etc.) under the same reaction conditions without isolation of intermediate. These reactions are viewed as environmentally benign and economically beneficial. On the other hand, Morita-Baylis-Hillman (MBH) reaction has been considered as the atom economy reaction for making C-C bond formation. Due to the versatility of MBH adducts, they have been widely using as synthons in several synthetic transformations and developing new molecules. In the recent year’s *trans*-β-nitro styrene derived MBH adducts have become interesting precursors in synthetic organic chemistry.

In continuation of our research interest towards spiropyrans using primary nitro allylic alcohol and fused heterocyclic skeletons, we envisioned that the synthesis of multisubstituted spirocyclic pyrans having four stereocenters *via* Oxa-Michael/Michael through formal [4+2] cycloaddition reaction can be accomplished using ambiphilic substrates (1C, 2C) 2-arylidene-1,3-indanedione and (1C, 4O) secondary nitroallylic alcohol.

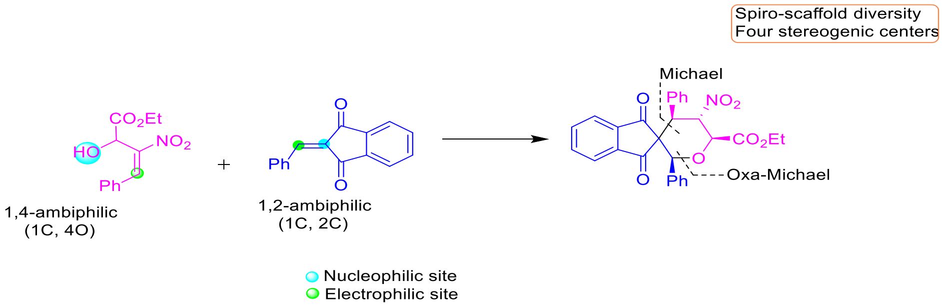

Figure-1: Construction of multisubtituted spiropyrans

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OP/PP-13

Water Based Thioamidation Reaction by Direct Installationof Amine and Elemental Sulfur at Room Temperature

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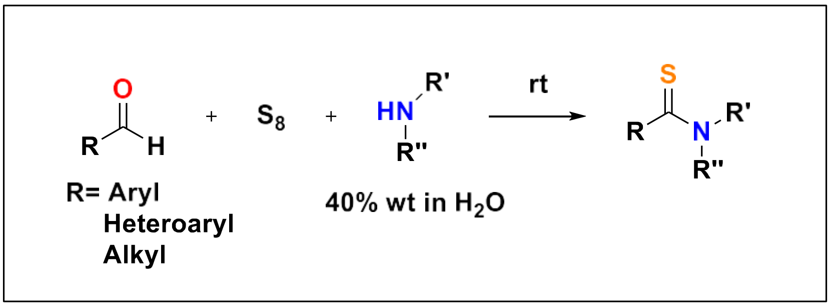
Abstract

Thioamides have an important role in the field of biochemistry and medicinal chemistry due to their highly pharmaceutical and biological activity. Recently, we reported the synthesis of Thioamides by direct installation of sulphur and amine in aldehyde at room temperature in aqueous medium. The present methodology demonstrate the substrate scope with different type of aliphatic, aromatic, heteroaromatic aldehyde with the use of different array amines with the scaled-up method. The use of no catalyst, oxidants or additives makesthis method unique. Biologically active molecules such as thionicotinamide, thioisonicotinamide which exhibit anticancer activity can be synthesized by our protocol.



Keywords: Thioamide, Elemental Sulfur, water based organic reaction and Amine.

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OP/PP-14

UPLC-MS/MS Quantitative analysis and structural fragmentation study of five *Parmotrema* lichens from the Eastern Ghats

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Abstract

Comparative Phytochemical analysis of five lichen species [*P. tinctorum* (Delise ex Nyl.) Hale, *P. andinum* (Mull. Arg.) Hale, *P. praesorediosum (Nyl.) Hale*, *P. grayanum* (Hue) Hale, *P. austrosinense* (Zahlbr.) Hale] of *Parmotrema* genus were performed using two complementary UPLC–MS systems. The first system consists of high resolution UPLC-QToF-MS/MS spectrometer and the second system consisted of UPLC-MS/MS in Multiple Reaction Monitoring (MRM) mode for quantitative analysis of major constituents in the selected lichen species.

The individual compounds (47 compounds) were identified using Q-ToF-MS/MS, via comparison of the exact molecular masses from their MS/MS spectra, the comparison of literature data and retention times to those of standard compounds which were isolated from crude extract of abundant lichen, *P. tinctorum*. The analysis also allowed us to identify unknown peaks/compounds, which were further characterized by their mass fragmentation studies. Moreover, the determination of antioxidant, AGE Inhibition, and antimicrobial activities were carried out for the crude extracts. To the best of our knowledge, this is the first report of comparative metabolite profilings on *Parmotrema* genus with these informative techniques to analyze secondary metabolites in lichens. Further, we believe that profiling patterns and these methods will be useful for chemotaxonomic classification, de-replication of secondary metabolites in the rare lichens.

OP/PP-15

Design, Synthesis, Biological Screening and Docking Studies of 1-(3-(Naphthalen-1-yl)-1-phenyl-1H-pyrazol-4-yl) Ethanone Hybrids as Cytotoxic Agents

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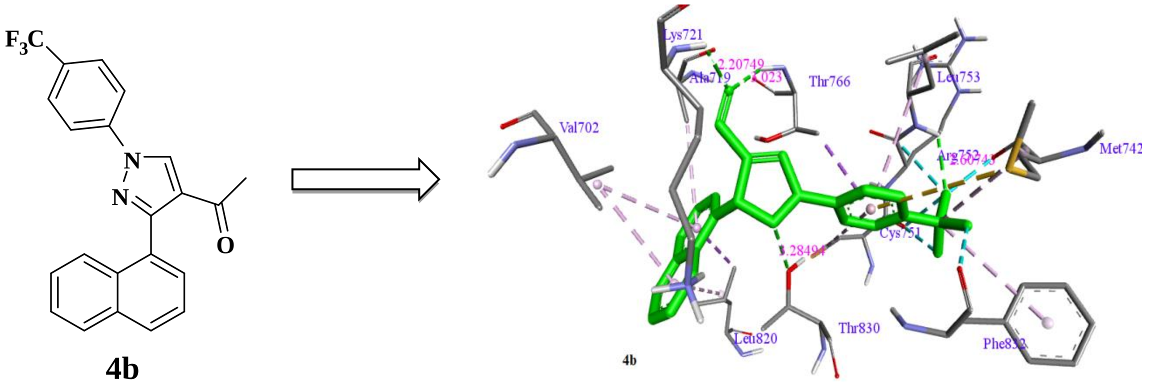
Abstract:

A series of 1-(3-(naphthalen-1-yl)-1-phenyl-1H-pyrazol-4-yl)ethanone hybrids (**4a-e**) have been designed and synthesized. The synthesized compounds were characterized by elemental analyses, FT-IR, ^{1}H &^{13}C-NMR and mass spectroscopic techniques. The entire target compounds were investigated for their in vitro cytotoxic activity by the MTT-based assay against four human cancer cell lines. Compared with the standard drug cisplatin, the compounds **4b** and **4e** displayed good cytotoxic activity against the growth of the tested cancer cell lines. Molecular docking studies were conducted against the EGFR protein receptor to illustrate the binding abilities of the synthesized compounds to the active site of the protein.The compounds **4b** and **4e** with -11.71 Kcal/mol, and -11.32 Kcal/mol, exhibited the lowest binding energies which correlate with cytotoxic activity results.

Graphical abstract



4b

Key words: Synthesis, Cytotoxic activity, EGFR protein, Molecular docking studies.

OP/PP-16

Green Synthesis of Schiff's Bases Derived from ortho Phthalaldehyde and their Pd (II) Complexes

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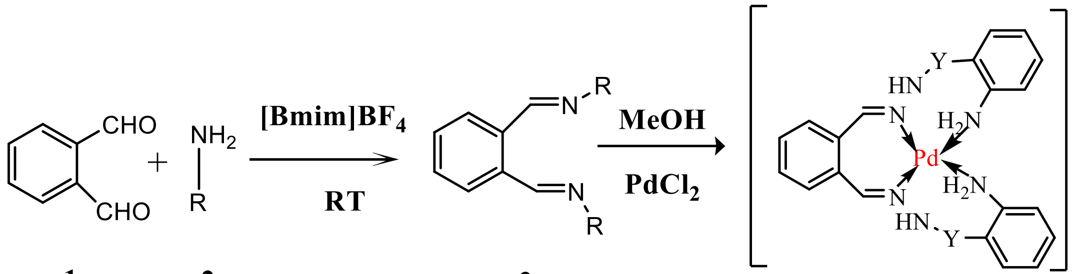
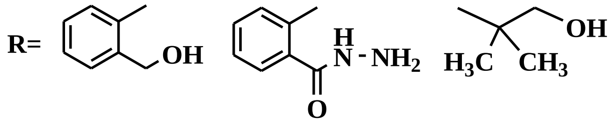
Abstract

Recently ionic liquids have emerged as very potential green alternatives to the volatile and hazardous organic solvents and have been used as efficient reaction media for organic synthesis due to their special properties such as good solvating capability, wide liquid range, negligible vapour pressure, easy recycling, and high thermal stability and rate enhancing ability. Schiff bases and their biologically active complexes have been often used as chelating ligands in the coordination chemistry of transition metals, radiopharmaceuticals for cancer targeting, agrochemicals, model systems for biological macromolecules, catalysts and as dioxygen carriers.

In continuation of our research work on the synthesis of Schiff's Bases using ionic liquids, herein, we have reported an efficient synthesis of novel tetradentate Schiff base ligands from the condensation of phthalaldehyde and 2-amino benzyl alcohol, 2-amino-2-methyl-1-propanol and 2-amino benzohydrazine respectively in the presence of ionic liquid [Bmim]BF_4 at RT in excellent yields with short reaction times. These ligands were reacted with $PdCl_2$ in methanol to form corresponding Pd metal complexes like [Pd(BDMAB)], [Pd(BDMAT)] and [Pd(BDMAZ)]Cl_2. The synthesized ligands and complexes are characterized by elemental analysis, IR, ^{1}H-NMR and mass spectral studies.



1 2 3 4(a-c)



2a 2b 2c

OP/PP-17

Design and Synthesis of cis-Stilbene-Thiazolidinedione Conjugates as Potential Tubulin Polymerization Inhibitors

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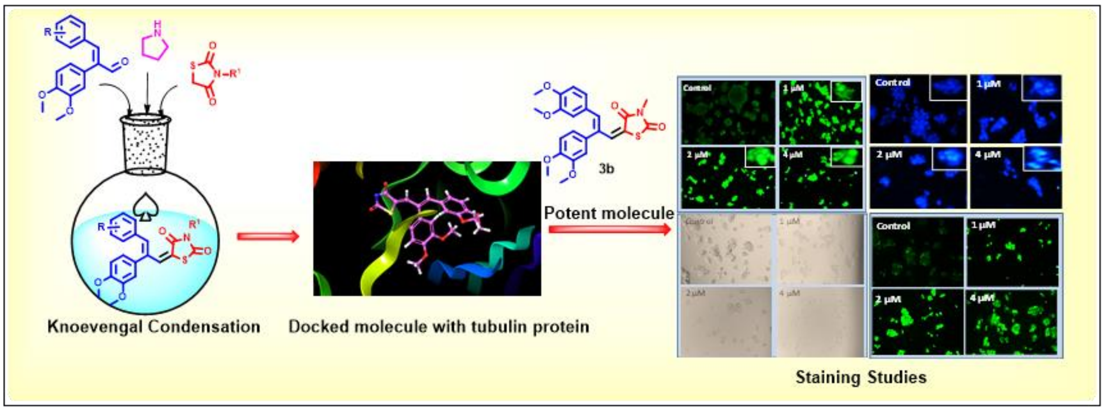
Abstract

Anticancer agents that target tubulin when used alone or in combination with other drugs have proved to one of the most effective treatments for cancer patients significantly increasing the survival rates. Combretastatin A-4 is a potent cytotoxic *cis*-stilbene derivative currently under phase III clinical trial, showing potent tubulin inhibitory action against broad spectrum of cancer cells. Next, thiazolidinedione, a privileged scaffold has been reported for its anticancer activity, which acts on PPARɣ and non-PPARɣ dependent signal cascade that controls the cell growth and apoptosis. With this background, we designed a series of stilbene-thiazolidinedione conjugates. Primarily, these conjugates were evaluated using *in-silico* studies such as glide docking studies, and binding energy. The glide score revealed that conjugates interact and binds efficiently in the colchicine binding site of tubulin. With this insight, we synthesized a series of stilbene-thiazolidinedione conjugates and evaluated their *in-vitro* cytotoxicity against different cancer celllines. Delightfully, one of the representative molecule **3b** showed potent cytoxicity against BT-474 cancer cell lines with IC_{50} = 2.14±0.38 µM. Further, cell morphology staining studies were also conducted.



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OP/PP-18

Synthesis of spirooxindolo-1,2,4-oxadiazoles *via* Et_3N catalyzed [3+2] cycloaddition Reaction

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Abstract

A convenient and metal free Et_3N catalyzed domino reaction of isatin schiff bases and hydroximoyl chlorides has been developed to achieve [3+2] cycloaddition of imines into aryl nitrile oxides at room temperature. In this transformation, spiro-1,2,4-oxadiazole skeleton was efficiently formed. The reaction proceeds through C-O and C-N bond formations under mild reaction conditions. A range of spirooxadiazoles were obtained in good to excellent yields from readily available starting materials.

Mild reactions conditions, operational simplicity and simple purification method make this protocol become environmentally benign and can be considered to be as green protocol. The structures of all the target compounds were in agreement with their spectroscopic (FT-IR, ^{1}H NMR, ^{13}C NMR) and mass spectral data. This protocol offers significant advantages for accessing biologically active spirooxadiazole derivatives.

Keywords: [3+2] cycloaddition,spiro-1,2,4-oxadiazole,biologically active.

Acknowledgments

The authors M.K, and S.B thank the Director, NIT Warangal for providing the facilities. M. K. thanks the Ministry of Education India (MoE), India for providing financial support.

Conflicts of Interest

No conflict of interest.

OP/PP-19

LC-MS-Guided Isolation of new Limonoids from *Trichilia connaroides* (Wight & Arn.)

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Abstract

Limonoids, a group of highly oxygenated and modified tetra nortriterpenoids are characteristic components of the plants of the Meliaceae and Rutaceae families. The diversified structures and wide range of biological activities of these limonoids have attracted much attention to both phytochemists and agrochemists. *Trichilia connaroides* (Wight et Arn.) is one of the important member in maleacae plant family and traditionally used for the treatment of cholera, arthritis, pharyngitis, tonsillitis and various other ailments. As part of our ongoing investigations on the maleaeceae plants, we conducted a LC-MS analysis of methanol extract from seeds of *T.connoroides* and analysis indicated the presencea various limonoids.

The aim of present study is to discover novel limonoids from *Trichilia connaroides by using* LC-MS powerful dereplication tool to facilitate compound identification. The present dereplication analysis is based on comparison of the molecular weight, MS/MS fragmentation and characteristic ^{1}H NMR signals with previously reported data in databases such as Reaxys, SciFinder Scholar, and also chemotaxonomic considerations that identify structurally similar compounds present in the same species, genus, or even family of the plant. From these results we identified three novel limonoids from *Trichilia connaroides.* The high sensitivity and selectivity of MS detection method effectively reduced the time of analysis and consequently enabled fast isolation of target constituents. All the isolated constituents were subjected to insecticidal activity against *spodoptera litura*

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OP/PP-20

Sulphated Al-MCM 41 Catalysts for the Effective Conversion of Bioglycerol to Solketal

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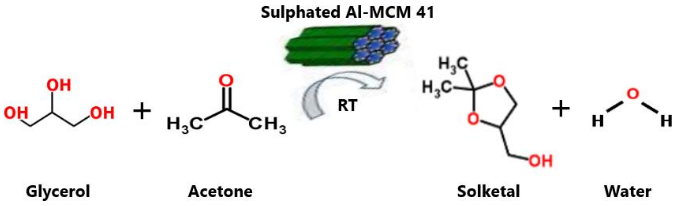
Abstract

Conversion of glycerol, a by-product in the biodiesel production to valuable chemicals can make it a sustainable process and at the same time glycerol can be exploited as a renewable chemical feedstock as well. Solketal is one such valuable product from acetalization of glycerol that is used as a fuel additive to reduce carbon emissions and enhance octane number. Further, solketal has several other applications in solvents, inks, paints and pharmaceuticals. Acetalization of glycerol involves carbocation production by the activation of ketone carbonyl group through a protonation step or polarization by the Lewis or Brønsted acid sites. The present work is a report of highly efficient sulphated Al-MCM 41 catalyst for the selective synthesis of Solketal by acetalization of glycerol at room temperature. Al-MCM41 was prepared by templating method followed by sulphonation with H_2SO_4 (1N) to obtain sulphated Al-MCM 41.

The catalyst was characterized by low angle XRD, BET-SA and Pore size measurements, SEM-EDAX and py-adsorbed FT-IR studies. The XRD patterns clearly show the mesoporous structure of MCM 41 from the low angle peak and BET-SA obtained was ~ 600 m^2g^{-1} with a typical adsorption isotherm of type-IV, a characteristic feature of mesoporous materials. The py-adsorbed FT-IR patterns of the Al-MCM 41and sulphated Al-MCM 41 clearly indicate the generation of enhanced Bronsted acidity on the surface of the catalyst which explains the higher activity of the sulphated catalyst over the non-sulphated one. The catalyst activity was compared with simple Al MCM41 and also sulphated zirconia and results have shown sulphated Al MCM 41 to be superior to the other two catalysts tested. This clearly indicates the role of mesoporous structure that gives a stable and enhanced surface.



Scheme: Solketal synthesis from Glycerol over sulphated Al-MCM 41 catalyst

OP/PP-21

Lewis Acids activated double bond of *S*-allyl α-enolic dithioester to form of 2-alkylidene1,3-dithiolane in mild condition

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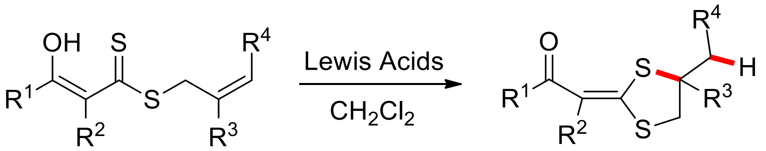
Abstract

The development of an atom-economical approach for the efficient construction of diversely functionalized molecules from easily accessible starting materials is continuously a special attention for synthetic organic chemists. Especially, Dithiolanes are well-known intermediates for some fundamental reactions in organic chemistry and in natural product synthesis.[1-3] 1,3-dithiolane derivatives with extended π-conjugation between the dithiolane rings have attributed an attraction in organic material synthesis as they have shown attention towards charge-transfer materials and some of them are electronic conductors.[4-7] There are various methods reported in the literature for the synthesis of 1,3-dithiolane. However these methods provide highly expensive and harsh reaction conditions. Therefore, it is still of great importance to develop alternative methods for the preparation of 1,3-dithiolane. In this context, we report inexpensive and environmentally benign, $AlCl_3$ catalyzed synthesis of various 1,3-dithiolane and 1,3-dithianes.



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OP/PP-22

An efficient one-pot synthesis of indolyl-4H-chromene derivatives

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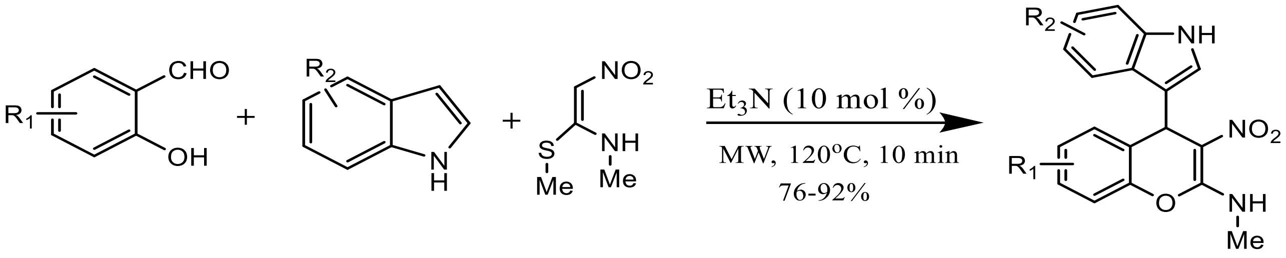
Abstract

A new one-pot three-component reaction for the synthesis of indolyl-4H-chromene derivatives has been developed. The synthesis was achieved by reacting salicylaldehydes, (E)-N-methyl-1-(methylsulfanyl)-2-nitroethenamine, and indoles in the absence of solvent using triethylamine as a catalyst. The final products were isolated by precipitation after the addition of ethanol to the reaction mixture. This transformation involves the formation of indole-substituted chromene ring by creation of two C–C bonds and one C–O bond in a single synthetic operation. This rapid one-pot reaction does not require chromatographic purification and provides the indolyl-4H-chromene derivatives in good yields.



R_1= H, Cl, Br etc; R_2 = H, Me, Br, I, OH, CN etc.

OP/PP-23

Knoevenagel-Friedel-Crafts-Hemiketalization Triple Cascade Reaction: A Diastereoselective Formal [1+2+3] Cyclization towards Indeno naphthopyran Scaffolds

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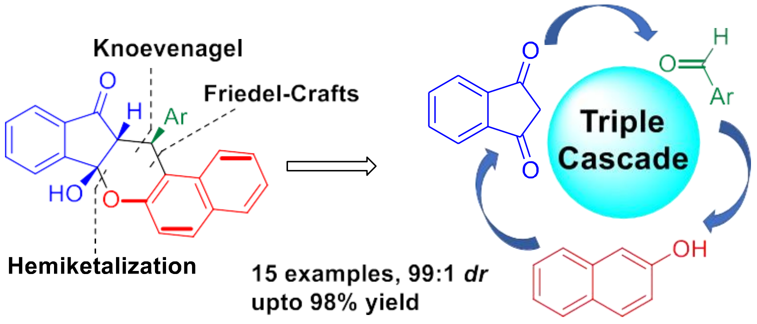
Abstract

A simple and efficient cascade reaction *via* formal [1+2+3] cyclization of 1,3- indanedione, aldehyde and 2-naphthol is reported using K_2CO_3 as a base. The advantage includes metal-free conditions, varied substrate scope and shortened reaction duration with high diastereoselectivity (i.e., 99:1) resulting in the formation of two carbon-carbon as well as two carbon-oxygen bonds through Knoevenagel-Friedel-Crafts-Hemiketalization sequence resulting in three contiguous stereocenters.

- KC-FC-HK: Triple Cascade Reaction
- Diastereoselective [1+2+3] Cyclisation
- Two [C-O] and Two [C-C] bonds formation
- Broad substrate scope with high yields
- Excellent *cis*- selectivity
- Three contiguous stereo centres
- Metal free conditions with divergent synthesis
- One pot protocol to complex products



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OP/PP-24

TBHP-mediated Selenocyclization of *N*-allylbenzamides/benzthioamides *via in situ* Generation of “PhSeOH” Species

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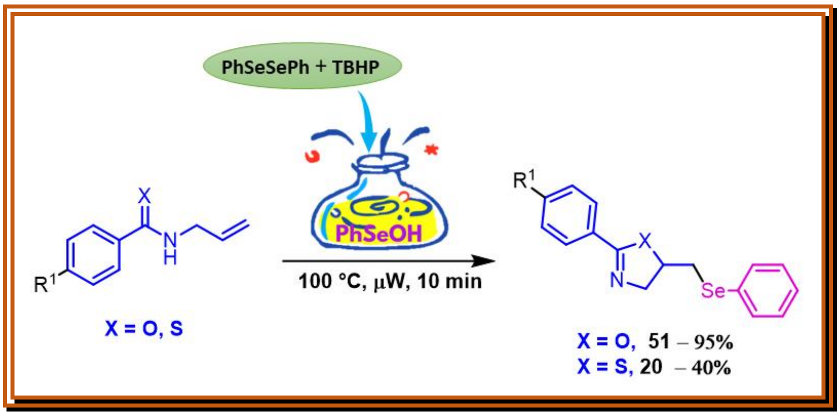
Abstract

Olefin functionalization presents us with a dynamic approach for the structuring of highly functionalized scaffolds. One such functionalization known as oxidative selenocyclization results in formation of a selenated heterocyclic scaffold, oxazoline, aided by an electrophilic selenium species. A simple *tert*-butyl hydroperoxide (TBHP)-mediated method has been developed for the construction of selenated oxazolines/thiazolines under microwave irradiation. The selenocyclization of *N*-allylbenzamides/benzthioamides could be achieved owing to the addition of an active electrophilic selenium species, generated *in situ* from diphenyl diselenide on reacting with TBHP, at their olefinic site. For the first time, the reaction mechanism was confirmed by intercepting and characterizing all the proposed intermediates by ESI-QTOF-MS and NMR study. This method offers several advantages which include simpler reaction conditions, short reaction time, catalyst-free, thus, rendering a competent alternative to the synthesis of selenated oxazolines/thiazolines in moderate to good yields (20-95%).



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OP/PP-25

Method Development and Validation for the Simultaneous Determination of Dolutegravir and Lamivudine in API Form and Marketed Pharmaceutical Tablet Dosage Form by Using RP-HPLC

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ABSTRACT

Analytical method development and validation for Dolutegravir and Lamivudine in bulk and combine dosage form by RP-HPLC, new method was established for simultaneous estimation of Dolutegravir and Lamivudine by RP-HPLC method. The chromatographic conditions were successfully developed for the separation of Dolutegravir and Lamivudine by using Symmetry C18 5µm (4.6 x 150mm), flow rate was 1.0 ml/min, mobile phase ratio was Phosphate buffer (0.02M) pH-3.8: Methanol: Acetonitrile (60:20:20%v/v), detection wavelength was 260nm.

The retention times of Dolutegravir and Lamivudine were found to be 2.324mins and 4.314mins respectively. The % purity of Dolutegravir and Lamivudine was found to be 99.865% and 99.658% respectively. The analytical method was validated according to ICH guidelines (ICH, Q2 (R1)). The linearity study of Dolutegravir and Lamivudine was found in concentration range of 0µg-36µg and 0µg-39µg and correlation coefficient (r2) was found to be 0.9995 and 0.9998, % recovery was found to be 100.280, %RSD for repeatability was 0.174 and 0.709, % RSD for intermediate precision was 0.093 and 0.937 respectively. The precision study was precise, robust, and repeatable. LOD value was 1.377 and 1.079, and LOQ value was 4.174 and 3.272 respectively. Hence the suggested RP-HPLC method can be used for routine analysis of Dolutegravir and Lamivudine in API and Pharmaceutical dosage form.

Keywords: Dolutegravir and Lamivudine, Method Development, Validation, Accuracy.

OP/PP-26

Fabrication of hollow spheres in self-assembly of hybrid oligomers

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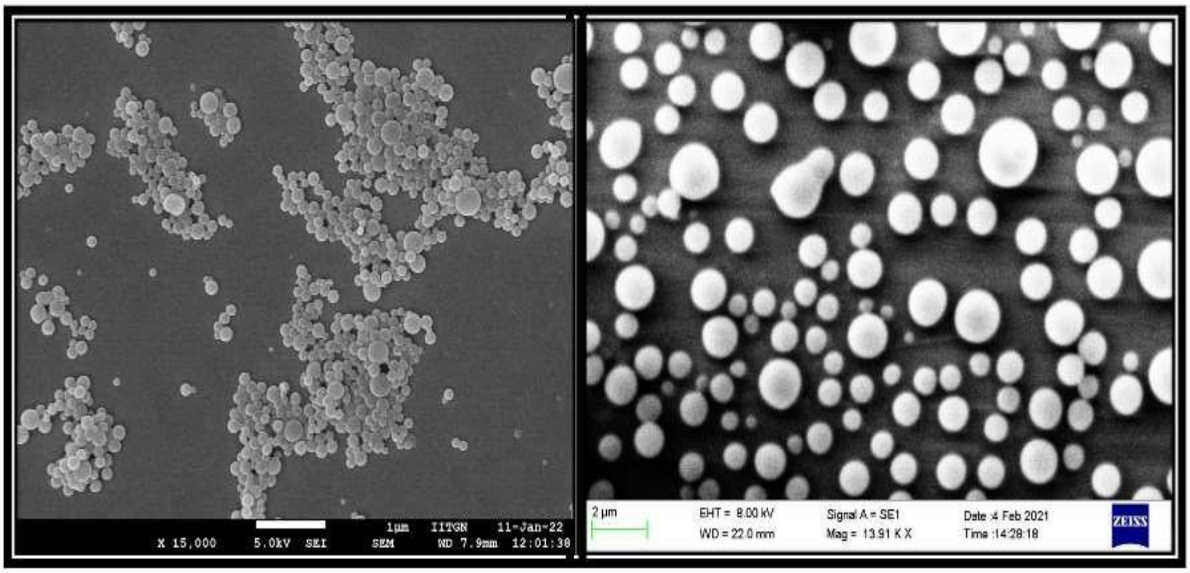
Abstract

Synthetic oligomers with well-defined conformational features ('foldamers') have attained considerable interest in recent years. They show interesting features such as structural tunability and predictability and find vast applications in various interdisciplinaryareas such as molecular recognition, catalysis and drug therapeutics.[1] They can act as structural /functional mimics of the biomolecules and are presented as promising candidates for biological applications. In addition, they show well defined self-assembly in different types of nanoarchitectures including wires, rods, sheets, spheres, fibres[2].

In this direction, the work describes the synthesis, characterization and conformational analysis and functional assessment of set oligomers with repeating units of natural and unnatural amino acid and study the effect of *O*-alkylation on the folding propensity of these oligomers and, their applications in self-assembled nanoarchitectures as drug loading agent.



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OP/PP-27

Vilsmeier-Haack Formylation and Acetylation Reactions with Anilines and Acetanilides under Solvent-free Conditions

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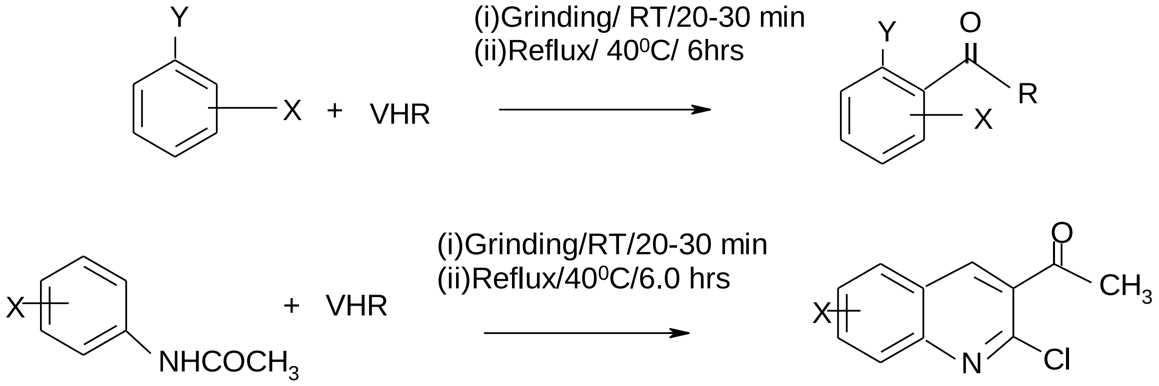
ABSTRACT

The Vilsmeier-Haack reaction with anilines and acetanilides has been carried out under solvent free conditions. The reactants are taken in a mortar and grounded with a pestle for about 20 to 30 min at room temperature. The reactions afforded formyl derivatives in fairly good yields when a mixture of dimethyl formamide (DMF) and $POCl_3$ is used as VH reagent. However acetyl derivatives were obtained when DMF was replaced by DMA in the composition of VH reagent. Results of solvent free reactions are more superior over solution phase reactions with very good yields and far lesser reaction times.

The present finding is more advantageous over solution phase reaction. It is conducted with economically cheap and readily available reagents. The reaction occurs under mild and under environmentally safe conditions with a simple work up at room temperature. Far less reaction times (about 12 times less than thermal reactions) coupled with enhanced reaction yields substantiate that the present work is a major breakthrough in the area of Vilsmeier-Haack synthesis.



Keywords: Vilsmeier-Haack reaction, Anilines, acetanilides, Formyl derivatives, Acetyl derivatives

OP/PP-28

Synthesis and anticancerevaluation of 1,2,3-Triazole Incorporated Thiazole-pyrimidine-isoxazoles derivatives

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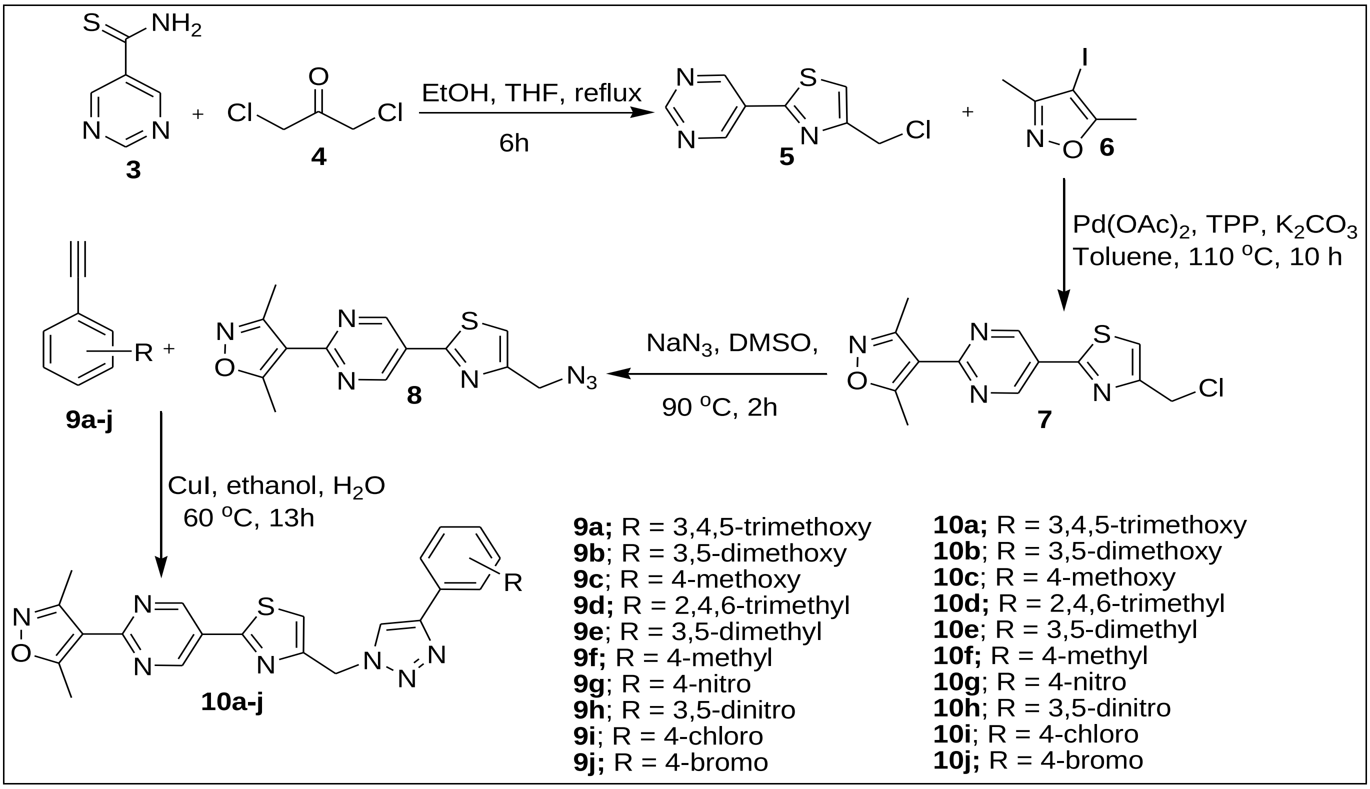
Abstract

A series of novel library of 1,2,3-triazole incorporated thiazole-pyrimidine-isoxazoles (**10a-j**) were designed, synthesized and characterized by ^{1}H NMR, ^{13}C NMR and mass spectral data. Further, these compounds were screened for their anticancer activities alongside a panel of human cancer cell lines like Prostate cancer (PC3 and DU-145), Lung cancer (A549) and Breast cancer (MCF-7) by using of MTT assay and etoposide used as standard drug. The outcome resulted were expressed in IC_{50} µM and to compared with standard drug as etoposide. The IC_{50} values ranges of compounds from 0.011±0.0017 µM to 33.7±9.32 µM and standard drug showed values ranges from 1.97 ± 0.45 µM to 3.08 ± 0.135 µM. Among the synthesized derivatives, five compounds **10a, 10g, 10h, 10i** and **10j** were proved most potent activity compared to etoposide.



Keywords: Imatinib, tazobactum, pyrimidine, 1,2,3-triazole, and anticancer activity.

OP/PP-29

Design, synthesis and anticancer evaluation of chalcone incorporated benzothiazole-imidazo[2,1-b]thiazole derivatives

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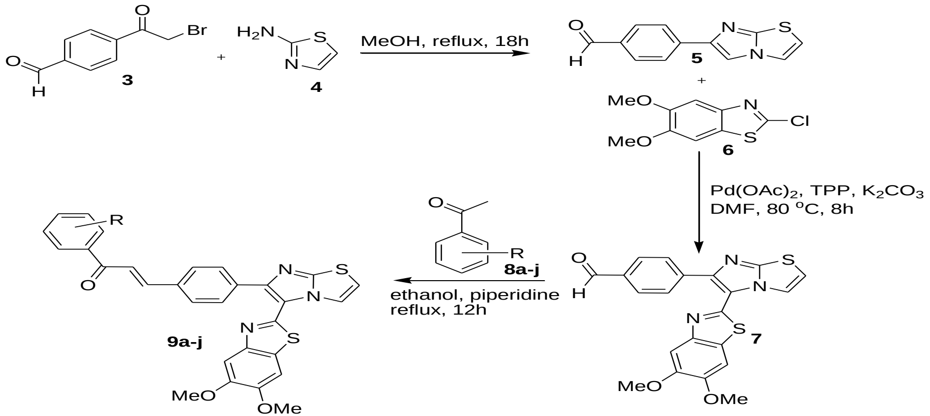
Abstract

A new library of chalcone incorporated imidazo[2,1-b]thiazole derivatives (**9a-j**) was developed and their structures were determined from their analytical data. Further, all were screened for their anticancer profile towards a panel of human cancer cell lines like prostate cancer (PC3), lung cancer (A549), breast cancer (MCF-7) and ovarian cancer (A2780) by utilizing of MTT assay and etoposide used as standard reference drug. All compounds were displayed good to moderate anticancer properties on four cell lines with IC_{50} values ranges from 0.012±0.0076 µM to 21.9±8.24 µM, and standard showed IC_{50} values range from 1.38 ± 0.56 µM to 3.08 ± 0.135 µM respectively. Amongst (**9a-j**), five compounds **9a, 9b, 9c, 9d** and **9e** were exhibited potent anticancer activities. In which, compound **9a** was demonstrated excellent anticancer activity.



9a; R = 3,4,5-trimethoxy
9b; R = 3,5-dimethoxy
9c; R = 4-methoxy
9d; R = 3,5-dinitro
9e; R = 4-nitro
9f; R = 4-chloro
9g; R = 4-bromo
9h; R = 4-methyl
9i; R = 4-cyano
9j; R = 4-(dimethylamino)

8a; R = 3,4,5-trimethoxy
8b; R = 3,5-dimethoxy
8c; R = 4-methoxy
8d; R = 3,5-dinitro
8e; R = 4-nitro
8f; R = 4-chloro
8g; R = 4-bromo
8h; R = 4-methyl
8i; R = 4-cyano
8j; R = 4-(dimethylamino)

Keywords**:** Levamisole, sofalcone, imidazo[2,1-b]thiazole, chalcone and anticancer.

OP/PP-30

Synthesis and Biological Evaluation of Thiourea Derivatives of structurally modifiedImidazo-pyridine as Anticancer Agents

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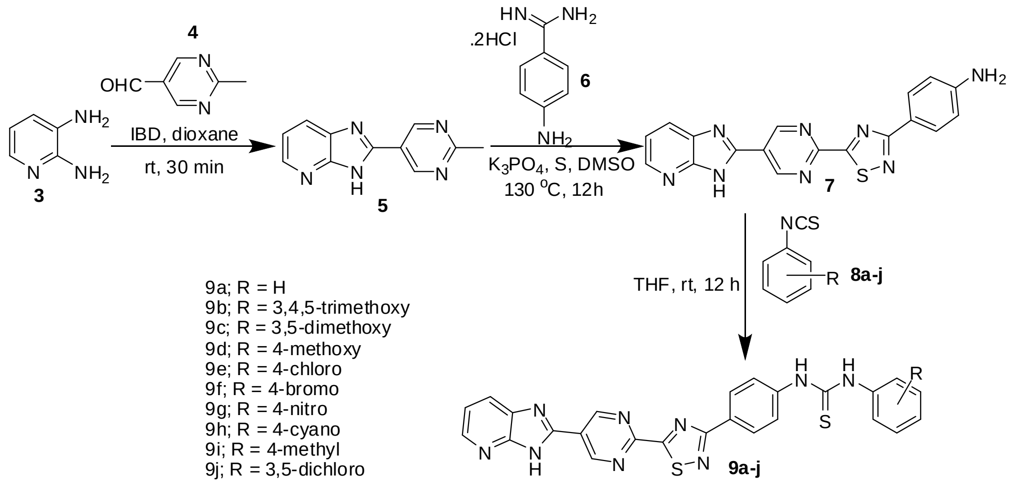
Abstract

A library of 4-(5-(5-(3H-imidazo[4,5-b]pyridin-2-yl)pyrimidin-2-yl)-1,2,4-thiadiazol-3-yl)benzene thiourea (**9a-j**) derivatives were designed and synthesized. The structures of the synthesized compounds were characterized by ^{1}H NMR, ^{13}C NMR and massspectroscopy techniques. Further, all these compounds investigated against a panel of human cancer cell lines comprised MCF-7, MDA MB-231 (breast cancer), A549 (lung cancer) and DU-145 (prostate cancer) by employing MTT assay, Etoposide used as positive control. Most of the newly prepared compounds exhibited more potent anticancer activities on four cancer cell lines with IC50 values ranging from 0.16±0.039 µM to 12.56±4.58 µM and positive control showed with 1.91 ± 0.84 µM to 3.08 ± 0.135 µM. Among them, compounds **9a, 9b, 9c, 9d, 9h** and **9i** were found to be more promising anticancer activity than positive control.



Keywords: Imatinib, pyrimidine, tenovin-1, thiourea and anticancer activity.

OP/PP-31

Synthesis of Tamarind gum-based pH responsive Hydrogel For Anticancer Drug delivery and antimicrobial Applications

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Abstract

This paper describes the development of pH-responsive hydrogel from tamarind gumand pH sensitive AGA monomers by a simple free radical polymerization method in presence of bis[2-(methacryloyloxy)ethyl] phosphate as a cross linker and potassium per sulphate as an initiator. In addition, these hydrogels have been used as templates for green synthesis of silver nanoparticles by using aqueous leaf extract as reducing agent. The synthesized and silver composites hydrogels were successfully characterized by the FTIR, UV-Vis, XRD, SEM and TEM, to know the chemical structure, crystalline behavior and surface morphology studies. The pH-sensitive swelling behavior of hydrogels were investigated in different pH solutions, and swelling kinetics.

These hydrogels anticancer drugs successfully encapsulated into hydrogel network. *in vitro* release studies in pH physiological and gastric environment at 37 °C. The drug release behavior is examined with kinetic models such as zero order, first order, Higuchi, Hixson-Crowell, Korsmeyer-Peppas. These release data was the best fitted with the Korsemeyer-Peppas transport mechanism. The Antimicrobial activity of Ag nanocomposites hydrogels is studied against to *Staphylococcus aureus* and *Klebsiella pneumonia.*

Keywords: Natural polysaccharide, tamarind gum, pH responsive behavior, Anticancer drug, Drug delivery and antimicrobial activity.

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OP/PP-32

Synthesis of sodium2-mercaptoethanesulfonate by using Mercapto ethanol

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Abstract

Sodium 2-mercapto ethanesulfonate is in a class of drugs known as chemoprotectants. Mesna is used for the prevention of urothelial toxicity in patients being treated with the antineoplastics ifosfamide or cyclophosphamide. In this study, a new method for synthesis of mesna from 2-mercaptoethanol using bromo intermediate was continuously developed by the scale of 50g per batch. The synthesis was carried out in 2 steps: Firstly, 2-bromoethanethiol was prepared from 2-mercaptoethanol by bromination. Secondly, sodium 2-chloroethanesulfonate was reacted with sodium sulfite, with the standard equivalent of sodium sulfite without any pH adjustment. Finally, mesna was obtained by HPLC in reaction mass ~97% compared with standard sample (~98% HPLC), which was cost and yield effective for industrial synthesis.

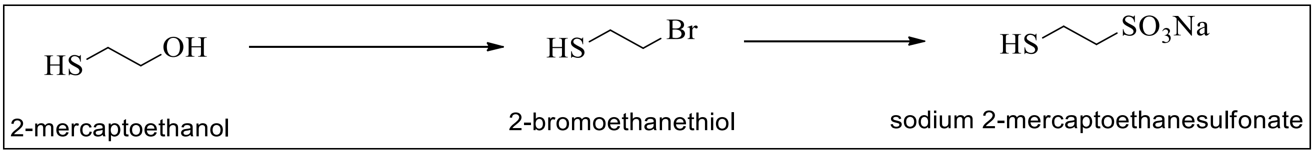

Figure-1: Synthesis of sodium 2-mercapto ethanesulfonate

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1). N.S.H. Dao1*, V. H. Nguyen1 , D.T. Do2 , D.L. Nguyen1 1 Department of Pharmaceutical Industry, Hanoi University of Pharmacy, Hanoi, Vietnam 2 Thai Nguyen Eye Hospital, Thai Nguyen, Vietnam.

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OP/PP-33

Design and Synthesis and Cytotoxicity Evaluation of 1,2,3-Triazole Conjugated *Cis*-Stilbene Analogues: Molecular Docking Studies

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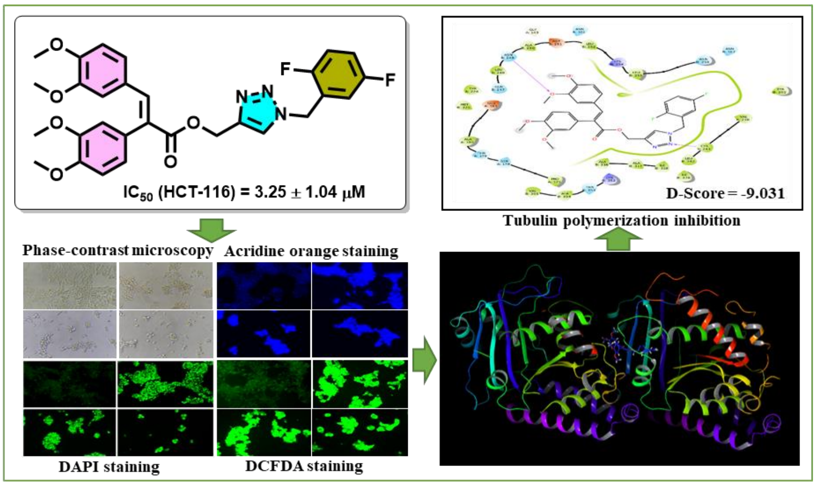
Abstract

The *cis* restricted stilbenes are of great importance in the field of medicinal chemistry and are found to possess potential anticancer activity by inhibiting tubulin polymerisation or selective estrogen receptor modulation. 1,2,3-Triazole is also considered as an attractive scaffold due to its ease of synthesis, act as a bridging unit and possess diverse biological activities. Therefore, in continuation of our earlier efforts in the development of new anticancer agents in the drug discovery program, herein, a series of novel *cis*-stilbene-1,2,3-triazole conjugates were designed and synthesised by reacting propargyl ester of substituted (*E*)-2,3-diphenylacrylic acid with phenacyl/benzyl azides using 'click' reaction and obtained in good to excellent yields.

The final conjugates were characterised by ^{1}HNMR, ^{13}C NMR, HRMS, and FT-IR spectroscopic techniques. Moreover, docking studies were also performed to interpret the interactions between synthesised conjugates and the target protein (PDB ID: 4O2B). Among all the conjugates, the compounds **9h**, **9j** and **10e** exhibited good docking scores (-8.406, -9.031 and -9.167 respectively). Conjugate **9j** also demonstrated a significant IC_{50} value (3.25 ±1.04 µM) against the HCT-116 (human colon cancer cell line) cell line with the potential of tubulin polymerisation inhibition.



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OP/PP-34

Stability Indicating RP-HPLC Method Development and Validation for the Simultaneous Determination of Empagliflozin and Linagliptin in Bulk Form and Marketed Pharmaceutical Dosage Form

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ABSTRACT

A Novel Analytical simple, reproducible and efficient RP-HPLC method was developed for simultaneous estimation of Empagliflozin and Linagliptin in pure form and marketed combined pharmaceutical dosage forms. A column having Develosil ODS HG-5 RP C18, 15cmx4.6mm, i.d. Column in isocratic mode with mobile phase containing Methanol: Acetonitrile in the ratio of 85:15% v/v was used. The flow rate was 1.0 ml/min and effluent was monitored at 258nm. The retention times and linearity range for Empagliflozin and Linagliptin was found to be (2.217, 5861min) and (0-14, 0-28), respectively.

The method has been validated for linearity, accuracy and precision, robustness and limit of detection and limit of quantitation. The limit of detection (LOD) and limit of quantification (LOQ) were found to be 0.08µg/ml and 0.24µg/ml for Empagliflozin and 0.1µg/ml 0.3µg/ml for Linagliptin respectively. The proposed method was found to be accurate, precise and selective for simultaneous estimation of Empagliflozin and Linagliptin in pure form and marketed combined pharmaceutical dosage forms.

Keywords: Empagliflozin, Linagliptin, RP-HPLC, Validation, Accuracy, Precision.

OP/PP-35

β-Nitrostyrenes as a valuable precursor for synthesis of β- aryl-γ-lactam and 2-oxo-1,2-dihydroquinoline derivatives.

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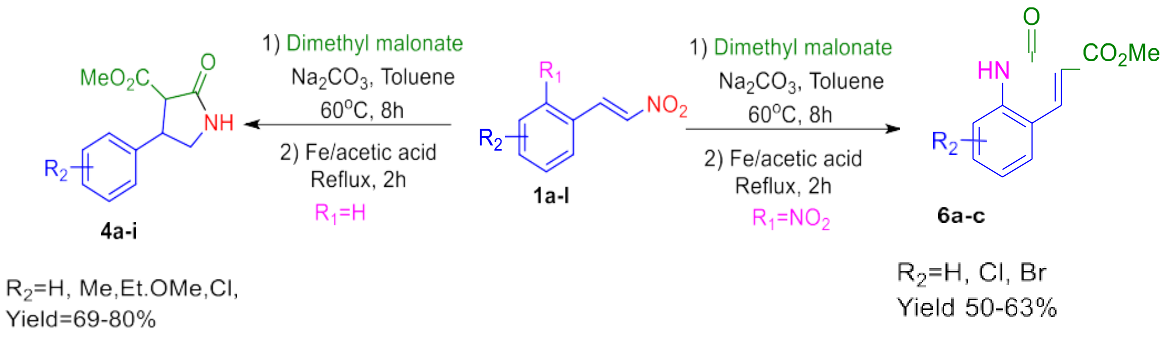
Abstract

We successfully demonstrated two different reaction pathways for the synthesis of β- aryl-γ-lactam and 2-oxo-1,2-dihydroquinoline derivatives using β-nitrostyrenes. The reaction strategy involves the Michael addition followed by reduction and cyclization reactions. Michael adducts containing two different nitro group such as one on aryl ring and another on side chain, selectively takes the path to involve nitro group on aryl to form β-aryl-γ-lactam derivatives as cyclized product. Michael adducts with nitro group on side chain alone forms 2-oxo-1,2-dihydroquinoline derivatives as cyclized product. This methodology is appealing with reliability and scalability with gram scale products can be synthesized. These heterocyclic compounds can be exploited for their biological activity.



Keywords: β-Aryl-γ-lactams, 2-oxo-1,2- dihydroquinolines Michael addition, dimethyl malonate, β-nitrostyrenes.

Reference:

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OP/PP-36

Computational, Equilibrium, Antimicrobial Studies of 1-Formyl-3-Thiosemicarbazide and Characterization of its Cd(II) And Hg(II) Complexes

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Abstract

1-formyl-3-thiosemicarbazide (FTSC) was synthesized and characterized by LC-MS, IR, UV,^{1}H- and ^{13}C-NMR spectroscopy. NMR studies revealed the existence of tautomeric forms. Computational studies were carried out using Gaussian-16W program package. Six possible keto-enol and thione-thiol forms of FTSC were constructed and geometry optimized in closed-shell three-parameter functional Becke-Lee-Yang-Parr hybrid exchange-correlation (B3LYP) in combination with 6-311G(d,p) basis setto derive the complete geometry. Thermodynamic parameters of all the forms were evaluated. The surfaces of HOMO, LUMO and Molecular electrostatic potential mappings have been generated. The quantum chemical descriptors like ionization potential (I), electron affinity (A), ΔEgap, electronegativity (χ), chemical potential (μ), global hardness (η), global softness (S) and global electrophilicity index (ω) have been calculated from E_{HOMO} and E_{LUMO} of the respective tautomers.

Equilibrium studies of FTSC with Cd(II) ion carried out by potentiometric Irving Rossetti titration technique in 70% v/v DMF-water medium at 303 K temperature and 0.1 M (KNO_3) ionic strength revealed the formation of 1:1 and 1:2 Cd(II)-FTSC complexes in the solution. The solid complexes of Cd(II) and Hg(II) with FTSC were synthesized and characterized by elemental analysis, TGA,LC-MS, IR, UV-visible and ^{1}H-NMR studies. Molar conductance measurements revealed their non-electrolytic nature. The formation of mononuclear five membered chelates with $ML_2(H_2O)_2$ composition and octahedral geometry have been predicted for both the complexes.The antimicrobial studies showed that the chelates have good activity than the ligand against gram negative bacteria.

Key words: Computational studies, Equilibrium studies, Antimicrobial studies

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OP/PP-37

Synthesis, Characterization and Biological applications of unsaturated diacyl and alkyl-acyl piperazine derivatives

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Abstract

In this study, we obtained new unsaturated piperazine compounds by the reactions of piperazine and piperazine derivatives with acylation reactive groups. Acyl chlorides were preparedfrom the reaction of thionyl chloride with carboxylic acids obtained as a result of the reaction. In addition, from the reaction of nitro substituted compoundand acyl chlorides, unsaturated piperazines were synthesized in good yields (63%–84%). Further, all these newly synthesized compounds structures were determined by NMR, Mass, FTIR and CHN analysis. These compounds were also screened for different biological studies.

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OP/PP-38

Biosynthesis of silver nanoparticles using *alternanthera sessilis*, phytochemical estimation, anti bacterial and anti fungal study.

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ABSTRACT

Green synthesis of nanoparticles has gained notable significance in the recent time because of the use of cost-effective and eco –friendly procedure. In the present study, one such simple cost-effective and eco-friendly biosynthesis of silver nanoparticles {AgNPs} was developed. The synthesis of AgNPs from aqueous leaf extract of *Alternantera sessilis* was assessed by varying different reaction parameters like concentration of plant extract, the ratio of reactants, temperature and reaction time. Characterization using UV-Visible Spectrophotometry revealed a Surface Plasmon Resonance [SPR] peak at 429nm confirming the formation of AgNPs. Further, characterization of the AgNPs was carried out using X-ray Difractometer{XRD}, it reveals the presence of face-centered cubic structure of AgNPs and confirms its crystalline nature and The crystallite size of the synthesized particle was 22.29 nm which was calculated using peak broadening profile of [111] peak at 37.72°. Nanoparticle analyzer helps in determining the size of the particle and size distribution. The SEM image of AgNPs synthesized from aqueous leaf extract of *Alternantera sessilis*, the particles are predominantly spherical in shape and the TEM results revealed well dispersed and mostly spherical AgNPs. Maximum particles were in the size range of 10-20 nm and few particles were found above the range of 30 nm. The Fourier Transform Infrared Spectroscopy {FTIR} study explained that Bimolecules in *Alternantera sessilis* leaf extract have acted as the reducing and stabilizing agents during the synthesis.

The *in-vitro* antimicrobial activity of the AgNPs was investigated against Bacillus subtilis, Escherichi coli, Klebsiella pneumonia and Staphylococcus aureus. In the present study, AgNPs showed greater antimicrobial activity in comparison with the standard antibiotic Ampicillin. The activity exhibited by AgNPs was found to be dose-dependent. With increase in concentration of the AgNPs, there was also a simultaneous increase in the zone of inhibition showing an increase in the Antibacterial activity exhibited by the green synthesized AgNPs.

The catalytic activity of the AgNPs thus synthesized was investigated by studying the degradation of methylene blue dye by sodium borohydide. The present study revealed significant catalytic activity of AgNPs in presence of sodium borohydride against methylene blue dye, and found that, dye completely degraded with in 25min. AgNPs synthesized from aqueous leaf extract of *Alternantera sessilis* showed effective antimicrobial and catalytic properties. The developed method can be used as substitute for the physical and chemical methods used for synthesis of AgNPs.

OP/PP-39

Design and synthesis Nanoparticle Composite- cluster core based Metal Organic Framework (MOFs) for electro- catalysts for water splitting applications

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Abstract

Porous coordination polymers (**PCPs**), or metal-organic frameworks (**MOFs**) are emerging as potential materials of the decade, particularly forgas storage, separation, catalysts, and sensors, etc. However, **PCPs** existing in the literature were mostly surface oriented porosity without any open metal sites (**OMSs**). Some of the **PCPs** are formed by the coordinated solvent in the pristine form are unstable after removal of the solvent leads collapse of the structure.

To overcome these problems, synthesized new MOFs using new 3,3’3’’-(Benzene -1,3,5- triyltris ethyne-2,1-diyl) tribezoic acid (H_3BETB). Later in these MOFs Metal Nano particles were incorporated for the splitting of water in hydrogen and Oxygen. In this study we present our latest results on MOFs for Metal Organic Framework (MOFs) for electro- catalysts for water splitting applications

OP/PP-40

Synthesis of Functionally ModifiedAlginate BasedPolymeric Hydrogel for Anticancer Drug Delivery

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Abstract

This paper describes the development of pH-responsivehydrogel from functionally modified alginate with pH sensitive monomers by a simple free radical polymerization method using phosphate crosslinker and potassium per sulphate as an initiator. These hydrogels were successfully characterized by the FTIR, XRD and SEM, to know the chemical structure, crystalline behavior and surface morphology studies. The pH-sensitive swelling behavior of hydrogels were investigated in different pH solutions and swelling kinetics. These hydrogel drug successfully encapsulated into hydrogel network. The *in-vitro* drug release profiles will be performed in both pH 1.2 & 7.4 and temperatures at 25 and 37 °C. The release of drug analyzed by various kinetics models. The drug release mechanism can be analyzed by evaluating the swelling release data using different empirical equations.

Keywords: Propylene glycol alginate, pH responsive behavior, Anticancer drug, Drug delivery.

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OP/PP-41

An Analogy between the Physical properties of transition metal ions doped with Mixed Alkali Borosilicate Glasses

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Abstract

Mixed alkali borosilicate glasses doped with transition metal ions Cu^{2+}, V^{4+}, Ti^{4+}, Mo^{4+} are prepared by melt quenching technique and their physical properties are studied. From the observed values of density of all the samples it is clear that Cu^{2+} doped borosilicate glasses have maximum value of density and for Mo^{4+} doped glasses have the minimum of density. There is a variation in inter ionic radius of transition metal ions in studied glasses.

The separation between Cu^{2+} ions is less and Molybdenum ions are more in studied glasses. Molar Polarizability has larger value for Cu^{2+} doped glasses and has smaller value for Molybdenum doped glasses. From the calculated values of Molar refraction per unit volume it is evident Cu^{2+} doped glasses have the more ionic nature and Molybdenum doped glasses have the less.

OP/PP-42

Effect of annealing on the nanocrystal embedment in B_2O_3-ZnO-CdO-BaO-MoO_3 glass matrix

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ABSTRACT

This paper reports the formation of spherical nanocrystals in the glass matrix of composition B_2O_3-ZnO-CdO-BaO-MoO_3 during the embedment process. The effect of annealing temperature and the temperature at which embedment was carried out is discussed. XRD, SEM, EDAX results support the size and shape of the nanocrystals formed in the glass matrix. The relation between melting temperature, addition temperature, and nanocrystal radius is discussed.

This paper gives the details of the rapid synthesis of embedding nanocrystals in the glass matrices. The effect of annealing temperature and addition temperatures on the luminescence properties of the Rare earth (Gd) ions in the nanocrystals is also discussed.

Keywords: Nanocrystals, glass matrix, embedment, XRD, SEM, EDAX, annealing and addition temperature, luminescence, rare earth ion.

OP/PP-43

RP-HPLC Method Development and Validation for the Simultaneous Estimation of Trifluridine and Tipiracil in Pure Form and Pharmaceutical Dosage Form

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ABSTRACT

A simple, rapid, precise, accurate and sensitive reverse phase liquid chromatographic method has been developed for the simultaneous determination of Trifluridine and Tipiracil in bulk and pharmaceutical dosage form dosage form. The chromatographic method was standardized using Waters ODS (C18) RP Column, 250 mm x 4.6 mm. 5µm i.d. column with UV detection at 251 nm and Phosphate Buffer (pH- 6.5): Acetonitrile with 65: 35% v/v ratios at a flow rate of 1.0 ml/ min. The Retention time of Trifluridine and Tipiracil in Optimized condition is 2.179 and 3.610.The proposed method was successfully applied to the simultaneous determination of Trifluridine and Tipiracil in bulk and pharmaceutical dosage form. The method was linear over the range of 0-60µg/ml for Trifluridine and 0-40µg/ml for Tipiracil. The recovery was in the range of 98% to 102%. The LOD was found to be 0.06 µg/ml and 0.08 µg/ml for Trifluridine and Tipiracil respectively. The LOQ was found to be 0.18 µg/ml and 0.24 µg/ml for Trifluridine and Tipiracil.

The results of the forced degradation studies indicated the specificity of the developed method that has been developed. Trifluridine and Tipiracil were stable only in acidic, basic and thermal stress conditions and photolytic stress conditions. Different analytical performance parameters such as precision, accuracy, limit of detection, limit of quantification and robustness were determined according to International Conference on Harmonization (ICH) guidelines.

Keywords: RP-HPLC, Trifluridine and Tipiracil, Accuracy, Precision, ICH Guidelines.

OP/PP-44

Green Synthesis of 5–aryl–2–[2-1, 1, 2, 2, 2 – Penta Fluoroethyl] (1, 8) naphthyridin–3–yl]-1, 3,4-exadiazoles using $FeCl_3.H_2O$ in the Solid State and their antibacterial activity

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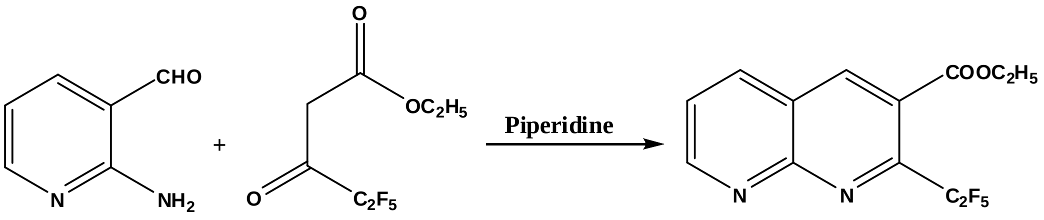
Abstract

Compounds containing 1, 8 naphthyridine moiety represents an important class of compounds and have attracted a great deal of attention, because of their wide range of biological and pharmacological properties, 1, 3, 4–Oxadiazole hetero cycles a Central position in modern hetero cycle chemistry and several methods available in the literature for the synthesis of 1, 3, 4 – Oxadiazoles consequently new and efficient methods for the preparation of this important hetero cyclic ring system. Flourine containing organic compounds constitutes an area of rapidly growing interest because of their unique physical and biological properties.

The Friedlander condensation of 2 – amino nicotinaldehyde with ethyl 4, 4, 5, 5 - Penta fluro – 3 – Oxopentanoate in the presence of piperidine in solvent free grinding condition at room temperature furnished Elhyl – 2 – (1, 12, 2, 2, 2 – Pentafluro ethyl (1, 5) naphthyridine – 3 – Carboxylate.



Keywords: Pharmacology, Biological importance, Green synthesis.

OP/PP-45

Synthesis of novel oxadiazole functionalized pyrazolo[3,4-*b*]pyridine derivatives and their anticancer activity

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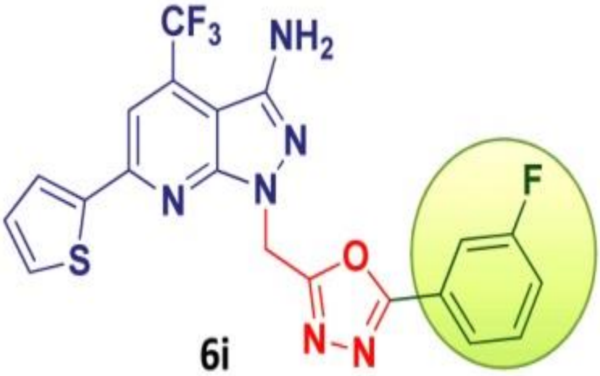
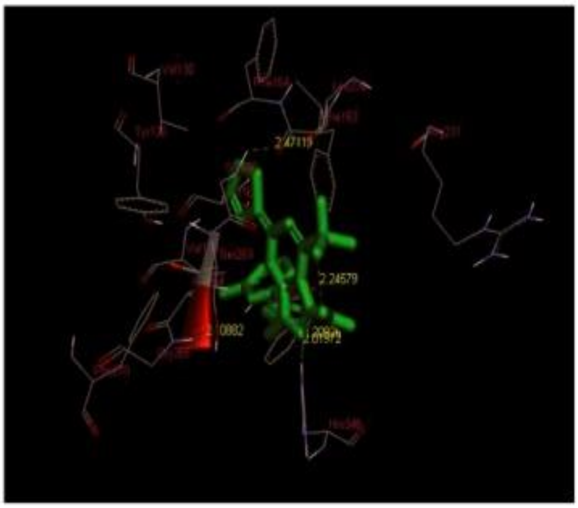
Abstract

A series of novel oxadiazole tagged pyrazolo[3,4-b]pyridine derivatives **6a-n** were prepared. All the final products **6a-n** were screened for anticancer activity against four cancer cell lines such as HeLa-Cervical cancer (CCL-2); COLO 205-Colon cancer (CCL-222); HepG2-Liver cancer (HB-8065); MCF7-Breast cancer (HTB-22); Compounds **6i, 6m** and **6n** are found to have promising anticancer activity at micro molar concentration.



6i



OP/PP-46

Design, synthesis and biological evaluation of some novel 1,3,4-oxadiazoles

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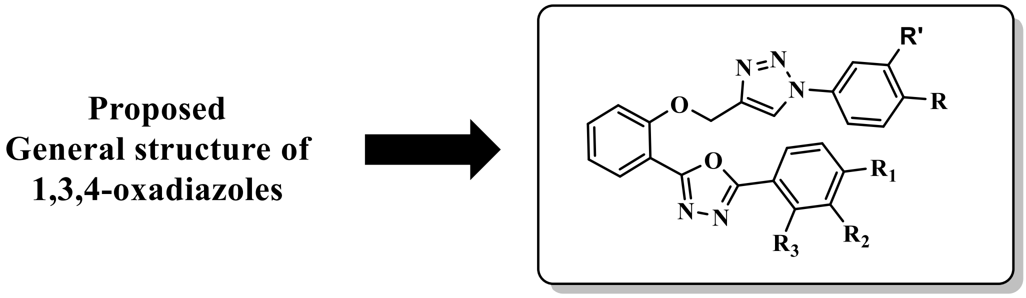
Abstract

Microbial infection is one of the major areas of concern in healthcare and community environments. As per the recent report of UN Ad hoc interagency coordinating Group on Antimicrobial resistances an estimated of 10millions deaths each year by 2050 due to drug resistance microbial diseases and could force up to 24 million people into extreme poverty by 2030. Effective antimicrobial drugs are prerequisites for both preventive and curative measures, protecting patients from potentially fatal diseases and ensuring that complex procedures, such as surgery and chemotherapy, can be provided at low risk. Of particular concern are severe infections caused Gram positive bacteria Staphylococcus aureus, Bacillus subtilis and Gram-negative bacteria Escherichia coli. At the same time reactive oxygen species (ROS) which is the product of normal cellular metabolism, can cause damage to the biomolecules at higher concentration which can lead to oxidative stress-related diseases like cancer, aging, atherosclerosis, and diabetes mellitus. Antioxidants supplements via diet or medicines are required to gain the equilibrium between ROS generation and defensive mechanism of humans, in order to protect against oxidative stress related diseases.

1,3,4-oxadiazoles, an important class of nitrogen and oxygen containing heterocyclic exhibiting a wide range of biological activities such as antibiotic(I), anticancer(II), anti-hypertensive(III) and antiretroviral(IV). On the other hand 1,2,3-triazoles which is continuously attracting the attention of medicinal chemists due to its simple synthetic protocol, and wide variety of pharmacological properties on combining with other heterocyclic moieties. Keeping the importance of 1,3,4-oxadoazole scaffold in view, as part of anongoing project, in search of finding useful novel bioactive molecules here in, we report the design and an efficient synthesis of some 1,3,4-oxadiazoles. Below figure shows the general structure of the synthesized compounds. All the synthesized compounds are analyzed spectroscopically and submitted for biological evaluation.



Keywords**:** 1,3,4-oxadiazoles, Antimicrobial, Molecular docking.

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OP/PP-47

Synthesis and Characterization Of Ru(II), Ru(III) Complexes and Their Catalytic Activity

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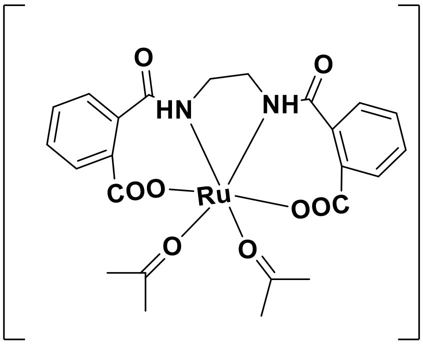
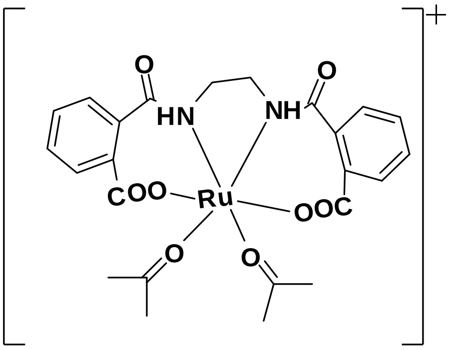
Abstract

A series of new ligands derived by Phthalic anhydride with different aliphatic diamines and substituted aromatic diamines were used to afford new Ru(I), Ru(III), coordination compounds. All the ligands, complexes were characterized by IR, ^{1}H NMR, ^{13}C NMR, mass, ESR in case Ru(III) complexes, magnetic, thermal studies with their structures have been proposed and further these complexes used in catalytic applications.





OP/PP-48

An Efficient $(TBA)_2S_2O_8$ Catalyzed Regioselective Solvent-Free One-Pot Synthesis of Fully Substituted Pyrazoles

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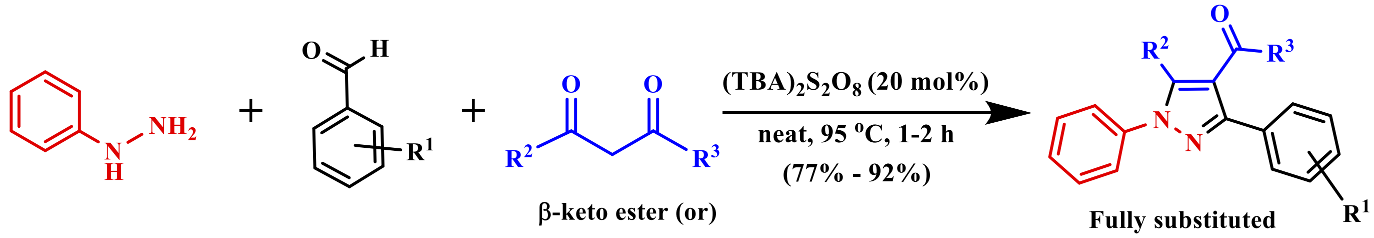
ABSTRACT

An efficient tetra-n-butyl ammonium peroxydisulphate $(TBA)_2S_2O_8$ catalyzed, direct one-pot synthesis of fully substituted pyrazoles in excellent yields with high regioselectivity has been described *via* a three-component cyclocondensation of aldehydes, aryl hydrazines with β-diketones or β-keto esters under solvent-free conditions. The structure of the target compound 4 m was confirmed by X-ray diffraction.



Phenyl hydrazine (2.1)

Aldehyde (2.2 a-i)

β-keto ester (or) β-diketone (2.3 a-c)

Fully substituted pyrazole (2.4 a-p)

Scheme - Synthesis of fully substituted pyrazoles

Keywords: Three-component, One-pot synthesis, Fully substituted pyrazoles, $(TBA)_2S_2O_8$.

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OP/PP-49

Synthesis and Biological Evaluation of Novel 2-Arylquinoline-3-fused thiazolo[2,3c]1,2,4-triazole Heterocycles as Potential Antiproliferative and Antimicrobial Agents

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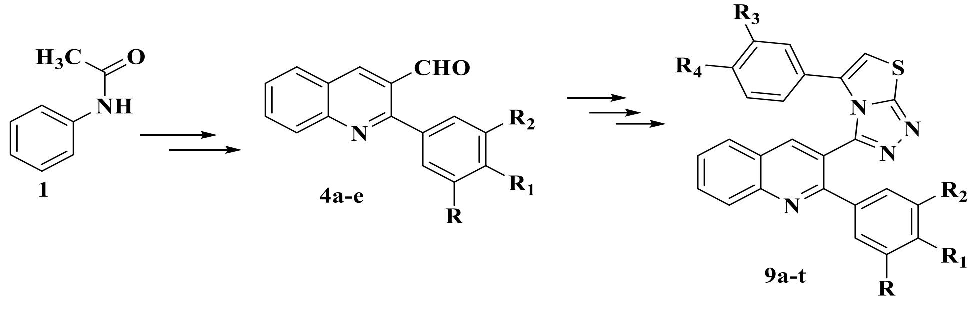
Abstract

An organic compound with at least one hetero atom are known as heterocyclic compounds, which were found to be structural moieties in many synthetic, medicinal chemistry, agrochemicals, also in biomolecules such as vitamins, enzymes and natural products. The widespread of heterocyclic compounds generally fused with nitrogen, oxygen and sulfur atoms. Heterocyclic compounds either naturally produced or synthetically derived often exhibit significant biological and industrial applications. According WHO studies, cancer is one of the major causes of deaths worldwide [1] due to its uncontrolled growth of cells, which exerts physical, mental and financial strain to individuals and of course rapid deadly disease in poor developed nations [2]. Apart from the cancer disease, microbial infections, mainly caused by bacteria, fungi and virus have been creating serious attention from the centuries [3].

A series of novel 2-arylqulinoline-3-fused thiazolo[2,3c]1,2,4-triazole heterocycles **9a-t** were efficiently synthesized using simple conventional methods in good yields. The structure of newly synthesized molecules was characterized on the basis of their IR, ^{1}H NMR, ^{13}C NMR and mass spectral data. Among **9a-t**, compounds **9h**, **9n**, **9b** and **9d** exhibited highly significant antiproliferative activity against two cancer cell lines C6 (nerve cells) and MCF-7 (human breast adenocarcinoma cells) when compared with standard reference *Doxorubicin*. *In vitro* antimicrobial activities of target compounds ***9h, 9b, 9d, 9m** and **9n*** were effectuated on Gram-positive *Staphylococcus aurus (ATCC 25923), Bacillussubtilis (ATCC 6633) and Gram-negative strains Klebsiella Pneumonia (ATCC 31488) and Escherichia coli (ATCC 25966)* strains and found to exhibit promising activity against standard *Ciprofloxacin* drug. Further, *in vitro* antifungal activity was conducted on *Aspergillus Flavus, Aspergillus Niger* strains among all the compounds ***9h, 9b, 9d** and **9n** shown* best activity against standard *Fluconazole* drug moiety.



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OP/PP-50

Synthesis, Characterization and Biological Screening of Metal (II) Complexes of NSO Donor Ligand Derived from 2-(1-(7-hydroxy-2-oxo-2H-chromen-8-yl) Ethylidene) Hydrazine Carbothioamide

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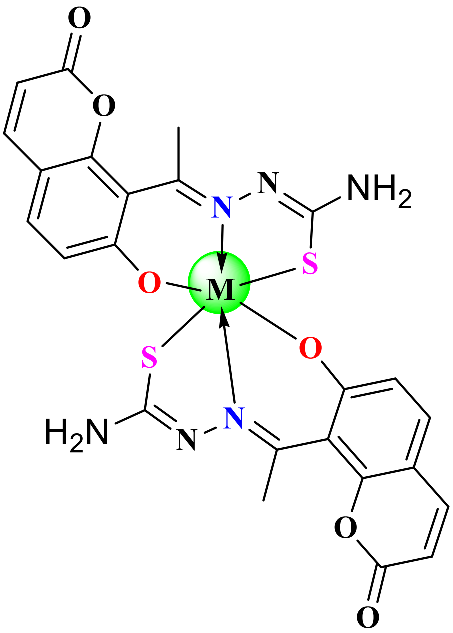
Abstract

The Complexes 2-(1-(7-hydroxy-2-oxo-2H-chromen-8-yl)ethylidene) hydrazine carbothio amide ligand with cobalt(II) (1), nickel(II) (2), copper(II) (3), and zinc(II) (4) are synthesized and characterized byusing different spectroscopic methods such as UV–Visible, infrared, ^{1}H, ^{13}C NMR, molar conductance, ESR and elemental analysis. The anti-proliferative activity of the compounds was evaluated against different human cancer cell lines (IMR-32, MCF-7, COLO205, A549, HeLa and HEK 293) and cisplatin was used as a reference drug. Compounds **1** and **4** showed remarkable cytotoxicity in five cancer cell lines tested, except MCF-7. Also, the compounds were examined for their in vitro antimicrobial and scavenging activities.



M= Co(II), Ni(II), Cu(II) and Zn(II)

OP/PP-51

Development of New RP-HPLC Method for Estimation of Lamivudine and Abacavir in Tablet Dosage Forms and Validation of Method

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Abstract

A sensitive & selective stability-indicating RP-HPLC method has been developed & validated for the analysis of lamivudine and abacavir tablets. In the case of RP-HPLC various columns are available, but here THERMOSIL C18, 150m x 4.6mm x 5µm, or equivalent column was preferred because using this column peak shape, resolution and absorbance were good. Mobile phase & diluent for preparation of various samples were finalized after studying the solubility of API in different solvents of our disposal (acetonitrile, chloroform, methanol, water, etc). The drug was found to be highly soluble in acetonitrile & water. Thus, using acetonitrile, water and phosphate buffer PH 2.5 solvents with appropriate composition newer method can be developed and validated. The chromatograms for lamivudine and abacavir were found to be satisfactory on THERMOSIL C18 150m x 4.6mm x 5µm, or equivalent column using Water: acetonitrile: buffer 2.5 (45:15:40) as mobile phase with flow rate 1.0ml/minute. Wavelength detection was selected after performing UV-spectroscopy of the standard solution of the drug at 232nm.

The calibration curve for Lamivudine & Abacavir was obtained by plotting peak area versus concentration over the range of 300-700 ppm & 600-1400ppm respectively. The regression equation so obtained for the calibration curve was $y= 6156x + 44283$, $r^2 = 0.998$ & $y=30832\ x\text{-}8E + 06$, $r^2= 0.999$ respectively for Lamivudine and Abacavir. Further, the proposed RP-HPLC method has excellent results for all the validation parameters such as Precision, Accuracy, Linearity, Ruggedness, and Specificity. The results shows that the developed method is yet another suitable method for assay and validation parameter studies that can help in the analysis of lamivudine and abacavir in different formulations. A recovery of 101.1% for lamivudine and 99.9% abacavir was found in the assay from tablet formulation. It can be concluded that the proposed RP-HPLC method is sensitive and reproducible for the analysis of Lamivudine and Abacavir in pharmaceutical dosage forms within a short analysis of time.

OP/PP-52

Preparation and characterization of PVA/PVDF/ZnO nanocomposite polymer blends for Electric and Dielectric applications

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Abstract

In this study polyvinyl alcohol (PVA) and polyvinylidene fluoride (PVDF) have been used as the host polymers and the polymer blend is doped with different concentrations of ZnO nanoparticles. Composite polymer blends are prepared by the solution casting technique. The formation of blend, polymer-polymer interactions, interaction between polymer and nanoparticles and role of the nanoparticles on the interactions among PVA/PVDF blend nanocomposites were studied by FTIR spectroscopy.

The crystallinity of the prepared nanocomposites was studied by the XRD characterisation technique and it is observed that there is an increase in amorphous nature, which is due to the addition of nanoparticles into the base matrix.The vibrational morphology and dielectric properties have been studied using UV-Visible, SEM and Impedance spectroscopy. Direct and indirect band gap was found from UV-visible spectrum. The conductivity of PVA/PVDF/ZnO composite is found to be increased with concentration of ZnO nanoparticles. Maximum conductivity was observed for the combination PVA/PVDF/0.5 % ZnO.

Keywords: Polymer blend, PVA, PVDF, PVA/PVDF, ZnO Nanoparticles, nanocomposites, electric and dielectric properties, impedance spectroscopy of the polymers, UV analysis and electrical conductivity of the polymer.

OP/PP-53

One-pot regioselective synthesis of 7-bromo-2H-benzo[b][1,4]oxazin-3(4H)-one linked isoxazole hybrids as anti-cancer agents

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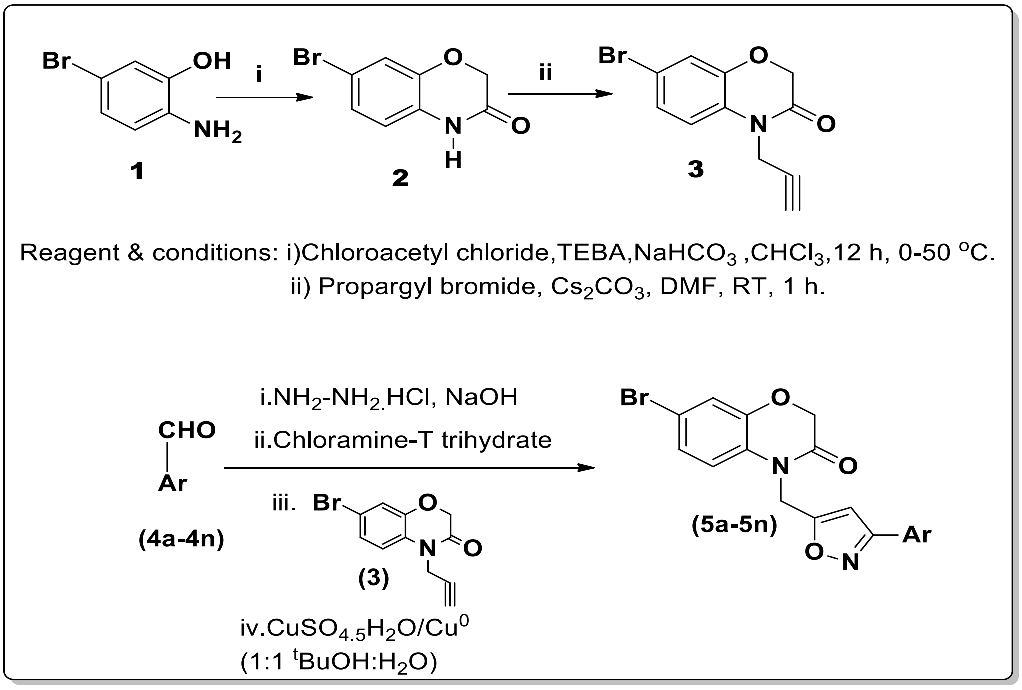
Abstract

Regioselective synthesis of some novel 7-bromo-2H-benzo[b][1,4]oxazin-3(4H)-one linked isoxazole hybrids (**5a-5n**)via copper(I) catalyzed one-pot reaction of various aromatic aldehydes with7-bromo-4-(prop-2-yn-1-yl)-2H-benzo[b][1,4]oxazin-3(4H)-oneis developed. The structures of the compounds that are synthesized are confirmed by ^{1}H-NMR, ^{13}C-NMR, Mass spectra. All the hybrids have been tested for their *in vitro* anticancer activity against four human cancer cell lines including HeLa, MCF-7, A549 and PC3. Among all the compounds 5g (Ar=4-CNC$_6$H$_4$), 5h (Ar=4-NO$_2$C$_6$H$_4$) and 5i (Ar=3,5-di-Cl-C$_6$H$_4$) exhibited remarkable anticancer activity compared to standard drug Etoposide. Molecular docking studies with EGFR (PDB ID- 4HJO) also strengthened the *in vitro* anticancer activity.



Reagent & conditions: i)Chloroacetyl chloride,TEBA,NaHCO$_3$,CHCl$_3$,12 h, 0-50 °C.
ii) Propargyl bromide, Cs$_2$CO$_3$, DMF, RT, 1 h.

OP/PP-54

Kinetics and Mechanistic Investigations in the Acid Bromate Oxidation of Anti-Inflammatory Drug Mefenamic Acid

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ABSTRACT

Mefenamic acid (MFA), a derivative of anthranilic acid is a non-steroidal anti-inflammatory medication (NSAID), belonging to the group of fenemates and exhibits anti-inflammatory, anti-pyretic and to treat many pathological conditions. The kinetics and mechanism of the oxidation of such anti-inflammatory drug mefenamic acid by acid bromate (unmixed with Br_2) in aqueous acetic acid medium was studied.

The reaction exhibited first order each in [bromate] and [mefenamic acid] and second order in [acid]. Variation of ionic strength had no effect on the reaction rate. The reaction rate has enhanced by lowering the dielectric constant of the reaction medium. The reaction has been carried out at six different temperatures and the activation and thermodynamic parameters were calculated. The mechanism proposed involves the decomposition of mefenamic acid-bromate complex leading to 2-((2,3-dimethylphenyl)hydroxyamine)benzoicacid.

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OP/PP-55

Synthesis, Characterization and Anticancer Activity of Cu (II) and Ni (II) Complexes of Novel Schiff Base Ligands.

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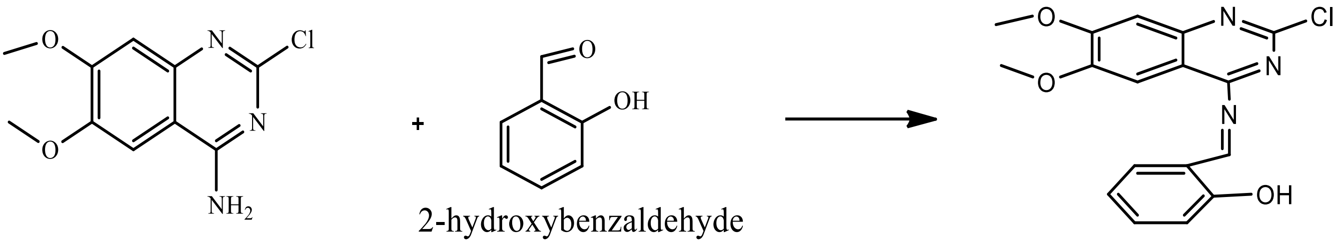
Abstract

Quinazolines are important scaffolds in medicinal chemistry, on account of a wide range of their anti-viral, anti-HIV, anti-malaria, anti-inflammatory, antifungal, anti-bacterial, anti-spasmodic, anti-cytotoxin, anti-virus, anti-analgesic, ***anticancer***, anti-oxidation, anti-hypertensive, anti-depressant, anti-psychotic, anti-diabetes, anti-tuberculosis activities, and also their inhibitory effects on thyrosine kinase, poly-(ADP-ribose) polymerase (PARP) and thymidylate synthase. There are several approved drugs with quinazoline structure in the market. Afatinib, Gefitinib, Vandetanib, Erlotinib, Lepatinib etc are the commercially available anticancer drugs which contain quinazoline motif.

A series of novel Schiff base ligands were synthesized by the condensation of substituted amino quinazolines and various aldehydes. The Schiff bases and their metal complexes were characterized by elemental analysis and various spectroscopic methods like I.R, UV-Vis etc. Further the ligands and their metal complexes were screened for anti cancer activity.



2-chloro-6,7-dimethoxyquinazolin-4-amine

2-hydroxybenzaldehyde

2-(((2-chloro-6,7-dimethoxyquinazolin-4-yl)imino)methyl)phenol

OP/PP-56

Efficient synthesis of 1-phenyl-4-(*m*-tolyl)[1,2,4]triazolo[4,3-a]quinoline

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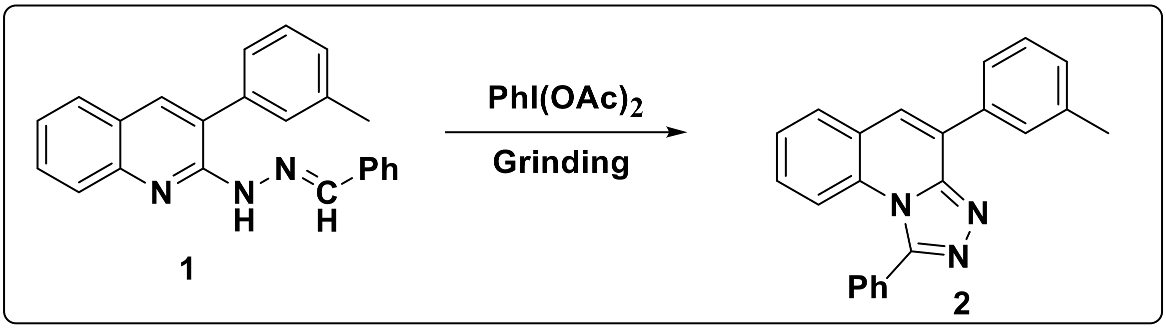
Abstract

A highly efficiently method for the synthesis of 1-phenyl-4-(*m*-tolyl)[1,2,4]triazolo[4,3-a]quinoline **2** by the oxidation of the corresponding (*E*)-2-(2-benzylidenehydrazinly)-3-(m-tolyl) quinoline **1** using Iodobenzene diacetate [$PhI(OAc)_2$] in the solid state at RT under grinding conditions is described. The yields are very good and purity is high. The structures of compounds 3-8 were confirmed by their spectroscopic (IR, 1H NMR and MS) and analytical data.



Keywords: 1,2,4-Triazole, quinoline, Iodobenzene diacetate, solid state.

OP/PP-57

Design, Synthesis and Biological Evaluation of Some New Quinoxaline Containing 1,2,4-thiadiazole Amide Hybrids as Anti-proliferative Agents

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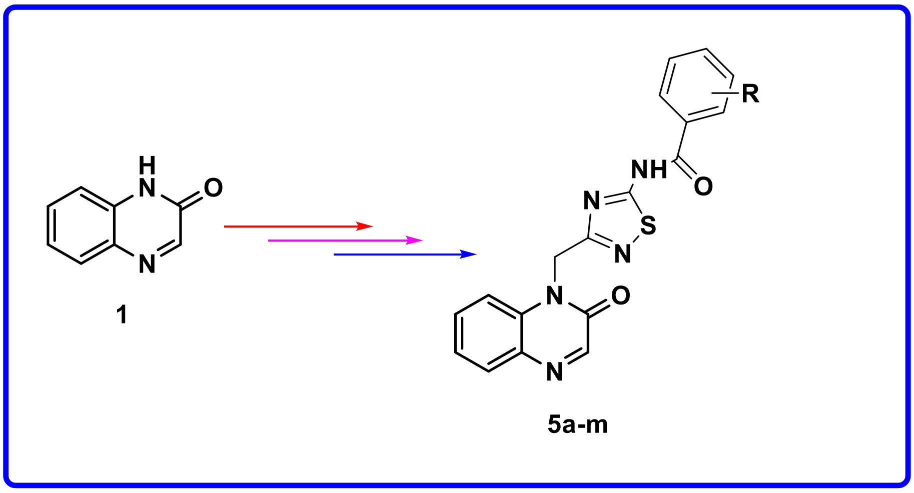
Abstract

A novel series of quinoxaline containing 1,2,4-thiadiazole amide derivatives were synthesized and evaluated for their ability to function as anti-proliferative agents on four different human cancer cell lines including breast cancer HeLa, A549, MCF-7 and HEK-293 and Etoposide as a standard drug. The results showed that **5d, 5e** and **5g** of the synthesized compounds showed promising anticancer activities against four cell lines. Predominantly, the compound **5e** was displayed greater activity on HeLa, A549, MCF-7, and HEK-293 with IC_{50} values of 1.25 ± 0.02, 3.00±0.01, 4.30 ±0.60 and 3.40±0.05μM than the standard drug Etoposide. Furthermore, the compounds **5d** and **5e** displayed promising inhibitory activity over tyrosine kinase EGFR when compared with the standard Erlotinib.



OP/PP-58

Charge Transfer dynamics of 5-BPY with DDQ: Synthesis, Spectrophotometric, Characterization, DNA binding, Anti-cancer activity and DFT/ Time-Dependent DFT Computational studies

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Abstract

The charge transfer (CT) interaction of donor 2, 3-diamino-5-bromo pyridine (5-BPY) and π-acceptor 2, 3-dichloro-5,6-dicyano-p-benzoquinon (DDQ) in acetonitrile (ACN) and methanol (MeOH) solvents at room temperature was studied spectrophotometrically. The stoichiometry proportion of the CT complex was determined by using Jobs and photometric titration methods and found to be 1:1. The association constant (K_{CT}), molar absorptivity (ε) and spectroscopic physical parameters were used to determine the stability of the charge transfer complex. The formation constant recorded higher values and the molar extinction coefficient recorded lower values in methanol compared with acetonitrile, confirming the strong interaction between the molecular orbitals of donor and acceptor in the ground state in a less polar solvent. The prepared complex was characterized by FT-IR, NMR, powder XRD, and SEM EDX analysis. The nature of the DNA binding ability of the complex was probed by using UV-visible spectroscopy, and the binding mode of the CT complex is intercalative. The intrinsic binding constant (K_b) value is 5.2×10^6 M^{-1}.

The CT complex may be used as a pharmaceutical drug in the future due to its high binding affinity. Anticancer activity was screened against breast cancer MDA-MB-231 and MCF-7 cell lines, the complex shows significant activity when compared to corresponding donor and acceptor. Moreover, density functional theory (DFT) studies are discussed for the charge transfer complex 5-BPY-DDQ, using the CAM-B3LYP with a 6-31 G (d, p) basis set. The bond lengths, bond angles, Mulliken and natural atomic charges, reactivity parameters, and FMO surfaces were also evaluated. The theoretical UV-visible spectrum of the compound and the electronic properties, such as HOMO and LUMO energies, were performed using the time-dependent (TD-DFT) approach with CAM-B3LYP, employing the 6-31 G (d, p) basis set, and good agreement with the theoretical and experimental UV-visible data was found.

OP/PP-59

DNA Binding, Cleavage, Docking, Biological and Kinetic Studies of Cr(III), Fe(III), Co(II) and Cu(II) Complexes with *ortho*-Vanillin Schiff Base Derivative.

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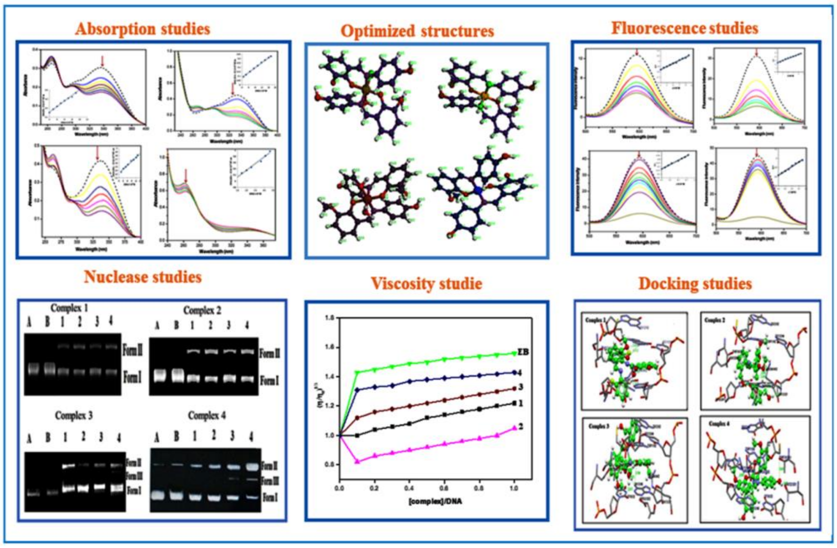
ABSTRACT

Schiff base (**HL**) was synthesized by refluxing of 2-hydroxy- 3-methoxybenzaldehyde with *p*-aminophenol in 1:1 molar ratio. The coordination behaviour of a series of transition metal ions with the synthesized HL ligand, $[Cr(HL)_2]$ (**1**), $[Fe(HL)_2]$ (**2**), $[Co(HL)_2]$ (**3**) and $[Cu(HL)_2]$ (**4**) is reported. The stereochemistry and the bonding behaviour of the complexes was deduced by sophisticated spectral techniques. These studies revealed that the metal centres were found to be octahedral for **1, 2** and **3** complexes and complex **4** with square planar geometry. Kinetic parameters of the complexes were estimated by Coats-Redfern method and the complexes were found to be thermally stable.

DNA binding affinity of these metal complexes was explored by means of fluorescence, UV-visible and viscosity studies and the studies suggested intercalative mode. The K_b values from the absorption studies are 2.98×10^3, 2.16×10^3, 4.66×10^3 and $5.46\times10^3 M^{-1}$ and K_{sv} values from fluorescence studies are 3.79×10^4, 2.14×10^4, 4.92×10^4 and $6.47\times10^4 M^{-1}$ for **1, 2, 3** and **4** complexes respectively. Nuclease studies in the presence of H_2O_2 were performed using *pUC19* supercoiled DNA. Docking studies were done using *human* DNA topoisomerase -I (DNA topoI) receptor protein. *In vitro* antimicrobial studies revealed higher activity for complexes than the ligand and *in vitro* anti-tumour studies showed that complexes **3** and **4** possess potential inhibitory efficiency with an IC_{50} of 49.13± 1.2μg/mL and 33.85± 2.2μg/mL correspondingly.



Key words: DNA binding, nuclease, *in- vitro* biological, docking studies.

OP/PP-60

Spectral, Structural and Biological applications of Piperazine Connected D-(-)-alpha-Phenylglycine: protease kinase inhibitor

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Abstract

The structural and biological mechanism of a drug material was investigated by spectroscopic techniques and molecular modeling methods. To explore the biological activities docking studies of D-(-)-alpha-Phenylglycine is performed with Prolactinoma and hyperprolactinemia diseases. The interpretation which affords good information about D-(-)-alpha-Phenylglycine's electronic properties with different solvation effects. Reactive sites were also analysed using topological studies. All the newly synthesized compounds structures were determined by NMR, Mass, FTIR and CHN analysis.

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OP/PP-61

Catalytic and Antioxidant Activity of biogenic Ni Nanoparticles using *Terminalia chebula* fruit aqueous extract: A Green Synthesis

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Abstract

In the present work, a green synthetic method was employed for a synthesis of Nickel/ Nickel Oxide (Ni/NiO) nanoparticles using Polyphenolic rich *Terminalia Chebula* fruit aqueous extract. The UV-Vis data revealed the formation and monodispersed nature of Nanoparticles. FTIR & EDX confirmed that polyphenolic and alkaloids were utilized in the formation of Nanoparticles. The XRD established formation of Ni & NiO nanoparticles of FCC. SEM indicated the agglomeration of nanoparticles and TEM established the spherical shape with an average size about 15.6 nm.

This study evaluated the antioxidant and catalytic activity of green synthesized Ni/NiO NPs against DPPH and Congo Red (CR) Dye respectively. Degradation of the Congo red dye found to be first order kinetics, the catalytic degradation of carcinogenic Congo red dye completed within 30 mints and assay of DPPH found maximum at 100 µg/ml and EC 50 as 65.01.

Keywords: Antioxidant activity, Aqueous extract, Catalytic, Green synthesis, Nanoparticles.

OP/PP-62

Application of FT-IR Spectroscopy for Quantitative determination of drugs

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Abstract

The most common pharmaceutical analysis is the quantitative measurement of the active ingredient and related compounds in the pharmaceutical product. These determinations require the highest accuracy, precision and reliability because of the intended use of the data, manufacturing control, stability evaluation. Pharmaceutical analysis is an important subject for the quality control of raw materials, drugs, food stuffs and pharmaceuticals. This is due to the fact that drug, pharmaceutical and foodstuffs of maximum purity are essential for the safeguard of the health of human beings. The purity and stability of the drugs are checked with the help of various physical, chemical and instrumental technologies.

FT-IR spectroscopy is a rapid technique, requires minimal sample and provides comparable accuracy to other established methods. The IR spectra of peak area, peak height or peak ratio which are most suitable for quantitative determination.

Aceclofenac is a class of non-steroidal anti-inflammatory drug. Aceclofenac concentration range (2-20 mg/mL), the calibration curves were constructed absorbances at 1149.53cm^{-1}, 1280.73 cm^{-1}, 1417.68 cm^{-1} and 1506.41 cm^{-1}. The limits of Beer's law, slope, intercept, correlation coefficient (0.994), sandell's sensitivity (0.033), LOD(2.167), LOQ(6.566) and regression equation for aceclofenac were calculated. Pharmaceutical formulation of aceclofenac was analysed with same concentration. The values like % RSD, % error, t- and F- tests values were determined.

Alfuzosin HCl is a selective α_1 adreno receptor antagonist used in the treatment of benign prostatic hyperplasia. Alfuzosin concentration range (1-10 mg/mL). The calibration curves were constructed absorbances at 1280.73 cm^{-1}, 1492.90 cm^{-1}, 1529.55 cm^{-1} and 1664.57cm^{-1}. The limits of Beer's law, slope, intercept, correlation coefficient (0.998), sandell's sensitivity (0.011), LOD(0.157), LOQ(0.357) and regression equation for alfuzosin were calculated. The values like % RSD, % error, t- and F- tests values were determined.

Keywords: Aceclofenac, Alfuzosin HCl, Chloroform, FT-IR Spectrometry.

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OP/PP-63

Green, One-pot, Four Component Synthesis of Novel N-Substituted 5-(2,4-Diphenyl-l-1H-Imidazol-1-yl)-1-Isopropyl-1H-1,2,4-Triazole as Anti-inflammatory Agents

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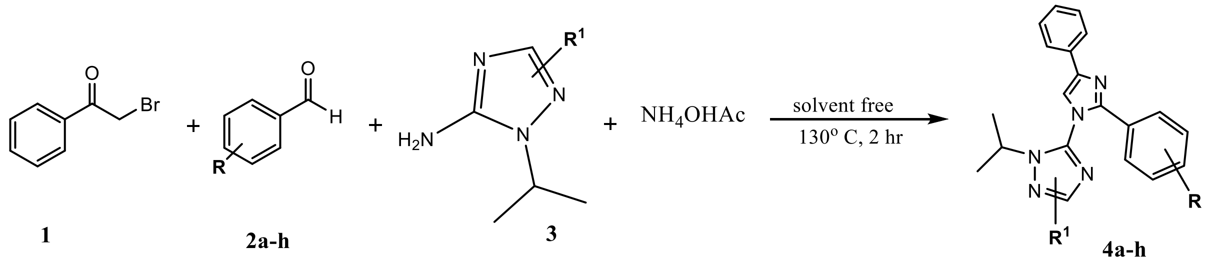
Abstract

A one-pot, four-component catalyst free synthesis of 5-(2,4-diphenyl-1H-imidazol-1-yl)-1-isopropyl-1H-1,2,4-triazole derivatives **(4a-h)** is described. Heating a mixture of a 2-bromoacetophenone, an aldehyde, a triazole amine, and ammonium acetate under solvent-free conditions affords functionalized triazole substituted imidazoles in good to excellent yields. The structures of all the synthetic derivatives were confirmed by ^{1}HNMR, ^{13}CNMR, and mass spectral data. Further, these compounds were tested for their anti-inflammatory activity.



1 **2a-h** **3** **4a-h**

R= **a**) 4-H, **b**) 4-Me, **c**) 4-OMe,
d) 4-NO_2, **e**) 4-CN,
f) 4- Cl, **g**) 3,5- di nitro, **h**) 3,5- di fluoro

Key words: one-pot, four-component, 1,2,4-trisubstituted imidazole's, solvent free,

Catalyst free, anti-inflammatory agents

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OP/PP-64

Development and Validation of RP-HPLC for the Simultaneous Estimation of Etoricoxib and Thiocolchicoside in API Form and Marketed Combined Tablet Dosage Form

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ABSTRACT

A new analytical simple, rapid, precise, accurate and sensitive reverse phase liquid chromatographic method has been developed for the simultaneous determination of Etoricoxib and Thiocolchicoside in bulk and pharmaceutical dosage form dosage form. The chromatographic method was standardized using Develosil ODS HG-5 RP C_{18}, 5µm, 15cmx4.6mm i.d. i.d. column with UV detection at 255nm and Methanol: Phosphate buffer (0.02M) with 55:45 (pH-2.6) ratios at a flow rate of 1.0 ml/ min. Different analytical performance parameters such as precision, accuracy, limit of detection, limit of quantification and robustness were determined according to International Conference on Harmonization (ICH) guidelines. The method was linear over the range of 0-14µg/ml for Etoricoxib and 0-28µg/ml for Thiocolchicoside. The recovery was in the range of 98% to 102%. The LOD was found to be 0.06 µg/ml and 0.09 µg/ml for Etoricoxib and Thiocolchicoside respectively. The LOQ was found to be 0.18 µg/ml and 0.27 µg/ml for Etoricoxib and Thiocolchicoside. The proposed method was successfully applied to the simultaneous determination of Etoricoxib and Thiocolchicoside in bulk and pharmaceutical dosage form.

Keywords: RP-HPLC, Etoricoxib and Thiocolchicoside, ICH Guidelines, Accuracy, Precision.

OP/PP-65

In vivo Anti-inflammatory, DNA Interaction, Molecular Docking, Biological and Thermal Studies of Schiff base Complexes Derived from o-Hydroxy Acetophenone and 2-Fluoroaniline.

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Abstract

Series of transition metal complexes were derived from Schiff base ligand **(HL)** obtained by condensation of o-hydroxy acetophenone with 2-fluoroaniline in 1:1 ratio. Structural and bonding parameters of the ligand and metal complexes [Fe $(HL)_2Cl(H_2O)$]**(1)**, [Co $(HL)_2$]**(2)**, [Ni$(HL)_2$]**(3)** and [Cu$(HL)_2$]**(4)** have been deduced by analytical and spectral studies which revealed octahedral geometry for complex **1** and square planar geometry for complexes **(2)**, **(3)** and **(4)**. Coats-Redfern calculations for deriving thermodynamic properties, suggest that all the complexes are non-spontaneous and thermally stable.

DNA binding studies revealed intercalation binding mode, while intrinsic binding constant (K_b), S*tern-Volmer* quenching constant (K_{sq}) support high binding abilities. The nuclease activity of the metal complexes was carried out by gel electrophoresis using CT-DNA. Docking studies were done using Accelry’s Discovery Studio 2.1 program to understand binding affinities. *In vivo* carrageenan induced inflammation studies in paw volume were carried out in rats and results show a higher rate of edema inhibition for complex**4**. *In vitro* cytotoxicity and antimicrobial assay reveal that complex **4** exhibited much cytotoxic and microbial activity over other complexes and the ligand.

Key words: DNA binding, *in-vivo,* carrageenan, *in- vitro* cytotoxicity, docking studies.

OP/PP-66

Regioselective synthesis of 1,3,5 triazine-1,2,3-triazolo-spiroxindoles *via* 1,3- dipolar cycloaddition reaction

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Abstract

The essential need for the anti-cancer agents with high selectivity towards the cancer cell lines has prompted us to synthesize a novel series of triazine-triazolo spirooxindoles. The title compounds were synthesized by using one-pot multicomponent reaction of 1,3,5 triazine-1,2,3- triazolo chalcones, oxindoles and *L*-proline in methanol at room temperature delivers triazine-triazolo spirooxindoles in good to excellent yields *via* 1,3-dipolar cycloaddition reaction. The azomethine ylide generated *in situ* from isatins and secondary aminoacids (*L*-proline) reacted with 1,3,5 triazine-1,2,3-triazole chalcones to produce spirooxindole derivatives. The structures of all the generated compounds were characterised by using FT-IR, ^{1}H NMR, ^{13}C NMR and Mass spectral data.

Keywords: Multicomponent reaction, triazine-triazole chalcones, Spiroxindoles, Isatin, L-proline.

Acknowledgments

We are thankful to the CSIR-HRDG for providing research fellowship and thankful to NIT-Warangal for providing fecilities.

Conflicts of Interest

No conflict of interest.

OP/PP-67

Synthesis of Carbohydrate Polymer/Graphene Oxide Nanocomposite for Anticancer Drug Delivery

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Abstract

The 5-fluorouracil loaded sodium alginate hydrogel beads coated with graphene oxide to increase the drug loading capacity by simple ionotropic gelation technique with different crosslinking agents for targeted drug delivery. The obtained beads were charecterised by FTIR, SEM, XRD, DSC, TGA. Drug release studies were performed at 1.2, 5.4 and 6.8 pH at 37º C. The outcomes of the analysis showed that increases the magnesium cross linker enhanced the swelling and drug release rate. Antitumor activity of drug loaded hydrogel beads were studied by using MTT assay. Finally concluded that the drug loaded hydrogel beads potential for cancer applications.

OP/PP-68

A New Charge Transfer Interaction between 6-Amino Indole and Chloranilic Acid: Spectrophotometric, Characterization, Computational, Antimicrobial and DNA Binding Properties

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ABSTRACT

The chemistry of a new charge and proton transfer hydrogen bonded complex (PT CT) between the donor 6-Aminoindole (6 AMI) and the π-acceptor Chloranilic acid (CLA) has been explored in acetonitrile (ACN), methanol (MeOH), and 50% acetonitrile + 50% methanol (ACN-MeOH) at 25 ℃ by

using electronic absorption spectroscopy. By exploiting Job’s and the photometric titration methods, the molar proportion of the PT CT complex was confirmed as 1:1. The modified Benesi-Hildebrand principle was used to evaluate the association constant (K_{CT}) and molar absorptivity ($\mathcal{E}_{CT}$) of the PT CT complex, and these values indicate that produced PT CT complex is more stable. In three different solvents, the effect of solvent polarity on charge transfer spectra was also observed. Different spectroscopic physical parameters were assessed in different polar solvents, including energy (E_{CT}), ionization potential (I_D), resonance energy (R_N), oscillator strength (f), dissociation energy (W), standard Gibbs free energy (ΔG^o), transition dipole movement (μ_{EN}), and these were also within the accepted values, confirming the stability of the formed PT CT complex.

The produced solid PT CT complex was analyzed by using FT-IR, NMR, TGA-DTA, and SEM-EDX spectra. Powder XRD analysis was used to determine the PT CT complex nature and crystalline size. The biological activity of the current PT CT complex has been screened in antimicrobial and DNA binding studies. The synthesized PT CT complex was shown to have excellent antimicrobial activity and DNA binding affinity. Therefore, in the future, it may be used as a pharmaceutical drug for bacterial and fungal infections. The computational studies were carried out by using DFT analysis, and the functions were used to B3LYP and CAM B3LYP in the gas phase, with the basis set being 6-31G + (d, p). The bond lengths, bond angles, Mulliken atomic charges, MEP maps, reactivity parameters, and FMO surfaces were also calculated. The computational analysis is additionally supported by the experimental studies of the PT CT complex.

OP/PP-69

One-pot Synthesis of 3-Aminoindolizines Using Readily Available and Recyclable CuCN/[bmim]PF_6 System

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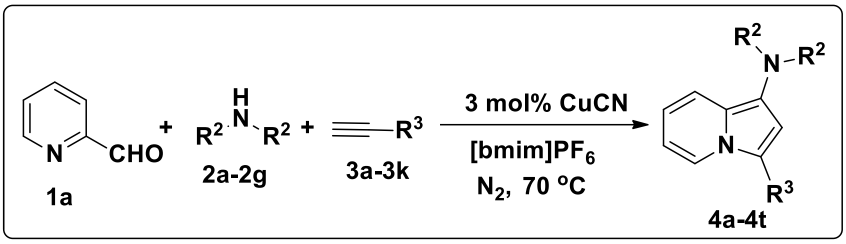
Abstract

A simple, readily available, clean and efficient CuCN/[bmim][PF_6] system to synthesize 3-aminoindolizines in one-pot from the pyridine-2-carbaldehyde, secondary amines, and terminal alkynes was developed for the first time. The desired 3-aminoindolizines were simply isolated by diethyl ether and the resulting CuCN/[bmim][PF_6] system was reused for six times without any appreciable change in the catalytic activity.



Keywords: 3-Aminoindolizines; CuCN/[bmim]PF_6; Intramolecular cyclization; Mannich-Grignard Addition; One-pot synthesis.

OP/PP-70

Convenient One-Pot Synthesis of Multi substituted thiazol-2-yl-1,2,3,6-tetrahydro pyrimidine-4,5-dicarboxylate via Catalyst-Free Multicomponent Reactions

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Abstract

A novel and convenient one-pot synthesis was developed for the synthesis of multisubstituted thiazolyl pyrimidine analogues via catalyst free from electron-deficient alkynes, anilines and formaldehyde by a domino reaction under optimized conditions. The multicomponent reactions were skilful with high regioselectivity and excellent yields. The structures of the synthesised derivatives were confirmed by ^{1}HNMR, ^{13}CNMR, and mass spectral data. Further, these compounds were tested for their antibacterial activity.

Key Words: One-pot, Catalyst free, Tetrahydro pyrimidine, antimicrobial activity,

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OP/PP-71

Synthesis and Biological Screening of 9-Aryl-6-[2-(trifluoromethyl)phenyl] [1,2,4]Triazolo [4,3-*a*][1,8]Naphthyridines as Antibacterial and Anti-inflammatory Agents

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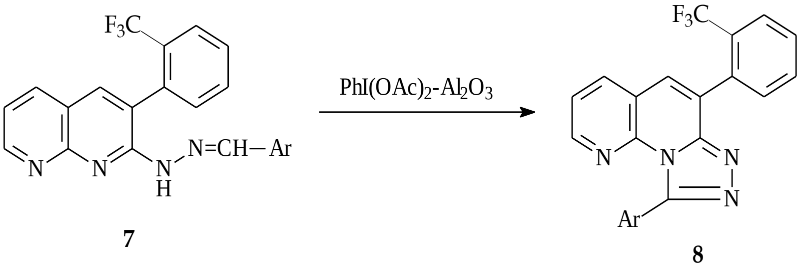
Abstract

Fused 1,2,4-triazoles constitute one of the most active class of compounds possessing diverse pharmacological and microbiological activity[1,2]. A simple, rapid and efficient protocol for the synthesis of 9-aryl-6-[2-(trifluoromethyl) phenyl] [1,2,4]triazolo[4,3-*a*][1,8] naphthyridines **8** is achieved by the oxidation of aryl aldehyde 1-{3-[2-(trifluoromethyl)phenyl][1,8]naphthyridin-2-yl}hydrazones **7** with alumina-supported iodobenzene diacetate [$PhI(OAc)_2$-Al_2O_3] in the solid state. The reaction proceeds efficiently at room temperature in high yields and in a state of high purity. The structures of compounds are assigned on the basis of their spectral (IR, ^{1}H NMR and MS) and analytical data. The compounds **8** have been evaluated for their antibacterial and anti-inflammatory activities.



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OP/PP-72

Design and Syntheses of New Flexible Metal-OrganicFrameworks (MOFs) for Heterogeneous Catalysts

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Abstract

Porous coordination polymers (**PCPs**), or metal-organic frameworks (**MOFs**) are emerging as potential materials of the decade, particularly forgas storage, separation, catalysts, and sensors, etc. However, **PCPs** existing in the literature were mostly surface oriented porosity without any open metal sites (**OMSs**). Some of the **PCPs** are formed by the coordinated solvent in the pristine form are unstable after removal of the solvent leads collapse of the structure.

To overcome these problems, we focused on flexible MOFs using ligands obtained by reacting Aromatic nitro compounds with the corresponding symmetrically substituted azo compounds. Later, these flexible MOFs were employed various applications including heterogeneous catalysts.

OP/PP-73

Design, synthesis and biological evaluation of the thiazolidinone based pyrrolidino-bisspiroxindoles as anti-cancer agents.

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Abstract

A novel series of thiazolidinone based pyrrolidino-bisspiroxindoles were designed and synthesized from thiazolidinone based chalcones (**7a-j**), isatin and sarcosine. The benzanilide substituted chalcones (**7a-j**) were synthesized from thiazolidindione and various benzaldehydes (**2a-j**). The synthesized target compounds thiazolidinone based pyrrolidino-bisspiroxindoles (**10a-j**) were characterized by IR, NMR and Mass spectral data.

In silico anti-cancer molecular docking studies were performed on these compounds and they were showing good binding affinity (-10.2 kcal/mol to -8.9 kcal/mol) towards cancer protein (PDB ID: 1VKG). *In vitro* anti-cancer studies of these target compounds are under progress.

OP/PP-74

Green synthesis of 6-Aryl-14H-Quinolino[2^1,3^1:4,5] pyrimido [1,2-A] Quinolin-14-one

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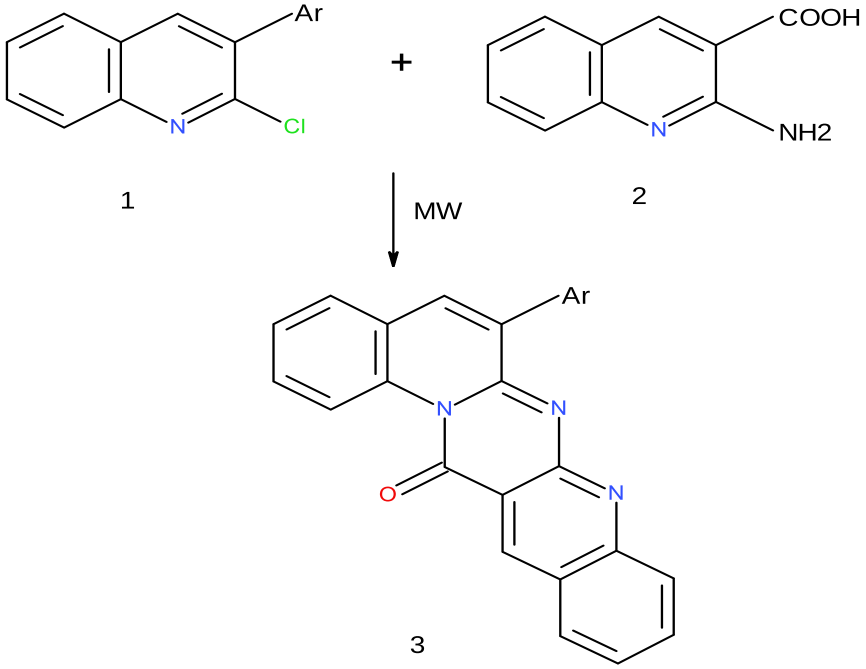
Abstract

An efficient and rapid method for the synthesis of 6-Aryl-14H-Quinolino[2^1,3^1:4,5] pyrimido [1,2-A]Quinolin-14-one (3) achieved by the reaction of 3-aryl-2-chloro Quinolines (1)with 2-amino Quinoline-3-carboxylic acid(2) in the presence of catalytic amount of DMF in solvent- free conditions Under microwave irradiation. The products are obtained in 6-Aryl-14H-Quinolino [2^1,3^1:4,5] pyrimido [1,2-A]Quinolin-14-one very good yields and in state of high purity.



OP/PP-75

Physico-chemical Studies and Biological Activity of Pyrimidine Based Schiff Base Complexes

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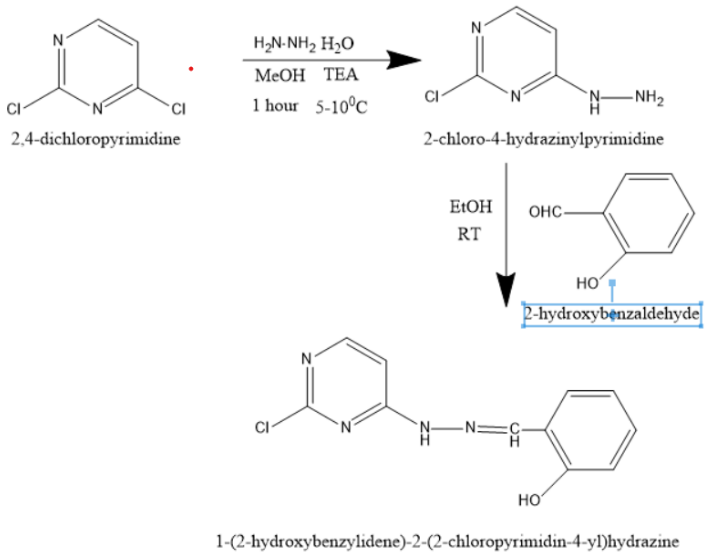
Abstract

A Schiff base derived from the condensation of 2-chloro-4-hydrazinylpyrimidine with 2-hydroxy benzaldehyde and its complexes with VO(IV), Cr(III), Mn(II), Fe(III), Co(II), Ni(II), Cu(II), Zn(II), Pd(II), Cd(II) and Hg(II) have been synthesized and characterized by elemental analysis, magnetic, thermal and infrared, UV-visible and ESR spectral data. The ligand acts as a mono negative, bidentate one towards VO(IV), Zn(II), Pd(II), Cd(II) and Hg(II) coordinating through nitrogen of free C=N and phenolic oxygen and as tridentate one coordinating additionally through nitrogen of pyrimidine ring C=N towards Cr(III), Mn(II), Fe(III), Co(II), Ni(II) and Cu(II).

The VO(IV), Cr(III), Mn(II), Fe(III), Co(II), Ni(II) and Cu(II) complexes are paramagnetic while the Zn(II), Pd(II), Cd(II) and Hg(II) complexes are diamagnetic. The Cr(III), Mn(II), Fe(III), Co(II) and Ni(II) complexes are octahedral, Cu(II) complex tetragonal, VO(IV) complex square pyramidal, Pd(II) complex square planar and the Zn(II), Cd(II) and Hg(II) complexes tetrahedral in geometry. Ligand field parameters in the case of Co(II) and Ni(II) complexes and the in-plane and out-of-plane bonding parameters in the case of Cu(II) complex have been evaluated and relevant conclusions drawn therefrom.



OP/PP-76

Design, Fe(III)-Catalysed Synthesis and Biological Evaluation of Novel 2-(4-Phenyl Quinolin-2-yl) Thiazole Derivatives as Anticancer Agents

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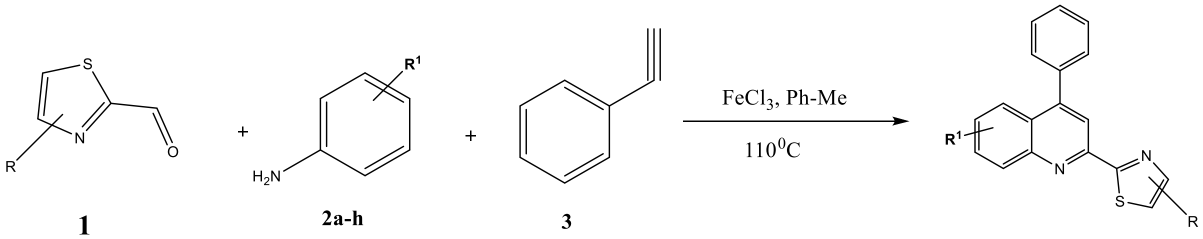
Abstract

We have designed and achieved a one-pot three-component synthesis of novel 2-(4-phenylquinolin-2-yl) thiazole Derivatives **(4a-h)** from substituted thiazole -2-carbaldehyde, an amine and a terminal alkyne with Fe(III)-catalyst. All the chemical structures were confirmed by ^{1}HNMR, ^{13}CNMR and mass spectral data. Further, these compounds were tested for their preliminary anticancer activity against four different human cancer cell lines such as A549 (lung), MCF-7 (breast), MDA MB-231 (breast), and DU-145 (prostate) by MTT assay and etoposide used as standard drug. All these derivatives were exhibited well to moderate anticancer activity compared to the standard drug. Among them, four compounds **(4d, 4e, 4g and 4h)** have showed more potent activity.



1 **2a-h** **3** **4a-h**

R^1= **a**) 4-H, **b**) 4-Me, **c**) 4-OMe,
d) 4-NO_2, **e**) 4-CN,
f) 4- Cl, **g**) 3,5- di nitro, **h**) 3,5- di fluoro

Keywords: one-pot three component reaction, Fe(III)-catalyst, quinolines, anticancer agents.

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OP/PP-77

Design, Synthesis and Molecular Docking Studies of Quinoxaline Linked 1, 2, 4-Oxadiazole Hybrids and Their Anti-Proliferative Activity

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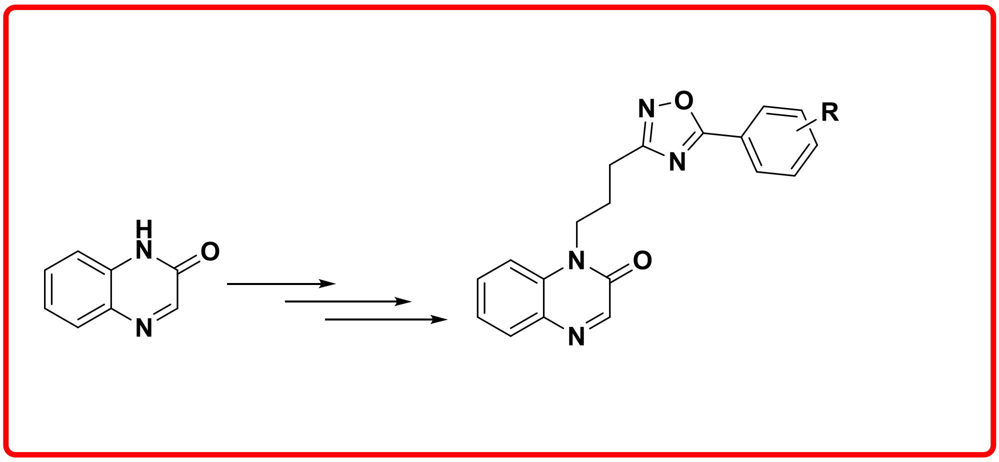
Abstract

We, herein, described the synthesis of some new quinoxaline-1, 2, 4-oxadiazole derivatives (**3a–n**) and their *in vitro* anti-cancer activity against four human cancer cell lines like MCF-7 (human breast), HeLa (human cervical), HCT116 (human colon carcinoma) HepG2 (liver hepato cellular carcinoma). The results revealed that the compounds **3d, 3e, 3i** and **3k** have shown promising activity as compared to etoposide. Predominantly, the compound **3d** was displayed greater activity on MCF-7, HeLa, HCT116 and HepG2 with IC_{50} values of 1.20±0.12, 2.20 ± 0.31, 2.34±0.32 and 2.67± 0.45 than the standard drug etoposide. Moreover, molecular docking studies of derivatives **(3a–n)** on EGFR receptor suggested that the most potent compound **3d** strongly binds to protein EGFR (pdbid: 4HJO). Furthermore, the compounds **3d** and **3k** displayed promising inhibitory activity over tyrosine kinase EGFR when compared with the standard erlotinib.



OP/PP-78

Fabrication of Levofloxacin Encapsulated Montmorillonite-Based Sodium Alginate/ Silver Nanoparticles Microbeads for Ph-Responsive Drug Delivery

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Abstract

The study reports the fabrication of montmorillonite (MMT)-based sodium alginate (SA)/silver nanoparticles (AgNPs) microbeads as potential drug vehicle for controlled release of levofloxacin (LVX). The microbeads were prepared using in situ ion-exchange followed by simple ionotropic gelation technique. The developed beads were characterized by fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), X-ray diffraction (XRD) and scanning electron microscopy (SEM). Swelling studies and in vitro release studies were investigated in pH 1.2, 5.0 and 7.4 at 37°C.

Results suggested that both the swelling and in-vitro release studies were influenced by the pH of test media, which might be suitable for intestinal drug delivery. The release mechanism was analyzed by fitting the release data into Korsmeyer-Peppas equation. Antibacterial activity of the synthesized microbeads was studied against gram-negative bacteria, namely *Escherichia coli* and gram-positive bacteria, namely *Bacillus cereus* by agar disc diffusion method. The results suggested that the developed dual drug-loaded 2-hydroxyethyl starch MPs could significantly inhibit bacteria development.

OP/PP-79

Biological Studies of 1-(4'-Chlorobenzoyl)-4-methyl-3-thiosemicarbazide and its Co(II), Ni(II) Binary Chelates

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Abstract

Binary chelates of 1-(4'-chlorobenzoyl)-4-methyl-3-thiosemicarbazide with Co(II) and Ni(II) ions have been synthesized and characterized by elemental analyses, TGA, conductivity and magnetic susceptibility measurements, LC-MS, IR, UV-Visible spectroscopy. Co(II) ion formed 1:1 polynuclear and Ni(II) ion formed mononuclear 1:2 chelates with $[ML(H_2O)_2]_n$ and $ML_2(H_2O)_2$ compositions respectively. Equilibrium studies of1-(4'-chlorobenzoyl)-4-methyl-3-thiosemicarbazide with Co(II) and Ni(II) ions have been carried outby Irving Rossetti pH titration technique in 70% v/v DMF-Water medium, 0.1M (KNO_3) ionic strength at 303K, which revealed the formation of 1:1 and 1:2 metal complexes in solution.

Interaction of the solid metal chelates with calf thymus DNA has been evaluated using absorption spectroscopy, spectro-fluorimetry and viscosity measurements. Both the complexes exhibited hypochromism and intercalation mode of binding. The cleavage studies of metal complexes with supercoiled pBR33 DNA using gel electrophoresis method showed hydrolytic cleavage of plasmid DNA. The synthesized complexes displayed antibacterial activity against Gram +ve and Gram -ve bacteria.

Keywords: Equilibrium studies, DNA interaction, DNA cleavage, antibacterial activity.

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OP/PP-80

Synthesis of some new Isoxazole-Piperidine-1, 2, 3-Triazoles as *in vitro* Anticancer Agents

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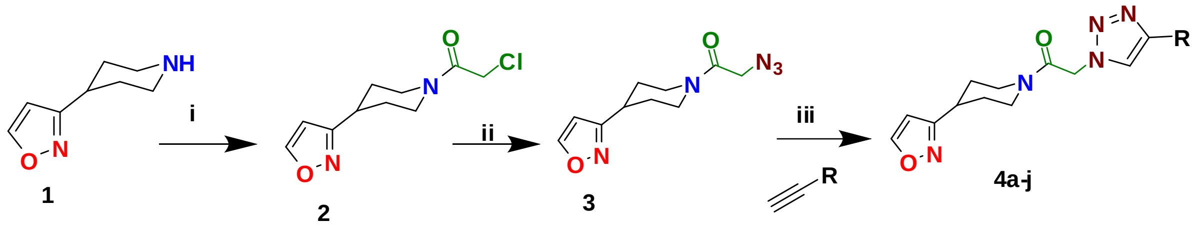
Abstract

The synthesis of some new isoxazole-piperidine-1,2,3-triazoles (4a-4j) was achieved using Sharpless Cu(I) catalyzed [3+2] cycloaddition as a key approach. The *in vitro* anticancer screening of all the compounds against four human cancer cell lines including MCF-7, HeLa, A549 and IMR32 revealed that the compounds **4c** and **4f** exhibited promising activity against all the cell lines as compared to etoposide. Rests of the compounds were shown good to zero activity against specific cell liens when compared with the positive control. Predominantly, the compound **4c** was shown superior activity against IMR32 which posses IC_{50} value 3.2±0.3 µM.



Reagents and conditions: (i) $ClCH_2COCl$, DCM,Et_3N, 0-5 ^0C, 30 mins **(ii)** NaN_3, Acetone,H_20, 30 ^0C, 3hr **(iii)** $CuSO_4$,Sodium ascorbate, MeOH,H_2O,30 ^0C, 9hr.

Scheme 1. Synthesis of isoxazole-piperidine-1, 2, 3-triazoles (4a-j)

Key words: piperidine, 1,2,3-triazole, *in vitro* anticancer activity.

OP/PP-81

Synthesis of novel DPP-4 active xanthine containing 1,2,3-triazoles

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Abstract

Inhibitors of dipeptidyl peptidase-4 (DPP-4) have been shown to be effective treatments for type 2 diabetes. A number of new xanthine containing 1,2,3-triazole derivativeswere designed and evaluated for *in vitro* dipeptidyl peptidase-4 (DPP-4) activity.Some of the derivatives have showed excellent inhibitory activity of DPP-4 with IC_{50} values ranging from 39.41 to 6.77 nM, respectively.

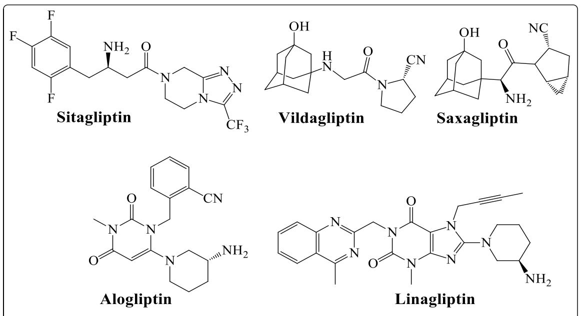


Figure 1. DPP4 inhibitors on the market and under development.

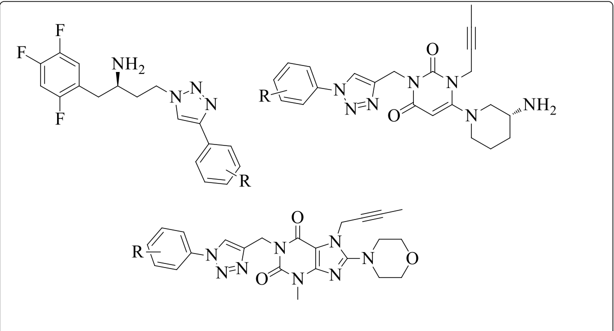
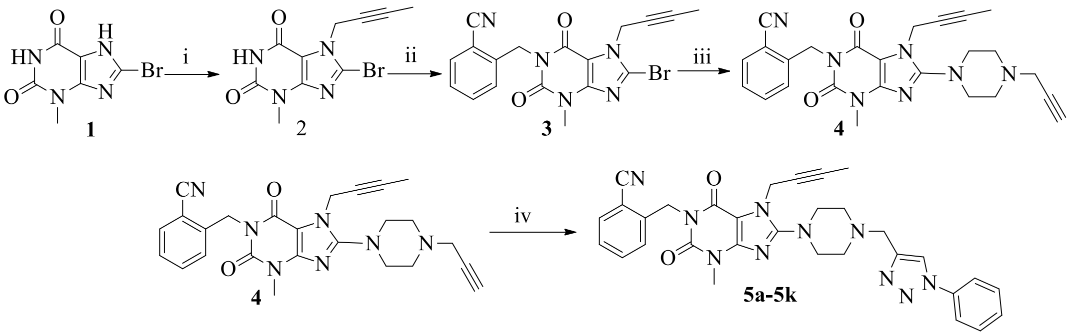


Figure 2. Sitagliptin, Alogliptin and Linagliptin analogues with a 1,2,3-triazole



Scheme

Keywords: Purine; 1,2,3-triazole; Piperzine; DPP-4 inhibitory activity.

Reference

S. Narsimha, B. K. Swamy, M. Ravinder, Y. N. Reddy, N. V. Reddy, *J. Chem. Sci.* (**2020**) *132*:59. https://doi.org/10.1007/s12039-020-1760-0

OP/PP-82

Synthesis of some new Indole-1,2,4-Oxadiazole hybrids as in vitro anticancer agents

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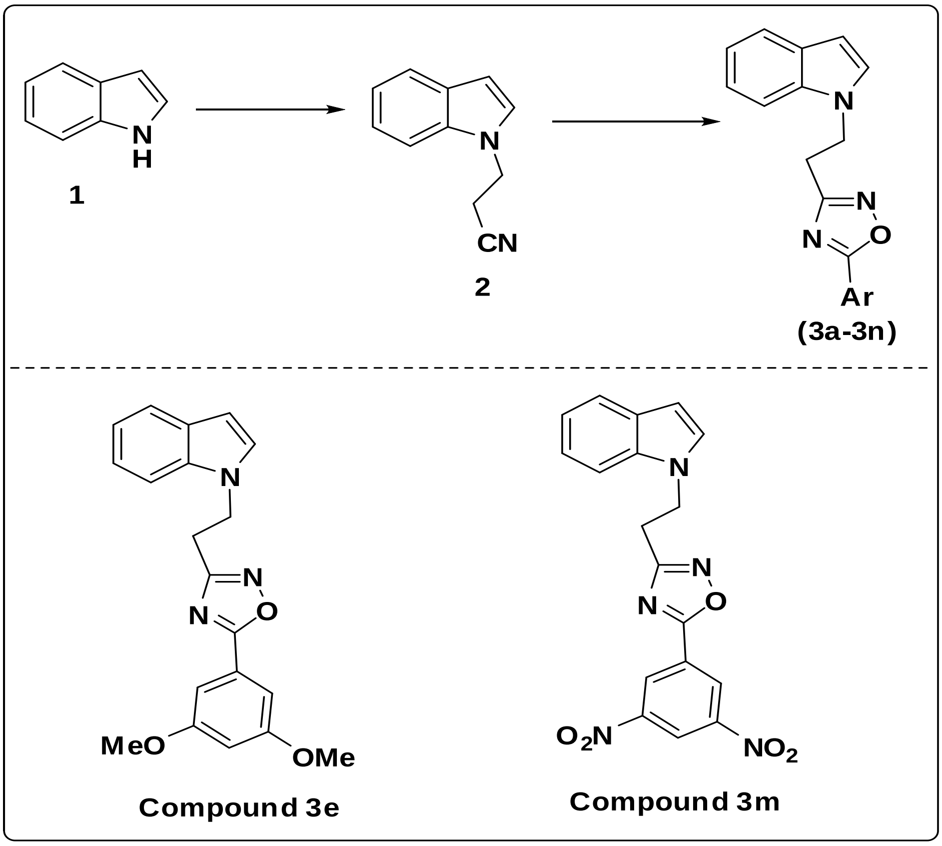
Abstract

Herein, we described the synthesis of some new indole-1,2,4-oxadiazole hybrids (**3a–3n**) using from the reaction between 3-(1H-indol-1-yl)propane nitrile and several readily available aromatic carboxylic acids. All the synthesized hybrids were further investigated for their *in vitro* anticancer activity against two human cancer cell lines like MCF7 (breast) and A549 (lung) using MTT assay and the results revealed that three compounds like **3e** and **3m** showed superior inhibitory activities against two cell lines than the standard etoposide. Predominantly, the compound **3m** showed outstanding activity in MCF-7 cell line possessing IC_{50} values 0.83 μM. Remaining compounds showed moderate to low activity against selected cell lines.



OP/PP-83

Carbon Dioxide Capture Using Cao Supported On Activated Carbon

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Abstract

A series (2, 4, 6, 8, 10 wt %) of CaO supported on activated carbon were prepared by impregnation method and tested for the Carbon dioxide capture. All the catalysts were characterized by PXRD, FT-IR, N_2 adsorption-desorption isotherms and elemental analysis. CO_2 capture was conducted by fixed bed method at different temperature and atmospheric pressure. 6 wt% CaO supported on activated carbon has shown high adsorption capacity of 105 μ mol/g at 303 K and good recyclability up to 10 cycles without loss of adsorption capacity.

CO_2 adsorption study

CO_2 capture study was conducted on fixed bed reactor by loading 0.2 g of adsorbent in between the two quartz plugs in stainless steel reactor having 8 mm I.D and 400 mm of length. Temperatures were controlled by PID controllers and gas flows maintained by Sevenstar MFC. Prior to adsorption of CO_2, the adsorbent was treated with helium gas flow 30 ml/min at 150 °C for 1 h to remove physisorbed gases and moisture then cooled to desired temperature and pass 10% CO_2 balanced helium with flow rate of 20 ml/min until the adsorbent is saturated. Effluent and influent gases were analyzed by gas chromatography Agilent technologies 7820A GC System having thermal conductivity detector with Porapak Q column 3 m length and 3 mm I.D. CO_2 capture capacity was calculated from break through curves.

Keywords: CaO, Activated carbon, fixed bed adsorption, Recyclability

OP/PP-84

Synthesis and Antimicrobial Activity of 1,2,3-Triazole-Isoxazole Hybrids

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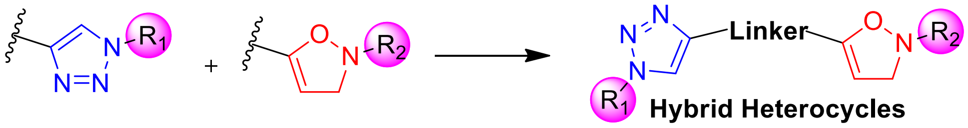
Abstract

Isoxazole derivatives have attracted considerable attention from organic and medicinal chemists due to their considerable biological activities. Ibotenic acid derived from the mushroom *Amanita muscaria* is a potent neurotoxin [1]. Muscimol, produced naturally in the *Amanita muscaria*, is an agonist of □-aminobutyric acid A receptor (GABAAR) which plays a role in regulating neuronal excitability in the central nervous system [2]. Isoxazole forms the basis for several drugs such as leflunomide (antirheumatic), valdecoxib (COX-2 inhibitor) and zonisamide (anticonvulsant). On the other hand, 1,2,3-triazoles are an important class of heterocyclic compounds that received considerable attention for the past few years since the wide range of their applications in biochemical, pharmaceutical, and material sciences [3] [4] [5]. Hence, these moieties can be shaped into powerful pharmacophores that can play an important role in bio-conjugation. Encouraged by the biological activities of isoxazoles and 1,2,3-triazoles we synthesized novel isoxazole-1,2,3-triazole hybrids. The purpose of this study was to investigate the antimicrobial activity of 1,2,3-triazole-isoxazole hybrids, with the ultimate aim of development of novel potent antimicrobial agents.



Key words: 1,2,3-triazoles, isoxazole, hybrid heterocyclic, antimicrobial activity

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OP/PP-85

Synthesis of Novel Coumarinyl-Thiazolyl Schiff Bases

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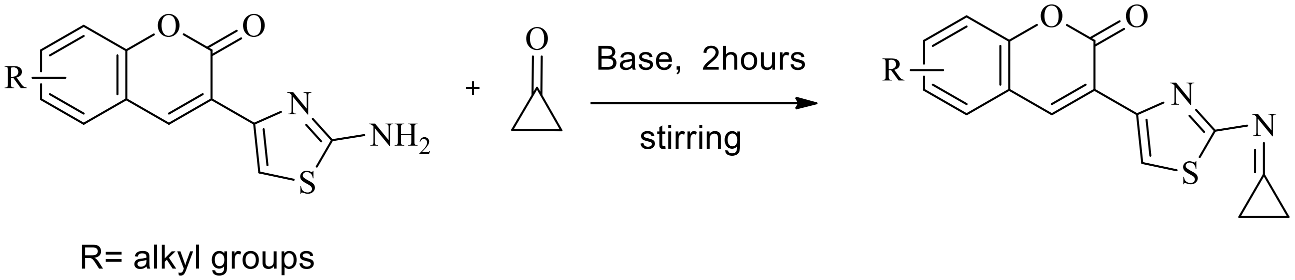
Abstract

A series of novel Schiff bases were synthesized by the reaction of 2-amino-4(3-coumainyl) thiazole with different carbonyl compounds in presence of a base. 2-Amino-4(3-coumainyl) thiazole reacting with cyclopropanone in presence of base, stirring for two hours gives 3-(2-(cyclopropylidene amino)thiazol-4-yl)-2H-chromen-2-one. Changing the substitutions on coumarin ring gives various Schiff bases, which are precursors for many heterocyclic compounds.



Scheme

OP/PP-86

Synthesis and Characterization of Copper Silver Ferrite / Poly Aniline Nano Composites by Sol-gel method & Photocatalytic activity

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Abstract

Polyaniline–$CuAgFe_2O_4$ nanocomposites (PANI–$CuAgFe_2O_4$) with different contents of $CuAgFe_2O_4$ (2.5, 5, 7.5, 10 and 50 wt%) were prepared via in situ chemical oxidation polymerization, while the nanoparticles copper Silver ferrite were synthesized by sol–gel method. The prepared samples were characterized by using some techniques such as Fourier transforms infrared (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Moreover, the electrical conductivity and optical properties and Photocatalytic activity of the nano composites were investigated. Pure (PANI) and the composites containing 2.5 and 5 wt% $CuAgFe_2O_4$ showed amorphous structures. UV studies also confirm the interactions of metals with polyaniline backbone chains. SEM studies have shown that the average size of the CuAgFe2O4 nano particles was of approximately 75±13. FTIR spectra evident the interactions between the polymer and poly nano particles.

The electrical conductivity of PANI–$CuAgFe_2O_4$ nano composite was found to increase with the rise in $CuAgFe_2O_4$ nano particle content. The ferromagnetic order in samples annealed at 700-900 ^{0}C, suggest the decomposition of the phase. The particle size of $CuAgFe_2O_4$ annealed at 400 ^{0}C was quite small [a nm]. The crystalline size of nano composites increased with increasing spinel ferrite contents in the PANI matrix due to amorphous structure of PANI.

Keywords: Nanoparticles, Composite materials, Polyaniline, Electrical conductivity, Photocatalytic activity.

OP/PP-87

Ultrasonically assisted synthesis of 1, 2, 3- triaozoles

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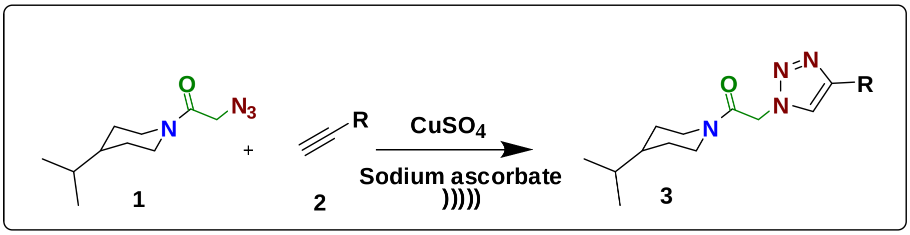
Abstract

In the present investigation, the synthesis of new class of triazole tethered piperidine hybrid heterocycles has been achieved in three good yielding employing Huisgen 1, 3-dipolar cycloaddition reaction *via* a click chemistry approach in between 2-azido-1-(4-isopropyl piperidin-1-yl) ethan-1-one **(1)** and terminal alkyne **(2)** by means of sharpless catalyst under Sonication. The synthetic strategy planned for the preparation of desired target (**3)** is summarized below.



Keywords: 1,2,3-triazole, cycloaddition, Sharpless catalyst

OP/PP-88

Cu(II) Complex of Schiff Base Ligand Containing Pyrazole Motif Synthesis, Characterization, Biological and Molecular Docking Studies.

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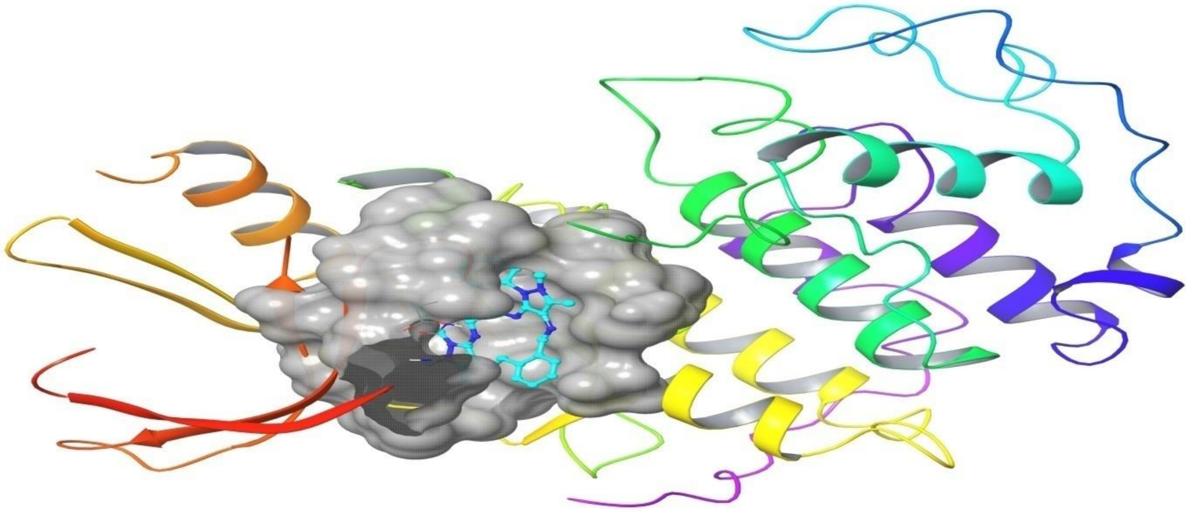
Abstract

Condensation of Ortho-phthalaldehyde,4-Amino antipyrene and diamines form a macrocyclic ligand which on further reaction with respective metal salts results in macrocyclic metal complexes. The newly formed Schiff base ligands and their Cu (II) complexes were characterized by thermal analysis, elemental analysis, mass, I.R, UV-Vis, and ESR spectral studies. Biological studies revealed that the Cu (II) complex of Schiff base ligands has increased activity than corresponding Schiff bases.

Molecular docking is the primary method for simulation of molecular interaction and is able to give insights into the interaction at the atomic level, offering the opportunity to fully characterize the binding site of each molecule. Molecular docking studies were performed for the new ligands and all of them have showed good results.



Molecular Docking image of new Schiff base ligand

OP/PP-89

Green Synthesis of Substituted Quinolne derivatives

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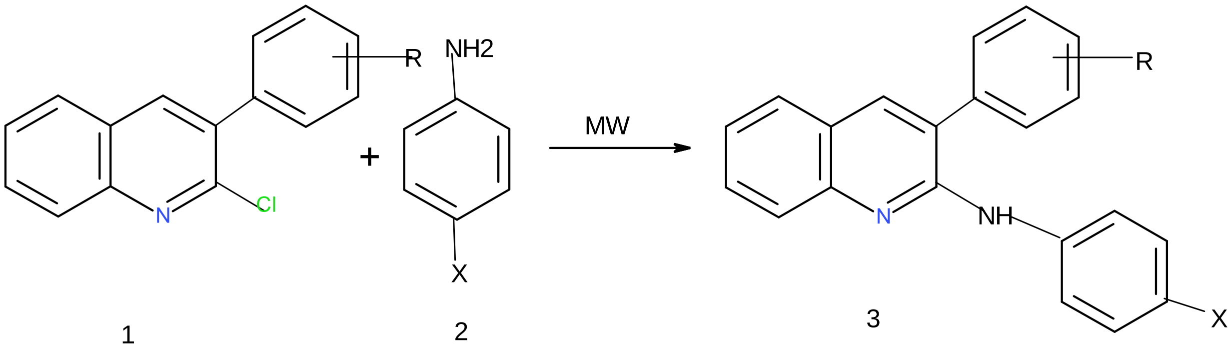
Abstract

An exceedingly and highly efficient method was developed for the synthesis of substituted N-3-diaryl-quinoline -2-amines (3) by the reaction of 2-chloro-3-aryl-quinolines (1) with various anilines (2) in the presence of N-methyl-2-pyrrolidone and K_2CO_3 under thermal green solvent-free conditions. The significant features of this green reaction include very good yields in purity, simple experimental, short reaction time, easy workability, and avoidance of toxic solvents.



OP/PP-90

Ultrasonically assisted Two step synthesis of 7-((1H-1,2,3-triazol-5-yl)-2H-chromen-2-one

Aileni Pranusha, Vanaparthi Akhil, Kanike Chandu and Kavitha Siddoju*
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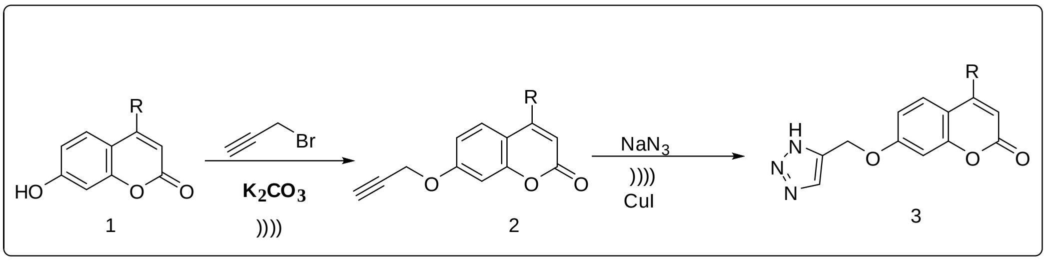
Email: kavithavbr@gmail.com

Abstract

The synthesis of a new class of triazol-chromen hybrid heterocycles has been achieved in three good yielding employing Huisgen 1, 3-dipolar cycloaddition reaction *via* a click chemistry approach in between 7-hydroxy-2*H*-chromen-2-one **(1)** and Propargyl bromide **(2)** followed by sodium azide under CuI viz ultra sonication by means of Sharpless catalyst under sonication. The synthetic strategy planned for the preparation of desired target 7-((1H-1,2,3-triazol-5-yl)-2H-chromen-2-one (**3)** is summarized below.



Keywords: triazole, chromones , cycloaddition, Sharpless catalyst.

OP/PP-91

Chloramine-T mediated synthesis of Quinolinyl 1,3,4-oxadiazoles under microwave irradiation

Sontireddy Surender Reddy and Jella Kumara Swamy*
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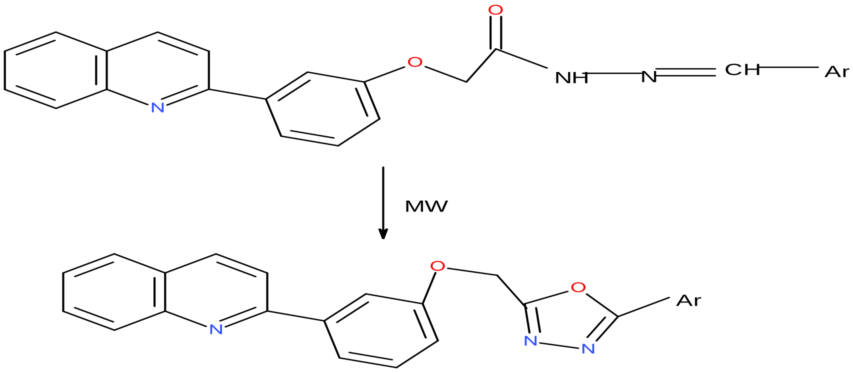
Abstract

An effective practical and simple approach towards the synthesis of 5-aryl-2-[3-(Quinolin-2-yl) phenoxy methyl]-1,3,4-oxadiazoles from the corresponding aryl aldehyde 3-(Quinolin-2-yl) phenoxy acetic acid arylidine hydrazides has been achieved, using chloramines-T in ethanol in combination with microwave irradiation. The yields are good and purity is high. The method is preparatively convenient and useful.



OP/PP-92

Copper-catalyzed hydroformylation of styrenes

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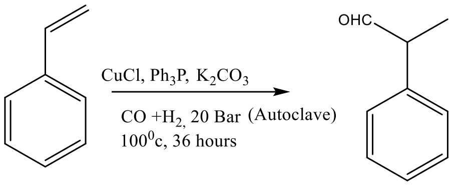
Abstract

Hydroformylation catalyzed by transition metals is one of the most important homogeneous catalytic reactions in industrial chemistry. Millions of tons of aldehydes and related chemicals are produced by this transformation per annum. However, most of the reactions scientists use rhodium as catalyst. In our research procedure we were preferred a copper-catalyzed hydroformylation of alkenes has been prepared, by using various copper catalysts, the obtained product is aldehyde.



OP/PP-93

Synthesis of novel Amino Pyridin-2-amine containing Schiff’s bases and divalent Cu, Co, Ni and Zn metal complexes

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Abstract

Reaction between Pyridin-2-amine (1) with aromatic various aldehydes (2a-j) according to the procedure depicted below. In a clean and dry round bottom flask, Pyridin-2-amine was dissolved in aqueous ethanol under continuous stirring on magnetic stirrer followed by slow addition of 30 cm^3 of hot solution of aromatic aldehydes in EtOH. The above reaction mass was refluxed for 2 hrs on water bath. Schiff’s base metal complexes were synthesized by adding of methanolic solution of 3a-j methanolic solution of metal (II) salts. The pH of reaction mass was maintained slightly basic by using 10% methanolic NaOH solution. It was refluxed for 2-3 hr. The reaction mass was concentrated to around and cooled at RT. The precipitated metal complexes were 4a-j containing Cu (II), Co (II), Ni (II), Zn(II) filtered out and washed with extra amount of MeOH.

Key words Pyridin-2-amine, aromatic aldehydes, Schiff’s bases, bivalent metal complexes

OP/PP-94

Catalytic activity of the Gallium metal complexes towards Ring-opening Polymerization (ROP) of Cyclic esters like ε-Caprolactone &Ethylene Brassylate

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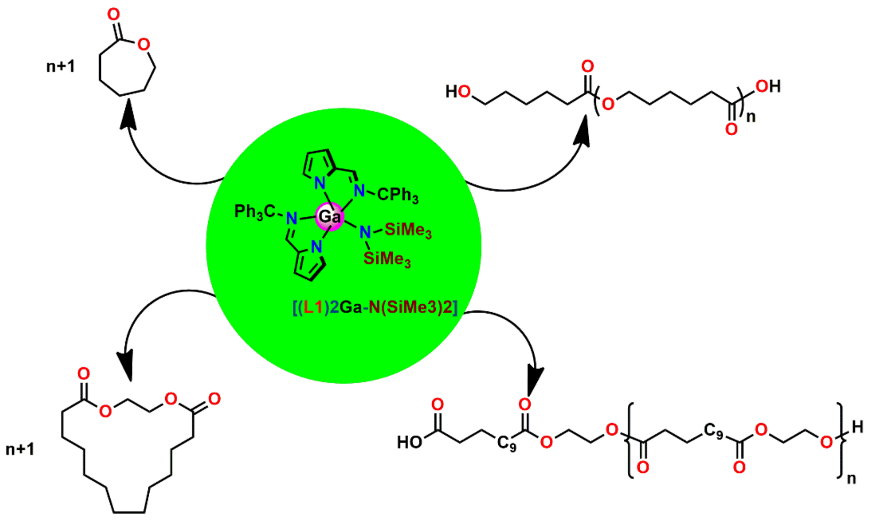
Abstract

The ring-opening polymerization (ROP) of cyclic esters like ε-Caprolactone & 1,4-Dioxacycloheptadecane-5,17-dione (ethylenebrassylate)by discrete organic/inorganic initiators has been intensively investigated over the past 10to 15 years[1].Over the past five years, Ga (III) have attracted a growing interest towards ROP of cyclic esters, like ε-Caprolactone.Motivated by these results we successfully established highly potential Gallium metal complexes$[(L1)_2Ga\text{-}N(SiMe_3)_2]$(1)&$[(L1)_2Ga(TBD)]$(2)(where $L1=[Ph_3CN=CH\text{-}C_4H_3NH]$ via one-pot slat metathesis route & ligand group exchange reactions under inert atmospheric conditions at ambient temperature.

All these complexes were initially characterized by using spectroscopic and analytical techniques. The crystal structure of Gallium complex (1) was further confirmed by single crystal X-ray diffraction analysis. The ring-opening polymerization of ε-Caprolactone and ethylenebrassylate were studied under various conditions and obtained polymers were characterized by using NMR analysis.



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OP/PP-95

Synthesis of thiazole ring containing chalcone and Dihydopyrazole Derivatives

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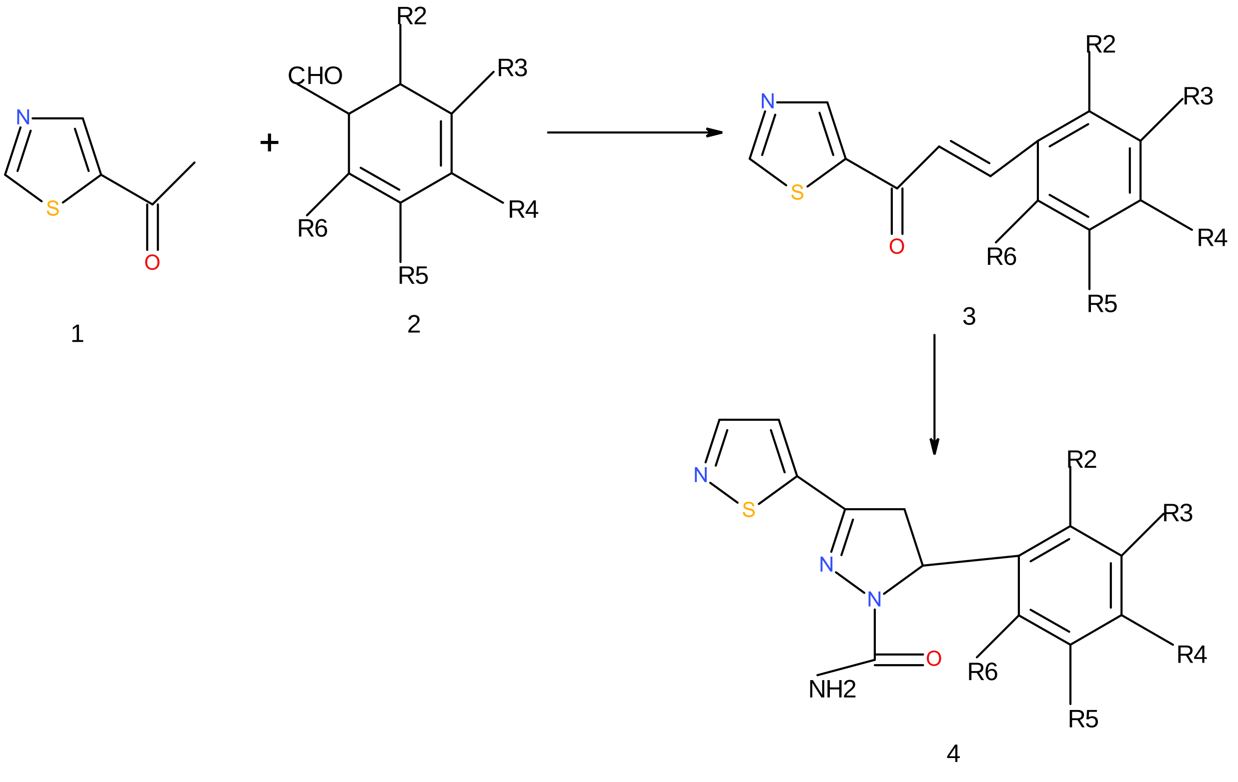
Abstract

The 1-(thiazole-5- yl)ethanone (1) was condensed with substituted benzaldehyde (2)under basic condition at room temperature . The crude precipitate was recrystallized using chloroform to afford chalcones (3). The target dihydropyrazoles (4) were obtained by treating the synthesized chalcones with semicarbazide in a catalytic amount of pyridine and purified using silica gel column chromatography.



Keywords: Thiazole; chalcones; dihydropyrazole

OP/PP-96

CSIR-CSMCRI Technology: Production of biodiesel using LDH derived oxides

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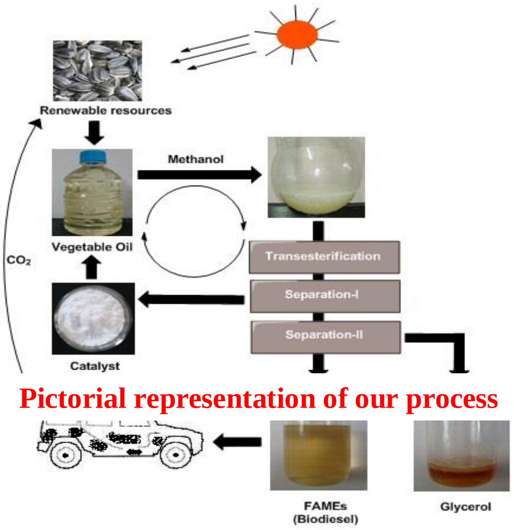
Abstract

Fatty acid alkyl esters (biodiesel) are widely accepted as alternative diesel fuels because of its non-toxic, biodegradable and renewable nature.[1] Complete burning property of biodiesel reduces emissions of SO_x, CO and unburnt hydrocarbons and thus resulting non-polluted environment.[2] Trans-esterification of triglycerides with short chain alcohols (mainly methanol) is a preferred approach for biodiesel production.[3] Generally, industrial processes are carried out by using homogeneous base catalysts such as NaOH (or) KOH due to their superior activity than acid (or) enzyme catalysts. But these catalysts are not reusable and create huge environmental impact and thus promoted an interest to look for heterogeneous base catalysts. Layered double hydroxides (LDHs; also referred as hydrotalcite-like [HT-like] materials) belongs the category of anionic clays, wherein both as-synthesized and modified forms are explored as heterogeneous base catalysts.[4] Because of their favorable physicochemical properties and tunable basicity; they are potential candidates in biodiesel production.



Pictorial representation of our process

CSIR-CSMCRI have been explored the mixed oxides derived from CaAl2-LDH as effective heterogeneous catalysts for fatty acid methyl esters (FAMEs) production from edible, non-edible and used cooking oils with methanol.[5,6] This catalyst showed highest activity with > 90% yield of FAME using low methanol:oil molar ratio (< 6:1) at 65 °C in 5 h. The activity of the catalyst was attributed to its optimum basicity as supported by Hammett and CO_2-TPD studies. The catalyst was successfully reused for up to four cycles and scaled up successfully with improved efficiency. Some of the fuel properties such as density, viscosity, neutralization number and glycerol contents of the obtained biodiesel matched well with the standard DIN values. They conclude, a scalable and environmentally friendly heterogeneously catalysed trans-esterification process for conversion of edible, non-edible and used cooking oils to biodiesel is demonstrated.

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OP/PP-97

Chemo- and regioselective synthesis of arylated γ-valerolactones from bio-based levulinic acid with aromatics using H-β zeolite catalyst

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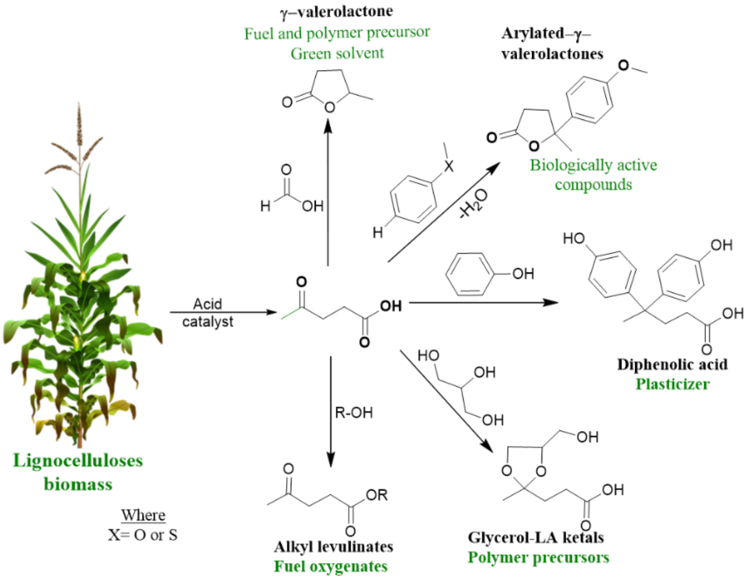
Abstract



Scheme: Industrial applications of LA

Levulinic acid (LA), a biomass derived keto carboxylic acid, serves as an important building block for the synthesis of valuable fuels and chemicals via several catalytic transformations. LA is easily obtained from abundant waste/surplus carbohydrate (C_6-Glucose/C_5-Xylose) biomass [1, 2]. Owing to multiple functionalities possessed by LA, it participates in facile manner in several organic transformations. Sreedhar et al. used the LA functionality (carbonyl and carboxylic) to obtain various important products by reacting with aromatics using H-β zeolite as an efficient C-C and C-O bond forming solid acid catalyst.

One-pot synthesis of arylated γ-valerolactones has been demonstrated by Sreedhar et al. from biomass derived levulinic acid (LA) using H-β zeolite as a catalyst. The conversion is specific for aromatic rings bearing heteroatom comprising oxygen or sulphur and is highly chemo- and regioselective. These arylated γ-valerolactones are stable in air for several months. The β-catalyst gets deactivated due to deposition of organic carbon during the reaction, and however, could be reactivated by calcination.

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OP/PP-98

A Novel approach of green synthesis and characterization of Zinc oxide nanoparticles from *Ficus amplissima* leaf extract

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Abstract

In the present day research, synthesis of metal nanoparticle from different medicinal plants has potential capacity to develop eco-friendly novel technologies. The novel green synthesis of zinc oxide natural product nanoparticles from the leaf extract of *Ficus amplissima* is reported in the present work. The green synthesized zinc oxide nanoparticles were characterized by various techniques like transmission electron microscope (TEM), Energy dispersive X-ray (EDX) analysis.

Keywords: Green Synthesis; Characterization; Zinc Oxide-natural product nanoparticles; XRD; EDX; TEM; Ficus amplissima.

OP/PP-99

Green synthetic Approaches for 1,2,4-triazoles

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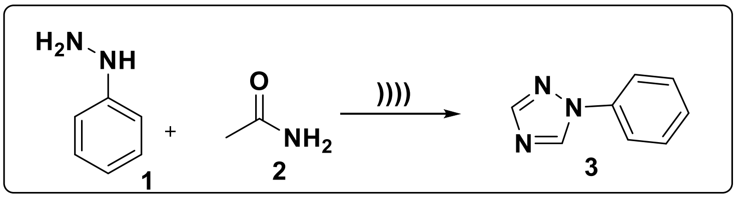
Abstract

A highly efficiently method for the synthesis of substituted 1,2,4-triazoles (3) from hydrazines (1) and formamide (2) proceeds smoothly under ultrasonication 3-6 min in the absence of a catalyst and shows excellent functional-group tolerance. The structures of compounds were confirmed by their spectroscopic (IR, 1H NMR and MS) and analytical data.



Keywords: 1,2,4-Triazole, ultrasonication reaction, hydrazine, formamide.

OP/PP-100

A Novel Analytical Development and Validation of a RP-HPLC Assay Method for the Quantification of Apalutamide in Bulk and its Marketed Formulation

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ABSTRACT

A simple, rapid, specific and accurate reverse phase high performance liquid chromatographic method has been developed for the validation of Apalutamide in bulk as well as in marketed pharmaceutical dosage form. This separation was performed on a Symmetry ODS C18 (4.6×250mm, 5µm) column with Methanol: Phosphate Buffer (35:65) V/V as mobile phase at a flow rate of 1.0 mL min^{-1} with UV detection at 235 nm; the constant column temperature was Ambient. The run time under these chromatographic conditions was less than 8 min. The retention time of Apalutamide was found to be 2.252.

The calibration plot was linear over the concentration range of 6–14 µg mL^{-1} with limits of detection and quantification values of 1.2 and 3.6 ng mL^{-1} respectively. The mean % assay of marketed formulation was found to be 99.86%, and % recovery was observed in the range of 98-100%. Relative standard deviation for the precision study was found <2%. The developed method is simple, precise, specific, accurate and rapid, making it suitable for estimation of Apalutamide in bulk and marketed pharmaceutical dosage form dosage form.

Keywords: Apalutamide, RP-HPLC, Validation, ICH Guidelines.

OP/PP-101

Synthesis of ZnO Nanoparticles Using Chemical Reduction Method

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Abstract

ZnO Nanoparticles were synthesised by Chemical Reduction synthesis method of Zinc Sulphate with $NaBH_4$ as reducing agent and DMF as Solvent. The ZnO Nanoparticles of average size range from 30 to 40 nm have been synthesized by Chemical reduction method. The prepared ZnO Nanoparticles is Characterized by SEM, TEM, XRD and FTIR. The powdered ZnO Nanoparticles are Spherical in nature and are Agglomerates as Nanoparticles. The XRD shows hexagonal wurtzite ZnO Nanoparticle, SEM can be used for recognize the Size and Shape of the ZnO Nanoproduct, TEM provides the Morphological, Compositional and Crystallographic information of the sample and FTIR enables the in-situ analysis of functional groups present in Nanoparticles.

Keywords: ZnO Nanoparticles, DMF, $NaBH_4$, SEM, TEM, XRD, FTIR and Chemical Reduction Method.

OP/PP-102

Development of A New Analytical Method and Validation of Encorafenib in Bulk Form and Pharmaceutical Dosage form by RP-HPLC

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ABSTRACT

A new, simple, robust, accurate, rapid and precise RP-HPLC method has been developed and validated for determination of Encorafenib in bulk and its pharmaceutical dosage forms. The developed method is isocratic method which gives retention time of Encorafenib as 2.497min. The separation was carried out on Symmetry ODS C18 (4.6mm×250mm, 5µm) column using Acetonitrile: Methanol as a mobile phase in the ratio of 35:65v/v. The flow rate was 1.0mL/min and wavelength used was 285nm.

The method has been validated according to ICH guidelines for specificity, linearity, accuracy, precision, robustness, ruggedness, LOD and LOQ. The method was validated as per ICH guideline and found to be linear between the ranges of 55-95µg/mL for Encorafenib. The limits of detection (LOD) and quantification (LOQ) values were 1.2 and 3.4 ng/mL respectively. The method was found to be specific, accurate and precise, robust, rugged and sensitive. The developed method was good linearity, novel, rapid for the estimation of Encorafenib in bulk and its pharmaceutical dosage forms. Thus it can be employed for the routine analysis.

Keywords: Encorafenib, RP-HPLC, Accuracy, Precision, Validation.

OP/PP-103

$Zr(OH)_2CO_3.ZrO_2$ Catalyzed Friedlander Synthesis of Quinolines in the Solid state

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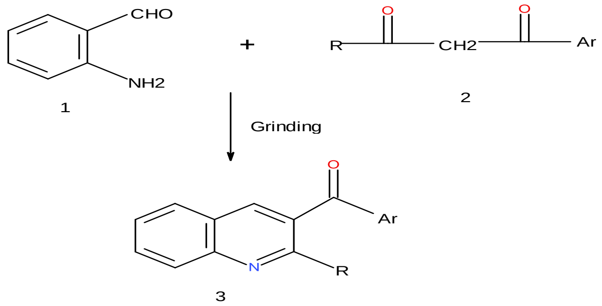
Abstract

The Friedlander condensation of 2-amino Benzaldehyde **1** with various carbonyl compounds containing alpha methylene group **2** in the presence of $Zr(OH)_2CO_3.ZrO_2$ in the solid state at RT furnished the corresponding Quinolines **3.** The condensation reaction is very clean and efficient and is devoid of any by-products, and the work-up procedure is simple and convenient. The experimental procedure is very simple. The process is environmentally benign.



OP/PP-104

A Novel Method for the Determination of Dacomitinib in Pure Form and Tablet Dosage Form by Using RP-HPLC

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ABSTRACT

A new simple, selective, rapid, precise RP- HPLC method is described for the determination of Dacomitinib in bulk and marketed pharmaceutical dosage form. Chromatography was carried on a Symmetry C18 (4.6×150mm) 5µm column using a mixture of Methanol: Phosphate Buffer (pH-4.6) (25:75) V/V as the mobile phase at a flow rate of 1.0mL/min with detection at 260 nm. The retention time of the drug was 2.379min. The detector response was linear in the concentration of 10-50mcg/mL the limit of detection and limit of quantification was 2.13 and 6.31mcg/mL respectively. The % recovery was observed in the range of 98-100%. Relative standard deviation for the precision study was found <2%. The percentage assay of Dacomitinib was 99.86%. The proposed method was validated by determining its sensitivity, accuracy and precision. The proposed method is simple, fast, accurate and precise and hence can be applied for routine quality control of Dacomitinib in bulk and marketed pharmaceutical dosage form.

Keywords: Dacomitinib, RP-HPLC, Method Development, Validation, ICH Guidelines

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OP/PP-105

A New Analytical Method Development and Validation of Baricitinib in Tablet Dosage Form by RP-HPLC Method

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ABSTRACT

A new simple, accurate, economic, rapid and precise reverse phase high performance liquid chromatographic method has been developed for the validated of Baricitinib in bulk and its marketed tablet form. Chromatography was carried out on Zodiac C18 (4.6mm×250mm) 5µm particle size column using a mixture of Acetonitrile: TEA Buffer pH-4.6 (35:65) as the mobile phase at a flow rate of 1.0ml/min, the detection was carried out at 258nm. The retention time of Baricitinib was found to be 3.213±0.02min.

The method was validated according to ICH guidelines for linearity, sensitivity, accuracy, precision, specificity and robustness. The response was found to be linear in the drug concentration range of 20-60 mcg/mL for Baricitinib. The correlation coefficient was found to be 0.999. The LOD and LOQ for Baricitinib were found to be 0.9µg/mL and 2.7µg/mL respectively. The proposed method was found to be good percentage recovery for Baricitinib, which indicates that the proposed method is highly accurate. The method precision for the determination of assay was below 2.0% RSD. The method is useful in the quality control of bulk and marketed pharmaceutical formulations.

Keywords: Baricitinib, RP-HPLC, Method Development, Accuracy, Precision.

OP/PP-106

A Simple Method Development and Validation for the Deterimination of Duvelisib by Using RP-HPLC

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ABSTRACT

A new, economical, simple, rapid, precise, accurate and reproducible RP-HPLC method was developed for the determination of Duvelisib in bulk form and marketed pharmaceutical formulation. Separation of Duvelisib was successfully achieved on a Develosil C18 (4.6mm × 250mm) 5µm column in an isocratic mode of separation utilizing Methanol: Acetonitrile in the ratio of 40:60% v/v at a flow rate of 1.0mL/min and the detection was carried out at 258nm. The method was validated according to ICH guidelines for linearity, sensitivity, accuracy, precision, specificity and robustness. The response was found to be linear in the drug concentration range of 15-35mcg/mL for Duvelisib. The correlation coefficient was found to be 0.999 for Duvelisib. The LOD and LOQ for Duvelisib were found to be 2.1µg/mL and 3.6µg/mL respectively.

The proposed method was found to be good with good percentage of recovery for Duvelisib, which indicates that the proposed method is highly accurate. The specificity of the method shows good correlation between retention times of standard solution with the sample solution. Therefore, the proposed method specifically determines the analyte in the sample without interference from excipients of pharmaceutical dosage forms.

Keywords: Duvelisib, RP-HPLC, Accuracy, Precision, ICH Guidelines.

OP/PP-107

Synthesis and Biological screening of Some Novel Quinazolin-Aminothiazole analogues as antioxidant, antibacterial agents

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ABSTRACT

In the present study, we report herewith synthesis of novel series Quinazolin-Aminothiazole analogues (**5a-j**). The synthesized compounds were characterized by elemental analyses, FT-IR, ^{1}H &^{13}C NMR and mass spectroscopic techniques. The compounds were screened for their anti-oxidant activity by DPPH radical scavenging assay. Out of all the tested compounds, **5c, 5d, 5f** and **5i** showed portent anti-oxidant activity. These synthesized compounds were also screened for their anti-bacterial activity. The compounds of **5b, 5e** and **5h** found to be the most potent activity and reaming compounds exhibited are moderate to poor activity against all the tested strains.

Keywords: Quinazolin-Aminothiazole, Anti-oxidant activity, Anti-bacterial activity, DPPH scavenging.

OP/PP-108

Efficient synthesis of novel methyl sulfones in eco-friendly manner

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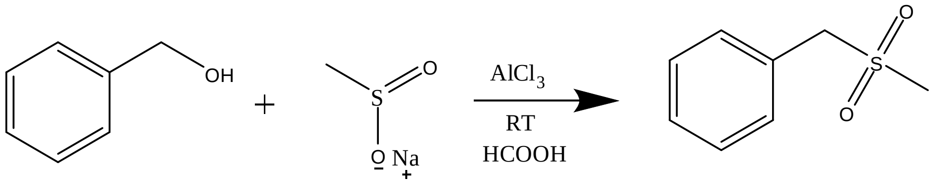
Abstract

A series of ten methyl sulfones (**3a-3j**) were synthesised in the eco-friendly method, by decreasing the rection conditions to room temperature from higher temperatures. A series of ten alcohols (**2a-2j**) were synthesised from the respective ally aldehydes (**1a-1j**) with the help of sodium borohydride reagent. The reaction conditions were simple with the excellent yields were obtained. All the synthesized compounds were characterized with the help of spectroscopic techniques.



Keywords: $AlCl_3$, allyl alcohols, methyl sulphones,

OP/PP-109

Design, synthesis and computational docking studies of *N*-(substituted)-8-methyl-1-nitro-10*H*-phenoxazine-3-sulphonamides as anti-inflammatory agents

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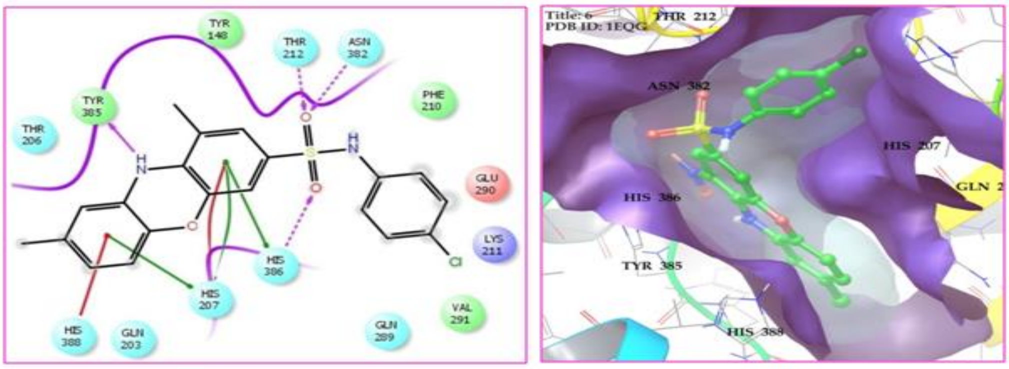
Abstract

A series of phenoxazine sulphonamides were synthesised and evaluated for their in-vitro and in-vivo anti-inflammatory activities. The results revealed that all the eleven compounds under investigation showed excellent percentage (above 70%) of inhibition in comparison with the standard drug ibuprofen. Among them six compounds showed above 80% inhibition. Sulphonamide with pyridine-2-yl group showed highest (84.7%) inhibition in-vitro. In-vivo experimental data revealed that compound with 4-chlorobenzene-1-yl groupinhibited the carrageenan induced edema to the extent of 93.5% whereas compound with pyridine-2-ylshowed only 90.7% inhibition.

Sulfonamides were also analyzed for their molecular docking studies against Ram Prostaglandin H_2 synthase-1 (*cyclooxygenase-1*, COX-1). Four compounds (PDB: 1EQG) strongly interacted with the active sites of protein H-bonds in close distances. The most active compound with 4-chlorobenzene-1-yl group(PDB: 1EQG) strongly interacted with the active sites of protein Gln289, Asn382, Tyr385 and Thr212 through four H-bonds in the close distances (1.89–3.42 A°).



2D Diagram

Surface

Figure: Top scorer **(**compound with 4-chloroaniline**)** for Ram Prostaglandin H_2 synthase-1 (cyclooxygenase-1 or COX-1) 1EQG.

Keywords: Celecoxib; Sulphonamide; Anti-infammatory; Computational docking.

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OP/PP-110

Prosopis Juliflora Charcoal as a Biosorbent to Remove Heavy Metals from Aqueous Solution

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ABSTRACT

P. juliflora charcoal considered to be as an important fuel resource in India. The wood biomass conversion into charcoal reduces the weight and increases the energy and economic value of the product. It can be converted into charcoal by pyrolysis. This conversion reduces the weight of biomass there by enhances the energy and economic value of the product. *P. juliflora* biomass is considered to be environmentally viable due to the low sulpher content when compare to other conventional sources such as coal [1]. Availability of abundant biomass of *P. jiliflora* at cheap price makes this plant is ideal for biosorption studies. Lead removal from aqueous solution using P. juliflora is known in literature [2]. Hence objectives of this study aimed at potential of *P. juliflora* wood charcoal for removal of heavy metals form aqueous solution.

P. juliflora considered to be an exotic weed in India. Effective management of these plants needs to be attention for potential usage of this plant. Hence PJWC (Prosopis juliflora Wood Charcol) was selected for studying Pb(II) removal from aqueous solution. The following conclusion can be drawn from present study. The adsorption process is pH dependent and the experimental kinetic data was best described by pseudo-second-order kinetic model.

References:

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OP/PP-111

Green Synthesis Of 2-(9-Phenyl-[1,2,4]Triazolo[4,3A] [1,8]Naphthyridin-6-Yl) Benzenesulfonic Acid

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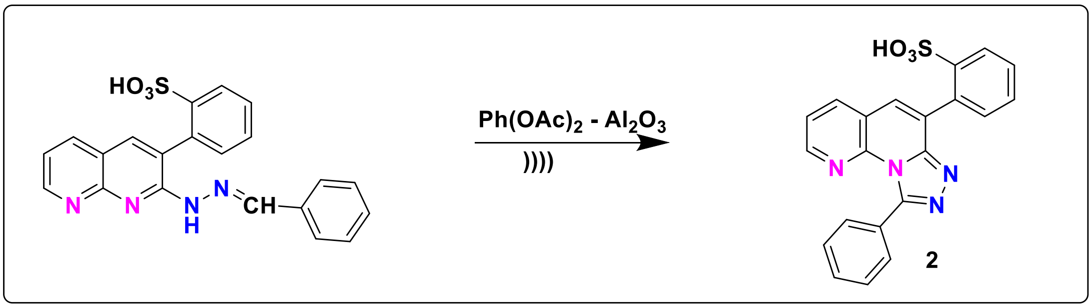
Abstract

Herein, an efficient, solvent-free synthesis of 9-aryl-6-[2-(trifluoromethyl)phenyl][1,2,4]triazolo [4,3-a][1,8]naphthyridines **2** is achieved by the oxidation of aryl aldehyde (E)-2-(2-(2-benzylidenehydrazinyl)-1,8-naphthyridin-3-yl)benzenesulfonic acid with alumina-supported Iodobenzene diacetate [$PhI(OAc)_2$-Al_2O_3] in the solid state. The reaction proceeds through sonication in high yields and in a state of high purity. The structures of compounds are assigned on the basis of their spectral and analytical data.



Scheme-1: Synthesis of 2-(9-phenyl-[1,2,4]triazolo[4,3-a][1,8]naphthyridin-6-yl)benzenesulfonic acid.

Keywords: 1,8-Naphthyridine, 1,2,4-Triazole, $PhI(OAc)_2$-Al_2O_3, Sonication.

OP/PP-112

Synthesis and characterization of Sm and Gd co-doped Calcium Tungstanate nanocrystals

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Abstract

We report the synthesis of co-doped calcium tungstate ($CaWO_4$) nanocrystals with Samarium (Sm) and Gadolinium (Gd) rare earth ions using hydrothermal synthesis method for the first time. The synthesised nanocrystals were characterized by X-ray diffraction (XRD) with energy dispersive X-ray analysis (EDAX) and field-emission scanning electron microscopy (FESEM). The phase of the nanocrystalsunder study was identified by X-ray diffraction (XRD).The field-emission scanning electron microscope (FESEM) image shows that the synthesized nanocrystals are in the size range of 55nm – 85nm. The presence of Sm and Gd rare earth ions in the Sm-Gd co-doped $CaWO_4$ nanocrystals was confirmed by the energy dispersive analysis of the X-rays (EDAX). The rare-earth co-doped calcium tungstate nanocrystals are highly significant for developing luminescent materials of tungstate systems.

Keywords: Nanocrystals, X-ray diffraction, field emission scanning electron microscopy.

OP/PP-113

Green synthesis of perimidine derivatives using heterogeneous catalyst

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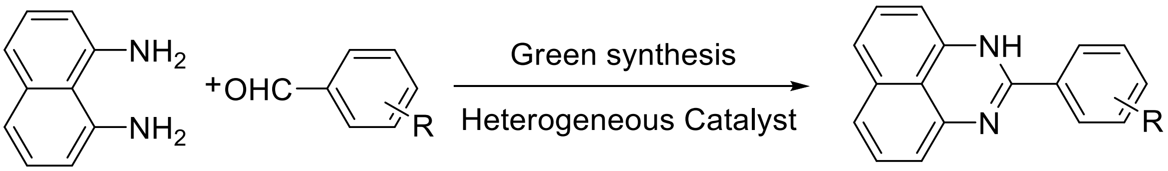
Abstract

Green chemistry is a design, advancement, use of chemical products and systems that minimize or remove the utilisation and formation of destructive and toxic materials. It is a universal method that is feasible to all areas of science. Synthetic process involves the use of various substances. Unfortunately majority of the chemical reagents and substances are applied in industrial and chemical laboratories which are hazardous toxic compoundsled to environmental pollution.Perimidine derivatives are very important and valuable compounds in the fields of medicine, biology and pharma.

A series of 2-phenyl-1*H*-perimidine derivatives were synthesised using heterogeneous catalyst and green chemistry approach. This study reveals effects and benefits of various green synthetic strategies to develop diversity-oriented perimidine nucleus through solid heterogeneous catalyst without solvent medium in MWI reducing negative impact on the environment and lively hood.All the synthesised compounds have been purified and characterized by IR, ^{1}H &^{13}C NMR, Mass spectral data and elemental analysis.



R= Phenyl, 4-methylphenyl, 4-fluorophenyl, 4-chlorophenyl, 4-bromophenyl, 4-hydroxyphenyl, 4-nitrophenyl, 2,4-dichlorophenyl.

Scheme: Synthesis of 2-phenyl-1*H*-perimidine derivatives

Keywords: Perimidine; Heterogeneous catalyst; Green synthesis.

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OP/PP-114

Mechanistic and Kinetic Studies of the Phenacylation of Benzimidazole

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Abstract

The nucleophilic substitution reaction of phenacyl bromide with benzimidazole has been studied conductometrically in methanol medium in the temperature range 303-318K. The reaction is observed to be first order with respect to both [bezimidazole] and [phenacyl bromide]. The reaction is overall second order.

Substituent effect on rate of the reaction suggests that electron withdrawing groups (*p*-NO_2, *p*-Cl, *m*-NO_2) enhance the rate of the reaction compared to the unsubstituted compound, while the electron donating group (*p*-OCH_3) decrease the rate of the reaction compared to unsubstituted compound. For the substituted (*p*-OCH_3, *p*-NO_2 and *p*-Cl) and the unsubstituted compound form a linear free energy relationship, from the intersection of lines in the Hammett and Arrhenius plots, the isokinetic temperature is discussed.

A point of great interest in kinetic and mechanistic studies is the influence of substituent present on the substrate on rate of reaction. To assess this effect the present system was studied using *p*-OCH_3, *p*-NO_2, *p*-Cl and *m*-NO_2 substituents on phenacyl bromide in methanol medium and second order rate constants k in the temperature range 303-318K have been evaluated. These values (Table-2) indicate that electron withdrawing groups (*p*-NO_2, *p*-Cl, *m*-NO_2) enhance the rate of the reaction compared to the unsubstituted compound, while the electron donating group (*p*-OCH_3) retards the rate of the reaction compared to unsubstituted compound. The order of the ractivity is *p*-NO_2 > *m*-NO_2 > *p*-Cl > -H > *p*-OCH_3. Correlation of log k with Hammett's subtituent constant σ[10] gives a linear plot with a positive slope. With exception to *m*-NO_2 the remaining three substituents fall on a straight line with a positive slope. To verify the applicability of Hammett's linear free energy relationship (LFER), log k_{II} is correlated with Hammett's substituent constant σ[12] in the temperature range 303-318K.

Keywords: Nucleophilic substitution, conductometric Studies, isokinetic temperature, Hammett and Arrhenius plots.

OP/PP-115

Saccharomyces cerevisiae as a biosorbent for heavy metal sequestration from aqueous systems

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ABSTRACT

Rapid ramification of industrial activity and massive urbanization results in release of large amounts of heavy metal containing effluent into the nature. Several industrial activities such as storage batteries, varnishes, paints, antiknock compounds in gasoline, solder, alloys, ammunition, zinc ores, fertilizers, metal plating, battery production, fertilizers industry, stabilizers, pigments and textile and mining contributing for the disposing of large quantities of heavy metals containing effluent into water streams. The metals with a density of 5.0 g/cm^3 or greater are called heavy metals. Heavy metals are toxic and persist in nature without any degradation [1]. These characteristics of heavy metals make them detrimental to human health and shows huge impact on environment. Hence it is necessary to clean up the metal contaminated sites in an effective manner. Conventional methods for removing metals from aqueous solutions include chemical precipitation, ion exchange, filtration, reverse osmosis, oxidation or reduction, membrane technologies and evaporation recovery are cost intensive, biosorption emerged as an important cost effective eco friendly alternative.

In biosorption there is no secondary pollutant production, as we see in the conventional methods in forms of toxic chemical sludge and again it needs disposal/treatment which is a costly process. Satisfying all the economic and environmental aspects biological materials have emerged as an effective substrates for sequestering heavy metals from water streams. The bio-sorbents of different origin shows a great affinity towards the heavy metals. So the metal-sorption by various types of biomaterials can find enormous applications for removing metals from solution and their recovery.

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OP/PP-116

Synthesis, characterization and evaluation of various novel isoquinoline analogues as efficient anticancer agents

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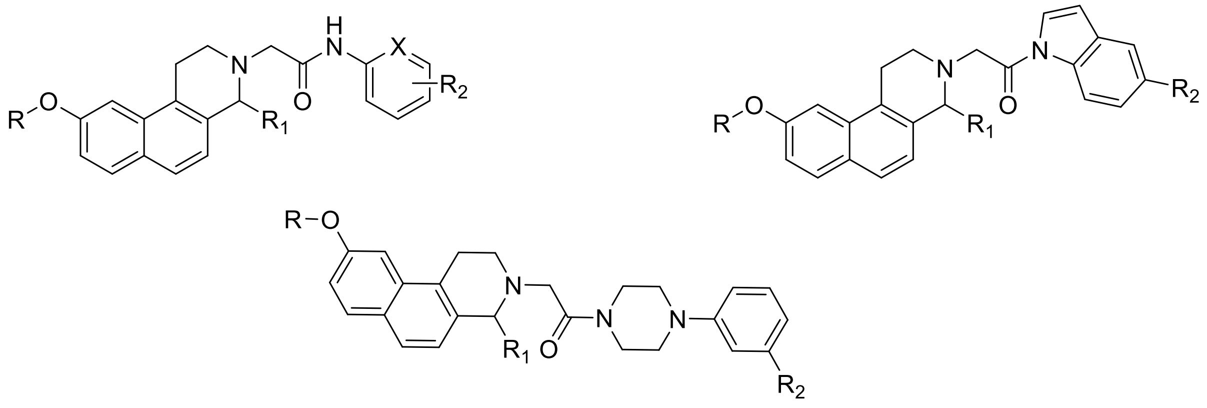
Abstract

A simple synthetic methodology has been devised for the preparation of numerous divergent and advanced 2-(1,2-dihydro-9-methoxy-4-methylbenzo[f] isoquinolin-3(*4H*)-yl)-*N*-phenylacetamides, 1-(4-(3-trifluoromethyl)phenyl) piperazin-1-yl)-2-(1,2-dihydro-9-methoxy-4-methylbenzo [f] isoquinolin-3-(*4H*)-yl) ethanones and 1-(2-(1,2-Dihydro-9-methoxy-4-methylbenzo[f]isoquinolin-3-(*4H*)-yl)acetyl) indoline-5-carbonitriles. The required essential intermediate 1,2,3,4-tetrahydro-9-methoxy-4-methylbenzo[f]isoquinoline was prepared from 2-(2-Methoxynaphthalen-8-yl)-ethanamine and acetyl chloride.

The synthesized compounds have been purified and characterized by IR, ^{1}H &^{13}C NMR, Mass spectral data and elemental analysis. Additionally, the final compounds have been examined for their preliminary anticancer activity. The compounds under investigation exhibited moderate to good activity.



Scheme: Structures of isoquinoline analogues

Key words: Isoquinoline; Phenylacetamide; Anticancer activity.

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OP/PP-117

Synthesis and Biological Activity of Novel Pyrimidine Derivatives

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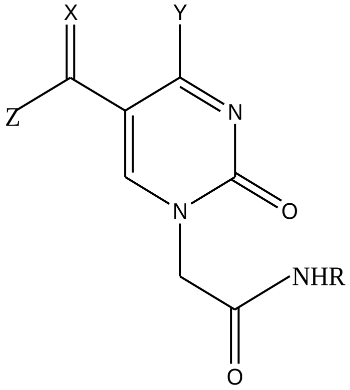
ABSTRACT

Pyrimidine and its derivatives play a wide role in drug discovery processes and have considerable chemical significance and biological activities. Pyrimidines are the building blocks of many natural compounds such as vitamins, liposaccharides, and antibiotics. Pyrimidine is used as parent substance for the synthesis of a wide variety of heterocyclic compounds and raw material for drug synthesis and is also crucial in the theoretical development of heterocyclic chemistry and in organic synthesis.

Contemplating the importance of nitrogen containing heterocycles as an important class of compounds in medicinal chemistry, we have synthesized a series of novel pyrimidine analogues (1) and planned to study their biological assay like anti-microbial and anti-bacterial activities.



Keywords: Pyrimidine, heterocyclic chemistry, biological assay.

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OP/PP-118

Novel Synthesis of Oxoindolyl Derivatives from Isatins and Propiolates through DIBAL-H

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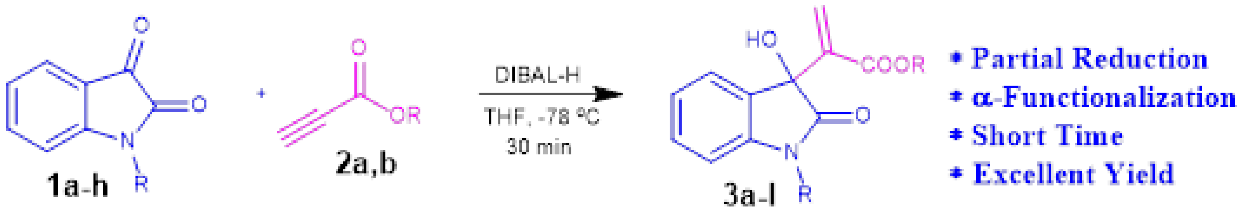
ABSTRACT

N-alkyl or N-aryl 3-hydroxyl oxindole derivatives (Morita-Baylis-Hilmann adduct) has been synthesized effectively with DIBAL-H as partial reducing agent to methyl and ethyl propiolate at lower temperature (-78 °C), which on nucleophilic addition to N-substituted isatins produces MBH carbonates (Oxoindolyl derivatives) in excellent yield with in short time through α-functionalisation, stable tetrahedral intermediate compound. These oxyindolyl compounds are biologically active and good intermediates in the construction of functionalized hetero cycle compounds.



Keywords: Morita-Baylis-Hilmann adduct, Oxoindolyl derivatives, functionalized hetero cycles.

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OP/PP-119

Synthesis of novel 1,3,4-oxadiazole derivatives and their biological properties

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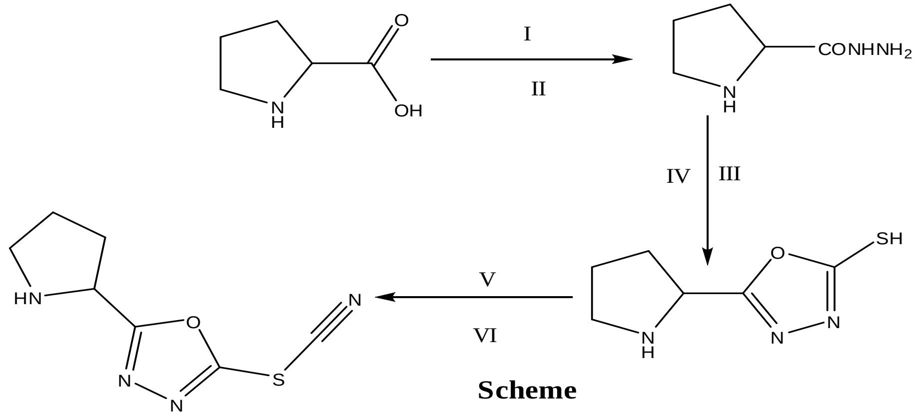
Abstract

Heterocyclic compounds containing the five-membered oxadiazole nucleus possess a diversity of useful biological effects. 1,3,4-Oxadiazole and 3-aroylpropionic acid moieties are important because of their versatile biological actions. In particular, compounds bearing the 1,3,4-oxadiazole nucleus are known to have unique anti-edema and anti-inflammatory activities (1). Differently substituted oxadiazole moieties have also been found to have other interesting activities such as analgesic (2), antimicrobial (3), antitubercular, anticonvulsant and anti-hepatitis B viral activities (4), some of them are commercially available; however, they are associated with gastrointestinal side effects. Studies suggest that direct tissue contact of these agents plays an important role in the production of side effects and the reported literature confirms that gastrointestinal side effects of aroylpropionic acids are due to the presence of a free carboxylic group in the parent drug.

Thus, developing new agents with minimum or without side effects is an extensive research area at present. Therefore, it was considered worthwhile to synthesize some new 3-(4-bromobenzoyl)propionic acid derivatives by incorporating the oxadiazolyl moiety, hoping to get better anti- -inflammatory molecules. In view of the reported activities of 1,3,4-oxadiazoles, we have synthesized pyrrolidine linked oxadiazole derivatives and also tested for their analgesic and antibacterial activities.



Scheme

Keywords: Heterocyclics, Oxadiazoles, biological activity.

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OP/PP-120

Defensive Chemistry of *Coridius janus* (Heteroptera: Pentatomidae)

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ABSTRACT

Insects of many varieties have developed various modes of chemical and behavioral defensive mechanisms. When disturbed, many hemipterans release a pungent and volatile fluid with an offensive odour. These secretions may be used by the *Coridius janus* as defensive substances. *C. janus* possesses abdominal scent glands in larvae and metathoracic scent glands in adults. The extraction of scent secretion from larvae and adults of *C. janus* was collected with the help of micro capillaries and subjected to analysis by Gas chromatographic and Mass spectra (GC-MS) and compared with authentic samples.

Seven chemical compounds were identified in the analysis of the metathoracic scent secretions of adults, 4,5-Dimethyl diazole, (E)-2-Hexenyl acetate, O-iso butenyl phenol, Undecane, Undecylamine, 1,12-Dodecane-diol and N-methyl dodec-6,10 diene amine. Five chemical compounds were identified in the analysis of the abdominal scent secretions of nymph, 5-iso-propenyl pentyl amine, 1-dodecane, Indole-3-acetic acid ethyl ester, N-methyl-dodec-6,10-diene-amine and 6,10-dodec-dienyl acetate. The function of the scent is defensive against predators.

Keywords: *C. janus*, abdominal scent glands, metathoracic scent glands, defensive secretions, chemical compounds.

OP/PP-121

Isolation and Purification of Metabolites

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Abstract

Ion-exchange chromatography is a technique for the separation and purification of various biomolecules that express both hydrophobic and ionic moieties because the column matrix can strongly interact with the biomolecules through long-distance electrostatic force. Thus, effective separation of biomolecular substances is achieved by introducing the opposite ionic moiety

A cellulose based ion exchange resin was synthesized by copolymerizing cellulose with electropositive metal alkyl sulfonate and styrene. The matrix was physicochemically and thermally stable and resistant to acids, bases, and enzymes. In static adsorption tests, the CIR had decolorization ratios .for mixed dyestuffs in wastewater of up to 87.79%, which was higher than the decolorization ratios for a synthetic ion exchange resin .In dynamic adsorption tests, the CIR bed had a decolorization ratios of 92.59% and a wastewater handling capacity 15 times the column volume. the adaptability of the CIR to continuous column adsorption, make the CIR suitable for removing dyestuffs from industrial wastewater and a potential substitute for traditional sorbents such as synthetic resins.

OP/PP-122

Spectrophotometric Determination of Drugs and Pharmaceuticals based onCharge Transfer Complexation with *p*-CA

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Abstract

A Simple, sensitive selective and Precise method is developed for the UV-Visible Spectrophotometric methods have been developed for the estimation of five drugs *VIZ* .,1). Aripiprazole 2). Astemizole 3). Carvedilol 4). Escitalopram oxalate and 5). Ketoconazole. In the present study area under curve(AUC) has been considered for the purpose of quantification of drugs as AUC is more accurate and precise than selecting one wavelength because AUC combines optical densities at the all the wave length. The AUC was calculated using Excel programme. This is taken between 400 to 700 nm as this area is minimally interfered by *p*-CA absorption.

After recording optical densities and calculating AUC for four replicates a commonly used analytical parameter called "relative response" (O.D / Conc. (μg mL^{-1}) and AUC / Conc. (μg mL^{-1}) have been calculated. This method has been applied for the estimation of drugs in their pure form as well as in tablet formulation. The results of analysis have been validated statistically for linearity, accuracy, precision, LOD and LOQ.

Key Words: UV-Visible Spectrophotometry, Drugs, *p*-CA , Quantification, Validation.

OP/PP-123

DNA Binding of Ruthenium (II) Polypyridyl Complexes containing Novel Ligand 4-(1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)-N,N-dimethylnaphthalen-1-amine

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Abstract

A new novel ligand dmnip (dmnip = {4-(1H-imidazo[4,5-f][1,10]phenanthrolin-2-yl)-N,N-dimethylnaphthalen-1-amine)} and its mononuclear Ru(II) polypyridyl complexes of $[Ru(phen)_2dmnip]^{2+}$ **(1)** (phen= 1,10-Phenanthrolene), $[Ru(bpy)_2dmnip]^{2+}$**(2)** (bpy=2,2' bipyridyl), $[Ru(dmb)_2dmnip]^{2+}$ **(3)** (dmb=4, 4'-dimethyl 2, 2'-bipyridine), have been synthesized successfully and characterized thoroughly by elemental analysis, UV-vis, IR, 1H, 13C-NMR, and ESI-MS.

The interaction of these complexes with CT-DNA was studied using absorption, emission spectroscopy, viscosity measurements and molecular docking studies. The docking study infers the binding ability of complexes with stability constants, similar to absorption, emission techniques. These studies reveal that the three Ru(II) polypyridyl complexes bind to CT-DNA through intercalation. The binding ability of these complexes in presence of different ions and solvents are also reported.

OP/PP-124

DFT & Thermo-Physical Studies of Binary Mixtures of Ethyl Salicylate (Es) with 1-Alkanols at Various Temperatures

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Abstract

The physical properties of a binary mixture such as density (ρ), viscosity (η) and speed of sound (u) are important from practical and theoretical points of view, to understand liquid theory. These properties are very useful for design of many types of transport and process equipment in chemical industries. These parameters afford valuable information regarding behavior of binary liquid systems, due to intra molecular and inter molecular associations, dipolar interactions, complex formation and related structural changes effect the compressibility of the system.

Experimental results of density and speed of sound at 293.15, 298.15, and 303.15K are presented for the binary mixture of Ethyl Salicylate (ES) with 1-propanol, 1-butanol, 1-pentanol and 1-hexanol over the whole composition. From these data, excess molar volume (V^E), deviation in viscosity ($\Delta\eta$) deviation in speed of sound (Δu) and isentropic compressibility (Δk_s) have been calculated. These results are fitted to a Redlich-Kister type of polynomial equation. These results further discussions in terms of the different types of molecular interactions between the unlike molecules. The bond characteristics, geometries, interaction energies and natural bonding orbital (NBO) analysis for the hydrogen bonded complex have been calculated using the density functional theory (DFT) method.

Key words: Density (ρ), viscosity (η), Speed of Sound (u), Binary liquid mixtures, molecular interactions, Redlich-Kister type of polynomial equation, DFT.

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